Full wwPDB EM Validation Report

Apr 21, 2025 – 05:38 PM EDT

PDB ID	:	9B0W / pdb_00009b0w
EMDB ID	:	EMD-44060
Title	:	In situ human eEF2-A/P-P/E state 80S ribosome
Authors	:	Wei, Z.; Yong, Z.
Deposited on	:	2024-03-12
Resolution	:	2.66 Å(reported)

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

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

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

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

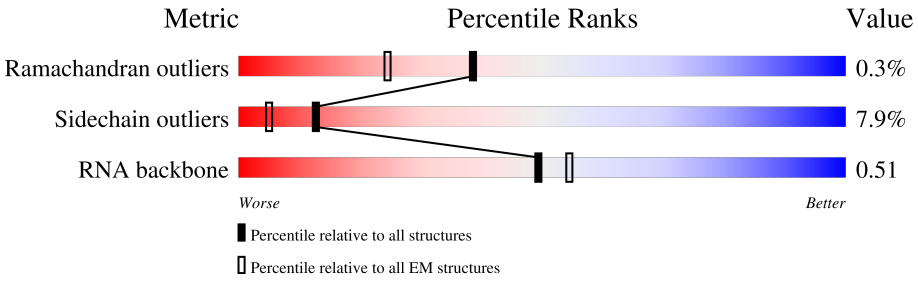
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.66 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	Se	58	24% 53% 26% • 19%
2	CH	132	47% 73% 25% •
3	LW	118	42% 92% 8%
4	SE	262	13% 90% 10%
5	SI	206	18% 92% 8%
6	SL	153	14% 88% 12%
7	SX	141	6% 94% 6%
8	SG	237	32% 92% 8%

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Mol	Chain	Length	Quality of chain
9	SJ	185	16% 92% 8%
10	SY	131	35% 89% 11%
11	SA	221	13% 95% 5%
12	SB	214	88% 12%
13	SH	186	34% 91% 9%
14	SV	83	5% 84% 16%
15	Sa	102	7% 92% 8%
16	SC	222	93% 7%
17	SN	150	95% 5%
18	SO	140	9% 91% 9%
19	SW	129	97%
20	Sb	83	14% 96%
21	L5	3740	9% 76% 23%
22	L7	120	91% 9%
23	L8	156	5% 80% 19%
24	LA	248	93% 7%
25	LB	402	93% 7%
26	LC	368	94% 6%
27	LD	293	5% 94% 6%
28	LE	236	11% 94% 6%
29	LF	225	96%
30	LG	241	11% 93% 7%
31	LH	190	96%
32	LI	202	96%
33	LJ	176	12% 94% 6%

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Mol	Chain	Length	Quality of chain
34	LL	210	7% 93% 7%
35	LM	139	93% 6%
36	LN	203	95% 5%
37	LO	201	97%
38	LP	153	93% 7%
39	LQ	187	96%
40	LR	187	12% 95% 5%
41	LS	175	97%
42	LT	159	95% 5%
43	LU	101	7% 87% 13%
44	LV	131	93% 7%
45	LX	120	92% 8%
46	LY	134	96%
47	LZ	135	93% 7%
48	La	147	99%
49	Lb	109	13% 92% 8%
50	Lc	98	7% 93% 7%
51	Ld	107	7% 94% 6%
52	Le	128	95% 5%
53	Lf	109	90% 10%
54	Lg	114	6% 96%
55	Lh	122	93% 7%
56	Li	102	91% 9%
57	Lj	86	91% 9%
58	Lk	69	96%

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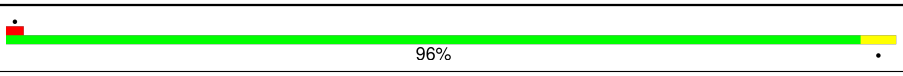
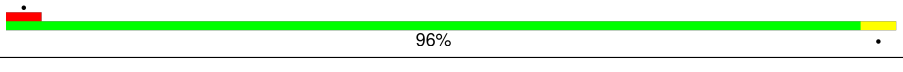
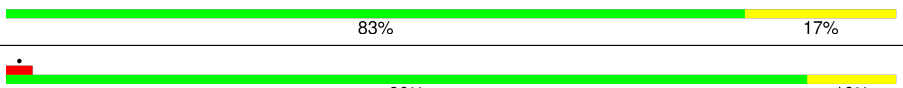
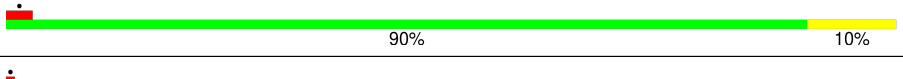
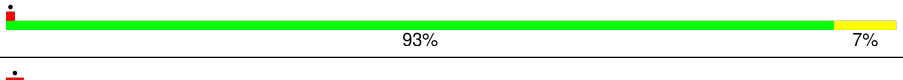
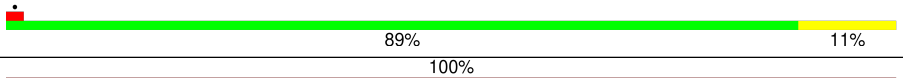
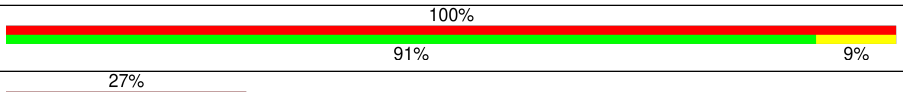
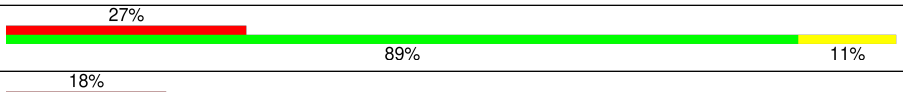
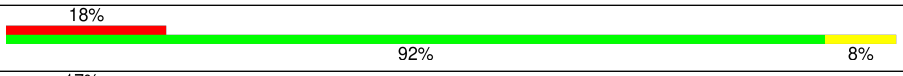
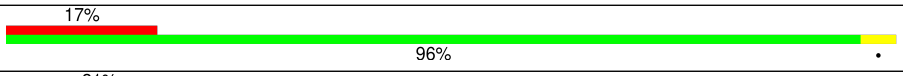
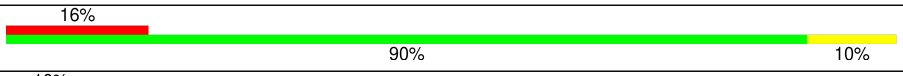
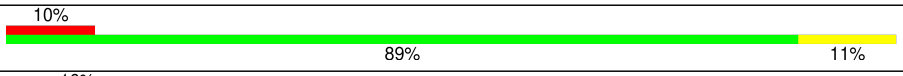
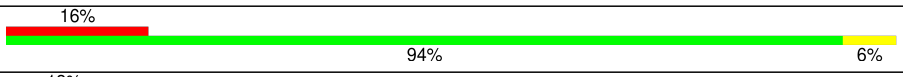
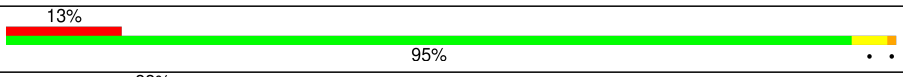
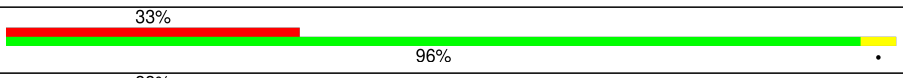
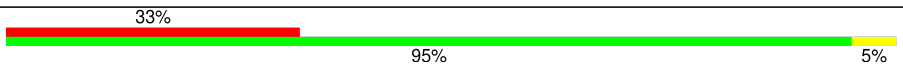
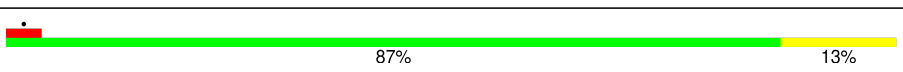
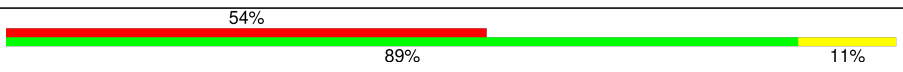
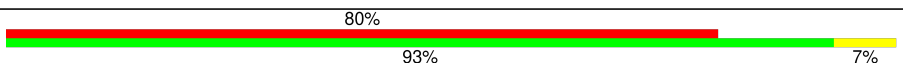
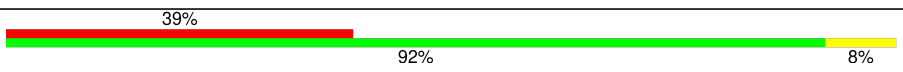
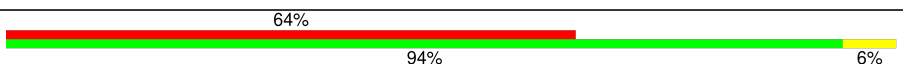
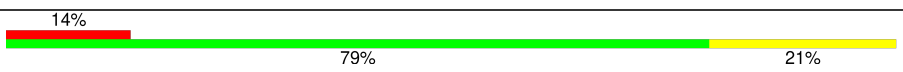
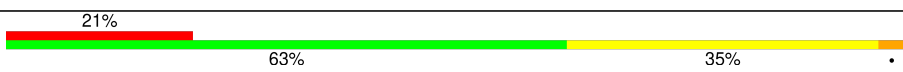
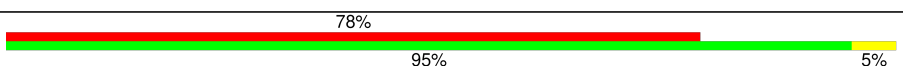
Mol	Chain	Length	Quality of chain
59	Ll	50	
60	Lm	52	
61	Ln	24	
62	Lo	105	
63	Lp	91	
64	Lr	125	
65	Lz	217	
66	SR	135	
67	SD	227	
68	SF	189	
69	SK	98	
70	SP	121	
71	SQ	144	
72	SS	145	
73	ST	143	
74	SU	104	
75	Sc	64	
76	Sd	55	
77	Sg	313	
78	SM	122	
79	SZ	75	
80	Sf	67	
81	AP	71	
82	PE	75	
83	Ls	196	

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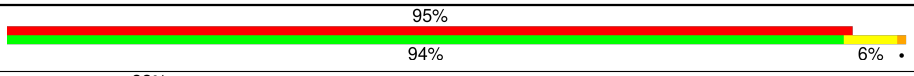
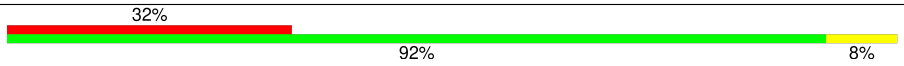
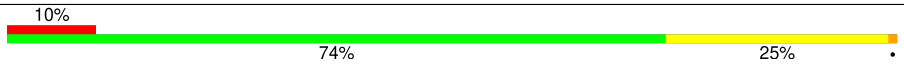
Mol	Chain	Length	Quality of chain
84	Lt	141	
85	CB	846	
86	S2	1740	

2 Entry composition (i)

There are 88 unique types of molecules in this entry. The entry contains 230194 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Small ribosomal subunit protein eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Se	47	378	234	84	59	1	0	0

- Molecule 2 is a protein called Endothelial differentiation-related factor 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	CH	132	1018	625	199	194	0	0

- Molecule 3 is a protein called 60S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	LW	118	965	604	199	158	4	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein eS4, X isoform.

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

- Molecule 5 is a protein called 40S ribosomal protein S8.

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

- Molecule 6 is a protein called 40S ribosomal protein S11.

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

- Molecule 7 is a protein called 40S ribosomal protein S23.

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

- Molecule 8 is a protein called 40S ribosomal protein S6.

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

- Molecule 9 is a protein called 40S ribosomal protein S9.

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

- Molecule 10 is a protein called 40S ribosomal protein S24.

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

- Molecule 11 is a protein called 40S ribosomal protein SA.

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

- Molecule 12 is a protein called 40S ribosomal protein S3a.

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

- Molecule 13 is a protein called 40S ribosomal protein S7.

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

- Molecule 14 is a protein called 40S ribosomal protein S21.

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

- Molecule 15 is a protein called 40S ribosomal protein S26.

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

- Molecule 16 is a protein called 40S ribosomal protein S2.

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

- Molecule 17 is a protein called 40S ribosomal protein S13.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

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

- Molecule 19 is a protein called 40S ribosomal protein S15a.

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

- Molecule 20 is a protein called Small ribosomal subunit protein eS27.

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

- Molecule 21 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L5	3740	Total	C	N	O	P	0	0
			79860	35549	14585	25987	3739		

- Molecule 22 is a RNA chain called 5S rRNA.

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

- Molecule 23 is a RNA chain called 5.8S rRNA.

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

- Molecule 24 is a protein called 60S ribosomal protein L8.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 26 is a protein called 60S ribosomal protein L4.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 28 is a protein called 60S ribosomal protein L6.

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

- Molecule 29 is a protein called 60S ribosomal protein L7.

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

- Molecule 30 is a protein called 60S ribosomal protein L7a.

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

- Molecule 31 is a protein called 60S ribosomal protein L9.

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

- Molecule 32 is a protein called 60S ribosomal protein L10-like.

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

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

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

- Molecule 34 is a protein called Large ribosomal subunit protein eL13.

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

- Molecule 35 is a protein called 60S ribosomal protein L14.

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

- Molecule 36 is a protein called 60S ribosomal protein L15.

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

- Molecule 37 is a protein called 60S ribosomal protein L13a.

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

- Molecule 38 is a protein called 60S ribosomal protein L17.

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

- Molecule 39 is a protein called 60S ribosomal protein L18.

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

- Molecule 40 is a protein called 60S ribosomal protein L19.

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

- Molecule 41 is a protein called 60S ribosomal protein L18a.

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

- Molecule 42 is a protein called 60S ribosomal protein L21.

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

- Molecule 43 is a protein called Heparin-binding protein HBp15.

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

- Molecule 44 is a protein called 60S ribosomal protein L23.

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

- Molecule 45 is a protein called 60S ribosomal protein L23a.

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

- Molecule 46 is a protein called 60S ribosomal protein L26.

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

- Molecule 47 is a protein called 60S ribosomal protein L27.

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

- Molecule 48 is a protein called 60S ribosomal protein L27a.

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

- Molecule 49 is a protein called 60S ribosomal protein L29.

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

- Molecule 50 is a protein called 60S ribosomal protein L30.

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

- Molecule 51 is a protein called 60S ribosomal protein L31.

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

- Molecule 52 is a protein called 60S ribosomal protein L32.

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

- Molecule 53 is a protein called 60S ribosomal protein L35a.

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

- Molecule 54 is a protein called 60S ribosomal protein L34.

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

- Molecule 55 is a protein called 60S ribosomal protein L35.

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

- Molecule 56 is a protein called 60S ribosomal protein L36.

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

- Molecule 57 is a protein called 60S ribosomal protein L37.

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

- Molecule 58 is a protein called 60S ribosomal protein L38.

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

- Molecule 59 is a protein called 60S ribosomal protein L39.

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

- Molecule 60 is a protein called Large ribosomal subunit protein eL40.

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

- Molecule 61 is a protein called 60S ribosomal protein L41.

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

- Molecule 62 is a protein called 60S ribosomal protein L36a.

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

- Molecule 63 is a protein called 60S ribosomal protein L37a.

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

- Molecule 64 is a protein called 60S ribosomal protein L28.

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

- Molecule 65 is a protein called 60S ribosomal protein L10a.

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

- Molecule 66 is a protein called 40S ribosomal protein S17.

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

- Molecule 67 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 68 is a protein called 40S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	SF	189	Total	C	N	O	S	0	0
			1495	934	284	270	7		

- Molecule 69 is a protein called 40S ribosomal protein S10.

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

- Molecule 70 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	SP	121	Total	C	N	O	S	0	0
			985	623	185	170	7		

- Molecule 71 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 72 is a protein called 40S ribosomal protein S18.

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

- Molecule 73 is a protein called 40S ribosomal protein S19.

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

- Molecule 74 is a protein called 40S ribosomal protein S20.

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

- Molecule 75 is a protein called 40S ribosomal protein S28.

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

- Molecule 76 is a protein called 40S ribosomal protein S29.

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

- Molecule 77 is a protein called Receptor of activated protein C kinase 1.

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

- Molecule 78 is a protein called Small ribosomal subunit protein eS12.

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

- Molecule 79 is a protein called Small ribosomal subunit protein eS25.

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

- Molecule 80 is a protein called Ubiquitin-40S ribosomal protein S27a.

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

- Molecule 81 is a RNA chain called A/P site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	AP	71	Total	C	N	O	P	0	0
			1514	677	275	492	70		

- Molecule 82 is a RNA chain called P/E site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	PE	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 83 is a protein called 60S acidic ribosomal protein P0.

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

- Molecule 84 is a protein called 60S ribosomal protein L12.

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

- Molecule 85 is a protein called eEF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	CB	846	Total	C	N	O	S	0	0
			6605	4193	1136	1232	44		

- Molecule 86 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	S2	1740	Total	C	N	O	P	0	0
			36898	16459	6599	12101	1739		

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
87	Sa	1	Total	Zn	0
			1	1	
87	Lg	1	Total	Zn	0
			1	1	
87	Lj	1	Total	Zn	0
			1	1	
87	Lm	1	Total	Zn	0
			1	1	
87	Lo	1	Total	Zn	0
			1	1	
87	Lp	1	Total	Zn	0
			1	1	

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
88	L5	211	Total	Mg	0
			211	211	
88	L7	3	Total	Mg	0
			3	3	
88	L8	4	Total	Mg	0
			4	4	

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Mol	Chain	Residues	Atoms	AltConf
88	LA	1	Total Mg 1 1	0
88	LB	1	Total Mg 1 1	0
88	LI	1	Total Mg 1 1	0
88	LP	1	Total Mg 1 1	0
88	LV	1	Total Mg 1 1	0
88	Le	1	Total Mg 1 1	0
88	Lg	1	Total Mg 1 1	0
88	S2	30	Total Mg 30 30	0

3 Residue-property plots (i)

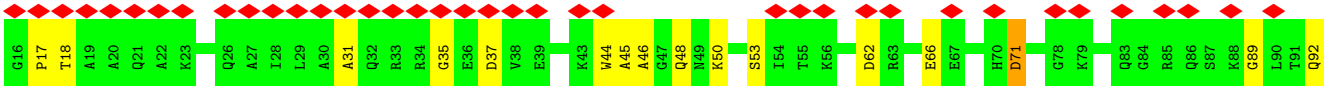
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

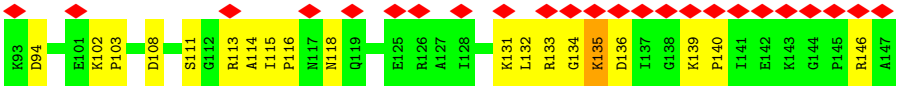
• Molecule 1: Small ribosomal subunit protein eS30

Chain Se:

• Molecule 2: Endothelial differentiation-related factor 1

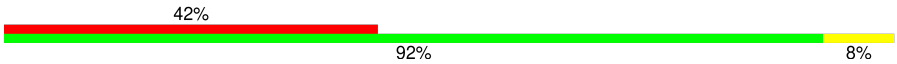
Chain CH:

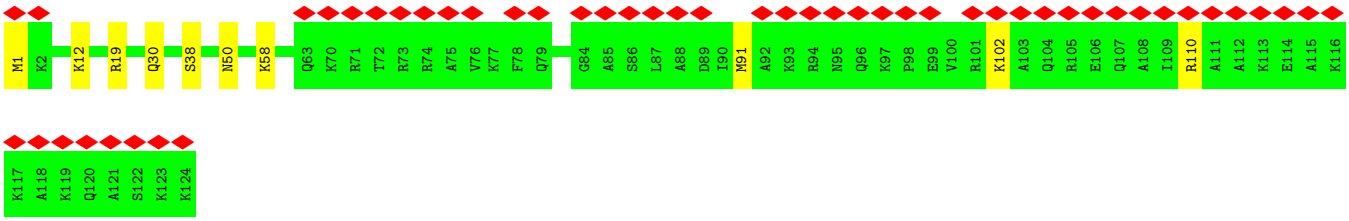




• Molecule 3: 60S ribosomal protein L24

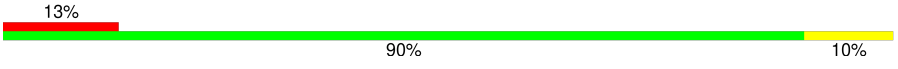
Chain LW:

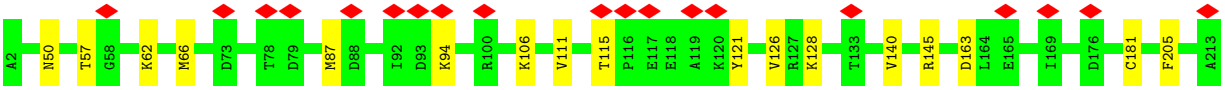


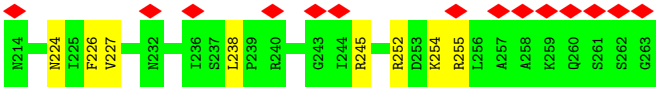


• Molecule 4: Small ribosomal subunit protein eS4, X isoform

Chain SE:

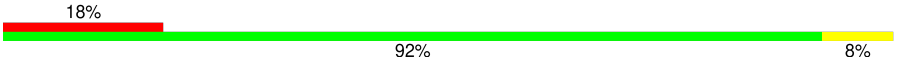


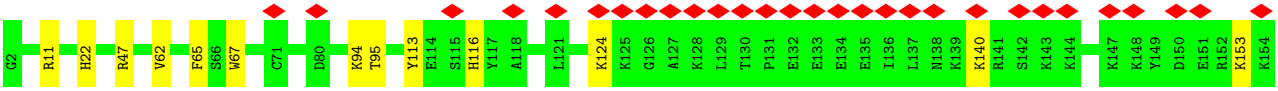


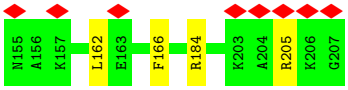


• Molecule 5: 40S ribosomal protein S8

Chain SI:

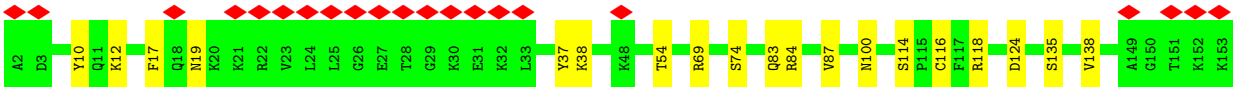






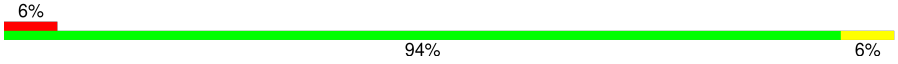
• Molecule 6: 40S ribosomal protein S11

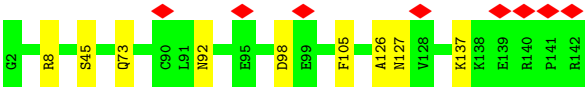
Chain SL:



• Molecule 7: 40S ribosomal protein S23

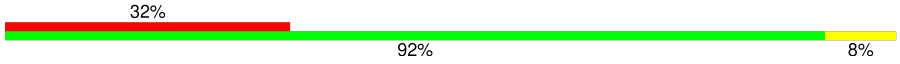
Chain SX:

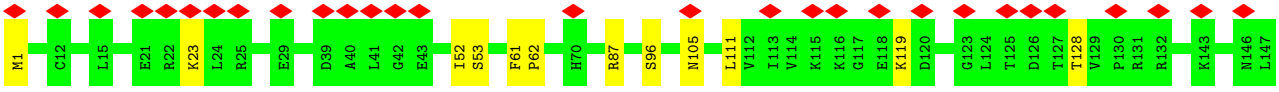


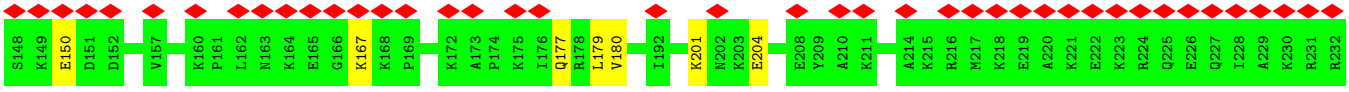


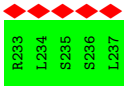
• Molecule 8: 40S ribosomal protein S6

Chain SG:



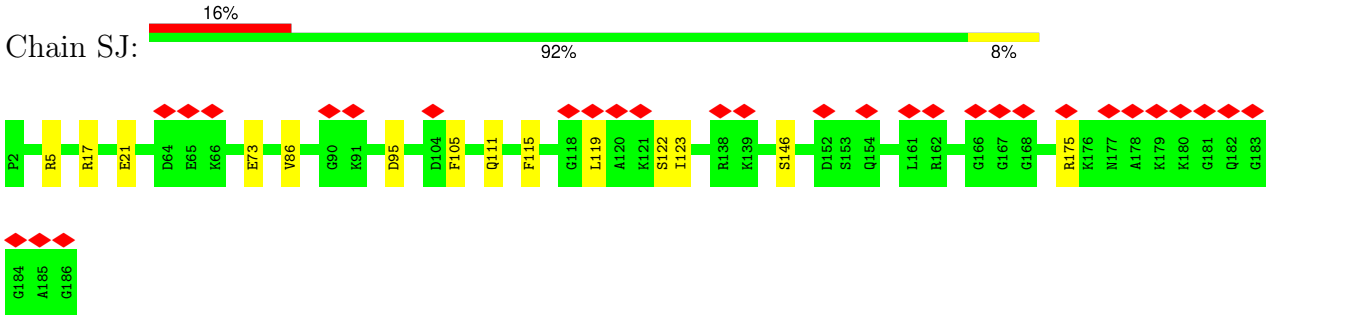






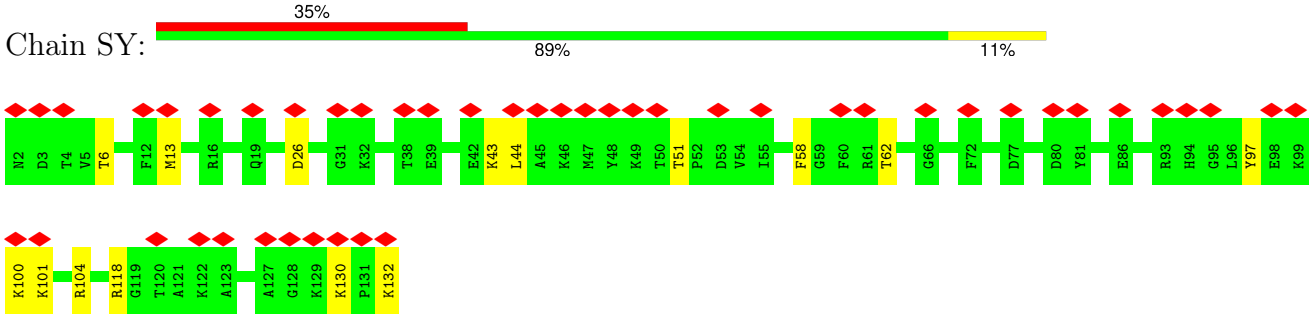
• Molecule 9: 40S ribosomal protein S9

Chain SJ:



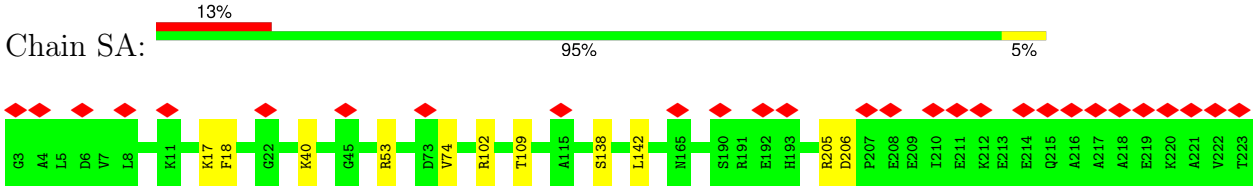
• Molecule 10: 40S ribosomal protein S24

Chain SY:



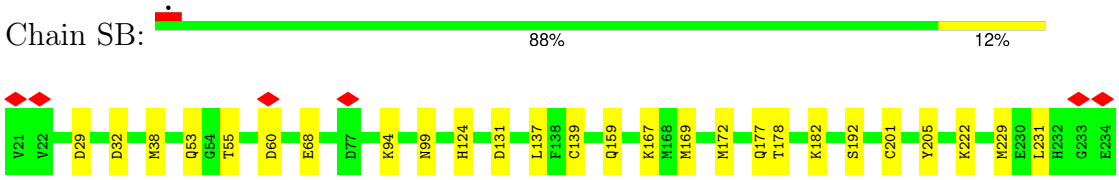
• Molecule 11: 40S ribosomal protein SA

Chain SA:



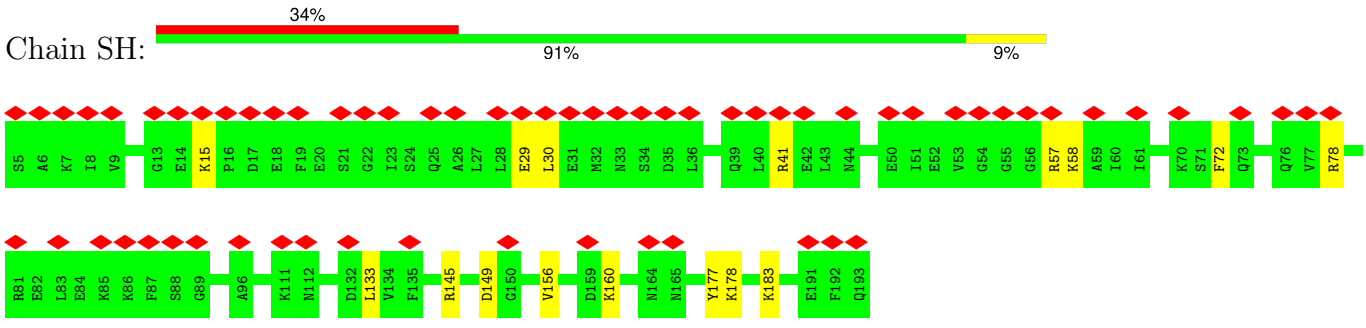
• Molecule 12: 40S ribosomal protein S3a

Chain SB:



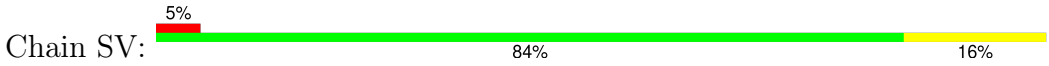
• Molecule 13: 40S ribosomal protein S7

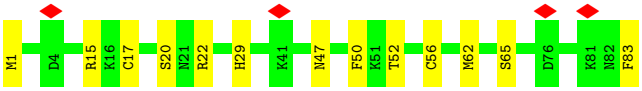
Chain SH:



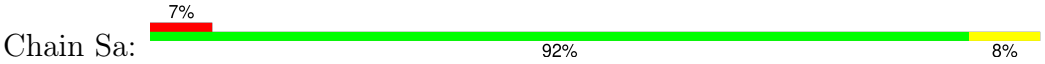
• Molecule 14: 40S ribosomal protein S21

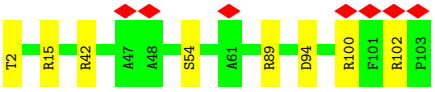
Chain SV:





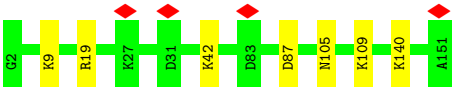
• Molecule 15: 40S ribosomal protein S26



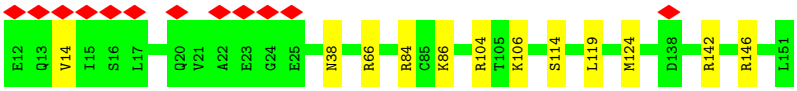


• Molecule 16: 40S ribosomal protein S2

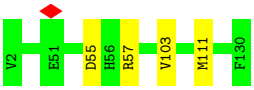
• Molecule 17: 40S ribosomal protein S13



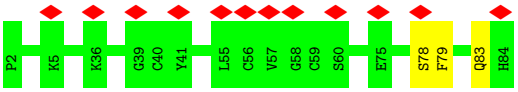
• Molecule 18: Small ribosomal subunit protein uS11



• Molecule 19: 40S ribosomal protein S15a

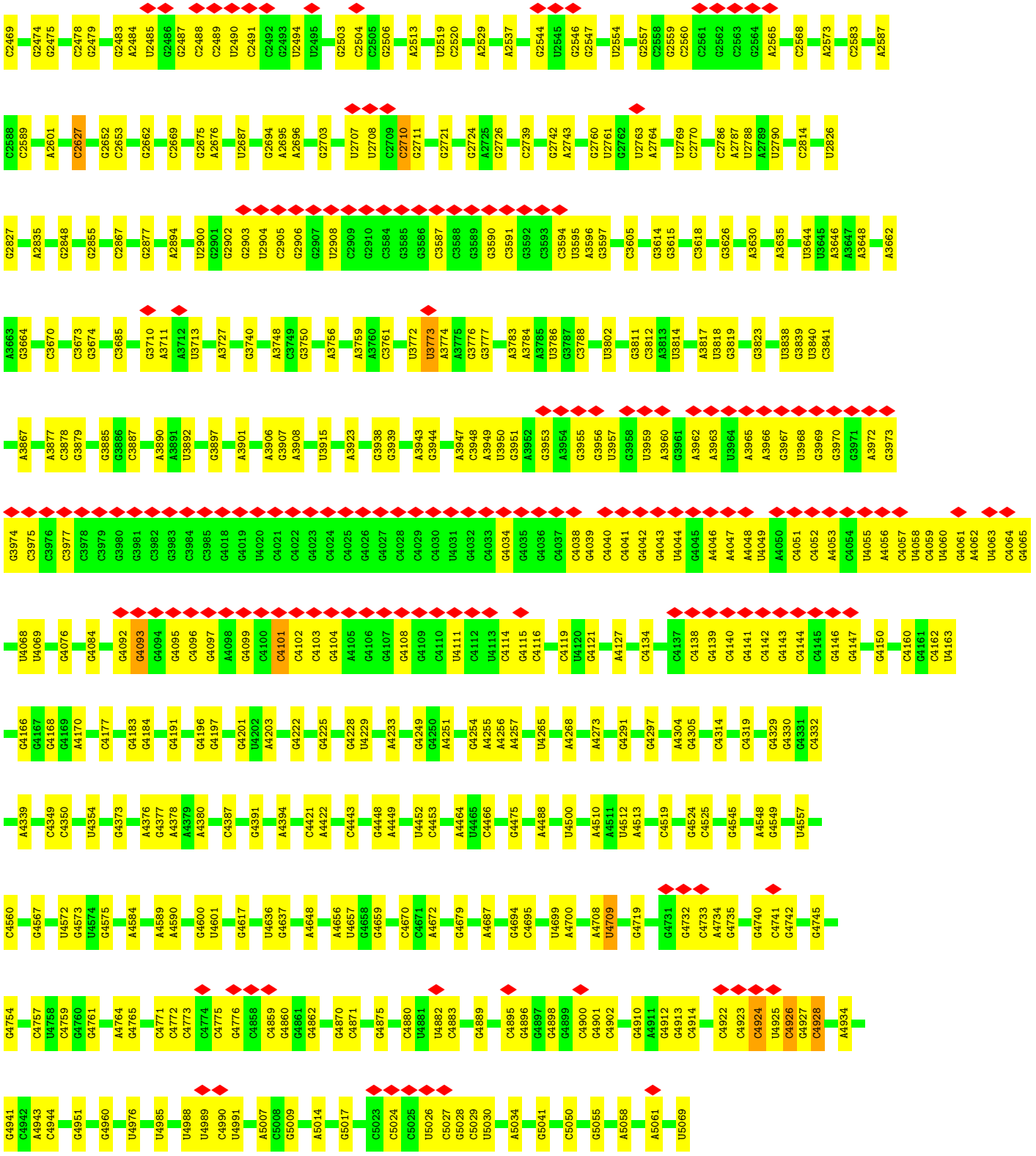


• Molecule 20: Small ribosomal subunit protein eS27



• Molecule 21: 28S rRNA

Chain L5:

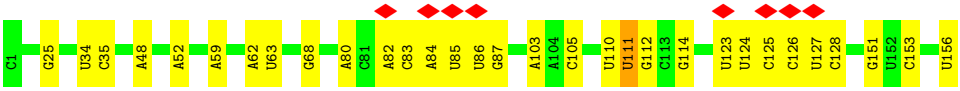


- Molecule 22: 5S rRNA

Chain L7:

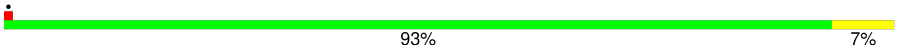
• Molecule 23: 5.8S rRNA

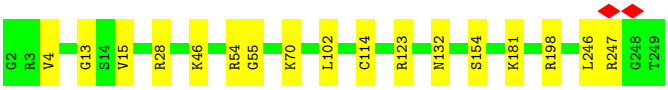
Chain L8:



• Molecule 24: 60S ribosomal protein L8

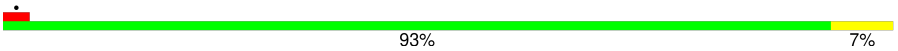
Chain LA:

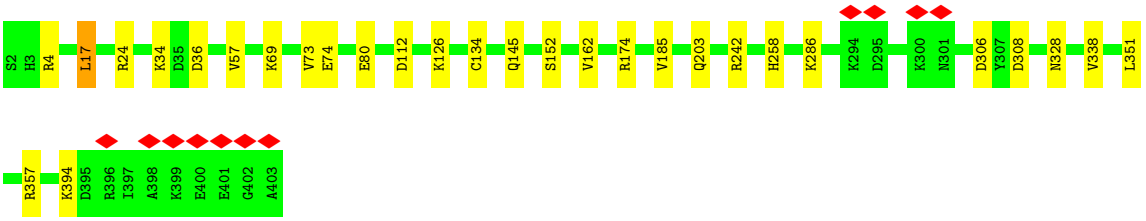




• Molecule 25: Large ribosomal subunit protein uL3

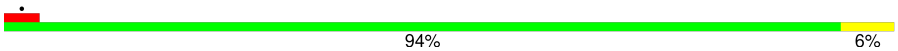
Chain LB:

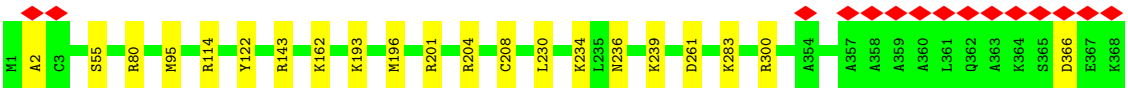




• Molecule 26: 60S ribosomal protein L4

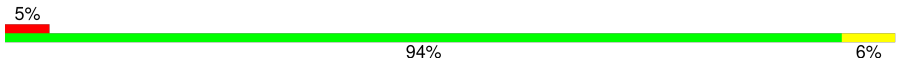
Chain LC:





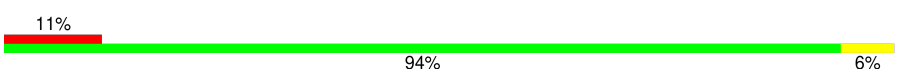
• Molecule 27: Large ribosomal subunit protein uL18

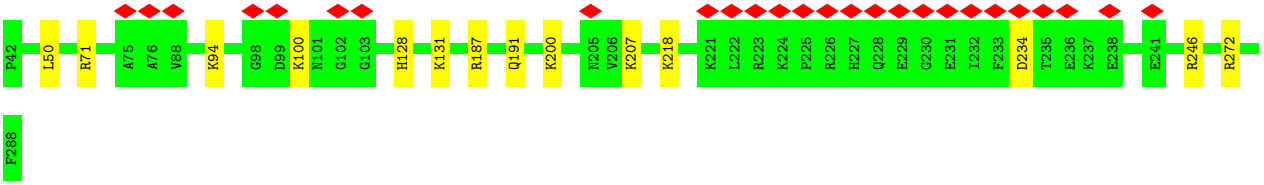
Chain LD:



• Molecule 28: 60S ribosomal protein L6

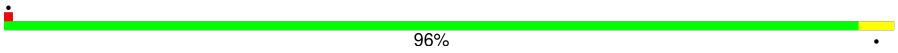
Chain LE:





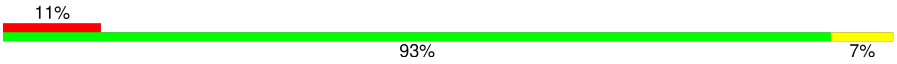
• Molecule 29: 60S ribosomal protein L7

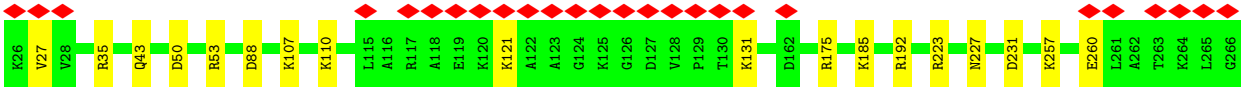
Chain LF:



• Molecule 30: 60S ribosomal protein L7a

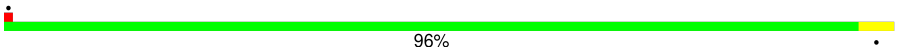
Chain LG:





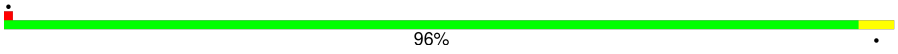
• Molecule 31: 60S ribosomal protein L9

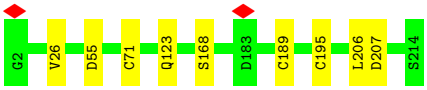
Chain LH:



• Molecule 32: 60S ribosomal protein L10-like

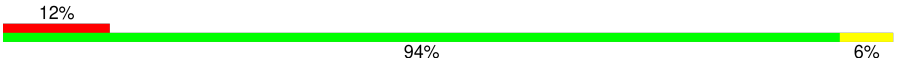
Chain LI:

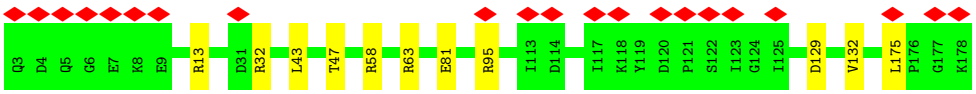




• Molecule 33: 60S ribosomal protein L11

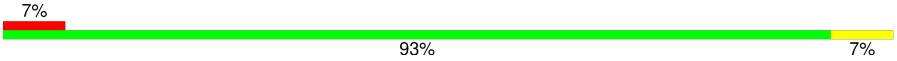
Chain LJ:

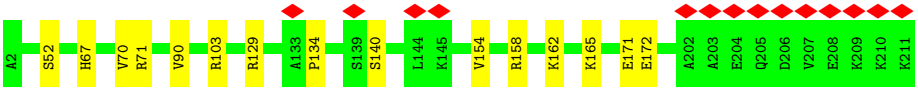




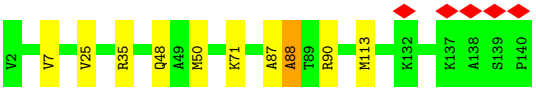
• Molecule 34: Large ribosomal subunit protein eL13

Chain LL:



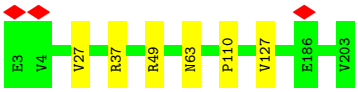


• Molecule 35: 60S ribosomal protein L14

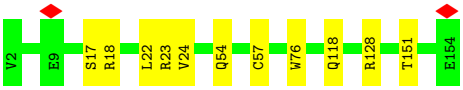


• Molecule 36: 60S ribosomal protein L15

• Molecule 37: 60S ribosomal protein L13a

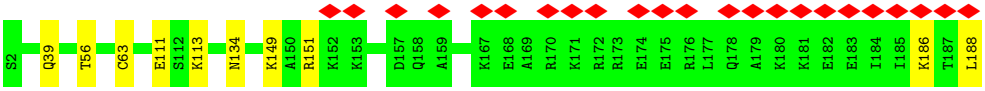


• Molecule 38: 60S ribosomal protein L17



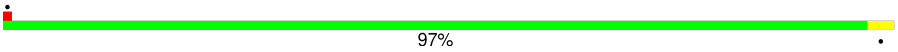
• Molecule 39: 60S ribosomal protein L18

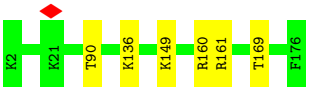
• Molecule 40: 60S ribosomal protein L19



• Molecule 41: 60S ribosomal protein L18a

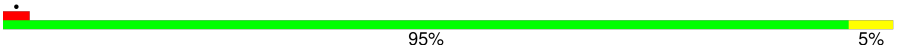
Chain LS:

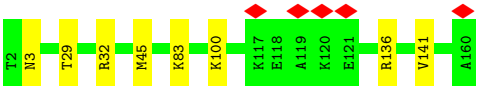




• Molecule 42: 60S ribosomal protein L21

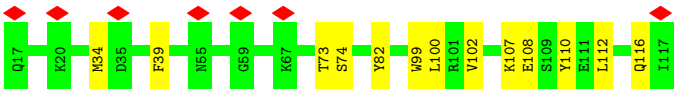
Chain LT:





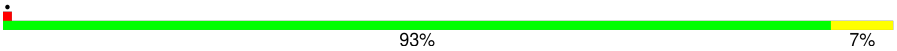
• Molecule 43: Heparin-binding protein HBp15

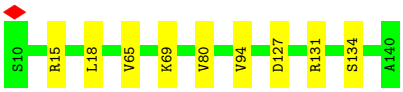
Chain LU:



• Molecule 44: 60S ribosomal protein L23

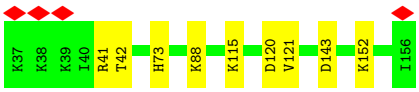
Chain LV:





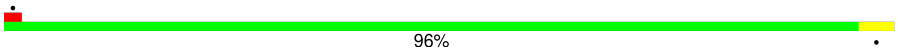
• Molecule 45: 60S ribosomal protein L23a

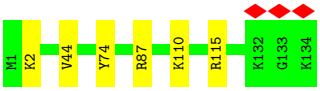
Chain LX:



• Molecule 46: 60S ribosomal protein L26

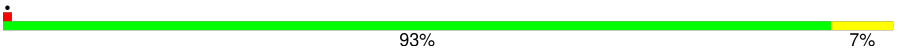
Chain LY:

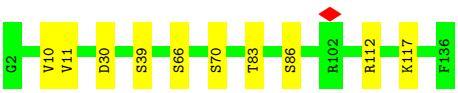




• Molecule 47: 60S ribosomal protein L27

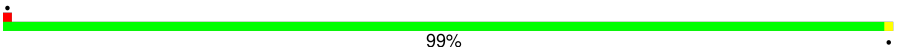
Chain LZ:

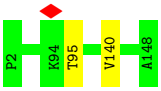




• Molecule 48: 60S ribosomal protein L27a

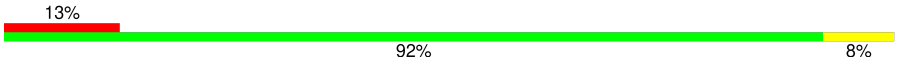
Chain La:

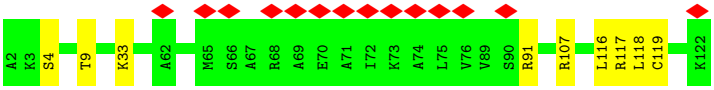




• Molecule 49: 60S ribosomal protein L29

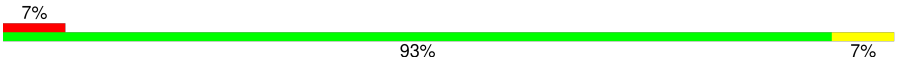
Chain Lb:

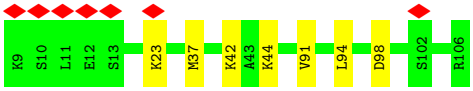




• Molecule 50: 60S ribosomal protein L30

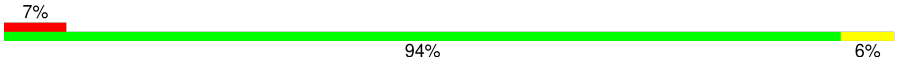
Chain Lc:

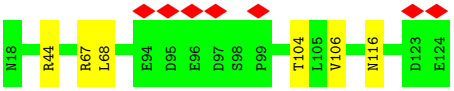




• Molecule 51: 60S ribosomal protein L31

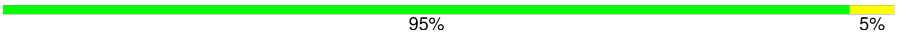
Chain Ld:





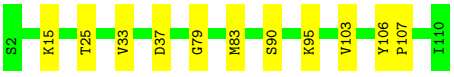
• Molecule 52: 60S ribosomal protein L32

Chain Le:



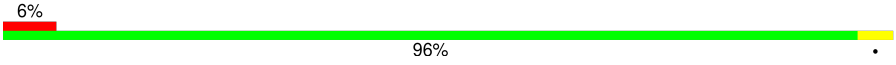
• Molecule 53: 60S ribosomal protein L35a

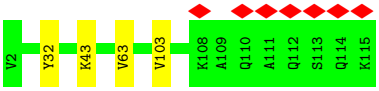
Chain Lf:



• Molecule 54: 60S ribosomal protein L34

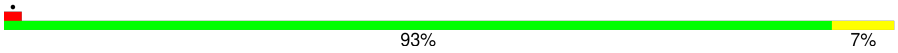
Chain Lg:

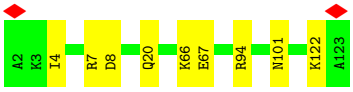




• Molecule 55: 60S ribosomal protein L35

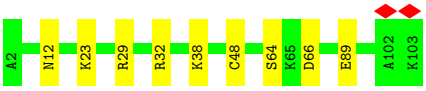
Chain Lh:





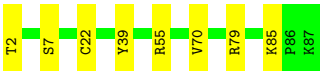
• Molecule 56: 60S ribosomal protein L36

Chain Li:



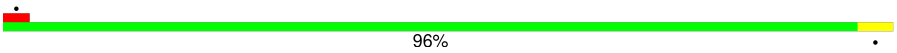
• Molecule 57: 60S ribosomal protein L37

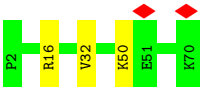
Chain Lj:



• Molecule 58: 60S ribosomal protein L38

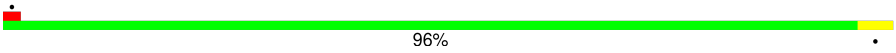
Chain Lk:

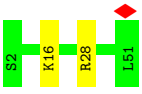




• Molecule 59: 60S ribosomal protein L39

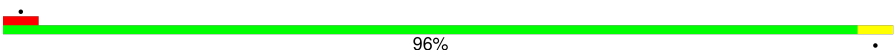
Chain Ll:

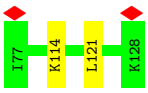




• Molecule 60: Large ribosomal subunit protein eL40

Chain Lm:



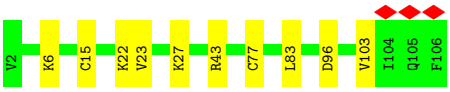


• Molecule 61: 60S ribosomal protein L41

Chain Ln:

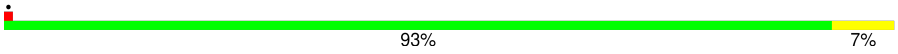
• Molecule 62: 60S ribosomal protein L36a

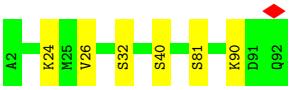
Chain Lo:



• Molecule 63: 60S ribosomal protein L37a

Chain Lp:



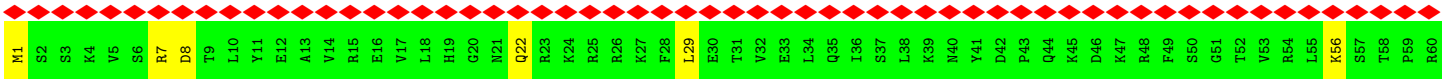


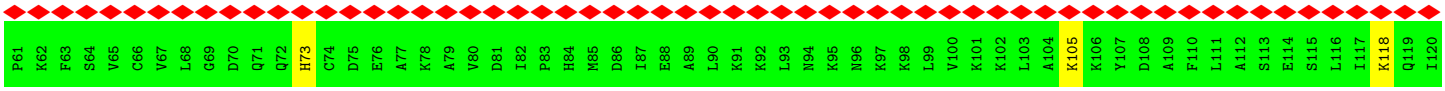
• Molecule 64: 60S ribosomal protein L28

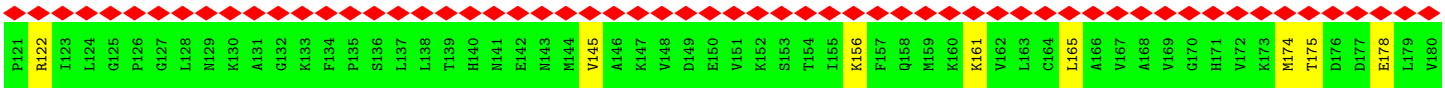
Chain Lr:

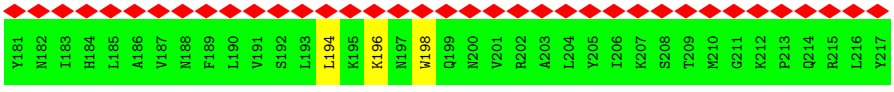
• Molecule 65: 60S ribosomal protein L10a

Chain Lz:



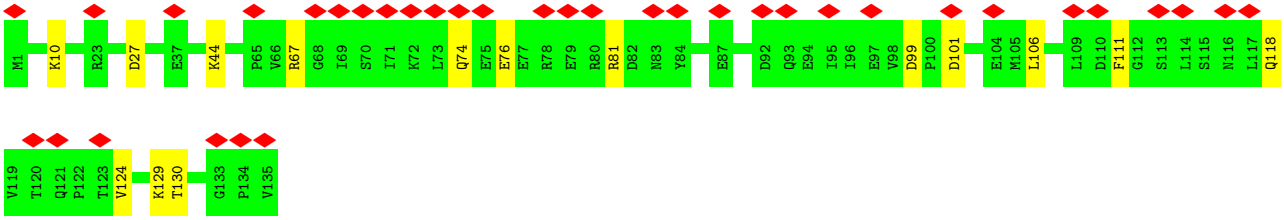




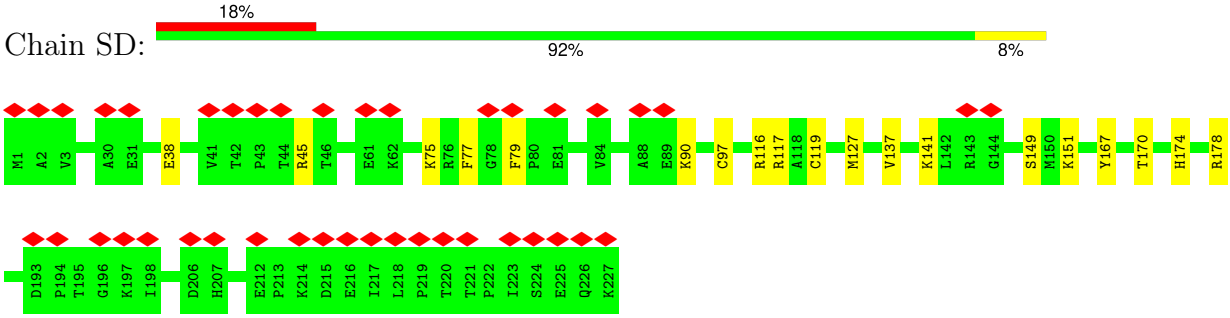


• Molecule 66: 40S ribosomal protein S17

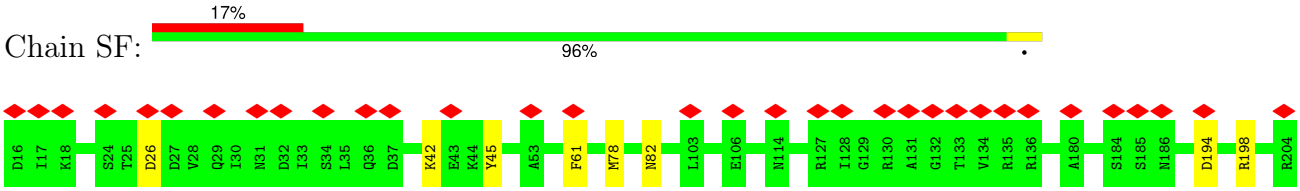
Chain SR:



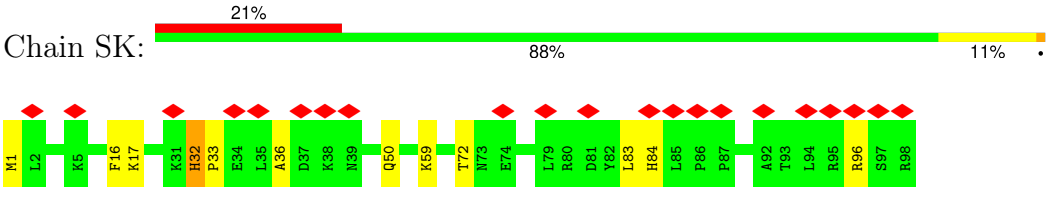
• Molecule 67: Small ribosomal subunit protein uS3



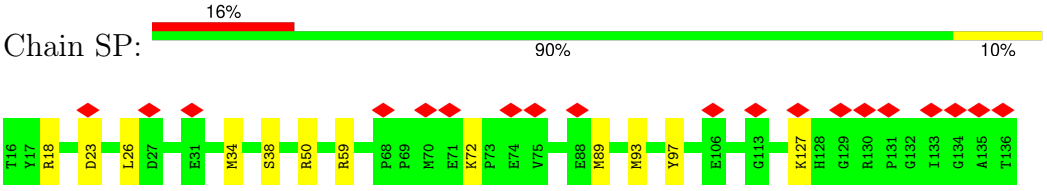
• Molecule 68: 40S ribosomal protein S5



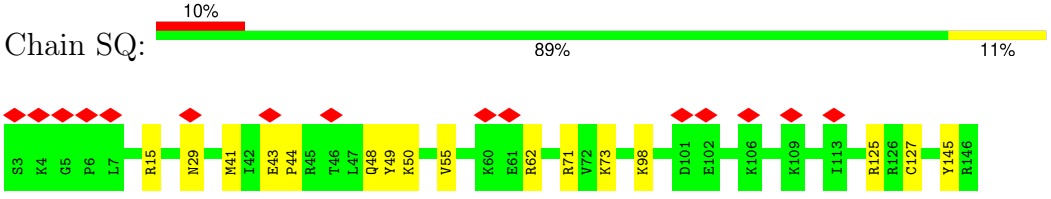
• Molecule 69: 40S ribosomal protein S10



• Molecule 70: Small ribosomal subunit protein uS19

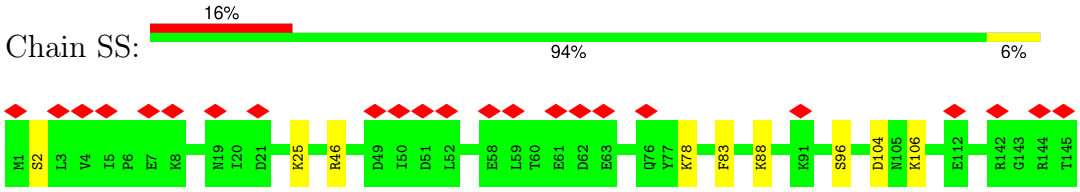


• Molecule 71: Small ribosomal subunit protein uS9



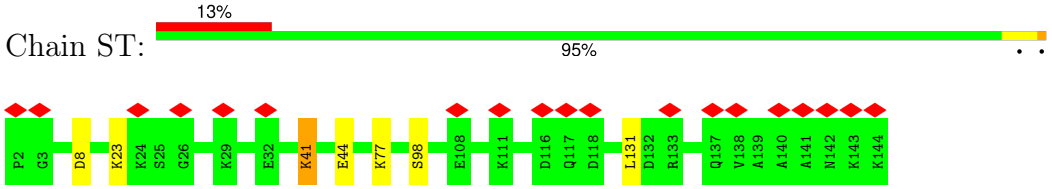
• Molecule 72: 40S ribosomal protein S18

Chain SS:



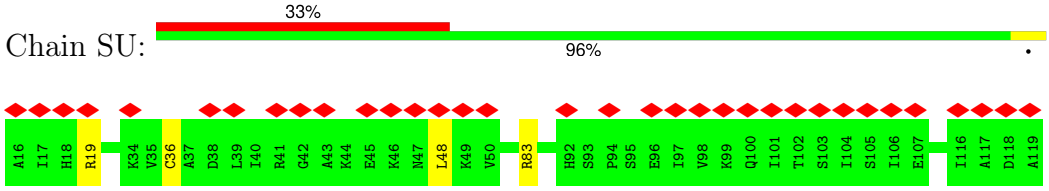
• Molecule 73: 40S ribosomal protein S19

Chain ST:



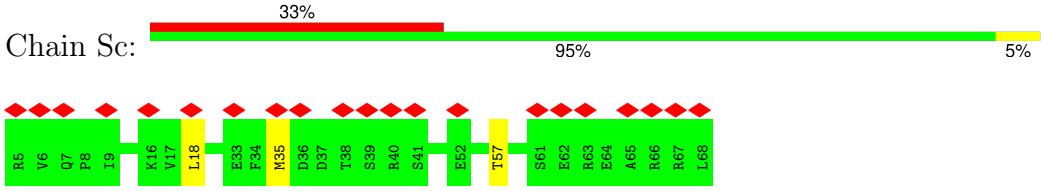
• Molecule 74: 40S ribosomal protein S20

Chain SU:



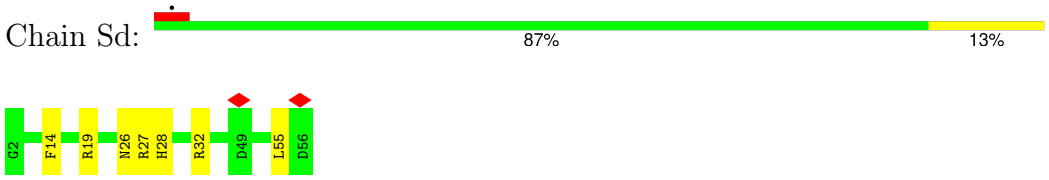
• Molecule 75: 40S ribosomal protein S28

Chain Sc:



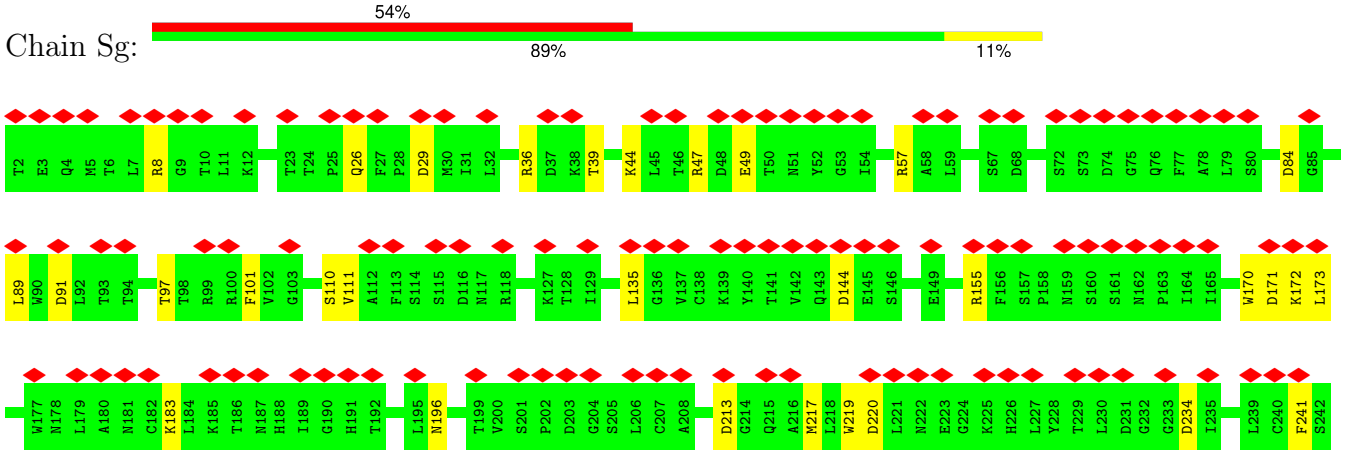
• Molecule 76: 40S ribosomal protein S29

Chain Sd:



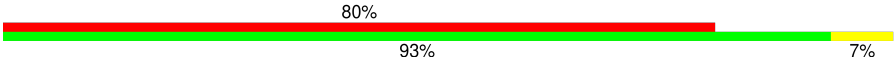
• Molecule 77: Receptor of activated protein C kinase 1

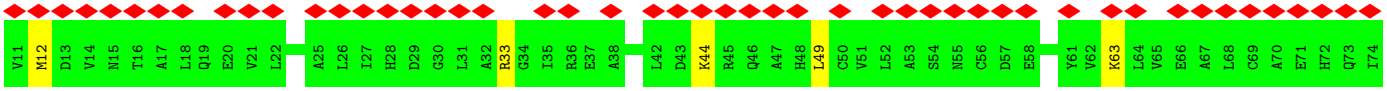
Chain Sg:

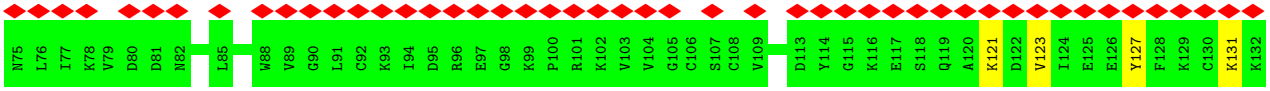


• Molecule 78: Small ribosomal subunit protein eS12

Chain SM:

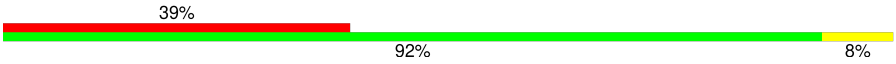


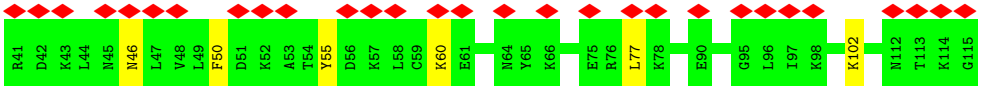




• Molecule 79: Small ribosomal subunit protein eS25

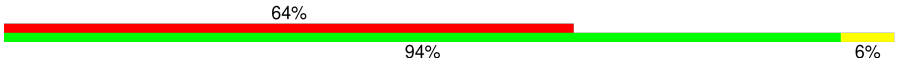
Chain SZ:

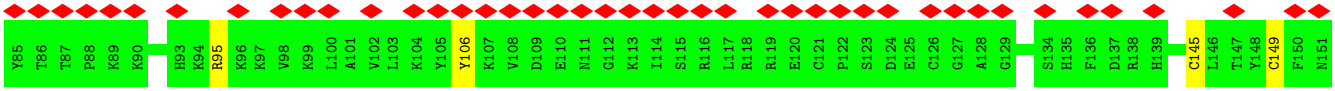




• Molecule 80: Ubiquitin-40S ribosomal protein S27a

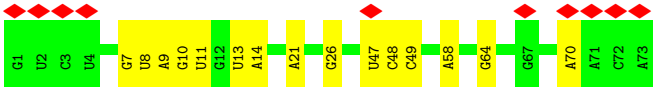
Chain Sf:





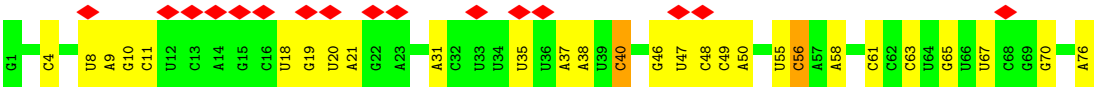
• Molecule 81: A/P site tRNA

Chain AP:



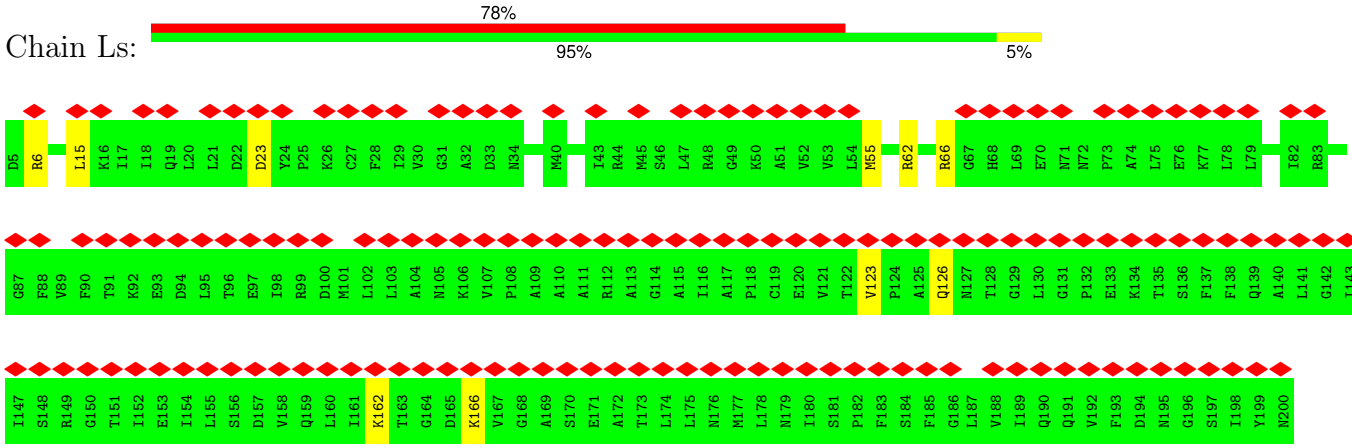
• Molecule 82: P/E site tRNA

Chain PE:



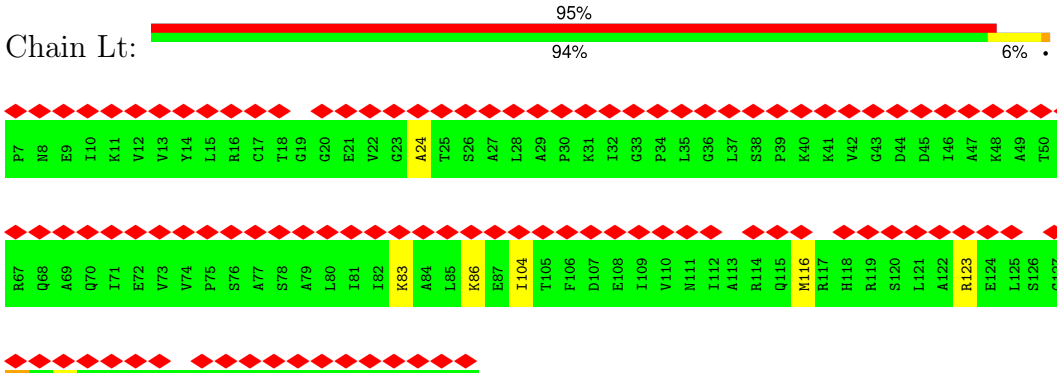
• Molecule 83: 60S acidic ribosomal protein P0

Chain Ls:



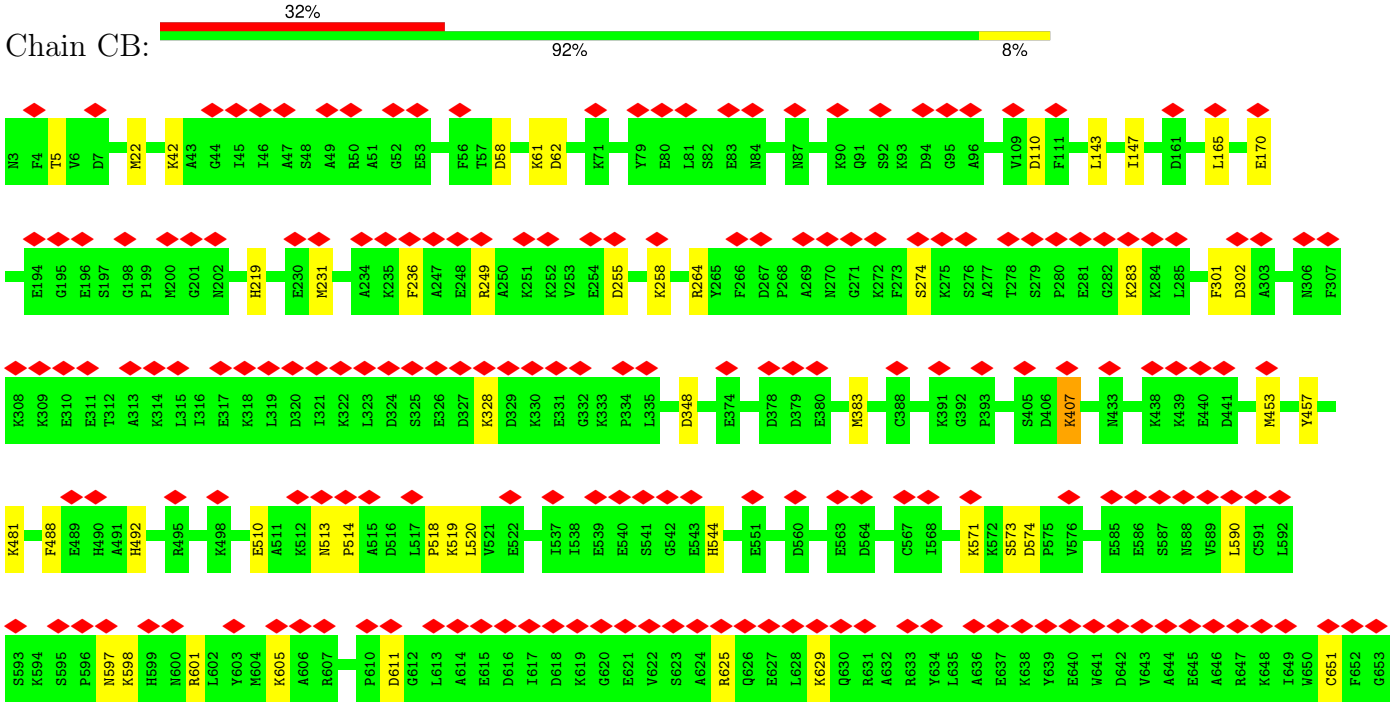
• Molecule 84: 60S ribosomal protein L12

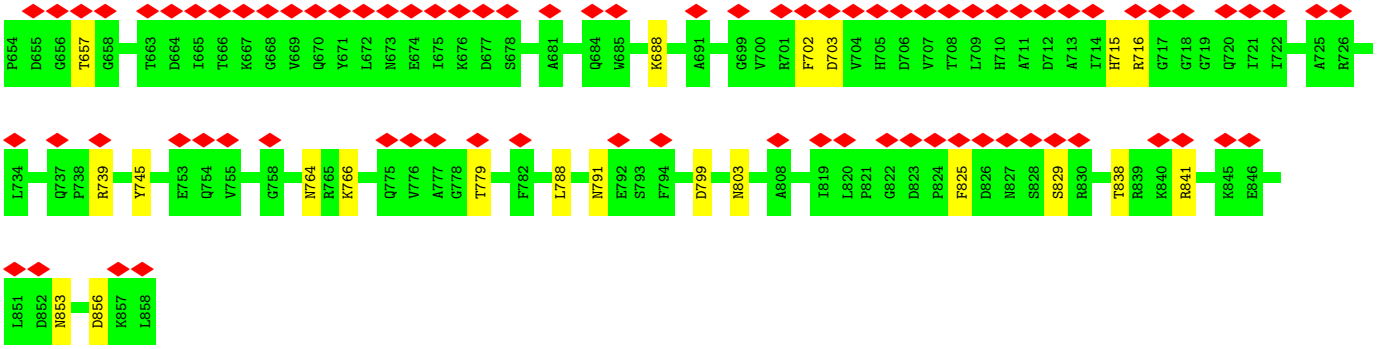
Chain Lt:



• Molecule 85: eEF2

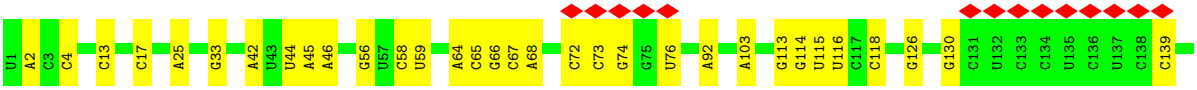
Chain CB:

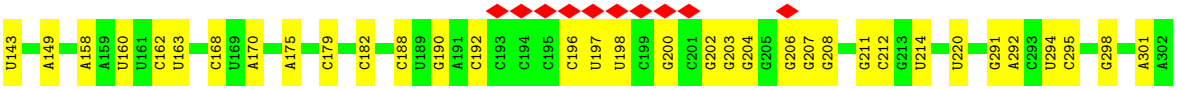


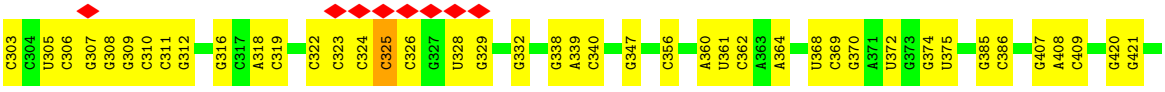


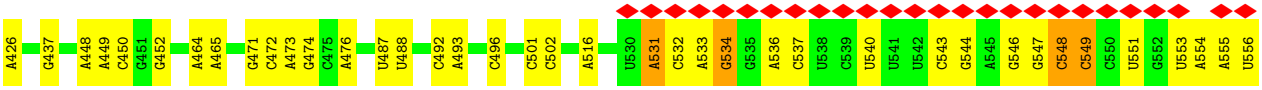
• Molecule 86: 18S rRNA

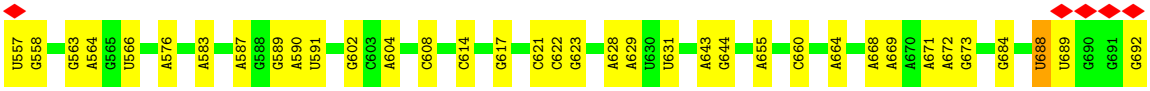
Chain S2:

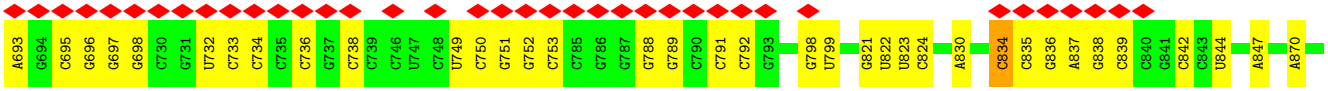


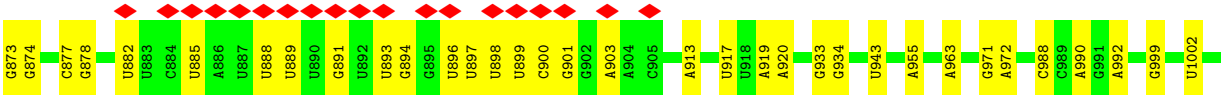


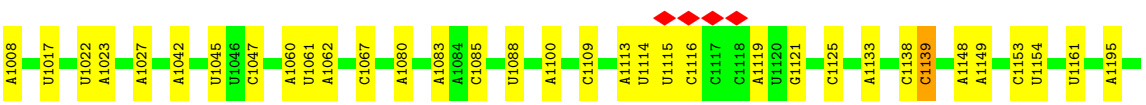


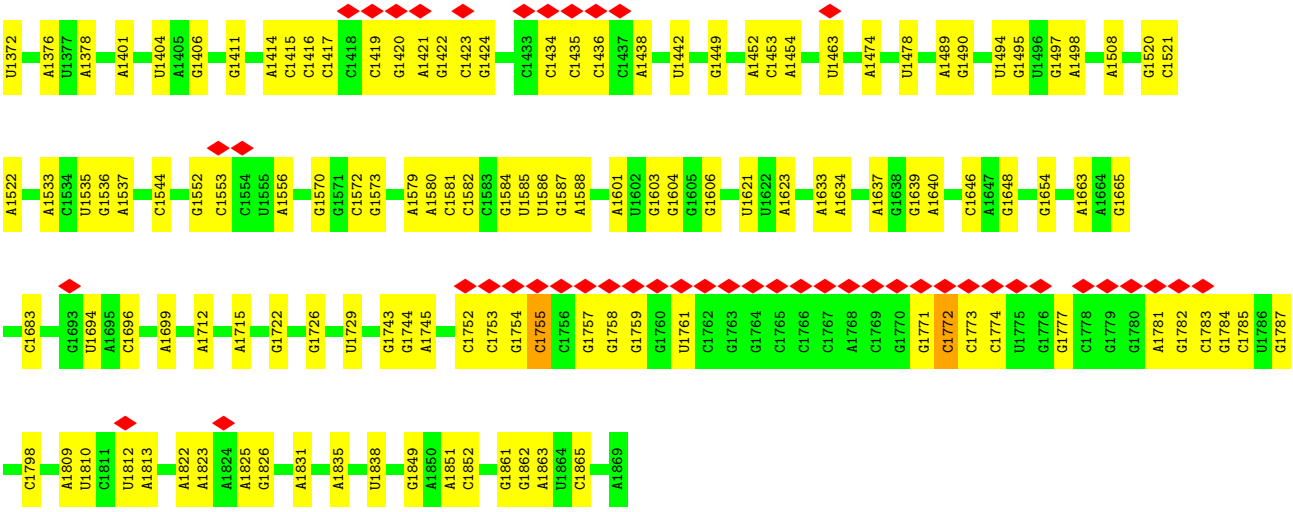











U1372 A1376 U1377 A1378 A1401 U1404 A1405 G1406 G1411 A1414 C1415 C1416 C1417 C1418 C1419 G1420 A1421 G1422 C1423 G1424 C1433 C1434 C1435 C1436 C1437 A1438 U1442 G1449 A1452 C1453 A1454 U1463 A1474 U1478 A1489 G1490 U1494 G1495 U1496 G1497 A1498 A1508 G1520 C1521
A1522 A1533 C1534 U1535 G1536 A1537 C1544 G1552 C1553 C1554 U1555 A1556 G1570 G1571 C1572 G1573 A1579 A1580 C1581 C1582 C1583 G1584 U1585 U1586 G1587 A1588 A1601 U1602 G1603 G1604 G1605 G1606 U1621 U1622 A1623 A1633 A1634 A1637 G1638 G1639 A1640 C1646 A1647 G1648 G1654 A1663 A1664 G1665
C1683 G1693 U1694 A1695 C1696 A1699 A1712 A1715 G1722 G1726 U1729 G1743 G1744 A1745 C1752 C1753 G1754 C1755 C1756 G1757 G1758 G1759 G1760 U1761 C1762 G1763 G1764 C1765 C1766 C1767 A1768 C1769 C1770 G1771 C1772 C1773 C1774 U1775 G1776 G1777 C1778 G1779 G1780 A1781 G1782 C1783 G1784 C1785 U1786 G1787
C1798 A1809 U1810 C1811 U1812 A1813 A1822 A1823 A1824 A1825 G1826 A1831 A1835 U1838 G1849 A1850 A1851 C1852 G1861 G1862 A1863 U1864 C1865 A1869

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	130154	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.563	Depositor
Minimum map value	-0.256	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.042	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	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: ZN, MG

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	Se	0.77	0/382	0.79	1/504 (0.2%)
2	CH	0.53	1/1028 (0.1%)	0.86	11/1376 (0.8%)
3	LW	0.26	0/979	0.57	0/1295
4	SE	0.28	0/2118	0.57	0/2849
5	SI	0.26	0/1715	0.56	0/2287
6	SL	0.26	0/1268	0.57	0/1696
7	SX	0.25	0/1116	0.53	0/1490
8	SG	0.40	2/1946 (0.1%)	0.75	5/2590 (0.2%)
9	SJ	0.28	0/1550	0.64	0/2069
10	SY	0.28	0/1083	0.61	1/1438 (0.1%)
11	SA	0.26	0/1778	0.56	0/2416
12	SB	0.27	0/1765	0.53	0/2362
13	SH	0.28	0/1519	0.57	1/2033 (0.0%)
14	SV	0.25	0/643	0.58	0/860
15	Sa	0.29	0/836	0.62	0/1121
16	SC	0.29	0/1762	0.54	0/2381
17	SN	0.26	0/1232	0.52	0/1656
18	SO	0.25	0/1062	0.64	2/1425 (0.1%)
19	SW	0.28	0/1051	0.56	0/1406
20	Sb	0.24	0/665	0.54	0/891
21	L5	0.33	0/89313	0.86	82/139291 (0.1%)
22	L7	0.30	0/2861	0.80	0/4459
23	L8	0.32	0/3701	0.79	1/5766 (0.0%)
24	LA	0.28	0/1936	0.61	1/2596 (0.0%)
25	LB	0.27	0/3306	0.56	1/4424 (0.0%)
26	LC	0.26	0/2981	0.56	1/4002 (0.0%)
27	LD	0.28	0/2428	0.53	0/3252
28	LE	0.26	0/1942	0.56	0/2606
29	LF	0.28	0/1905	0.54	0/2539
30	LG	0.26	0/1960	0.54	0/2637
31	LH	0.27	0/1537	0.57	0/2066
32	LI	0.30	0/1673	0.56	0/2233

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	LJ	0.28	0/1433	0.61	0/1915
34	LL	0.26	0/1732	0.58	0/2315
35	LM	0.27	0/1161	0.56	0/1554
36	LN	0.26	0/1746	0.57	0/2338
37	LO	0.27	0/1682	0.53	0/2250
38	LP	0.26	0/1268	0.52	0/1701
39	LQ	0.31	0/1537	0.64	0/2052
40	LR	0.25	0/1582	0.58	0/2091
41	LS	0.26	0/1493	0.55	0/2003
42	LT	0.27	0/1326	0.54	0/1770
43	LU	0.27	0/839	0.61	1/1126 (0.1%)
44	LV	0.28	0/993	0.54	0/1332
45	LX	0.26	0/1002	0.56	0/1345
46	LY	0.27	0/1132	0.56	0/1504
47	LZ	0.28	0/1130	0.57	0/1507
48	La	0.27	0/1191	0.54	0/1591
49	Lb	0.24	0/889	0.62	1/1175 (0.1%)
50	Lc	0.26	0/774	0.55	0/1038
51	Ld	0.26	0/903	0.59	0/1216
52	Le	0.26	0/1071	0.55	0/1429
53	Lf	0.27	0/895	0.59	0/1198
54	Lg	0.28	0/916	0.59	0/1220
55	Lh	0.25	0/1023	0.54	0/1351
56	Li	0.25	0/843	0.58	0/1115
57	Lj	0.26	0/720	0.60	0/952
58	Lk	0.26	0/575	0.54	0/761
59	Ll	0.24	0/454	0.57	0/599
60	Lm	0.25	0/435	0.55	0/575
61	Ln	0.24	0/231	0.70	0/294
62	Lo	0.30	0/876	0.59	0/1156
63	Lp	0.34	0/718	0.53	0/953
64	Lr	0.42	1/1017 (0.1%)	0.78	2/1364 (0.1%)
65	Lz	0.25	0/1769	0.53	1/2371 (0.0%)
66	SR	0.26	0/1105	0.64	1/1484 (0.1%)
67	SD	0.26	0/1793	0.56	0/2414
68	SF	0.26	0/1516	0.53	0/2037
69	SK	0.64	4/851 (0.5%)	0.92	6/1147 (0.5%)
70	SP	0.25	0/1003	0.55	0/1342
71	SQ	0.27	0/1160	0.61	0/1553
72	SS	0.25	0/1216	0.58	0/1628
73	ST	0.26	0/1131	0.56	0/1515
74	SU	0.25	0/831	0.61	0/1115
75	Sc	0.25	0/508	0.65	0/680

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	Sd	0.25	0/470	0.60	0/623
77	Sg	0.32	1/2493 (0.0%)	0.59	1/3394 (0.0%)
78	SM	0.24	0/950	0.53	0/1275
79	SZ	0.27	0/604	0.63	0/810
80	Sf	0.26	0/560	0.56	0/745
81	AP	0.19	0/1692	0.78	0/2634
82	PE	0.26	0/1778	0.89	2/2767 (0.1%)
83	Ls	0.27	0/1519	0.54	1/2052 (0.0%)
84	Lt	0.28	0/1058	0.58	0/1430
85	CB	0.40	3/6734 (0.0%)	0.64	6/9094 (0.1%)
86	S2	0.25	0/41241	0.82	40/64251 (0.1%)
All	All	0.30	12/246610 (0.0%)	0.75	169/361167 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	SX	0	1
13	SH	0	1
24	LA	0	1
25	LB	0	2
34	LL	0	1
35	LM	0	2
37	LO	0	1
42	LT	0	1
53	Lf	0	3
57	Lj	0	1
70	SP	0	1
71	SQ	0	1
All	All	0	16

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	CB	514	PRO	CG-CD	-20.58	0.82	1.50
69	SK	33	PRO	CG-CD	-10.86	1.14	1.50
8	SG	62	PRO	CG-CD	-10.65	1.15	1.50
85	CB	513	ASN	C-N	7.86	1.49	1.34
85	CB	513	ASN	C-O	7.84	1.38	1.23
69	SK	32	HIS	C-N	7.47	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
77	Sg	101	PHE	CE1-CZ	7.29	1.51	1.37
69	SK	32	HIS	C-O	7.07	1.36	1.23
64	Lr	122	LYS	C-N	6.95	1.47	1.34
2	CH	116	PRO	N-CD	5.51	1.55	1.47
69	SK	33	PRO	N-CD	5.20	1.55	1.47
8	SG	61	PHE	C-O	5.14	1.33	1.23

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
85	CB	514	PRO	N-CD-CG	-21.13	71.50	103.20
85	CB	514	PRO	CB-CG-CD	18.81	179.86	106.50
8	SG	62	PRO	N-CD-CG	-16.20	78.89	103.20
69	SK	33	PRO	N-CD-CG	-14.78	81.03	103.20
64	Lr	123	PRO	CA-N-CD	-14.04	91.84	111.50
64	Lr	122	LYS	C-N-CD	11.44	152.43	128.40
85	CB	514	PRO	CA-CB-CG	-10.23	84.57	104.00
69	SK	33	PRO	N-CA-CB	-9.80	91.53	103.30
8	SG	62	PRO	CA-CB-CG	-9.70	85.58	104.00
2	CH	116	PRO	CA-N-CD	-9.66	97.97	111.50
21	L5	129	C	N3-C2-O2	-9.55	115.22	121.90
21	L5	485	C	C2-N1-C1'	9.52	129.28	118.80
21	L5	174	C	N3-C2-O2	-9.24	115.43	121.90
69	SK	32	HIS	C-N-CD	9.19	147.70	128.40
85	CB	513	ASN	C-N-CD	9.06	147.44	128.40
49	Lb	118	LEU	CA-CB-CG	8.75	135.42	115.30
21	L5	2710	C	C2-N1-C1'	8.74	128.41	118.80
85	CB	514	PRO	N-CA-CB	-8.68	92.88	103.30
1	Se	121	PRO	CA-N-CD	-8.67	99.37	111.50
21	L5	2710	C	N1-C2-O2	8.66	124.10	118.90
2	CH	103	PRO	CA-N-CD	-8.55	99.53	111.50
2	CH	17	PRO	CA-N-CD	-8.46	99.65	111.50
2	CH	140	PRO	CA-N-CD	-8.44	99.69	111.50
21	L5	4138	C	N3-C2-O2	-8.26	116.12	121.90
86	S2	1453	C	C2-N1-C1'	8.08	127.69	118.80
86	S2	356	C	C2-N1-C1'	8.04	127.65	118.80
86	S2	356	C	N1-C2-O2	7.93	123.66	118.90
21	L5	1447	C	N3-C2-O2	-7.84	116.41	121.90
21	L5	456	C	O4'-C1'-N1	7.78	114.43	108.20
21	L5	130	C	N3-C2-O2	-7.78	116.45	121.90
21	L5	456	C	N3-C2-O2	-7.75	116.47	121.90
86	S2	1453	C	N1-C2-O2	7.64	123.48	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L5	1252	C	N3-C2-O2	-7.62	116.57	121.90
86	S2	1416	C	N3-C2-O2	-7.54	116.62	121.90
86	S2	1772	C	N1-C2-O2	7.47	123.39	118.90
21	L5	3773	U	N3-C2-O2	-7.34	117.06	122.20
21	L5	2710	C	N3-C2-O2	-7.31	116.78	121.90
86	S2	1424	G	N3-C4-N9	7.27	130.36	126.00
86	S2	1772	C	N3-C2-O2	-7.27	116.81	121.90
21	L5	1082	C	O4'-C1'-N1	7.25	114.00	108.20
21	L5	485	C	C6-N1-C1'	-7.22	112.13	120.80
21	L5	1182	C	C2-N1-C1'	7.17	126.69	118.80
21	L5	490	C	N3-C2-O2	-7.01	116.99	121.90
8	SG	61	PHE	C-N-CD	6.99	143.08	128.40
21	L5	417	G	O4'-C1'-N9	6.86	113.69	108.20
86	S2	602	G	N3-C4-N9	-6.86	121.89	126.00
21	L5	1994	C	N3-C2-O2	-6.83	117.12	121.90
2	CH	102	LYS	C-N-CD	-6.76	105.73	120.60
85	CB	518	PRO	CA-N-CD	-6.73	102.08	111.50
21	L5	1182	C	N1-C2-O2	6.70	122.92	118.90
86	S2	548	C	C2-N1-C1'	6.69	126.16	118.80
69	SK	33	PRO	CA-CB-CG	-6.68	91.30	104.00
21	L5	925	C	N1-C2-O2	6.64	122.88	118.90
8	SG	62	PRO	CA-N-CD	-6.51	102.38	111.50
21	L5	2710	C	C6-N1-C2	-6.48	117.71	120.30
21	L5	175	C	N3-C2-O2	-6.46	117.38	121.90
86	S2	356	C	N3-C2-O2	-6.42	117.41	121.90
21	L5	1082	C	N3-C2-O2	-6.38	117.43	121.90
21	L5	4147	G	N1-C6-O6	-6.33	116.10	119.90
24	LA	246	LEU	CA-CB-CG	6.28	129.74	115.30
86	S2	1022	U	C2-N1-C1'	6.26	125.21	117.70
21	L5	4709	U	C2-N1-C1'	6.26	125.21	117.70
69	SK	33	PRO	CA-N-CD	-6.25	102.74	111.50
21	L5	925	C	N3-C2-O2	-6.24	117.53	121.90
21	L5	1414	C	N1-C2-O2	6.18	122.61	118.90
8	SG	180	VAL	C-N-CA	6.17	137.12	121.70
21	L5	4147	G	C5-C6-O6	6.17	132.30	128.60
82	PE	56	C	N3-C2-O2	-6.16	117.59	121.90
18	SO	14	VAL	C-N-CA	6.14	137.05	121.70
86	S2	1424	G	C4-N9-C1'	6.14	134.48	126.50
18	SO	119	LEU	CA-CB-CG	6.11	129.34	115.30
21	L5	100	C	C2-N1-C1'	6.09	125.50	118.80
21	L5	489	C	N1-C2-O2	6.09	122.55	118.90
21	L5	138	G	N3-C4-N9	6.08	129.65	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L5	209	U	C2-N1-C1'	6.08	124.99	117.70
21	L5	1191	C	N3-C2-O2	-6.07	117.65	121.90
21	L5	1414	C	N3-C2-O2	-6.04	117.67	121.90
2	CH	139	LYS	C-N-CD	-6.03	107.33	120.60
86	S2	621	C	N3-C2-O2	-6.03	117.68	121.90
21	L5	2410	C	C2-N1-C1'	6.02	125.42	118.80
86	S2	1453	C	N3-C2-O2	-5.99	117.70	121.90
86	S2	688	U	P-O3'-C3'	5.99	126.89	119.70
21	L5	4709	U	C5-C4-O4	-5.96	122.33	125.90
21	L5	4928	C	C2-N1-C1'	5.91	125.30	118.80
86	S2	1424	G	C8-N9-C1'	-5.89	119.34	127.00
86	S2	531	A	OP1-P-O3'	5.87	118.11	105.20
21	L5	904	C	C2-N1-C1'	5.83	125.21	118.80
21	L5	2710	C	C6-N1-C1'	-5.81	113.83	120.80
86	S2	356	C	C6-N1-C2	-5.79	117.99	120.30
21	L5	4924	C	N3-C2-O2	-5.78	117.85	121.90
69	SK	83	LEU	CA-CB-CG	5.78	128.60	115.30
21	L5	3761	C	C2-N1-C1'	5.77	125.14	118.80
86	S2	834	C	N3-C2-O2	-5.73	117.89	121.90
86	S2	549	C	C6-N1-C2	-5.72	118.01	120.30
86	S2	602	G	N9-C4-C5	5.64	107.66	105.40
21	L5	985	C	C2-N1-C1'	5.62	124.98	118.80
10	SY	44	LEU	CA-CB-CG	5.61	128.19	115.30
66	SR	106	LEU	CA-CB-CG	5.60	128.18	115.30
86	S2	1520	G	C4-N9-C1'	5.60	133.78	126.50
21	L5	2627	C	C2-N1-C1'	5.58	124.94	118.80
21	L5	4926	C	C2-N1-C1'	5.57	124.92	118.80
21	L5	654	C	N1-C2-O2	5.54	122.22	118.90
21	L5	3773	U	C2-N1-C1'	5.54	124.35	117.70
86	S2	1453	C	C6-N1-C1'	-5.53	114.16	120.80
21	L5	485	C	N1-C2-O2	5.50	122.20	118.90
21	L5	262	G	N1-C6-O6	-5.48	116.61	119.90
86	S2	602	G	C8-N9-C1'	5.48	134.12	127.00
21	L5	1182	C	N3-C2-O2	-5.46	118.08	121.90
86	S2	322	C	N1-C2-O2	5.45	122.17	118.90
86	S2	534	G	N3-C4-N9	-5.45	122.73	126.00
21	L5	1216	C	C2-N1-C1'	5.44	124.78	118.80
86	S2	356	C	C6-N1-C1'	-5.42	114.29	120.80
21	L5	138	G	N3-C4-C5	-5.41	125.89	128.60
21	L5	1367	C	C2-N1-C1'	5.41	124.75	118.80
86	S2	1453	C	C6-N1-C2	-5.39	118.14	120.30
21	L5	2627	C	N1-C2-O2	5.39	122.14	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	LU	112	LEU	CA-CB-CG	5.38	127.67	115.30
86	S2	118	C	C2-N1-C1'	5.37	124.70	118.80
21	L5	129	C	C6-N1-C2	-5.36	118.16	120.30
86	S2	549	C	C6-N1-C1'	5.33	127.19	120.80
21	L5	4093	G	O4'-C1'-N9	5.33	112.46	108.20
21	L5	4926	C	N1-C2-O2	5.31	122.08	118.90
86	S2	534	G	C5-C6-O6	5.30	131.78	128.60
21	L5	1994	C	N1-C2-O2	5.28	122.07	118.90
25	LB	306	ASP	CB-CG-OD1	5.28	123.05	118.30
86	S2	1424	G	C6-C5-N7	-5.28	127.23	130.40
21	L5	3773	U	N1-C2-O2	5.27	126.49	122.80
86	S2	1424	G	N3-C4-C5	-5.25	125.98	128.60
86	S2	1755	C	N1-C2-O2	5.24	122.05	118.90
21	L5	739	G	N3-C4-N9	5.23	129.14	126.00
13	SH	30	LEU	CA-CB-CG	5.23	127.32	115.30
77	Sg	89	LEU	CD1-CG-CD2	5.23	126.18	110.50
21	L5	262	G	C5-C6-O6	5.22	131.73	128.60
2	CH	71	ASP	CB-CG-OD2	5.22	123.00	118.30
2	CH	108	ASP	CB-CG-OD2	5.21	122.99	118.30
2	CH	62	ASP	CB-CG-OD2	5.21	122.99	118.30
21	L5	4898	G	C5-C6-O6	5.21	131.72	128.60
2	CH	37	ASP	CB-CG-OD2	5.19	122.97	118.30
21	L5	4101	C	N3-C4-C5	5.17	123.97	121.90
65	Lz	194	LEU	CA-CB-CG	5.17	127.19	115.30
21	L5	1447	C	N1-C2-O2	5.17	122.00	118.90
83	Ls	15	LEU	CA-CB-CG	5.16	127.17	115.30
21	L5	963	G	C4-N9-C1'	5.15	133.20	126.50
2	CH	94	ASP	CB-CG-OD2	5.14	122.93	118.30
21	L5	1082	C	C6-N1-C1'	5.13	126.95	120.80
26	LC	2	ALA	C-N-CA	5.12	134.49	121.70
82	PE	40	C	C2-N1-C1'	5.11	124.42	118.80
86	S2	602	G	C4-N9-C1'	-5.11	119.86	126.50
21	L5	4928	C	N1-C2-O2	5.11	121.97	118.90
86	S2	1520	G	N3-C4-N9	5.11	129.06	126.00
21	L5	129	C	N1-C2-N3	5.10	122.77	119.20
21	L5	914	U	C5-C4-O4	-5.10	122.84	125.90
21	L5	4898	G	N1-C6-O6	-5.08	116.85	119.90
86	S2	549	C	C5-C4-N4	5.08	123.76	120.20
86	S2	325	C	C2-N1-C1'	5.08	124.39	118.80
21	L5	140	G	C5-C6-O6	5.07	131.64	128.60
21	L5	1082	C	P-O3'-C3'	5.07	125.78	119.70
21	L5	664	G	N1-C6-O6	-5.07	116.86	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	L5	3761	C	N1-C2-O2	5.07	121.94	118.90
86	S2	1139	C	C2-N1-C1'	5.06	124.37	118.80
21	L5	1998	A	N1-C6-N6	-5.06	115.56	118.60
23	L8	111	U	C2-N1-C1'	5.04	123.75	117.70
21	L5	263	G	C5-C6-O6	5.03	131.62	128.60
21	L5	664	G	C5-C6-O6	5.03	131.62	128.60
21	L5	1241	C	C2-N1-C1'	5.03	124.33	118.80
21	L5	1241	C	N1-C2-O2	5.03	121.92	118.90
21	L5	2257	C	C2-N1-C1'	5.02	124.32	118.80
21	L5	115	C	C2-N1-C1'	5.01	124.31	118.80
21	L5	174	C	N1-C2-O2	5.00	121.90	118.90

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	LA	13	GLY	Peptide
25	LB	17	LEU	Peptide
25	LB	258	HIS	Peptide
34	LL	154	VAL	Peptide
35	LM	87	ALA	Peptide
35	LM	88	ALA	Peptide
37	LO	110	PRO	Peptide
42	LT	136	ARG	Peptide
53	Lf	103	VAL	Peptide
53	Lf	106	TYR	Peptide
53	Lf	79	GLY	Peptide
57	Lj	39	TYR	Peptide
13	SH	15	LYS	Peptide
70	SP	127	LYS	Peptide
71	SQ	43	GLU	Peptide
7	SX	126	ALA	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Se	45/58 (78%)	29 (64%)	12 (27%)	4 (9%)	0 0
2	CH	130/132 (98%)	53 (41%)	57 (44%)	20 (15%)	0 0
3	LW	114/118 (97%)	111 (97%)	3 (3%)	0	100 100
4	SE	260/262 (99%)	250 (96%)	10 (4%)	0	100 100
5	SI	204/206 (99%)	198 (97%)	6 (3%)	0	100 100
6	SL	151/153 (99%)	139 (92%)	12 (8%)	0	100 100
7	SX	139/141 (99%)	124 (89%)	14 (10%)	1 (1%)	19 31
8	SG	235/237 (99%)	221 (94%)	14 (6%)	0	100 100
9	SJ	183/185 (99%)	175 (96%)	7 (4%)	1 (0%)	25 40
10	SY	129/131 (98%)	121 (94%)	8 (6%)	0	100 100
11	SA	219/221 (99%)	201 (92%)	18 (8%)	0	100 100
12	SB	212/214 (99%)	205 (97%)	7 (3%)	0	100 100
13	SH	182/186 (98%)	163 (90%)	19 (10%)	0	100 100
14	SV	81/83 (98%)	74 (91%)	7 (9%)	0	100 100
15	Sa	100/102 (98%)	89 (89%)	11 (11%)	0	100 100
16	SC	220/222 (99%)	207 (94%)	13 (6%)	0	100 100
17	SN	148/150 (99%)	144 (97%)	4 (3%)	0	100 100
18	SO	138/140 (99%)	127 (92%)	11 (8%)	0	100 100
19	SW	127/129 (98%)	124 (98%)	3 (2%)	0	100 100
20	Sb	81/83 (98%)	72 (89%)	9 (11%)	0	100 100
24	LA	246/248 (99%)	226 (92%)	19 (8%)	1 (0%)	30 46
25	LB	400/402 (100%)	377 (94%)	22 (6%)	1 (0%)	37 53
26	LC	366/368 (100%)	346 (94%)	20 (6%)	0	100 100
27	LD	291/293 (99%)	275 (94%)	16 (6%)	0	100 100
28	LE	232/236 (98%)	209 (90%)	23 (10%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	LF	223/225 (99%)	215 (96%)	8 (4%)	0	100	100
30	LG	239/241 (99%)	225 (94%)	14 (6%)	0	100	100
31	LH	188/190 (99%)	177 (94%)	11 (6%)	0	100	100
32	LI	198/202 (98%)	191 (96%)	7 (4%)	0	100	100
33	LJ	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
34	LL	208/210 (99%)	191 (92%)	17 (8%)	0	100	100
35	LM	137/139 (99%)	128 (93%)	8 (6%)	1 (1%)	19	31
36	LN	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	25	40
37	LO	199/201 (99%)	193 (97%)	6 (3%)	0	100	100
38	LP	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
39	LQ	185/187 (99%)	179 (97%)	6 (3%)	0	100	100
40	LR	185/187 (99%)	181 (98%)	4 (2%)	0	100	100
41	LS	173/175 (99%)	164 (95%)	9 (5%)	0	100	100
42	LT	157/159 (99%)	146 (93%)	11 (7%)	0	100	100
43	LU	99/101 (98%)	82 (83%)	17 (17%)	0	100	100
44	LV	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
45	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
46	LY	132/134 (98%)	129 (98%)	3 (2%)	0	100	100
47	LZ	133/135 (98%)	124 (93%)	9 (7%)	0	100	100
48	La	145/147 (99%)	138 (95%)	7 (5%)	0	100	100
49	Lb	105/109 (96%)	98 (93%)	7 (7%)	0	100	100
50	Lc	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
51	Ld	105/107 (98%)	100 (95%)	5 (5%)	0	100	100
52	Le	126/128 (98%)	120 (95%)	6 (5%)	0	100	100
53	Lf	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	14	25
54	Lg	112/114 (98%)	112 (100%)	0	0	100	100
55	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
56	Li	100/102 (98%)	95 (95%)	5 (5%)	0	100	100
57	Lj	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
58	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
59	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
60	Lm	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
61	Ln	22/24 (92%)	22 (100%)	0	0	100	100
62	Lo	103/105 (98%)	100 (97%)	3 (3%)	0	100	100
63	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
64	Lr	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
65	Lz	215/217 (99%)	176 (82%)	39 (18%)	0	100	100
66	SR	133/135 (98%)	122 (92%)	10 (8%)	1 (1%)	16	28
67	SD	225/227 (99%)	206 (92%)	19 (8%)	0	100	100
68	SF	187/189 (99%)	166 (89%)	21 (11%)	0	100	100
69	SK	96/98 (98%)	87 (91%)	7 (7%)	2 (2%)	5	10
70	SP	119/121 (98%)	115 (97%)	4 (3%)	0	100	100
71	SQ	142/144 (99%)	125 (88%)	16 (11%)	1 (1%)	19	31
72	SS	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
73	ST	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	19	31
74	SU	102/104 (98%)	97 (95%)	5 (5%)	0	100	100
75	Sc	62/64 (97%)	51 (82%)	11 (18%)	0	100	100
76	Sd	53/55 (96%)	51 (96%)	1 (2%)	1 (2%)	6	11
77	Sg	311/313 (99%)	275 (88%)	36 (12%)	0	100	100
78	SM	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
79	SZ	73/75 (97%)	57 (78%)	16 (22%)	0	100	100
80	Sf	65/67 (97%)	59 (91%)	6 (9%)	0	100	100
83	Ls	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
84	Lt	137/141 (97%)	111 (81%)	24 (18%)	2 (2%)	8	14
85	CB	842/846 (100%)	792 (94%)	47 (6%)	3 (0%)	30	46
All	All	12824/13009 (99%)	11907 (93%)	875 (7%)	42 (0%)	38	53

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	CH	48	GLN
2	CH	66	GLU
85	CB	779	THR
1	Se	85	LYS
2	CH	50	LYS

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Mol	Chain	Res	Type
2	CH	111	SER
2	CH	113	ARG
2	CH	135	LYS
7	SX	127	ASN
36	LN	124	ASP
66	SR	124	VAL
69	SK	36	ALA
69	SK	96	ARG
84	Lt	144	ASP
85	CB	407	LYS
1	Se	79	SER
2	CH	31	ALA
2	CH	44	TRP
2	CH	89	GLY
2	CH	114	ALA
35	LM	88	ALA
2	CH	18	THR
2	CH	35	GLY
2	CH	45	ALA
2	CH	46	ALA
2	CH	53	SER
2	CH	71	ASP
2	CH	118	ASN
25	LB	4	ARG
84	Lt	24	ALA
85	CB	611	ASP
1	Se	84	GLY
1	Se	92	LYS
2	CH	115	ILE
73	ST	41	LYS
76	Sd	14	PHE
2	CH	92	GLN
2	CH	134	GLY
9	SJ	123	ILE
24	LA	55	GLY
53	Lf	107	PRO
71	SQ	44	PRO

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	Se	39/47 (83%)	27 (69%)	12 (31%)	0 0
2	CH	106/106 (100%)	100 (94%)	6 (6%)	17 29
3	LW	97/97 (100%)	87 (90%)	10 (10%)	6 9
4	SE	224/224 (100%)	199 (89%)	25 (11%)	5 8
5	SI	178/178 (100%)	161 (90%)	17 (10%)	7 10
6	SL	137/137 (100%)	118 (86%)	19 (14%)	3 4
7	SX	113/113 (100%)	106 (94%)	7 (6%)	15 26
8	SG	207/207 (100%)	191 (92%)	16 (8%)	10 17
9	SJ	161/161 (100%)	148 (92%)	13 (8%)	9 16
10	SY	113/113 (100%)	99 (88%)	14 (12%)	4 5
11	SA	183/183 (100%)	172 (94%)	11 (6%)	16 28
12	SB	195/195 (100%)	169 (87%)	26 (13%)	3 4
13	SH	166/166 (100%)	152 (92%)	14 (8%)	9 14
14	SV	67/67 (100%)	54 (81%)	13 (19%)	1 1
15	Sa	89/89 (100%)	81 (91%)	8 (9%)	8 12
16	SC	188/188 (100%)	172 (92%)	16 (8%)	8 13
17	SN	130/130 (100%)	123 (95%)	7 (5%)	18 32
18	SO	110/110 (100%)	100 (91%)	10 (9%)	7 12
19	SW	112/112 (100%)	108 (96%)	4 (4%)	30 48
20	Sb	75/75 (100%)	72 (96%)	3 (4%)	27 44
24	LA	190/190 (100%)	176 (93%)	14 (7%)	11 19
25	LB	348/348 (100%)	322 (92%)	26 (8%)	11 19
26	LC	306/306 (100%)	286 (94%)	20 (6%)	14 24
27	LD	246/247 (100%)	227 (92%)	19 (8%)	10 17
28	LE	209/209 (100%)	195 (93%)	14 (7%)	13 22
29	LF	194/194 (100%)	185 (95%)	9 (5%)	23 38
30	LG	203/205 (99%)	185 (91%)	18 (9%)	8 12
31	LH	169/169 (100%)	162 (96%)	7 (4%)	26 43
32	LI	172/172 (100%)	163 (95%)	9 (5%)	19 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
33	LJ	148/148 (100%)	137 (93%)	11 (7%)	11 19
34	LL	176/176 (100%)	162 (92%)	14 (8%)	10 16
35	LM	118/118 (100%)	110 (93%)	8 (7%)	13 22
36	LN	171/171 (100%)	162 (95%)	9 (5%)	19 33
37	LO	173/173 (100%)	168 (97%)	5 (3%)	37 58
38	LP	134/134 (100%)	123 (92%)	11 (8%)	9 15
39	LQ	164/164 (100%)	156 (95%)	8 (5%)	21 36
40	LR	166/166 (100%)	156 (94%)	10 (6%)	16 28
41	LS	156/156 (100%)	150 (96%)	6 (4%)	28 47
42	LT	139/139 (100%)	132 (95%)	7 (5%)	20 35
43	LU	91/91 (100%)	79 (87%)	12 (13%)	3 4
44	LV	101/101 (100%)	92 (91%)	9 (9%)	8 12
45	LX	108/108 (100%)	99 (92%)	9 (8%)	9 15
46	LY	124/124 (100%)	118 (95%)	6 (5%)	21 36
47	LZ	117/117 (100%)	107 (92%)	10 (8%)	8 13
48	La	120/120 (100%)	118 (98%)	2 (2%)	56 75
49	Lb	88/90 (98%)	80 (91%)	8 (9%)	7 12
50	Lc	83/83 (100%)	76 (92%)	7 (8%)	9 14
51	Ld	98/98 (100%)	92 (94%)	6 (6%)	15 27
52	Le	114/114 (100%)	107 (94%)	7 (6%)	15 27
53	Lf	88/88 (100%)	81 (92%)	7 (8%)	10 16
54	Lg	98/98 (100%)	94 (96%)	4 (4%)	26 43
55	Lh	109/109 (100%)	100 (92%)	9 (8%)	9 15
56	Li	86/86 (100%)	77 (90%)	9 (10%)	5 9
57	Lj	73/73 (100%)	66 (90%)	7 (10%)	7 10
58	Lk	64/64 (100%)	61 (95%)	3 (5%)	22 37
59	Ll	47/47 (100%)	45 (96%)	2 (4%)	25 41
60	Lm	48/48 (100%)	46 (96%)	2 (4%)	25 42
61	Ln	23/23 (100%)	19 (83%)	4 (17%)	1 2
62	Lo	93/93 (100%)	83 (89%)	10 (11%)	5 8
63	Lp	74/74 (100%)	68 (92%)	6 (8%)	9 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
64	Lr	109/109 (100%)	97 (89%)	12 (11%)	5 8
65	Lz	195/196 (100%)	176 (90%)	19 (10%)	6 10
66	SR	122/122 (100%)	109 (89%)	13 (11%)	5 8
67	SD	190/190 (100%)	171 (90%)	19 (10%)	6 10
68	SF	159/159 (100%)	151 (95%)	8 (5%)	20 35
69	SK	89/89 (100%)	81 (91%)	8 (9%)	8 12
70	SP	107/107 (100%)	96 (90%)	11 (10%)	6 9
71	SQ	119/119 (100%)	105 (88%)	14 (12%)	4 6
72	SS	126/126 (100%)	117 (93%)	9 (7%)	12 20
73	ST	113/113 (100%)	106 (94%)	7 (6%)	15 26
74	SU	94/94 (100%)	90 (96%)	4 (4%)	25 41
75	Sc	57/57 (100%)	54 (95%)	3 (5%)	19 33
76	Sd	48/48 (100%)	42 (88%)	6 (12%)	3 5
77	Sg	272/272 (100%)	240 (88%)	32 (12%)	4 6
78	SM	102/104 (98%)	93 (91%)	9 (9%)	8 12
79	SZ	66/66 (100%)	60 (91%)	6 (9%)	7 12
80	Sf	60/60 (100%)	56 (93%)	4 (7%)	13 22
83	Ls	162/164 (99%)	153 (94%)	9 (6%)	17 30
84	Lt	112/115 (97%)	104 (93%)	8 (7%)	12 20
85	CB	722/723 (100%)	656 (91%)	66 (9%)	7 12
All	All	11143/11165 (100%)	10261 (92%)	882 (8%)	13 17

All (882) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Se	80	LEU
1	Se	90	THR
1	Se	92	LYS
1	Se	95	LYS
1	Se	98	LYS
1	Se	100	LYS
1	Se	101	LYS
1	Se	105	ARG
1	Se	108	ARG
1	Se	109	ARG

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Mol	Chain	Res	Type
1	Se	114	ARG
1	Se	115	ARG
2	CH	131	LYS
2	CH	132	LEU
2	CH	133	ARG
2	CH	135	LYS
2	CH	136	ASP
2	CH	146	ARG
3	LW	1	MET
3	LW	12	LYS
3	LW	19	ARG
3	LW	30	GLN
3	LW	38	SER
3	LW	50	ASN
3	LW	58	LYS
3	LW	91	MET
3	LW	102	LYS
3	LW	110	ARG
4	SE	50	ASN
4	SE	57	THR
4	SE	62	LYS
4	SE	66	MET
4	SE	87	MET
4	SE	94	LYS
4	SE	106	LYS
4	SE	111	VAL
4	SE	115	THR
4	SE	121	TYR
4	SE	126	VAL
4	SE	128	LYS
4	SE	140	VAL
4	SE	145	ARG
4	SE	163	ASP
4	SE	181	CYS
4	SE	205	PHE
4	SE	224	ASN
4	SE	226	PHE
4	SE	227	VAL
4	SE	238	LEU
4	SE	245	ARG
4	SE	252	ARG
4	SE	254	LYS

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Mol	Chain	Res	Type
4	SE	255	ARG
5	SI	11	ARG
5	SI	22	HIS
5	SI	47	ARG
5	SI	62	VAL
5	SI	65	PHE
5	SI	67	TRP
5	SI	94	LYS
5	SI	95	THR
5	SI	113	TYR
5	SI	116	HIS
5	SI	124	LYS
5	SI	140	LYS
5	SI	153	LYS
5	SI	162	LEU
5	SI	166	PHE
5	SI	184	ARG
5	SI	205	ARG
6	SL	10	TYR
6	SL	12	LYS
6	SL	17	PHE
6	SL	19	ASN
6	SL	37	TYR
6	SL	38	LYS
6	SL	54	THR
6	SL	69	ARG
6	SL	74	SER
6	SL	83	GLN
6	SL	84	ARG
6	SL	87	VAL
6	SL	100	ASN
6	SL	114	SER
6	SL	116	CYS
6	SL	118	ARG
6	SL	124	ASP
6	SL	135	SER
6	SL	138	VAL
7	SX	8	ARG
7	SX	45	SER
7	SX	73	GLN
7	SX	92	ASN
7	SX	98	ASP

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Mol	Chain	Res	Type
7	SX	105	PHE
7	SX	137	LYS
8	SG	1	MET
8	SG	23	LYS
8	SG	52	ILE
8	SG	53	SER
8	SG	87	ARG
8	SG	96	SER
8	SG	105	ASN
8	SG	111	LEU
8	SG	119	LYS
8	SG	128	THR
8	SG	150	GLU
8	SG	167	LYS
8	SG	177	GLN
8	SG	179	LEU
8	SG	201	LYS
8	SG	204	GLU
9	SJ	5	ARG
9	SJ	17	ARG
9	SJ	21	GLU
9	SJ	73	GLU
9	SJ	86	VAL
9	SJ	95	ASP
9	SJ	105	PHE
9	SJ	111	GLN
9	SJ	115	PHE
9	SJ	119	LEU
9	SJ	122	SER
9	SJ	146	SER
9	SJ	175	ARG
10	SY	6	THR
10	SY	13	MET
10	SY	26	ASP
10	SY	43	LYS
10	SY	51	THR
10	SY	58	PHE
10	SY	62	THR
10	SY	97	TYR
10	SY	100	LYS
10	SY	101	LYS
10	SY	104	ARG

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Mol	Chain	Res	Type
10	SY	118	ARG
10	SY	130	LYS
10	SY	132	LYS
11	SA	17	LYS
11	SA	18	PHE
11	SA	40	LYS
11	SA	53	ARG
11	SA	74	VAL
11	SA	102	ARG
11	SA	109	THR
11	SA	138	SER
11	SA	142	LEU
11	SA	205	ARG
11	SA	206	ASP
12	SB	29	ASP
12	SB	32	ASP
12	SB	38	MET
12	SB	53	GLN
12	SB	55	THR
12	SB	60	ASP
12	SB	68	GLU
12	SB	94	LYS
12	SB	99	ASN
12	SB	124	HIS
12	SB	131	ASP
12	SB	137	LEU
12	SB	139	CYS
12	SB	159	GLN
12	SB	167	LYS
12	SB	169	MET
12	SB	172	MET
12	SB	177	GLN
12	SB	178	THR
12	SB	182	LYS
12	SB	192	SER
12	SB	201	CYS
12	SB	205	TYR
12	SB	222	LYS
12	SB	229	MET
12	SB	231	LEU
13	SH	29	GLU
13	SH	41	ARG

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Mol	Chain	Res	Type
13	SH	57	ARG
13	SH	58	LYS
13	SH	72	PHE
13	SH	78	ARG
13	SH	133	LEU
13	SH	145	ARG
13	SH	149	ASP
13	SH	156	VAL
13	SH	160	LYS
13	SH	177	TYR
13	SH	178	LYS
13	SH	183	LYS
14	SV	1	MET
14	SV	15	ARG
14	SV	17	CYS
14	SV	20	SER
14	SV	22	ARG
14	SV	29	HIS
14	SV	47	ASN
14	SV	50	PHE
14	SV	52	THR
14	SV	56	CYS
14	SV	62	MET
14	SV	65	SER
14	SV	83	PHE
15	Sa	2	THR
15	Sa	15	ARG
15	Sa	42	ARG
15	Sa	54	SER
15	Sa	89	ARG
15	Sa	94	ASP
15	Sa	100	ARG
15	Sa	102	ARG
16	SC	73	MET
16	SC	77	SER
16	SC	78	LEU
16	SC	80	GLU
16	SC	105	GLU
16	SC	117	ARG
16	SC	152	ARG
16	SC	167	ARG
16	SC	173	LYS

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Mol	Chain	Res	Type
16	SC	194	ARG
16	SC	206	SER
16	SC	220	ASP
16	SC	250	TYR
16	SC	259	THR
16	SC	271	ASP
16	SC	279	ARG
17	SN	9	LYS
17	SN	19	ARG
17	SN	42	LYS
17	SN	87	ASP
17	SN	105	ASN
17	SN	109	LYS
17	SN	140	LYS
18	SO	38	ASN
18	SO	66	ARG
18	SO	84	ARG
18	SO	86	LYS
18	SO	104	ARG
18	SO	106	LYS
18	SO	114	SER
18	SO	124	MET
18	SO	142	ARG
18	SO	146	ARG
19	SW	55	ASP
19	SW	57	ARG
19	SW	103	VAL
19	SW	111	MET
20	Sb	78	SER
20	Sb	79	PHE
20	Sb	83	GLN
24	LA	4	VAL
24	LA	15	VAL
24	LA	28	ARG
24	LA	46	LYS
24	LA	54	ARG
24	LA	70	LYS
24	LA	102	LEU
24	LA	114	CYS
24	LA	123	ARG
24	LA	132	ASN
24	LA	154	SER

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Mol	Chain	Res	Type
24	LA	181	LYS
24	LA	198	ARG
24	LA	247	ARG
25	LB	17	LEU
25	LB	24	ARG
25	LB	34	LYS
25	LB	36	ASP
25	LB	57	VAL
25	LB	69	LYS
25	LB	73	VAL
25	LB	74	GLU
25	LB	80	GLU
25	LB	112	ASP
25	LB	126	LYS
25	LB	134	CYS
25	LB	145	GLN
25	LB	152	SER
25	LB	162	VAL
25	LB	174	ARG
25	LB	185	VAL
25	LB	203	GLN
25	LB	242	ARG
25	LB	286	LYS
25	LB	308	ASP
25	LB	328	ASN
25	LB	338	VAL
25	LB	351	LEU
25	LB	357	ARG
25	LB	394	LYS
26	LC	55	SER
26	LC	80	ARG
26	LC	95	MET
26	LC	114	ARG
26	LC	122	TYR
26	LC	143	ARG
26	LC	162	LYS
26	LC	193	LYS
26	LC	196	MET
26	LC	201	ARG
26	LC	204	ARG
26	LC	208	CYS
26	LC	230	LEU

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Mol	Chain	Res	Type
26	LC	234	LYS
26	LC	236	ASN
26	LC	239	LYS
26	LC	261	ASP
26	LC	283	LYS
26	LC	300	ARG
26	LC	366	ASP
27	LD	28	THR
27	LD	48	LYS
27	LD	50	ARG
27	LD	59	ASP
27	LD	76	CYS
27	LD	86	TYR
27	LD	90	VAL
27	LD	110	LEU
27	LD	112	ARG
27	LD	118	ILE
27	LD	176	SER
27	LD	189	GLU
27	LD	197	LYS
27	LD	209	ARG
27	LD	229	ASN
27	LD	235	MET
27	LD	254	GLU
27	LD	291	GLN
27	LD	292	GLU
28	LE	50	LEU
28	LE	71	ARG
28	LE	94	LYS
28	LE	100	LYS
28	LE	128	HIS
28	LE	131	LYS
28	LE	187	ARG
28	LE	191	GLN
28	LE	200	LYS
28	LE	207	LYS
28	LE	218	LYS
28	LE	234	ASP
28	LE	246	ARG
28	LE	272	ARG
29	LF	77	LYS
29	LF	96	ARG

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Mol	Chain	Res	Type
29	LF	99	ASN
29	LF	196	THR
29	LF	200	ARG
29	LF	232	ASP
29	LF	236	ARG
29	LF	237	GLU
29	LF	247	MET
30	LG	27	VAL
30	LG	35	ARG
30	LG	43	GLN
30	LG	50	ASP
30	LG	53	ARG
30	LG	88	ASP
30	LG	107	LYS
30	LG	110	LYS
30	LG	121	LYS
30	LG	131	LYS
30	LG	175	ARG
30	LG	185	LYS
30	LG	192	ARG
30	LG	223	ARG
30	LG	227	ASN
30	LG	231	ASP
30	LG	257	LYS
30	LG	260	GLU
31	LH	5	LEU
31	LH	50	LYS
31	LH	112	VAL
31	LH	136	VAL
31	LH	146	LEU
31	LH	150	ASP
31	LH	177	ASP
32	LI	26	VAL
32	LI	55	ASP
32	LI	71	CYS
32	LI	123	GLN
32	LI	168	SER
32	LI	189	CYS
32	LI	195	CYS
32	LI	206	LEU
32	LI	207	ASP
33	LJ	13	ARG

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Mol	Chain	Res	Type
33	LJ	32	ARG
33	LJ	43	LEU
33	LJ	47	THR
33	LJ	58	ARG
33	LJ	63	ARG
33	LJ	81	GLU
33	LJ	95	ARG
33	LJ	129	ASP
33	LJ	132	VAL
33	LJ	175	LEU
34	LL	52	SER
34	LL	67	HIS
34	LL	70	VAL
34	LL	71	ARG
34	LL	90	VAL
34	LL	103	ARG
34	LL	129	ARG
34	LL	134	PRO
34	LL	140	SER
34	LL	158	ARG
34	LL	162	LYS
34	LL	165	LYS
34	LL	171	GLU
34	LL	172	GLU
35	LM	7	VAL
35	LM	25	VAL
35	LM	35	ARG
35	LM	48	GLN
35	LM	50	MET
35	LM	71	LYS
35	LM	90	ARG
35	LM	113	MET
36	LN	41	ARG
36	LN	50	ARG
36	LN	110	CYS
36	LN	115	VAL
36	LN	118	SER
36	LN	126	THR
36	LN	140	LYS
36	LN	184	ILE
36	LN	189	ARG
37	LO	27	VAL

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Mol	Chain	Res	Type
37	LO	37	ARG
37	LO	49	ARG
37	LO	63	ASN
37	LO	127	VAL
38	LP	17	SER
38	LP	18	ARG
38	LP	22	LEU
38	LP	23	ARG
38	LP	24	VAL
38	LP	54	GLN
38	LP	57	CYS
38	LP	76	TRP
38	LP	118	GLN
38	LP	128	ARG
38	LP	151	THR
39	LQ	16	LYS
39	LQ	19	LYS
39	LQ	54	SER
39	LQ	92	VAL
39	LQ	107	SER
39	LQ	124	ASP
39	LQ	137	VAL
39	LQ	176	ARG
40	LR	39	GLN
40	LR	56	THR
40	LR	63	CYS
40	LR	111	GLU
40	LR	113	LYS
40	LR	134	ASN
40	LR	149	LYS
40	LR	151	ARG
40	LR	186	LYS
40	LR	188	LEU
41	LS	90	THR
41	LS	136	LYS
41	LS	149	LYS
41	LS	160	ARG
41	LS	161	ARG
41	LS	169	THR
42	LT	3	ASN
42	LT	29	THR
42	LT	32	ARG

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Mol	Chain	Res	Type
42	LT	45	MET
42	LT	83	LYS
42	LT	100	LYS
42	LT	141	VAL
43	LU	34	MET
43	LU	39	PHE
43	LU	73	THR
43	LU	74	SER
43	LU	82	TYR
43	LU	99	TRP
43	LU	100	LEU
43	LU	102	VAL
43	LU	107	LYS
43	LU	108	GLU
43	LU	110	TYR
43	LU	116	GLN
44	LV	15	ARG
44	LV	18	LEU
44	LV	65	VAL
44	LV	69	LYS
44	LV	80	VAL
44	LV	94	VAL
44	LV	127	ASP
44	LV	131	ARG
44	LV	134	SER
45	LX	41	ARG
45	LX	42	THR
45	LX	73	HIS
45	LX	88	LYS
45	LX	115	LYS
45	LX	120	ASP
45	LX	121	VAL
45	LX	143	ASP
45	LX	152	LYS
46	LY	2	LYS
46	LY	44	VAL
46	LY	74	TYR
46	LY	87	ARG
46	LY	110	LYS
46	LY	115	ARG
47	LZ	10	VAL
47	LZ	11	VAL

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Mol	Chain	Res	Type
47	LZ	30	ASP
47	LZ	39	SER
47	LZ	66	SER
47	LZ	70	SER
47	LZ	83	THR
47	LZ	86	SER
47	LZ	112	ARG
47	LZ	117	LYS
48	La	95	THR
48	La	140	VAL
49	Lb	4	SER
49	Lb	9	THR
49	Lb	33	LYS
49	Lb	91	ARG
49	Lb	107	ARG
49	Lb	116	LEU
49	Lb	117	ARG
49	Lb	119	CYS
50	Lc	23	LYS
50	Lc	37	MET
50	Lc	42	LYS
50	Lc	44	LYS
50	Lc	91	VAL
50	Lc	94	LEU
50	Lc	98	ASP
51	Ld	44	ARG
51	Ld	67	ARG
51	Ld	68	LEU
51	Ld	104	THR
51	Ld	106	VAL
51	Ld	116	ASN
52	Le	5	ARG
52	Le	34	ASN
52	Le	87	VAL
52	Le	102	ASN
52	Le	113	GLU
52	Le	126	ASN
52	Le	129	LEU
53	Lf	15	LYS
53	Lf	25	THR
53	Lf	33	VAL
53	Lf	37	ASP

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Mol	Chain	Res	Type
53	Lf	83	MET
53	Lf	90	SER
53	Lf	95	LYS
54	Lg	32	TYR
54	Lg	43	LYS
54	Lg	63	VAL
54	Lg	103	VAL
55	Lh	4	ILE
55	Lh	7	ARG
55	Lh	8	ASP
55	Lh	20	GLN
55	Lh	66	LYS
55	Lh	67	GLU
55	Lh	94	ARG
55	Lh	101	ASN
55	Lh	122	LYS
56	Li	12	ASN
56	Li	23	LYS
56	Li	29	ARG
56	Li	32	ARG
56	Li	38	LYS
56	Li	48	CYS
56	Li	64	SER
56	Li	66	ASP
56	Li	89	GLU
57	Lj	2	THR
57	Lj	7	SER
57	Lj	22	CYS
57	Lj	55	ARG
57	Lj	70	VAL
57	Lj	79	ARG
57	Lj	85	LYS
58	Lk	16	ARG
58	Lk	32	VAL
58	Lk	50	LYS
59	Ll	16	LYS
59	Ll	28	ARG
60	Lm	114	LYS
60	Lm	121	LEU
61	Ln	9	ARG
61	Ln	10	MET
61	Ln	16	LYS

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Mol	Chain	Res	Type
61	Ln	23	ARG
62	Lo	6	LYS
62	Lo	15	CYS
62	Lo	22	LYS
62	Lo	23	VAL
62	Lo	27	LYS
62	Lo	43	ARG
62	Lo	77	CYS
62	Lo	83	LEU
62	Lo	96	ASP
62	Lo	103	VAL
63	Lp	24	LYS
63	Lp	26	VAL
63	Lp	32	SER
63	Lp	40	SER
63	Lp	81	SER
63	Lp	90	LYS
64	Lr	14	SER
64	Lr	15	SER
64	Lr	21	ASN
64	Lr	37	SER
64	Lr	49	VAL
64	Lr	61	VAL
64	Lr	67	ARG
64	Lr	71	ARG
64	Lr	84	LYS
64	Lr	98	ARG
64	Lr	119	ARG
64	Lr	125	MET
65	Lz	1	MET
65	Lz	7	ARG
65	Lz	8	ASP
65	Lz	22	GLN
65	Lz	29	LEU
65	Lz	56	LYS
65	Lz	73	HIS
65	Lz	105	LYS
65	Lz	118	LYS
65	Lz	122	ARG
65	Lz	145	VAL
65	Lz	156	LYS
65	Lz	161	LYS

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Mol	Chain	Res	Type
65	Lz	165	LEU
65	Lz	174	MET
65	Lz	175	THR
65	Lz	178	GLU
65	Lz	196	LYS
65	Lz	198	TRP
66	SR	10	LYS
66	SR	27	ASP
66	SR	44	LYS
66	SR	67	ARG
66	SR	74	GLN
66	SR	76	GLU
66	SR	81	ARG
66	SR	99	ASP
66	SR	101	ASP
66	SR	111	PHE
66	SR	118	GLN
66	SR	129	LYS
66	SR	130	THR
67	SD	38	GLU
67	SD	45	ARG
67	SD	75	LYS
67	SD	77	PHE
67	SD	79	PHE
67	SD	90	LYS
67	SD	97	CYS
67	SD	116	ARG
67	SD	117	ARG
67	SD	119	CYS
67	SD	127	MET
67	SD	137	VAL
67	SD	141	LYS
67	SD	149	SER
67	SD	151	LYS
67	SD	167	TYR
67	SD	170	THR
67	SD	174	HIS
67	SD	178	ARG
68	SF	26	ASP
68	SF	42	LYS
68	SF	45	TYR
68	SF	61	PHE

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Mol	Chain	Res	Type
68	SF	78	MET
68	SF	82	ASN
68	SF	194	ASP
68	SF	198	ARG
69	SK	1	MET
69	SK	16	PHE
69	SK	17	LYS
69	SK	32	HIS
69	SK	50	GLN
69	SK	59	LYS
69	SK	72	THR
69	SK	84	HIS
70	SP	18	ARG
70	SP	23	ASP
70	SP	26	LEU
70	SP	34	MET
70	SP	38	SER
70	SP	50	ARG
70	SP	59	ARG
70	SP	72	LYS
70	SP	89	MET
70	SP	93	MET
70	SP	97	TYR
71	SQ	15	ARG
71	SQ	29	ASN
71	SQ	41	MET
71	SQ	48	GLN
71	SQ	49	TYR
71	SQ	50	LYS
71	SQ	55	VAL
71	SQ	62	ARG
71	SQ	71	ARG
71	SQ	73	LYS
71	SQ	98	LYS
71	SQ	125	ARG
71	SQ	127	CYS
71	SQ	145	TYR
72	SS	2	SER
72	SS	25	LYS
72	SS	46	ARG
72	SS	78	LYS
72	SS	83	PHE

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Mol	Chain	Res	Type
72	SS	88	LYS
72	SS	96	SER
72	SS	104	ASP
72	SS	106	LYS
73	ST	8	ASP
73	ST	23	LYS
73	ST	41	LYS
73	ST	44	GLU
73	ST	77	LYS
73	ST	98	SER
73	ST	131	LEU
74	SU	19	ARG
74	SU	36	CYS
74	SU	48	LEU
74	SU	83	ARG
75	Sc	18	LEU
75	Sc	35	MET
75	Sc	57	THR
76	Sd	19	ARG
76	Sd	26	ASN
76	Sd	27	ARG
76	Sd	28	HIS
76	Sd	32	ARG
76	Sd	55	LEU
77	Sg	8	ARG
77	Sg	26	GLN
77	Sg	29	ASP
77	Sg	36	ARG
77	Sg	39	THR
77	Sg	44	LYS
77	Sg	47	ARG
77	Sg	49	GLU
77	Sg	57	ARG
77	Sg	84	ASP
77	Sg	91	ASP
77	Sg	97	THR
77	Sg	110	SER
77	Sg	111	VAL
77	Sg	135	LEU
77	Sg	144	ASP
77	Sg	155	ARG
77	Sg	170	TRP

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Mol	Chain	Res	Type
77	Sg	171	ASP
77	Sg	172	LYS
77	Sg	173	LEU
77	Sg	183	LYS
77	Sg	196	ASN
77	Sg	213	ASP
77	Sg	217	MET
77	Sg	219	TRP
77	Sg	220	ASP
77	Sg	234	ASP
77	Sg	241	PHE
77	Sg	259	TRP
77	Sg	271	LYS
77	Sg	310	TRP
78	SM	12	MET
78	SM	33	ARG
78	SM	44	LYS
78	SM	49	LEU
78	SM	63	LYS
78	SM	121	LYS
78	SM	123	VAL
78	SM	127	TYR
78	SM	131	LYS
79	SZ	46	ASN
79	SZ	50	PHE
79	SZ	55	TYR
79	SZ	60	LYS
79	SZ	77	LEU
79	SZ	102	LYS
80	Sf	95	ARG
80	Sf	106	TYR
80	Sf	145	CYS
80	Sf	149	CYS
83	Ls	6	ARG
83	Ls	23	ASP
83	Ls	55	MET
83	Ls	62	ARG
83	Ls	66	ARG
83	Ls	123	VAL
83	Ls	126	GLN
83	Ls	162	LYS
83	Ls	166	LYS

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Mol	Chain	Res	Type
84	Lt	57	ARG
84	Lt	83	LYS
84	Lt	86	LYS
84	Lt	104	ILE
84	Lt	116	MET
84	Lt	123	ARG
84	Lt	144	ASP
84	Lt	146	ARG
85	CB	5	THR
85	CB	22	MET
85	CB	42	LYS
85	CB	58	ASP
85	CB	61	LYS
85	CB	62	ASP
85	CB	110	ASP
85	CB	143	LEU
85	CB	147	ILE
85	CB	165	LEU
85	CB	170	GLU
85	CB	219	HIS
85	CB	231	MET
85	CB	236	PHE
85	CB	249	ARG
85	CB	255	ASP
85	CB	258	LYS
85	CB	264	ARG
85	CB	274	SER
85	CB	283	LYS
85	CB	301	PHE
85	CB	302	ASP
85	CB	328	LYS
85	CB	348	ASP
85	CB	383	MET
85	CB	407	LYS
85	CB	453	MET
85	CB	457	TYR
85	CB	481	LYS
85	CB	488	PHE
85	CB	492	HIS
85	CB	510	GLU
85	CB	519	LYS
85	CB	520	LEU

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Mol	Chain	Res	Type
85	CB	544	HIS
85	CB	571	LYS
85	CB	573	SER
85	CB	574	ASP
85	CB	590	LEU
85	CB	597	ASN
85	CB	598	LYS
85	CB	601	ARG
85	CB	605	LYS
85	CB	625	ARG
85	CB	629	LYS
85	CB	651	CYS
85	CB	657	THR
85	CB	688	LYS
85	CB	702	PHE
85	CB	703	ASP
85	CB	715	HIS
85	CB	716	ARG
85	CB	739	ARG
85	CB	745	TYR
85	CB	764	ASN
85	CB	766	LYS
85	CB	788	LEU
85	CB	791	ASN
85	CB	799	ASP
85	CB	803	ASN
85	CB	825	PHE
85	CB	829	SER
85	CB	838	THR
85	CB	841	ARG
85	CB	853	ASN
85	CB	856	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	CH	51	GLN
2	CH	57	ASN
2	CH	118	ASN
4	SE	17	HIS
4	SE	157	ASN
4	SE	161	GLN

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Mol	Chain	Res	Type
5	SI	116	HIS
9	SJ	111	GLN
11	SA	141	ASN
16	SC	113	GLN
18	SO	32	HIS
18	SO	113	GLN
19	SW	90	GLN
19	SW	113	HIS
24	LA	215	ASN
26	LC	236	ASN
27	LD	195	HIS
30	LG	29	ASN
32	LI	177	ASN
33	LJ	71	HIS
36	LN	8	GLN
41	LS	36	ASN
42	LT	114	GLN
43	LU	50	ASN
50	Lc	51	ASN
53	Lf	78	HIS
54	Lg	3	GLN
59	Ll	33	ASN
63	Lp	92	GLN
66	SR	118	GLN
67	SD	22	ASN
67	SD	101	GLN
69	SK	44	HIS
71	SQ	48	GLN
72	SS	73	ASN
77	Sg	26	GLN
77	Sg	196	ASN
77	Sg	222	ASN
77	Sg	285	GLN
77	Sg	311	GLN
83	Ls	42	GLN
85	CB	8	GLN
85	CB	18	ASN
85	CB	21	ASN
85	CB	101	ASN
85	CB	179	GLN
85	CB	553	HIS
85	CB	626	GLN

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Mol	Chain	Res	Type
85	CB	660	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	L5	3705/3740 (99%)	855 (23%)	21 (0%)
22	L7	119/120 (99%)	11 (9%)	0
23	L8	155/156 (99%)	31 (20%)	0
81	AP	69/71 (97%)	15 (21%)	0
82	PE	74/75 (98%)	27 (36%)	1 (1%)
86	S2	1714/1740 (98%)	436 (25%)	8 (0%)
All	All	5836/5902 (98%)	1375 (23%)	30 (0%)

All (1375) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	L5	2	G
21	L5	13	U
21	L5	17	A
21	L5	25	A
21	L5	30	C
21	L5	39	A
21	L5	42	A
21	L5	48	G
21	L5	56	A
21	L5	59	A
21	L5	64	A
21	L5	65	A
21	L5	66	A
21	L5	69	A
21	L5	73	A
21	L5	91	G
21	L5	104	G
21	L5	108	A
21	L5	109	G
21	L5	110	C
21	L5	119	G
21	L5	120	A
21	L5	132	G
21	L5	133	C
21	L5	134	G

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Mol	Chain	Res	Type
21	L5	135	G
21	L5	144	G
21	L5	151	G
21	L5	152	U
21	L5	159	C
21	L5	165	A
21	L5	172	C
21	L5	181	C
21	L5	183	C
21	L5	184	U
21	L5	185	C
21	L5	187	U
21	L5	188	G
21	L5	189	G
21	L5	200	U
21	L5	209	U
21	L5	216	C
21	L5	218	A
21	L5	234	G
21	L5	237	G
21	L5	253	G
21	L5	255	C
21	L5	256	G
21	L5	261	G
21	L5	263	G
21	L5	264	C
21	L5	265	C
21	L5	266	C
21	L5	267	G
21	L5	275	C
21	L5	276	C
21	L5	278	G
21	L5	280	G
21	L5	281	U
21	L5	297	U
21	L5	306	A
21	L5	310	G
21	L5	315	G
21	L5	316	U
21	L5	340	C
21	L5	350	C
21	L5	373	G

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Mol	Chain	Res	Type
21	L5	385	A
21	L5	387	G
21	L5	388	A
21	L5	396	A
21	L5	401	G
21	L5	407	A
21	L5	409	G
21	L5	410	A
21	L5	411	G
21	L5	412	G
21	L5	413	G
21	L5	415	G
21	L5	431	G
21	L5	432	U
21	L5	449	C
21	L5	450	G
21	L5	452	A
21	L5	453	G
21	L5	454	U
21	L5	456	C
21	L5	457	G
21	L5	467	U
21	L5	468	U
21	L5	485	C
21	L5	486	C
21	L5	489	C
21	L5	494	U
21	L5	495	C
21	L5	497	G
21	L5	498	C
21	L5	499	G
21	L5	501	C
21	L5	502	C
21	L5	503	C
21	L5	504	G
21	L5	505	G
21	L5	506	C
21	L5	509	A
21	L5	510	U
21	L5	512	U
21	L5	513	U
21	L5	514	U

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Mol	Chain	Res	Type
21	L5	517	C
21	L5	518	G
21	L5	643	C
21	L5	644	G
21	L5	646	G
21	L5	653	U
21	L5	654	C
21	L5	655	C
21	L5	656	C
21	L5	657	C
21	L5	658	C
21	L5	659	G
21	L5	666	G
21	L5	667	A
21	L5	668	C
21	L5	669	C
21	L5	673	C
21	L5	685	C
21	L5	686	A
21	L5	687	U
21	L5	696	C
21	L5	703	G
21	L5	704	C
21	L5	706	C
21	L5	708	G
21	L5	730	G
21	L5	731	G
21	L5	738	C
21	L5	739	G
21	L5	741	C
21	L5	742	G
21	L5	753	C
21	L5	758	G
21	L5	759	G
21	L5	760	G
21	L5	904	C
21	L5	905	C
21	L5	906	C
21	L5	910	G
21	L5	911	U
21	L5	912	G
21	L5	913	U

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Mol	Chain	Res	Type
21	L5	914	U
21	L5	915	A
21	L5	917	A
21	L5	918	G
21	L5	923	C
21	L5	924	C
21	L5	926	G
21	L5	932	A
21	L5	933	G
21	L5	935	A
21	L5	936	C
21	L5	942	G
21	L5	943	A
21	L5	944	A
21	L5	945	U
21	L5	946	C
21	L5	958	G
21	L5	959	G
21	L5	960	A
21	L5	961	G
21	L5	962	C
21	L5	965	G
21	L5	966	A
21	L5	967	C
21	L5	968	C
21	L5	969	C
21	L5	970	G
21	L5	982	U
21	L5	985	C
21	L5	989	U
21	L5	990	C
21	L5	992	C
21	L5	993	G
21	L5	995	C
21	L5	996	G
21	L5	1048	G
21	L5	1049	C
21	L5	1050	C
21	L5	1051	G
21	L5	1070	G
21	L5	1072	C
21	L5	1075	G

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Mol	Chain	Res	Type
21	L5	1082	C
21	L5	1083	U
21	L5	1095	A
21	L5	1168	G
21	L5	1171	G
21	L5	1172	C
21	L5	1173	G
21	L5	1178	G
21	L5	1179	U
21	L5	1180	C
21	L5	1182	C
21	L5	1183	C
21	L5	1193	C
21	L5	1202	C
21	L5	1203	G
21	L5	1210	C
21	L5	1211	G
21	L5	1214	C
21	L5	1215	C
21	L5	1216	C
21	L5	1217	G
21	L5	1218	G
21	L5	1219	G
21	L5	1222	A
21	L5	1235	G
21	L5	1241	C
21	L5	1242	G
21	L5	1245	C
21	L5	1246	G
21	L5	1253	G
21	L5	1254	A
21	L5	1257	A
21	L5	1258	G
21	L5	1262	G
21	L5	1266	G
21	L5	1267	C
21	L5	1269	G
21	L5	1270	A
21	L5	1271	G
21	L5	1272	C
21	L5	1273	G
21	L5	1274	A

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Mol	Chain	Res	Type
21	L5	1275	G
21	L5	1277	G
21	L5	1280	C
21	L5	1284	G
21	L5	1285	U
21	L5	1287	G
21	L5	1293	G
21	L5	1294	A
21	L5	1295	C
21	L5	1296	G
21	L5	1301	C
21	L5	1314	C
21	L5	1326	A
21	L5	1337	A
21	L5	1354	A
21	L5	1358	G
21	L5	1359	G
21	L5	1365	C
21	L5	1367	C
21	L5	1387	A
21	L5	1394	G
21	L5	1397	A
21	L5	1398	A
21	L5	1404	G
21	L5	1405	C
21	L5	1407	C
21	L5	1409	C
21	L5	1410	U
21	L5	1411	C
21	L5	1414	C
21	L5	1415	G
21	L5	1417	C
21	L5	1420	A
21	L5	1433	A
21	L5	1437	C
21	L5	1439	C
21	L5	1443	A
21	L5	1446	C
21	L5	1447	C
21	L5	1482	G
21	L5	1483	C
21	L5	1493	G

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Mol	Chain	Res	Type
21	L5	1497	A
21	L5	1498	G
21	L5	1502	G
21	L5	1517	G
21	L5	1518	A
21	L5	1534	A
21	L5	1547	A
21	L5	1562	G
21	L5	1564	A
21	L5	1566	C
21	L5	1578	U
21	L5	1591	U
21	L5	1596	U
21	L5	1624	G
21	L5	1631	A
21	L5	1633	G
21	L5	1634	A
21	L5	1638	A
21	L5	1640	C
21	L5	1641	G
21	L5	1642	A
21	L5	1654	G
21	L5	1661	C
21	L5	1663	C
21	L5	1676	C
21	L5	1677	U
21	L5	1678	C
21	L5	1681	G
21	L5	1685	G
21	L5	1694	C
21	L5	1699	A
21	L5	1700	G
21	L5	1703	C
21	L5	1704	C
21	L5	1705	G
21	L5	1707	C
21	L5	1718	C
21	L5	1726	U
21	L5	1731	C
21	L5	1734	G
21	L5	1740	C
21	L5	1741	G

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Mol	Chain	Res	Type
21	L5	1742	A
21	L5	1750	G
21	L5	1757	U
21	L5	1758	G
21	L5	1760	G
21	L5	1761	G
21	L5	1762	C
21	L5	1763	C
21	L5	1764	G
21	L5	1765	A
21	L5	1766	A
21	L5	1767	A
21	L5	1768	C
21	L5	1770	A
21	L5	1787	A
21	L5	1803	G
21	L5	1804	A
21	L5	1806	G
21	L5	1810	G
21	L5	1815	G
21	L5	1820	C
21	L5	1821	G
21	L5	1822	U
21	L5	1836	G
21	L5	1837	A
21	L5	1842	G
21	L5	1843	A
21	L5	1855	G
21	L5	1869	G
21	L5	1882	U
21	L5	1892	A
21	L5	1893	C
21	L5	1897	A
21	L5	1917	A
21	L5	1918	U
21	L5	1919	G
21	L5	1920	C
21	L5	1921	C
21	L5	1922	G
21	L5	1925	G
21	L5	1931	C
21	L5	1932	A

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Mol	Chain	Res	Type
21	L5	1940	G
21	L5	1948	G
21	L5	1951	G
21	L5	1959	U
21	L5	1960	A
21	L5	1961	G
21	L5	1962	A
21	L5	1965	G
21	L5	1974	U
21	L5	1975	G
21	L5	1978	C
21	L5	1980	U
21	L5	1981	G
21	L5	1982	G
21	L5	1983	A
21	L5	1984	A
21	L5	1985	G
21	L5	1986	U
21	L5	1989	G
21	L5	1991	A
21	L5	1992	U
21	L5	1993	C
21	L5	1997	U
21	L5	1998	A
21	L5	2000	G
21	L5	2001	G
21	L5	2002	A
21	L5	2004	U
21	L5	2011	C
21	L5	2014	C
21	L5	2017	A
21	L5	2018	C
21	L5	2024	G
21	L5	2026	A
21	L5	2033	A
21	L5	2034	G
21	L5	2046	G
21	L5	2048	U
21	L5	2052	G
21	L5	2055	G
21	L5	2056	G
21	L5	2062	C

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Mol	Chain	Res	Type
21	L5	2069	A
21	L5	2084	C
21	L5	2092	G
21	L5	2093	A
21	L5	2095	A
21	L5	2096	G
21	L5	2097	U
21	L5	2098	G
21	L5	2101	C
21	L5	2102	G
21	L5	2106	G
21	L5	2107	C
21	L5	2108	G
21	L5	2112	G
21	L5	2250	C
21	L5	2252	G
21	L5	2253	A
21	L5	2256	C
21	L5	2258	C
21	L5	2259	G
21	L5	2260	C
21	L5	2262	G
21	L5	2263	A
21	L5	2289	C
21	L5	2300	A
21	L5	2301	G
21	L5	2313	A
21	L5	2331	G
21	L5	2332	A
21	L5	2333	G
21	L5	2345	G
21	L5	2348	G
21	L5	2351	C
21	L5	2360	A
21	L5	2395	A
21	L5	2397	G
21	L5	2402	G
21	L5	2412	A
21	L5	2417	A
21	L5	2421	G
21	L5	2425	U
21	L5	2441	C

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Mol	Chain	Res	Type
21	L5	2447	U
21	L5	2453	A
21	L5	2464	C
21	L5	2465	C
21	L5	2467	U
21	L5	2469	C
21	L5	2474	G
21	L5	2475	G
21	L5	2478	C
21	L5	2479	G
21	L5	2483	G
21	L5	2484	A
21	L5	2485	U
21	L5	2487	G
21	L5	2488	C
21	L5	2489	C
21	L5	2490	U
21	L5	2491	C
21	L5	2494	U
21	L5	2503	G
21	L5	2504	C
21	L5	2506	G
21	L5	2513	A
21	L5	2519	U
21	L5	2520	C
21	L5	2529	A
21	L5	2537	A
21	L5	2544	G
21	L5	2546	G
21	L5	2547	G
21	L5	2554	U
21	L5	2557	G
21	L5	2559	G
21	L5	2560	C
21	L5	2565	A
21	L5	2568	C
21	L5	2573	A
21	L5	2583	C
21	L5	2587	A
21	L5	2589	C
21	L5	2601	A
21	L5	2627	C

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Mol	Chain	Res	Type
21	L5	2652	G
21	L5	2653	C
21	L5	2662	G
21	L5	2669	C
21	L5	2675	G
21	L5	2676	A
21	L5	2687	U
21	L5	2694	G
21	L5	2695	A
21	L5	2696	A
21	L5	2703	G
21	L5	2707	U
21	L5	2708	U
21	L5	2710	C
21	L5	2711	G
21	L5	2721	G
21	L5	2724	G
21	L5	2726	G
21	L5	2739	C
21	L5	2742	G
21	L5	2743	A
21	L5	2761	U
21	L5	2763	U
21	L5	2764	A
21	L5	2769	U
21	L5	2770	C
21	L5	2787	A
21	L5	2788	U
21	L5	2790	U
21	L5	2814	C
21	L5	2826	U
21	L5	2827	G
21	L5	2835	A
21	L5	2848	G
21	L5	2855	G
21	L5	2867	C
21	L5	2877	G
21	L5	2894	A
21	L5	2900	U
21	L5	2902	G
21	L5	2903	G
21	L5	2904	U

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Mol	Chain	Res	Type
21	L5	2905	C
21	L5	2906	G
21	L5	2908	U
21	L5	3587	C
21	L5	3590	G
21	L5	3591	C
21	L5	3594	C
21	L5	3595	U
21	L5	3596	A
21	L5	3597	G
21	L5	3605	C
21	L5	3615	G
21	L5	3618	C
21	L5	3626	G
21	L5	3630	A
21	L5	3635	A
21	L5	3644	U
21	L5	3646	A
21	L5	3648	A
21	L5	3662	A
21	L5	3664	G
21	L5	3670	C
21	L5	3673	C
21	L5	3674	G
21	L5	3685	C
21	L5	3710	G
21	L5	3711	A
21	L5	3713	U
21	L5	3727	A
21	L5	3740	G
21	L5	3748	A
21	L5	3750	G
21	L5	3756	A
21	L5	3759	A
21	L5	3772	U
21	L5	3773	U
21	L5	3774	A
21	L5	3776	G
21	L5	3777	G
21	L5	3783	A
21	L5	3784	A
21	L5	3786	U

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Mol	Chain	Res	Type
21	L5	3788	C
21	L5	3802	U
21	L5	3811	G
21	L5	3812	C
21	L5	3814	U
21	L5	3817	A
21	L5	3818	U
21	L5	3819	G
21	L5	3823	G
21	L5	3838	U
21	L5	3839	G
21	L5	3840	U
21	L5	3841	C
21	L5	3867	A
21	L5	3877	A
21	L5	3878	C
21	L5	3879	G
21	L5	3885	G
21	L5	3887	C
21	L5	3890	A
21	L5	3892	U
21	L5	3897	G
21	L5	3901	A
21	L5	3906	A
21	L5	3907	G
21	L5	3908	A
21	L5	3915	U
21	L5	3923	A
21	L5	3938	G
21	L5	3939	G
21	L5	3943	A
21	L5	3944	G
21	L5	3947	A
21	L5	3948	C
21	L5	3949	A
21	L5	3950	U
21	L5	3951	G
21	L5	3953	G
21	L5	3955	G
21	L5	3956	G
21	L5	3957	U
21	L5	3959	U

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Mol	Chain	Res	Type
21	L5	3960	A
21	L5	3962	A
21	L5	3963	A
21	L5	3965	A
21	L5	3966	A
21	L5	3967	G
21	L5	3968	U
21	L5	3969	G
21	L5	3970	G
21	L5	3972	A
21	L5	3973	G
21	L5	3974	G
21	L5	3975	C
21	L5	3977	C
21	L5	4034	G
21	L5	4038	C
21	L5	4039	G
21	L5	4040	C
21	L5	4041	C
21	L5	4042	G
21	L5	4043	G
21	L5	4044	U
21	L5	4046	A
21	L5	4047	A
21	L5	4048	A
21	L5	4049	U
21	L5	4051	C
21	L5	4052	C
21	L5	4053	A
21	L5	4055	U
21	L5	4056	A
21	L5	4057	C
21	L5	4058	U
21	L5	4059	C
21	L5	4060	U
21	L5	4061	G
21	L5	4062	A
21	L5	4063	U
21	L5	4064	C
21	L5	4065	G
21	L5	4068	U
21	L5	4069	U

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Mol	Chain	Res	Type
21	L5	4076	G
21	L5	4084	G
21	L5	4092	G
21	L5	4093	G
21	L5	4095	G
21	L5	4096	C
21	L5	4097	G
21	L5	4099	G
21	L5	4101	C
21	L5	4102	C
21	L5	4103	C
21	L5	4104	G
21	L5	4108	G
21	L5	4111	U
21	L5	4114	C
21	L5	4115	G
21	L5	4116	C
21	L5	4119	C
21	L5	4121	G
21	L5	4127	A
21	L5	4134	C
21	L5	4139	G
21	L5	4140	C
21	L5	4141	G
21	L5	4142	C
21	L5	4143	G
21	L5	4144	C
21	L5	4146	G
21	L5	4150	G
21	L5	4160	C
21	L5	4162	C
21	L5	4163	U
21	L5	4166	G
21	L5	4168	G
21	L5	4170	A
21	L5	4177	C
21	L5	4183	G
21	L5	4184	G
21	L5	4191	G
21	L5	4196	G
21	L5	4197	G
21	L5	4201	G

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Mol	Chain	Res	Type
21	L5	4203	A
21	L5	4222	G
21	L5	4225	G
21	L5	4228	G
21	L5	4229	U
21	L5	4233	A
21	L5	4249	G
21	L5	4251	A
21	L5	4254	G
21	L5	4255	A
21	L5	4256	A
21	L5	4257	A
21	L5	4265	U
21	L5	4268	A
21	L5	4273	A
21	L5	4291	G
21	L5	4297	G
21	L5	4304	A
21	L5	4305	G
21	L5	4314	C
21	L5	4319	C
21	L5	4329	G
21	L5	4330	G
21	L5	4332	C
21	L5	4339	A
21	L5	4349	C
21	L5	4350	C
21	L5	4354	U
21	L5	4373	G
21	L5	4376	A
21	L5	4377	G
21	L5	4378	A
21	L5	4380	A
21	L5	4387	C
21	L5	4391	G
21	L5	4394	A
21	L5	4421	C
21	L5	4422	A
21	L5	4443	C
21	L5	4448	G
21	L5	4449	A
21	L5	4452	U

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Mol	Chain	Res	Type
21	L5	4453	C
21	L5	4464	A
21	L5	4466	C
21	L5	4475	G
21	L5	4488	A
21	L5	4500	U
21	L5	4510	A
21	L5	4512	U
21	L5	4513	A
21	L5	4519	C
21	L5	4524	G
21	L5	4525	C
21	L5	4545	G
21	L5	4548	A
21	L5	4549	G
21	L5	4557	U
21	L5	4560	C
21	L5	4567	G
21	L5	4572	U
21	L5	4573	G
21	L5	4575	G
21	L5	4584	A
21	L5	4589	A
21	L5	4590	A
21	L5	4600	G
21	L5	4601	U
21	L5	4617	G
21	L5	4636	U
21	L5	4637	G
21	L5	4648	A
21	L5	4656	A
21	L5	4657	U
21	L5	4659	G
21	L5	4670	C
21	L5	4672	A
21	L5	4679	G
21	L5	4687	A
21	L5	4694	G
21	L5	4695	C
21	L5	4700	A
21	L5	4708	A
21	L5	4709	U

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Mol	Chain	Res	Type
21	L5	4719	G
21	L5	4732	G
21	L5	4733	C
21	L5	4734	A
21	L5	4735	G
21	L5	4740	G
21	L5	4741	C
21	L5	4742	G
21	L5	4745	G
21	L5	4754	G
21	L5	4757	C
21	L5	4759	C
21	L5	4761	G
21	L5	4764	A
21	L5	4765	G
21	L5	4771	C
21	L5	4772	C
21	L5	4773	C
21	L5	4775	C
21	L5	4776	G
21	L5	4859	C
21	L5	4860	G
21	L5	4862	G
21	L5	4870	G
21	L5	4871	C
21	L5	4875	G
21	L5	4880	C
21	L5	4882	U
21	L5	4883	C
21	L5	4889	G
21	L5	4895	C
21	L5	4896	G
21	L5	4900	C
21	L5	4901	G
21	L5	4902	C
21	L5	4910	G
21	L5	4912	G
21	L5	4914	C
21	L5	4922	C
21	L5	4923	C
21	L5	4924	C
21	L5	4925	U

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Mol	Chain	Res	Type
21	L5	4926	C
21	L5	4927	G
21	L5	4928	C
21	L5	4934	A
21	L5	4941	G
21	L5	4943	A
21	L5	4944	C
21	L5	4951	G
21	L5	4960	G
21	L5	4976	U
21	L5	4985	U
21	L5	4988	U
21	L5	4989	U
21	L5	4990	C
21	L5	4991	U
21	L5	5007	A
21	L5	5009	G
21	L5	5014	A
21	L5	5017	G
21	L5	5024	C
21	L5	5026	U
21	L5	5027	C
21	L5	5028	G
21	L5	5029	C
21	L5	5030	U
21	L5	5034	A
21	L5	5041	G
21	L5	5050	C
21	L5	5055	G
21	L5	5058	A
21	L5	5061	A
21	L5	5069	U
22	L7	33	U
22	L7	38	U
22	L7	53	U
22	L7	54	A
22	L7	63	C
22	L7	64	G
22	L7	97	G
22	L7	100	A
22	L7	102	U
22	L7	110	G

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Mol	Chain	Res	Type
22	L7	111	C
23	L8	25	G
23	L8	34	U
23	L8	35	C
23	L8	48	A
23	L8	52	A
23	L8	59	A
23	L8	62	A
23	L8	63	U
23	L8	68	G
23	L8	80	A
23	L8	82	A
23	L8	83	C
23	L8	84	A
23	L8	85	U
23	L8	86	U
23	L8	87	G
23	L8	103	A
23	L8	105	C
23	L8	110	U
23	L8	111	U
23	L8	112	G
23	L8	114	G
23	L8	123	U
23	L8	124	U
23	L8	125	C
23	L8	126	C
23	L8	127	U
23	L8	128	C
23	L8	151	G
23	L8	153	C
23	L8	156	U
81	AP	7	G
81	AP	8	U
81	AP	9	A
81	AP	10	G
81	AP	11	U
81	AP	13	U
81	AP	14	A
81	AP	21	A
81	AP	26	G
81	AP	47	U

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Mol	Chain	Res	Type
81	AP	48	C
81	AP	49	C
81	AP	58	A
81	AP	64	G
81	AP	70	A
82	PE	4	C
82	PE	8	U
82	PE	9	A
82	PE	10	G
82	PE	11	C
82	PE	19	G
82	PE	20	U
82	PE	21	A
82	PE	31	A
82	PE	35	U
82	PE	37	A
82	PE	38	A
82	PE	40	C
82	PE	46	G
82	PE	47	U
82	PE	48	C
82	PE	49	C
82	PE	50	A
82	PE	55	U
82	PE	56	C
82	PE	58	A
82	PE	61	C
82	PE	63	C
82	PE	65	G
82	PE	67	U
82	PE	70	G
82	PE	76	A
86	S2	2	A
86	S2	4	C
86	S2	13	C
86	S2	17	C
86	S2	25	A
86	S2	33	G
86	S2	42	A
86	S2	44	U
86	S2	45	A
86	S2	46	A

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Mol	Chain	Res	Type
86	S2	56	G
86	S2	58	C
86	S2	59	U
86	S2	64	A
86	S2	65	C
86	S2	66	G
86	S2	67	C
86	S2	68	A
86	S2	72	C
86	S2	73	C
86	S2	74	G
86	S2	76	U
86	S2	92	A
86	S2	103	A
86	S2	113	G
86	S2	114	G
86	S2	115	U
86	S2	116	U
86	S2	126	G
86	S2	130	G
86	S2	139	C
86	S2	143	U
86	S2	149	A
86	S2	158	A
86	S2	160	U
86	S2	162	C
86	S2	163	U
86	S2	168	C
86	S2	170	A
86	S2	175	A
86	S2	179	C
86	S2	182	C
86	S2	188	C
86	S2	190	G
86	S2	192	C
86	S2	196	C
86	S2	197	U
86	S2	198	U
86	S2	200	G
86	S2	202	G
86	S2	203	G
86	S2	204	G

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Mol	Chain	Res	Type
86	S2	206	G
86	S2	207	G
86	S2	208	G
86	S2	211	G
86	S2	212	C
86	S2	214	U
86	S2	220	U
86	S2	291	G
86	S2	292	A
86	S2	294	U
86	S2	295	C
86	S2	298	G
86	S2	301	A
86	S2	303	C
86	S2	305	U
86	S2	306	C
86	S2	307	G
86	S2	308	G
86	S2	309	G
86	S2	310	C
86	S2	311	C
86	S2	312	G
86	S2	316	G
86	S2	318	A
86	S2	319	C
86	S2	323	C
86	S2	324	C
86	S2	325	C
86	S2	326	C
86	S2	328	U
86	S2	329	G
86	S2	332	G
86	S2	338	G
86	S2	339	A
86	S2	340	C
86	S2	347	G
86	S2	360	A
86	S2	361	U
86	S2	362	C
86	S2	364	A
86	S2	368	U
86	S2	369	C

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Mol	Chain	Res	Type
86	S2	370	G
86	S2	372	U
86	S2	374	G
86	S2	375	U
86	S2	385	G
86	S2	386	C
86	S2	407	G
86	S2	408	A
86	S2	409	C
86	S2	421	G
86	S2	426	A
86	S2	437	G
86	S2	448	A
86	S2	449	A
86	S2	450	C
86	S2	452	G
86	S2	464	A
86	S2	465	A
86	S2	471	G
86	S2	472	C
86	S2	473	A
86	S2	474	G
86	S2	476	A
86	S2	487	U
86	S2	488	U
86	S2	492	C
86	S2	493	A
86	S2	496	C
86	S2	501	C
86	S2	502	C
86	S2	516	A
86	S2	531	A
86	S2	532	C
86	S2	533	A
86	S2	534	G
86	S2	536	A
86	S2	537	C
86	S2	540	U
86	S2	543	C
86	S2	544	G
86	S2	546	G
86	S2	547	G

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Mol	Chain	Res	Type
86	S2	548	C
86	S2	549	C
86	S2	551	U
86	S2	553	U
86	S2	554	A
86	S2	555	A
86	S2	556	U
86	S2	557	U
86	S2	558	G
86	S2	563	G
86	S2	564	A
86	S2	566	U
86	S2	576	A
86	S2	583	A
86	S2	587	A
86	S2	589	G
86	S2	590	A
86	S2	591	U
86	S2	604	A
86	S2	608	C
86	S2	614	C
86	S2	617	G
86	S2	622	C
86	S2	623	G
86	S2	628	A
86	S2	629	A
86	S2	631	U
86	S2	643	A
86	S2	644	G
86	S2	655	A
86	S2	660	C
86	S2	664	A
86	S2	668	A
86	S2	669	A
86	S2	671	A
86	S2	672	A
86	S2	673	G
86	S2	684	G
86	S2	688	U
86	S2	689	U
86	S2	692	G
86	S2	693	A

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Mol	Chain	Res	Type
86	S2	695	C
86	S2	696	G
86	S2	697	G
86	S2	698	G
86	S2	732	U
86	S2	733	C
86	S2	734	C
86	S2	736	C
86	S2	738	C
86	S2	749	U
86	S2	750	C
86	S2	751	G
86	S2	752	G
86	S2	753	C
86	S2	788	G
86	S2	789	G
86	S2	791	C
86	S2	792	C
86	S2	798	G
86	S2	799	U
86	S2	821	G
86	S2	822	U
86	S2	823	U
86	S2	824	C
86	S2	830	A
86	S2	834	C
86	S2	835	C
86	S2	836	G
86	S2	837	A
86	S2	838	G
86	S2	839	C
86	S2	842	C
86	S2	844	U
86	S2	847	A
86	S2	870	A
86	S2	873	G
86	S2	874	G
86	S2	877	C
86	S2	878	G
86	S2	882	U
86	S2	885	U
86	S2	888	U

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Mol	Chain	Res	Type
86	S2	889	U
86	S2	891	G
86	S2	893	U
86	S2	894	G
86	S2	896	U
86	S2	897	U
86	S2	898	U
86	S2	899	U
86	S2	900	C
86	S2	901	G
86	S2	903	A
86	S2	913	A
86	S2	917	U
86	S2	919	A
86	S2	920	A
86	S2	933	G
86	S2	934	G
86	S2	943	U
86	S2	955	A
86	S2	963	A
86	S2	971	G
86	S2	972	A
86	S2	988	C
86	S2	990	A
86	S2	992	A
86	S2	999	G
86	S2	1002	U
86	S2	1008	A
86	S2	1017	U
86	S2	1023	A
86	S2	1027	A
86	S2	1042	A
86	S2	1045	U
86	S2	1047	C
86	S2	1060	A
86	S2	1061	U
86	S2	1062	A
86	S2	1067	C
86	S2	1080	A
86	S2	1083	A
86	S2	1085	C
86	S2	1088	U

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Mol	Chain	Res	Type
86	S2	1100	A
86	S2	1109	C
86	S2	1113	A
86	S2	1114	U
86	S2	1115	U
86	S2	1116	C
86	S2	1119	A
86	S2	1121	G
86	S2	1125	C
86	S2	1133	A
86	S2	1138	C
86	S2	1139	C
86	S2	1148	A
86	S2	1149	A
86	S2	1153	C
86	S2	1154	U
86	S2	1161	U
86	S2	1195	A
86	S2	1207	G
86	S2	1208	A
86	S2	1215	C
86	S2	1216	C
86	S2	1217	A
86	S2	1220	A
86	S2	1224	G
86	S2	1227	G
86	S2	1237	C
86	S2	1240	A
86	S2	1242	U
86	S2	1243	U
86	S2	1251	A
86	S2	1253	A
86	S2	1256	G
86	S2	1257	G
86	S2	1259	A
86	S2	1264	C
86	S2	1274	G
86	S2	1275	G
86	S2	1283	C
86	S2	1284	A
86	S2	1286	G
86	S2	1287	A

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Mol	Chain	Res	Type
86	S2	1290	G
86	S2	1294	G
86	S2	1295	A
86	S2	1301	A
86	S2	1302	G
86	S2	1303	C
86	S2	1308	U
86	S2	1333	U
86	S2	1342	U
86	S2	1357	A
86	S2	1358	U
86	S2	1371	U
86	S2	1372	U
86	S2	1376	A
86	S2	1378	A
86	S2	1401	A
86	S2	1404	U
86	S2	1406	G
86	S2	1411	G
86	S2	1414	A
86	S2	1415	C
86	S2	1417	C
86	S2	1419	C
86	S2	1420	G
86	S2	1421	A
86	S2	1422	G
86	S2	1423	C
86	S2	1434	C
86	S2	1435	C
86	S2	1436	C
86	S2	1438	A
86	S2	1442	U
86	S2	1449	G
86	S2	1452	A
86	S2	1454	A
86	S2	1463	U
86	S2	1474	A
86	S2	1478	U
86	S2	1489	A
86	S2	1490	G
86	S2	1494	U
86	S2	1495	G

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Mol	Chain	Res	Type
86	S2	1497	G
86	S2	1498	A
86	S2	1508	A
86	S2	1521	C
86	S2	1522	A
86	S2	1533	A
86	S2	1535	U
86	S2	1536	G
86	S2	1537	A
86	S2	1544	C
86	S2	1552	G
86	S2	1553	C
86	S2	1556	A
86	S2	1570	G
86	S2	1572	C
86	S2	1573	G
86	S2	1579	A
86	S2	1580	A
86	S2	1581	C
86	S2	1582	C
86	S2	1584	G
86	S2	1585	U
86	S2	1586	U
86	S2	1587	G
86	S2	1588	A
86	S2	1601	A
86	S2	1603	G
86	S2	1604	G
86	S2	1606	G
86	S2	1621	U
86	S2	1623	A
86	S2	1633	A
86	S2	1634	A
86	S2	1637	A
86	S2	1639	G
86	S2	1640	A
86	S2	1646	C
86	S2	1648	G
86	S2	1654	G
86	S2	1663	A
86	S2	1665	G
86	S2	1683	C

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Mol	Chain	Res	Type
86	S2	1694	U
86	S2	1696	C
86	S2	1699	A
86	S2	1712	A
86	S2	1715	A
86	S2	1722	G
86	S2	1726	G
86	S2	1729	U
86	S2	1743	G
86	S2	1744	G
86	S2	1745	A
86	S2	1752	C
86	S2	1753	C
86	S2	1754	G
86	S2	1755	C
86	S2	1757	G
86	S2	1758	G
86	S2	1759	G
86	S2	1761	U
86	S2	1771	G
86	S2	1772	C
86	S2	1773	C
86	S2	1774	C
86	S2	1777	G
86	S2	1782	G
86	S2	1783	C
86	S2	1784	G
86	S2	1785	C
86	S2	1787	G
86	S2	1798	C
86	S2	1809	A
86	S2	1810	U
86	S2	1812	U
86	S2	1813	A
86	S2	1822	A
86	S2	1823	A
86	S2	1825	A
86	S2	1826	G
86	S2	1831	A
86	S2	1835	A
86	S2	1838	U
86	S2	1849	G

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Mol	Chain	Res	Type
86	S2	1851	A
86	S2	1852	C
86	S2	1861	G
86	S2	1862	G
86	S2	1863	A
86	S2	1865	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	L5	406	C
21	L5	493	G
21	L5	914	U
21	L5	1049	C
21	L5	1082	C
21	L5	1590	C
21	L5	1633	G
21	L5	1977	C
21	L5	2033	A
21	L5	2055	G
21	L5	2416	G
21	L5	2675	G
21	L5	2760	G
21	L5	2786	C
21	L5	3614	G
21	L5	3673	C
21	L5	3948	C
21	L5	4061	G
21	L5	4600	G
21	L5	4699	U
21	L5	4913	G
82	PE	18	U
86	S2	291	G
86	S2	420	G
86	S2	531	A
86	S2	557	U
86	S2	563	G
86	S2	688	U
86	S2	1434	C
86	S2	1781	A

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 261 ligands modelled in this entry, 261 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	L5	11
86	S2	7
49	Lb	1
28	LE	1
3	LW	1
85	CB	1
13	SH	1
81	AP	1
84	Lt	1
32	LI	1
82	PE	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Lb	76:VAL	C	89:VAL	N	34.34
1	S2	753:C	O3'	785:C	P	28.13
1	LE	76:ALA	C	88:VAL	N	24.39
1	L5	2910:G	O3'	3584:C	P	20.70
1	L5	760:G	O3'	903:C	P	17.25
1	LW	63:GLN	C	70:LYS	N	17.10
1	L5	519:C	O3'	642:G	P	16.92
1	L5	4776:G	O3'	4858:C	P	16.29
1	S2	698:G	O3'	730:C	P	15.90
1	CB	236:PHE	C	247:ALA	N	15.24
1	L5	996:G	O3'	1047:C	P	14.32
1	L5	2112:G	O3'	2249:C	P	14.01
1	S2	739:C	O3'	746:C	P	13.50
1	L5	1222:A	O3'	1234:G	P	11.16
1	SH	107:LYS	C	111:LYS	N	11.06
1	AP	15:G	O3'	18:G	P	10.95
1	Lt	87:GLU	C	104:ILE	N	10.64
1	L5	1051:G	O3'	1064:G	P	8.44
1	S2	225:G	O3'	287:U	P	7.29
1	LI	102:MET	C	114:GLY	N	6.92
1	L5	1100:U	O3'	1167:C	P	6.56
1	PE	16:C	O3'	18:U	P	6.10
1	L5	1709:C	O3'	1714:C	P	5.96
1	L5	3985:C	O3'	4018:G	P	4.55
1	S2	527:C	O3'	528:A	P	3.34
1	S2	559:G	O3'	560:A	P	3.29
1	S2	1210:G	O3'	1211:G	P	3.25

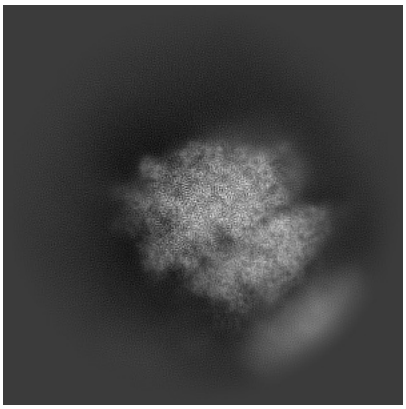
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-44060. These allow visual inspection of the internal detail of the map and identification of artifacts.

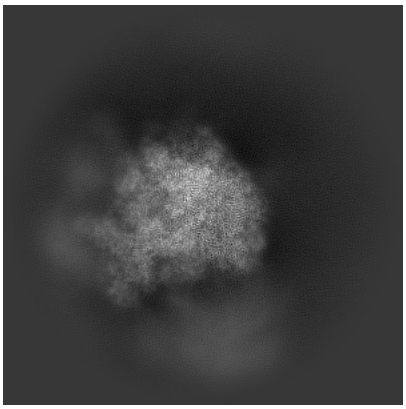
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

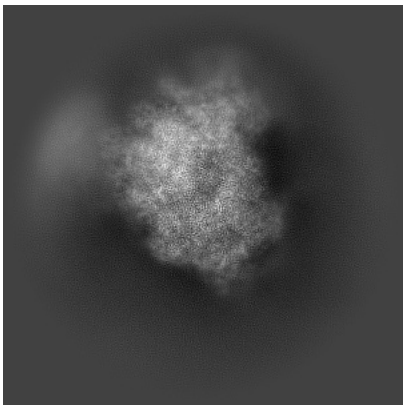
6.1.1 Primary map



X

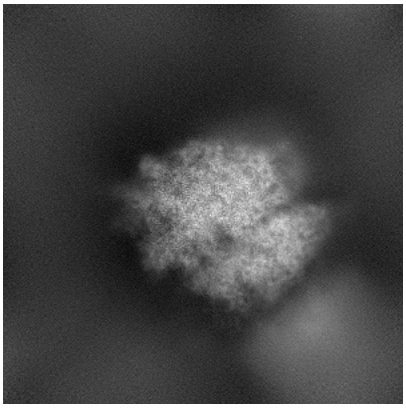


Y

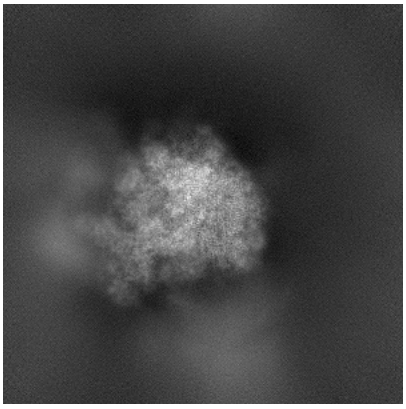


Z

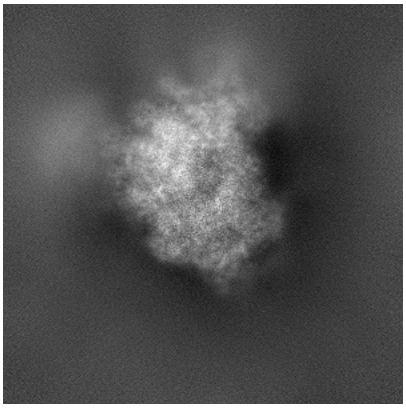
6.1.2 Raw map



X



Y

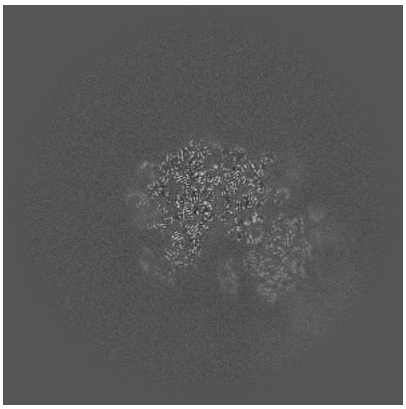


Z

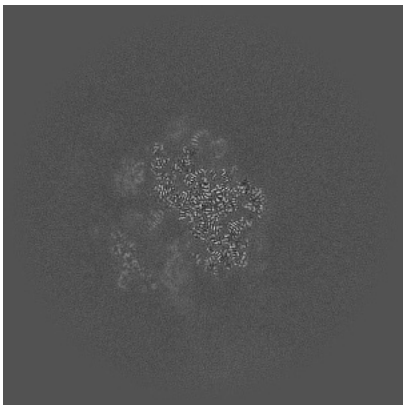
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

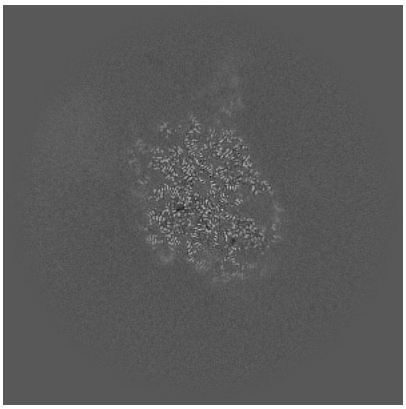
6.2.1 Primary map



X Index: 256

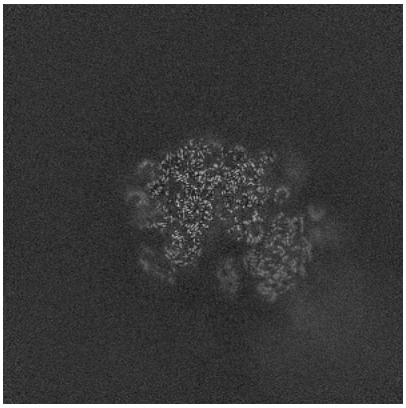


Y Index: 256

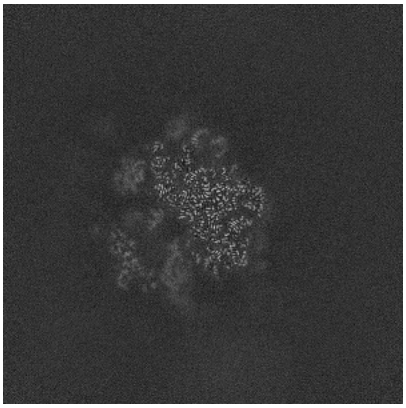


Z Index: 256

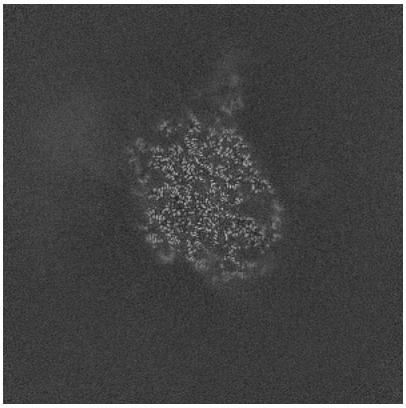
6.2.2 Raw map



X Index: 256



Y Index: 256

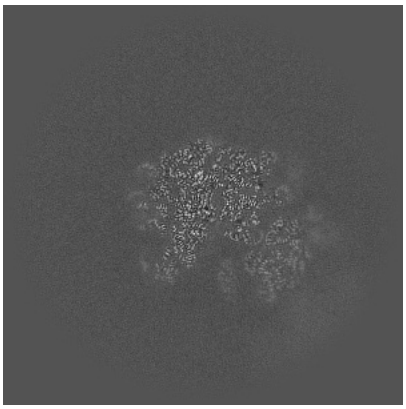


Z Index: 256

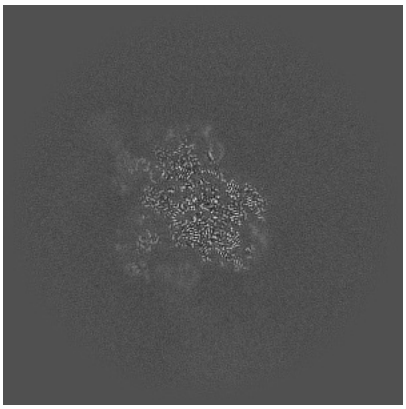
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

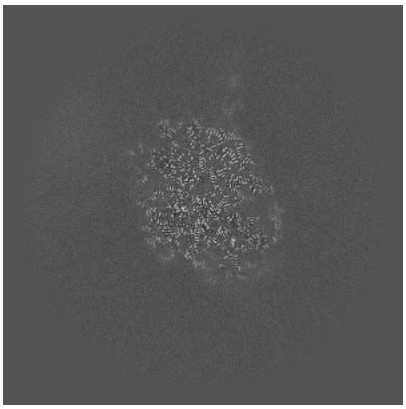
6.3.1 Primary map



X Index: 253

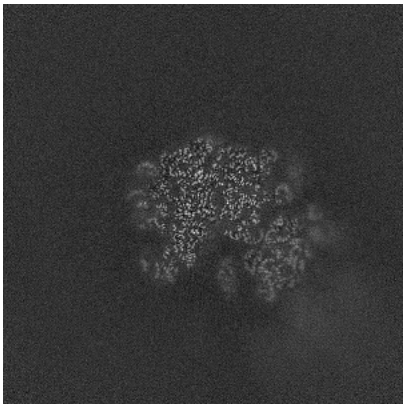


Y Index: 243

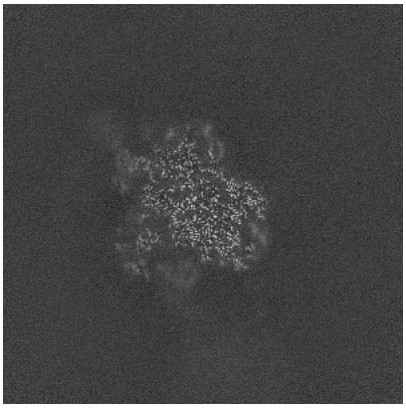


Z Index: 258

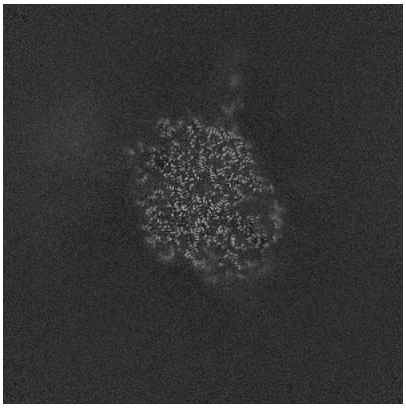
6.3.2 Raw map



X Index: 253



Y Index: 243

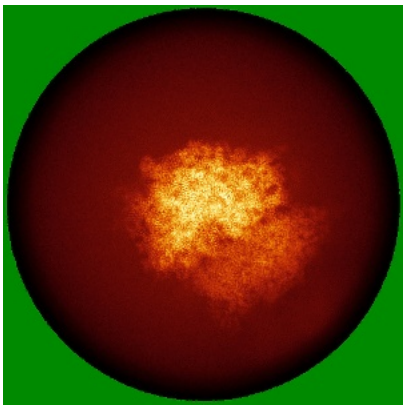


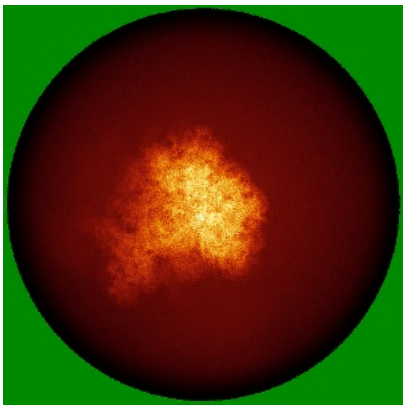
Z Index: 258

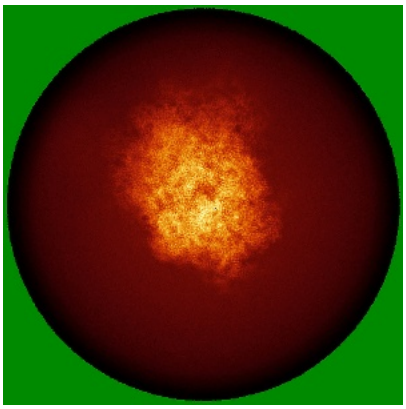
The images above show the largest variance slices of the map in three orthogonal directions.

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

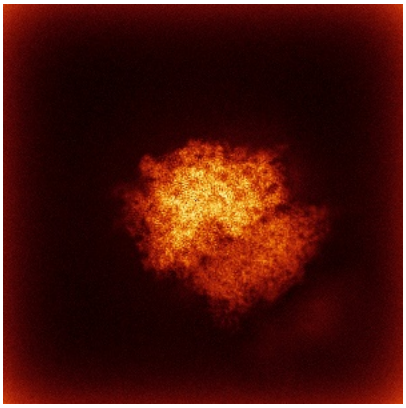
6.4.1 Primary map

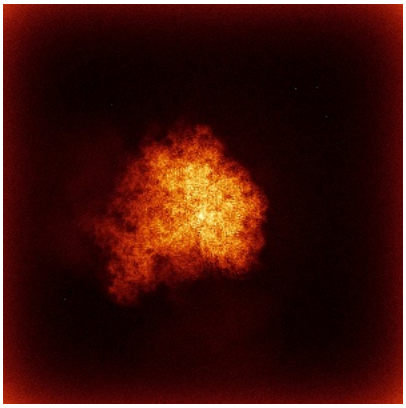

X

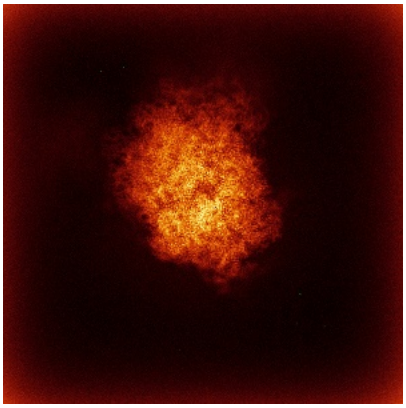

Y


Z

6.4.2 Raw map


X

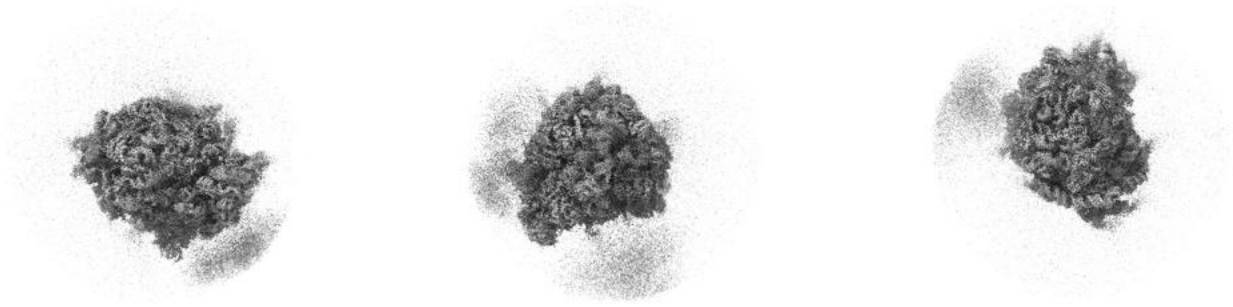

Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.042. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

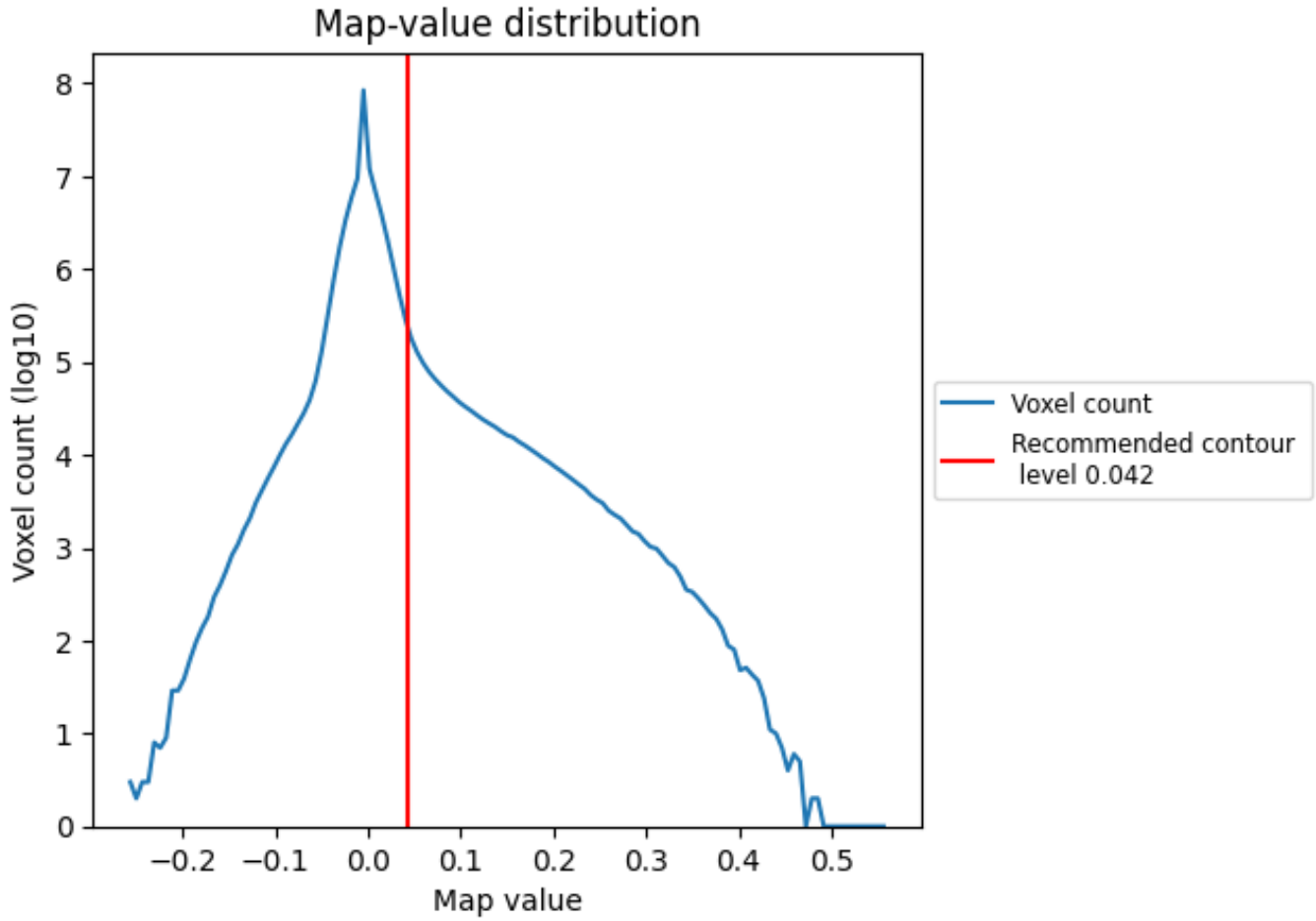
6.6 Mask visualisation (i)

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

7 Map analysis

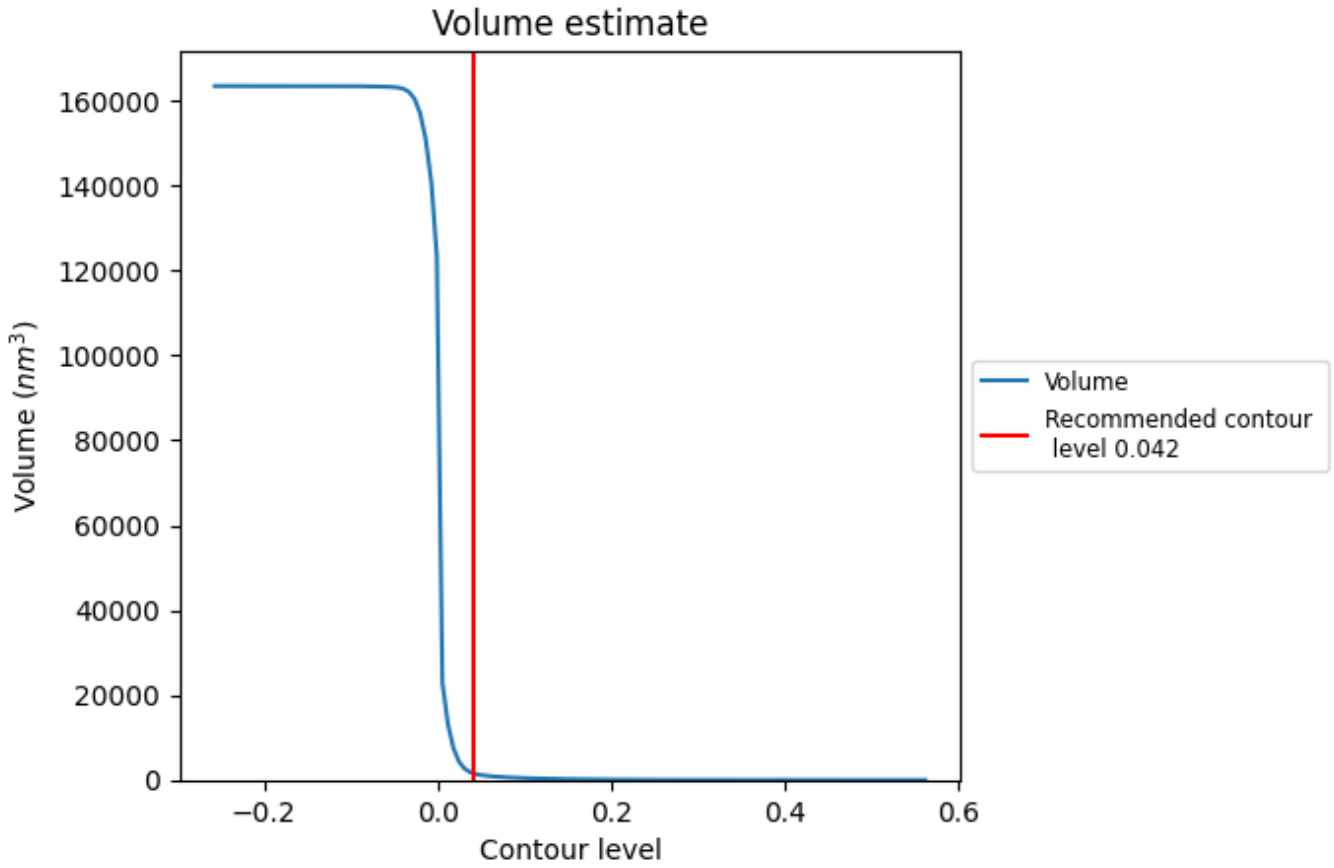
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

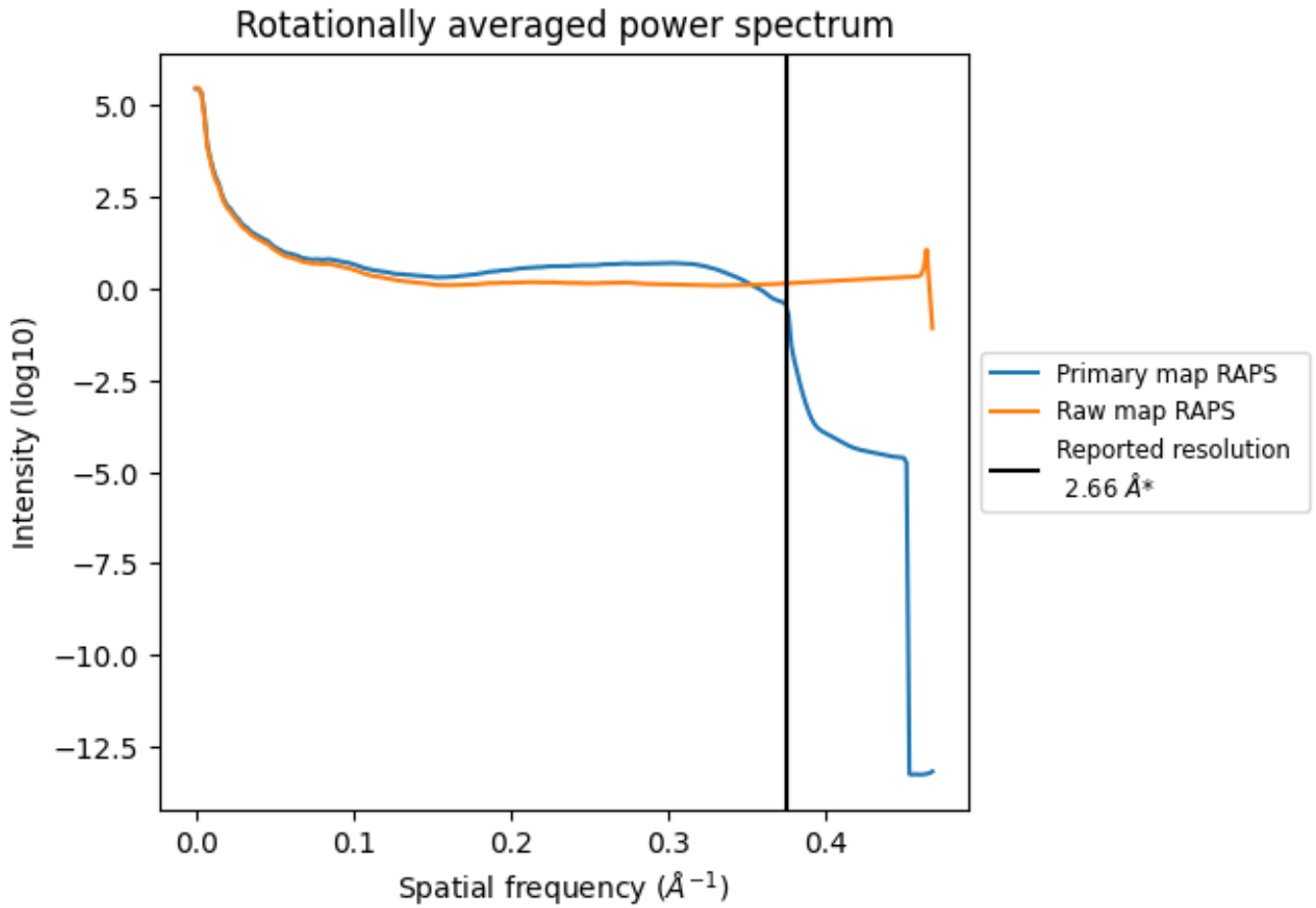
7.2 Volume estimate



The volume at the recommended contour level is 1562 nm^3; this corresponds to an approximate mass of 1411 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)

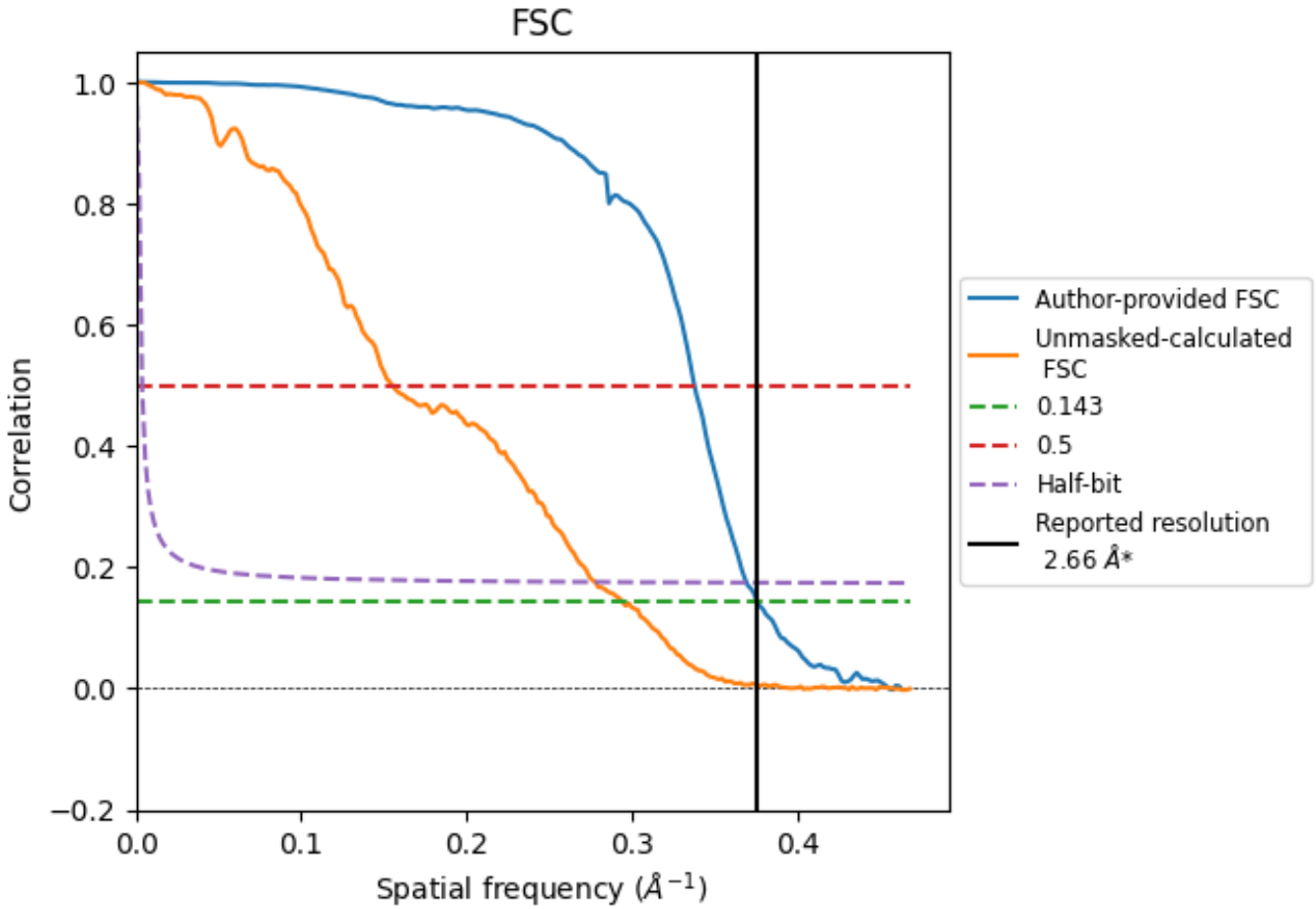


*Reported resolution corresponds to spatial frequency of 0.376 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.376 Å^{-1}

8.2 Resolution estimates (i)

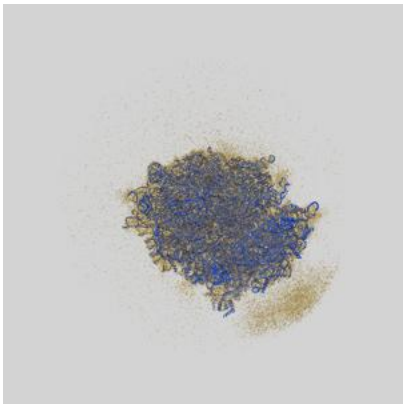
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.66	-	-
Author-provided FSC curve	2.66	2.96	2.71
Unmasked-calculated*	3.40	6.45	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.40 differs from the reported value 2.66 by more than 10 %

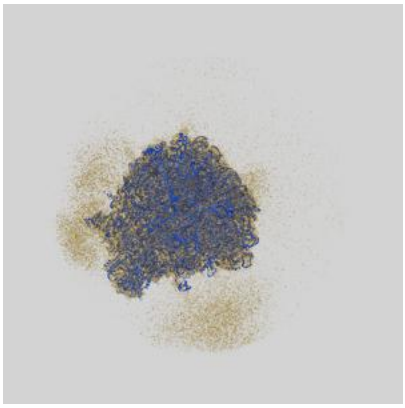
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-44060 and PDB model 9B0W. Per-residue inclusion information can be found in section 3 on page 21.

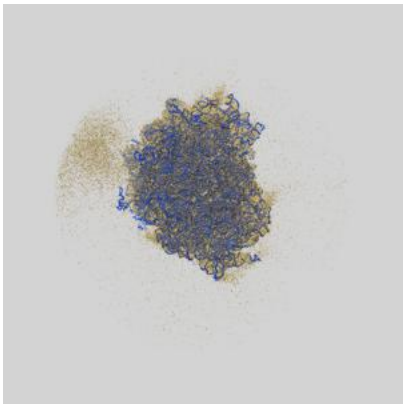
9.1 Map-model overlay



X



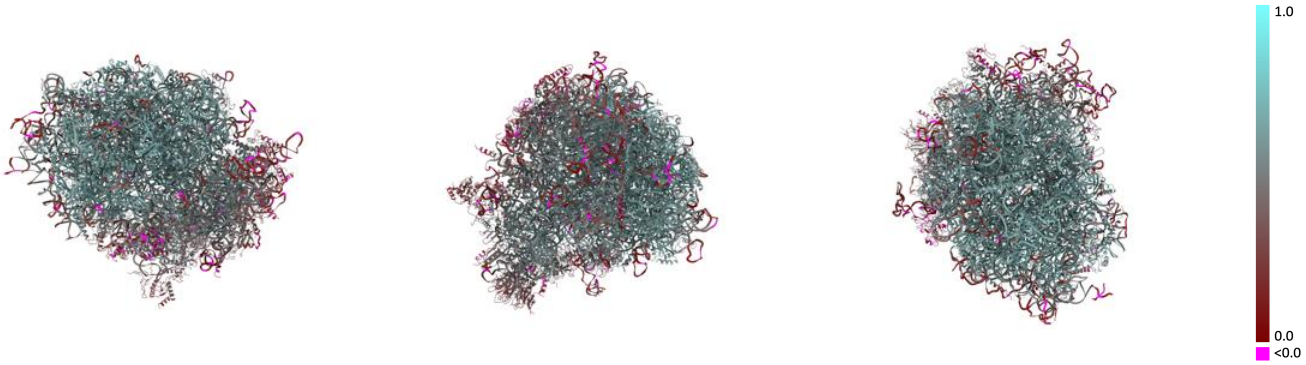
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.042 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.

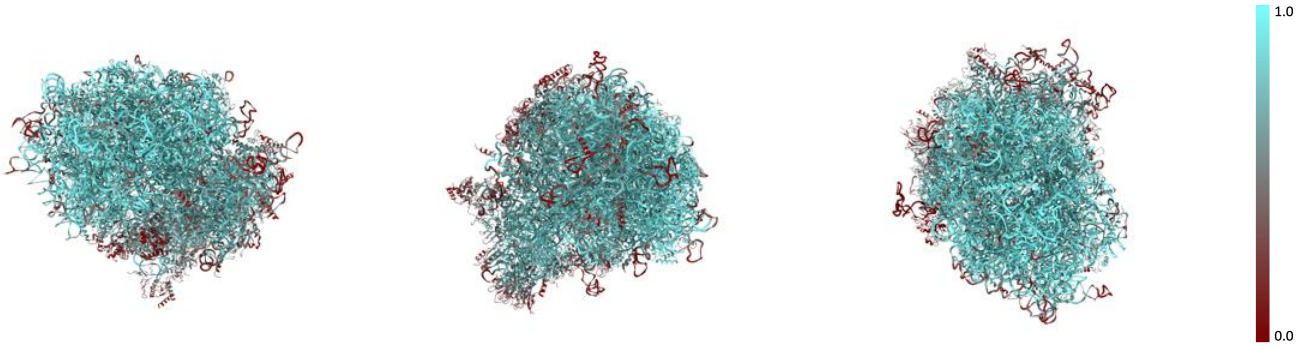
9.2 Q-score mapped to coordinate model (i)



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.

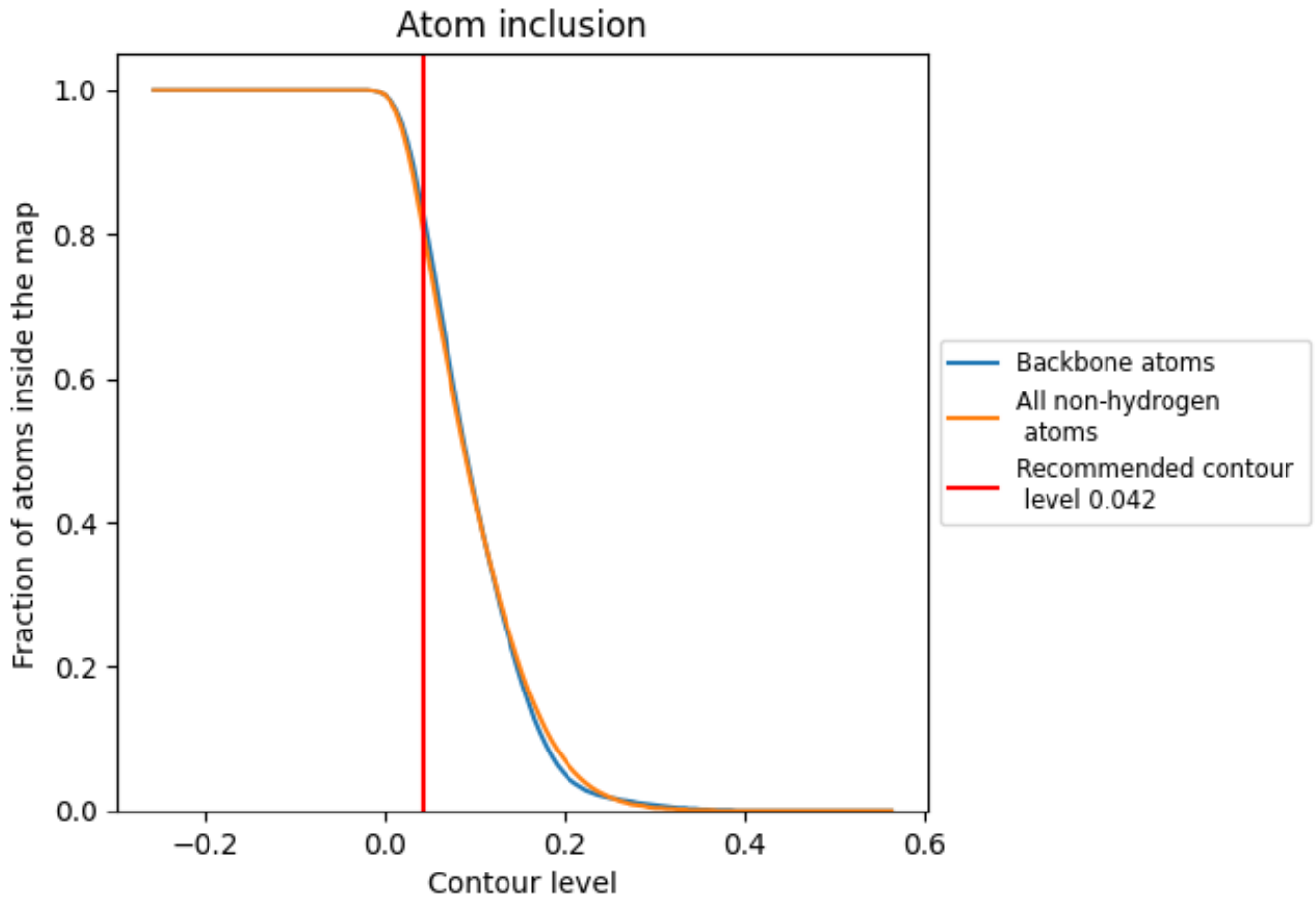
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.042).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.042) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.5230
AP	0.6160	0.3940
CB	0.5300	0.4080
CH	0.3920	0.3130
L5	0.8790	0.5500
L7	0.9840	0.6250
L8	0.9300	0.5900
LA	0.9580	0.6320
LB	0.9140	0.6100
LC	0.9160	0.6150
LD	0.8620	0.5800
LE	0.8050	0.5460
LF	0.9460	0.6240
LG	0.8080	0.5640
LH	0.8950	0.5950
LI	0.9240	0.6180
LJ	0.7530	0.5060
LL	0.8700	0.5890
LM	0.9050	0.5930
LN	0.9820	0.6440
LO	0.9440	0.6280
LP	0.9380	0.6330
LQ	0.9640	0.6390
LR	0.8240	0.5420
LS	0.9620	0.6360
LT	0.8890	0.5920
LU	0.7530	0.4940
LV	0.9370	0.6190
LW	0.5890	0.4250
LX	0.8960	0.6100
LY	0.9000	0.6130
LZ	0.8970	0.5930
La	0.9600	0.6420
Lb	0.8020	0.5440
Lc	0.8720	0.5680

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Chain	Atom inclusion	Q-score
Ld	0.8690	0.5910
Le	0.9620	0.6370
Lf	0.9630	0.6360
Lg	0.9020	0.6040
Lh	0.9110	0.6140
Li	0.9000	0.6080
Lj	0.9660	0.6340
Lk	0.7810	0.5560
Ll	0.9340	0.6250
Lm	0.9060	0.6120
Ln	0.8950	0.5960
Lo	0.9030	0.6100
Lp	0.9420	0.6220
Lr	0.9430	0.6290
Ls	0.2310	0.2220
Lt	0.1220	0.1540
Lz	0.0320	0.1050
PE	0.6220	0.2960
S2	0.8420	0.4990
SA	0.6970	0.4820
SB	0.7770	0.5480
SC	0.8050	0.5360
SD	0.6380	0.4600
SE	0.6670	0.4490
SF	0.6490	0.4600
SG	0.5310	0.3980
SH	0.5340	0.3940
SI	0.6580	0.4620
SJ	0.6660	0.4460
SK	0.6510	0.4220
SL	0.7370	0.4910
SM	0.2310	0.2550
SN	0.8130	0.5470
SO	0.7690	0.5210
SP	0.6850	0.4880
SQ	0.6740	0.4630
SR	0.5830	0.4080
SS	0.6860	0.4790
ST	0.6870	0.4680
SU	0.5420	0.3870
SV	0.7120	0.4900
SW	0.8620	0.5610

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Chain	Atom inclusion	Q-score
SX	0.7710	0.5250
SY	0.5050	0.3590
SZ	0.5110	0.3900
Sa	0.8250	0.5450
Sb	0.6950	0.4870
Sc	0.5000	0.3310
Sd	0.8440	0.5460
Se	0.5650	0.3570
Sf	0.3170	0.2480
Sg	0.3910	0.3370