Full wwPDB EM Validation Report ⓘ

Jul 12, 2023 – 02:28 PM JST

PDB ID	:	8I9W
EMDB ID	:	EMD-35286
Title	:	Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - Dbp10-3
Authors	:	Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on	:	2023-02-07
Resolution	:	3.10 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:

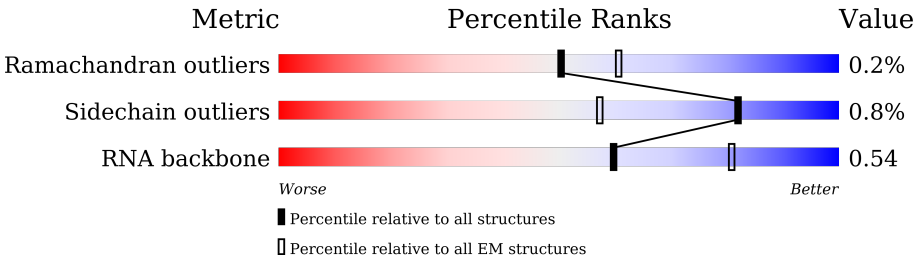
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance

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

The reported resolution of this entry is 3.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	C1	3341	50% 14% 35%
2	C2	319	61% 19% 20%
3	CA	316	78% 21%
4	CB	391	66% 34%
5	CC	801	36% 64%
6	CE	598	77% 23%
7	CF	270	90% 9%
8	CG	184	96%

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Mol	Chain	Length	Quality of chain
9	CH	661	75% 24%
10	CI	414	35% 65%
11	CJ	679	56% 44%
12	CK	261	91% 9%
13	CL	558	51% 71% 29%
14	CM	249	15% 90% 10%
14	LF	249	98%
15	CN	246	100%
16	CO	120	52% 48%
17	CP	751	46% 53%
18	CQ	225	56% 44%
19	CR	237	70% 30%
20	CS	834	5% 28% 72%
21	CT	688	13% 70% 29%
22	CU	451	39% 61%
23	CV	147	94% 5%
24	CX	203	43% 57%
25	CY	788	10% 45% 54%
26	Cb	924	67% 31%
27	Cz	123	11% 57% 43%
28	LB	392	85% 14%
29	LC	365	99%
30	LE	200	85% 10%
31	LG	262	77% 22%
32	LH	192	98%

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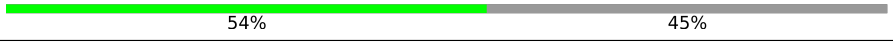
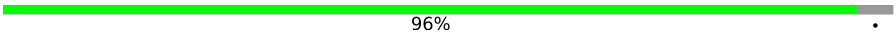
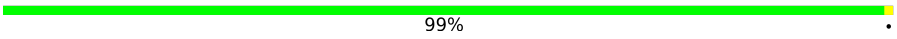
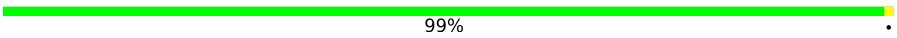
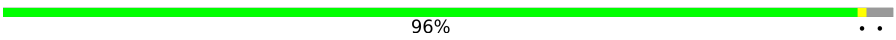
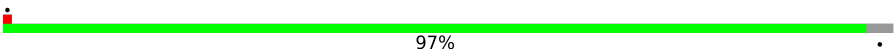
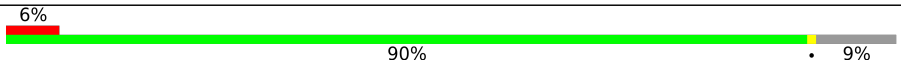
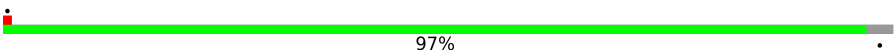
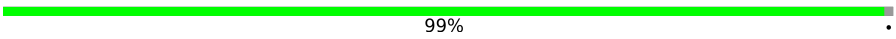
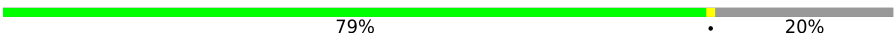
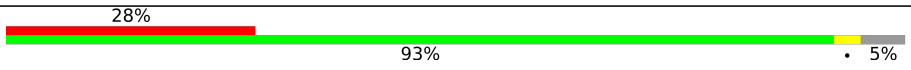
Mol	Chain	Length	Quality of chain
33	LK	165	
34	LL	213	
35	LM	142	
36	LN	203	
37	LO	204	
38	LP	187	
39	LQ	213	
40	LS	174	
41	LT	160	
42	LV	139	
43	LX	156	
44	LY	138	
45	Ld	120	
46	Le	131	
47	Lf	109	
48	Lh	935	
49	Li	110	
50	Lj	95	
51	Lq	217	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 136840 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	C1	2163	46266	20653	8376	15074	2163	0	0

- Molecule 2 is a RNA chain called RNA (319-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	256	5456	2435	974	1791	256	0	0

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	CA	251	2069	1324	381	357	7	0	0

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CB	260	2063	1322	367	371	3	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	CC	291	2413	1530	403	471	2	7	0	0

- Molecule 6 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CE	463	3673	2352	643	667	11	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 7 is a protein called Ribosome assembly factor mrt4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CF	245	Total	C	N	O	S	0	0
			1945	1222	352	362	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CF	13	ILE	THR	conflict	UNP G0S616
CF	139	THR	PRO	conflict	UNP G0S616
CF	228	ASN	SER	conflict	UNP G0S616
CF	259	ILE	MET	conflict	UNP G0S616

- Molecule 8 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CG	177	Total	C	N	O	S	0	0
			1396	884	247	253	12		

- Molecule 9 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CH	503	Total	C	N	O	S	0	0
			4085	2594	712	763	16		

- Molecule 10 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 11 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CJ	379	Total	C	N	O	S	0	0
			3092	1991	543	548	10		

- Molecule 12 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CK	238	Total	C	N	O	S	0	0
			1908	1199	375	330	4		

- Molecule 13 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	CL	397	Total	C	N	O	0	0
			2239	1350	459	430		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CL	69	ARG	ILE	conflict	UNP G0SEW3

- Molecule 14 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CM	223	Total	C	N	O	S	0	0
			1820	1169	340	308	3		
14	LF	247	Total	C	N	O	S	0	0
			2017	1294	376	344	3		

- Molecule 15 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	CN	246	Total	C	N	O	S	0	0
			1856	1158	322	369	7		

- Molecule 16 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 17 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	CP	356	Total	C	N	O	S	0	0
			2798	1777	495	510	16		

- Molecule 18 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CQ	125	Total	C	N	O	S	0	0
			1056	664	219	163	10		

- Molecule 19 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 20 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	CS	235	Total	C	N	O	S	0	0
			1891	1186	359	341	5		

- Molecule 21 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	CT	488	Total	C	N	O	S	0	0
			3911	2486	690	719	16		

- Molecule 22 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	CU	178	Total	C	N	O	S	0	0
			1415	876	265	271	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
23	CV	139	Total	C	N	O	0	0
			1073	672	213	188		

- Molecule 24 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CX	88	Total	C	N	O	S	0	0
			701	435	128	135	3		

- Molecule 25 is a protein called Putative NOC2 family protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CY	361	Total	C	N	O	S	0	0
			2919	1874	525	509	11		

- Molecule 26 is a protein called ATP-dependent RNA helicase DBP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Cb	634	Total	C	N	O	S	0	0
			5005	3183	907	902	13		

- Molecule 27 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Cz	70	Total	C	N	O	S	0	0
			592	368	120	101	3		

- Molecule 28 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LB	339	Total	C	N	O	S	0	0
			2696	1713	491	480	12		

- Molecule 29 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LC	362	Total	C	N	O	S	0	0
			2752	1738	526	479	9		

- Molecule 30 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LE	179	Total	C	N	O	S	0	0
			1403	898	255	247	3		

- Molecule 31 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LG	204	Total	C	N	O	S	0	0
			1644	1060	297	282	5		

- Molecule 32 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LH	190	Total	C	N	O	S	0	0
			1496	950	268	272	6		

There are 37 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	TYR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	PHE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ARG	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	THR	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	SER	deletion	UNP G0S0E5
LH	?	-	LYS	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5
LH	?	-	GLU	deletion	UNP G0S0E5
LH	?	-	LEU	deletion	UNP G0S0E5
LH	?	-	ASP	deletion	UNP G0S0E5
LH	?	-	ILE	deletion	UNP G0S0E5
LH	?	-	ASN	deletion	UNP G0S0E5
LH	?	-	GLY	deletion	UNP G0S0E5

- Molecule 33 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LK	146	Total	C	N	O	S	0	0
			1112	701	203	206	2		

- Molecule 34 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LL	117	Total	C	N	O	S	0	0
			964	608	206	148	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LM	137	Total	C	N	O	S	0	0
			1101	699	211	190	1		

- Molecule 36 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LN	183	Total	C	N	O	S	0	0
			1563	974	332	253	4		

- Molecule 37 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LO	204	Total	C	N	O	S	0	0
			1618	1039	306	267	6		

- Molecule 38 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LP	153	Total	C	N	O	S	0	0
			1200	747	238	213	2		

- Molecule 39 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LQ	129	Total	C	N	O	S	0	0
			1021	646	200	173	2		

- Molecule 40 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LS	174	Total	C	N	O	S	0	0
			1433	922	267	239	5		

- Molecule 41 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	LT	126	Total	C	N	O	S	0	0
			1014	643	196	173	2		

- Molecule 42 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LV	135	Total	C	N	O	S	0	0
			995	633	185	170	7		

- Molecule 43 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	LX	47	Total	C	N	O	0	0
			354	224	72	58		

- Molecule 44 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Ld	109	Total	C	N	O	S	0	0
			890	563	171	155	1		

- Molecule 46 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Le	127	Total	C	N	O	S	0	0
			1025	645	209	164	7		

- Molecule 47 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 48 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	Lh	121	Total	C	N	O	0	0
			995	633	196	166		

- Molecule 49 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Li	88	Total	C	N	O	S	0	0
			731	449	162	119	1		

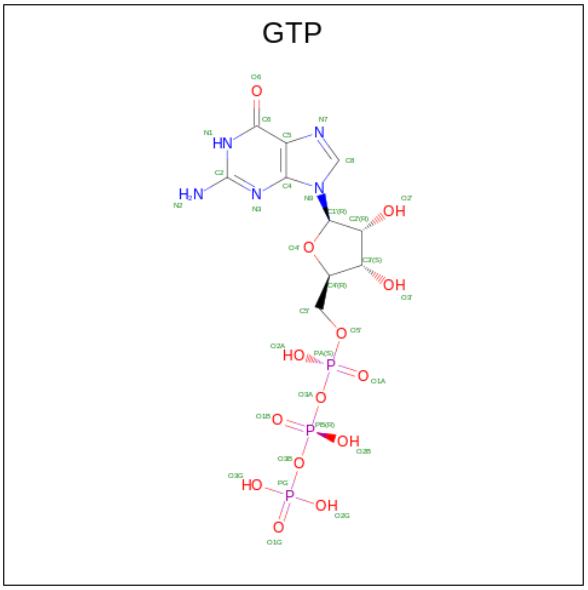
- Molecule 50 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lj	74	Total	C	N	O	S	0	0
			595	365	132	93	5		

- Molecule 51 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Lq	207	Total	C	N	O	S	0	0
			1600	1016	285	291	8		

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

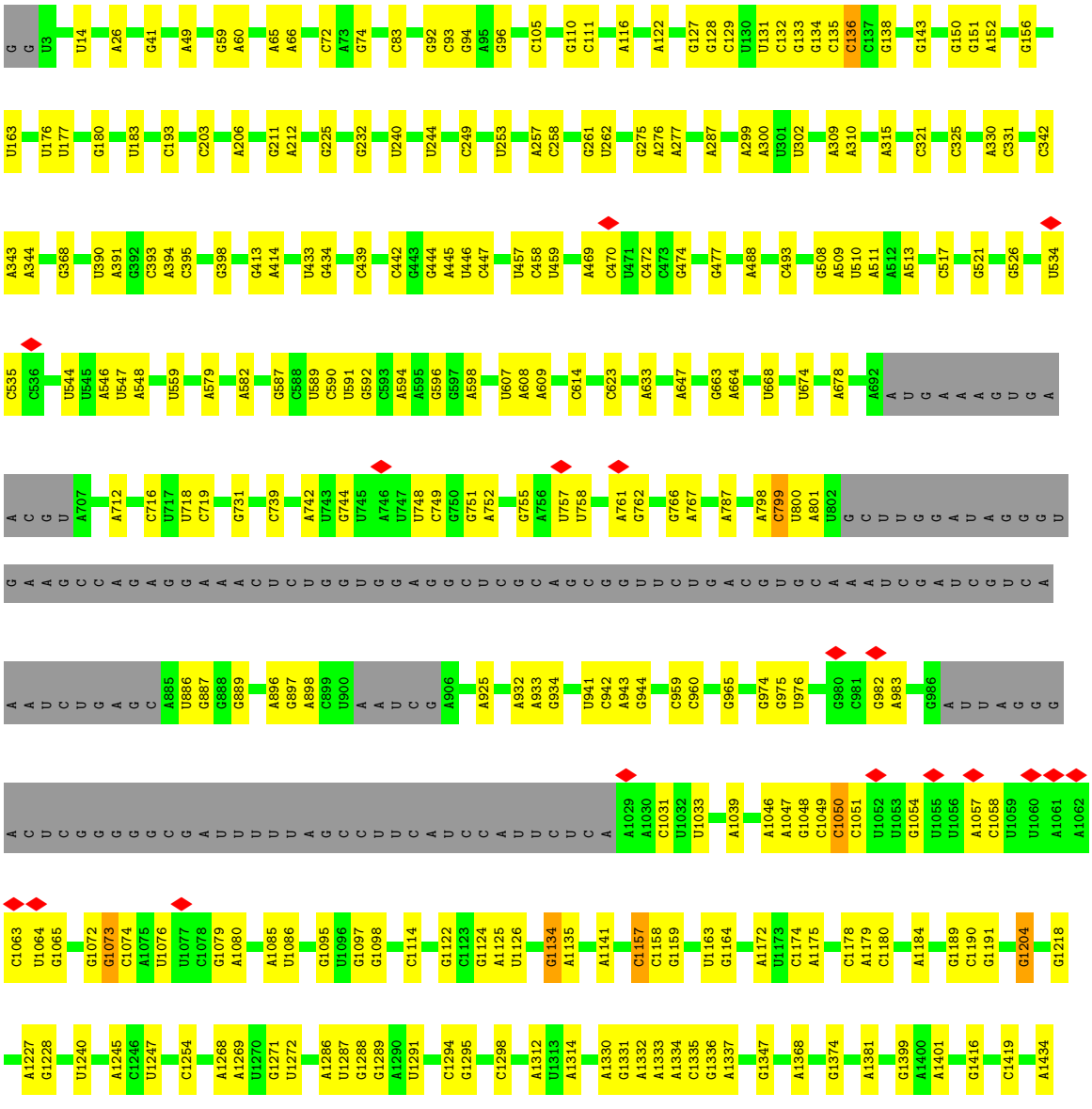
Mol	Chain	Residues	Atoms	AltConf
53	CQ	1	Total Zn 1 1	0
53	Lj	1	Total Zn 1 1	0

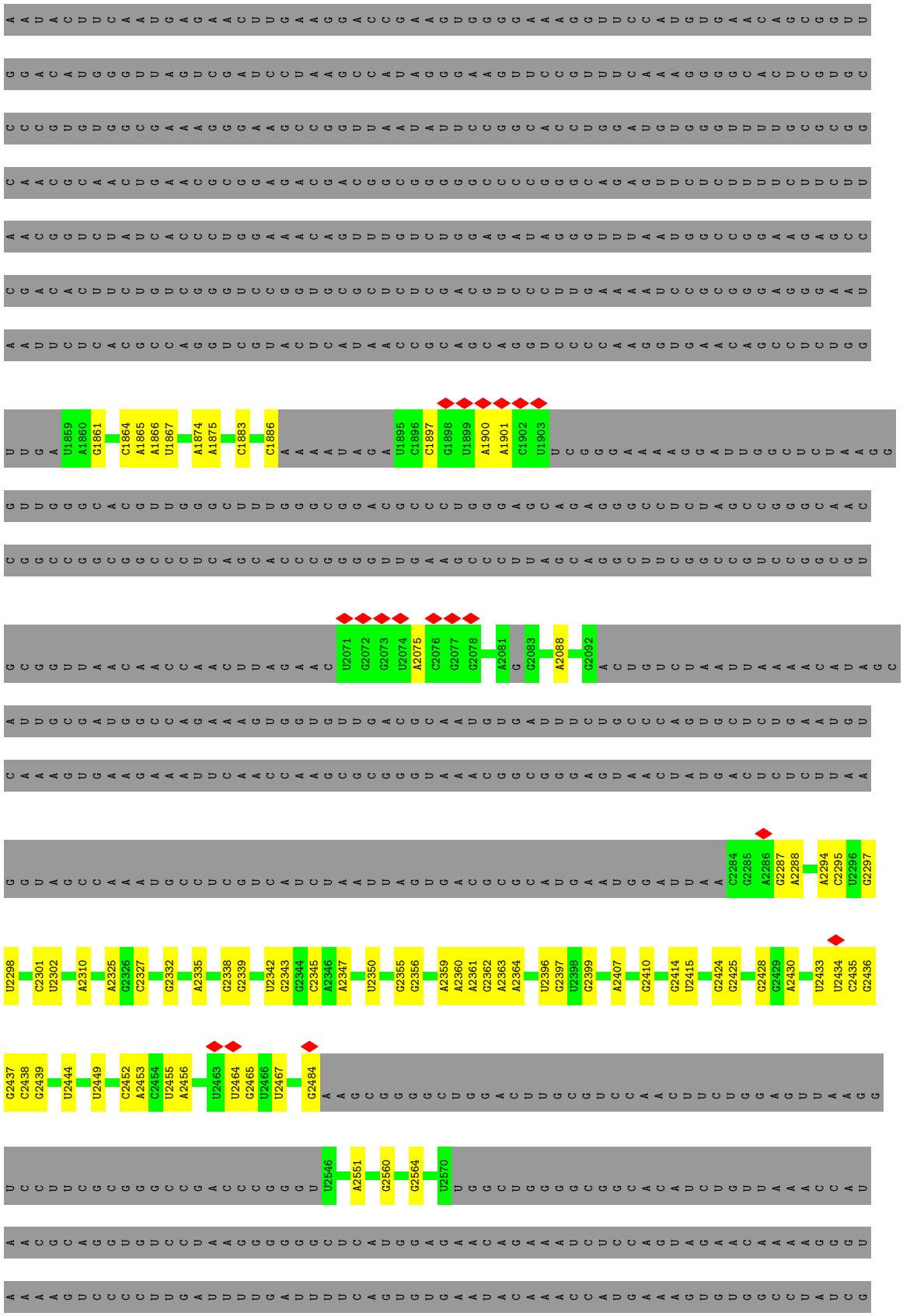
3 Residue-property plots (i)

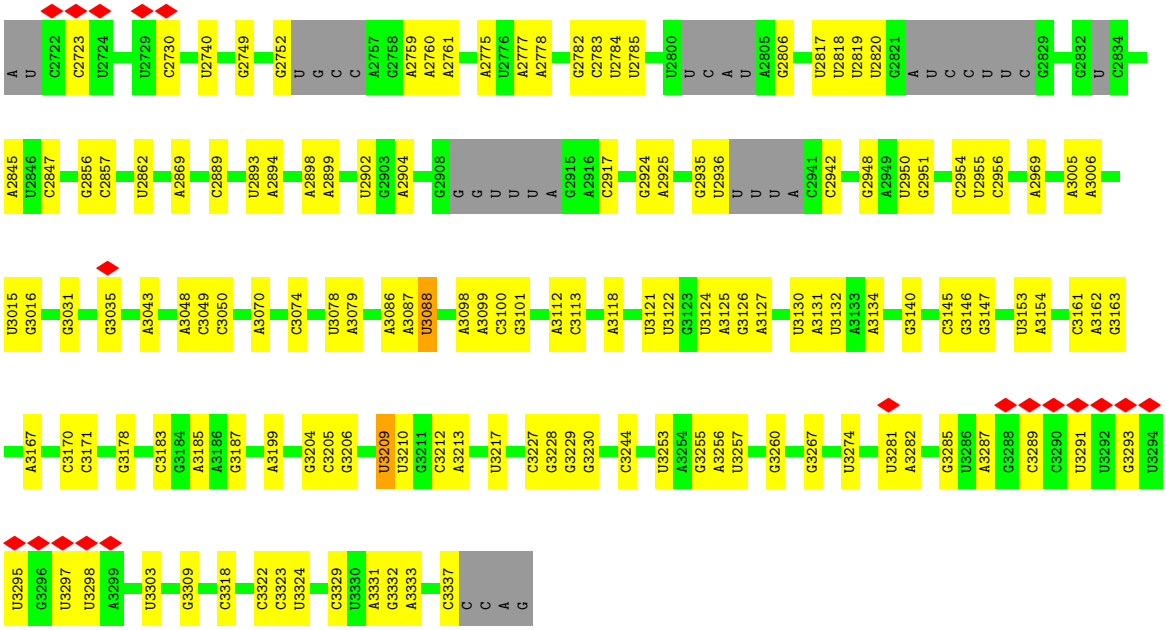
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: RNA (3341-MER)

Chain C1:

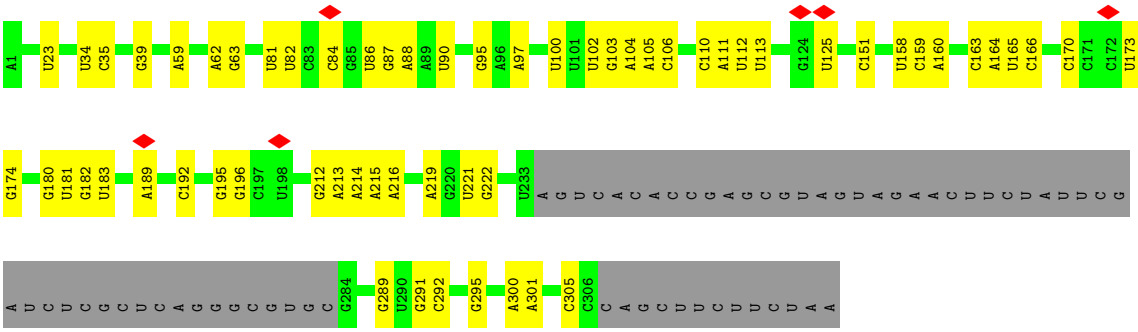



U1859 A1860 G1861 C1864 A1865 A1866 U1867 A1874 A1875 C1883 C1886 U1895 C1896 C1897 G1898 U1899 A1900 A1901 C1902 U1903
U2071 G2072 G2073 U2074 A2075 C2076 G2077 G2078 A2081 G2083 A2088 G2092
C2284 G2285 A2286 G2287 A2288 A2294 C2295 U2296 G2297
U2298 C2301 U2302 A2310 A2325 G2326 C2327 G2332 A2335 G2338 G2339 U2342 G2343 G2344 C2345 A2346 A2347 U2350 G2355 G2356 A2359 A2360 A2361 G2362 A2363 A2364 U2396 G2397 U2398 G2399 A2407 G2410 G2414 U2415 G2424 G2425 G2428 G2429 A2430 U2433 U2434 C2435 G2436
G2437 C2438 G2439 U2444 U2449 C2452 A2453 C2454 U2455 A2456 U2463 U2464 G2465 U2466 U2467 G2484
U2546 A2551 G2560 G2564 U2570



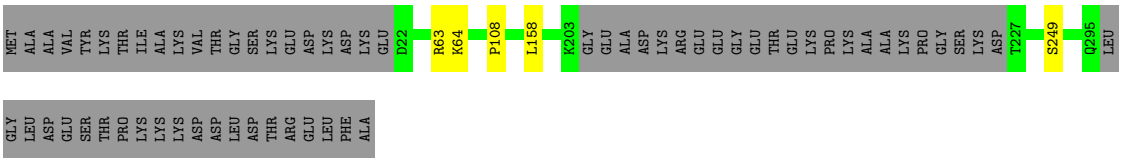
• Molecule 2: RNA (319-MER)

Chain C2:



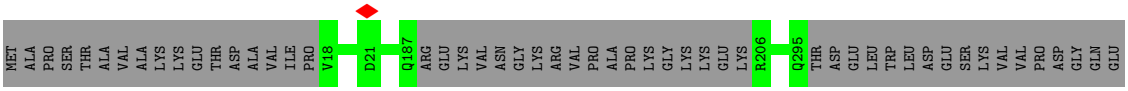
• Molecule 3: Brix domain-containing protein

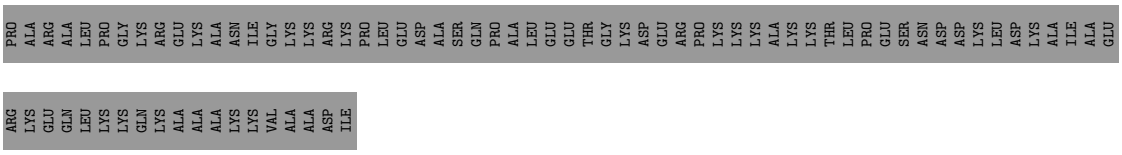
Chain CA:



• Molecule 4: Ribosome biogenesis protein C8F11.04

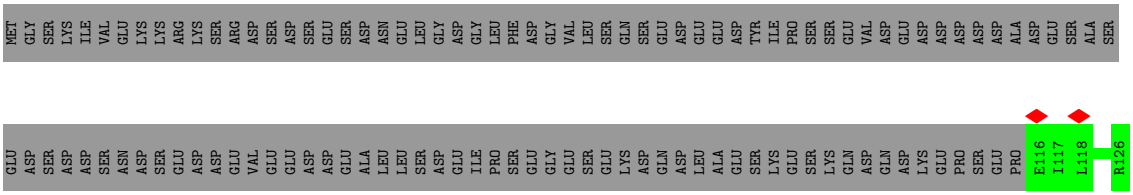
Chain CB:

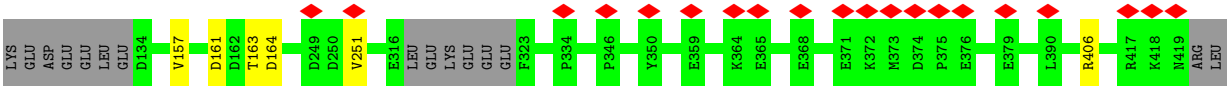


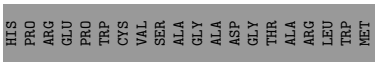


• Molecule 5: Ribosome biogenesis protein ERB1

Chain CC:

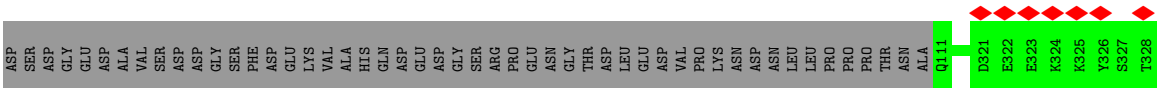


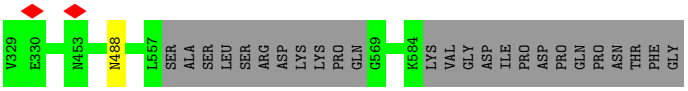




• Molecule 6: RNA helicase

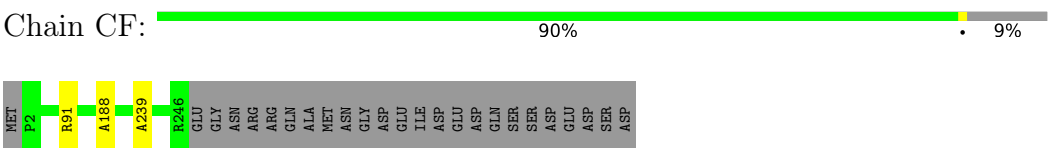
Chain CE:





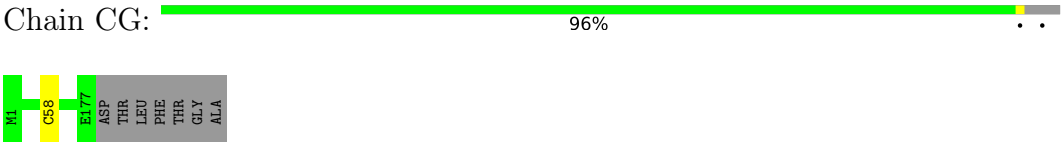
• Molecule 7: Ribosome assembly factor mrt4

Chain CF:



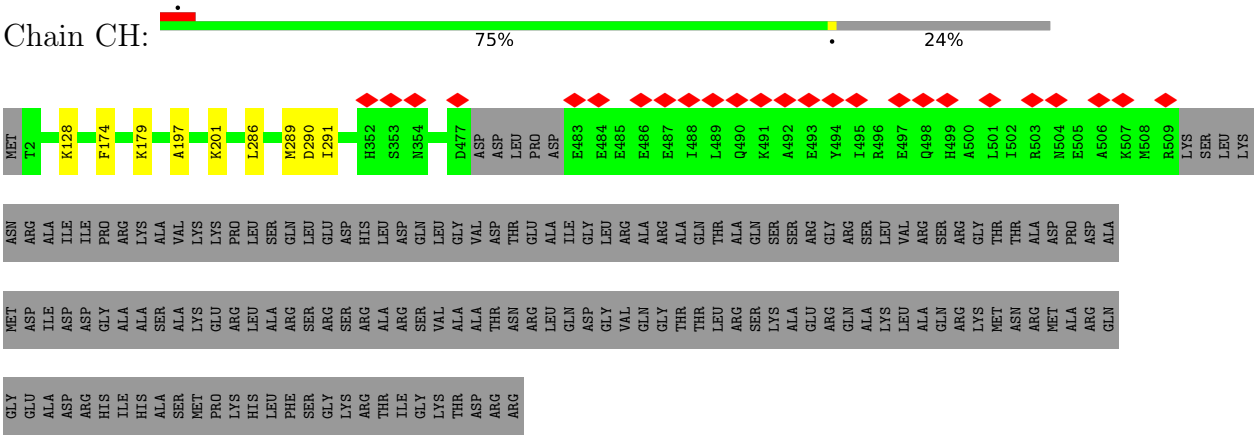
• Molecule 8: 60S ribosome subunit biogenesis protein NIP7

Chain CG:



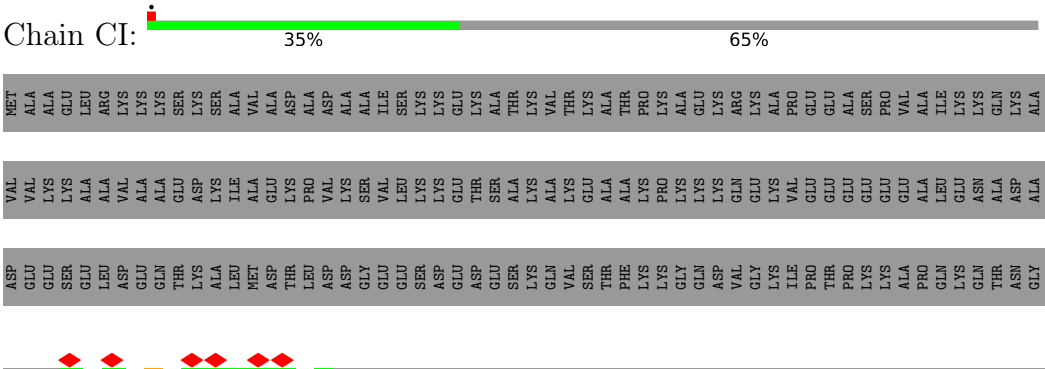
• Molecule 9: Nucleolar GTP-binding protein 1

Chain CH:



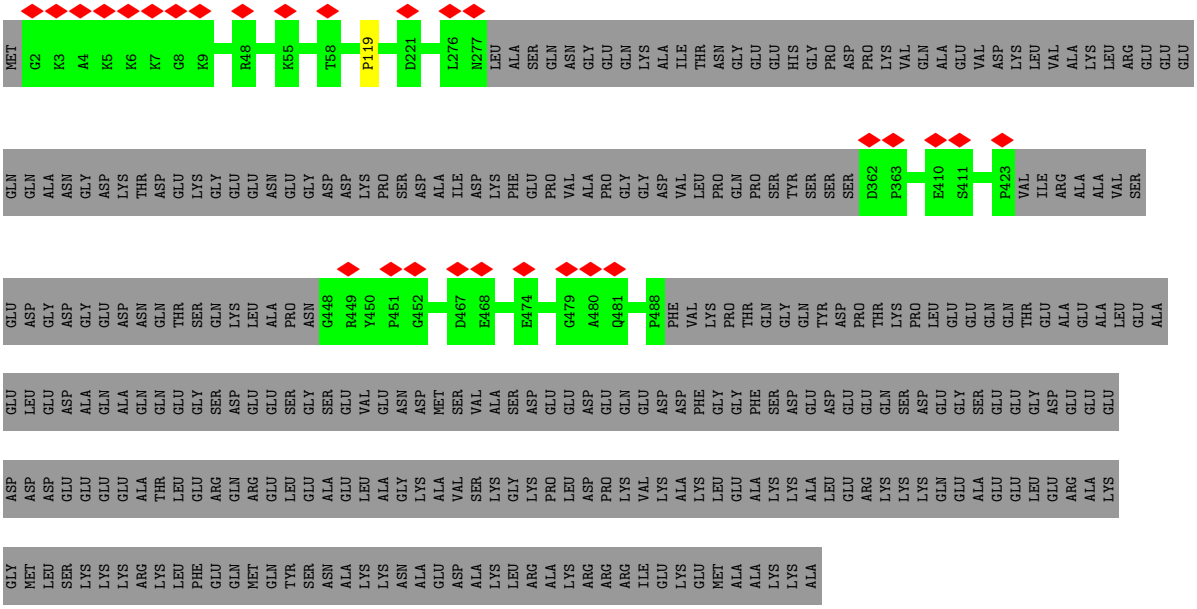
• Molecule 10: Putative RNA-binding protein

Chain CI:



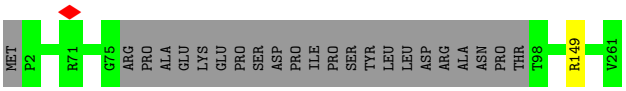
• Molecule 11: Pescadillo homolog

Chain CJ:



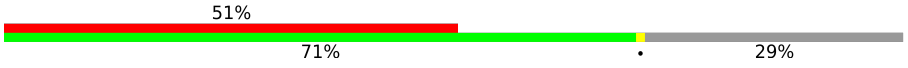
• Molecule 12: Ribosome biogenesis protein NSA2 homolog

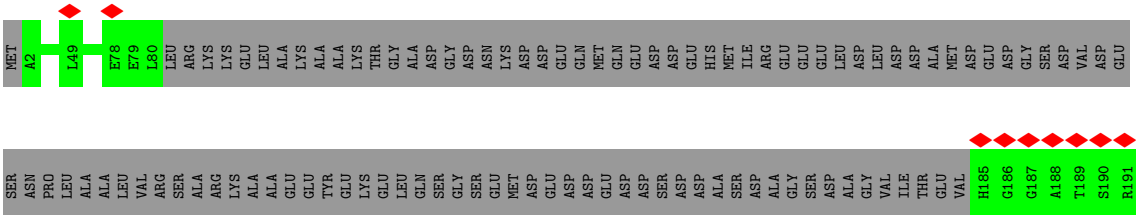
Chain CK:

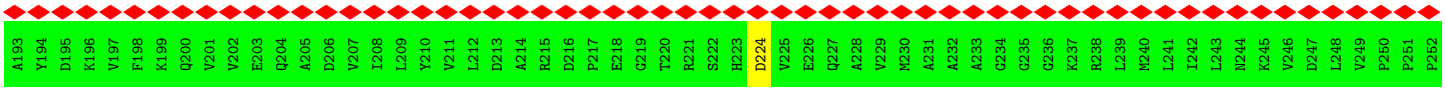


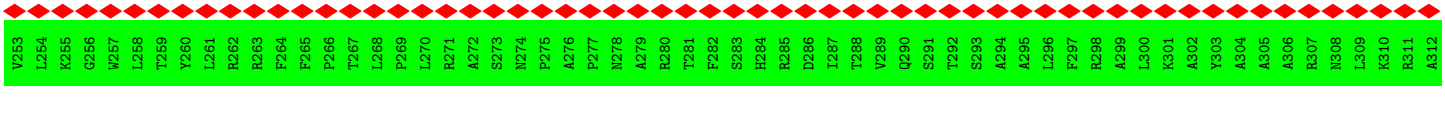
• Molecule 13: Putative GTP binding protein

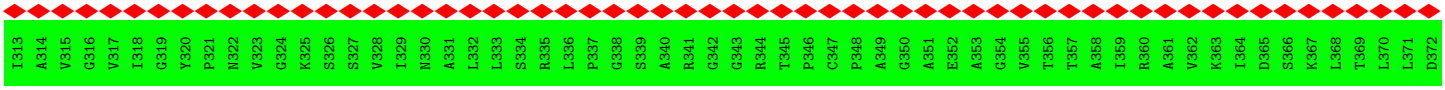
Chain CL:

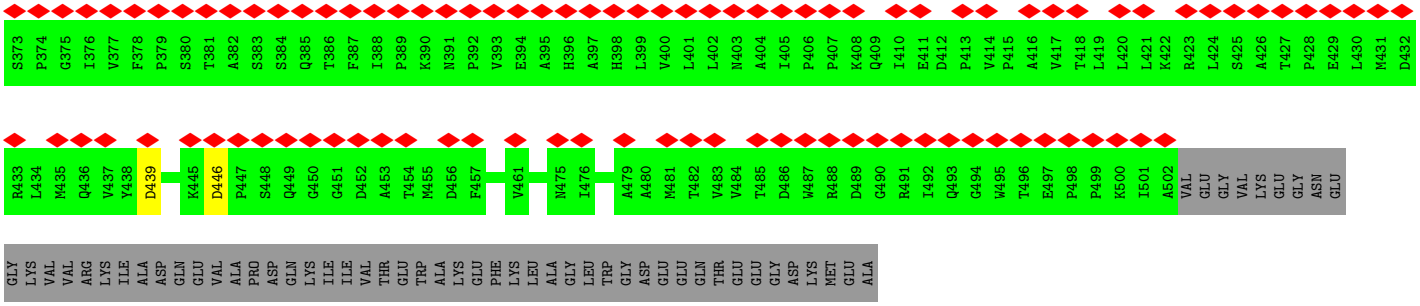






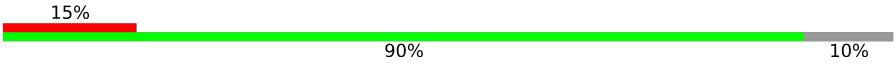


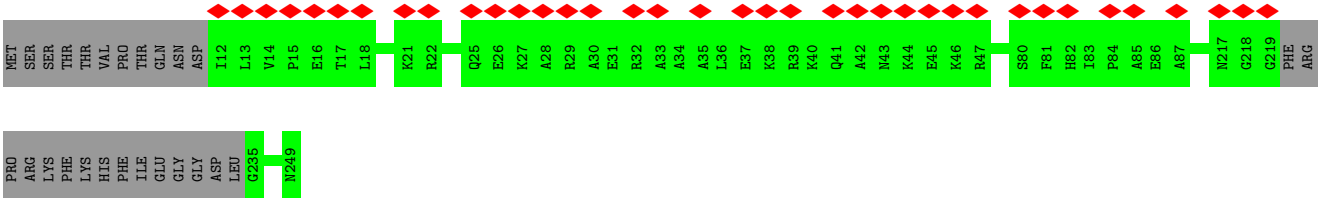




• Molecule 14: 60S ribosomal protein l7-like protein

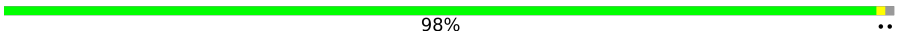
Chain CM:





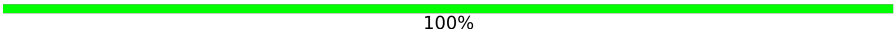
• Molecule 14: 60S ribosomal protein l7-like protein

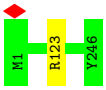
Chain LF:



• Molecule 15: Eukaryotic translation initiation factor 6

Chain CN:





• Molecule 16: DUF2423 domain-containing protein

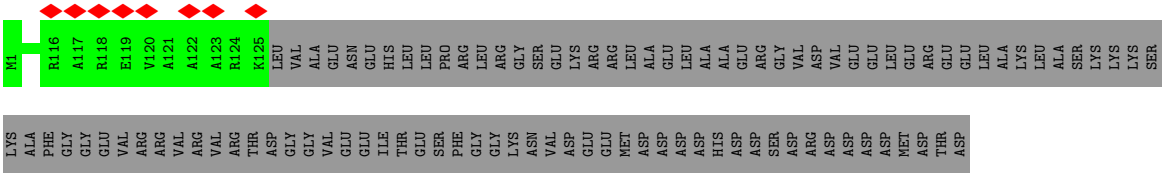
Chain CO:

• Molecule 17: RNA methyltransferase nop2-like protein

Chain CP:

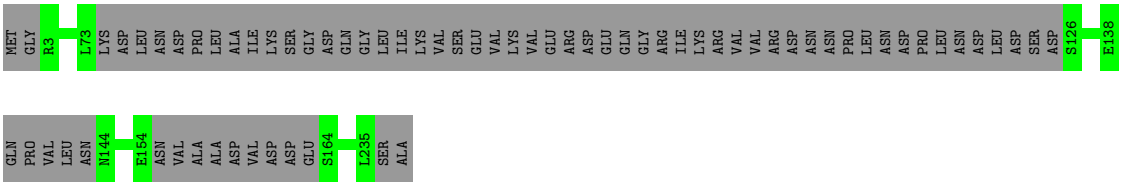
• Molecule 18: Ribosome biogenesis protein RLP24

Chain CQ:



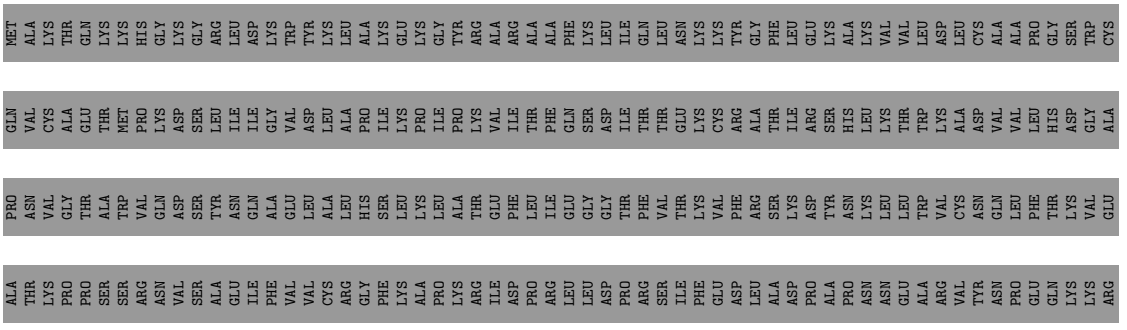
• Molecule 19: Nucleolar protein 16

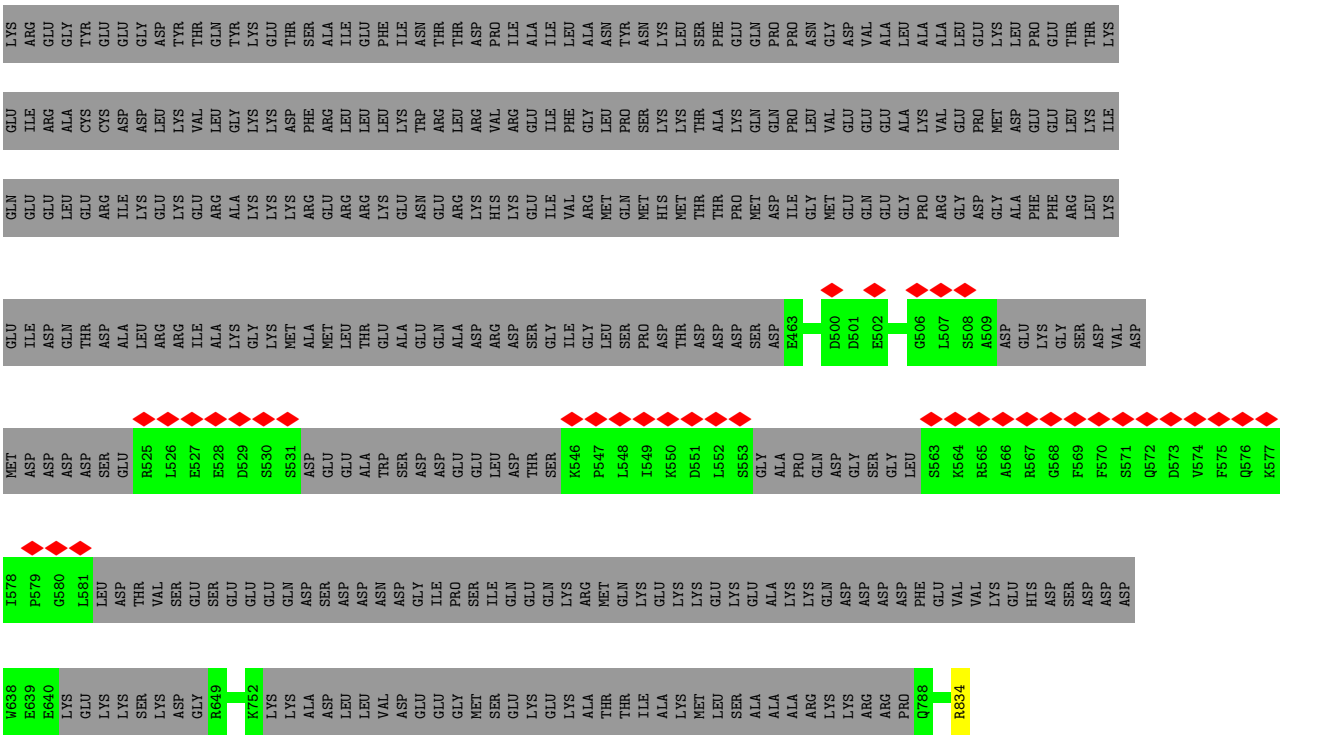
Chain CR:



• Molecule 20: AdoMet-dependent rRNA methyltransferase SPB1

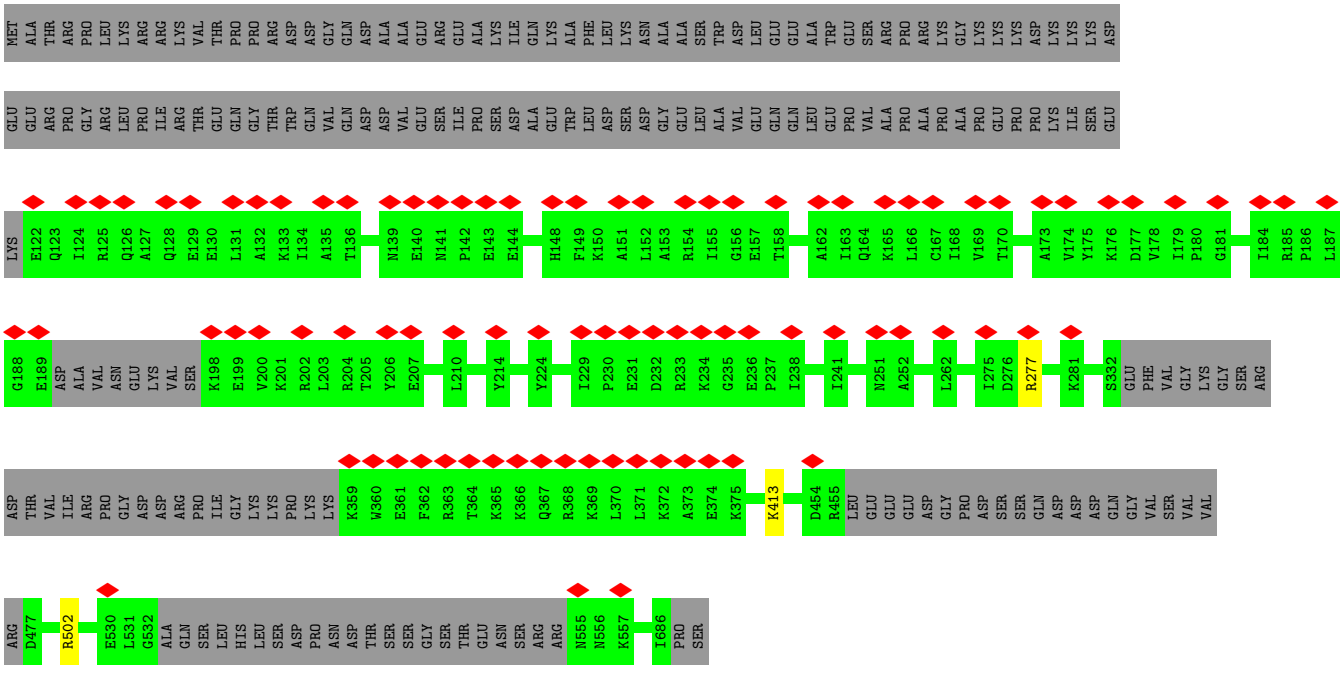
Chain CS:





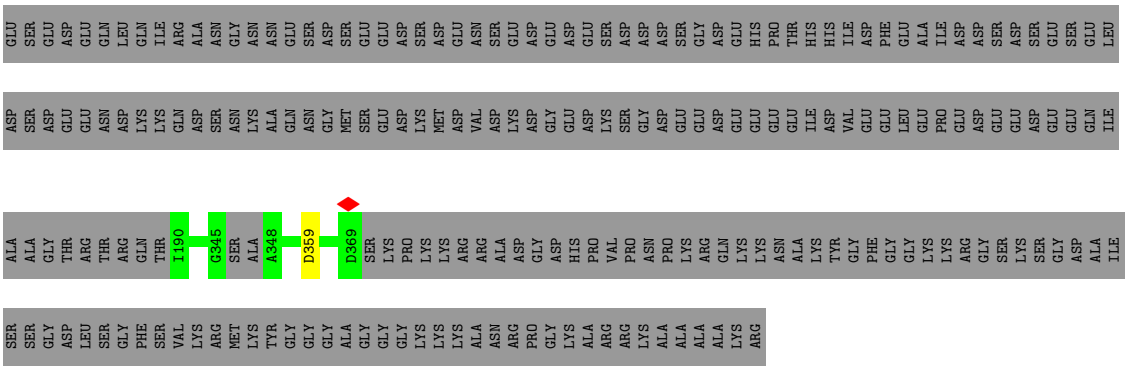
• Molecule 21: Nucleolar complex-associated protein 3

Chain CT:



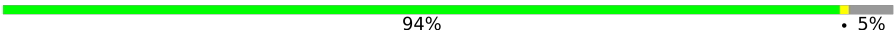
• Molecule 22: rRNA-processing protein EBP2

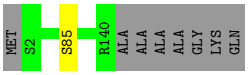
Chain CU:



• Molecule 23: Putative 60S ribosomal protein

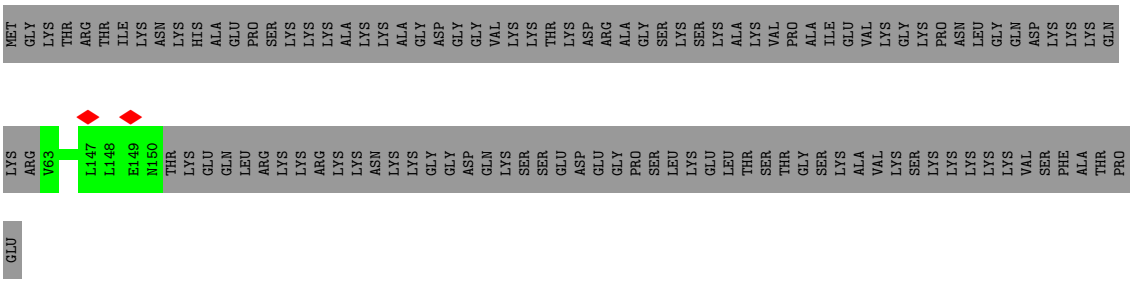
Chain CV:





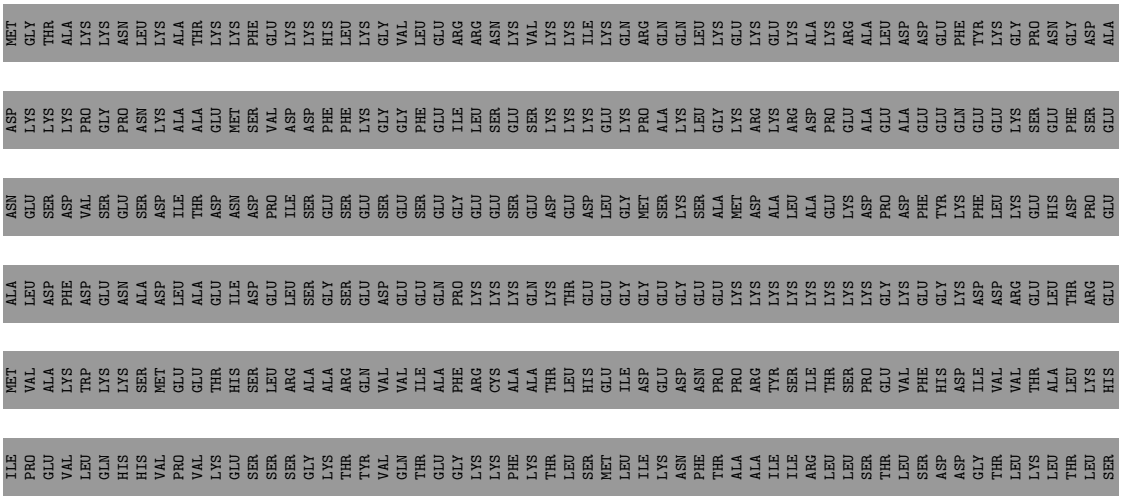
• Molecule 24: 60S ribosomal subunit-like protein

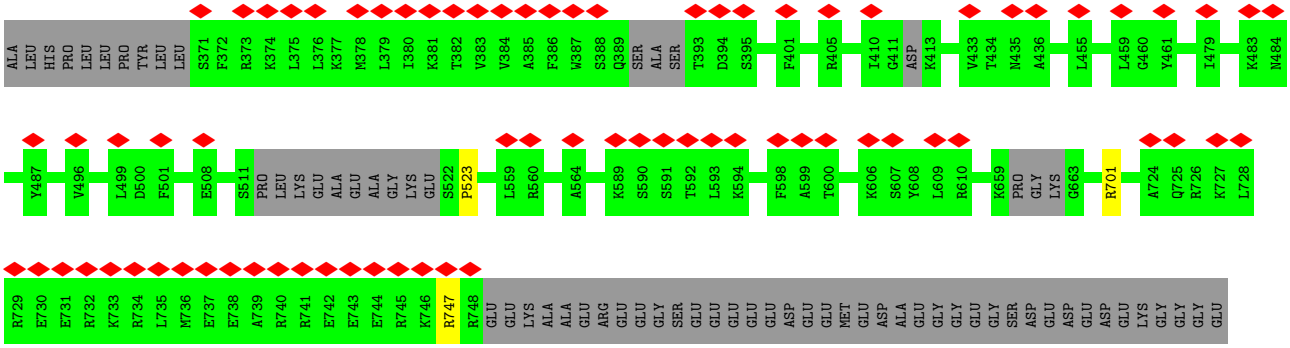
Chain CX:



• Molecule 25: Putative NOC2 family protein

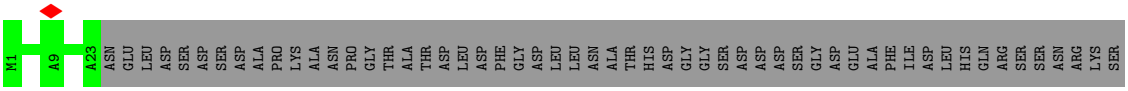
Chain CY:

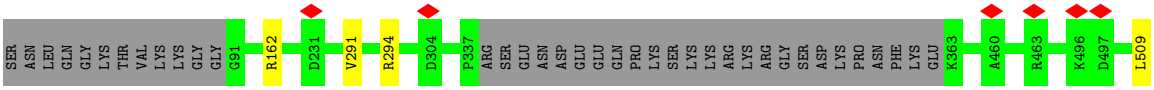


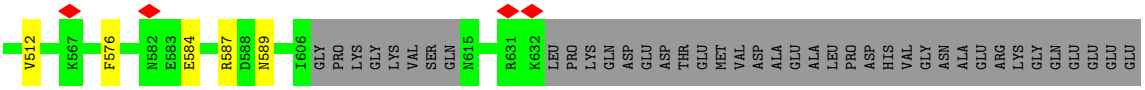


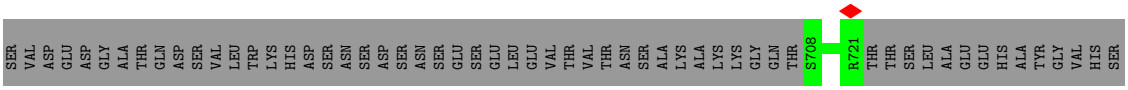
• Molecule 26: ATP-dependent RNA helicase DBP10

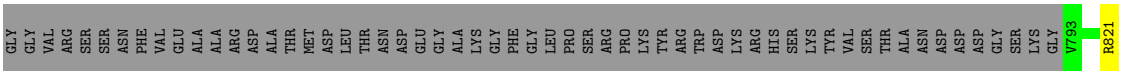
Chain Cb:

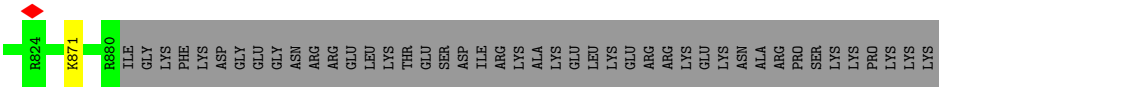


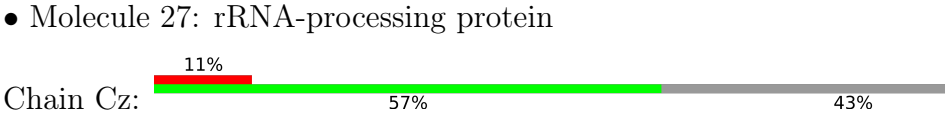






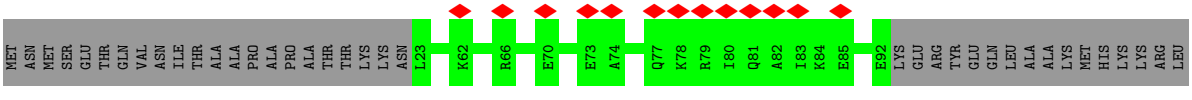


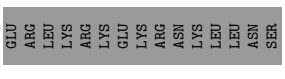




• Molecule 27: rRNA-processing protein

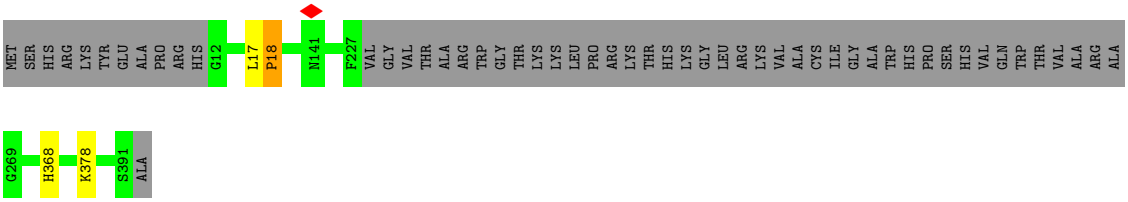
Chain Cz:





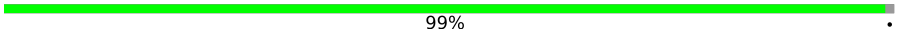
• Molecule 28: 60S ribosomal protein L3-like protein

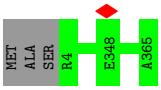
Chain LB:



• Molecule 29: 60S ribosomal protein L4-like protein

Chain LC:



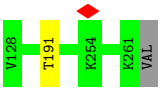


• Molecule 30: 60S ribosomal protein L6

Chain LE:

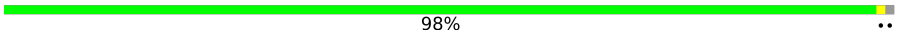
• Molecule 31: 60S ribosomal protein L8

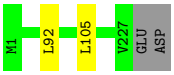
Chain LG:



• Molecule 32: 60S ribosomal protein l9-like protein

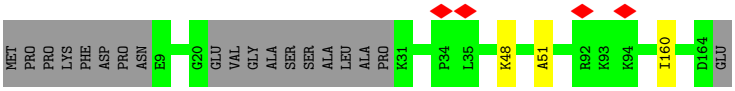
Chain LH:





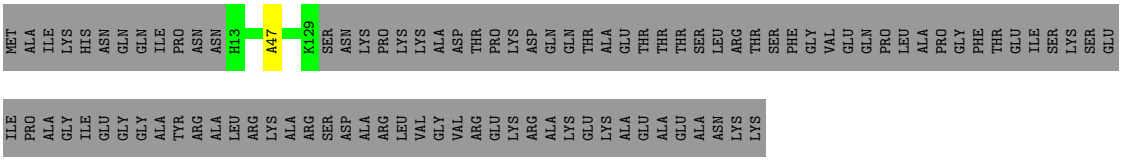
• Molecule 33: 60S ribosomal protein L12-like protein

Chain LK:



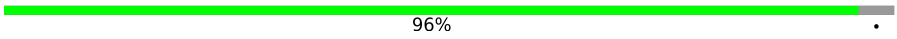
• Molecule 34: 60S ribosomal protein L13

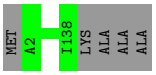
Chain LL:



• Molecule 35: 60S ribosomal protein L14-like protein

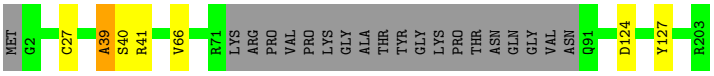
Chain LM:





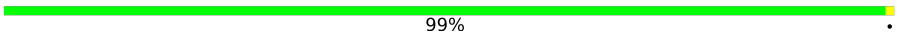
• Molecule 36: Ribosomal protein L15

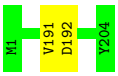
Chain LN:



• Molecule 37: 60S ribosomal protein L16-like protein

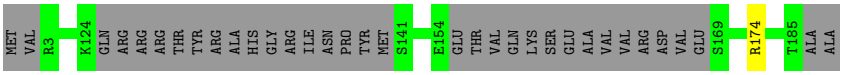
Chain LO:





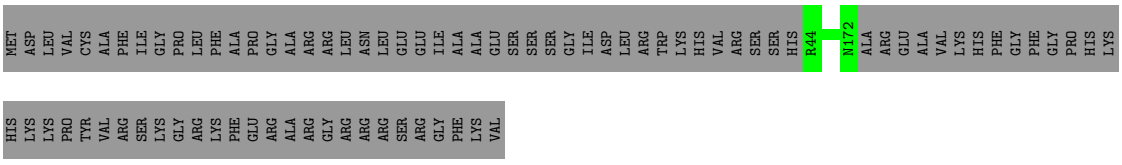
• Molecule 38: 60S ribosomal protein l17-like protein

Chain LP:



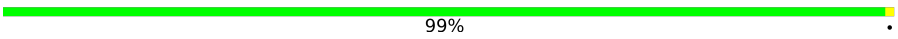
• Molecule 39: Ribosomal protein L18-like protein

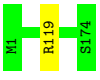
Chain LQ:



• Molecule 40: 60S ribosomal protein L20

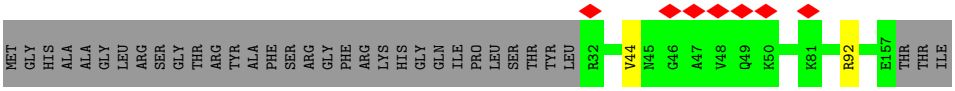
Chain LS:





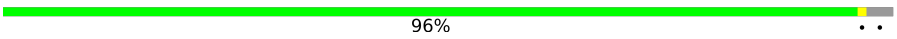
• Molecule 41: 60S ribosomal protein l21-like protein

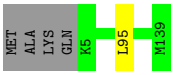
Chain LT:



• Molecule 42: 60S ribosomal protein l23-like protein

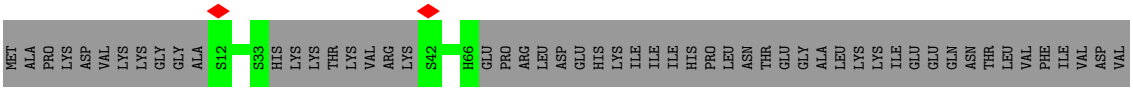
Chain LV:





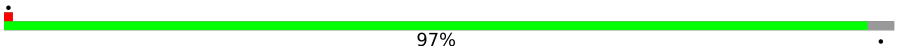
• Molecule 43: 60S ribosomal protein L25-like protein

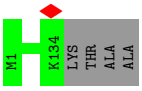
Chain LX:



• Molecule 44: 60S ribosomal protein L26-like protein

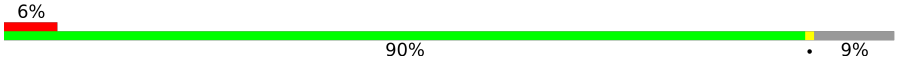
Chain LY:

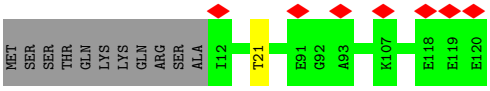




• Molecule 45: Putative 60S ribosomal protein

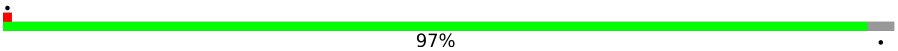
Chain Ld:

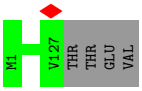




• Molecule 46: 60S ribosomal protein L32-like protein

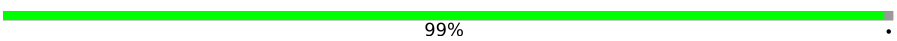
Chain Le:





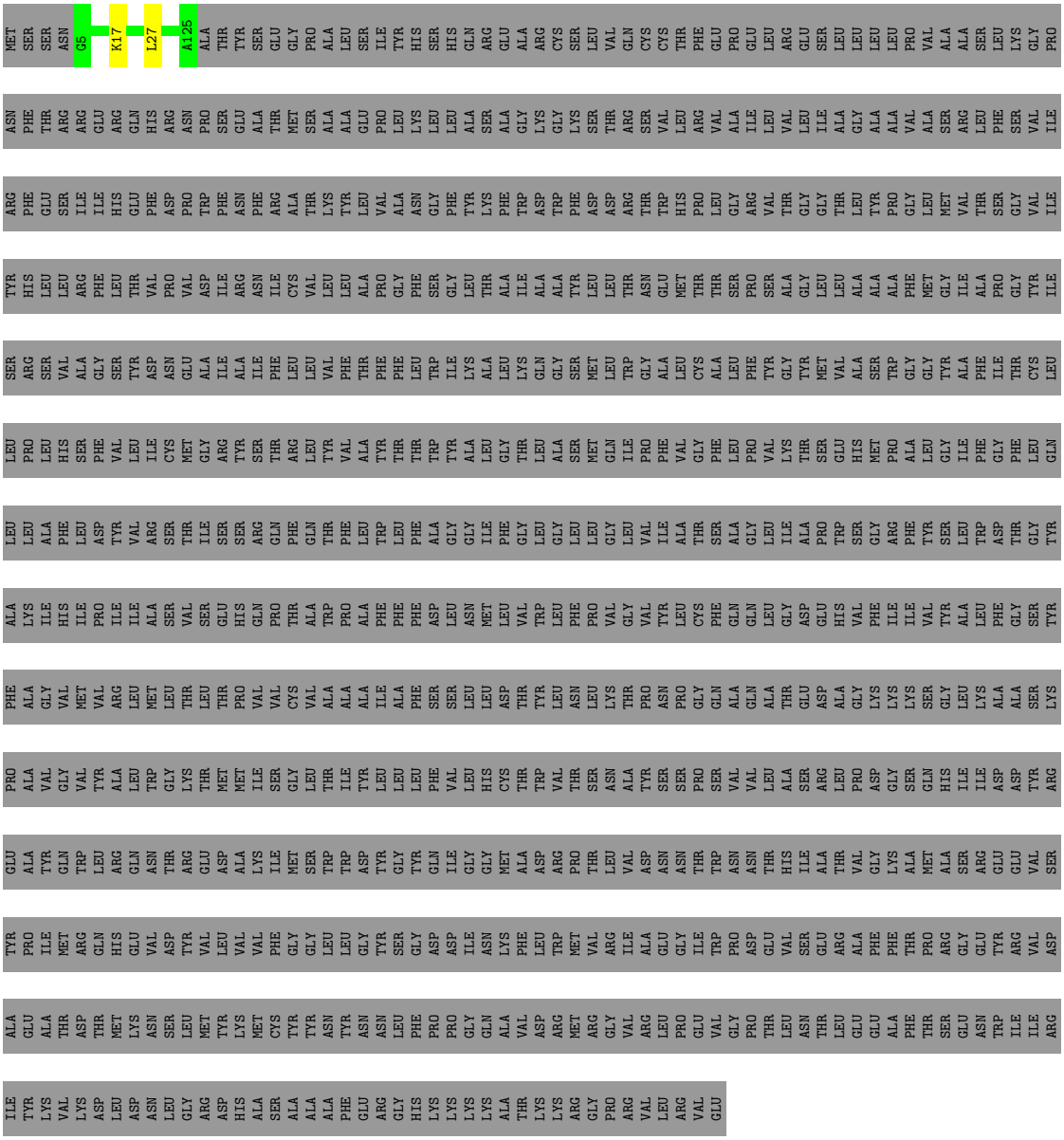
• Molecule 47: 60S ribosomal protein l33-like protein

Chain Lf:



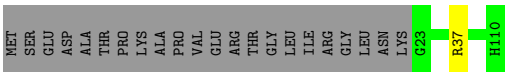
• Molecule 48: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:



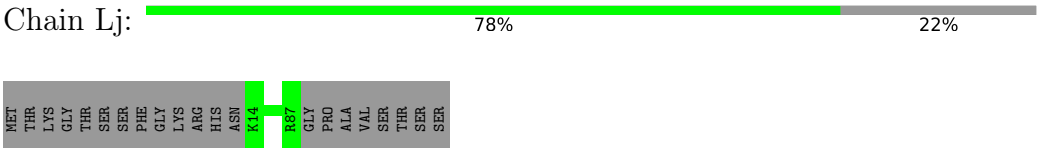
• Molecule 49: 60S ribosomal protein L36

Chain Li:



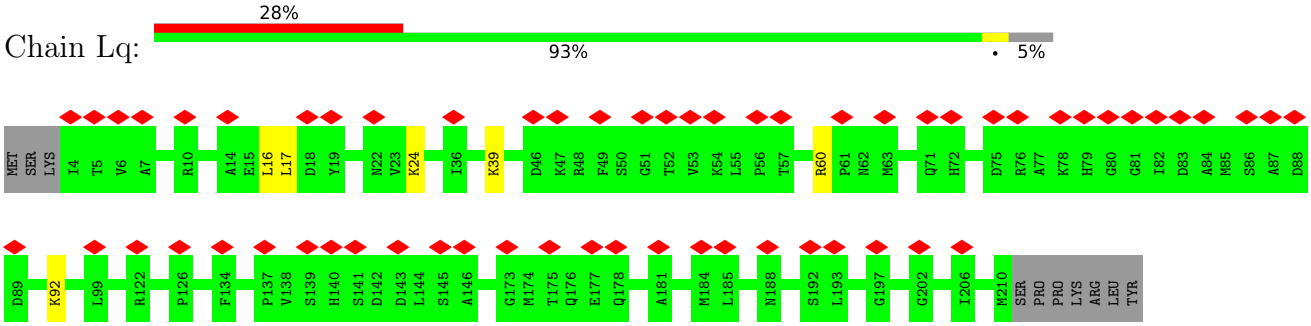
• Molecule 50: Ribosomal protein L37

Chain Lj:



• Molecule 51: Ribosomal protein

Chain Lq:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30333	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.497	Depositor
Minimum map value	-0.266	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.045, 1.045, 1.045	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: TPO, SEP, GTP, ZN

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	C1	0.31	0/51760	0.82	35/80668 (0.0%)
2	C2	0.31	0/6097	0.77	0/9499
3	CA	0.33	0/2115	0.58	1/2840 (0.0%)
4	CB	0.30	0/2109	0.58	0/2866
5	CC	0.28	0/2461	0.54	0/3348
6	CE	0.28	0/3743	0.53	0/5045
7	CF	0.27	0/1982	0.60	0/2671
8	CG	0.33	0/1422	0.59	0/1920
9	CH	0.32	0/4162	0.56	0/5618
10	CI	0.30	0/1225	0.66	1/1645 (0.1%)
11	CJ	0.27	0/3171	0.56	1/4286 (0.0%)
12	CK	0.28	0/1940	0.57	0/2601
13	CL	0.25	0/2247	0.49	0/3076
14	CM	0.29	0/1851	0.58	0/2481
14	LF	0.31	0/2055	0.56	1/2758 (0.0%)
15	CN	0.27	0/1881	0.56	0/2560
16	CO	0.26	0/470	0.54	0/619
17	CP	0.36	0/2859	0.62	1/3870 (0.0%)
18	CQ	0.31	0/1077	0.67	0/1427
19	CR	0.26	0/1369	0.56	0/1828
20	CS	0.25	0/1912	0.51	0/2534
21	CT	0.27	0/3974	0.54	0/5357
22	CU	0.30	0/1428	0.57	0/1910
23	CV	0.27	0/1091	0.54	0/1468
24	CX	0.29	0/705	0.54	0/938
25	CY	0.28	0/2971	0.60	0/4006
26	Cb	0.29	0/5097	0.56	0/6868
27	Cz	0.26	0/598	0.55	0/785
28	LB	0.33	0/2748	0.59	0/3684
29	LC	0.29	0/2809	0.54	0/3787
30	LE	0.44	0/1428	0.67	0/1921
31	LG	0.34	0/1667	0.60	0/2230

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LH	0.34	0/1516	0.59	0/2038
33	LK	0.27	0/1124	0.56	0/1507
34	LL	0.31	0/983	0.63	0/1318
35	LM	0.30	0/1120	0.57	0/1507
36	LN	0.34	0/1595	0.65	2/2132 (0.1%)
37	LO	0.32	0/1652	0.56	0/2215
38	LP	0.24	0/1217	0.54	0/1636
39	LQ	0.28	0/1033	0.59	0/1391
40	LS	0.28	0/1468	0.56	0/1975
41	LT	0.24	0/1033	0.51	0/1389
42	LV	0.29	0/1013	0.52	0/1361
43	LX	0.25	0/361	0.50	0/482
44	LY	0.26	0/1079	0.57	0/1443
45	Ld	0.34	0/904	0.55	0/1209
46	Le	0.27	0/1043	0.55	0/1389
47	Lf	0.29	0/883	0.59	0/1187
48	Lh	0.31	0/1006	0.64	1/1338 (0.1%)
49	Li	0.28	0/738	0.61	0/971
50	Lj	0.29	0/606	0.63	0/803
51	Lq	0.28	0/1621	0.59	0/2180
All	All	0.30	0/144419	0.69	43/206585 (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
28	LB	0	1
36	LN	0	1
51	Lq	0	1
All	All	0	3

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1050	C	N3-C2-O2	-12.14	113.41	121.90
1	C1	1050	C	N1-C2-O2	10.77	125.36	118.90
1	C1	136	C	N3-C2-O2	-8.71	115.80	121.90
1	C1	2723	C	N3-C2-O2	-7.43	116.70	121.90
1	C1	2452	C	N3-C2-O2	-7.21	116.85	121.90

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	3209	U	P-O3'-C3'	7.18	128.31	119.70
1	C1	1051	C	N3-C2-O2	-6.91	117.06	121.90
1	C1	3267	G	C4'-C3'-C2'	-6.61	96.00	102.60
1	C1	1051	C	C6-N1-C2	-6.57	117.67	120.30
1	C1	83	C	C2-N3-C4	-6.50	116.65	119.90
1	C1	127	G	N3-C4-N9	6.49	129.89	126.00
1	C1	249	C	N3-C2-O2	-6.35	117.46	121.90
1	C1	72	C	C2-N3-C4	-6.30	116.75	119.90
1	C1	3015	U	C2-N1-C1'	6.29	125.25	117.70
1	C1	136	C	N1-C2-O2	6.23	122.64	118.90
1	C1	799	C	N3-C2-O2	-6.16	117.59	121.90
10	CI	313	ARG	CB-CG-CD	6.12	127.52	111.60
48	Lh	27	LEU	CA-CB-CG	5.87	128.79	115.30
1	C1	1050	C	C6-N1-C2	-5.76	118.00	120.30
14	LF	13	LEU	CA-CB-CG	5.74	128.51	115.30
1	C1	249	C	N1-C2-O2	5.69	122.31	118.90
36	LN	39	ALA	C-N-CA	5.67	135.88	121.70
1	C1	1157	C	C6-N1-C2	5.63	122.55	120.30
1	C1	2752	G	C5-C6-O6	5.54	131.92	128.60
1	C1	83	C	N1-C2-N3	5.51	123.06	119.20
1	C1	127	G	C8-N9-C1'	-5.48	119.88	127.00
1	C1	127	G	C4-N9-C1'	5.42	133.55	126.50
1	C1	1134	G	O4'-C1'-N9	5.36	112.49	108.20
17	CP	576	PHE	CB-CA-C	-5.32	99.75	110.40
1	C1	2752	G	N1-C6-O6	-5.32	116.71	119.90
1	C1	442	C	C2-N1-C1'	5.27	124.60	118.80
1	C1	3015	U	N1-C2-O2	5.27	126.49	122.80
36	LN	127	TYR	CB-CA-C	-5.26	99.87	110.40
1	C1	799	C	N1-C2-O2	5.26	122.06	118.90
3	CA	108	PRO	CB-CA-C	-5.26	98.84	112.00
11	CJ	119	PRO	CA-N-CD	-5.23	104.17	111.50
1	C1	1204	G	O4'-C1'-N9	5.14	112.31	108.20
1	C1	398	G	O4'-C1'-N9	5.13	112.30	108.20
1	C1	136	C	C6-N1-C2	-5.09	118.26	120.30
1	C1	1072	G	N1-C2-N2	-5.08	111.63	116.20
1	C1	3289	C	N1-C2-O2	5.08	121.95	118.90
1	C1	3088	U	C2-N1-C1'	5.07	123.79	117.70
1	C1	1073	G	N1-C2-N2	-5.05	111.65	116.20

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	LB	17	LEU	Peptide
36	LN	39	ALA	Peptide
51	Lq	60	ARG	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	
3	CA	247/316 (78%)	232 (94%)	15 (6%)	0	100	100
4	CB	256/391 (66%)	239 (93%)	17 (7%)	0	100	100
5	CC	283/801 (35%)	268 (95%)	14 (5%)	1 (0%)	34	69
6	CE	459/598 (77%)	444 (97%)	15 (3%)	0	100	100
7	CF	243/270 (90%)	230 (95%)	11 (4%)	2 (1%)	19	54
8	CG	175/184 (95%)	167 (95%)	8 (5%)	0	100	100
9	CH	499/661 (76%)	470 (94%)	28 (6%)	1 (0%)	47	79
10	CI	144/414 (35%)	134 (93%)	10 (7%)	0	100	100
11	CJ	373/679 (55%)	355 (95%)	18 (5%)	0	100	100
12	CK	234/261 (90%)	221 (94%)	13 (6%)	0	100	100
13	CL	393/558 (70%)	361 (92%)	29 (7%)	3 (1%)	19	54
14	CM	219/249 (88%)	209 (95%)	10 (5%)	0	100	100
14	LF	245/249 (98%)	237 (97%)	7 (3%)	1 (0%)	34	69
15	CN	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
16	CO	56/120 (47%)	55 (98%)	1 (2%)	0	100	100
17	CP	354/751 (47%)	332 (94%)	21 (6%)	1 (0%)	41	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CQ	123/225 (55%)	119 (97%)	4 (3%)	0	100	100
19	CR	159/237 (67%)	156 (98%)	3 (2%)	0	100	100
20	CS	221/834 (26%)	213 (96%)	8 (4%)	0	100	100
21	CT	478/688 (70%)	456 (95%)	21 (4%)	1 (0%)	47	79
22	CU	174/451 (39%)	169 (97%)	4 (2%)	1 (1%)	25	59
23	CV	137/147 (93%)	134 (98%)	2 (2%)	1 (1%)	22	57
24	CX	86/203 (42%)	84 (98%)	2 (2%)	0	100	100
25	CY	351/788 (44%)	323 (92%)	27 (8%)	1 (0%)	41	73
26	Cb	622/924 (67%)	575 (92%)	45 (7%)	2 (0%)	41	73
27	Cz	68/123 (55%)	66 (97%)	2 (3%)	0	100	100
28	LB	335/392 (86%)	315 (94%)	18 (5%)	2 (1%)	25	59
29	LC	360/365 (99%)	344 (96%)	16 (4%)	0	100	100
30	LE	175/200 (88%)	167 (95%)	7 (4%)	1 (1%)	25	59
31	LG	200/262 (76%)	192 (96%)	8 (4%)	0	100	100
32	LH	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
33	LK	142/165 (86%)	134 (94%)	6 (4%)	2 (1%)	11	40
34	LL	115/213 (54%)	106 (92%)	8 (7%)	1 (1%)	17	52
35	LM	135/142 (95%)	128 (95%)	7 (5%)	0	100	100
36	LN	179/203 (88%)	168 (94%)	9 (5%)	2 (1%)	14	46
37	LO	202/204 (99%)	190 (94%)	10 (5%)	2 (1%)	15	49
38	LP	147/187 (79%)	144 (98%)	3 (2%)	0	100	100
39	LQ	127/213 (60%)	122 (96%)	5 (4%)	0	100	100
40	LS	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
41	LT	124/160 (78%)	119 (96%)	4 (3%)	1 (1%)	19	54
42	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
43	LX	43/156 (28%)	43 (100%)	0	0	100	100
44	LY	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
45	Ld	107/120 (89%)	102 (95%)	5 (5%)	0	100	100
46	Le	125/131 (95%)	120 (96%)	5 (4%)	0	100	100
47	Lf	106/109 (97%)	103 (97%)	3 (3%)	0	100	100
48	Lh	119/935 (13%)	111 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
49	Li	86/110 (78%)	85 (99%)	1 (1%)	0	100 100
50	Lj	72/95 (76%)	69 (96%)	3 (4%)	0	100 100
51	Lq	205/217 (94%)	180 (88%)	25 (12%)	0	100 100
All	All	10572/16590 (64%)	10025 (95%)	521 (5%)	26 (0%)	50 79

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	CF	239	ALA
21	CT	502	ARG
36	LN	40	SER
37	LO	191	VAL
17	CP	442	GLU
22	CU	359	ASP
25	CY	523	PRO
26	Cb	294	ARG
28	LB	18	PRO
33	LK	51	ALA
7	CF	188	ALA
13	CL	224	ASP
13	CL	439	ASP
26	Cb	576	PHE
28	LB	368	HIS
9	CH	197	ALA
23	CV	85	SER
30	LE	85	GLY
14	LF	118	ASN
36	LN	124	ASP
13	CL	446	ASP
33	LK	160	ILE
37	LO	192	ASP
41	LT	44	VAL
34	LL	47	ALA
5	CC	251	VAL

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
3	CA	223/276 (81%)	219 (98%)	4 (2%)	59 82
4	CB	222/329 (68%)	222 (100%)	0	100 100
5	CC	266/708 (38%)	262 (98%)	4 (2%)	65 85
6	CE	398/517 (77%)	397 (100%)	1 (0%)	92 96
7	CF	214/236 (91%)	213 (100%)	1 (0%)	88 94
8	CG	150/155 (97%)	149 (99%)	1 (1%)	84 93
9	CH	448/575 (78%)	440 (98%)	8 (2%)	59 82
10	CI	121/336 (36%)	120 (99%)	1 (1%)	81 92
11	CJ	330/579 (57%)	330 (100%)	0	100 100
12	CK	204/225 (91%)	203 (100%)	1 (0%)	88 94
13	CL	72/458 (16%)	72 (100%)	0	100 100
14	CM	191/215 (89%)	191 (100%)	0	100 100
14	LF	213/215 (99%)	212 (100%)	1 (0%)	88 94
15	CN	206/206 (100%)	205 (100%)	1 (0%)	88 94
16	CO	48/99 (48%)	48 (100%)	0	100 100
17	CP	302/632 (48%)	297 (98%)	5 (2%)	60 83
18	CQ	107/192 (56%)	107 (100%)	0	100 100
19	CR	144/206 (70%)	144 (100%)	0	100 100
20	CS	188/716 (26%)	187 (100%)	1 (0%)	88 94
21	CT	427/600 (71%)	425 (100%)	2 (0%)	88 94
22	CU	149/376 (40%)	149 (100%)	0	100 100
23	CV	109/112 (97%)	109 (100%)	0	100 100
24	CX	76/172 (44%)	76 (100%)	0	100 100
25	CY	313/686 (46%)	311 (99%)	2 (1%)	86 94
26	Cb	535/779 (69%)	526 (98%)	9 (2%)	60 83
27	Cz	60/107 (56%)	60 (100%)	0	100 100
28	LB	289/331 (87%)	287 (99%)	2 (1%)	84 93
29	LC	283/285 (99%)	283 (100%)	0	100 100
30	LE	151/166 (91%)	143 (95%)	8 (5%)	22 54
31	LG	175/222 (79%)	174 (99%)	1 (1%)	86 94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
32	LH	167/169 (99%)	165 (99%)	2 (1%)	71 88
33	LK	121/136 (89%)	120 (99%)	1 (1%)	81 92
34	LL	99/176 (56%)	99 (100%)	0	100 100
35	LM	115/117 (98%)	115 (100%)	0	100 100
36	LN	164/180 (91%)	161 (98%)	3 (2%)	59 82
37	LO	163/163 (100%)	163 (100%)	0	100 100
38	LP	123/152 (81%)	122 (99%)	1 (1%)	81 92
39	LQ	110/178 (62%)	110 (100%)	0	100 100
40	LS	154/154 (100%)	153 (99%)	1 (1%)	86 94
41	LT	109/135 (81%)	108 (99%)	1 (1%)	78 91
42	LV	99/102 (97%)	98 (99%)	1 (1%)	76 90
43	LX	36/129 (28%)	36 (100%)	0	100 100
44	LY	117/119 (98%)	117 (100%)	0	100 100
45	Ld	95/105 (90%)	94 (99%)	1 (1%)	73 89
46	Le	110/114 (96%)	110 (100%)	0	100 100
47	Lf	89/90 (99%)	89 (100%)	0	100 100
48	Lh	108/781 (14%)	107 (99%)	1 (1%)	78 91
49	Li	75/93 (81%)	74 (99%)	1 (1%)	69 87
50	Lj	61/78 (78%)	61 (100%)	0	100 100
51	Lq	179/189 (95%)	174 (97%)	5 (3%)	43 73
All	All	8908/14071 (63%)	8837 (99%)	71 (1%)	82 92

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	63	ARG
3	CA	64	LYS
3	CA	158	LEU
3	CA	249	SER
5	CC	157	VAL
5	CC	161	ASP
5	CC	164	ASP
5	CC	406	ARG
6	CE	488	ASN
7	CF	91	ARG

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Mol	Chain	Res	Type
8	CG	58	CYS
9	CH	128	LYS
9	CH	174	PHE
9	CH	179	LYS
9	CH	201	LYS
9	CH	286	LEU
9	CH	289	MET
9	CH	290	ASP
9	CH	291	ILE
10	CI	313	ARG
12	CK	149	ARG
15	CN	123	ARG
17	CP	286	ASN
17	CP	397	HIS
17	CP	517	VAL
17	CP	562	LEU
17	CP	563	THR
20	CS	834	ARG
21	CT	277	ARG
21	CT	413	LYS
25	CY	701	ARG
25	CY	747	ARG
26	Cb	162	ARG
26	Cb	291	VAL
26	Cb	509	LEU
26	Cb	512	VAL
26	Cb	584	GLU
26	Cb	587	ARG
26	Cb	589	ASN
26	Cb	821	ARG
26	Cb	871	LYS
28	LB	18	PRO
28	LB	378	LYS
30	LE	66	ARG
30	LE	68	LYS
30	LE	74	LYS
30	LE	107	VAL
30	LE	154	VAL
30	LE	169	LEU
30	LE	170	ILE
30	LE	176	VAL
14	LF	94	ARG

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Mol	Chain	Res	Type
31	LG	191	THR
32	LH	92	LEU
32	LH	105	LEU
33	LK	48	LYS
36	LN	27	CYS
36	LN	41	ARG
36	LN	66	VAL
38	LP	174	ARG
40	LS	119	ARG
41	LT	92	ARG
42	LV	95	LEU
45	Ld	21	THR
48	Lh	17	LYS
49	Li	37	ARG
51	Lq	16	LEU
51	Lq	17	LEU
51	Lq	24	LYS
51	Lq	39	LYS
51	Lq	92	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
3	CA	193	ASN
4	CB	234	HIS
4	CB	277	ASN
7	CF	38	GLN
9	CH	73	GLN
9	CH	258	GLN
10	CI	269	HIS
11	CJ	259	GLN
11	CJ	381	GLN
12	CK	4	ASN
15	CN	162	HIS
16	CO	42	GLN
17	CP	343	GLN
17	CP	437	ASN
17	CP	474	ASN
19	CR	148	GLN
20	CS	744	GLN
21	CT	436	GLN
21	CT	602	GLN

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Mol	Chain	Res	Type
22	CU	217	HIS
22	CU	305	GLN
23	CV	17	ASN
23	CV	23	GLN
24	CX	102	ASN
25	CY	443	ASN
25	CY	481	ASN
25	CY	509	HIS
26	Cb	210	ASN
26	Cb	437	ASN
26	Cb	517	ASN
29	LC	280	ASN
14	LF	99	ASN
14	LF	116	GLN
14	LF	119	ASN
14	LF	178	ASN
33	LK	70	GLN
35	LM	106	GLN
40	LS	8	GLN
40	LS	62	ASN
51	Lq	200	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2145/3341 (64%)	455 (21%)	27 (1%)
2	C2	254/319 (79%)	60 (23%)	6 (2%)
All	All	2399/3660 (65%)	515 (21%)	33 (1%)

All (515) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	14	U
1	C1	26	A
1	C1	41	G
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	74	G

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Mol	Chain	Res	Type
1	C1	92	G
1	C1	93	C
1	C1	94	G
1	C1	96	G
1	C1	105	C
1	C1	110	G
1	C1	111	C
1	C1	116	A
1	C1	122	A
1	C1	128	G
1	C1	129	C
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	135	C
1	C1	136	C
1	C1	138	G
1	C1	143	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G
1	C1	163	U
1	C1	176	U
1	C1	177	U
1	C1	180	G
1	C1	183	U
1	C1	193	C
1	C1	203	C
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	225	G
1	C1	232	G
1	C1	240	U
1	C1	244	U
1	C1	253	U
1	C1	257	A
1	C1	258	C
1	C1	261	G
1	C1	262	U

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Mol	Chain	Res	Type
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	299	A
1	C1	300	A
1	C1	302	U
1	C1	309	A
1	C1	310	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	330	A
1	C1	331	C
1	C1	342	C
1	C1	343	A
1	C1	344	A
1	C1	368	G
1	C1	390	U
1	C1	391	A
1	C1	393	C
1	C1	394	A
1	C1	395	C
1	C1	413	G
1	C1	414	A
1	C1	433	U
1	C1	434	G
1	C1	439	C
1	C1	444	G
1	C1	446	U
1	C1	447	C
1	C1	457	U
1	C1	458	C
1	C1	459	U
1	C1	469	A
1	C1	470	C
1	C1	472	C
1	C1	474	G
1	C1	477	G
1	C1	488	A
1	C1	493	C
1	C1	508	G

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Mol	Chain	Res	Type
1	C1	509	A
1	C1	510	U
1	C1	511	A
1	C1	513	A
1	C1	517	C
1	C1	521	G
1	C1	526	G
1	C1	534	U
1	C1	535	C
1	C1	544	U
1	C1	546	A
1	C1	547	U
1	C1	548	A
1	C1	559	U
1	C1	579	A
1	C1	582	A
1	C1	587	G
1	C1	589	U
1	C1	590	C
1	C1	591	U
1	C1	592	G
1	C1	594	A
1	C1	596	G
1	C1	598	A
1	C1	607	U
1	C1	608	A
1	C1	609	A
1	C1	614	C
1	C1	623	C
1	C1	633	A
1	C1	647	A
1	C1	663	G
1	C1	664	A
1	C1	668	U
1	C1	674	U
1	C1	678	A
1	C1	712	A
1	C1	716	C
1	C1	718	U
1	C1	719	C
1	C1	731	G
1	C1	739	C

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Mol	Chain	Res	Type
1	C1	742	A
1	C1	744	G
1	C1	748	U
1	C1	749	C
1	C1	751	G
1	C1	752	A
1	C1	755	G
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	766	G
1	C1	767	A
1	C1	787	A
1	C1	798	A
1	C1	799	C
1	C1	800	U
1	C1	801	A
1	C1	887	G
1	C1	889	G
1	C1	896	A
1	C1	898	A
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G
1	C1	941	U
1	C1	942	C
1	C1	943	A
1	C1	944	G
1	C1	959	C
1	C1	960	C
1	C1	965	G
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1046	A

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Mol	Chain	Res	Type
1	C1	1047	A
1	C1	1048	G
1	C1	1049	C
1	C1	1050	C
1	C1	1054	G
1	C1	1057	A
1	C1	1058	C
1	C1	1063	C
1	C1	1064	U
1	C1	1065	G
1	C1	1073	G
1	C1	1074	C
1	C1	1076	U
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1095	G
1	C1	1097	G
1	C1	1098	G
1	C1	1114	C
1	C1	1122	G
1	C1	1124	G
1	C1	1125	A
1	C1	1126	U
1	C1	1135	A
1	C1	1141	A
1	C1	1157	C
1	C1	1158	C
1	C1	1159	G
1	C1	1163	U
1	C1	1164	G
1	C1	1172	A
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1179	A
1	C1	1180	C
1	C1	1184	A
1	C1	1189	G
1	C1	1190	C
1	C1	1191	G

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Mol	Chain	Res	Type
1	C1	1204	G
1	C1	1218	G
1	C1	1227	A
1	C1	1228	G
1	C1	1240	U
1	C1	1245	A
1	C1	1247	U
1	C1	1254	C
1	C1	1268	A
1	C1	1269	A
1	C1	1271	G
1	C1	1272	U
1	C1	1286	A
1	C1	1287	U
1	C1	1288	G
1	C1	1289	G
1	C1	1291	U
1	C1	1294	C
1	C1	1295	G
1	C1	1298	C
1	C1	1312	A
1	C1	1314	A
1	C1	1330	A
1	C1	1331	G
1	C1	1332	A
1	C1	1333	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1347	G
1	C1	1368	A
1	C1	1374	G
1	C1	1381	A
1	C1	1399	G
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1434	A
1	C1	1861	G
1	C1	1864	C
1	C1	1865	A

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Mol	Chain	Res	Type
1	C1	1866	A
1	C1	1867	U
1	C1	1874	A
1	C1	1875	A
1	C1	1883	C
1	C1	1886	C
1	C1	1897	C
1	C1	1900	A
1	C1	1901	A
1	C1	2075	A
1	C1	2088	A
1	C1	2287	G
1	C1	2288	A
1	C1	2294	A
1	C1	2295	C
1	C1	2297	G
1	C1	2298	U
1	C1	2302	U
1	C1	2310	A
1	C1	2325	A
1	C1	2327	C
1	C1	2332	G
1	C1	2335	A
1	C1	2338	G
1	C1	2339	G
1	C1	2342	U
1	C1	2343	G
1	C1	2345	C
1	C1	2347	A
1	C1	2350	U
1	C1	2355	G
1	C1	2356	G
1	C1	2359	A
1	C1	2361	A
1	C1	2362	G
1	C1	2363	A
1	C1	2364	A
1	C1	2396	U
1	C1	2397	G
1	C1	2399	G
1	C1	2407	A
1	C1	2410	G

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Mol	Chain	Res	Type
1	C1	2414	G
1	C1	2415	U
1	C1	2424	G
1	C1	2425	G
1	C1	2428	G
1	C1	2430	A
1	C1	2433	U
1	C1	2434	U
1	C1	2435	C
1	C1	2436	G
1	C1	2437	G
1	C1	2438	C
1	C1	2439	G
1	C1	2444	U
1	C1	2449	U
1	C1	2453	A
1	C1	2455	U
1	C1	2456	A
1	C1	2464	U
1	C1	2465	G
1	C1	2467	U
1	C1	2484	G
1	C1	2551	A
1	C1	2560	G
1	C1	2564	G
1	C1	2730	C
1	C1	2740	U
1	C1	2749	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2775	A
1	C1	2777	A
1	C1	2778	A
1	C1	2782	G
1	C1	2783	C
1	C1	2784	U
1	C1	2785	U
1	C1	2806	G
1	C1	2818	U
1	C1	2819	U
1	C1	2820	U

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Mol	Chain	Res	Type
1	C1	2845	A
1	C1	2847	C
1	C1	2856	G
1	C1	2857	C
1	C1	2862	U
1	C1	2869	A
1	C1	2889	C
1	C1	2893	U
1	C1	2894	A
1	C1	2899	A
1	C1	2902	U
1	C1	2904	A
1	C1	2917	C
1	C1	2924	G
1	C1	2925	A
1	C1	2935	G
1	C1	2936	U
1	C1	2942	C
1	C1	2948	G
1	C1	2950	U
1	C1	2951	G
1	C1	2954	C
1	C1	2955	U
1	C1	2956	C
1	C1	2969	A
1	C1	3005	A
1	C1	3006	A
1	C1	3016	G
1	C1	3031	G
1	C1	3035	G
1	C1	3043	A
1	C1	3048	A
1	C1	3049	C
1	C1	3050	C
1	C1	3070	A
1	C1	3074	C
1	C1	3079	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3098	A
1	C1	3099	A

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Mol	Chain	Res	Type
1	C1	3100	C
1	C1	3101	G
1	C1	3112	A
1	C1	3113	C
1	C1	3118	A
1	C1	3121	U
1	C1	3122	U
1	C1	3124	U
1	C1	3125	A
1	C1	3126	G
1	C1	3127	A
1	C1	3130	U
1	C1	3131	A
1	C1	3132	U
1	C1	3134	A
1	C1	3140	G
1	C1	3145	C
1	C1	3146	G
1	C1	3147	G
1	C1	3153	U
1	C1	3154	A
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3167	A
1	C1	3170	C
1	C1	3171	C
1	C1	3178	G
1	C1	3183	C
1	C1	3185	A
1	C1	3187	G
1	C1	3199	A
1	C1	3205	C
1	C1	3206	G
1	C1	3210	U
1	C1	3212	C
1	C1	3213	A
1	C1	3217	U
1	C1	3227	C
1	C1	3228	G
1	C1	3229	G
1	C1	3230	G

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Mol	Chain	Res	Type
1	C1	3244	C
1	C1	3253	U
1	C1	3255	G
1	C1	3256	A
1	C1	3257	U
1	C1	3260	G
1	C1	3274	U
1	C1	3281	U
1	C1	3282	A
1	C1	3285	G
1	C1	3287	A
1	C1	3291	U
1	C1	3293	G
1	C1	3295	U
1	C1	3298	U
1	C1	3303	U
1	C1	3309	G
1	C1	3318	C
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3329	C
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
1	C1	3337	C
2	C2	23	U
2	C2	34	U
2	C2	35	C
2	C2	39	G
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	81	U
2	C2	82	U
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	88	A
2	C2	90	U
2	C2	95	G
2	C2	97	A

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Mol	Chain	Res	Type
2	C2	100	U
2	C2	103	G
2	C2	104	A
2	C2	105	A
2	C2	106	C
2	C2	110	C
2	C2	111	A
2	C2	112	U
2	C2	113	U
2	C2	125	U
2	C2	151	C
2	C2	158	U
2	C2	159	C
2	C2	160	A
2	C2	163	C
2	C2	164	A
2	C2	165	U
2	C2	166	C
2	C2	170	C
2	C2	173	U
2	C2	174	G
2	C2	180	G
2	C2	181	U
2	C2	182	G
2	C2	183	U
2	C2	189	A
2	C2	192	C
2	C2	195	G
2	C2	196	G
2	C2	212	G
2	C2	213	A
2	C2	214	A
2	C2	215	A
2	C2	216	A
2	C2	219	A
2	C2	221	U
2	C2	222	G
2	C2	289	G
2	C2	291	G
2	C2	292	C
2	C2	295	G
2	C2	300	A

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Mol	Chain	Res	Type
2	C2	301	A
2	C2	305	C

All (33) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	445	A
1	C1	446	U
1	C1	508	G
1	C1	510	U
1	C1	886	U
1	C1	897	G
1	C1	959	C
1	C1	1063	C
1	C1	1134	G
1	C1	2301	C
1	C1	2360	A
1	C1	2777	A
1	C1	2817	U
1	C1	2898	A
1	C1	3005	A
1	C1	3078	U
1	C1	3112	A
1	C1	3131	A
1	C1	3162	A
1	C1	3204	G
1	C1	3209	U
1	C1	3212	C
1	C1	3229	G
1	C1	3255	G
1	C1	3257	U
1	C1	3297	U
2	C2	87	G
2	C2	102	U
2	C2	163	C
2	C2	164	A
2	C2	180	G
2	C2	181	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	TPO	CC	163	5	8,10,11	0.66	0	10,14,16	1.01	1 (10%)
5	SEP	CC	160	5	8,9,10	0.62	0	8,12,14	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	TPO	CC	163	5	-	1/9/11/13	-
5	SEP	CC	160	5	-	4/5/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	CC	163	TPO	O-C-CA	-2.42	118.43	124.78

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	CC	160	SEP	CB-OG-P-O1P
5	CC	160	SEP	CB-OG-P-O2P
5	CC	160	SEP	CB-OG-P-O3P
5	CC	160	SEP	N-CA-CB-OG
5	CC	163	TPO	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	GTP	CH	1001	-	26,34,34	0.97	2 (7%)	32,54,54	0.78	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	GTP	CH	1001	-	-	7/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	CH	1001	GTP	C5-C6	-2.63	1.42	1.47
52	CH	1001	GTP	C8-N7	-2.07	1.31	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	CH	1001	GTP	O6-C6-C5	2.08	128.44	124.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

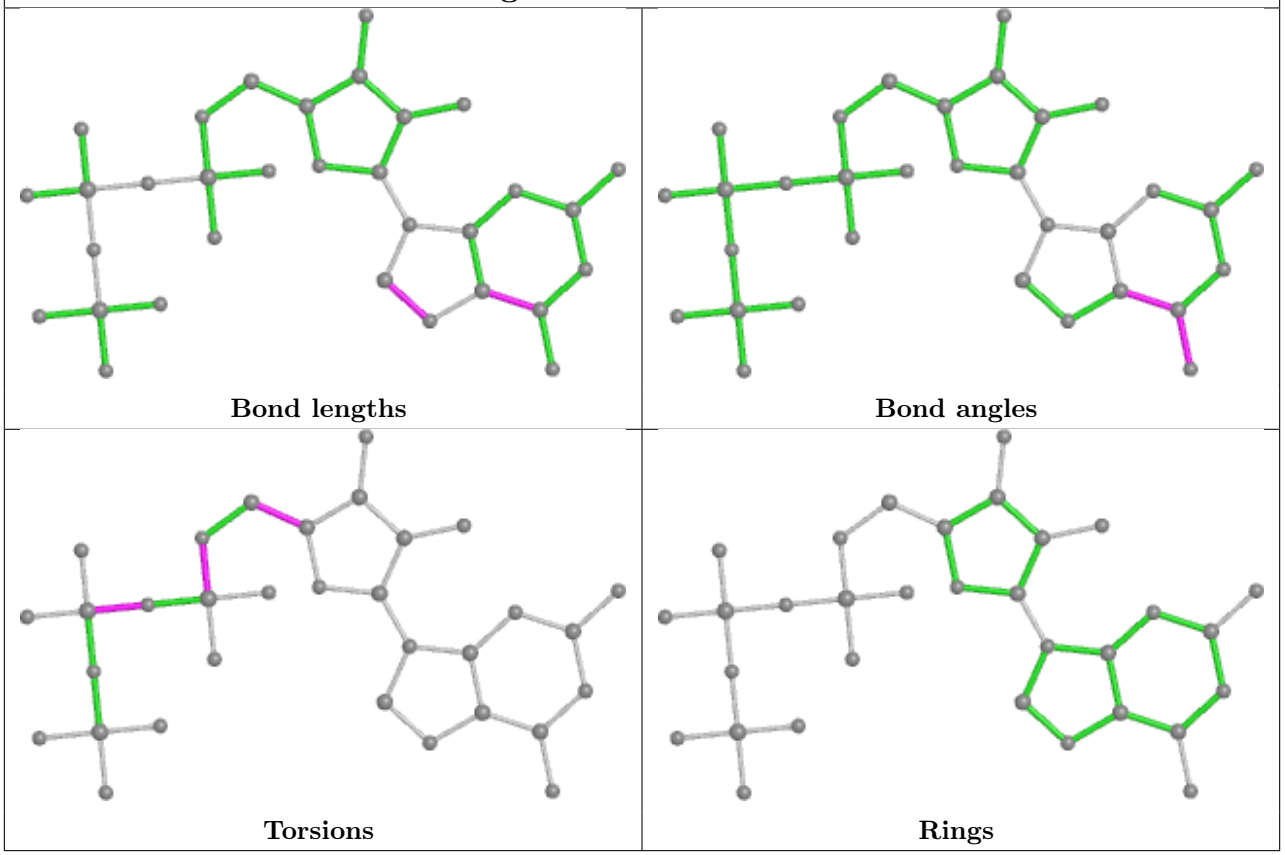
Mol	Chain	Res	Type	Atoms
52	CH	1001	GTP	C5'-O5'-PA-O1A
52	CH	1001	GTP	C5'-O5'-PA-O2A
52	CH	1001	GTP	O4'-C4'-C5'-O5'
52	CH	1001	GTP	C3'-C4'-C5'-O5'
52	CH	1001	GTP	C5'-O5'-PA-O3A
52	CH	1001	GTP	PA-O3A-PB-O2B
52	CH	1001	GTP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GTP CH 1001



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

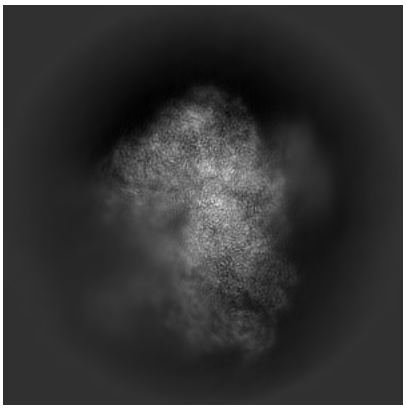
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-35286. These allow visual inspection of the internal detail of the map and identification of artifacts.

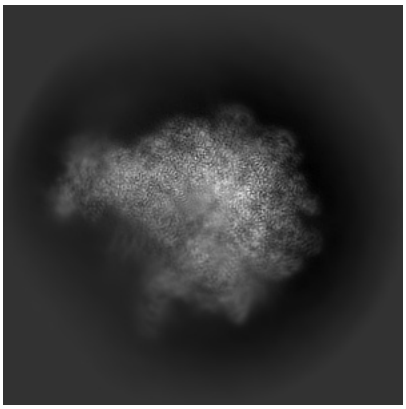
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

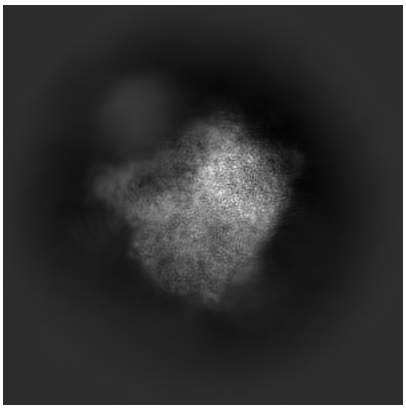
6.1.1 Primary map



X

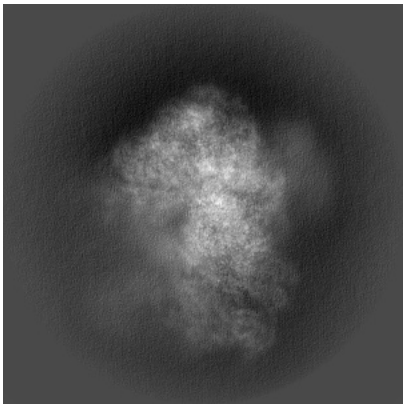


Y

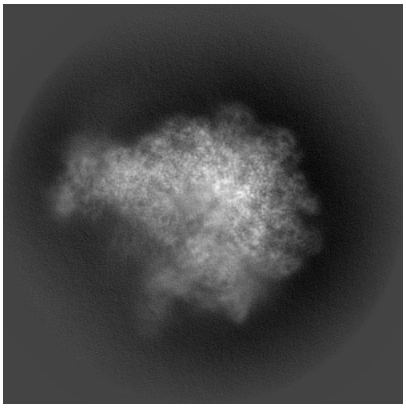


Z

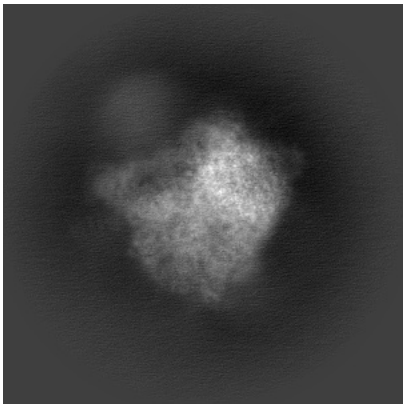
6.1.2 Raw map



X



Y

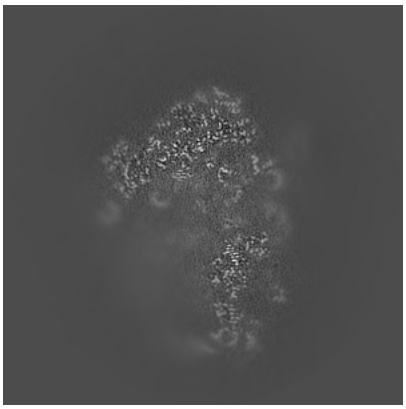


Z

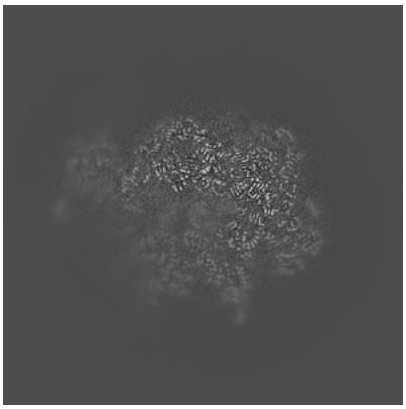
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

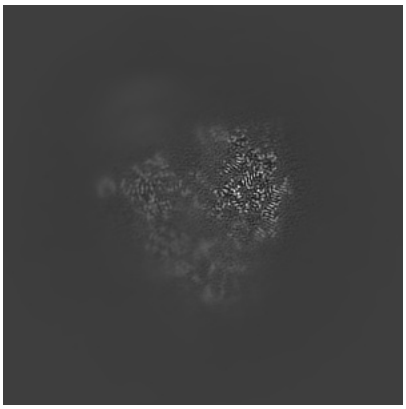
6.2.1 Primary map



X Index: 210

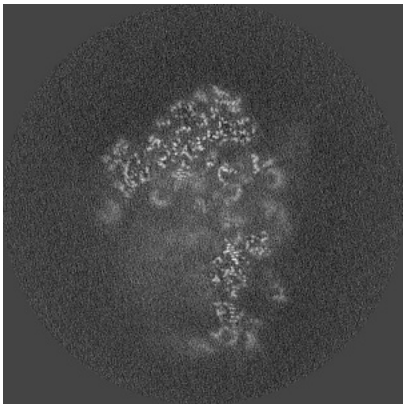


Y Index: 210

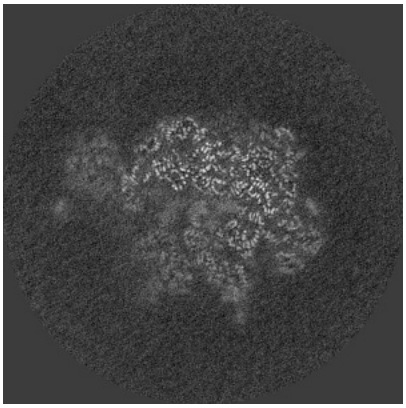


Z Index: 210

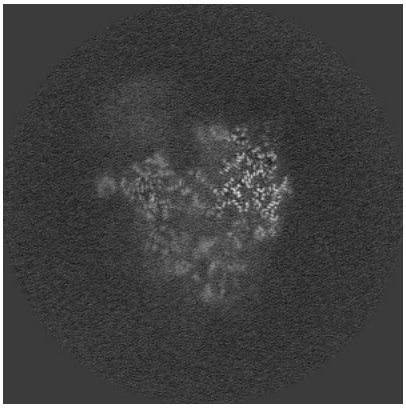
6.2.2 Raw map



X Index: 210



Y Index: 210

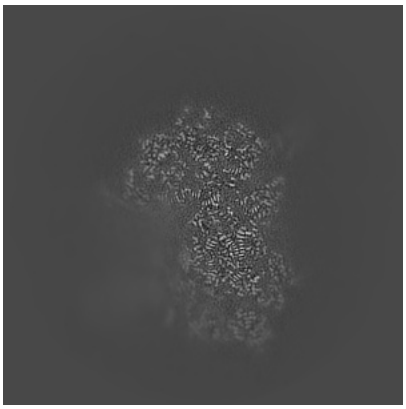


Z Index: 210

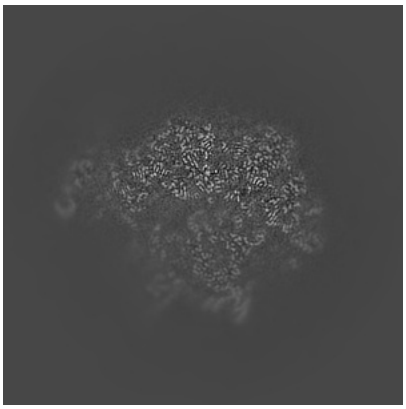
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

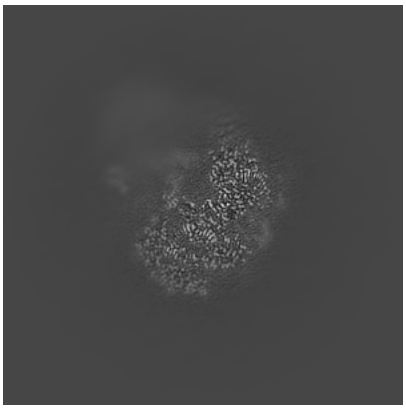
6.3.1 Primary map



X Index: 243

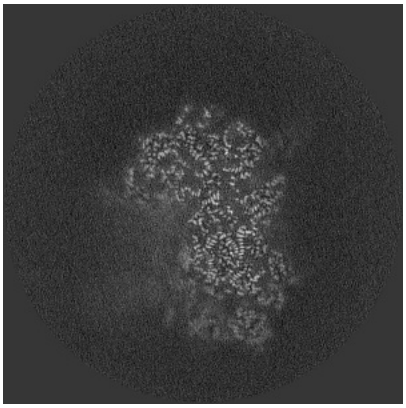


Y Index: 219

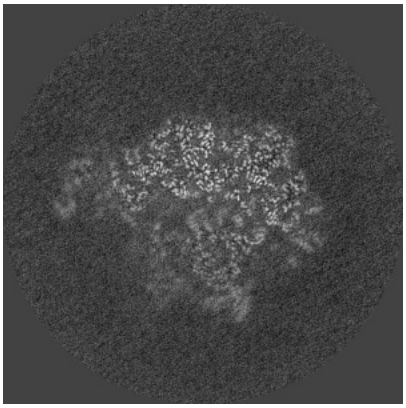


Z Index: 267

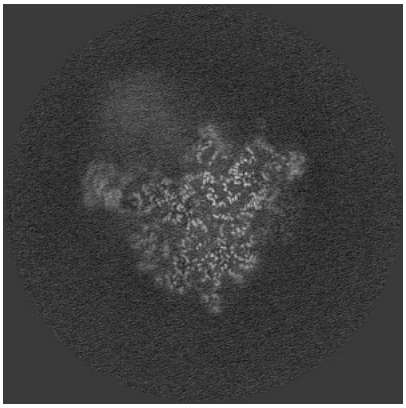
6.3.2 Raw map



X Index: 243



Y Index: 219

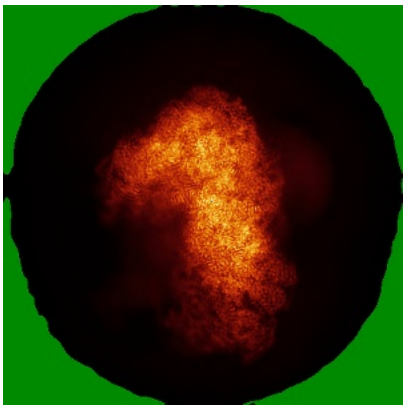


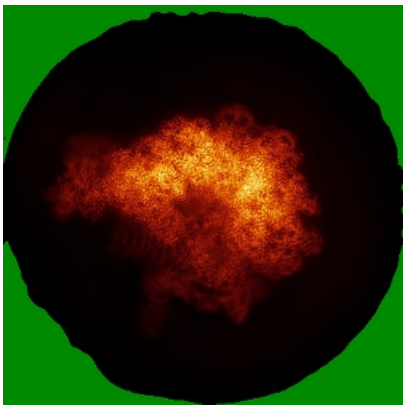
Z Index: 246

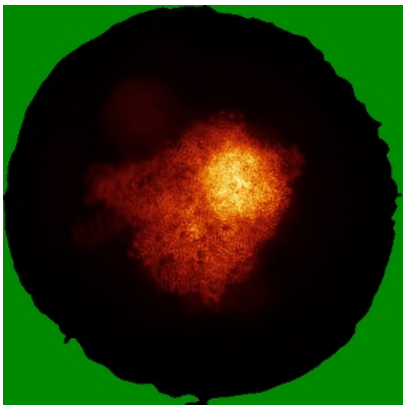
The images above show the largest variance slices of the map in three orthogonal directions.

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

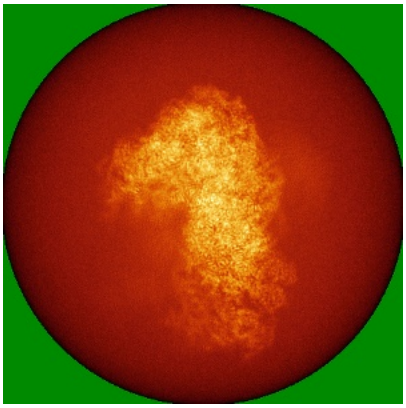
6.4.1 Primary map

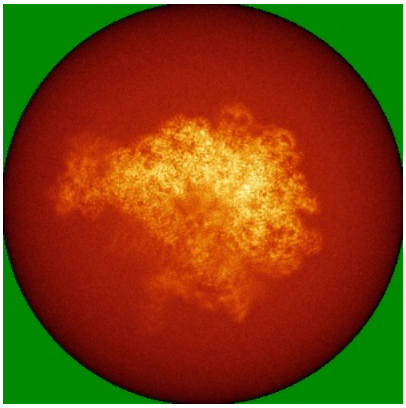

X

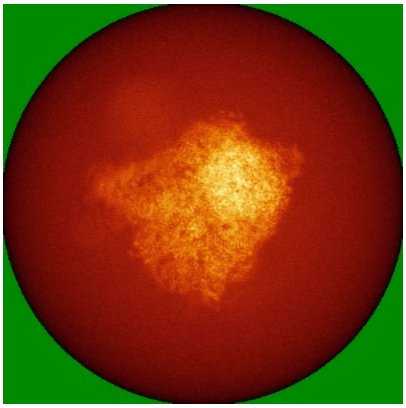

Y


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.

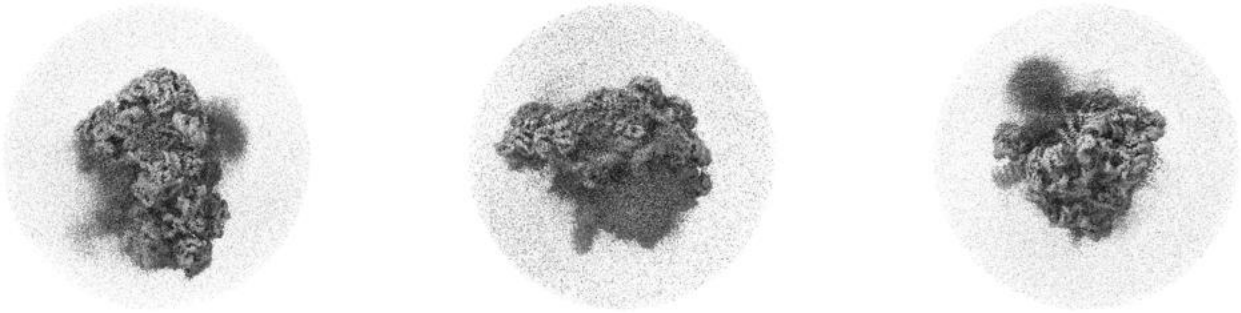
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

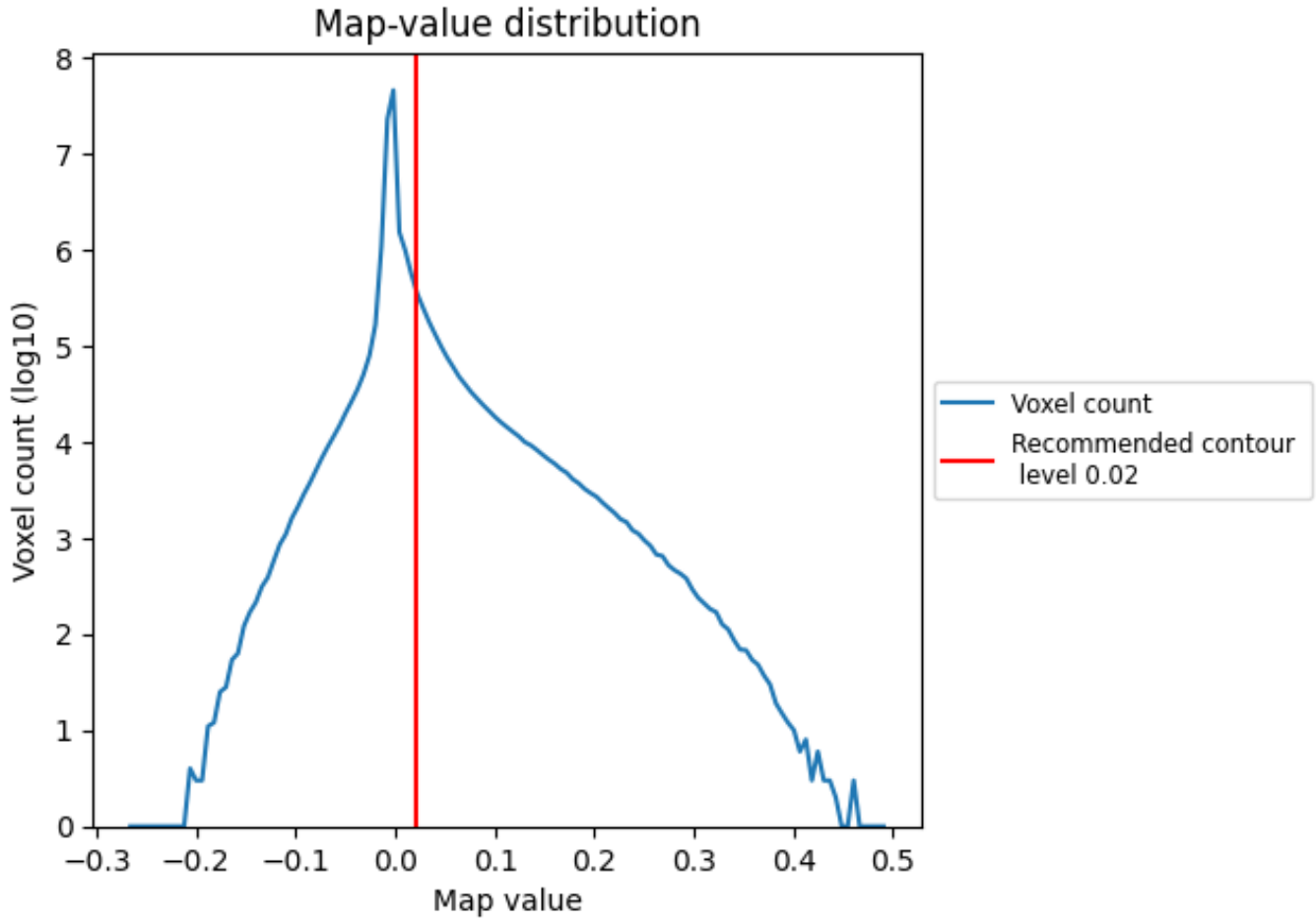
6.6 Mask visualisation (i)

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

7 Map analysis

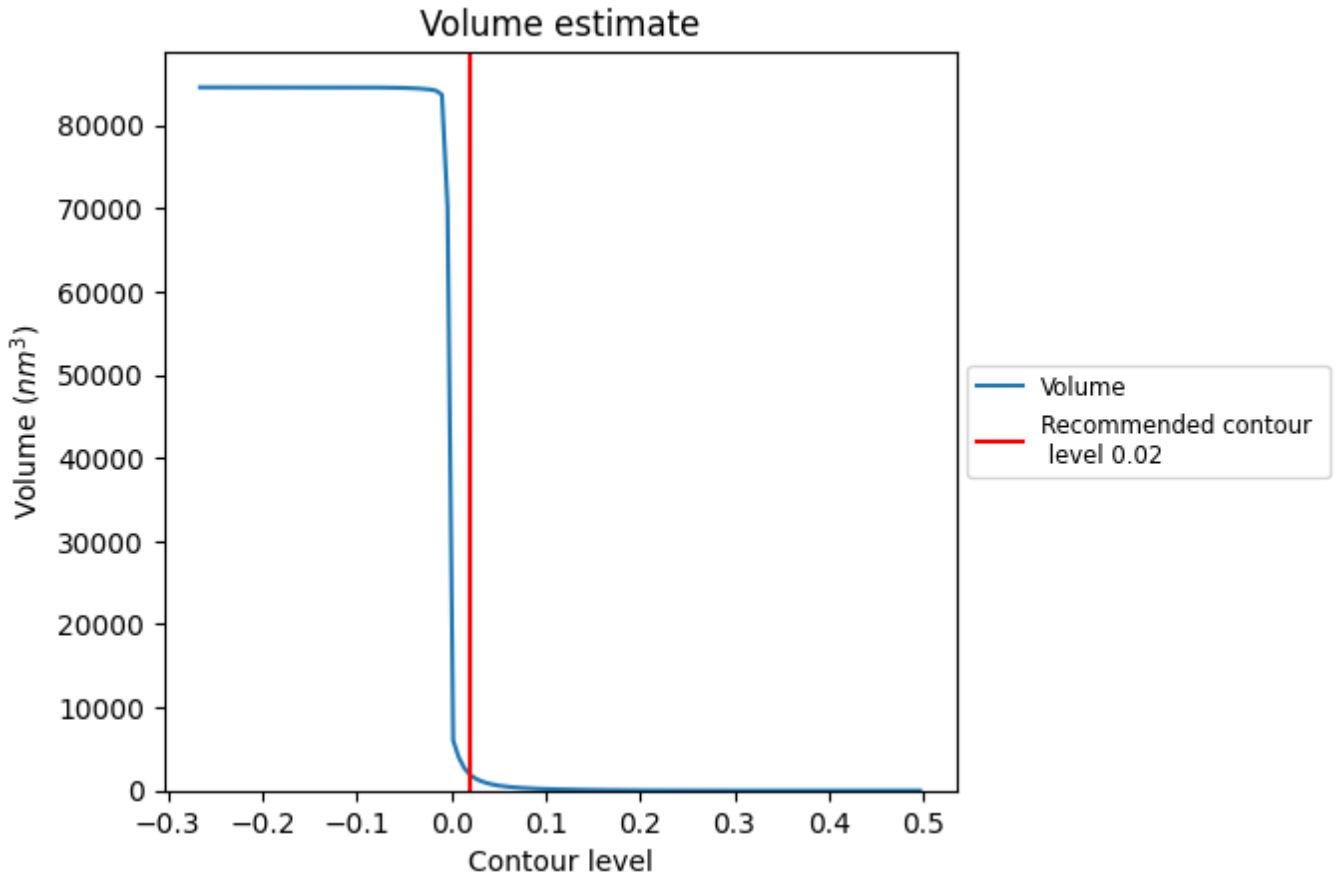
This section contains the results of statistical analysis of the map.

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.

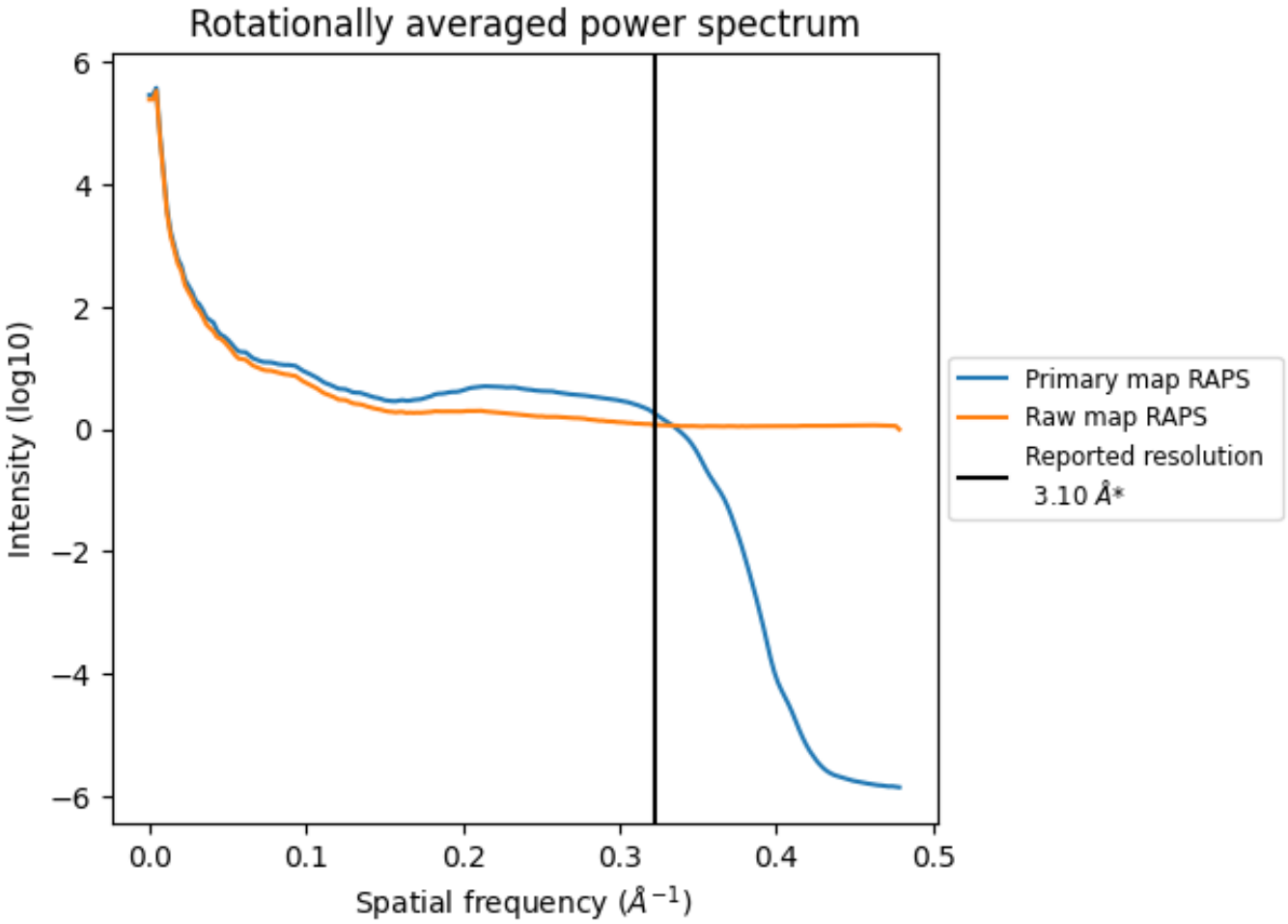
7.2 Volume estimate



The volume at the recommended contour level is 1891 nm^3; this corresponds to an approximate mass of 1708 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)

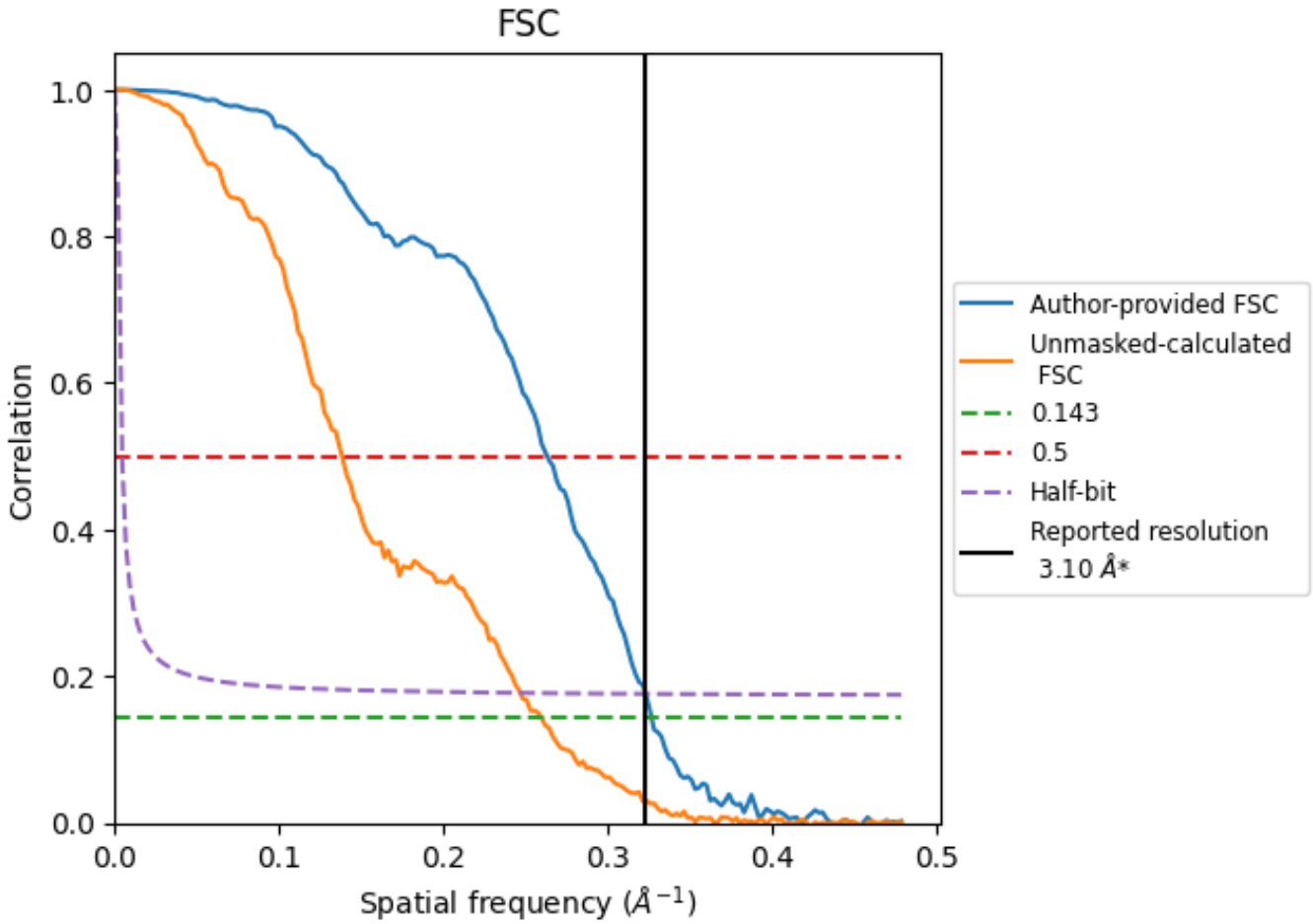


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 $Å^{-1}$

8.2 Resolution estimates (i)

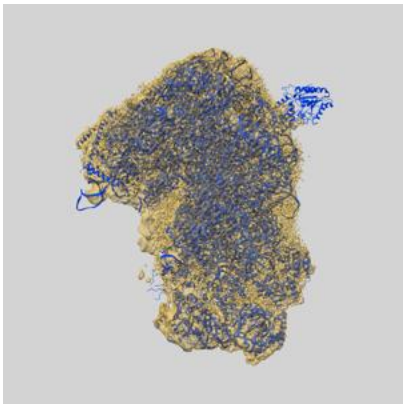
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.06	3.80	3.10
Unmasked-calculated*	3.85	7.23	4.05

*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 3.85 differs from the reported value 3.1 by more than 10 %

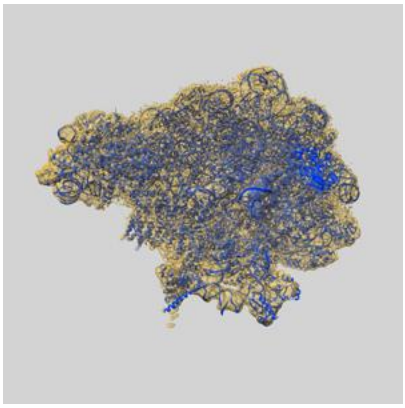
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-35286 and PDB model 8I9W. Per-residue inclusion information can be found in section 3 on page 16.

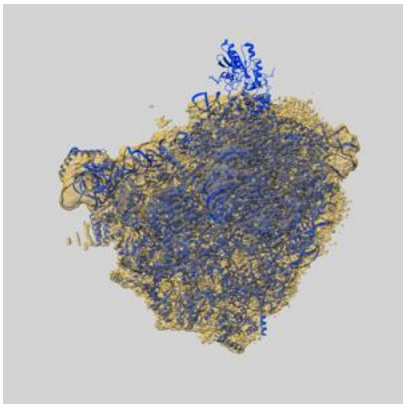
9.1 Map-model overlay



X



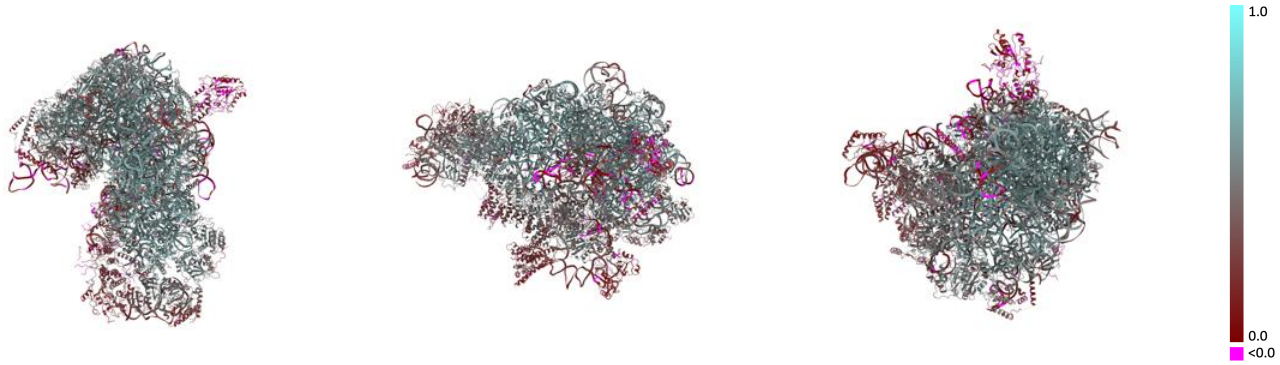
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

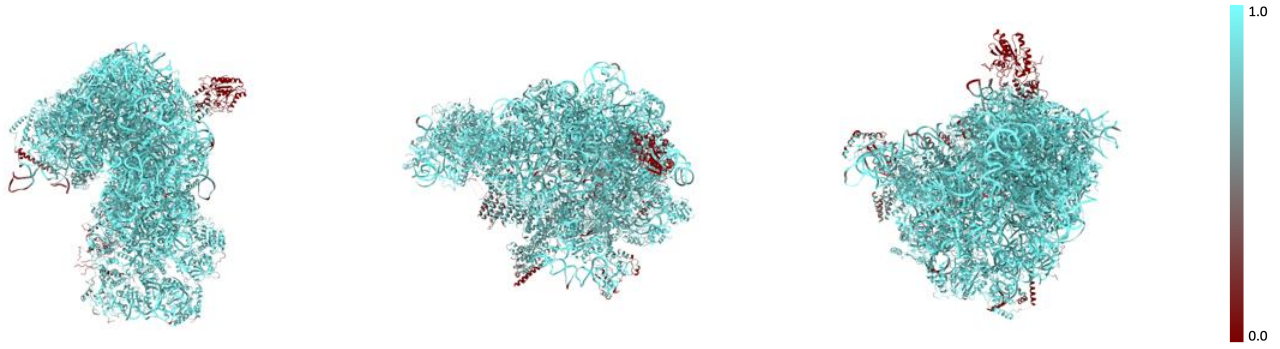
9.2 Q-score mapped to coordinate model (i)



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.

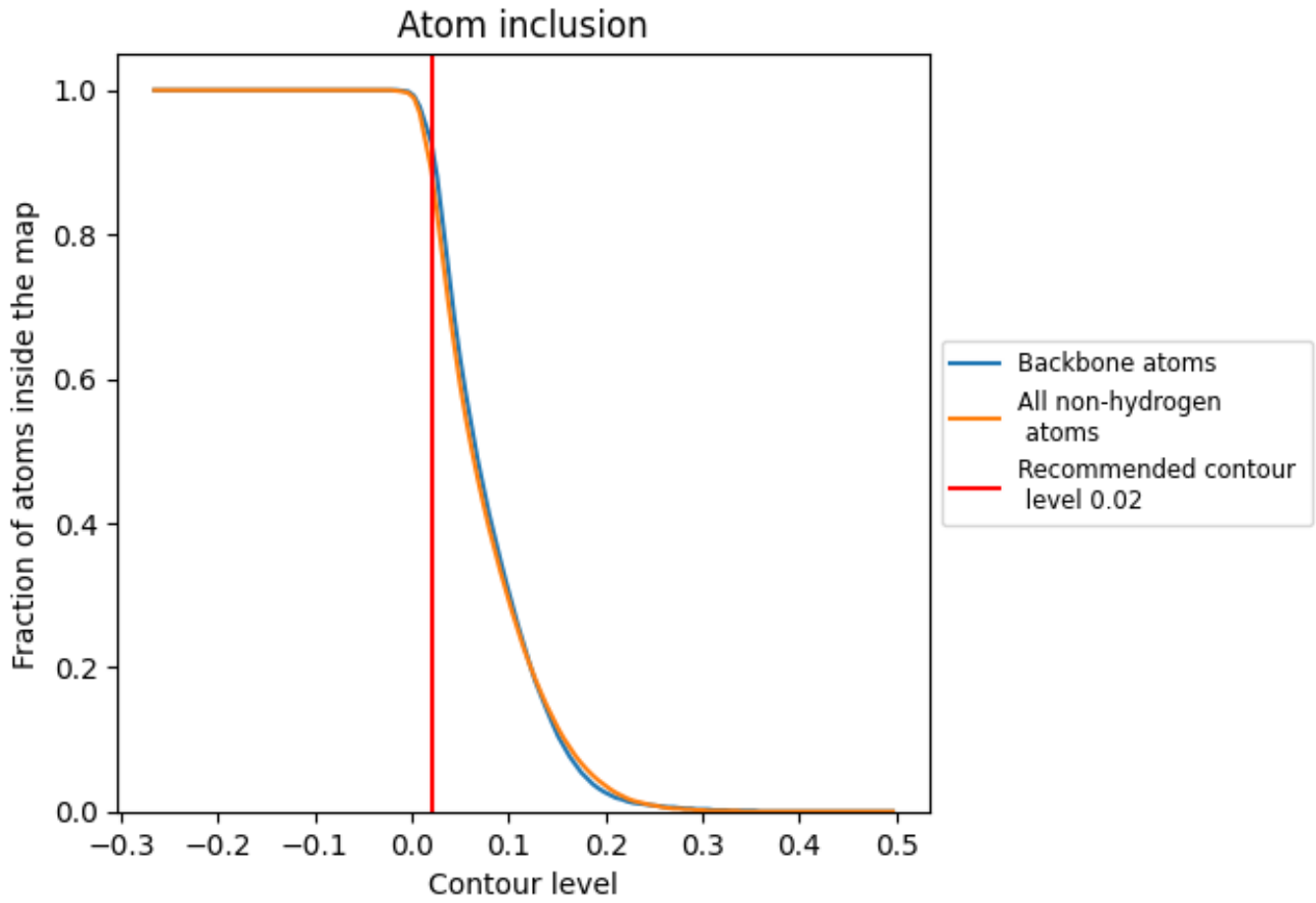
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 89% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8890	0.4410
C1	0.9440	0.4660
C2	0.9490	0.4500
CA	0.9510	0.5300
CB	0.8570	0.3860
CC	0.8170	0.3860
CE	0.8850	0.4780
CF	0.8860	0.4300
CG	0.9290	0.4430
CH	0.8650	0.4490
CI	0.8710	0.4080
CJ	0.8090	0.2690
CK	0.9230	0.4750
CL	0.3220	0.1720
CM	0.7400	0.2780
CN	0.9180	0.4870
CO	0.9670	0.5290
CP	0.9200	0.4450
CQ	0.8820	0.4350
CR	0.9400	0.5290
CS	0.7260	0.3300
CT	0.6890	0.2780
CU	0.9090	0.4630
CV	0.9460	0.5250
CX	0.8400	0.4060
CY	0.6120	0.2110
Cb	0.8170	0.3210
Cz	0.7220	0.2600
LB	0.9550	0.5380
LC	0.9610	0.5660
LE	0.9160	0.5060
LF	0.9420	0.5390
LG	0.9330	0.5310
LH	0.9440	0.5380
LK	0.8240	0.3220

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Chain	Atom inclusion	Q-score
LL	0.9720	0.5770
LM	0.9590	0.5440
LN	0.9730	0.5910
LO	0.9600	0.5680
LP	0.9540	0.5160
LQ	0.9520	0.5200
LS	0.9500	0.5400
LT	0.8320	0.2950
LV	0.9330	0.4830
LX	0.8390	0.3900
LY	0.9330	0.5340
Ld	0.8300	0.3610
Le	0.9600	0.5730
Lf	0.9770	0.5930
Lh	0.9070	0.4800
Li	0.9370	0.5200
Lj	0.9680	0.5690
Lq	0.6320	0.1540