Full wwPDB EM Validation Report (i)

Jul 12, 2023 – 02:49 PM JST

PDB ID	:	8I9V
EMDB ID	:	EMD-35285
Title	:	Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit - State Dbp10-2
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 (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

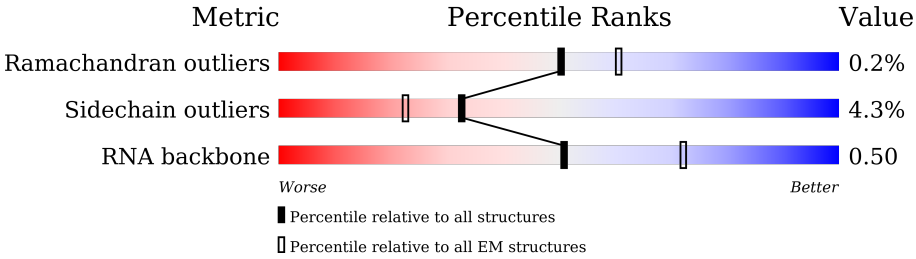
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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	48% 15% • 36%
2	C2	256	49% 12% 38%
3	C3	161	5% 37% 23% • 39%
4	CA	316	78% 5% 18%
5	CB	391	61% 5% • 34%
6	CC	801	15% 34% • 64%
7	CE	598	73% 5% 23%
8	CF	270	86% • 9%

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Mol	Chain	Length	Quality of chain
9	CG	184	91% 5%
10	CH	661	68% 28%
11	CI	414	34% 65%
12	CJ	679	28% 55% 44%
13	CK	261	84% 5% 11%
14	CL	558	51% 68% 30%
15	CM	249	17% 71% 25%
15	LF	249	94%
16	CN	246	97%
17	CO	120	51% 48%
18	CP	751	40% 57%
19	CQ	225	46% 50%
20	CR	237	67% 30%
21	CS	834	33% 35% 64%
22	CT	688	49% 66% 33%
23	CU	451	39% 61%
24	CX	203	21% 42% 57%
25	CY	788	22% 41% 59%
26	Cz	123	16% 56% 43%
27	Cb	924	67% 31%
28	LB	392	84% 13%
29	LC	365	97%
30	LE	200	83% 15%
31	LG	262	7% 73% 25%
32	LH	192	92% 7%

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Mol	Chain	Length	Quality of chain
33	LK	165	84% 12%
34	LL	213	54% 45%
35	LM	142	94%
36	LN	203	87% 10%
37	LO	204	98%
38	LP	187	78% 5% 18%
39	LQ	213	60% 39%
40	LS	174	94% 6%
41	LT	160	11% 76% 21%
42	LV	139	94%
43	LX	156	9% 14% 86%
44	LY	138	92% 5%
45	Ld	120	22% 88% 9%
46	Le	131	98%
47	Lf	109	94% 5%
48	Lh	935	13% 87%
49	Li	110	76% 20%
50	Lj	95	74% 22%
51	Lq	217	59% 94% 5%
52	Cc	282	82% 16%
53	Cd	436	76% 22%
54	Ce	336	55% 42%
55	Cf	570	10% 90%

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 138001 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	2152	46025	20547	8331	14995	2152	0	0

- Molecule 2 is a RNA chain called RNA (256-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C2	158	3359	1502	593	1106	158	0	0

- Molecule 3 is a RNA chain called RNA (161-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	C3	98	2097	933	381	685	98	0	0

- Molecule 4 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	CA	260	2144	1371	393	373	7	0	0

- Molecule 5 is a protein called Ribosome biogenesis protein C8F11.04.

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

- Molecule 6 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	CC	289	2388	1520	399	462	7	0	0

- Molecule 7 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 8 is a protein called Ribosome assembly factor mrt4.

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

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 9 is a protein called 60S ribosome subunit biogenesis protein NIP7.

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

- Molecule 10 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	CH	476	3851	2451	669	716	15	0	0

- Molecule 11 is a protein called Putative RNA-binding protein.

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

- Molecule 12 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	CJ	380	3109	2003	547	549	10	0	0

- Molecule 13 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	CK	232	1855	1165	363	323	4	0	0

- Molecule 14 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	CL	390	2173	1307	446	420	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 15 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	CM	187	1525	987	278	257	3	0	0
15	LF	240	1967	1264	368	332	3	0	0

- Molecule 16 is a protein called Eukaryotic translation initiation factor 6.

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

- Molecule 17 is a protein called DUF2423 domain-containing protein.

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

- Molecule 18 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	CP	324	2535	1618	445	457	15	0	0

- Molecule 19 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	CQ	112	960	607	195	148	10	0	0

- Molecule 20 is a protein called Nucleolar protein 16.

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

- Molecule 21 is a protein called AdoMet-dependent rRNA methyltransferase SPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	CS	298	1750	1072	330	347	1	0	0

- Molecule 22 is a protein called Nucleolar complex-associated protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	CT	458	2269	1353	458	458	0	0

- Molecule 23 is a protein called rRNA-processing protein EBP2.

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	CY	324	1608	960	324	324	0	0

- Molecule 26 is a protein called rRNA-processing protein.

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

- Molecule 27 is a protein called ATP-dependent RNA helicase DBP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Cb	642	5058	3216	918	911	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	LB	341	2708	1721	493	482	12	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	LE	170	1338	861	241	233	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	LG	196	1583	1021	287	270	5	0	0

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

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

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
			Total	C	N	O	S		
33	LK	146	1112	701	203	206	2	0	0

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

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

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

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

- Molecule 36 is a protein called Ribosomal protein L15.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	LP	154	1212	758	233	218	3	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	LX	22	148	91	31	26	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	Le	131	1055	663	213	172	7	0	0

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

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

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

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

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

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

- Molecule 50 is a protein called Ribosomal protein L37.

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

- Molecule 51 is a protein called Ribosomal protein.

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

- Molecule 52 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	Cc	236	1898	1208	337	343	10	0	0

- Molecule 53 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	Cd	342	2763	1743	533	483	4	0	0

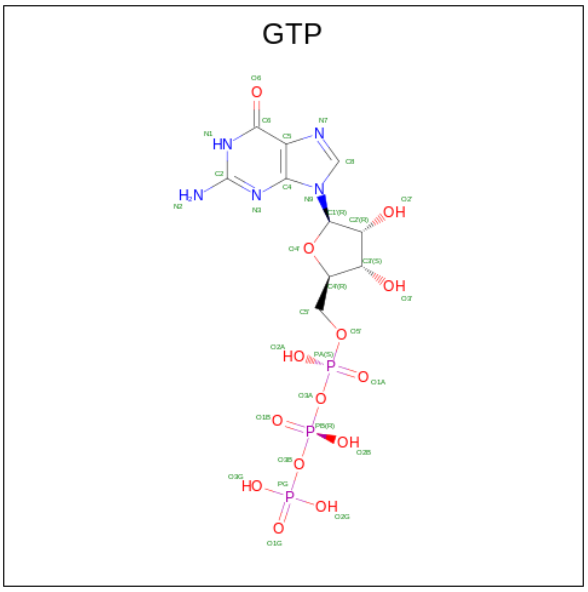
- Molecule 54 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	Ce	194	1609	1020	304	276	9	0	0

- Molecule 55 is a protein called 60S ribosome biogenesis protein Rrp14.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
55	Cf	59	513	310	111	92	0	0

- Molecule 56 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

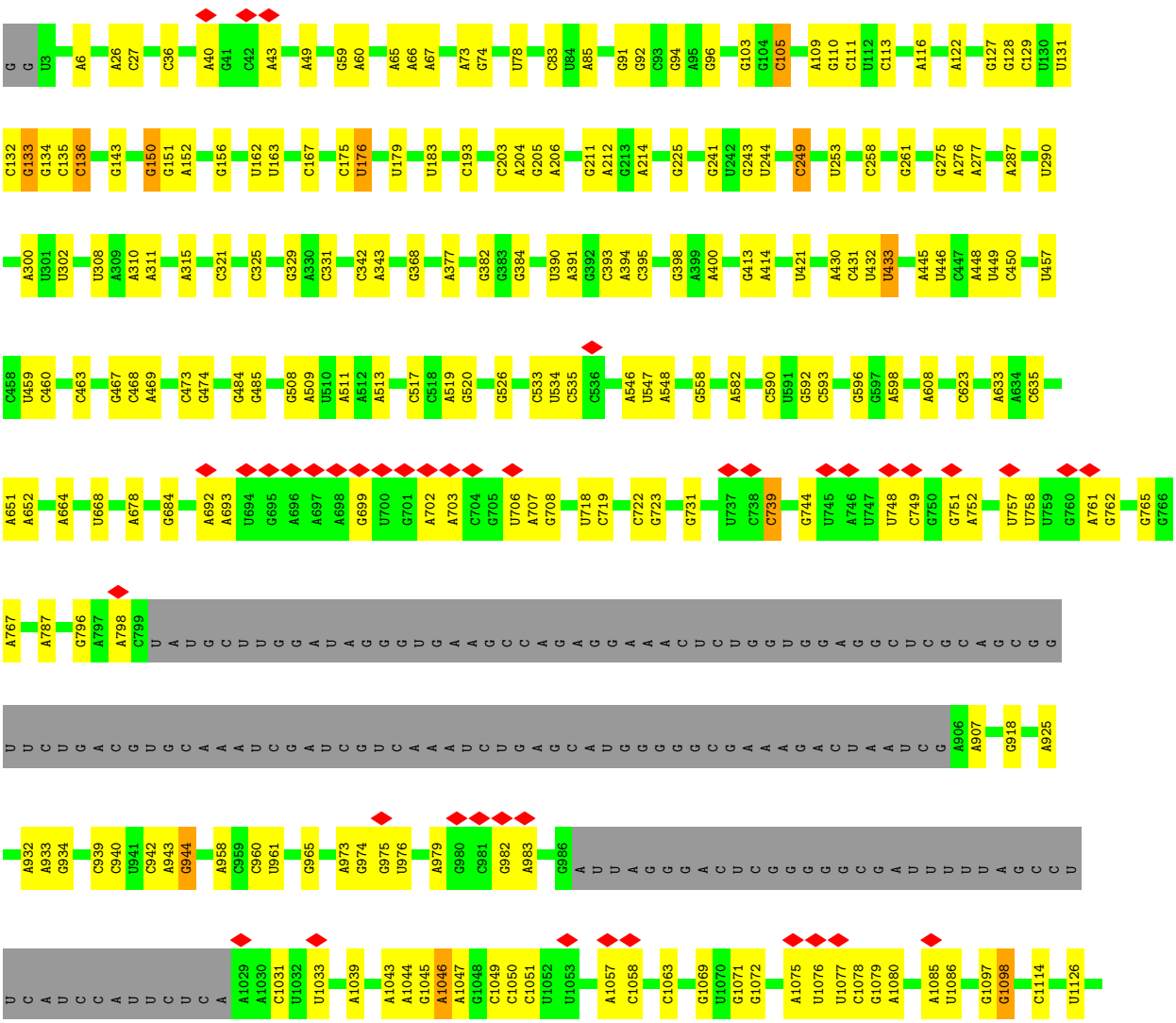
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	CQ	1	1	1	0
57	Lj	1	1	1	0
57	Ce	1	1	1	0

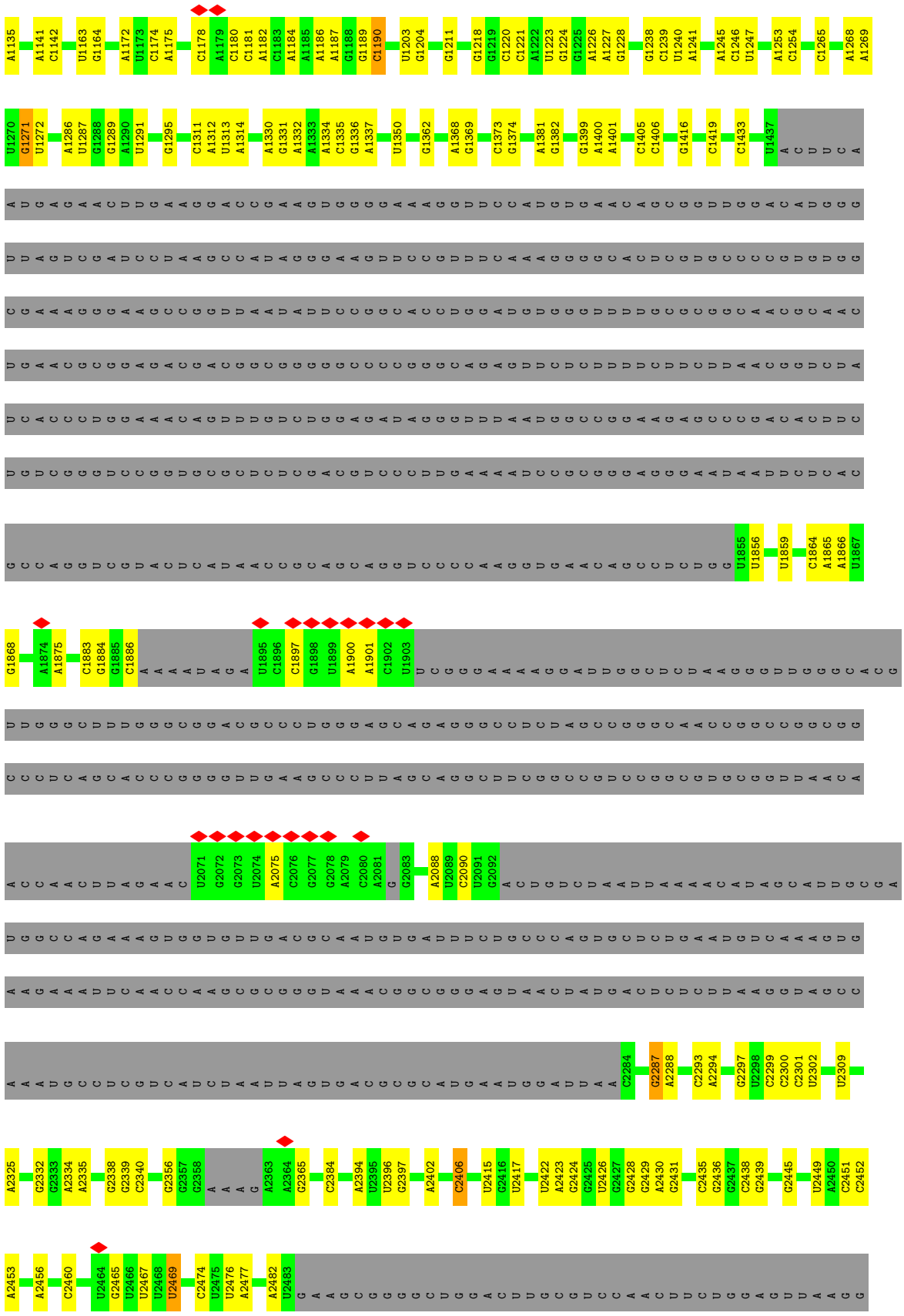
3 Residue-property plots (i)

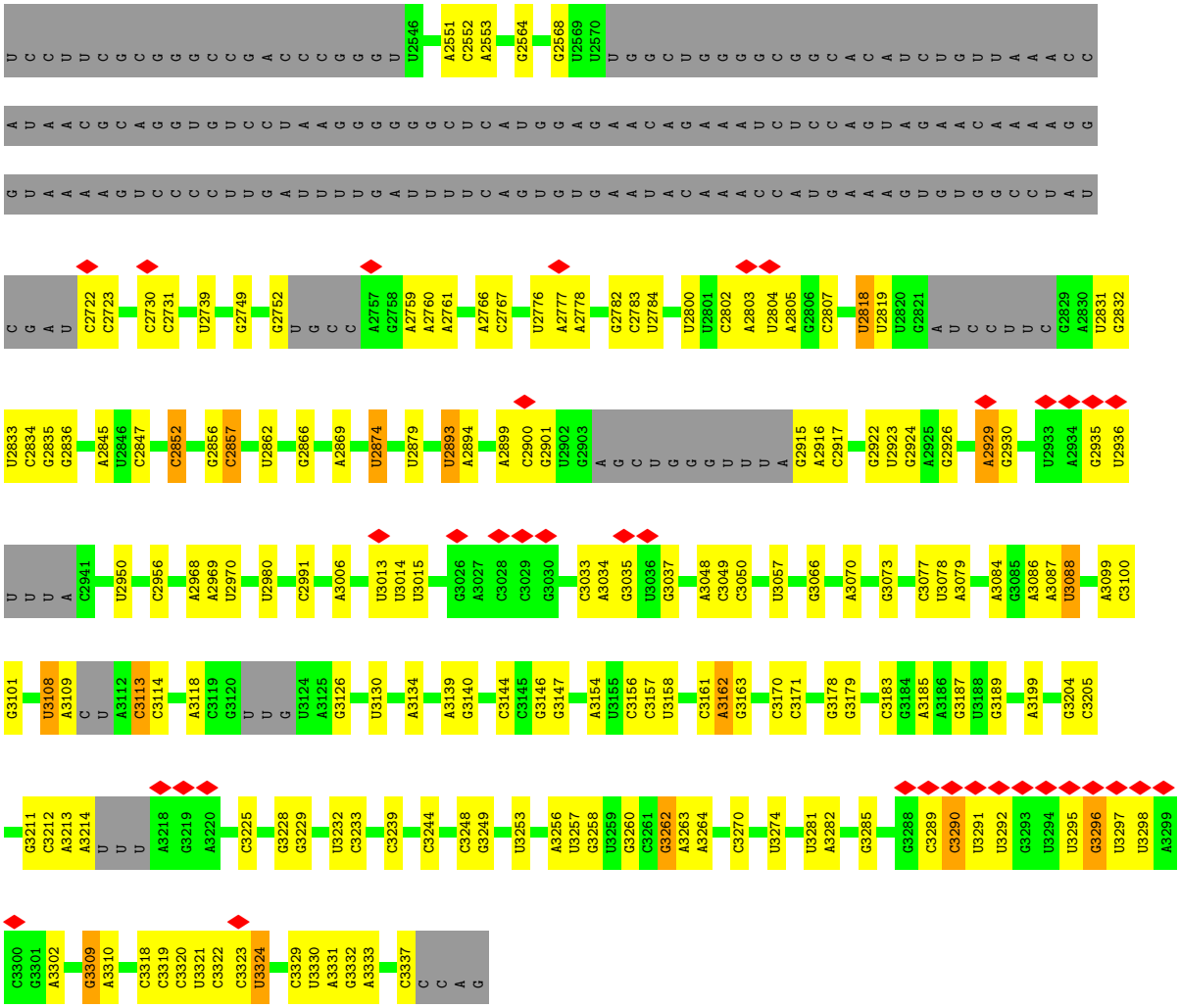
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 48% 15% 36%

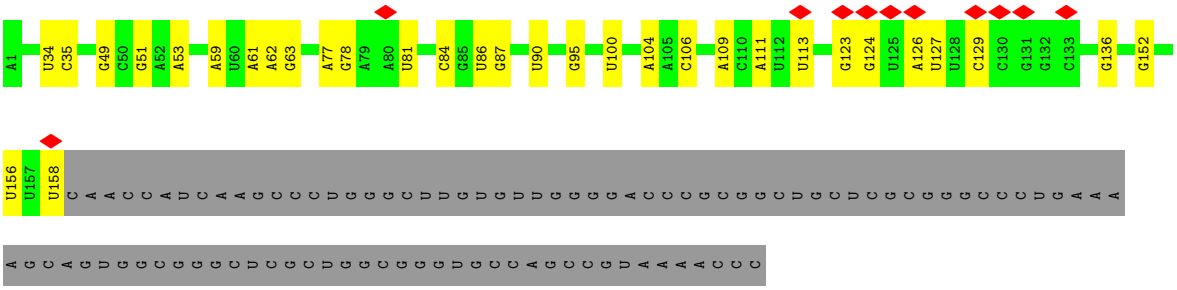



A1135 A1141 C1142 U1163 G1164 A1172 U1173 C1174 A1175 C1178 A1179 C1180 C1181 A1182 C1183 A1184 A1185 A1186 A1187 G1188 G1189 C1190 U1203 G1204 G1211 G1218 G1219 C1220 C1221 A1222 U1223 G1224 G1225 A1226 A1227 G1228 G1238 C1239 U1240 A1241 A1245 C1246 U1247 A1253 C1254 C1265 A1268 A1269
U1270 G1271 U1272 A1286 U1287 G1288 G1289 A1290 U1291 G1295 C1311 A1312 U1313 A1314 A1330 G1331 A1332 A1333 A1334 C1335 G1336 A1337 U1350 G1362 A1368 G1369 C1373 G1374 A1381 G1382 G1399 A1400 A1401 C1405 C1406 G1416 C1419 C1433 U1437 A C U U C A
U1855 U1856 U1859 C1864 A1865 A1866 U1867
G1868 A1874 A1875 C1883 G1884 G1885 C1886 U1895 C1896 C1897 G1898 U1899 A1900 A1901 C1902 U1903
U2071 G2072 G2073 U2074 A2075 C2076 G2077 G2078 A2079 C2080 A2081 G2083 A2088 U2089 C2090 U2091 G2092
C2284 G2287 A2288 C2293 A2294 G2297 U2298 C2299 C2300 C2301 U2302 U2309
A2325 G2332 G2333 A2334 A2335 G2338 G2339 C2340 G2356 G2357 G2358 A2363 A2364 G2365 C2384 A2394 U2395 U2396 G2397 A2402 C2406 U2415 G2416 U2417 U2422 A2423 G2424 G2425 U2426 G2427 G2428 G2429 A2430 G2431 C2435 G2436 G2437 C2438 G2439 G2445 U2449 A2450 C2451 C2452
A2453 A2456 C2460 U2464 G2465 U2466 U2467 U2468 U2469 C2474 U2475 U2476 A2477 A2482 U2483



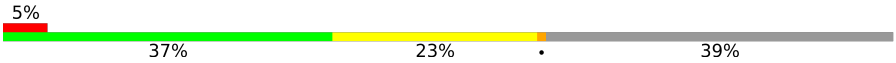
• Molecule 2: RNA (256-MER)

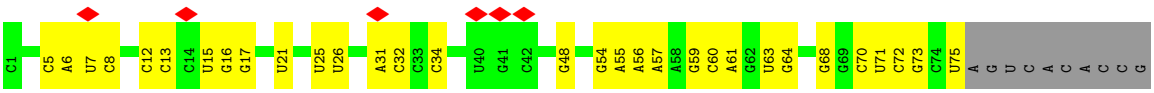
Chain C2:

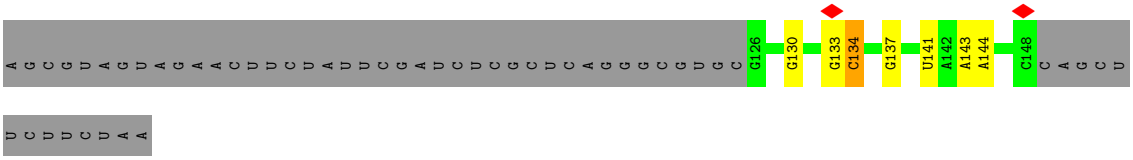


• Molecule 3: RNA (161-MER)

Chain C3:

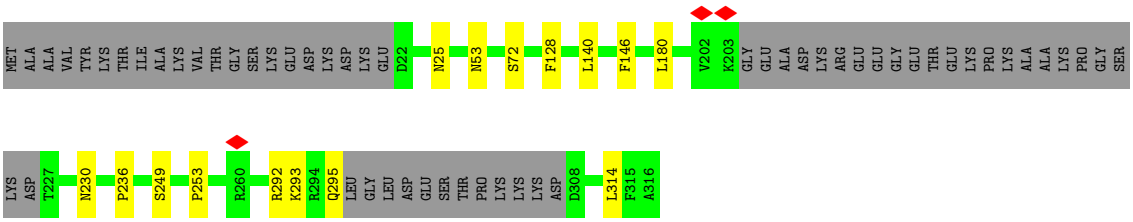






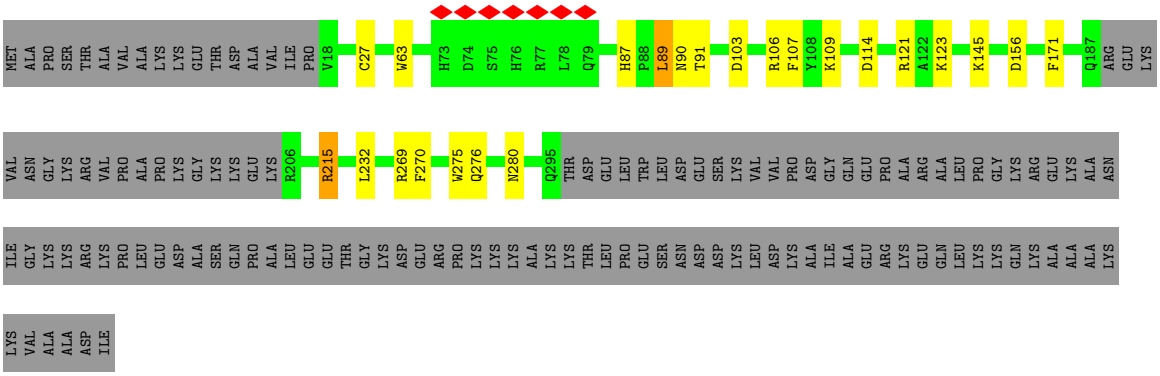
• Molecule 4: Brix domain-containing protein

Chain CA:



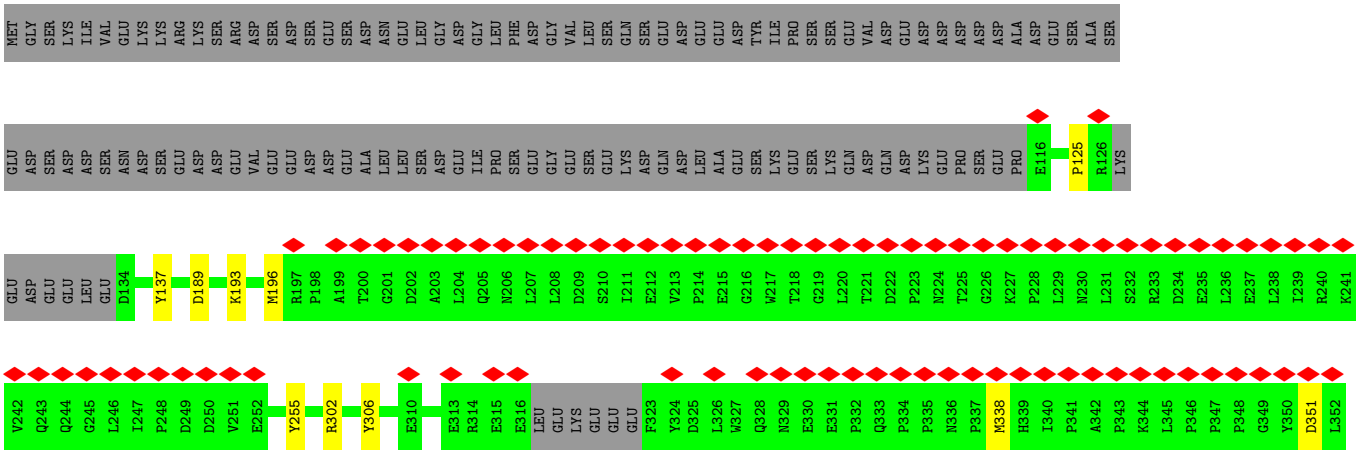
• Molecule 5: Ribosome biogenesis protein C8F11.04

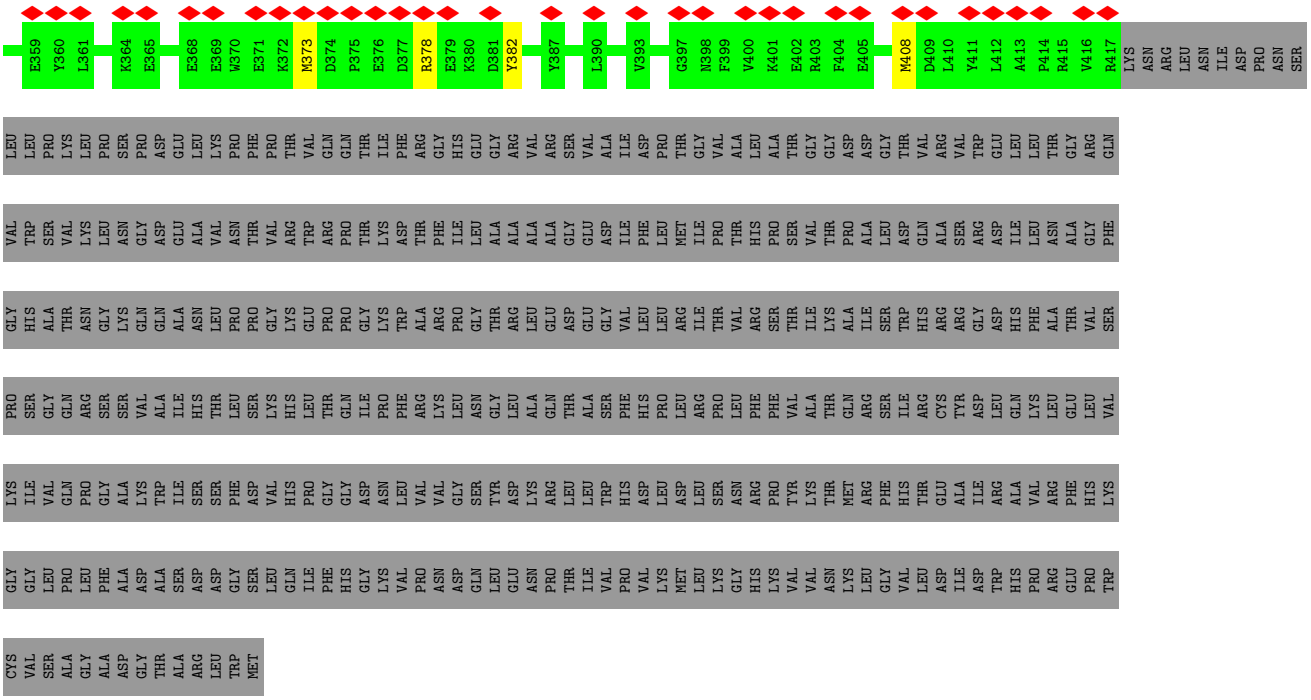
Chain CB:



• Molecule 6: Ribosome biogenesis protein ERB1

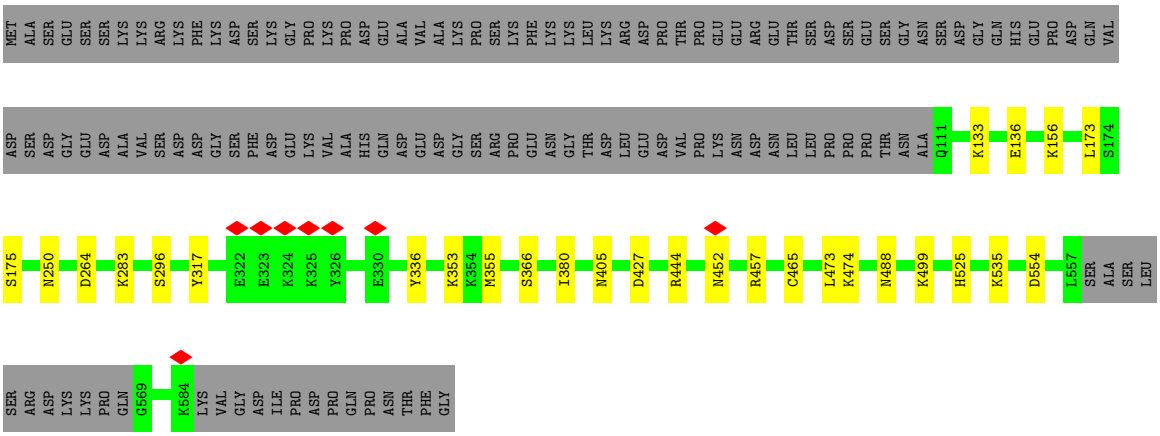
Chain CC:





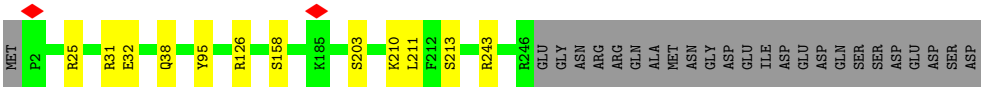
- Molecule 7: RNA helicase

Chain CE:



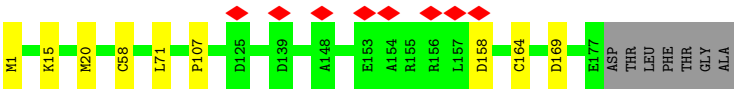
- Molecule 8: Ribosome assembly factor mrt4

Chain CF:



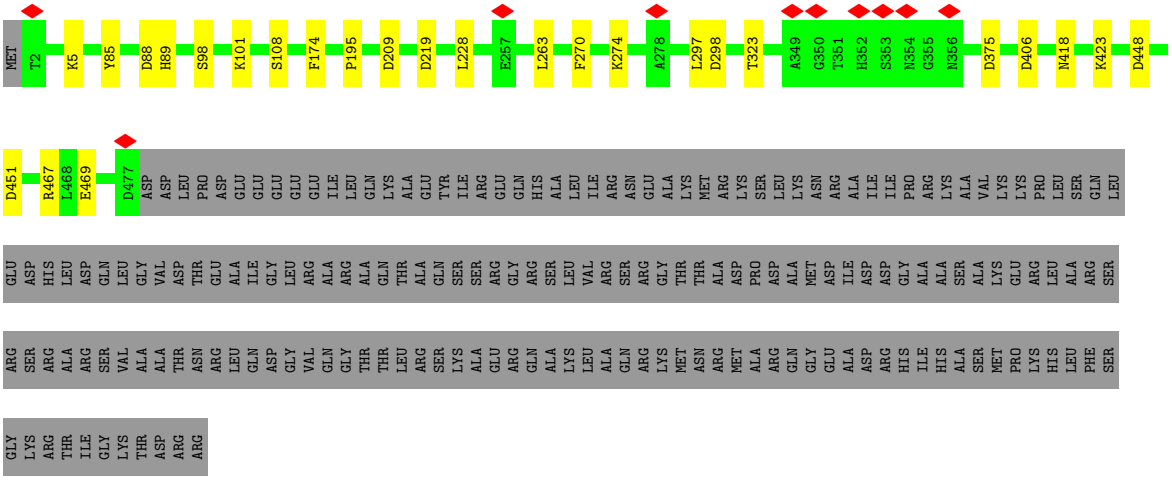
- Molecule 9: 60S ribosome subunit biogenesis protein NIP7

Chain CG:



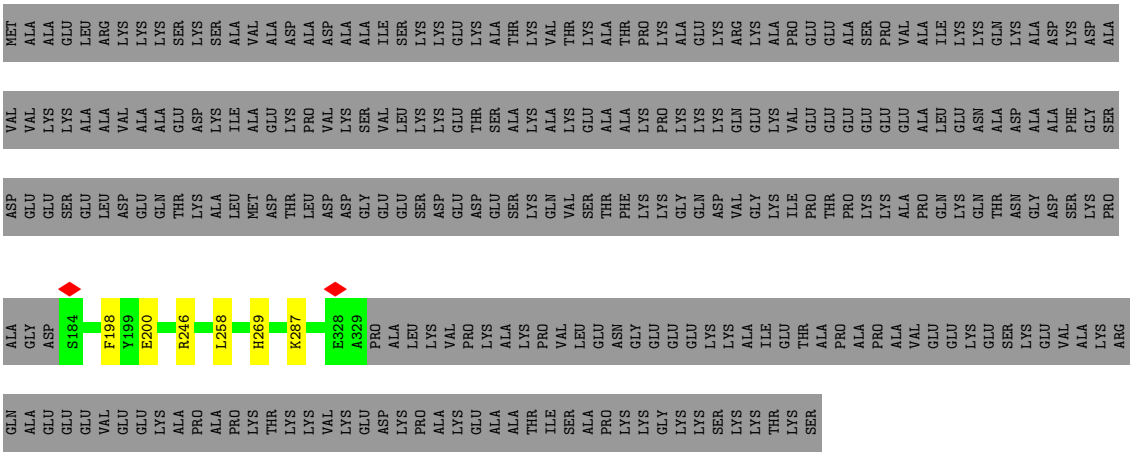
• Molecule 10: Nucleolar GTP-binding protein 1

Chain CH:



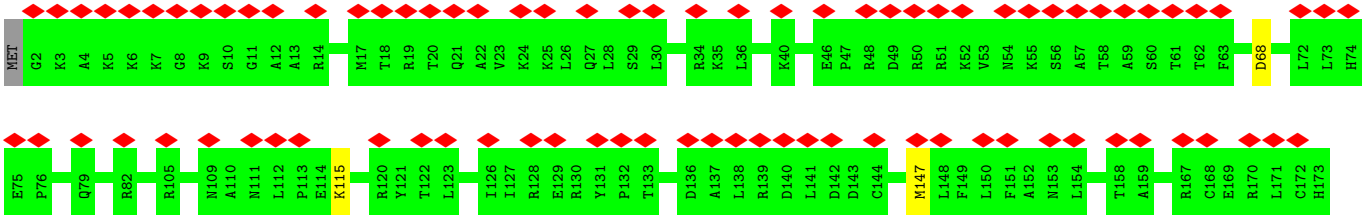
• Molecule 11: Putative RNA-binding protein

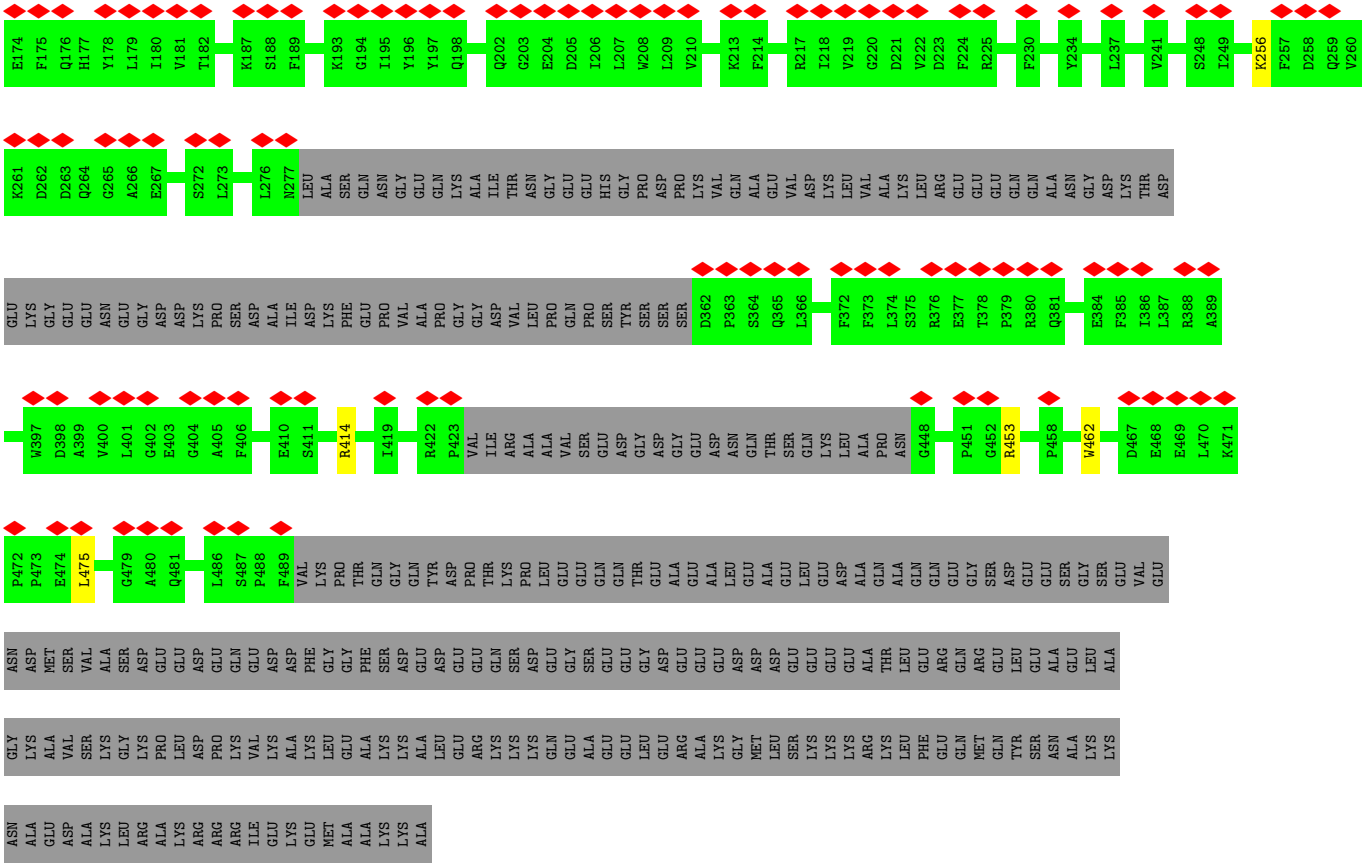
Chain CI:



• Molecule 12: Pescadillo homolog

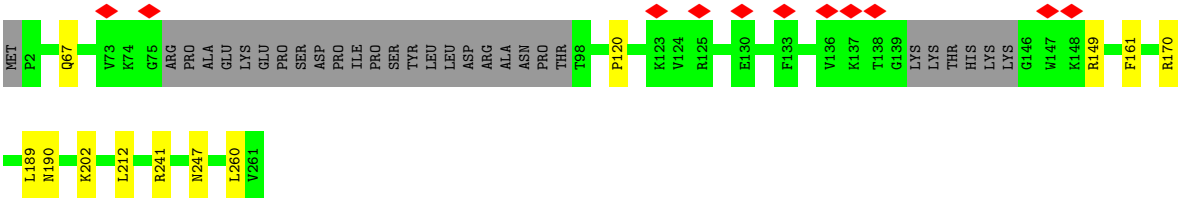
Chain CJ:





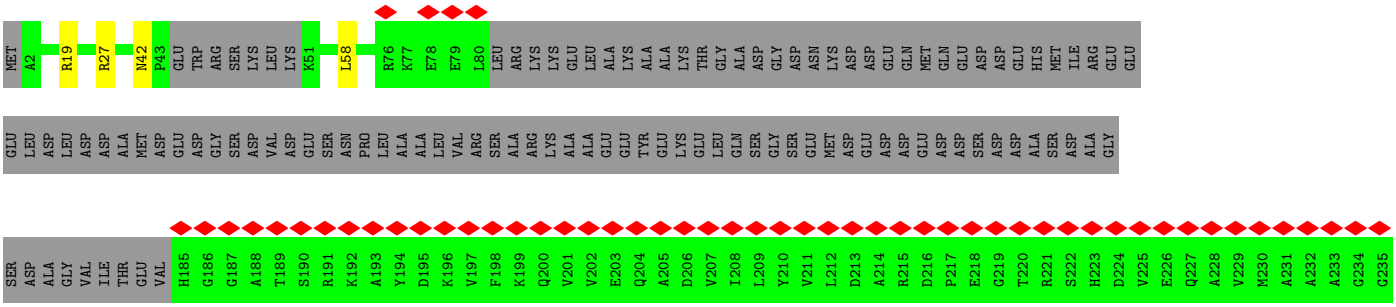
• Molecule 13: Ribosome biogenesis protein NSA2 homolog

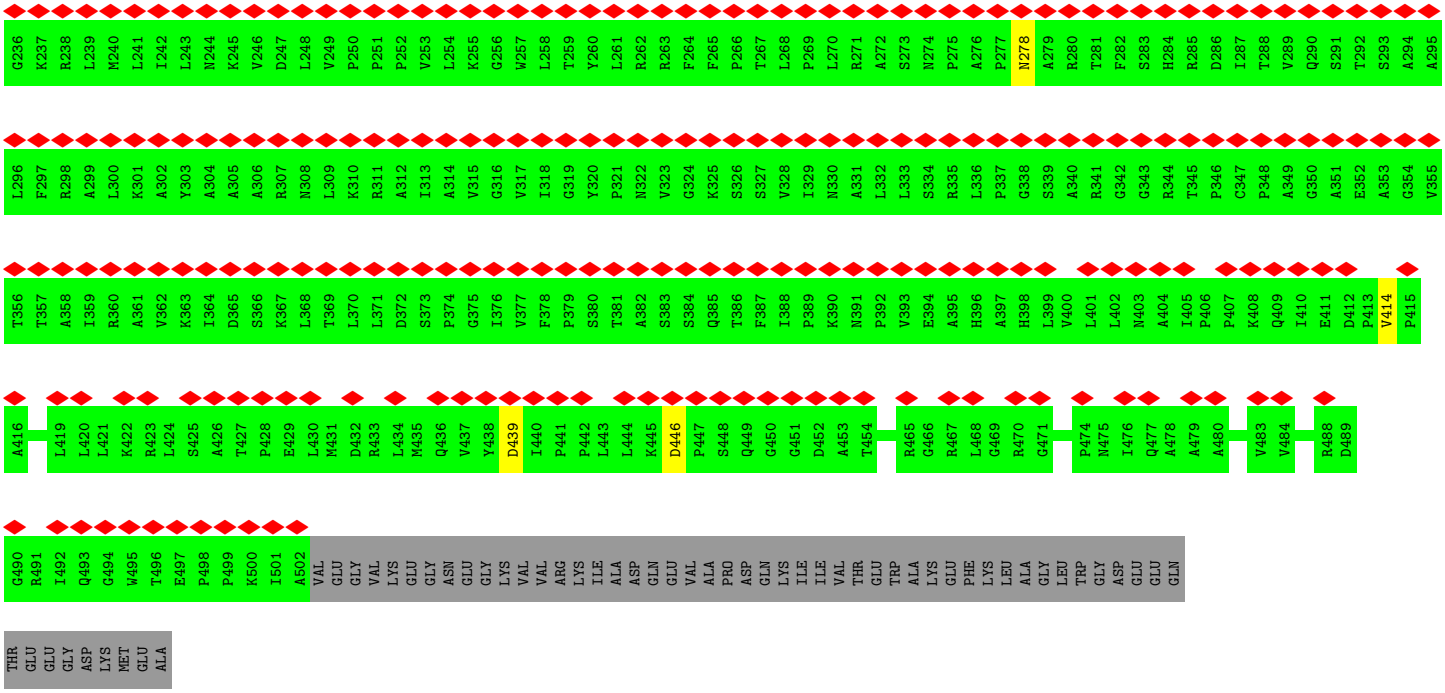
Chain CK:



• Molecule 14: Putative GTP binding protein

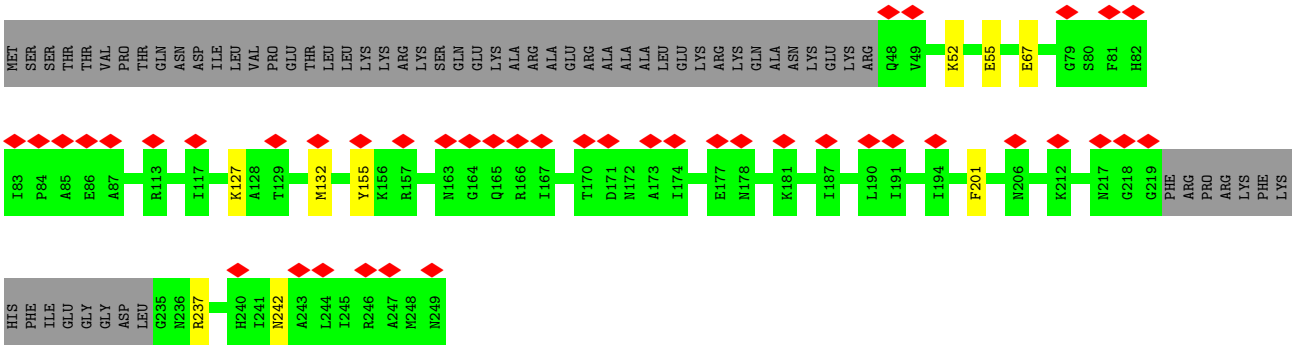
Chain CL:





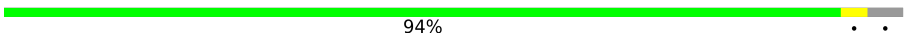
- Molecule 15: 60S ribosomal protein l7-like protein

Chain CM:



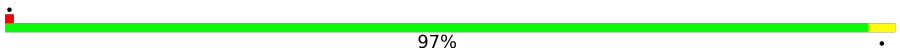
- Molecule 15: 60S ribosomal protein l7-like protein

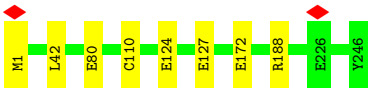
Chain LF:



- Molecule 16: Eukaryotic translation initiation factor 6

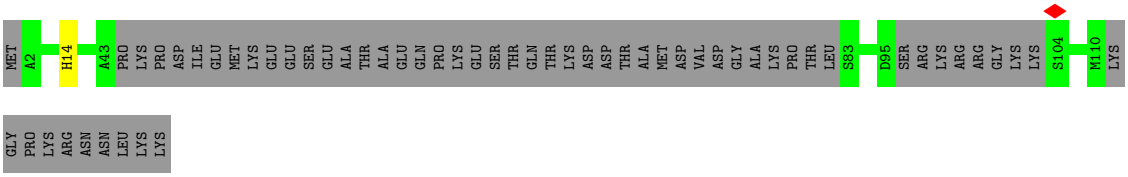
Chain CN:





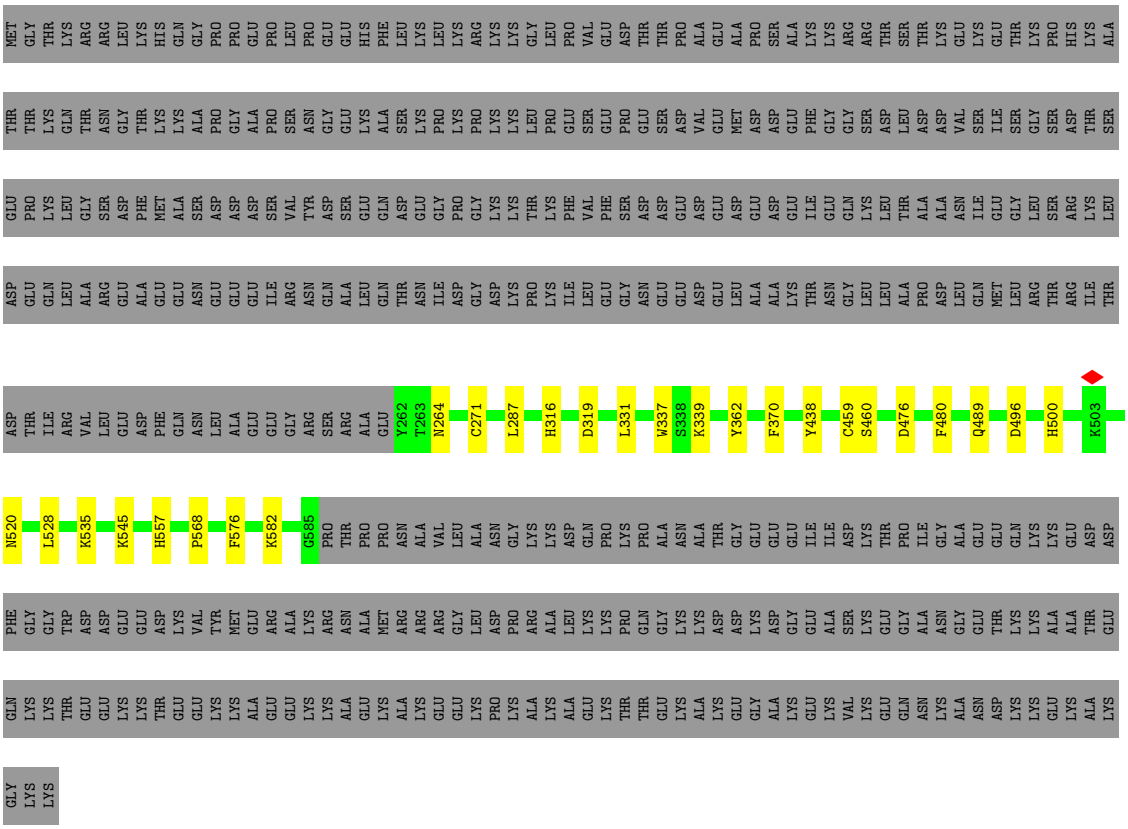
- Molecule 17: DUF2423 domain-containing protein

Chain CO: 51% 48%



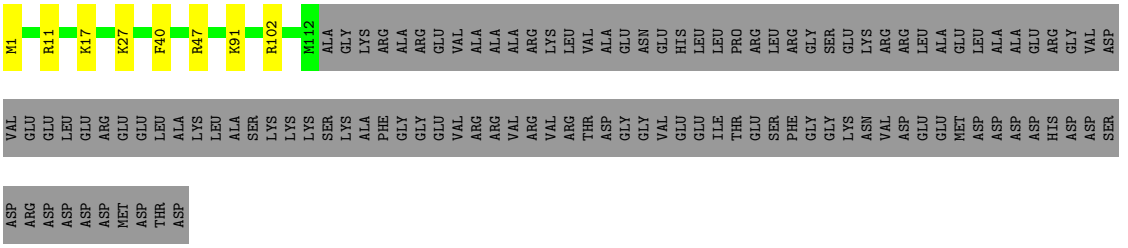
- Molecule 18: RNA methyltransferase nop2-like protein

Chain CP: 40% 57%



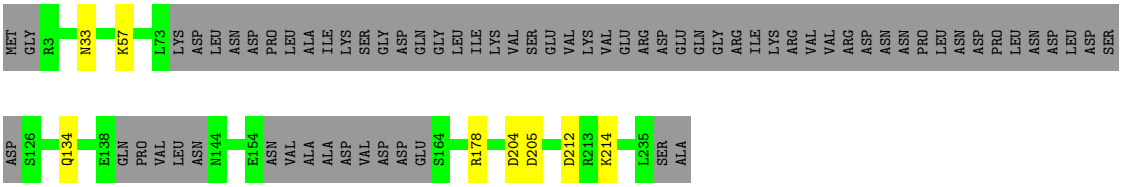
- Molecule 19: Ribosome biogenesis protein RLP24

Chain CQ: 46% 50%



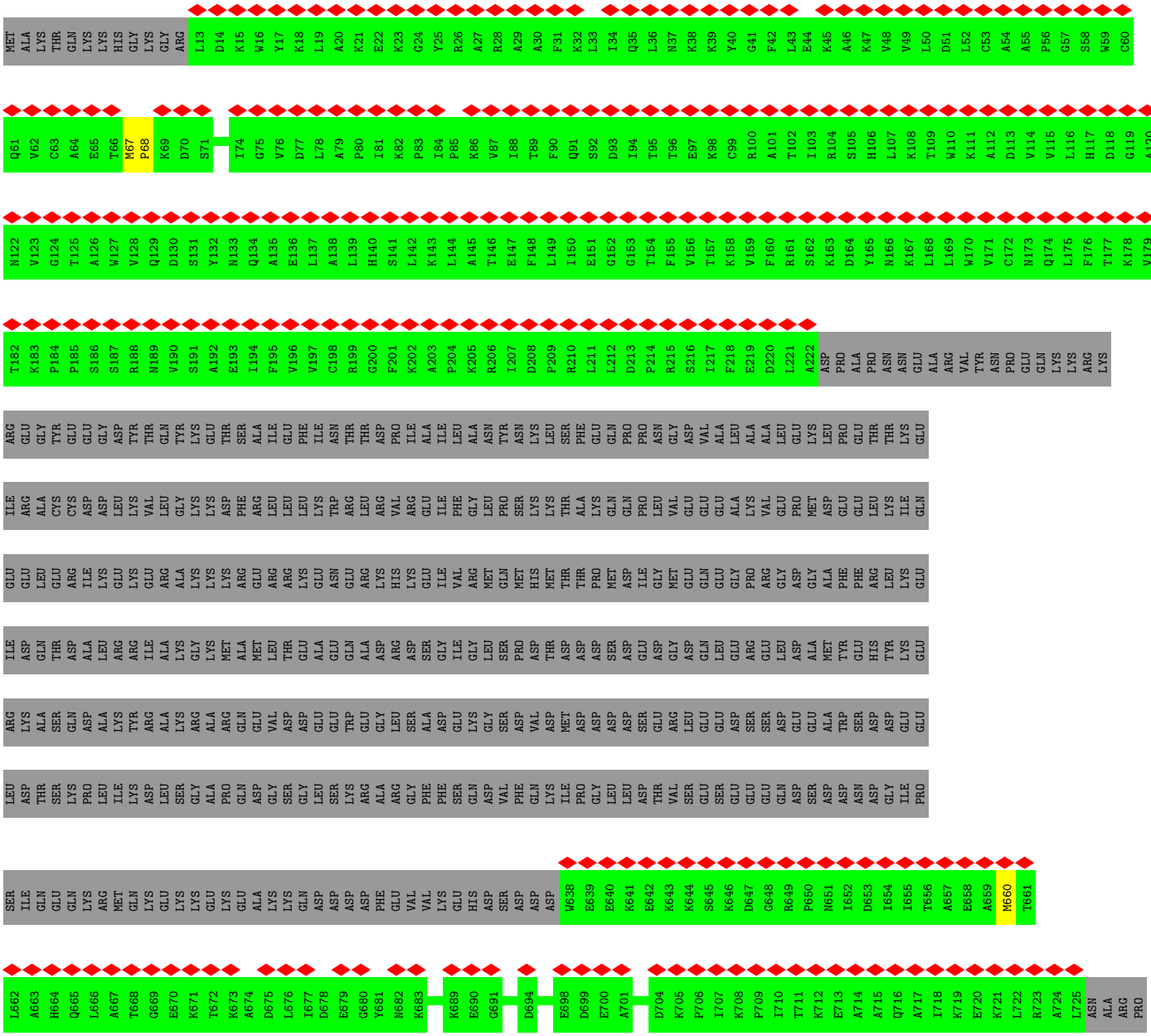
• Molecule 20: Nucleolar protein 16

Chain CR:



• Molecule 21: AdoMet-dependent rRNA methyltransferase SPB1

Chain CS:



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

LYS VAL VAL LYS ALA THR GLY ALA ASN ARG GLY ILE LYS GLY ARG PRO LYS GLY VAL LYS GLY ARG TYR LYS MET VAL ASP GLY ARG MET LYS LYS GLU MET ARG ALA LEU LYS ARG LEU ALA LYS LYS LYS ARG

- Molecule 22: Nucleolar complex-associated protein 3

Chain CT: 49% 66% 33%

MET ALA THR ARG PRO LEU LYS ARG ARG LYS VAL THR PRO PRO ARG ASP ASP GLY GLN ASP ALA ALA GLU ARG GLU ALA LYS ILE GLN LYS ALA PHE LEU LYS ASN ALA ALA SER TRP ASP LEU GLU GLU ALA TRP GLU SER ARG PRO ARG LYS GLY LYS LYS LYS ASP LYS LYS ASP

GLU GLU ARG PRO GLY ARG LEU PRO ILE ARG THR GLU GLN GLY THR TRP GLN VAL GLN ASP ASP VAL GLU SER ILE PRO SER ASP GLU TRP LEU ASP SER ASP GLY GLU LEU ALA VAL GLU GLN GLN LEU GLU PRO VAL ALA PRO ALA PRO ALA PRO GLU PRO PRO LYS ILE SER GLU

LYS E122 Q123 I124 R125 Q126 A127 Q128 E129 E130 L131 A132 K133 I134 A135 T136 Q137 L138 N139 E140 N141 P142 E143 E144 Y145 P146 G147 H148 F149 K150 A151 L152 A153 R154 I155 G156 E157 T158 P159 I160 L161 A162 I163 Q164 K165 L166 C167 I168 V169 T170 Q171 M172 A173 V174 Y175 K176 D177 V178 I179 P180

G181 Y182 R183 I184 R185 P186 L187 G188 E189 ASP ALA VAL ASN GLU LYS VAL SER K198 E199 V200 K201 R202 L203 R204 T205 Y206 E207 Q208 A209 L210 V211 A212 G213 G216 Y217 L218 K219 T220 L221 A222 T223 Y224 A225 A226 S227 S228 I229 P230 E231 D232 R233 K234 G235 E236 P237 I238 S239 S240 I241

A242 F243 T244 C245 A246 C247 E248 L249 V250 N251 A252 V253 P254 H255 F256 N257 F258 R259 G260 D261 L262 L263 R264 I265 L266 V267 K268 K269 L270 S271 T272 R273 K274 I275 D276 R277 D278 F279 V280 K281 C282 R283 E284 A285 L286 E287 K288 L289 F290 Q291 D292 D293 E294 E295 G296 N297 A298 S299 Q300 E301

A302 V303 S304 L305 L306 S307 K308 M309 M310 K311 A312 R313 E314 Y315 R316 V317 D318 E319 S320 V321 L322 N323 L324 F325 L326 H327 L328 R329 L330 L331 S332 GLU PHE VAL GLY LYS GLY SER ARG ASP THR VAL ILE ARG PRO GLY ASP ARG PRO ILE GLY LYS LYS PRO LYS LYS LYS TRP GLU

PHE ARG THR LYS LYS GLN ARG LYS LEU LEU LYS ALA GLU LYS GLU ALA GLN LYS VAL MET GLU GLN ALA ASP ALA THR VAL S389 H390 E391 E392 R393 E394 R395 I396 Q397 S398 E399 I400 L401 K402 M403 V404 F405 A406 T407 Y408 F409 R410 I411 L412 K413 A414 R415 V416 P417 H418 L419 M420 G421

A422 V423 L424 E425 G426 L427 A428 K429 Y430 A431 H432 L433 I434 M435 Q436 D437 F438 F439 G440 D441 L442 L443 E444 A445 L446 K447 D448 L449 I450 R451 D452 T453 D454 R455 LEU GLU GLU GLU ASP GLY PRO ASP SER SER GLN ASP ASP ASP GLN GLY VAL SER VAL VAL ARG D477 T478 E481 S482

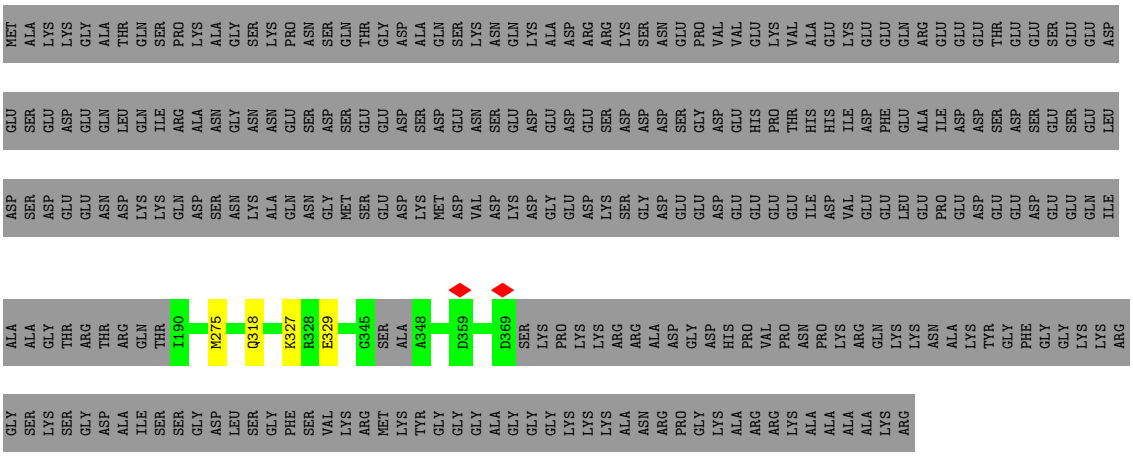
L483 L484 C485 A489 G495 Q496 D497 A498 H499 N500 A501 R502 S503 D504 L505 H506 L507 D508 L509 S510 F511 S519 S522 L523 S524 L525 N526 P527 D528 L529 E530 L531 G532 ALA GLN SER LEU HIS LEU SER ASP PRO ASN ASP THR SER SER GLY SER THR GLU ASN SER ARG ARG N555

N556 K557 I558 N559 L560 Q561 T562 T563 L566 R569 R582 S583 Q602 V603 P604 E605 K606 S607 A610 G613 L614 G623 E634 G639 T640 Y641 K642 E646 T647 V648 E649 G650 T657 E660 G661 E662 L663 L664 H667 F670 K671 E674 G675 A678

E682 S685 I686 PRO SER

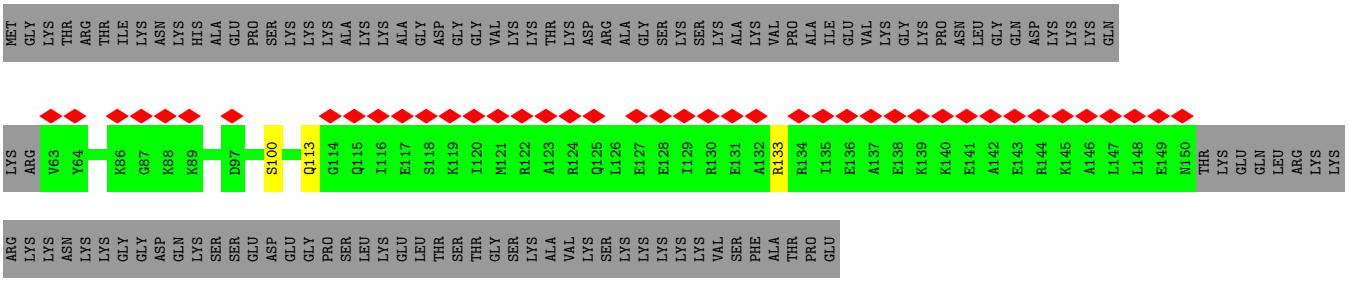
- Molecule 23: rRNA-processing protein EBP2

Chain CU: 39% 61%



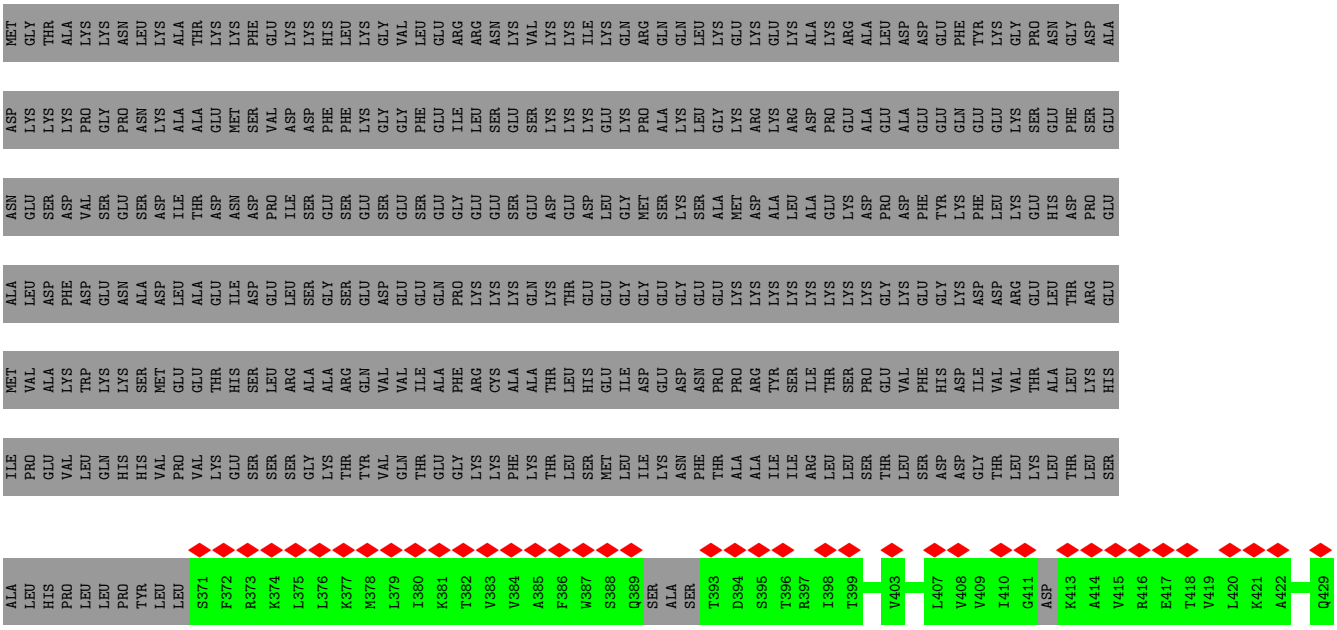
• Molecule 24: 60S ribosomal subunit-like protein

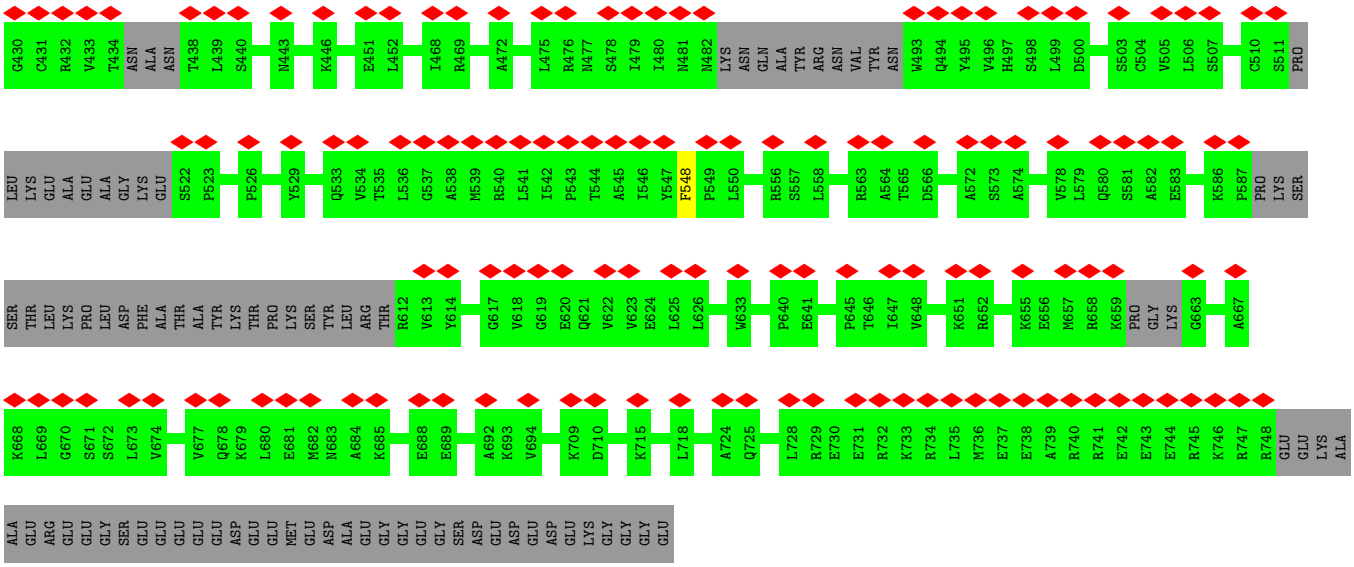
Chain CX:



• Molecule 25: Putative NOC2 family protein

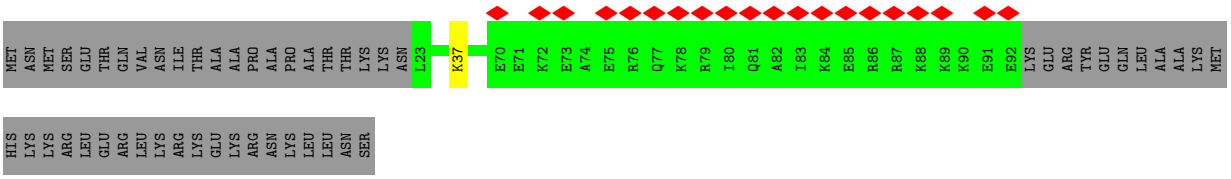
Chain CY:





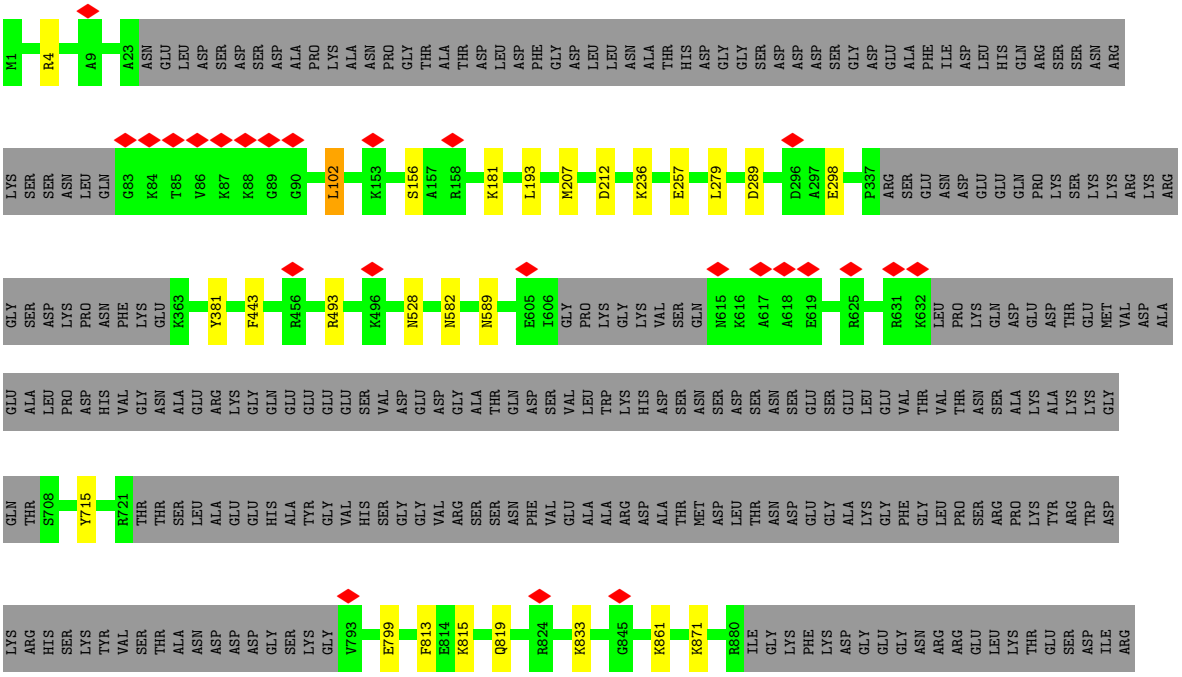
- Molecule 26: rRNA-processing protein

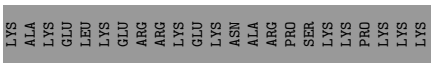
Chain Cz:



- Molecule 27: ATP-dependent RNA helicase DBP10

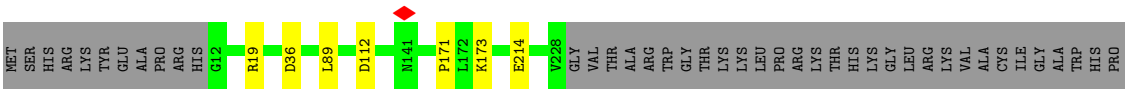
Chain Cb:

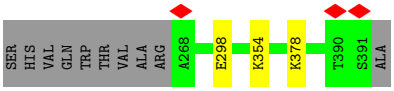




• Molecule 28: 60S ribosomal protein L3-like protein

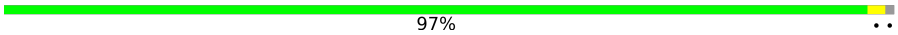
Chain LB:





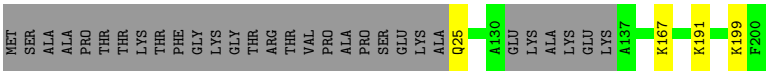
• Molecule 29: 60S ribosomal protein L4-like protein

Chain LC:



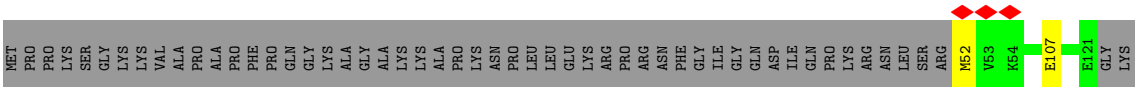
• Molecule 30: 60S ribosomal protein L6

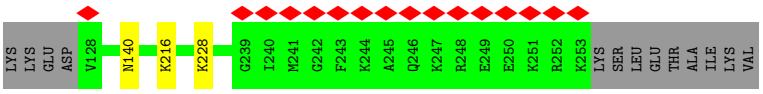
Chain LE:



• Molecule 31: 60S ribosomal protein L8

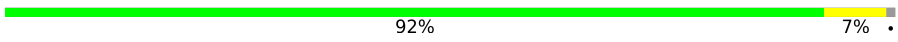
Chain LG:

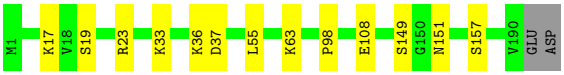




• Molecule 32: 60S ribosomal protein l9-like protein

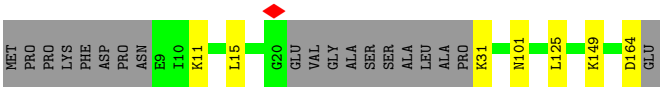
Chain LH:





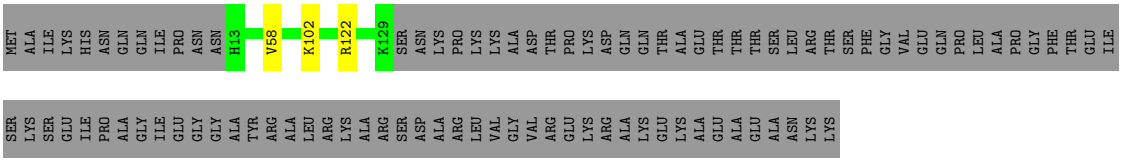
• Molecule 33: 60S ribosomal protein L12-like protein

Chain LK:



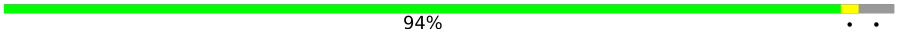
• Molecule 34: 60S ribosomal protein L13

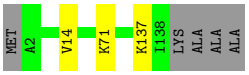
Chain LL:



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

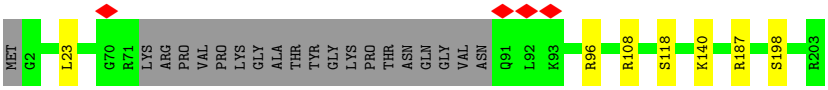
Chain LM:





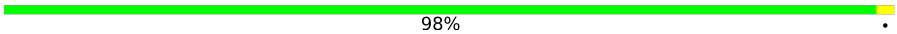
• Molecule 36: Ribosomal protein L15

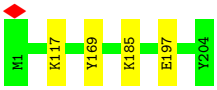
Chain LN:



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

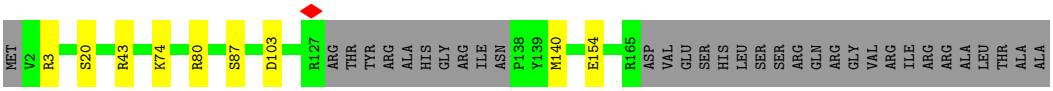
Chain LO:





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

Chain LP:



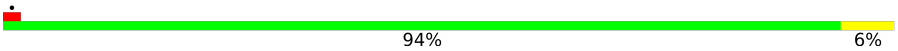
• Molecule 39: Ribosomal protein L18-like protein

Chain LQ:

HIS LYS HIS LYS LYS PRO TYR VAL ARG SER LYS GLY ARG LYS PHE GLU ARG ALA ARG GLY ARG ARG ARG SER ARG GLY PHE LYS VAL

- Molecule 40: 60S ribosomal protein L20

Chain LS:



M1 K50 N62 K71 S83 R84 S85 Y94 S98 R113 E130 K131 S149 S160 S174

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

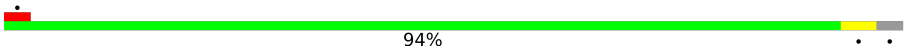
Chain LT:

MET GLY HIS ALA ALA GLY LEU ARG SER GLY THR ARG TYR ALA PHE SER ARG GLY PHE ARG LYS HIS GLY GLN ILE PRO LEU SER THR TYR LEU R32 V44 N45 G46 A47 V48 Q49 K50 G51 M52 P53 H54 K55 F56 Y57 K69 S70 A71 R83 R102 E103 D104 K118

E157 THR THR ILE

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

Chain LV:



MET ALA LYS GLN K5 M15 K42 G45 A46 R47 L48 N49 K68 K88 M139

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

Chain LX:

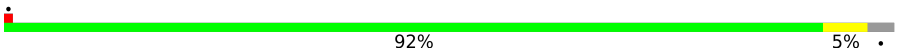
MET ALA PRO LYS ASP VAL LYS LYS GLY GLY ALA S12 K13 A14 A15 K16 G17 A18 K21 Q25 L28 K29 G30 V31 H32 S33 HIS LYS LYS THR LYS VAL ARG LYS SER THR THR PHE HIS ARG PRO LYS THR LEU VAL LEU SER ARG ALA PRO LYS TYR PRO ARG LYS SER ILE

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

THR LEU ILE ARG PRO ASP GLY THR LYS LYS ALA PHE ALA ARG LEU THR PRO ASP VAL ASP ALA LEU ASP ILE ALA ALA THR LYS LEU GLY LEU VAL

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

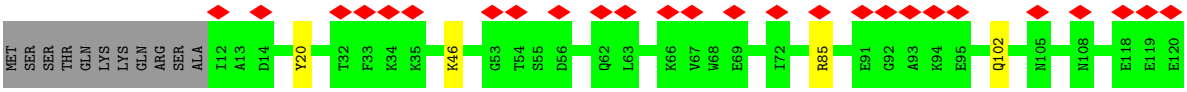
Chain LY:



M1 S8 Y73 K76 Y77 V78 R86 K122 G133 K134 LYS THR ALA ALA

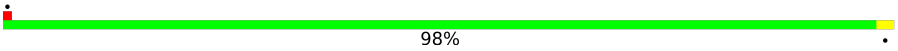
- Molecule 45: Putative 60S ribosomal protein

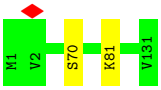
Chain Ld:



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

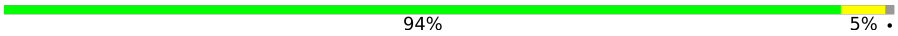
Chain Le:

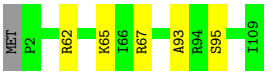




• Molecule 47: 60S ribosomal protein l33-like protein

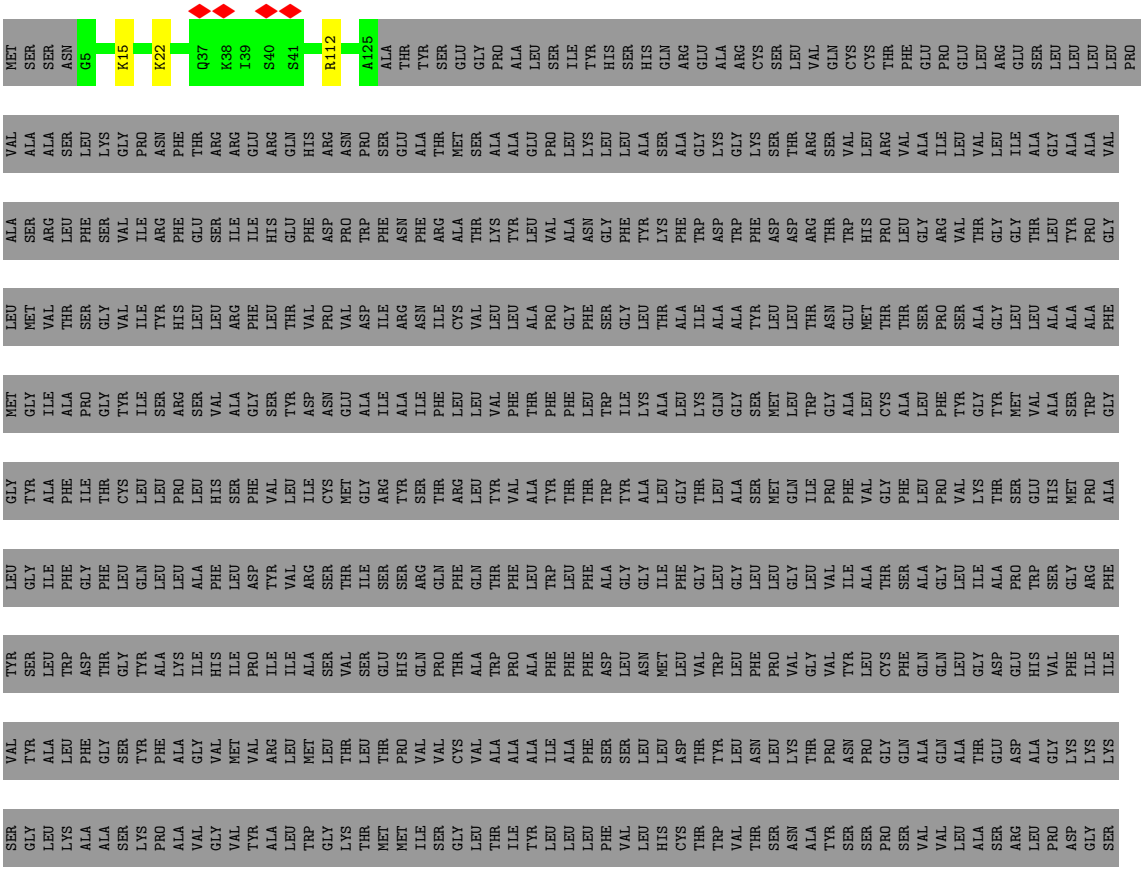
Chain Lf:





• Molecule 48: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:



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

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

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

THR SER GLU ASN TRP ILE ILE ARG ILE TYR LYS VAL LYS ASP LEU ASP ASN LEU GLY ARG ASP HIS ALA SER ALA ALA ALA PHE GLU ARG GLY HIS LYS LYS LYS LYS ALA THR LYS LYS ARG GLY PRO ARG VAL LEU ARG VAL GLU

- Molecule 49: 60S ribosomal protein L36

Chain Li:

MET SER GLU ASP ALA THR PRO LYS ALA PRO VAL GLU ARG THR GLY LEU ILE ARG GLY LEU ASN LYS G23 H24 K25 G40 A41 Y62 K83 R94 H110

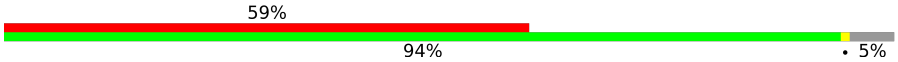
- Molecule 50: Ribosomal protein L37

Chain Lj:

MET THR LYS GLY THR SER SER PHE GLY LYS ARG HIS ASN K14 S26 S36 K52 S68 R87 GLY PRO ALA VAL SER THR SER SER

- Molecule 51: Ribosomal protein

Chain Lq:



MET SER LYS I4 T5 V6 A7 N12 L16 L17 D18 K24 K25 L29 E30 E33 L34 Q35 I36 G37 L38 K39 N40 Y41 Q44 R45 D46 K47 R48 F49 S50 G51 T52 V53 K54 L55 P56 T57 P61 N62 M63 S64 L68 G69 D70 Q71 H72 D73 I74 D75 R76 A77

K78 H79 G80 G81 I82 D83 A84 M85 S86 A87 D88 D89 L90 K91 K92 K95 N96 L99 I100 L103 K106 Y107 F110 S113 E114 S115 L116 I117 K118 Q119 I120 P121 R122 L123 P126 G127 L128 S129 K133 F134 P135 S139 H140 S141 D142 D143 L144 S145 A146 K147 V148

V151 K152 S153 T154 V155 K156 F157 Q158 L159 K160 K161 V162 L163 C164 M165 G166 V167 A168 N171 V172 G173 M174 T175 Q176 E177 Q178 L179 V180 A181 M184 L185 A186 I187 N188 Y189 L190 V191 S192 L193 L194 K195 K196 G197 W198 G202 S203 L204 T205 I206 M210 SER PRO PRO PRO LYS ARG

LEU TYR

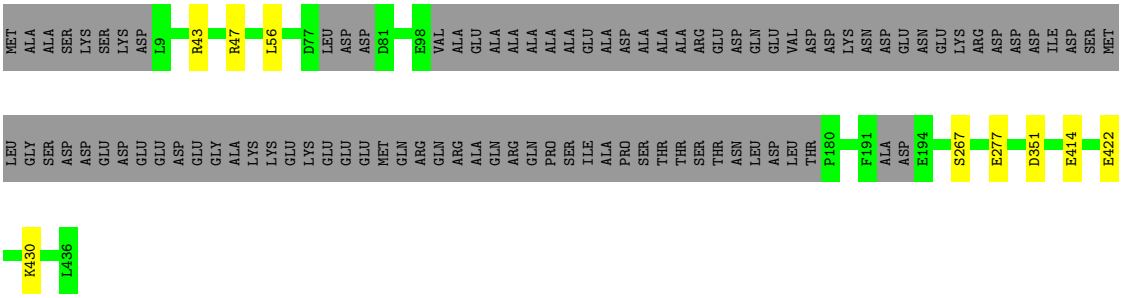
- Molecule 52: Ribosomal RNA-processing protein 1

Chain Cc:

MET THR SER GLN E5 K20 V38 A39 S40 K129 ASP GLY SER LEU GLY LYS ARG THR HIS ASP GLY GLN GLU LYS ALA VAL LYS THR G148 D151 Q177 S178 S179 E180 K181 E204 D230 D247 R258 ARG PRO ASN SER SER GLN ASP HIS ASP THR LYS ASP

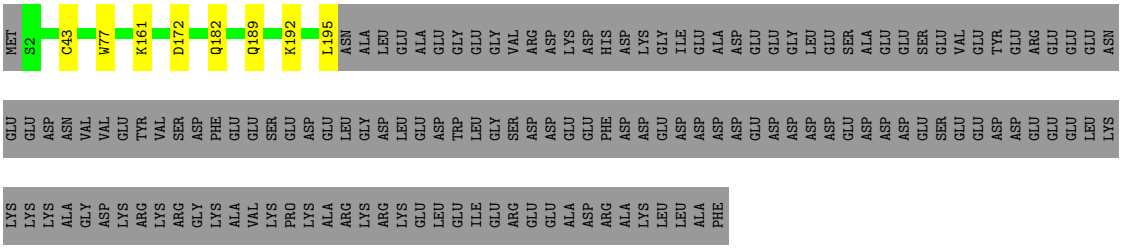
• Molecule 53: Brix domain-containing protein

Chain Cd:



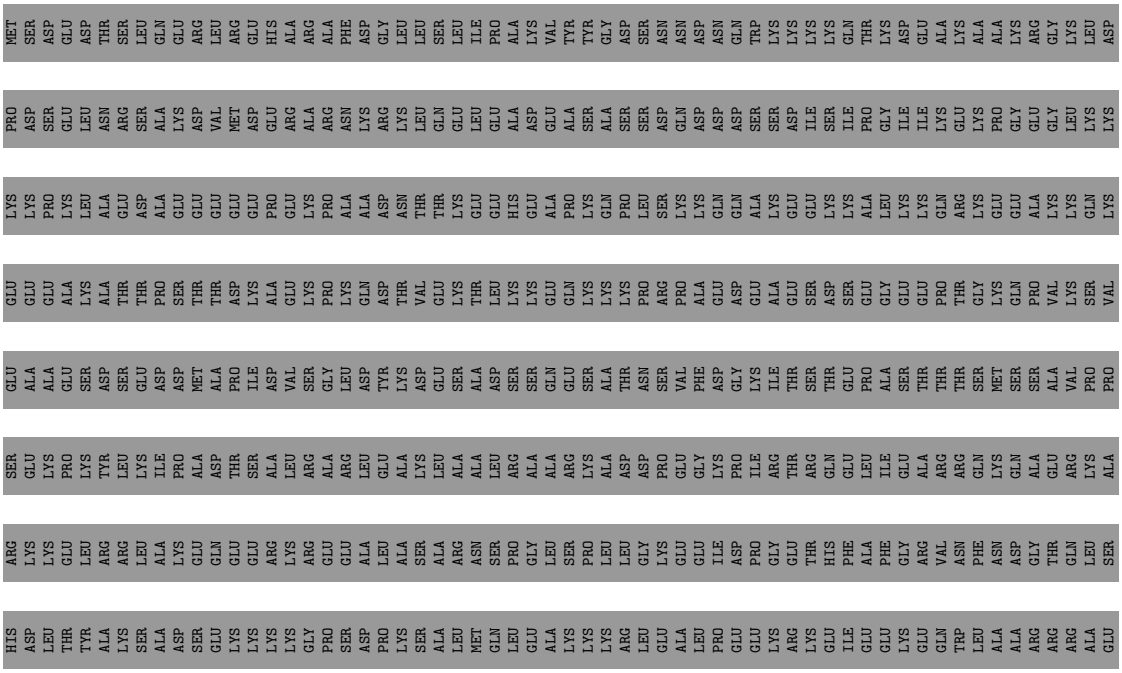
• Molecule 54: Protein MAK16

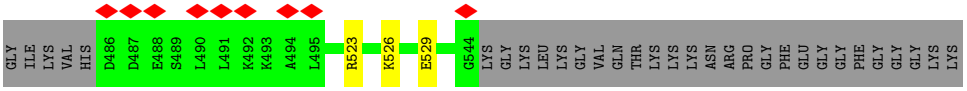
Chain Ce:



• Molecule 55: 60S ribosome biogenesis protein Rrp14

Chain Cf:




GLY
ILE
LYS
VAL
HIS
D486
D487
E488
S489
L490
L491
K492
K493
A494
L495
R523
K526
E529
G544
LYS
GLY
LYS
LEU
LYS
GLY
VAL
GLN
THR
LYS
LYS
LYS
ASN
ARG
PRO
GLY
PHE
GLU
GLY
GLY
PHE
GLY
GLY
GLY
LYS
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16465	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	0.458	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.010	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: 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	0.43	0/51490	1.00	169/80245 (0.2%)
2	C2	0.39	0/3754	0.90	1/5846 (0.0%)
3	C3	0.39	0/2342	1.07	11/3649 (0.3%)
4	CA	0.30	0/2190	0.61	1/2940 (0.0%)
5	CB	0.36	0/2109	0.72	3/2866 (0.1%)
6	CC	0.29	0/2459	0.56	0/3350
7	CE	0.31	0/3743	0.64	5/5045 (0.1%)
8	CF	0.30	0/1982	0.65	0/2671
9	CG	0.32	0/1422	0.70	2/1920 (0.1%)
10	CH	0.35	0/3927	0.70	7/5307 (0.1%)
11	CI	0.33	0/1225	0.68	1/1645 (0.1%)
12	CJ	0.27	0/3189	0.53	0/4309
13	CK	0.30	0/1885	0.64	2/2529 (0.1%)
14	CL	0.26	0/2178	0.48	0/2983
15	CM	0.32	0/1555	0.67	2/2091 (0.1%)
15	LF	0.29	0/2004	0.56	0/2686
16	CN	0.29	0/1881	0.64	1/2560 (0.0%)
17	CO	0.29	0/470	0.55	0/619
18	CP	0.33	0/2594	0.68	4/3514 (0.1%)
19	CQ	0.32	0/981	0.70	1/1301 (0.1%)
20	CR	0.29	0/1369	0.64	1/1828 (0.1%)
21	CS	0.26	0/1762	0.45	0/2417
22	CT	0.28	0/2264	0.47	0/3149
23	CU	0.33	0/1428	0.66	1/1910 (0.1%)
24	CX	0.27	0/705	0.57	0/938
25	CY	0.31	0/1600	0.47	0/2220
26	Cz	0.29	0/598	0.56	0/785
27	Cb	0.32	0/5150	0.68	4/6936 (0.1%)
28	LB	0.33	0/2760	0.65	2/3701 (0.1%)
29	LC	0.32	0/2809	0.57	0/3787
30	LE	0.30	0/1363	0.55	0/1833
31	LG	0.32	0/1606	0.57	0/2149

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	LH	0.29	0/1516	0.58	1/2038 (0.0%)
33	LK	0.30	0/1124	0.70	2/1507 (0.1%)
34	LL	0.34	0/983	0.65	0/1318
35	LM	0.29	0/1120	0.57	0/1507
36	LN	0.30	0/1595	0.62	0/2132
37	LO	0.31	0/1652	0.56	0/2215
38	LP	0.31	0/1231	0.61	0/1658
39	LQ	0.30	0/1033	0.63	0/1391
40	LS	0.31	0/1468	0.61	0/1975
41	LT	0.28	0/1033	0.68	1/1389 (0.1%)
42	LV	0.32	0/1013	0.57	0/1361
43	LX	0.24	0/148	0.35	0/194
44	LY	0.29	0/1079	0.61	0/1443
45	Ld	0.26	0/904	0.61	0/1209
46	Le	0.29	0/1073	0.56	0/1431
47	Lf	0.33	0/883	0.63	0/1187
48	Lh	0.28	0/1006	0.59	0/1338
49	Li	0.30	0/738	0.64	0/971
50	Lj	0.32	0/606	0.65	0/803
51	Lq	0.25	0/1621	0.55	0/2180
52	Cc	0.31	0/1934	0.57	0/2614
53	Cd	0.31	0/2818	0.61	0/3786
54	Ce	0.30	0/1638	0.56	0/2196
55	Cf	0.27	0/514	0.57	0/669
All	All	0.36	0/145524	0.80	222/208241 (0.1%)

There are no bond length outliers.

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	1050	C	N3-C2-O2	-11.53	113.83	121.90
1	C1	136	C	N3-C2-O2	-10.12	114.82	121.90
1	C1	2852	C	N3-C2-O2	-10.01	114.89	121.90
1	C1	939	C	N3-C2-O2	-9.73	115.09	121.90
28	LB	171	PRO	CA-N-CD	-9.15	98.69	111.50
1	C1	1190	C	N1-C2-O2	8.92	124.25	118.90
1	C1	2723	C	N3-C2-O2	-8.72	115.79	121.90
10	CH	451	ASP	CB-CG-OD2	8.60	126.03	118.30
1	C1	3320	C	C6-N1-C2	-8.46	116.92	120.30
1	C1	1050	C	N1-C2-O2	8.45	123.97	118.90
1	C1	2300	C	N3-C2-O2	-8.42	116.01	121.90
28	LB	36	ASP	CB-CG-OD1	8.34	125.80	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	3290	C	N3-C2-O2	-8.19	116.17	121.90
1	C1	2438	C	C6-N1-C2	-8.18	117.03	120.30
1	C1	36	C	N1-C2-O2	8.07	123.74	118.90
1	C1	136	C	N1-C2-O2	7.98	123.69	118.90
18	CP	476	ASP	CB-CG-OD1	7.95	125.45	118.30
1	C1	3114	C	N3-C2-O2	-7.84	116.41	121.90
1	C1	1050	C	C6-N1-C2	-7.84	117.17	120.30
1	C1	1190	C	N3-C2-O2	-7.78	116.45	121.90
3	C3	70	C	C5-C6-N1	7.72	124.86	121.00
1	C1	2406	C	C5-C6-N1	7.71	124.85	121.00
10	CH	195	PRO	CA-N-CD	-7.70	100.72	111.50
10	CH	375	ASP	CB-CG-OD1	7.70	125.23	118.30
10	CH	228	LEU	CA-CB-CG	7.67	132.95	115.30
1	C1	2406	C	C2-N1-C1'	7.61	127.17	118.80
1	C1	249	C	N1-C2-O2	7.60	123.46	118.90
1	C1	1051	C	N3-C2-O2	-7.59	116.59	121.90
1	C1	249	C	N3-C2-O2	-7.56	116.61	121.90
18	CP	568	PRO	CA-N-CD	-7.46	101.06	111.50
1	C1	2852	C	C6-N1-C2	-7.44	117.32	120.30
1	C1	2417	U	C2-N1-C1'	7.43	126.61	117.70
1	C1	635	C	N1-C2-O2	7.35	123.31	118.90
1	C1	3320	C	N3-C2-O2	-7.27	116.81	121.90
1	C1	2300	C	C6-N1-C2	-7.26	117.40	120.30
1	C1	739	C	C2-N1-C1'	7.17	126.69	118.80
1	C1	3088	U	C2-N1-C1'	7.15	126.28	117.70
1	C1	1190	C	C2-N1-C1'	7.14	126.66	118.80
1	C1	1406	C	N3-C2-O2	-7.05	116.96	121.90
1	C1	2866	G	N3-C2-N2	-6.95	115.03	119.90
10	CH	219	ASP	CB-CG-OD2	6.92	124.53	118.30
1	C1	2406	C	C6-N1-C2	-6.83	117.57	120.30
3	C3	34	C	N3-C2-O2	-6.80	117.14	121.90
7	CE	264	ASP	CB-CG-OD1	6.73	124.36	118.30
1	C1	3113	C	N1-C2-O2	6.72	122.93	118.90
1	C1	433	U	C2-N1-C1'	6.71	125.75	117.70
1	C1	2406	C	N1-C2-O2	6.71	122.92	118.90
1	C1	127	G	N3-C4-N9	6.64	129.98	126.00
1	C1	1049	C	N1-C2-O2	6.62	122.87	118.90
27	Cb	102	LEU	CA-CB-CG	6.54	130.35	115.30
1	C1	2818	U	N1-C2-O2	6.46	127.32	122.80
1	C1	1098	G	C4-N9-C1'	6.45	134.88	126.50
1	C1	1049	C	N3-C2-O2	-6.44	117.39	121.90
1	C1	136	C	C6-N1-C2	-6.43	117.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	3319	C	N1-C2-O2	6.42	122.75	118.90
1	C1	1406	C	C6-N1-C2	-6.40	117.74	120.30
3	C3	70	C	C6-N1-C2	-6.37	117.75	120.30
1	C1	2929	A	P-O3'-C3'	6.37	127.34	119.70
9	CG	107	PRO	CA-N-CD	-6.36	102.59	111.50
1	C1	2818	U	N3-C2-O2	-6.36	117.75	122.20
1	C1	3290	C	N1-C2-O2	6.35	122.71	118.90
1	C1	722	C	C2-N1-C1'	6.34	125.77	118.80
1	C1	3113	C	C2-N1-C1'	6.33	125.76	118.80
1	C1	2731	C	N1-C2-O2	6.30	122.68	118.90
1	C1	113	C	C2-N1-C1'	6.29	125.72	118.80
1	C1	463	C	C2-N1-C1'	6.29	125.72	118.80
1	C1	473	C	C2-N1-C1'	6.25	125.68	118.80
32	LH	37	ASP	CB-CG-OD1	6.24	123.92	118.30
1	C1	1051	C	C6-N1-C2	-6.23	117.81	120.30
5	CB	232	LEU	CA-CB-CG	6.22	129.61	115.30
27	Cb	289	ASP	CB-CG-OD1	6.18	123.86	118.30
1	C1	2991	C	N1-C2-O2	6.15	122.59	118.90
1	C1	2866	G	N9-C4-C5	6.11	107.84	105.40
1	C1	2417	U	N1-C2-O2	6.11	127.07	122.80
1	C1	2417	U	N3-C2-O2	-6.09	117.94	122.20
1	C1	635	C	C2-N1-C1'	6.07	125.48	118.80
16	CN	42	LEU	CA-CB-CG	6.07	129.25	115.30
1	C1	167	C	C2-N1-C1'	6.04	125.45	118.80
23	CU	275	MET	CB-CG-SD	6.03	130.50	112.40
10	CH	298	ASP	CB-CG-OD2	6.02	123.72	118.30
1	C1	398	G	O4'-C1'-N9	6.02	113.01	108.20
3	C3	12	C	C2-N1-C1'	5.99	125.39	118.80
1	C1	83	C	C6-N1-C1'	5.97	127.97	120.80
1	C1	1271	G	O4'-C1'-N9	5.97	112.97	108.20
1	C1	83	C	N3-C2-O2	-5.94	117.75	121.90
1	C1	1265	C	N1-C2-O2	5.94	122.46	118.90
18	CP	287	LEU	CA-CB-CG	5.94	128.95	115.30
1	C1	939	C	C6-N1-C2	-5.85	117.96	120.30
1	C1	433	U	N1-C2-O2	5.84	126.89	122.80
1	C1	83	C	C2-N1-C1'	-5.83	112.38	118.80
1	C1	1265	C	N3-C2-O2	-5.83	117.82	121.90
1	C1	2438	C	N3-C2-O2	-5.82	117.83	121.90
3	C3	70	C	C2-N1-C1'	5.82	125.20	118.80
1	C1	2857	C	C2-N1-C1'	5.81	125.19	118.80
1	C1	635	C	N3-C2-O2	-5.80	117.84	121.90
1	C1	36	C	N3-C2-O2	-5.80	117.84	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	2287	G	C4-C5-N7	5.80	113.12	110.80
1	C1	3229	G	N3-C4-N9	5.77	129.46	126.00
1	C1	243	G	C4-N9-C1'	5.75	133.98	126.50
1	C1	2287	G	N9-C4-C5	-5.75	103.10	105.40
7	CE	427	ASP	CB-CG-OD1	5.75	123.48	118.30
1	C1	1071	G	N1-C2-N2	-5.75	111.02	116.20
1	C1	1072	G	N1-C2-N2	-5.75	111.03	116.20
1	C1	1072	G	N1-C6-O6	-5.75	116.45	119.90
5	CB	156	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C1	2287	G	C6-C5-N7	-5.72	126.97	130.40
1	C1	3108	U	N1-C2-O2	5.71	126.80	122.80
27	Cb	207	MET	CB-CG-SD	5.70	129.50	112.40
10	CH	263	LEU	CA-CB-CG	5.68	128.37	115.30
1	C1	1350	U	N1-C2-O2	5.67	126.77	122.80
1	C1	939	C	N1-C2-N3	5.67	123.17	119.20
1	C1	1071	G	N3-C2-N2	5.63	123.84	119.90
1	C1	2287	G	C8-N9-C1'	-5.61	119.71	127.00
1	C1	3108	U	N3-C2-O2	-5.61	118.27	122.20
1	C1	1098	G	C8-N9-C1'	-5.59	119.73	127.00
3	C3	70	C	N1-C2-O2	5.59	122.25	118.90
1	C1	3319	C	C2-N1-C1'	5.58	124.94	118.80
1	C1	83	C	N3-C4-N4	-5.58	114.09	118.00
3	C3	13	C	N3-C2-O2	-5.57	118.00	121.90
1	C1	1239	C	C6-N1-C2	-5.56	118.08	120.30
1	C1	243	G	N3-C4-N9	5.54	129.32	126.00
1	C1	2287	G	C4-N9-C1'	5.54	133.70	126.50
1	C1	2340	C	C2-N1-C1'	5.54	124.89	118.80
1	C1	2866	G	N3-C4-N9	-5.53	122.68	126.00
7	CE	380	ILE	CG1-CB-CG2	-5.53	99.23	111.40
1	C1	944	G	N1-C6-O6	-5.53	116.58	119.90
1	C1	2731	C	C2-N1-C1'	5.51	124.87	118.80
1	C1	1405	C	N1-C2-O2	5.51	122.21	118.90
1	C1	150	G	P-O3'-C3'	5.51	126.31	119.70
1	C1	3309	G	N3-C4-C5	-5.49	125.86	128.60
20	CR	205	ASP	CB-CG-OD1	5.47	123.22	118.30
1	C1	127	G	N9-C4-C5	-5.46	103.22	105.40
1	C1	2474	C	N3-C2-O2	-5.46	118.08	121.90
1	C1	3320	C	N1-C2-N3	5.46	123.02	119.20
1	C1	127	G	C8-N9-C1'	-5.45	119.92	127.00
1	C1	83	C	C5-C4-N4	5.43	124.00	120.20
2	C2	156	U	C2-N1-C1'	5.43	124.21	117.70
3	C3	134	C	N3-C2-O2	-5.40	118.12	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C1	3324	U	C2-N1-C1'	5.39	124.17	117.70
3	C3	34	C	C6-N1-C1'	5.39	127.27	120.80
1	C1	2893	U	N3-C2-O2	-5.39	118.43	122.20
1	C1	3296	G	N1-C2-N2	-5.38	111.36	116.20
1	C1	27	C	N3-C2-O2	-5.38	118.14	121.90
13	CK	120	PRO	CA-N-CD	-5.37	103.99	111.50
1	C1	105	C	C2-N1-C1'	5.36	124.70	118.80
1	C1	133	G	N3-C4-C5	-5.36	125.92	128.60
5	CB	215	ARG	CA-CB-CG	5.36	125.19	113.40
1	C1	3233	C	N1-C2-O2	5.35	122.11	118.90
1	C1	2299	C	N1-C2-O2	5.34	122.10	118.90
1	C1	3162	A	P-O3'-C3'	5.33	126.09	119.70
27	Cb	279	LEU	CA-CB-CG	5.33	127.55	115.30
1	C1	2723	C	C6-N1-C2	-5.32	118.17	120.30
1	C1	2460	C	C2-N1-C1'	5.32	124.65	118.80
1	C1	27	C	N1-C2-O2	5.32	122.09	118.90
15	CM	132	MET	CG-SD-CE	5.32	108.71	100.20
3	C3	134	C	N1-C2-O2	5.31	122.09	118.90
1	C1	2991	C	N3-C2-O2	-5.31	118.19	121.90
1	C1	3114	C	C6-N1-C2	-5.31	118.18	120.30
1	C1	176	U	N1-C2-O2	5.30	126.51	122.80
1	C1	2915	G	C4-N9-C1'	5.30	133.39	126.50
1	C1	1190	C	C6-N1-C2	-5.29	118.18	120.30
19	CQ	102	ARG	CG-CD-NE	5.29	122.92	111.80
1	C1	2752	G	C5-C6-O6	5.29	131.78	128.60
1	C1	3289	C	N1-C2-O2	5.28	122.06	118.90
1	C1	162	U	N3-C2-O2	-5.27	118.51	122.20
1	C1	2922	G	C4-N9-C1'	5.27	133.36	126.50
1	C1	243	G	N3-C4-C5	-5.27	125.96	128.60
1	C1	175	C	C2-N1-C1'	5.26	124.59	118.80
1	C1	3156	C	C2-N1-C1'	5.26	124.59	118.80
1	C1	3158	U	C2-N1-C1'	5.26	124.02	117.70
1	C1	2866	G	C5-C6-O6	5.25	131.75	128.60
1	C1	1406	C	N1-C2-N3	5.25	122.88	119.20
1	C1	2915	G	N3-C4-C5	-5.24	125.98	128.60
4	CA	314	LEU	CA-CB-CG	5.24	127.36	115.30
1	C1	2893	U	N1-C2-O2	5.24	126.47	122.80
1	C1	3088	U	N1-C2-O2	5.24	126.47	122.80
1	C1	2287	G	N3-C4-N9	5.23	129.14	126.00
9	CG	20	MET	CB-CG-SD	5.21	128.04	112.40
1	C1	3296	G	P-O3'-C3'	5.21	125.95	119.70
1	C1	2874	U	C5-C6-N1	5.20	125.30	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	CE	173	LEU	CA-CB-CG	5.19	127.24	115.30
1	C1	1172	A	C4-N9-C1'	5.19	135.63	126.30
1	C1	3309	G	N3-C4-N9	5.19	129.11	126.00
1	C1	78	U	N3-C2-O2	-5.18	118.57	122.20
1	C1	135	C	N1-C2-O2	5.18	122.01	118.90
1	C1	3239	C	C2-N1-C1'	5.17	124.49	118.80
1	C1	1046	A	P-O3'-C3'	5.17	125.90	119.70
1	C1	2866	G	N1-C6-O6	-5.16	116.80	119.90
1	C1	421	U	C2-N1-C1'	5.16	123.89	117.70
1	C1	2722	C	N1-C2-O2	5.16	121.99	118.90
1	C1	2731	C	C6-N1-C2	-5.14	118.24	120.30
1	C1	1051	C	N1-C2-O2	5.14	121.98	118.90
33	LK	15	LEU	CA-CB-CG	5.13	127.09	115.30
1	C1	103	G	C5-C6-O6	5.11	131.67	128.60
1	C1	1239	C	C5-C6-N1	5.11	123.56	121.00
1	C1	127	G	C4-N9-C1'	5.11	133.14	126.50
13	CK	260	LEU	CB-CG-CD2	5.09	119.66	111.00
1	C1	2469	U	C2-N1-C1'	5.09	123.81	117.70
3	C3	13	C	N1-C2-O2	5.09	121.95	118.90
1	C1	2731	C	N3-C2-O2	-5.08	118.34	121.90
1	C1	2417	U	O4'-C1'-N1	5.08	112.27	108.20
1	C1	1311	C	O4'-C1'-N1	5.08	112.27	108.20
11	CI	200	GLU	CA-CB-CG	5.08	124.58	113.40
18	CP	528	LEU	CA-CB-CG	5.08	126.98	115.30
1	C1	2090	C	C5-C6-N1	5.07	123.54	121.00
41	LT	104	ASP	CB-CG-OD2	5.07	122.87	118.30
1	C1	3229	G	C8-N9-C1'	-5.07	120.41	127.00
1	C1	421	U	N3-C2-O2	-5.06	118.66	122.20
7	CE	133	LYS	CA-CB-CG	5.06	124.54	113.40
1	C1	133	G	C2-N3-C4	5.05	114.43	111.90
1	C1	1058	C	N1-C2-O2	5.05	121.93	118.90
1	C1	3113	C	C5-C6-N1	5.05	123.52	121.00
1	C1	3262	G	O4'-C1'-N9	5.04	112.23	108.20
1	C1	3229	G	C4-N9-C1'	5.04	133.05	126.50
33	LK	125	LEU	CA-CB-CG	5.04	126.89	115.30
1	C1	3073	G	N1-C6-O6	-5.03	116.88	119.90
1	C1	2406	C	C2-N3-C4	5.03	122.41	119.90
15	CM	132	MET	CA-CB-CG	5.01	121.82	113.30
1	C1	2818	U	C2-N1-C1'	5.01	123.71	117.70
1	C1	517	C	C2-N1-C1'	5.00	124.30	118.80
1	C1	2451	C	C2-N1-C1'	5.00	124.31	118.80
1	C1	179	U	N3-C2-O2	-5.00	118.70	122.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CA	254/316 (80%)	234 (92%)	19 (8%)	1 (0%)	34	69
5	CB	256/391 (66%)	244 (95%)	10 (4%)	2 (1%)	19	54
6	CC	283/801 (35%)	272 (96%)	11 (4%)	0	100	100
7	CE	459/598 (77%)	445 (97%)	13 (3%)	1 (0%)	47	79
8	CF	243/270 (90%)	234 (96%)	9 (4%)	0	100	100
9	CG	175/184 (95%)	167 (95%)	8 (5%)	0	100	100
10	CH	474/661 (72%)	456 (96%)	18 (4%)	0	100	100
11	CI	144/414 (35%)	136 (94%)	8 (6%)	0	100	100
12	CJ	374/679 (55%)	365 (98%)	9 (2%)	0	100	100
13	CK	226/261 (87%)	216 (96%)	10 (4%)	0	100	100
14	CL	384/558 (69%)	357 (93%)	22 (6%)	5 (1%)	12	42
15	CM	183/249 (74%)	175 (96%)	8 (4%)	0	100	100
15	LF	238/249 (96%)	228 (96%)	9 (4%)	1 (0%)	34	69
16	CN	244/246 (99%)	236 (97%)	8 (3%)	0	100	100
17	CO	56/120 (47%)	56 (100%)	0	0	100	100
18	CP	322/751 (43%)	307 (95%)	15 (5%)	0	100	100
19	CQ	110/225 (49%)	106 (96%)	4 (4%)	0	100	100
20	CR	159/237 (67%)	155 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	CS	294/834 (35%)	286 (97%)	6 (2%)	2 (1%)	22	57
22	CT	448/688 (65%)	425 (95%)	21 (5%)	2 (0%)	34	69
23	CU	174/451 (39%)	166 (95%)	8 (5%)	0	100	100
24	CX	86/203 (42%)	82 (95%)	4 (5%)	0	100	100
25	CY	308/788 (39%)	292 (95%)	15 (5%)	1 (0%)	41	73
26	Cz	68/123 (55%)	67 (98%)	1 (2%)	0	100	100
27	Cb	630/924 (68%)	597 (95%)	33 (5%)	0	100	100
28	LB	337/392 (86%)	320 (95%)	17 (5%)	0	100	100
29	LC	360/365 (99%)	348 (97%)	12 (3%)	0	100	100
30	LE	166/200 (83%)	160 (96%)	6 (4%)	0	100	100
31	LG	192/262 (73%)	188 (98%)	4 (2%)	0	100	100
32	LH	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
33	LK	142/165 (86%)	132 (93%)	10 (7%)	0	100	100
34	LL	115/213 (54%)	109 (95%)	6 (5%)	0	100	100
35	LM	135/142 (95%)	131 (97%)	4 (3%)	0	100	100
36	LN	179/203 (88%)	174 (97%)	5 (3%)	0	100	100
37	LO	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
38	LP	150/187 (80%)	149 (99%)	1 (1%)	0	100	100
39	LQ	127/213 (60%)	123 (97%)	4 (3%)	0	100	100
40	LS	172/174 (99%)	166 (96%)	6 (4%)	0	100	100
41	LT	124/160 (78%)	117 (94%)	6 (5%)	1 (1%)	19	54
42	LV	133/139 (96%)	131 (98%)	2 (2%)	0	100	100
43	LX	20/156 (13%)	20 (100%)	0	0	100	100
44	LY	132/138 (96%)	130 (98%)	2 (2%)	0	100	100
45	Ld	107/120 (89%)	102 (95%)	5 (5%)	0	100	100
46	Le	129/131 (98%)	126 (98%)	3 (2%)	0	100	100
47	Lf	106/109 (97%)	102 (96%)	3 (3%)	1 (1%)	17	52
48	Lh	119/935 (13%)	117 (98%)	2 (2%)	0	100	100
49	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
50	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
51	Lq	205/217 (94%)	186 (91%)	19 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	Cc	232/282 (82%)	226 (97%)	6 (3%)	0	100	100
53	Cd	334/436 (77%)	323 (97%)	11 (3%)	0	100	100
54	Ce	192/336 (57%)	185 (96%)	7 (4%)	0	100	100
55	Cf	57/570 (10%)	57 (100%)	0	0	100	100
All	All	11105/18067 (62%)	10656 (96%)	432 (4%)	17 (0%)	50	79

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CA	236	PRO
5	CB	103	ASP
14	CL	414	VAL
21	CS	67	MET
22	CT	254	PRO
25	CY	548	PHE
14	CL	446	ASP
15	LF	12	ILE
47	Lf	93	ALA
14	CL	42	ASN
14	CL	278	ASN
14	CL	439	ASP
5	CB	89	LEU
7	CE	452	ASN
41	LT	44	VAL
21	CS	68	PRO
22	CT	237	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	
4	CA	231/276 (84%)	218 (94%)	13 (6%)	21	52
5	CB	222/329 (68%)	202 (91%)	20 (9%)	9	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	CC	266/710 (38%)	252 (95%)	14 (5%)	22	54
7	CE	398/517 (77%)	376 (94%)	22 (6%)	21	53
8	CF	214/236 (91%)	202 (94%)	12 (6%)	21	52
9	CG	150/155 (97%)	143 (95%)	7 (5%)	26	59
10	CH	424/575 (74%)	405 (96%)	19 (4%)	27	60
11	CI	121/336 (36%)	116 (96%)	5 (4%)	30	64
12	CJ	332/579 (57%)	324 (98%)	8 (2%)	49	76
13	CK	198/225 (88%)	188 (95%)	10 (5%)	24	56
14	CL	65/458 (14%)	62 (95%)	3 (5%)	27	59
15	CM	161/215 (75%)	153 (95%)	8 (5%)	24	57
15	LF	206/215 (96%)	200 (97%)	6 (3%)	42	72
16	CN	206/206 (100%)	199 (97%)	7 (3%)	37	69
17	CO	48/99 (48%)	47 (98%)	1 (2%)	53	79
18	CP	273/632 (43%)	251 (92%)	22 (8%)	11	39
19	CQ	100/192 (52%)	93 (93%)	7 (7%)	15	45
20	CR	144/206 (70%)	137 (95%)	7 (5%)	25	57
21	CS	73/716 (10%)	72 (99%)	1 (1%)	67	86
23	CU	149/376 (40%)	146 (98%)	3 (2%)	55	80
24	CX	76/172 (44%)	73 (96%)	3 (4%)	32	65
26	Cz	60/107 (56%)	59 (98%)	1 (2%)	60	83
27	Cb	540/779 (69%)	517 (96%)	23 (4%)	29	62
28	LB	290/331 (88%)	282 (97%)	8 (3%)	43	73
29	LC	283/285 (99%)	275 (97%)	8 (3%)	43	73
30	LE	143/166 (86%)	139 (97%)	4 (3%)	43	73
31	LG	168/222 (76%)	163 (97%)	5 (3%)	41	71
32	LH	167/169 (99%)	155 (93%)	12 (7%)	14	44
33	LK	121/136 (89%)	116 (96%)	5 (4%)	30	64
34	LL	99/176 (56%)	96 (97%)	3 (3%)	41	71
35	LM	115/117 (98%)	112 (97%)	3 (3%)	46	74
36	LN	164/180 (91%)	157 (96%)	7 (4%)	29	62
37	LO	163/163 (100%)	159 (98%)	4 (2%)	47	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	LP	125/152 (82%)	116 (93%)	9 (7%)	14	44
39	LQ	110/178 (62%)	109 (99%)	1 (1%)	78	91
40	LS	154/154 (100%)	144 (94%)	10 (6%)	17	47
41	LT	109/135 (81%)	107 (98%)	2 (2%)	59	82
42	LV	99/102 (97%)	94 (95%)	5 (5%)	24	56
43	LX	12/129 (9%)	12 (100%)	0	100	100
44	LY	117/119 (98%)	110 (94%)	7 (6%)	19	49
45	Ld	95/105 (90%)	91 (96%)	4 (4%)	30	62
46	Le	114/114 (100%)	112 (98%)	2 (2%)	59	82
47	Lf	89/90 (99%)	85 (96%)	4 (4%)	27	60
48	Lh	108/781 (14%)	105 (97%)	3 (3%)	43	73
49	Li	75/93 (81%)	71 (95%)	4 (5%)	22	54
50	Lj	61/78 (78%)	57 (93%)	4 (7%)	16	47
51	Lq	179/189 (95%)	176 (98%)	3 (2%)	60	83
52	Cc	204/244 (84%)	199 (98%)	5 (2%)	47	75
53	Cd	291/367 (79%)	282 (97%)	9 (3%)	40	70
54	Ce	173/297 (58%)	165 (95%)	8 (5%)	27	59
55	Cf	53/482 (11%)	50 (94%)	3 (6%)	20	52
All	All	8538/14065 (61%)	8174 (96%)	364 (4%)	33	62

All (364) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	CA	25	ASN
4	CA	53	ASN
4	CA	72	SER
4	CA	128	PHE
4	CA	140	LEU
4	CA	146	PHE
4	CA	180	LEU
4	CA	230	ASN
4	CA	249	SER
4	CA	253	PRO
4	CA	292	ARG
4	CA	293	LYS
4	CA	295	GLN

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Mol	Chain	Res	Type
5	CB	27	CYS
5	CB	63	TRP
5	CB	87	HIS
5	CB	89	LEU
5	CB	90	ASN
5	CB	91	THR
5	CB	106	ARG
5	CB	107	PHE
5	CB	109	LYS
5	CB	114	ASP
5	CB	121	ARG
5	CB	123	LYS
5	CB	145	LYS
5	CB	171	PHE
5	CB	215	ARG
5	CB	269	ARG
5	CB	270	PHE
5	CB	275	TRP
5	CB	276	GLN
5	CB	280	ASN
6	CC	125	PRO
6	CC	137	TYR
6	CC	189	ASP
6	CC	193	LYS
6	CC	196	MET
6	CC	255	TYR
6	CC	302	ARG
6	CC	306	TYR
6	CC	338	MET
6	CC	351	ASP
6	CC	373	MET
6	CC	378	ARG
6	CC	382	TYR
6	CC	408	MET
7	CE	136	GLU
7	CE	156	LYS
7	CE	175	SER
7	CE	250	ASN
7	CE	283	LYS
7	CE	296	SER
7	CE	317	TYR
7	CE	336	TYR

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Mol	Chain	Res	Type
7	CE	353	LYS
7	CE	355	MET
7	CE	366	SER
7	CE	405	ASN
7	CE	444	ARG
7	CE	457	ARG
7	CE	465	CYS
7	CE	473	LEU
7	CE	474	LYS
7	CE	488	ASN
7	CE	499	LYS
7	CE	525	HIS
7	CE	535	LYS
7	CE	554	ASP
8	CF	25	ARG
8	CF	31	ARG
8	CF	32	GLU
8	CF	38	GLN
8	CF	95	TYR
8	CF	126	ARG
8	CF	158	SER
8	CF	203	SER
8	CF	210	LYS
8	CF	211	LEU
8	CF	213	SER
8	CF	243	ARG
9	CG	1	MET
9	CG	15	LYS
9	CG	58	CYS
9	CG	71	LEU
9	CG	158	ASP
9	CG	164	CYS
9	CG	169	ASP
10	CH	5	LYS
10	CH	85	TYR
10	CH	88	ASP
10	CH	89	HIS
10	CH	98	SER
10	CH	101	LYS
10	CH	108	SER
10	CH	174	PHE
10	CH	209	ASP

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Mol	Chain	Res	Type
10	CH	270	PHE
10	CH	274	LYS
10	CH	297	LEU
10	CH	323	THR
10	CH	406	ASP
10	CH	418	ASN
10	CH	423	LYS
10	CH	448	ASP
10	CH	467	ARG
10	CH	469	GLU
11	CI	198	PHE
11	CI	246	ARG
11	CI	258	LEU
11	CI	269	HIS
11	CI	287	LYS
12	CJ	68	ASP
12	CJ	115	LYS
12	CJ	147	MET
12	CJ	256	LYS
12	CJ	414	ARG
12	CJ	453	ARG
12	CJ	462	TRP
12	CJ	475	LEU
13	CK	67	GLN
13	CK	149	ARG
13	CK	161	PHE
13	CK	170	ARG
13	CK	189	LEU
13	CK	190	ASN
13	CK	202	LYS
13	CK	212	LEU
13	CK	241	ARG
13	CK	247	ASN
14	CL	19	ARG
14	CL	27	ARG
14	CL	58	LEU
15	CM	52	LYS
15	CM	55	GLU
15	CM	67	GLU
15	CM	127	LYS
15	CM	155	TYR
15	CM	201	PHE

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Mol	Chain	Res	Type
15	CM	237	ARG
15	CM	242	ASN
16	CN	1	MET
16	CN	80	GLU
16	CN	110	CYS
16	CN	124	GLU
16	CN	127	GLU
16	CN	172	GLU
16	CN	188	ARG
17	CO	14	HIS
18	CP	264	ASN
18	CP	271	CYS
18	CP	316	HIS
18	CP	319	ASP
18	CP	331	LEU
18	CP	337	TRP
18	CP	339	LYS
18	CP	362	TYR
18	CP	370	PHE
18	CP	438	TYR
18	CP	459	CYS
18	CP	460	SER
18	CP	480	PHE
18	CP	489	GLN
18	CP	496	ASP
18	CP	500	HIS
18	CP	520	ASN
18	CP	535	LYS
18	CP	545	LYS
18	CP	557	HIS
18	CP	576	PHE
18	CP	582	LYS
19	CQ	1	MET
19	CQ	11	ARG
19	CQ	17	LYS
19	CQ	27	LYS
19	CQ	40	PHE
19	CQ	47	ARG
19	CQ	91	LYS
20	CR	33	ASN
20	CR	57	LYS
20	CR	134	GLN

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Mol	Chain	Res	Type
20	CR	178	ARG
20	CR	204	ASP
20	CR	212	ASP
20	CR	214	LYS
21	CS	660	MET
23	CU	318	GLN
23	CU	327	LYS
23	CU	329	GLU
24	CX	100	SER
24	CX	113	GLN
24	CX	133	ARG
26	Cz	37	LYS
27	Cb	4	ARG
27	Cb	102	LEU
27	Cb	156	SER
27	Cb	181	LYS
27	Cb	193	LEU
27	Cb	212	ASP
27	Cb	236	LYS
27	Cb	257	GLU
27	Cb	298	GLU
27	Cb	381	TYR
27	Cb	443	PHE
27	Cb	493	ARG
27	Cb	528	ASN
27	Cb	582	ASN
27	Cb	589	ASN
27	Cb	715	TYR
27	Cb	799	GLU
27	Cb	813	PHE
27	Cb	815	LYS
27	Cb	819	GLN
27	Cb	833	LYS
27	Cb	861	LYS
27	Cb	871	LYS
28	LB	19	ARG
28	LB	89	LEU
28	LB	112	ASP
28	LB	173	LYS
28	LB	214	GLU
28	LB	298	GLU
28	LB	354	LYS

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Mol	Chain	Res	Type
28	LB	378	LYS
29	LC	62	SER
29	LC	64	GLU
29	LC	70	ARG
29	LC	121	PHE
29	LC	271	SER
29	LC	321	ARG
29	LC	359	LYS
29	LC	360	GLU
30	LE	25	GLN
30	LE	167	LYS
30	LE	191	LYS
30	LE	199	LYS
15	LF	32	ARG
15	LF	52	LYS
15	LF	100	LYS
15	LF	134	LYS
15	LF	181	LYS
15	LF	246	ARG
31	LG	52	MET
31	LG	107	GLU
31	LG	140	ASN
31	LG	216	LYS
31	LG	228	LYS
32	LH	17	LYS
32	LH	19	SER
32	LH	23	ARG
32	LH	33	LYS
32	LH	36	LYS
32	LH	55	LEU
32	LH	63	LYS
32	LH	98	PRO
32	LH	108	GLU
32	LH	149	SER
32	LH	151	ASN
32	LH	157	SER
33	LK	11	LYS
33	LK	31	LYS
33	LK	101	ASN
33	LK	149	LYS
33	LK	164	ASP
34	LL	58	VAL

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Mol	Chain	Res	Type
34	LL	102	LYS
34	LL	122	ARG
35	LM	14	VAL
35	LM	71	LYS
35	LM	137	LYS
36	LN	23	LEU
36	LN	96	ARG
36	LN	108	ARG
36	LN	118	SER
36	LN	140	LYS
36	LN	187	ARG
36	LN	198	SER
37	LO	117	LYS
37	LO	169	TYR
37	LO	185	LYS
37	LO	197	GLU
38	LP	3	ARG
38	LP	20	SER
38	LP	43	ARG
38	LP	74	LYS
38	LP	80	ARG
38	LP	87	SER
38	LP	103	ASP
38	LP	140	MET
38	LP	154	GLU
39	LQ	149	LEU
40	LS	62	ASN
40	LS	71	LYS
40	LS	83	SER
40	LS	85	SER
40	LS	94	TYR
40	LS	98	SER
40	LS	113	ARG
40	LS	131	LYS
40	LS	149	SER
40	LS	160	SER
41	LT	57	TYR
41	LT	118	LYS
42	LV	15	MET
42	LV	42	LYS
42	LV	68	LYS
42	LV	88	LYS

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Mol	Chain	Res	Type
42	LV	139	MET
44	LY	1	MET
44	LY	8	SER
44	LY	73	TYR
44	LY	76	LYS
44	LY	78	VAL
44	LY	86	ARG
44	LY	122	LYS
45	Ld	20	TYR
45	Ld	46	LYS
45	Ld	85	ARG
45	Ld	102	GLN
46	Le	70	SER
46	Le	81	LYS
47	Lf	62	ARG
47	Lf	65	LYS
47	Lf	67	ARG
47	Lf	95	SER
48	Lh	15	LYS
48	Lh	22	LYS
48	Lh	112	ARG
49	Li	25	LYS
49	Li	62	TYR
49	Li	83	LYS
49	Li	94	ARG
50	Lj	26	SER
50	Lj	36	SER
50	Lj	52	LYS
50	Lj	68	SER
51	Lq	25	LYS
51	Lq	34	LEU
51	Lq	184	MET
52	Cc	20	LYS
52	Cc	151	ASP
52	Cc	204	GLU
52	Cc	230	ASP
52	Cc	247	ASP
53	Cd	43	ARG
53	Cd	47	ARG
53	Cd	56	LEU
53	Cd	267	SER
53	Cd	277	GLU

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Mol	Chain	Res	Type
53	Cd	351	ASP
53	Cd	414	GLU
53	Cd	422	GLU
53	Cd	430	LYS
54	Ce	43	CYS
54	Ce	77	TRP
54	Ce	161	LYS
54	Ce	172	ASP
54	Ce	182	GLN
54	Ce	189	GLN
54	Ce	192	LYS
54	Ce	195	LEU
55	Cf	523	ARG
55	Cf	526	LYS
55	Cf	529	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
7	CE	334	GLN
10	CH	258	GLN
12	CJ	485	HIS
13	CK	203	ASN
15	CM	119	ASN
16	CN	79	GLN
16	CN	156	ASN
19	CQ	58	ASN
20	CR	133	GLN
20	CR	148	GLN
31	LG	140	ASN
40	LS	21	ASN
41	LT	146	ASN
42	LV	76	HIS
48	Lh	37	GLN
49	Li	42	GLN
54	Ce	185	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2134/3341 (63%)	479 (22%)	15 (0%)
2	C2	157/256 (61%)	30 (19%)	1 (0%)
3	C3	96/161 (59%)	34 (35%)	0
All	All	2387/3758 (63%)	543 (22%)	16 (0%)

All (543) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	A
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	67	A
1	C1	73	A
1	C1	74	G
1	C1	85	A
1	C1	91	G
1	C1	92	G
1	C1	94	G
1	C1	96	G
1	C1	105	C
1	C1	109	A
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	136	C
1	C1	143	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G

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Mol	Chain	Res	Type
1	C1	163	U
1	C1	176	U
1	C1	183	U
1	C1	193	C
1	C1	203	C
1	C1	204	A
1	C1	205	G
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	214	A
1	C1	225	G
1	C1	241	G
1	C1	244	U
1	C1	249	C
1	C1	253	U
1	C1	258	C
1	C1	261	G
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	290	U
1	C1	300	A
1	C1	302	U
1	C1	308	U
1	C1	310	A
1	C1	311	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	329	G
1	C1	331	C
1	C1	342	C
1	C1	343	A
1	C1	368	G
1	C1	377	A
1	C1	382	G
1	C1	384	G
1	C1	390	U
1	C1	391	A
1	C1	393	C

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Mol	Chain	Res	Type
1	C1	394	A
1	C1	395	C
1	C1	400	A
1	C1	413	G
1	C1	414	A
1	C1	430	A
1	C1	431	C
1	C1	432	U
1	C1	433	U
1	C1	445	A
1	C1	446	U
1	C1	448	A
1	C1	449	U
1	C1	450	C
1	C1	457	U
1	C1	459	U
1	C1	460	C
1	C1	467	G
1	C1	468	C
1	C1	469	A
1	C1	474	G
1	C1	484	G
1	C1	485	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	520	G
1	C1	526	G
1	C1	533	C
1	C1	534	U
1	C1	535	C
1	C1	546	A
1	C1	547	U
1	C1	548	A
1	C1	558	G
1	C1	582	A
1	C1	590	C
1	C1	592	G
1	C1	593	C
1	C1	596	G
1	C1	598	A

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Mol	Chain	Res	Type
1	C1	608	A
1	C1	623	C
1	C1	633	A
1	C1	651	A
1	C1	652	A
1	C1	664	A
1	C1	668	U
1	C1	678	A
1	C1	684	G
1	C1	692	A
1	C1	693	A
1	C1	699	G
1	C1	702	A
1	C1	703	A
1	C1	706	U
1	C1	707	A
1	C1	708	G
1	C1	718	U
1	C1	719	C
1	C1	723	G
1	C1	731	G
1	C1	739	C
1	C1	744	G
1	C1	748	U
1	C1	749	C
1	C1	751	G
1	C1	752	A
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	765	G
1	C1	767	A
1	C1	787	A
1	C1	796	G
1	C1	798	A
1	C1	907	A
1	C1	918	G
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G

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Mol	Chain	Res	Type
1	C1	940	C
1	C1	942	C
1	C1	943	A
1	C1	944	G
1	C1	958	A
1	C1	960	C
1	C1	961	U
1	C1	965	G
1	C1	973	A
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	979	A
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1033	U
1	C1	1039	A
1	C1	1043	A
1	C1	1045	G
1	C1	1046	A
1	C1	1047	A
1	C1	1057	A
1	C1	1063	C
1	C1	1069	G
1	C1	1075	A
1	C1	1076	U
1	C1	1077	U
1	C1	1078	C
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1086	U
1	C1	1097	G
1	C1	1098	G
1	C1	1114	C
1	C1	1126	U
1	C1	1135	A
1	C1	1141	A
1	C1	1142	C
1	C1	1163	U
1	C1	1164	G

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Mol	Chain	Res	Type
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1180	C
1	C1	1181	C
1	C1	1182	A
1	C1	1184	A
1	C1	1186	A
1	C1	1187	A
1	C1	1189	G
1	C1	1190	C
1	C1	1203	U
1	C1	1204	G
1	C1	1211	G
1	C1	1218	G
1	C1	1221	C
1	C1	1223	U
1	C1	1224	G
1	C1	1226	A
1	C1	1227	A
1	C1	1228	G
1	C1	1238	G
1	C1	1240	U
1	C1	1241	A
1	C1	1245	A
1	C1	1246	C
1	C1	1247	U
1	C1	1253	A
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	1289	G
1	C1	1291	U
1	C1	1295	G
1	C1	1312	A
1	C1	1313	U
1	C1	1314	A
1	C1	1330	A

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Mol	Chain	Res	Type
1	C1	1331	G
1	C1	1332	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1362	G
1	C1	1368	A
1	C1	1369	G
1	C1	1373	C
1	C1	1374	G
1	C1	1381	A
1	C1	1382	G
1	C1	1399	G
1	C1	1400	A
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1433	C
1	C1	1856	U
1	C1	1859	U
1	C1	1864	C
1	C1	1865	A
1	C1	1866	A
1	C1	1868	G
1	C1	1875	A
1	C1	1883	C
1	C1	1884	G
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	2293	C
1	C1	2294	A
1	C1	2297	G
1	C1	2302	U
1	C1	2309	U
1	C1	2325	A

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Mol	Chain	Res	Type
1	C1	2332	G
1	C1	2334	A
1	C1	2335	A
1	C1	2338	G
1	C1	2339	G
1	C1	2356	G
1	C1	2365	G
1	C1	2384	C
1	C1	2394	A
1	C1	2396	U
1	C1	2397	G
1	C1	2402	A
1	C1	2406	C
1	C1	2415	U
1	C1	2422	U
1	C1	2423	A
1	C1	2424	G
1	C1	2426	U
1	C1	2428	G
1	C1	2429	G
1	C1	2430	A
1	C1	2431	G
1	C1	2435	C
1	C1	2436	G
1	C1	2439	G
1	C1	2445	G
1	C1	2449	U
1	C1	2452	C
1	C1	2453	A
1	C1	2456	A
1	C1	2465	G
1	C1	2467	U
1	C1	2469	U
1	C1	2476	U
1	C1	2477	A
1	C1	2482	A
1	C1	2551	A
1	C1	2552	C
1	C1	2553	A
1	C1	2564	G
1	C1	2568	G
1	C1	2730	C

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Mol	Chain	Res	Type
1	C1	2739	U
1	C1	2749	G
1	C1	2759	A
1	C1	2760	A
1	C1	2761	A
1	C1	2766	A
1	C1	2767	C
1	C1	2776	U
1	C1	2777	A
1	C1	2778	A
1	C1	2782	G
1	C1	2783	C
1	C1	2784	U
1	C1	2800	U
1	C1	2802	C
1	C1	2803	A
1	C1	2804	U
1	C1	2805	A
1	C1	2807	C
1	C1	2818	U
1	C1	2819	U
1	C1	2831	U
1	C1	2832	G
1	C1	2833	U
1	C1	2834	C
1	C1	2835	G
1	C1	2836	G
1	C1	2845	A
1	C1	2847	C
1	C1	2852	C
1	C1	2856	G
1	C1	2857	C
1	C1	2862	U
1	C1	2869	A
1	C1	2874	U
1	C1	2879	U
1	C1	2893	U
1	C1	2894	A
1	C1	2899	A
1	C1	2900	C
1	C1	2901	G
1	C1	2916	A

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Mol	Chain	Res	Type
1	C1	2917	C
1	C1	2923	U
1	C1	2924	G
1	C1	2926	G
1	C1	2929	A
1	C1	2930	G
1	C1	2935	G
1	C1	2936	U
1	C1	2950	U
1	C1	2956	C
1	C1	2968	A
1	C1	2969	A
1	C1	2970	U
1	C1	2980	U
1	C1	3006	A
1	C1	3013	U
1	C1	3014	U
1	C1	3015	U
1	C1	3033	C
1	C1	3034	A
1	C1	3035	G
1	C1	3037	G
1	C1	3048	A
1	C1	3049	C
1	C1	3050	C
1	C1	3057	U
1	C1	3066	G
1	C1	3070	A
1	C1	3077	C
1	C1	3079	A
1	C1	3084	A
1	C1	3086	A
1	C1	3087	A
1	C1	3088	U
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3108	U
1	C1	3109	A
1	C1	3113	C
1	C1	3118	A
1	C1	3126	G

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Mol	Chain	Res	Type
1	C1	3130	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G
1	C1	3144	C
1	C1	3146	G
1	C1	3147	G
1	C1	3154	A
1	C1	3157	C
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3170	C
1	C1	3171	C
1	C1	3178	G
1	C1	3179	G
1	C1	3183	C
1	C1	3185	A
1	C1	3187	G
1	C1	3189	G
1	C1	3199	A
1	C1	3205	C
1	C1	3211	G
1	C1	3212	C
1	C1	3213	A
1	C1	3214	A
1	C1	3225	C
1	C1	3228	G
1	C1	3232	U
1	C1	3244	C
1	C1	3248	C
1	C1	3249	G
1	C1	3253	U
1	C1	3256	A
1	C1	3257	U
1	C1	3258	G
1	C1	3260	G
1	C1	3262	G
1	C1	3263	A
1	C1	3264	A
1	C1	3270	C
1	C1	3274	U

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Mol	Chain	Res	Type
1	C1	3281	U
1	C1	3282	A
1	C1	3285	G
1	C1	3290	C
1	C1	3291	U
1	C1	3292	U
1	C1	3295	U
1	C1	3296	G
1	C1	3297	U
1	C1	3298	U
1	C1	3302	A
1	C1	3309	G
1	C1	3310	A
1	C1	3318	C
1	C1	3321	U
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3329	C
1	C1	3330	U
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
1	C1	3337	C
2	C2	34	U
2	C2	35	C
2	C2	49	G
2	C2	51	G
2	C2	53	A
2	C2	59	A
2	C2	61	A
2	C2	62	A
2	C2	63	G
2	C2	77	A
2	C2	78	G
2	C2	81	U
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	100	U

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Mol	Chain	Res	Type
2	C2	104	A
2	C2	106	C
2	C2	109	A
2	C2	111	A
2	C2	113	U
2	C2	124	G
2	C2	126	A
2	C2	127	U
2	C2	129	C
2	C2	136	G
2	C2	152	G
2	C2	158	U
3	C3	5	C
3	C3	6	A
3	C3	7	U
3	C3	8	C
3	C3	15	U
3	C3	16	G
3	C3	17	G
3	C3	21	U
3	C3	25	U
3	C3	26	U
3	C3	31	A
3	C3	32	C
3	C3	48	G
3	C3	54	G
3	C3	55	A
3	C3	56	A
3	C3	57	A
3	C3	59	G
3	C3	60	C
3	C3	61	A
3	C3	63	U
3	C3	64	G
3	C3	68	G
3	C3	71	U
3	C3	72	C
3	C3	73	G
3	C3	75	U
3	C3	130	G
3	C3	133	G
3	C3	134	C

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Mol	Chain	Res	Type
3	C3	137	G
3	C3	141	U
3	C3	143	A
3	C3	144	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	308	U
1	C1	519	A
1	C1	1044	A
1	C1	1046	A
1	C1	1220	C
1	C1	2301	C
1	C1	2929	A
1	C1	3078	U
1	C1	3162	A
1	C1	3204	G
1	C1	3257	U
1	C1	3263	A
1	C1	3296	G
1	C1	3297	U
2	C2	123	G

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 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	$\#\|Z\| > 2$
56	GTP	CH	701	-	26,34,34	1.16	2 (7%)	32,54,54	1.60	7 (21%)

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
56	GTP	CH	701	-	-	6/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CH	701	GTP	C5-C6	-4.17	1.38	1.47
56	CH	701	GTP	C2-N3	2.11	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	CH	701	GTP	PB-O3B-PG	-3.73	120.02	132.83
56	CH	701	GTP	PA-O3A-PB	-3.20	121.86	132.83
56	CH	701	GTP	C5-C6-N1	3.15	119.51	113.95
56	CH	701	GTP	C3'-C2'-C1'	2.97	105.46	100.98
56	CH	701	GTP	C8-N7-C5	2.92	108.55	102.99
56	CH	701	GTP	C2-N1-C6	-2.87	119.81	125.10
56	CH	701	GTP	O6-C6-C5	-2.08	120.31	124.37

There are no chirality outliers.

All (6) torsion outliers are listed below:

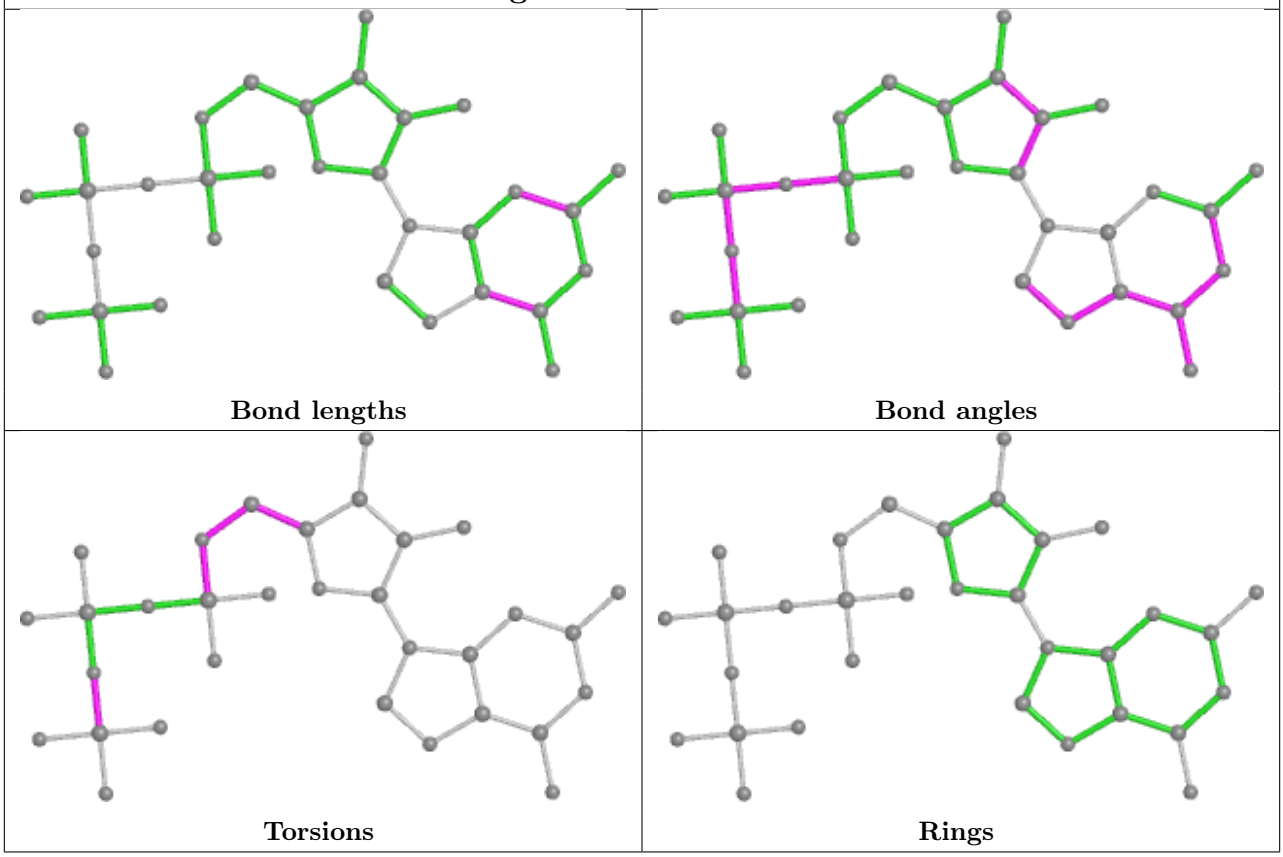
Mol	Chain	Res	Type	Atoms
56	CH	701	GTP	PB-O3B-PG-O2G
56	CH	701	GTP	PB-O3B-PG-O3G
56	CH	701	GTP	C5'-O5'-PA-O3A
56	CH	701	GTP	C4'-C5'-O5'-PA
56	CH	701	GTP	C5'-O5'-PA-O2A
56	CH	701	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand GTP CH 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

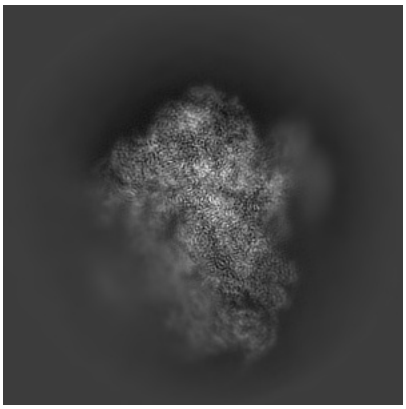
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-35285. These allow visual inspection of the internal detail of the map and identification of artifacts.

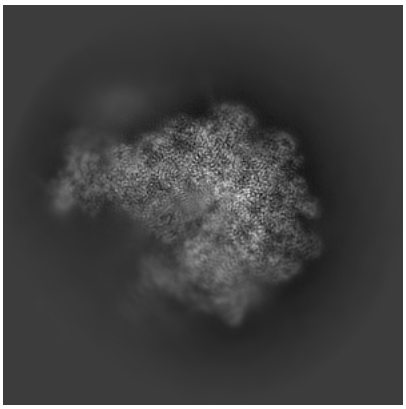
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

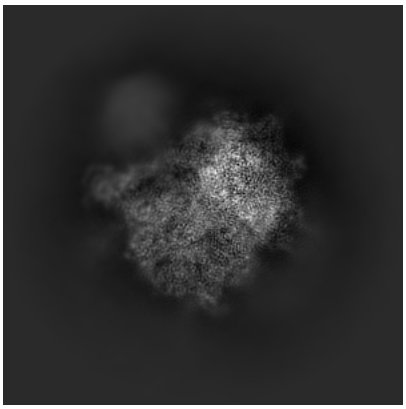
6.1.1 Primary map



X

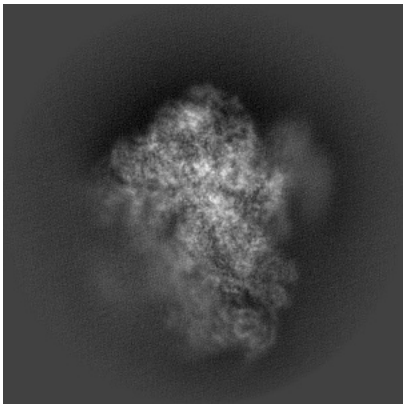


Y

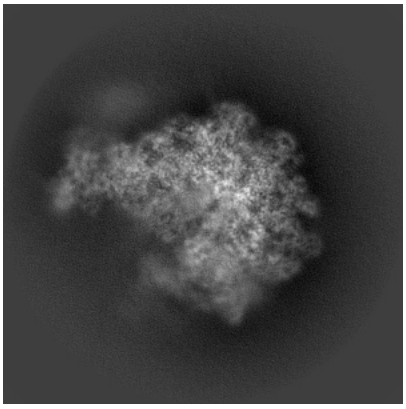


Z

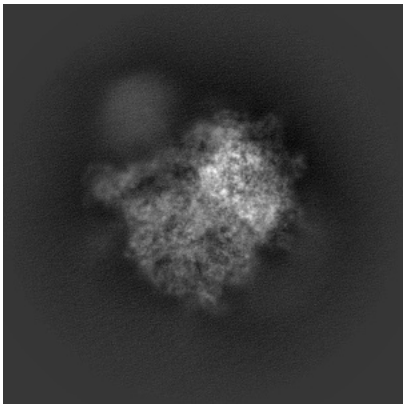
6.1.2 Raw map



X



Y

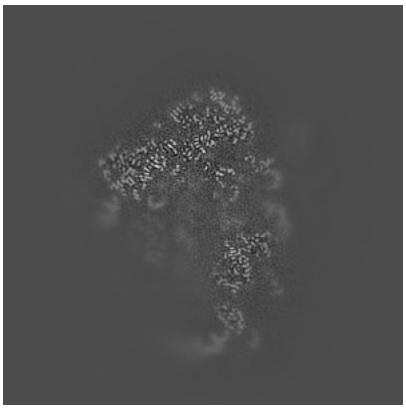


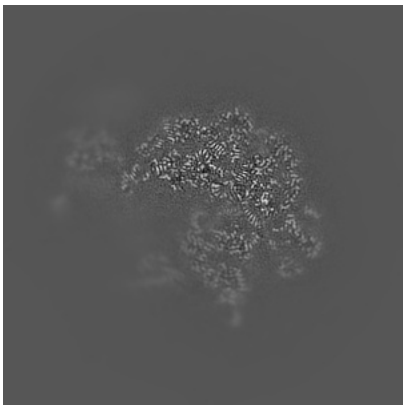
Z

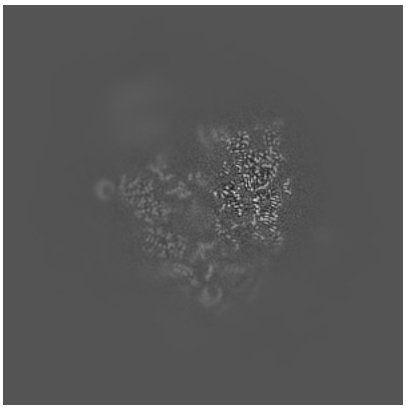
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

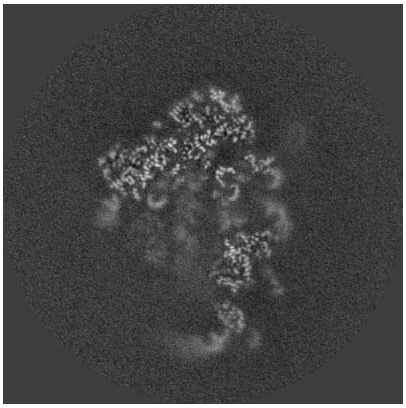
6.2.1 Primary map

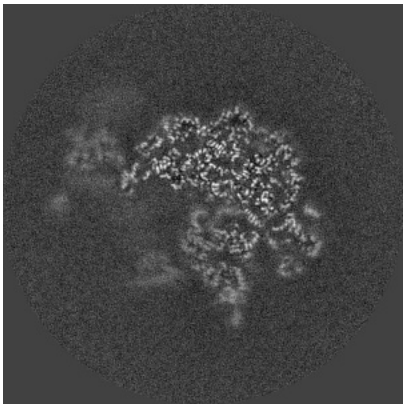

X Index: 210

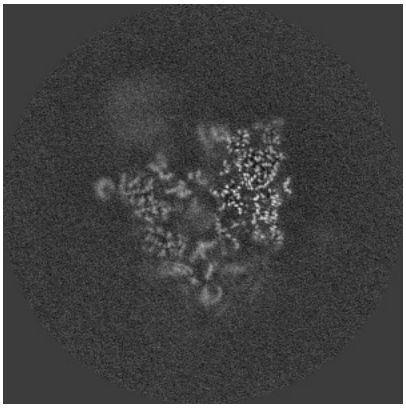

Y Index: 210


Z Index: 210

6.2.2 Raw map


X Index: 210


Y Index: 210

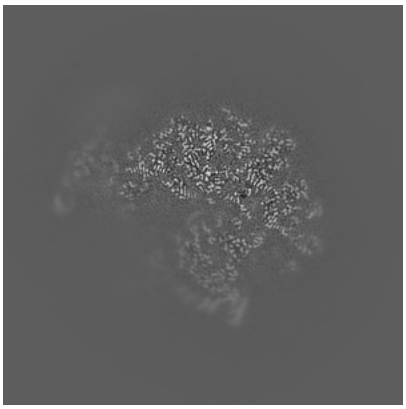

Z Index: 210

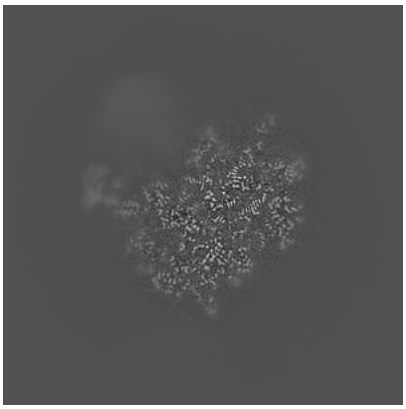
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

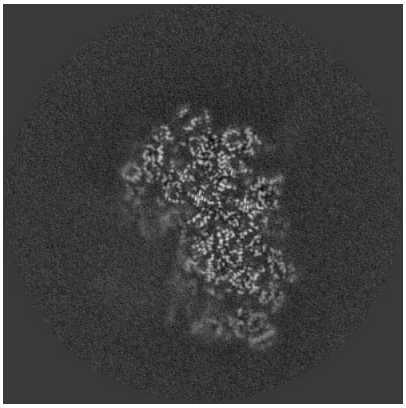
6.3.1 Primary map

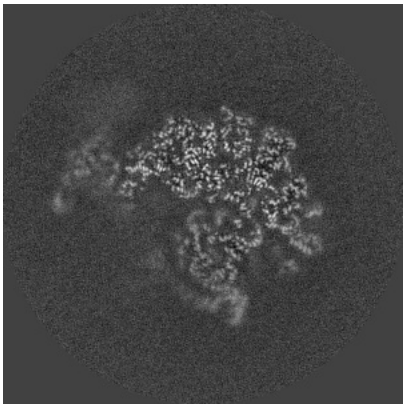
X Index: 247

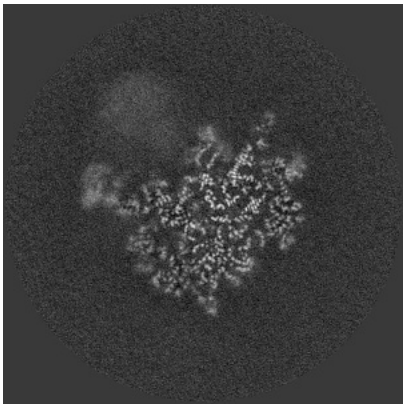

Y Index: 217


Z Index: 247

6.3.2 Raw map


X Index: 247

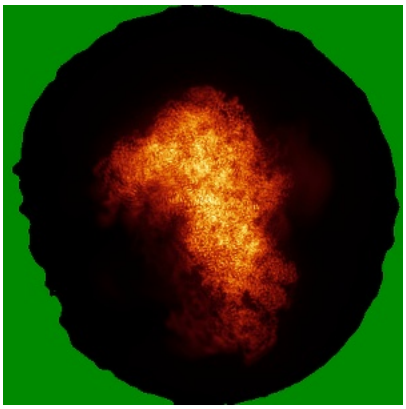

Y Index: 216

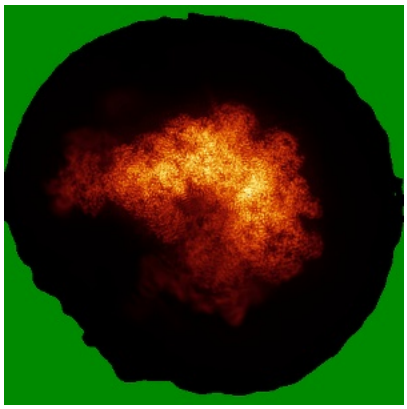

Z Index: 246

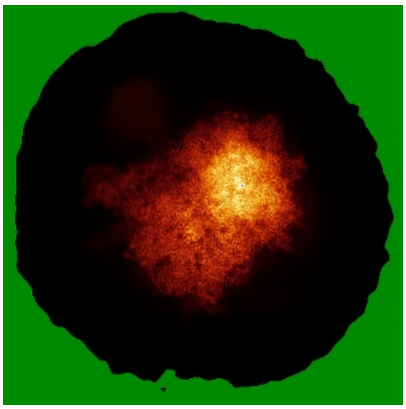
The images above show the largest variance slices of the map in three orthogonal directions.

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

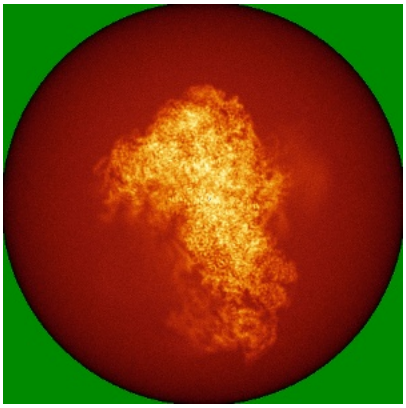
6.4.1 Primary map

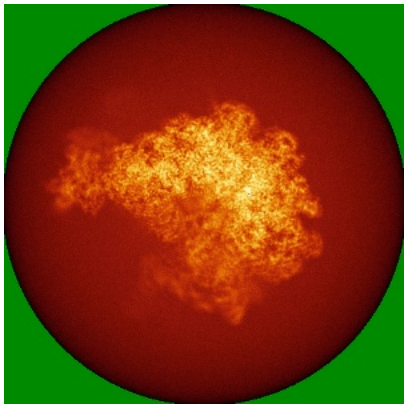

X

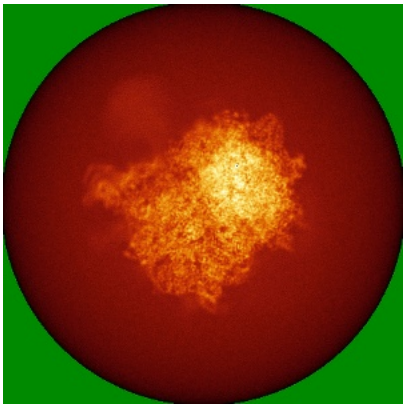

Y


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.

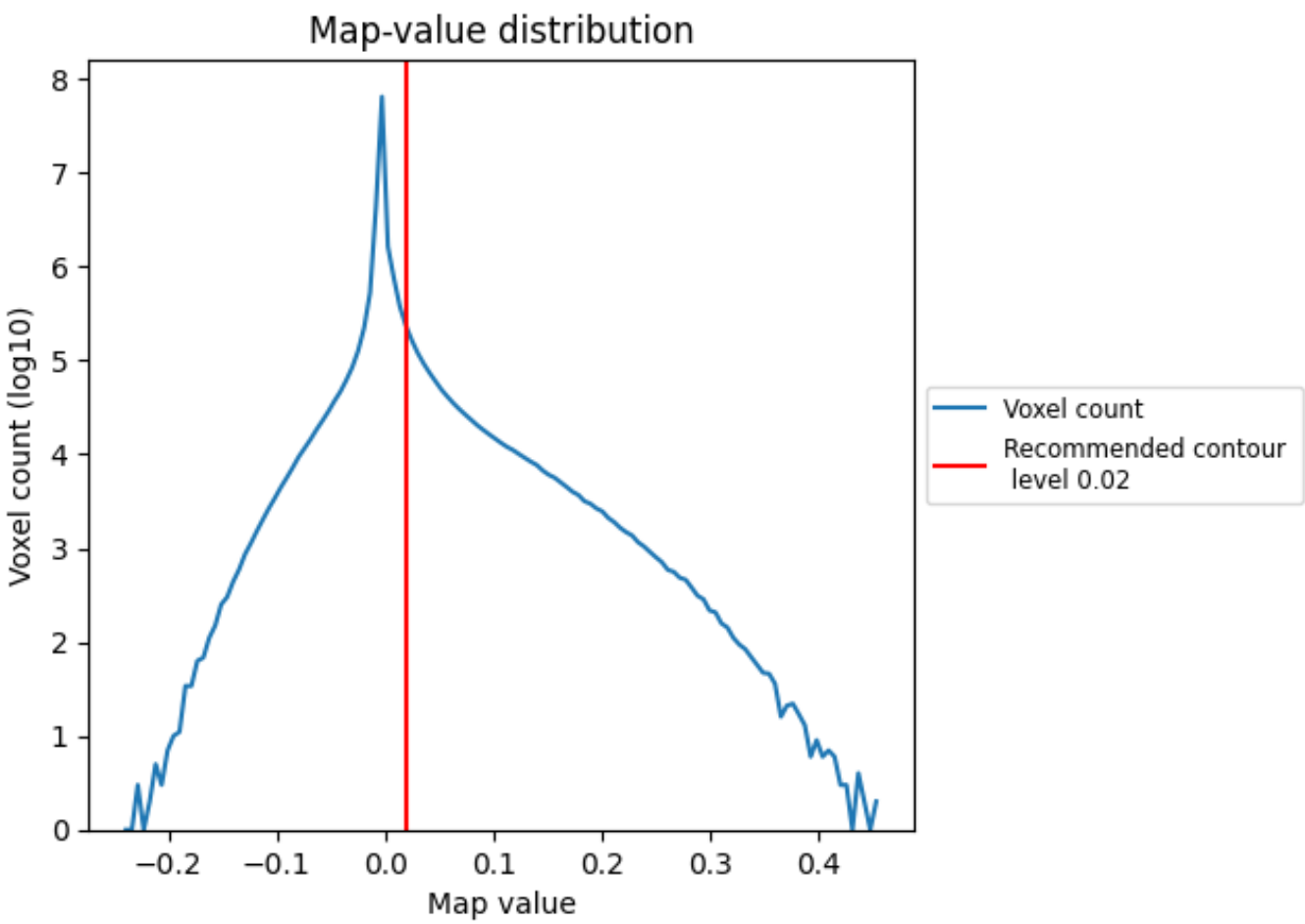
6.6 Mask visualisation (i)

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

7 Map analysis (i)

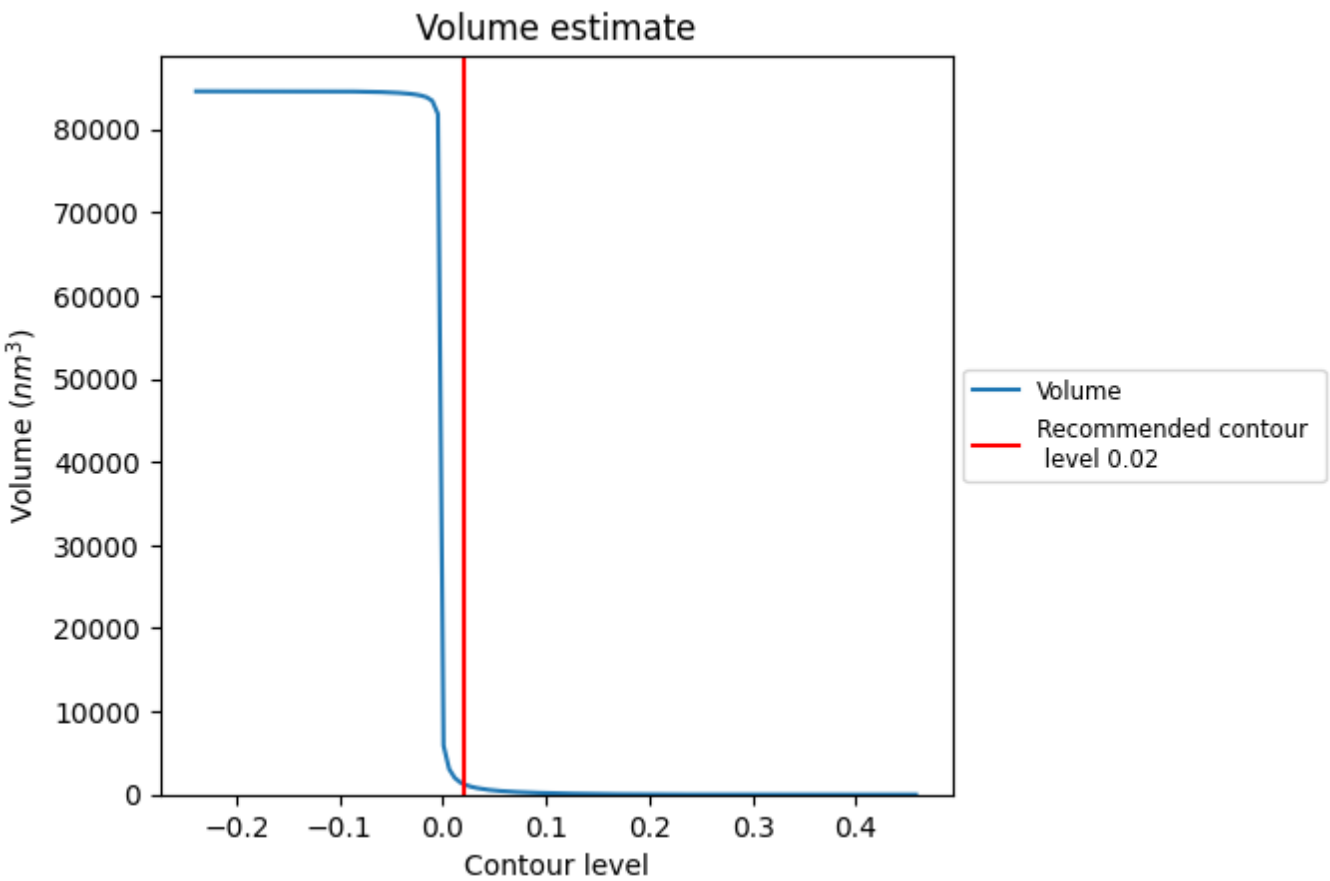
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

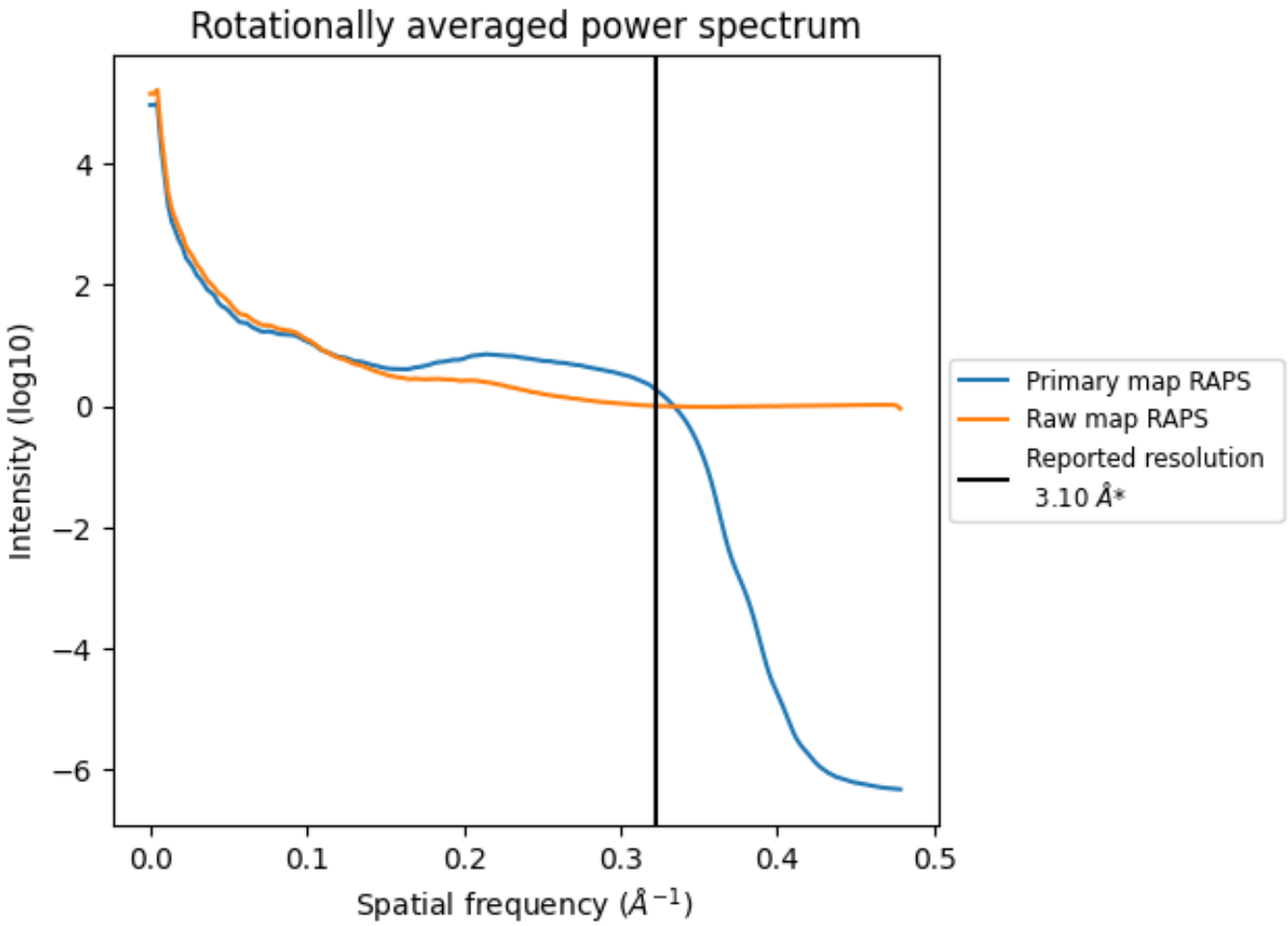
7.2 Volume estimate (i)



The volume at the recommended contour level is 1277 nm^3; this corresponds to an approximate mass of 1154 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)

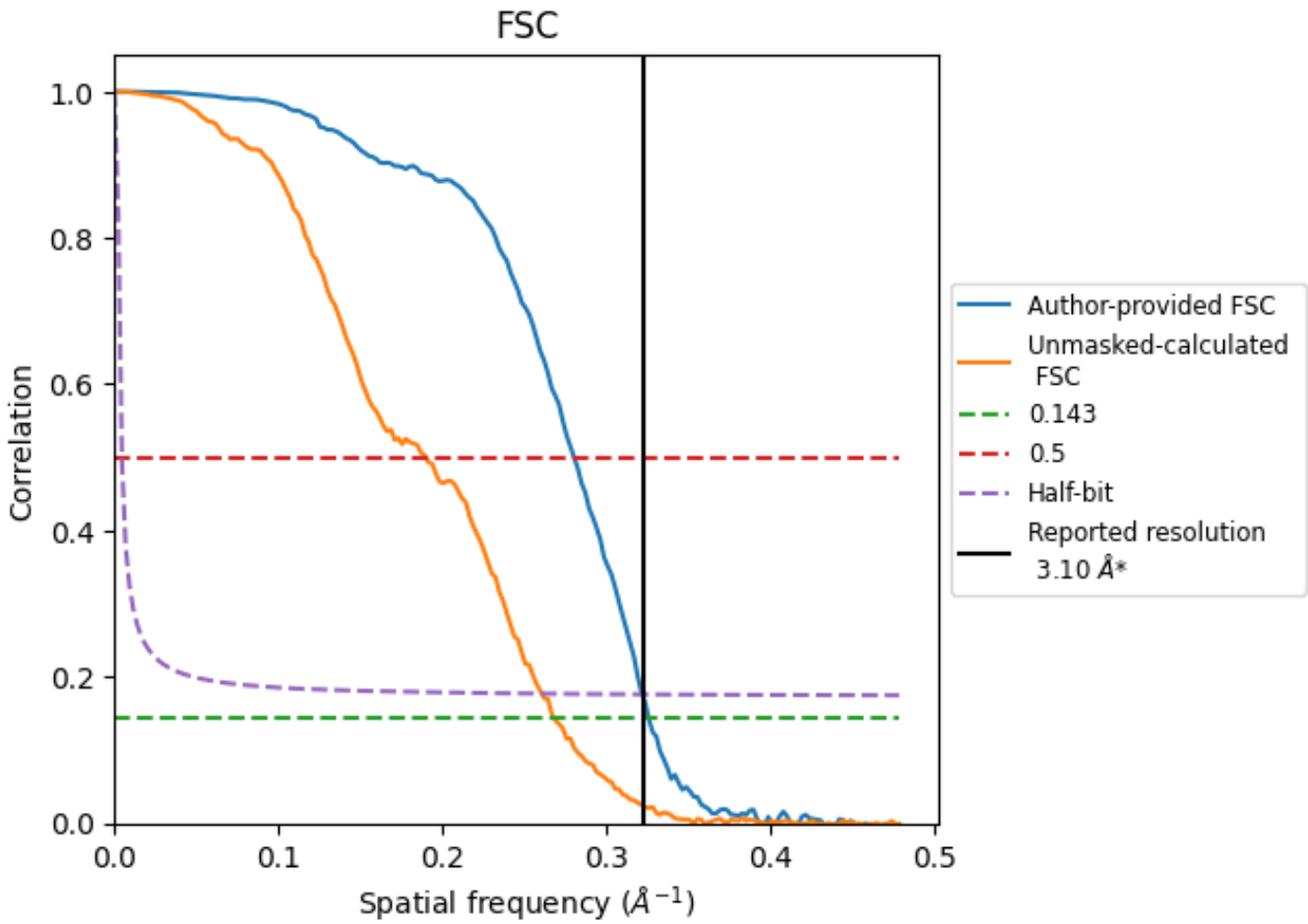


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



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

8.2 Resolution estimates (i)

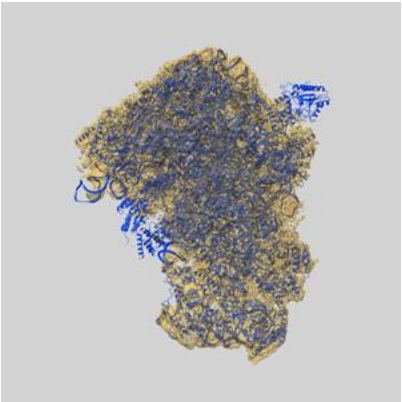
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.07	3.57	3.11
Unmasked-calculated*	3.73	5.27	3.84

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

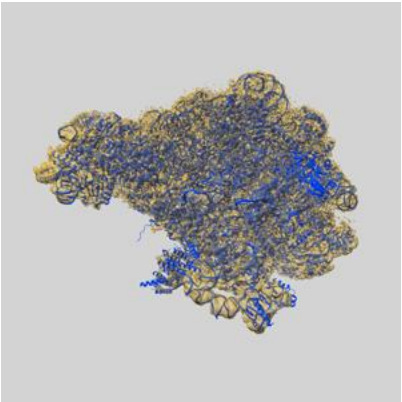
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-35285 and PDB model 8I9V. Per-residue inclusion information can be found in section 3 on page 16.

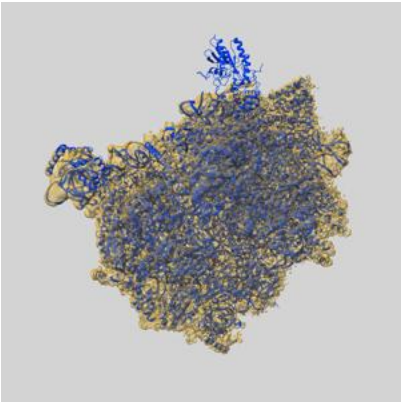
9.1 Map-model overlay (i)



X



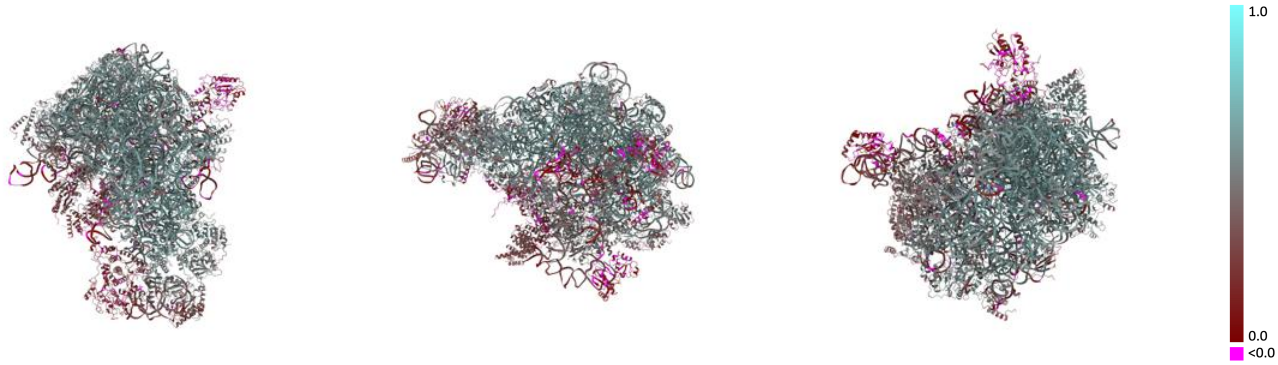
Y



Z

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

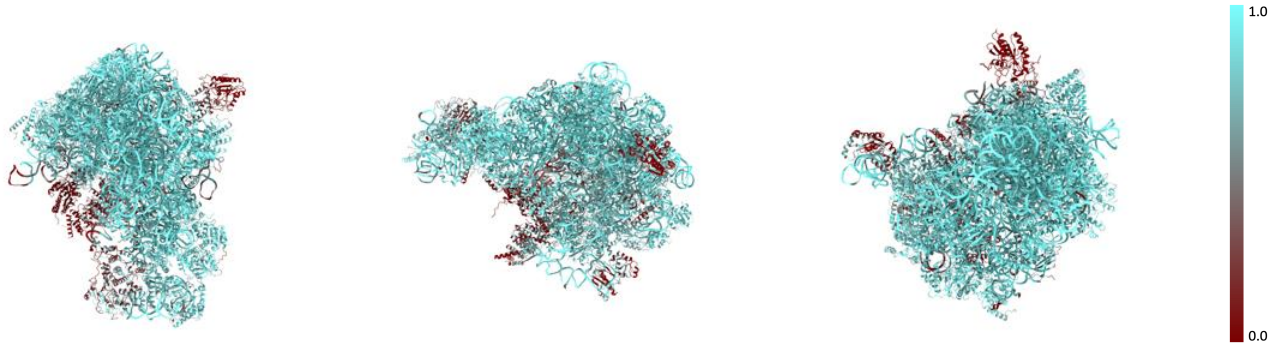
9.2 Q-score mapped to coordinate model (i)



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.

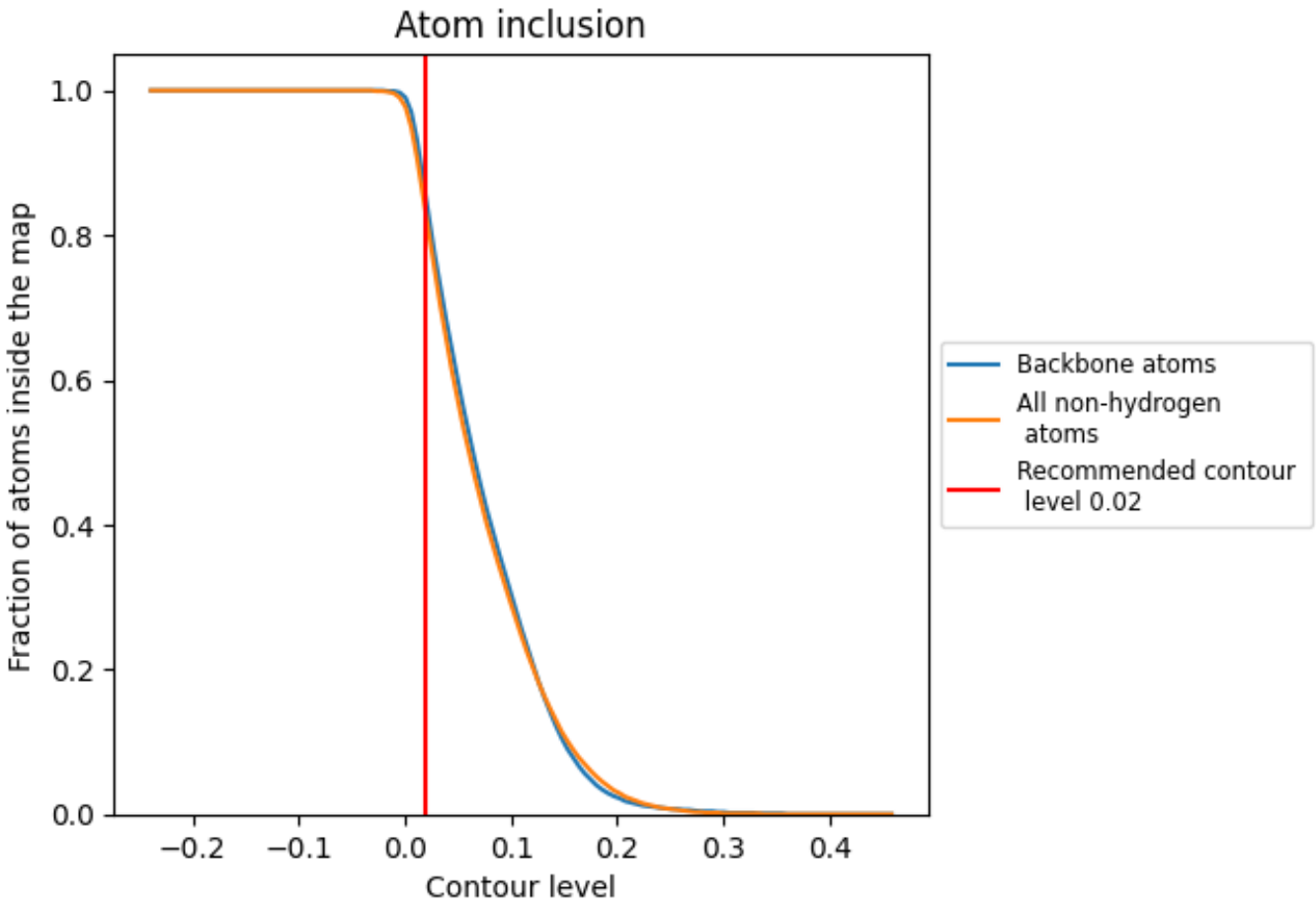
9.3 Atom inclusion mapped to coordinate model (i)



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, 85% of all backbone atoms, 83% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8270	0.4600
C1	0.9160	0.4920
C2	0.8890	0.4890
C3	0.8700	0.3460
CA	0.9100	0.5190
CB	0.7890	0.3810
CC	0.5130	0.2890
CE	0.8820	0.4970
CF	0.8700	0.4630
CG	0.7850	0.4060
CH	0.8810	0.4950
CI	0.8400	0.4180
CJ	0.4520	0.1900
CK	0.8500	0.4840
CL	0.3040	0.1920
CM	0.6100	0.2570
CN	0.8960	0.5130
CO	0.9340	0.5560
CP	0.8240	0.4390
CQ	0.9170	0.5070
CR	0.9130	0.5330
CS	0.0980	0.2140
CT	0.2590	0.2500
CU	0.8290	0.4480
CX	0.3990	0.1990
CY	0.4070	0.2780
Cb	0.7750	0.4150
Cc	0.8570	0.5040
Cd	0.9220	0.5390
Ce	0.9420	0.5730
Cf	0.6860	0.3770
Cz	0.6190	0.3280
LB	0.9320	0.5570
LC	0.9480	0.5860
LE	0.9180	0.5360

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Chain	Atom inclusion	Q-score
LF	0.9230	0.5600
LG	0.8410	0.5040
LH	0.9300	0.5580
LK	0.8110	0.3740
LL	0.9530	0.5840
LM	0.9440	0.5590
LN	0.9430	0.5890
LO	0.9520	0.5830
LP	0.9240	0.5510
LQ	0.9390	0.5720
LS	0.9310	0.5570
LT	0.7100	0.3300
LV	0.8870	0.5150
LX	0.3240	0.2180
LY	0.9190	0.5550
Ld	0.6000	0.2850
Le	0.9510	0.5970
Lf	0.9530	0.5990
Lh	0.8630	0.4980
Li	0.8880	0.5080
Lj	0.9590	0.5960
Lq	0.3400	0.0810