



wwPDB EM Validation Summary Report ⓘ

Dec 18, 2022 – 01:01 am GMT

PDB ID : 6ZQD
EMDB ID : EMD-11360
Title : Cryo-EM structure of the 90S pre-ribosome from *Saccharomyces cerevisiae*, state Post-A1
Authors : Cheng, J.; Lau, B.; Venuta, G.L.; Berninghausen, O.; Hurt, E.; Beckmann, R.
Deposited on : 2020-07-09
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

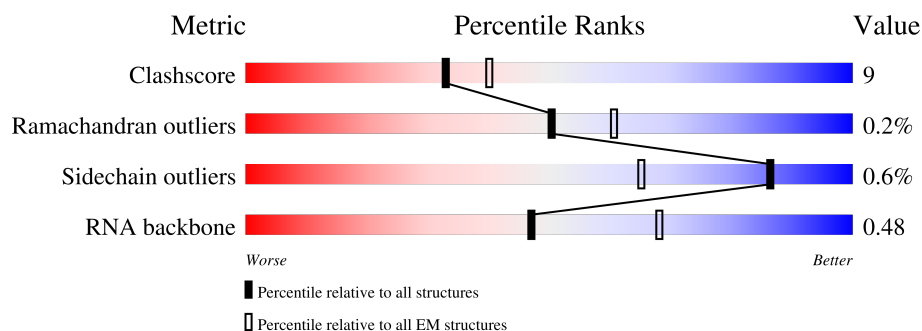
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)
Clashscore	158937	4297
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 $\leq 5\%$. 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	UA	923	68% 18% 14%
2	UB	810	16% 54% 14% 32%
3	UC	610	13% 86%
4	UD	776	62% 22% 15%
5	UE	643	56% 17% 26%
6	UF	440	55% 12% 33%
7	UG	554	64% 20% 15%





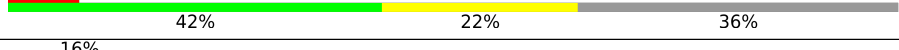

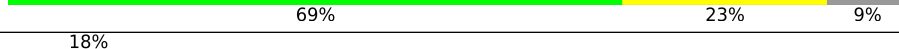
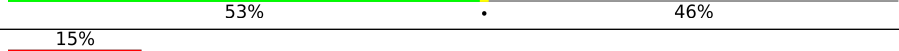
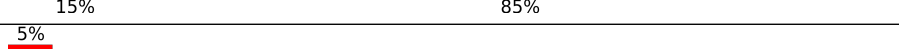
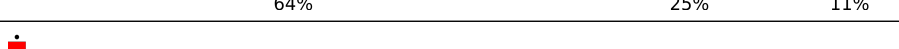
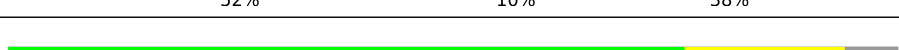

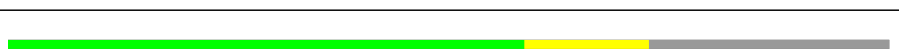

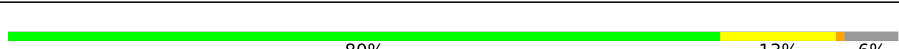





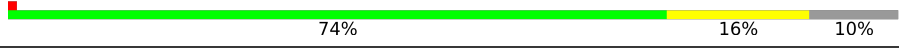
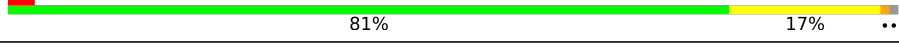



Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	UH	713	
9	UI	575	
10	UJ	1769	
11	UK	250	
12	UL	943	
13	UM	817	
14	UN	899	
15	UO	513	
16	UP	214	
17	UQ	896	
18	UR	594	
19	US	552	
20	UT	2493	
21	UU	939	
22	UV	1237	
23	UX	189	
24	CA	327	
24	CB	327	
25	CD	504	
26	CE	511	
27	CF	126	
27	CG	126	
28	CH	573	
29	CI	183	
30	CJ	290	



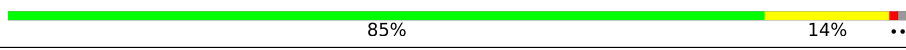


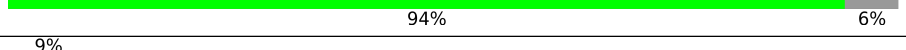

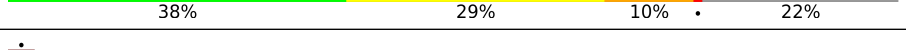
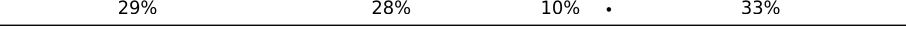
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	CK	593	
32	CL	1183	
33	CM	367	
34	CN	297	
35	JD	1267	
36	JF	252	
36	JG	252	
37	JH	483	
38	JI	1729	
39	JL	318	
40	JM	217	
41	JP	489	
42	Db	82	
43	JJ	274	
44	DA	255	
45	DE	261	
46	DF	225	
47	DG	236	
48	DH	190	
49	DI	200	
50	DJ	197	
51	DL	156	
52	DN	151	
53	DO	137	
54	DQ	143	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
55	DS	146	
56	DT	144	
57	DW	130	
58	DX	145	
59	DY	135	
60	Dc	67	
61	D2	81	
62	D3	1802	
63	D4	333	

2 Entry composition

There are 66 unique types of molecules in this entry. The entry contains 220657 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Periodic tryptophan protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	UA	792	Total	C	N	O	S	0	0
			6322	4040	1083	1181	18		

- Molecule 2 is a protein called Nucleolar complex protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	UB	553	Total	C	N	O	S	0	0
			4105	2602	736	756	11		

- Molecule 3 is a protein called Something about silencing protein 10.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	UC	86	Total	C	N	O	0	0
			694	430	139	125		

- Molecule 4 is a protein called U3 small nucleolar RNA-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	UD	663	Total	C	N	O	S	0	0
			5269	3339	915	994	21		

- Molecule 5 is a protein called U3 small nucleolar RNA-associated protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	UE	475	Total	C	N	O	S	0	0
			3772	2400	649	710	13		

- Molecule 6 is a protein called U3 small nucleolar RNA-associated protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	UF	293	Total	C	N	O	S	0	0
			2487	1605	435	434	13		

- Molecule 7 is a protein called U3 small nucleolar RNA-associated protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	UG	470	Total	C	N	O	S	0	0
			3718	2345	664	698	11		

- Molecule 8 is a protein called U3 small nucleolar RNA-associated protein 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	UH	474	Total	C	N	O	S	0	0
			2771	1706	513	549	3		

- Molecule 9 is a protein called U3 small nucleolar RNA-associated protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	UI	88	Total	C	N	O	S	0	0
			723	462	131	128	2		

- Molecule 10 is a protein called U3 small nucleolar RNA-associated protein 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	UJ	1116	Total	C	N	O	S	0	0
			8961	5802	1468	1666	25		

- Molecule 11 is a protein called U3 small nucleolar RNA-associated protein 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	UK	219	Total	C	N	O	S	0	0
			1845	1150	356	332	7		

- Molecule 12 is a protein called U3 small nucleolar RNA-associated protein 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	UL	779	Total	C	N	O	S	0	0
			6199	3974	1034	1164	27		

- Molecule 13 is a protein called U3 small nucleolar RNA-associated protein 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	UM	762	Total	C	N	O	S	0	0
			5970	3787	1007	1148	28		

- Molecule 14 is a protein called U3 small nucleolar RNA-associated protein 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	UN	203	Total	C	N	O	S	0	0
			1667	1038	313	314	2		

- Molecule 15 is a protein called U3 small nucleolar RNA-associated protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	UO	493	Total	C	N	O	S	0	0
			3911	2462	702	735	12		

- Molecule 16 is a protein called Bud site selection protein 21.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	UP	60	Total	C	N	O	0	0
			495	310	101	84		

- Molecule 17 is a protein called NET1-associated nuclear protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	UQ	820	Total	C	N	O	S	0	0
			6557	4171	1107	1260	19		

- Molecule 18 is a protein called U3 small nucleolar RNA-associated protein 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	UR	481	Total	C	N	O	S	0	0
			3791	2399	668	714	10		

- Molecule 19 is a protein called Nucleolar complex protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	US	487	Total	C	N	O	S	0	0
			3587	2305	610	660	12		

- Molecule 20 is a protein called U3 small nucleolar RNA-associated protein 20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	UT	2313	Total	C	N	O	S	0	0
			18789	12100	3144	3479	66		

- Molecule 21 is a protein called U3 small nucleolar RNA-associated protein 21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	UU	878	Total	C	N	O	S	0	0
			6922	4386	1198	1316	22		

- Molecule 22 is a protein called U3 small nucleolar RNA-associated protein 22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	UV	1083	Total	C	N	O	S	0	0
			8753	5692	1442	1595	24		

- Molecule 23 is a protein called rRNA-processing protein FCF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	UX	167	Total	C	N	O	S	0	0
			1330	854	241	225	10		

- Molecule 24 is a protein called rRNA 2'-O-methyltransferase fibrillarin.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	CA	242	Total	C	N	O	S	0	0
			1881	1193	338	340	10		
24	CB	228	Total	C	N	O	S	0	0
			1782	1131	320	321	10		

- Molecule 25 is a protein called Nucleolar protein 56.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	CD	380	Total	C	N	O	S	0	0
			2994	1898	513	574	9		

- Molecule 26 is a protein called Nucleolar protein 58.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CE	436	Total	C	N	O	S	0	0
			3326	2093	571	654	8		

- Molecule 27 is a protein called 13 kDa ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	CF	121	Total	C	N	O	S	0	0
			916	583	158	171	4		
27	CG	121	Total	C	N	O	S	0	0
			916	583	158	171	4		

- Molecule 28 is a protein called Ribosomal RNA-processing protein 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	CH	467	Total	C	N	O	S	0	0
			3736	2371	655	700	10		

- Molecule 29 is a protein called U3 small nucleolar ribonucleoprotein protein IMP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CI	175	Total	C	N	O	S	0	0
			1468	929	276	256	7		

- Molecule 30 is a protein called U3 small nucleolar ribonucleoprotein protein IMP4.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	CJ	256	Total	C	N	O	S	0	0
			2081	1306	394	374	7		

- Molecule 31 is a protein called U3 small nucleolar RNA-associated protein MPP10.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	CK	222	Total	C	N	O	S	0	0
			1789	1111	311	363	4		

- Molecule 32 is a protein called Ribosome biogenesis protein BMS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	CL	808	Total	C	N	O	S	0	0
			6551	4187	1171	1165	28		

- Molecule 33 is a protein called RNA 3'-terminal phosphate cyclase-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	CM	360	Total	C	N	O	S	0	0
			2781	1781	473	516	11		

- Molecule 34 is a protein called Ribosomal RNA-processing protein 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	CN	229	Total	C	N	O	S	0	0
			1868	1197	317	347	7		

- Molecule 35 is a protein called Probable ATP-dependent RNA helicase DHR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	JD	811	Total	C	N	O	S	0	0
			6509	4163	1151	1160	35		

- Molecule 36 is a protein called Ribosomal RNA small subunit methyltransferase NEP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	JF	216	Total	C	N	O	S	0	0
			1701	1079	296	315	11		
36	JG	230	Total	C	N	O	S	0	0
			1799	1142	313	333	11		

- Molecule 37 is a protein called Essential nuclear protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	JH	261	Total	C	N	O	0	0
			1295	773	261	261		

- Molecule 38 is a protein called rRNA biogenesis protein RRP5.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	JI	265	Total	C	N	O	0	0
			1314	784	265	265		

- Molecule 39 is a protein called Dimethyladenosine transferase.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	JL	283	Total	C	N	O	S	0	0
			2262	1439	401	408	14		

- Molecule 40 is a protein called rRNA-processing protein FCF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	JM	134	Total	C	N	O	S	0	0
			1131	715	206	207	3		

- Molecule 41 is a protein called Protein SOF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	JP	461	Total	C	N	O	S	0	0
			3765	2354	686	709	16		

- Molecule 42 is a protein called 40S ribosomal protein S27-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Db	81	Total	C	N	O	S	0	0
			610	382	110	113	5		

- Molecule 43 is a protein called Pre-rRNA-processing protein PNO1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	JJ	199	Total	C	N	O	S	0	0
			1573	1001	285	283	4		

- Molecule 44 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	DA	240	Total	C	N	O	S	0	0
			1912	1209	354	345	4		

- Molecule 45 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	DE	246	Total	C	N	O	S	0	0
			1950	1248	361	338	3		

- Molecule 46 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	DF	213	Total	C	N	O	S	0	0
			1669	1045	307	314	3		

- Molecule 47 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	DG	218	Total	C	N	O	S	0	0
			1755	1102	337	313	3		

- Molecule 48 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	DH	170	Total	C	N	O		0	0
			1361	880	235	246			

- Molecule 49 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	DI	177	Total	C	N	O	S	0	0
			1399	869	279	249	2		

- Molecule 50 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	DJ	185	Total	C	N	O	S	0	0
			1494	943	289	261	1		

- Molecule 51 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	DL	140	Total	C	N	O	S	0	0
			1129	724	215	187	3		

- Molecule 52 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	DN	150	Total	C	N	O	S	0	0
			1192	759	224	207	2		

- Molecule 53 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	DO	127	Total	C	N	O	S	0	0
			922	567	185	167	3		

- Molecule 54 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	DQ	125	Total	C	N	O	0	0
			969	623	174	172		

- Molecule 55 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	DS	105	Total	C	N	O	S	0	0
			861	545	160	154	2		

- Molecule 56 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	DT	143	Total	C	N	O	S	0	0
			1112	694	208	208	2		

- Molecule 57 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	DW	129	Total	C	N	O	S	0	0
			1021	650	188	180	3		

- Molecule 58 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	DX	143	Total	C	N	O	S	0	0
			1115	705	219	189	2		

- Molecule 59 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	DY	134	Total	C	N	O	S	0	0
			1073	676	208	189			

- Molecule 60 is a protein called 40S ribosomal protein S28-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Dc	63	Total	C	N	O	S	0	0
			497	306	99	91	1		

- Molecule 61 is a RNA chain called 5ETS RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	D2	81	Total	C	N	O	P	0	0
			1741	777	319	564	81		

- Molecule 62 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	D3	1409	Total	C	N	O	P	0	0
			30041	13429	5342	9861	1409		

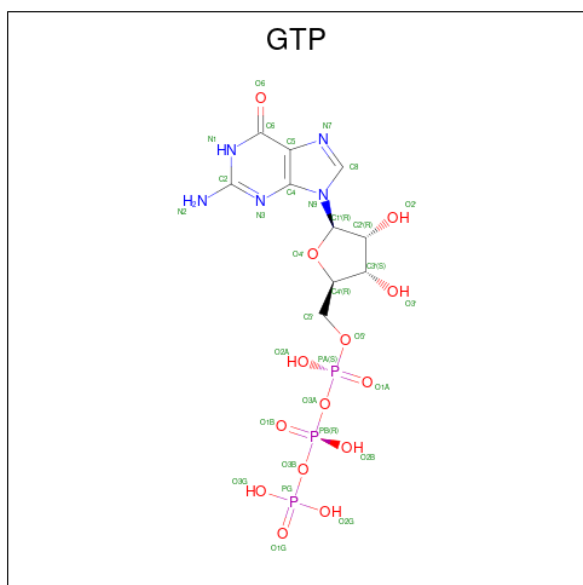
- Molecule 63 is a RNA chain called U3 snoRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	D4	223	Total	C	N	O	P	0	0
			4723	2114	819	1567	223		

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
64	UX	1	Total	Zn	0
			1	1	
64	Db	1	Total	Zn	0
			1	1	

- Molecule 65 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

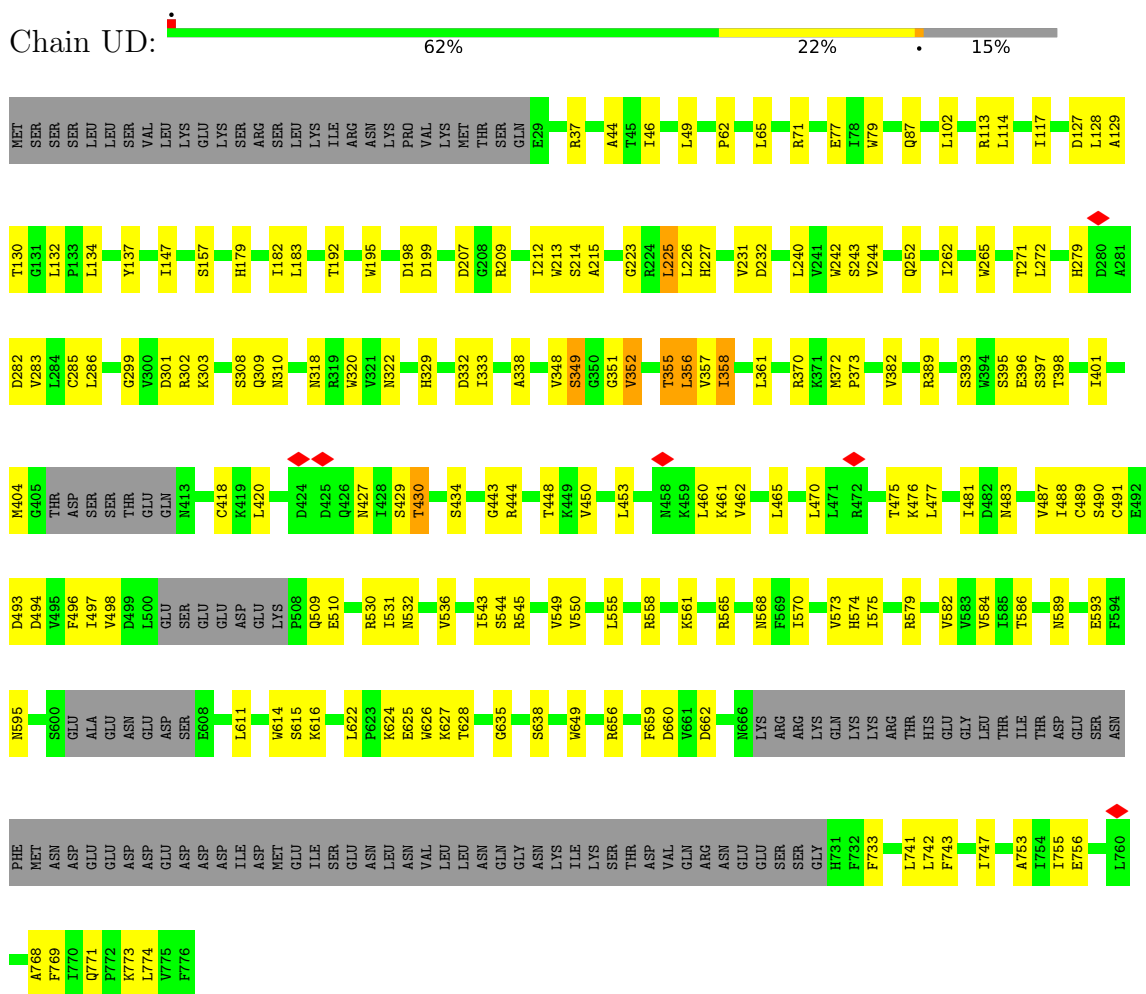


Mol	Chain	Residues	Atoms					AltConf
65	CL	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 66 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
66	CL	1	Total	Mg	0
			1	1	

- Molecule 4: U3 small nucleolar RNA-associated protein 4



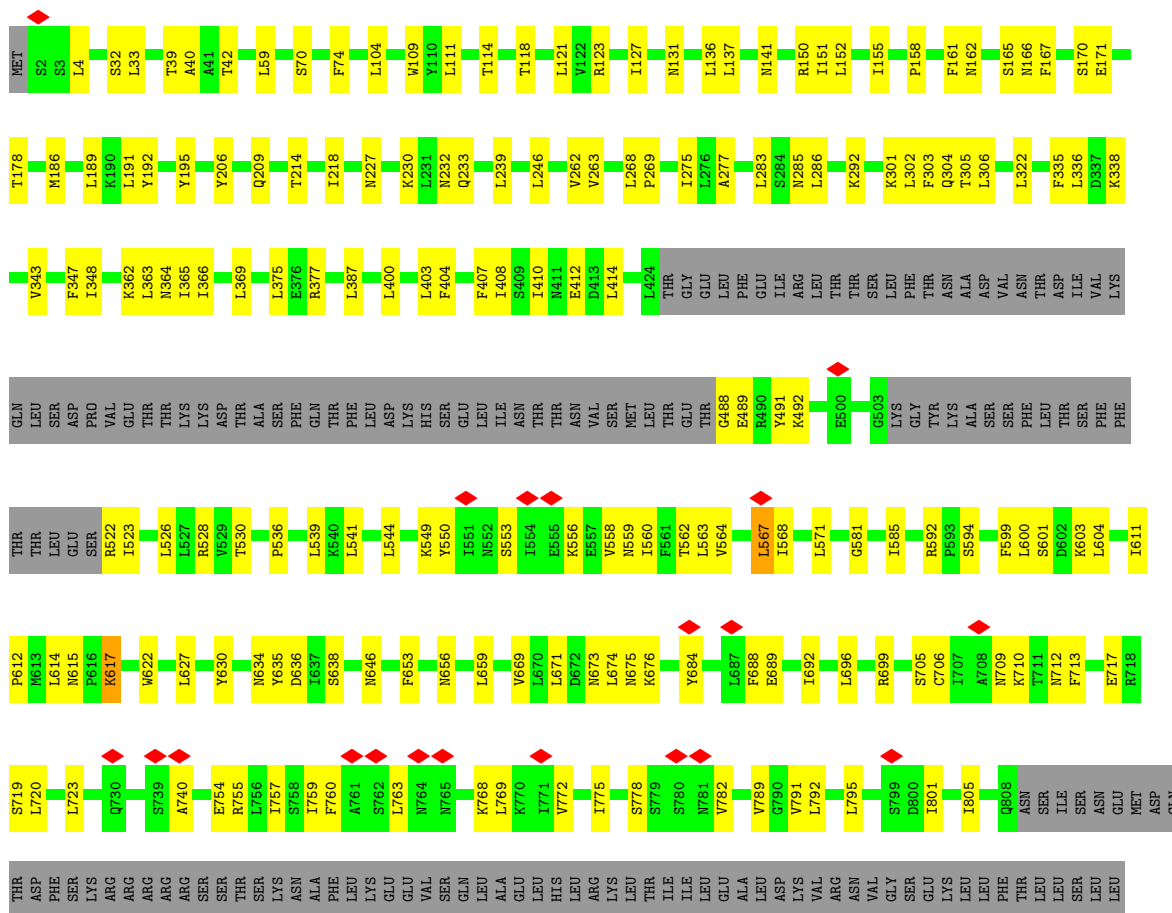
- Molecule 5: U3 small nucleolar RNA-associated protein 5





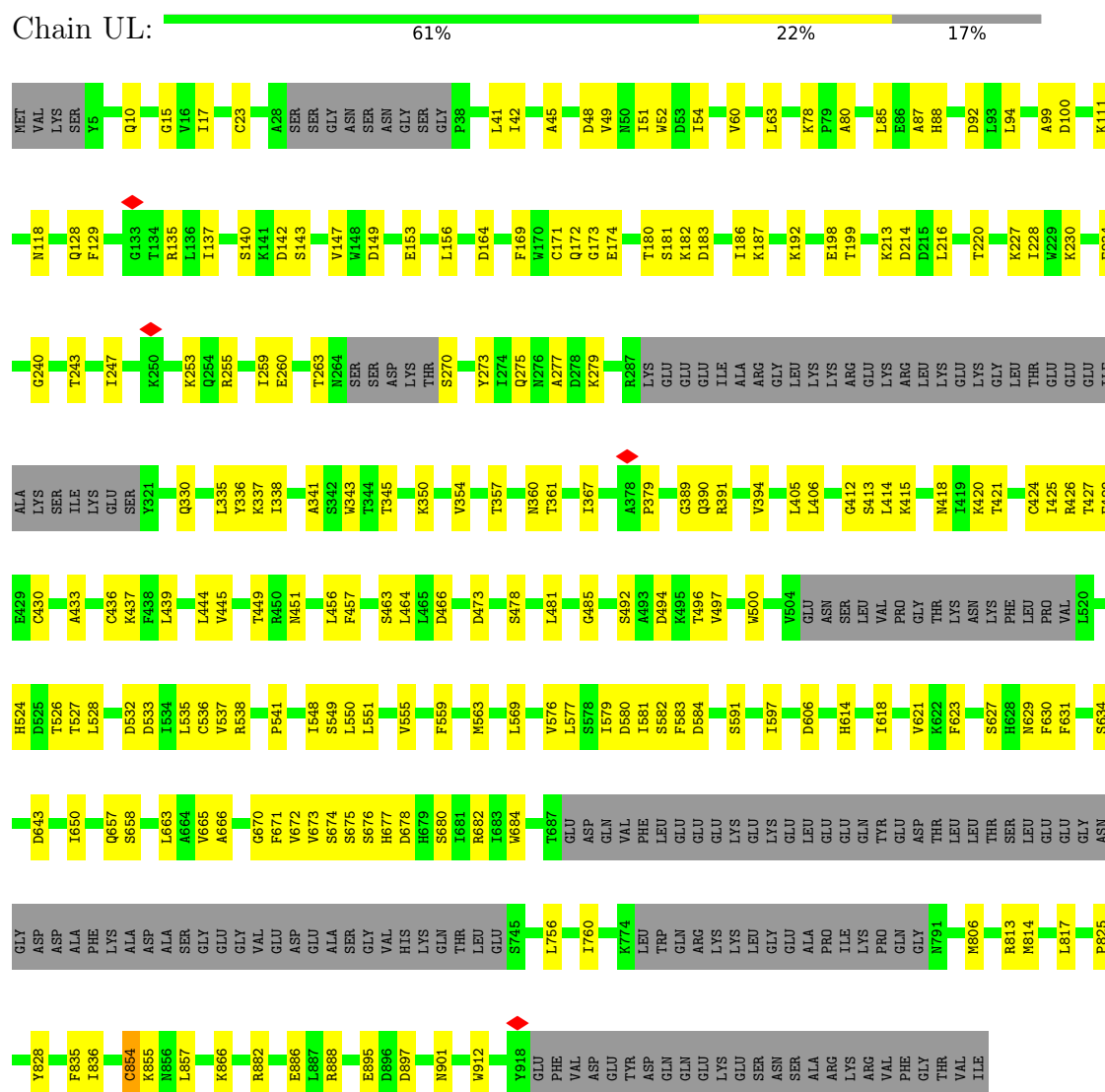
[illegible]

- Molecule 10: U3 small nucleolar RNA-associated protein 10



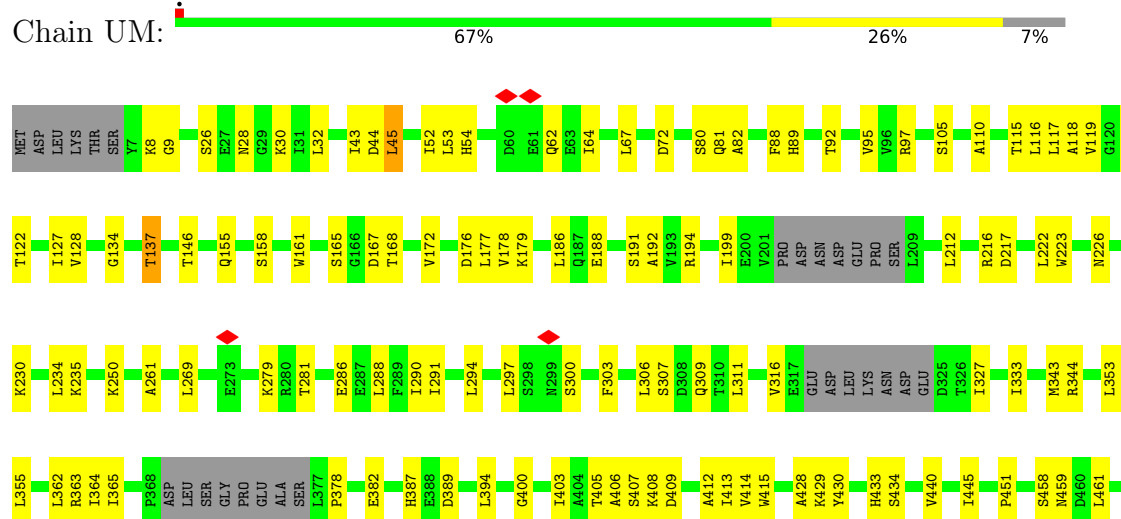


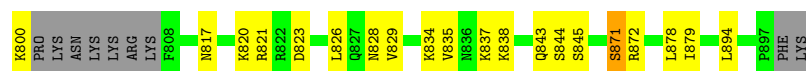
Chain UL:



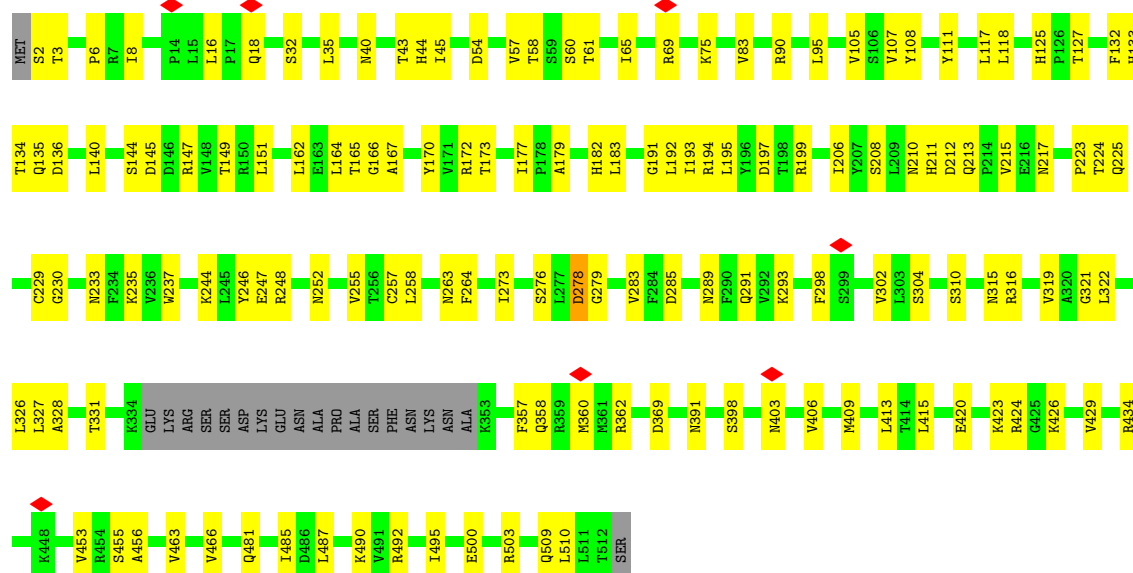
- Molecule 13: U3 small nucleolar RNA-associated protein 13

Chain UM:

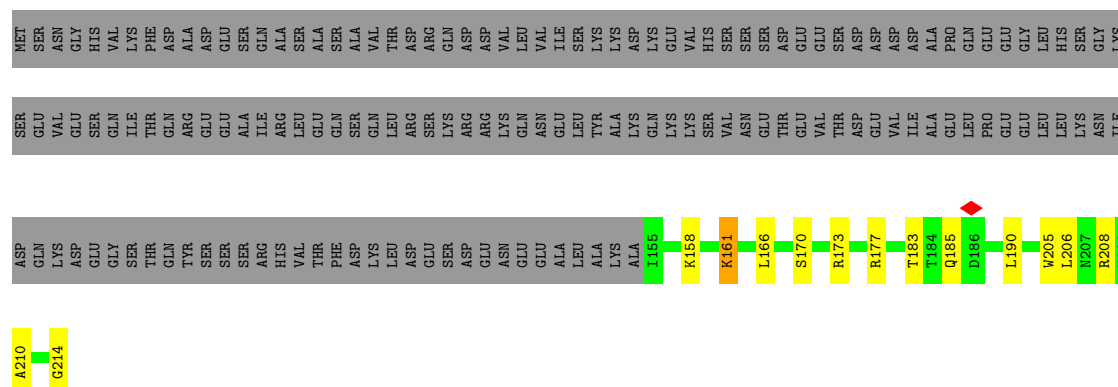




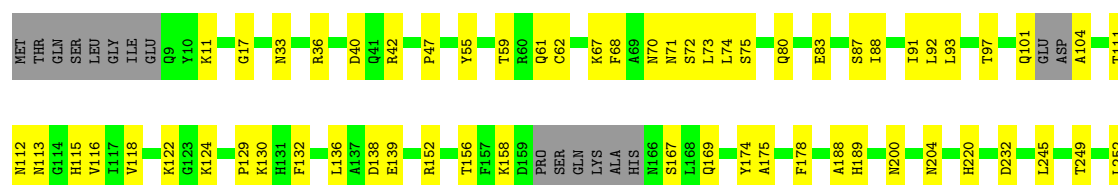
- Molecule 15: U3 small nucleolar RNA-associated protein 15

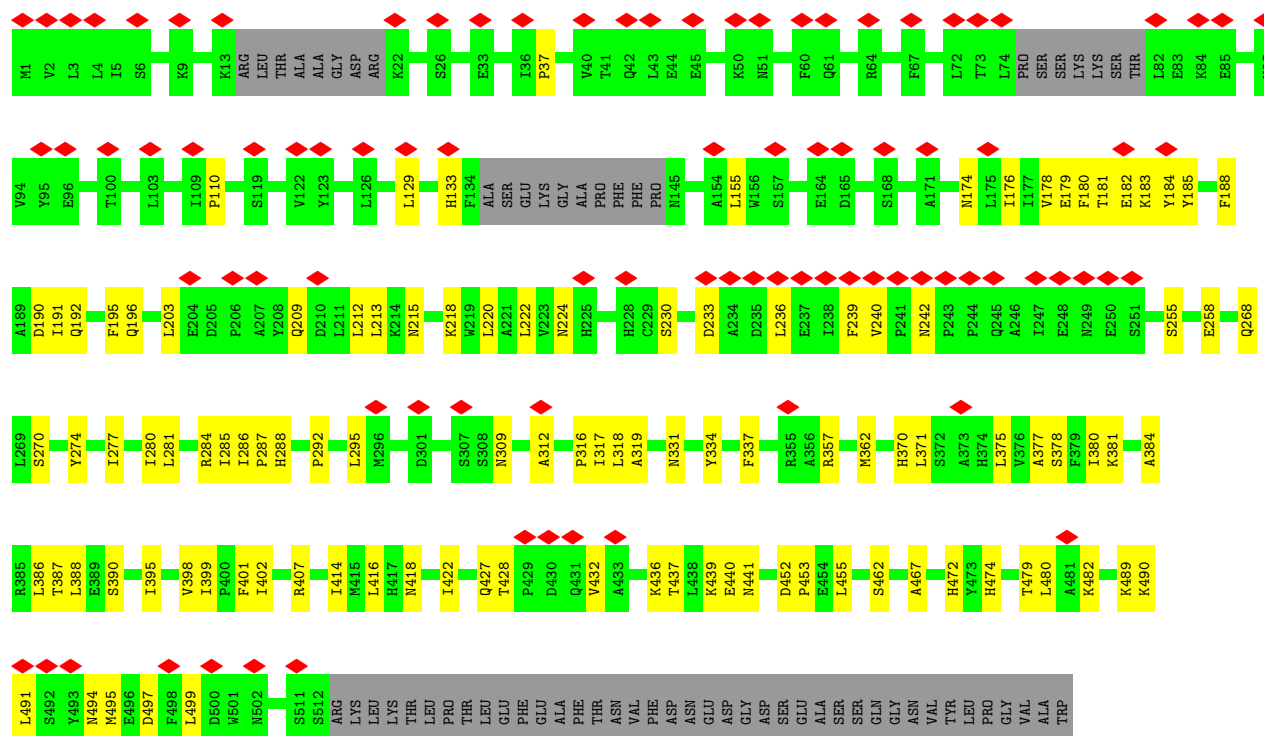


- Molecule 16: Bud site selection protein 21



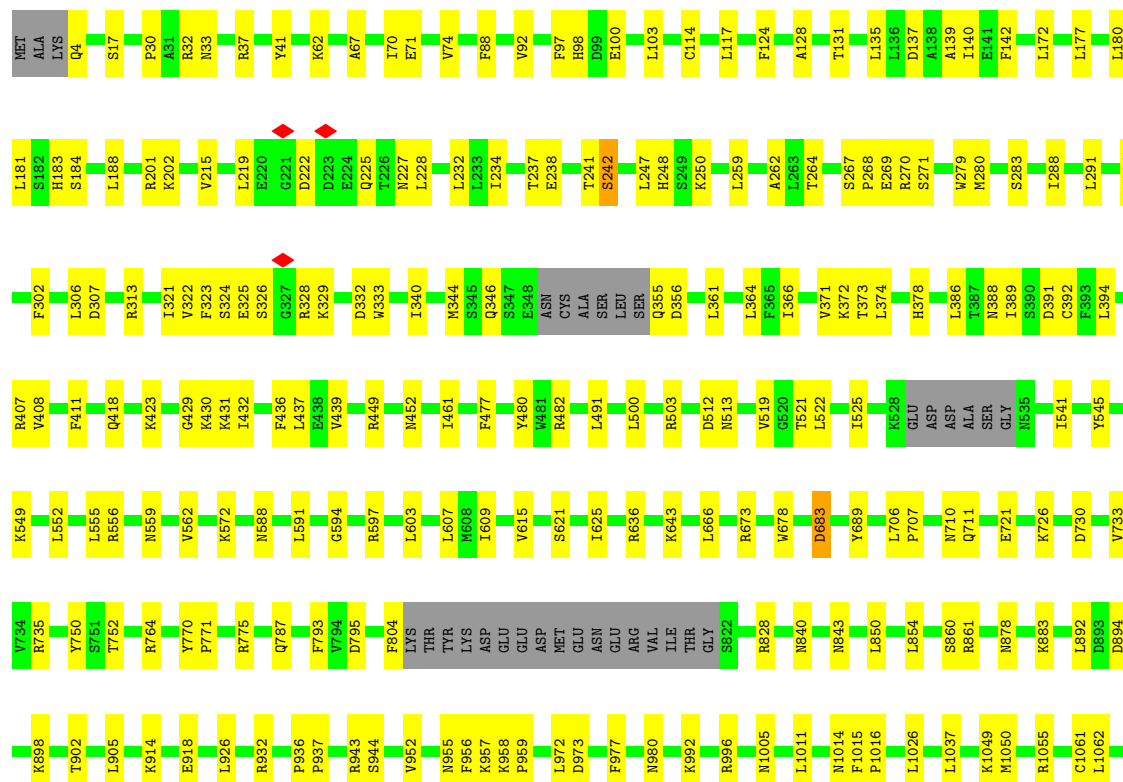
- Molecule 17: NET1-associated nuclear protein 1





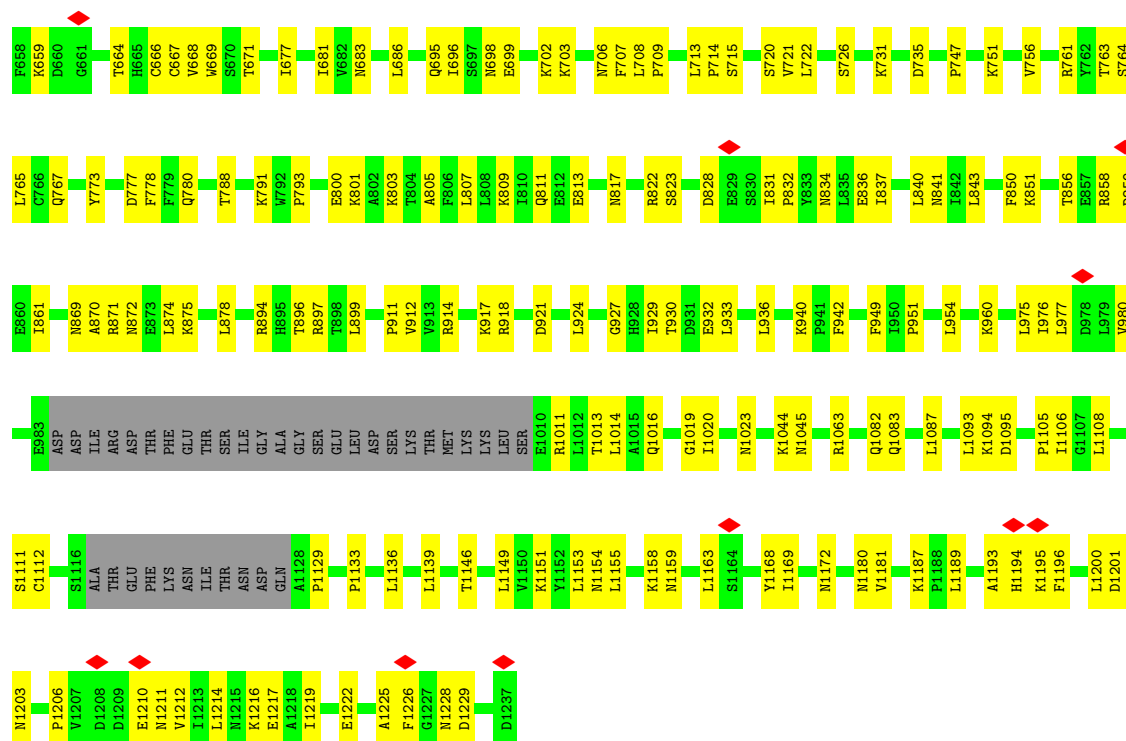
• Molecule 20: U3 small nucleolar RNA-associated protein 20

Chain UT: 71% 22% 7%

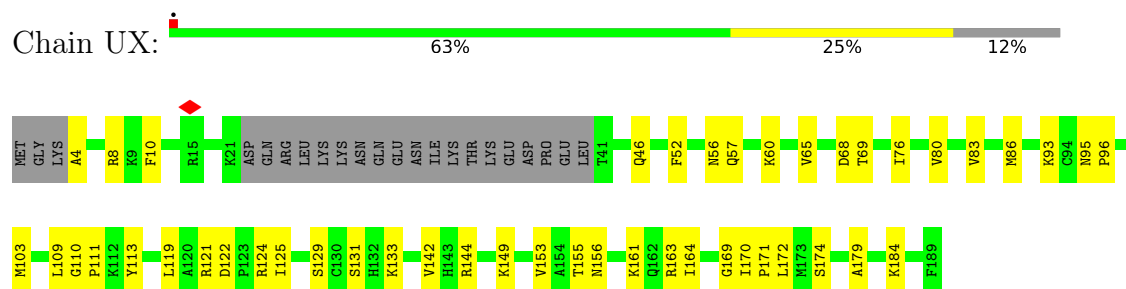




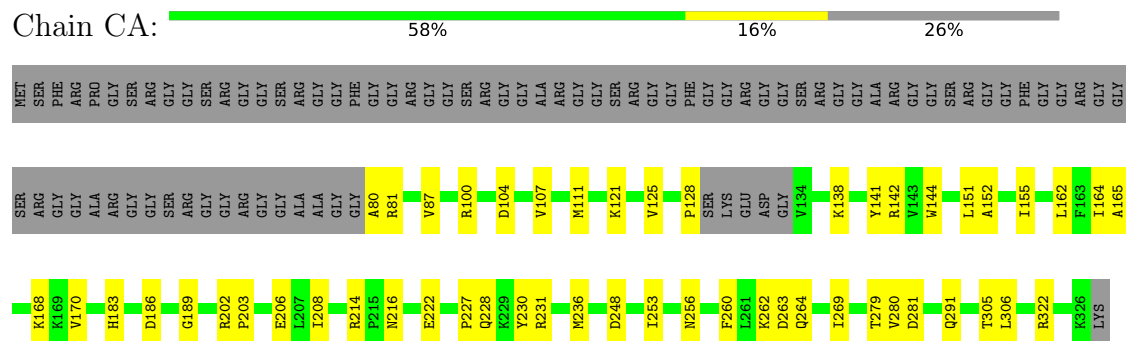




- Molecule 23: rRNA-processing protein FCF1

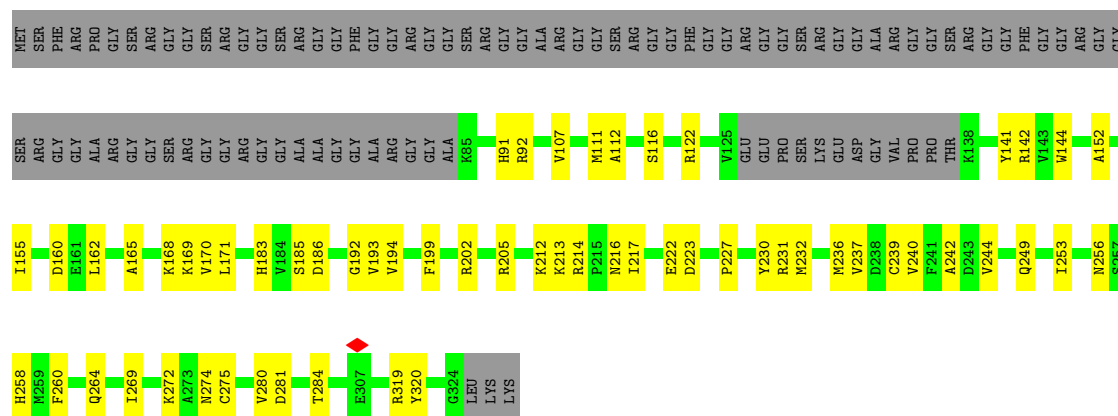


- Molecule 24: rRNA 2'-O-methyltransferase fibrillar

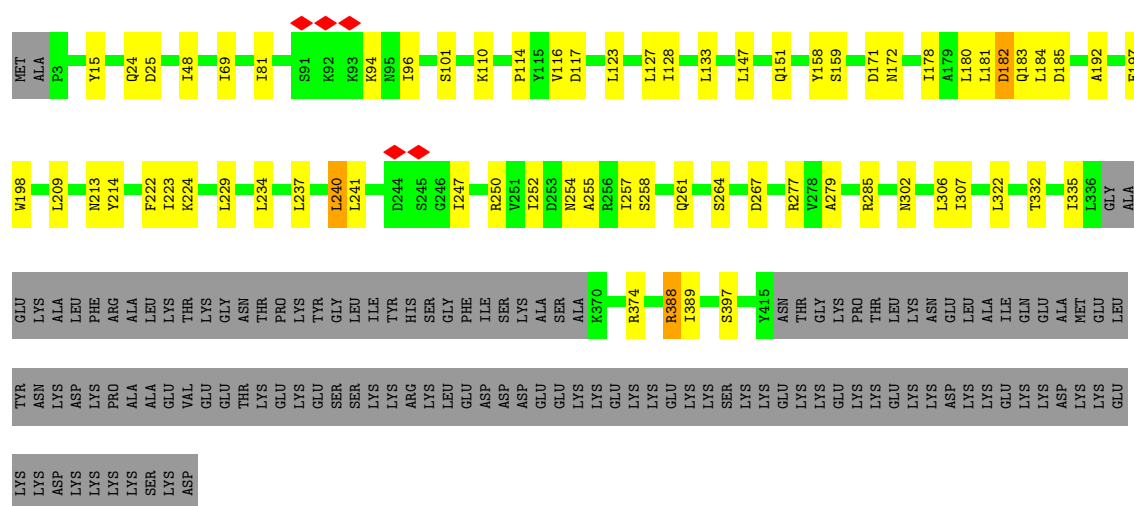


- Molecule 24: rRNA 2'-O-methyltransferase fibrillar

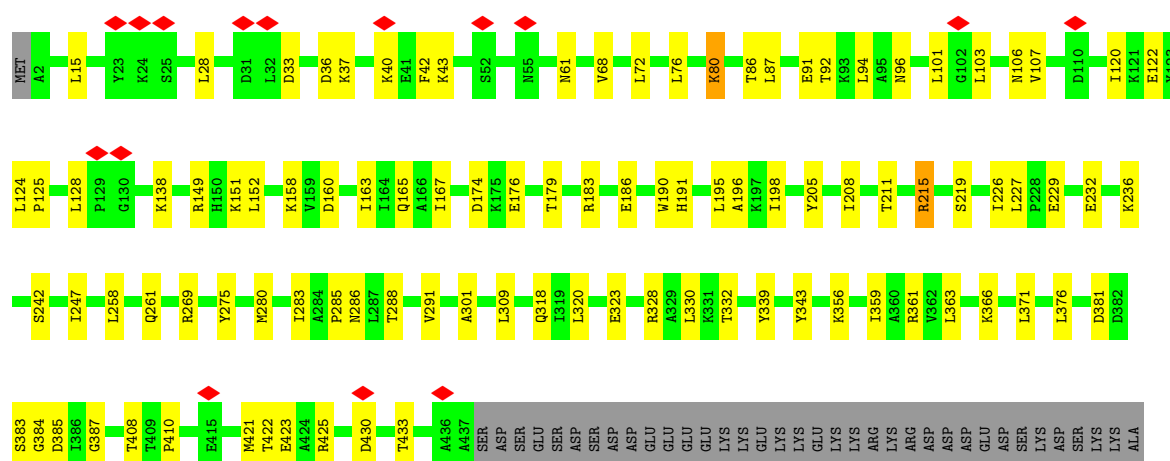




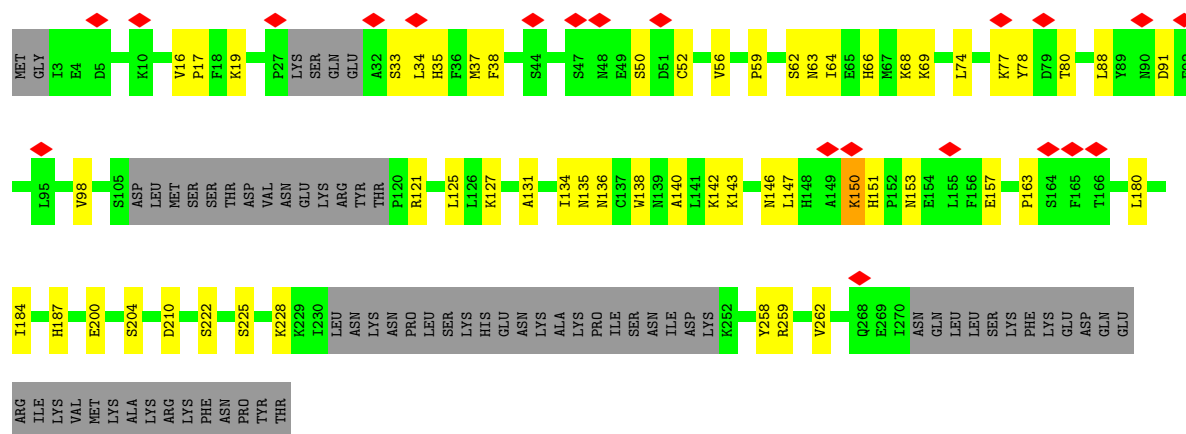
• Molecule 25: Nucleolar protein 56



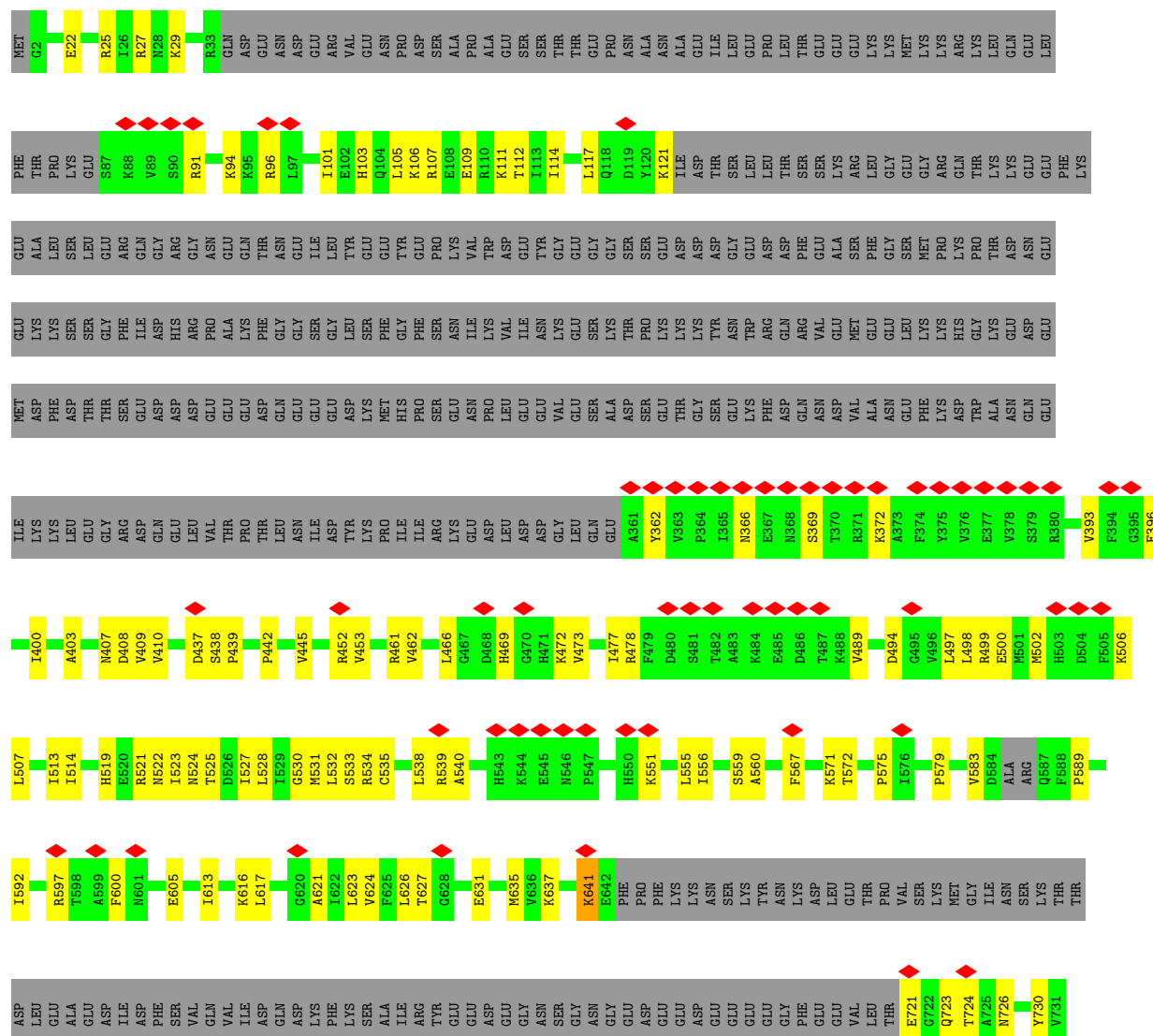
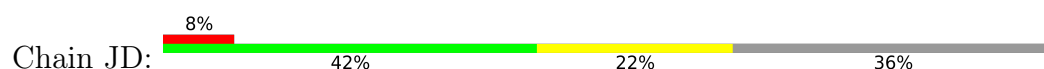
• Molecule 26: Nucleolar protein 58



-
- MET E2 N5 K6 Q7 H8 R9 K10 L21 N27 A28 K29 R45 L54 H55 P69 V72 P77 P78 G79 T80 G81 K82 T83 T84 L85 L86 S88 R87 L89 V90 R91 R92 R93 M93 L98 N99 I105 T106 V107 I108 I109 G110 K111 R114 F117 L118 E119 P120 D123 N126 I129 D130 I131 A132 K133 I134 A135 D136 L137 L140 L141 T152 M153 I158 V170 A171 T172 H173 L174 S179 Q180 S181 T182 V195 T196 Q200 K203 Y206 L207 S208 G209 V210 R214 Y215 R218 E219 L220 L221 N222 R225 K231 P238

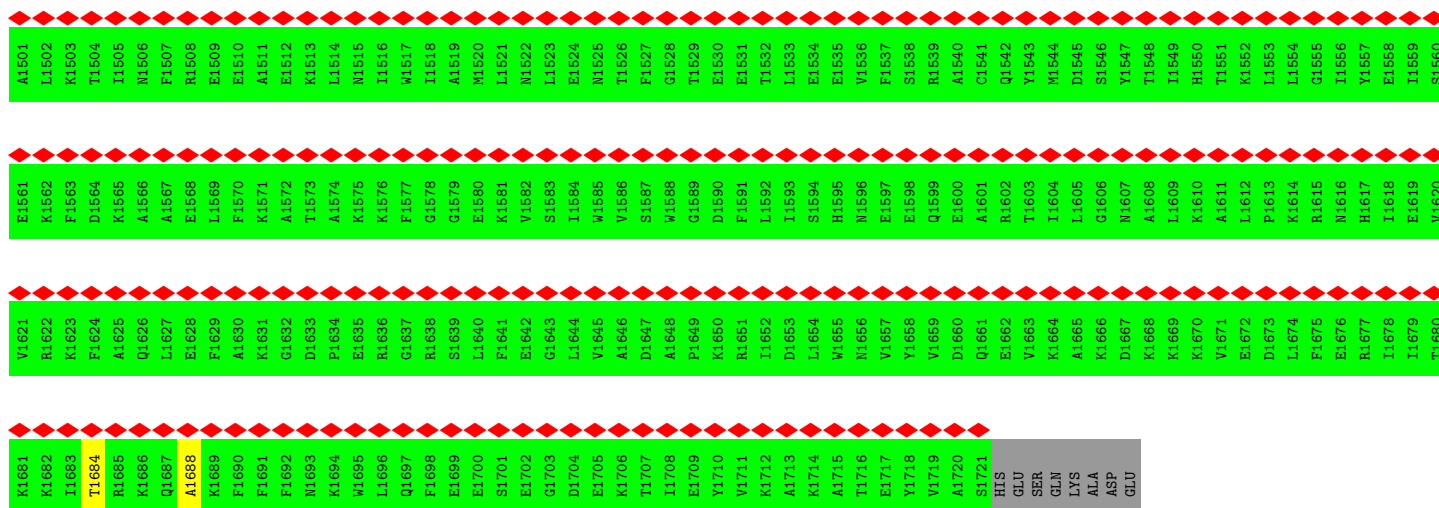


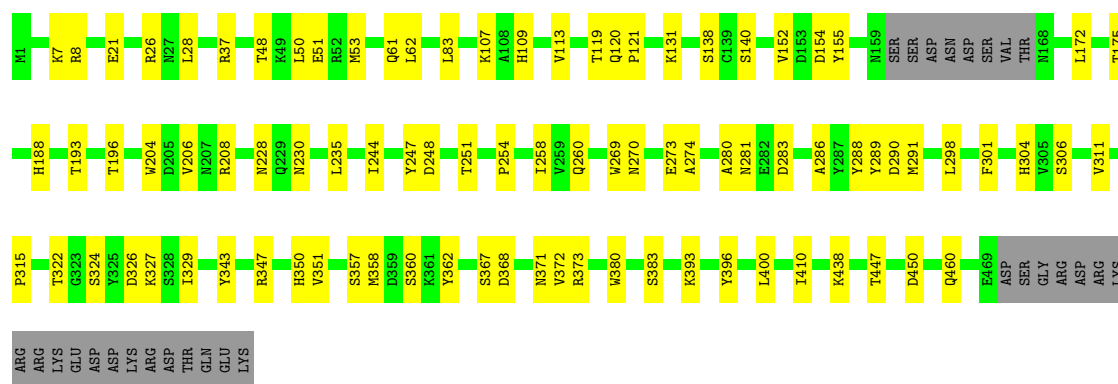
● Molecule 35: Probable ATP-dependent RNA helicase DHR1











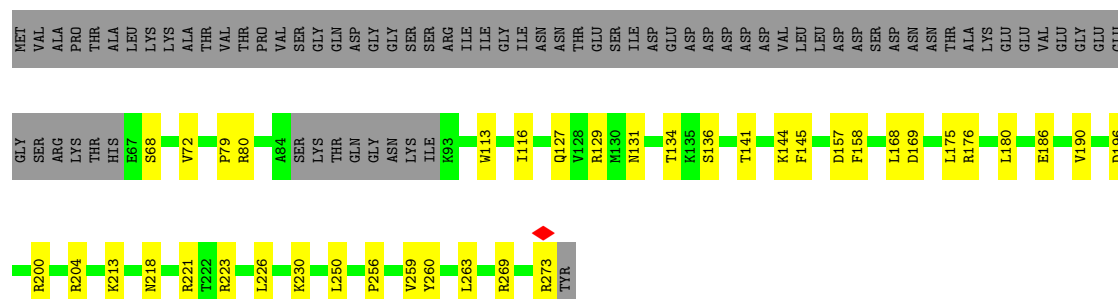
• Molecule 42: 40S ribosomal protein S27-A

Chain Db: 99% .



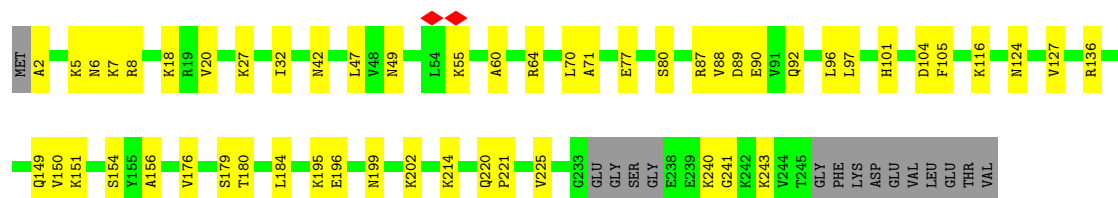
• Molecule 43: Pre-rRNA-processing protein PNO1

Chain JJ: 58% 14% 27%



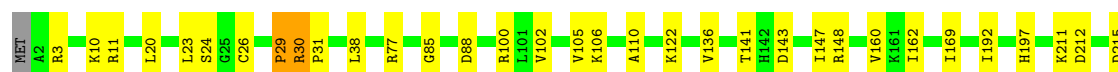
• Molecule 44: 40S ribosomal protein S1-A

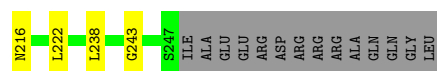
Chain DA: 73% 21% 6%



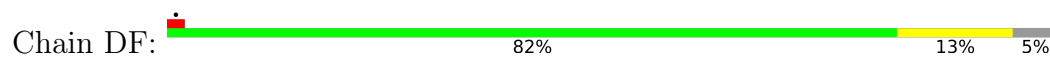
• Molecule 45: 40S ribosomal protein S4-A

Chain DE: 80% 13% 6%

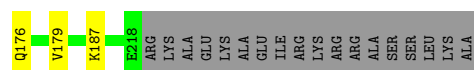
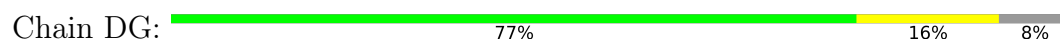




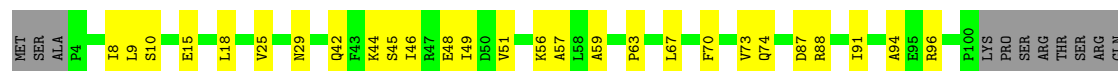
• Molecule 46: Rps5p



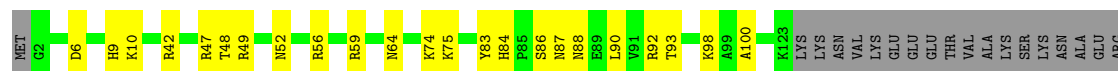
• Molecule 47: 40S ribosomal protein S6-A



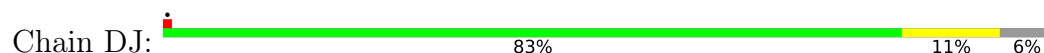
• Molecule 48: 40S ribosomal protein S7-A



• Molecule 49: 40S ribosomal protein S8-A

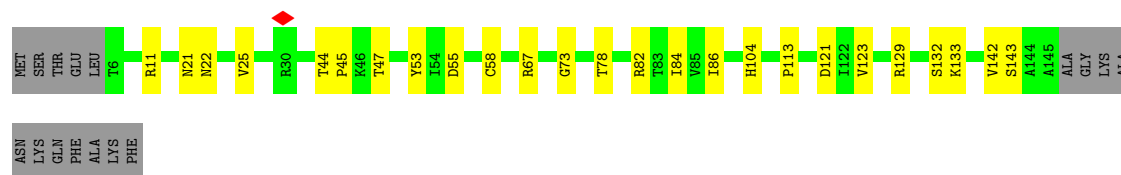
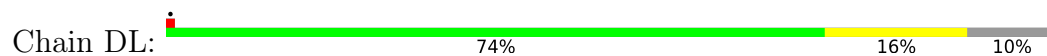


• Molecule 50: 40S ribosomal protein S9-A

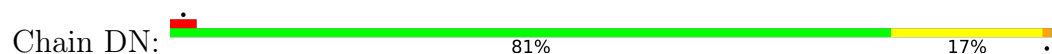




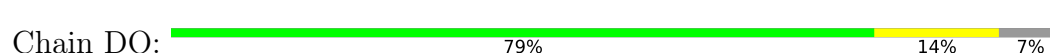
- Molecule 51: 40S ribosomal protein S11-A



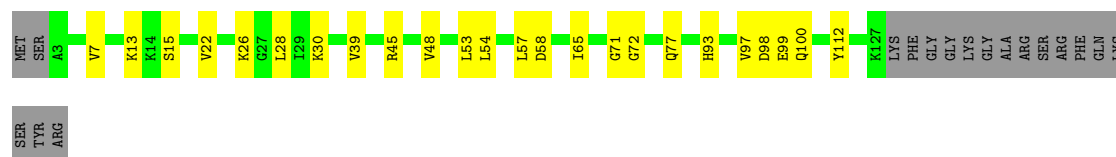
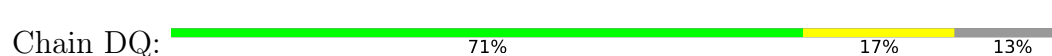
- Molecule 52: 40S ribosomal protein S13



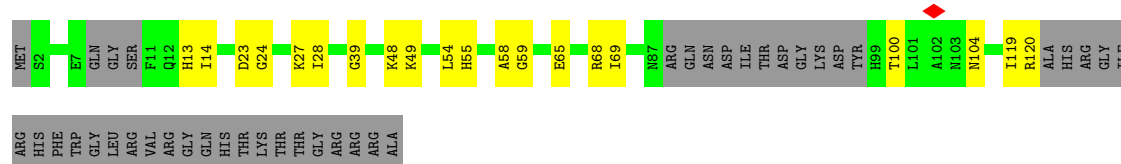
- Molecule 53: 40S ribosomal protein S14-A




- Molecule 54: 40S ribosomal protein S16-A



- Molecule 55: 40S ribosomal protein S18-A




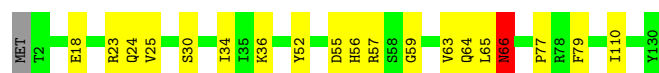
- Molecule 56: 40S ribosomal protein S19-A

Chain DT:  83% 17%




- Molecule 57: 40S ribosomal protein S22-A

Chain DW:  85% 14%



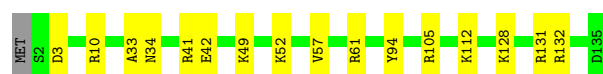
- Molecule 58: 40S ribosomal protein S23-A

Chain DX:  83% 15%



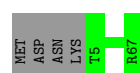
- Molecule 59: 40S ribosomal protein S24-A

Chain DY:  87% 12%



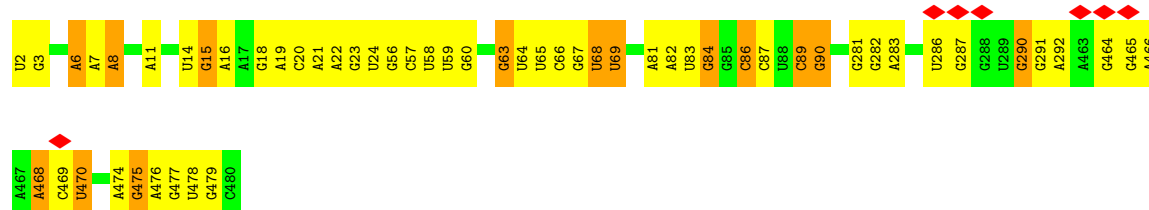
- Molecule 60: 40S ribosomal protein S28-A

Chain Dc:  94% 6%



- Molecule 61: 5ETS RNA

Chain D2:  9% 31% 52% 17%



- Molecule 62: 18S rRNA

Chain D3:  38% 29% 10% 22%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	176136	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 ($e^-/\text{\AA}^2$)	44, 28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k), FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.126	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	520.32, 520.32, 520.32	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, 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	UA	0.47	0/6465	0.57	1/8752 (0.0%)
2	UB	0.28	0/4158	0.53	4/5607 (0.1%)
3	UC	0.52	0/699	0.55	0/919
4	UD	0.33	0/5369	0.55	1/7272 (0.0%)
5	UE	0.35	0/3840	0.55	0/5208
6	UF	0.36	0/2538	0.47	0/3405
7	UG	0.41	0/3796	0.55	0/5126
8	UH	0.26	0/2773	0.58	12/3798 (0.3%)
9	UI	0.26	0/735	0.56	0/987
10	UJ	0.33	0/9111	0.53	1/12323 (0.0%)
11	UK	0.35	0/1869	0.50	0/2472
12	UL	0.34	0/6324	0.56	0/8546
13	UM	0.33	0/6071	0.58	2/8218 (0.0%)
14	UN	0.38	0/1697	0.50	0/2284
15	UO	0.31	0/3993	0.55	0/5413
16	UP	0.26	0/499	0.57	0/659
17	UQ	0.30	0/6688	0.53	1/9062 (0.0%)
18	UR	0.39	0/3875	0.54	0/5254
19	US	0.28	0/3667	0.53	3/5001 (0.1%)
20	UT	0.37	0/19132	0.53	3/25831 (0.0%)
21	UU	0.41	0/7059	0.52	0/9536
22	UV	0.30	0/8962	0.53	0/12120
23	UX	0.55	0/1353	0.61	0/1819
24	CA	0.60	1/1917 (0.1%)	0.58	0/2588
24	CB	0.36	0/1815	0.54	0/2448
25	CD	0.41	0/3041	0.52	1/4098 (0.0%)
26	CE	0.36	0/3364	0.54	0/4539
27	CF	0.45	0/928	0.59	1/1262 (0.1%)
27	CG	0.45	0/928	0.59	1/1262 (0.1%)
28	CH	0.49	0/3809	0.56	0/5128
29	CI	0.35	0/1494	0.57	0/2008
30	CJ	0.45	0/2118	0.60	0/2855

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	CK	0.34	0/1808	0.48	0/2424
32	CL	0.49	0/6691	0.57	1/9000 (0.0%)
33	CM	0.41	0/2832	0.53	0/3825
34	CN	0.30	0/1909	0.51	0/2571
35	JD	0.31	0/6634	0.58	0/8927
36	JF	0.29	0/1727	0.60	1/2329 (0.0%)
36	JG	0.29	0/1828	0.54	0/2470
37	JH	0.23	0/1293	0.36	0/1801
38	JI	0.27	0/1313	0.54	0/1830
39	JL	0.29	0/2305	0.53	0/3116
40	JM	0.40	0/1151	0.52	0/1535
41	JP	0.52	0/3844	0.58	2/5174 (0.0%)
42	Db	0.42	0/620	0.53	0/838
43	JJ	0.37	0/1600	0.53	1/2154 (0.0%)
44	DA	0.38	0/1937	0.52	0/2593
45	DE	0.60	0/1991	0.61	0/2683
46	DF	0.41	0/1690	0.52	0/2285
47	DG	0.44	0/1779	0.52	0/2379
48	DH	0.37	0/1383	0.54	0/1863
49	DI	0.50	0/1422	0.53	0/1899
50	DJ	0.59	0/1519	0.60	0/2035
51	DL	0.58	0/1155	0.54	0/1557
52	DN	0.45	0/1215	0.51	1/1638 (0.1%)
53	DO	0.39	0/933	0.55	0/1256
54	DQ	0.47	0/986	0.59	0/1330
55	DS	0.29	0/871	0.52	0/1171
56	DT	0.35	0/1130	0.49	0/1517
57	DW	0.58	0/1038	0.57	0/1395
58	DX	0.49	0/1133	0.56	0/1510
59	DY	0.61	0/1087	0.54	0/1449
60	Dc	0.43	0/499	0.57	0/670
61	D2	0.43	0/1946	1.08	3/3024 (0.1%)
62	D3	0.95	11/33585 (0.0%)	1.21	296/52288 (0.6%)
63	D4	0.63	0/5267	1.17	42/8178 (0.5%)
All	All	0.52	12/228208 (0.0%)	0.72	378/316514 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	UM	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
15	UO	0	1
20	UT	0	1
21	UU	0	1
23	UX	0	1
25	CD	0	1
35	JD	0	2
49	DI	0	1
59	DY	0	1
All	All	0	10

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	D3	355	G	N3-C4	-6.66	1.30	1.35
62	D3	118	U	C2-N3	-6.49	1.33	1.37
62	D3	355	G	C2-N3	-6.38	1.27	1.32
62	D3	622	A	N9-C4	-6.38	1.34	1.37
62	D3	545	A	C5-C4	-6.18	1.34	1.38

The worst 5 of 378 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	D3	1104	U	C2-N3-C4	-13.68	118.79	127.00
62	D3	850	A	OP1-P-OP2	12.73	138.70	119.60
62	D3	629	U	N3-C2-O2	-12.59	113.39	122.20
62	D3	355	G	N3-C2-N2	-12.17	111.38	119.90
13	UM	45	LEU	C-N-CA	11.65	150.84	121.70

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	UM	400	GLY	Peptide
15	UO	278	ASP	Peptide
20	UT	1925	ASP	Peptide
21	UU	94	TYR	Peptide
23	UX	52	PHE	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	UA	6322	0	6223	108	0
2	UB	4105	0	3846	77	0
3	UC	694	0	742	8	0
4	UD	5269	0	5281	126	0
5	UE	3772	0	3806	83	0
6	UF	2487	0	2533	32	0
7	UG	3718	0	3721	86	0
8	UH	2771	0	1817	33	0
9	UI	723	0	770	17	0
10	UJ	8961	0	9273	178	0
11	UK	1845	0	1926	38	0
12	UL	6199	0	6221	140	0
13	UM	5970	0	6008	146	0
14	UN	1667	0	1658	28	0
15	UO	3911	0	3906	100	0
16	UP	495	0	561	11	0
17	UQ	6557	0	6489	158	0
18	UR	3791	0	3772	67	0
19	US	3587	0	3200	64	0
20	UT	18789	0	19126	362	0
21	UU	6922	0	6886	123	0
22	UV	8753	0	8867	212	0
23	UX	1330	0	1416	29	0
24	CA	1881	0	1928	38	0
24	CB	1782	0	1826	52	0
25	CD	2994	0	3018	53	0
26	CE	3326	0	3406	70	0
27	CF	916	0	964	13	0
27	CG	916	0	964	16	0
28	CH	3736	0	3756	67	0
29	CI	1468	0	1519	28	0
30	CJ	2081	0	2112	58	0
31	CK	1789	0	1801	34	0
32	CL	6551	0	6706	117	0
33	CM	2781	0	2878	50	0
34	CN	1868	0	1845	37	0
35	JD	6509	0	6724	181	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	JF	1701	0	1767	47	0
36	JG	1799	0	1872	41	0
37	JH	1295	0	570	2	0
38	JI	1314	0	610	4	0
39	JL	2262	0	2330	53	0
40	JM	1131	0	1161	15	0
41	JP	3765	0	3714	59	0
42	Db	610	0	629	0	0
43	JJ	1573	0	1650	29	0
44	DA	1912	0	2023	42	0
45	DE	1950	0	2035	29	0
46	DF	1669	0	1724	19	0
47	DG	1755	0	1846	30	0
48	DH	1361	0	1437	22	0
49	DI	1399	0	1431	23	0
50	DJ	1494	0	1573	14	0
51	DL	1129	0	1196	14	0
52	DN	1192	0	1255	20	0
53	DO	922	0	946	13	0
54	DQ	969	0	1025	23	0
55	DS	861	0	896	16	0
56	DT	1112	0	1124	17	0
57	DW	1021	0	1060	12	0
58	DX	1115	0	1191	18	0
59	DY	1073	0	1132	13	0
60	Dc	497	0	535	0	0
61	D2	1741	0	876	60	0
62	D3	30041	0	15138	476	0
63	D4	4723	0	2398	104	0
64	Db	1	0	0	0	0
64	UX	1	0	0	0	0
65	CL	32	0	12	1	0
66	CL	1	0	0	0	0
All	All	220657	0	202651	3829	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 3829 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:UD:356:LEU:HD23	4:UD:372:MET:CB	1.55	1.35
1:UA:77:GLY:HA3	1:UA:95:PHE:O	1.26	1.31
32:CL:964:ALA:O	32:CL:975:GLU:HA	1.29	1.30
62:D3:618:U:C2	62:D3:1086:A:N6	2.03	1.26
15:UO:191:GLY:HA3	15:UO:211:HIS:O	1.07	1.25

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	UA	786/923 (85%)	717 (91%)	69 (9%)	0	100	100
2	UB	535/810 (66%)	509 (95%)	24 (4%)	2 (0%)	34	70
3	UC	82/610 (13%)	72 (88%)	10 (12%)	0	100	100
4	UD	653/776 (84%)	598 (92%)	55 (8%)	0	100	100
5	UE	465/643 (72%)	426 (92%)	39 (8%)	0	100	100
6	UF	283/440 (64%)	277 (98%)	6 (2%)	0	100	100
7	UG	464/554 (84%)	421 (91%)	43 (9%)	0	100	100
8	UH	446/713 (63%)	372 (83%)	54 (12%)	20 (4%)	2	25
9	UI	86/575 (15%)	83 (96%)	3 (4%)	0	100	100
10	UJ	1092/1769 (62%)	1040 (95%)	52 (5%)	0	100	100
11	UK	213/250 (85%)	198 (93%)	14 (7%)	1 (0%)	29	66
12	UL	765/943 (81%)	707 (92%)	58 (8%)	0	100	100
13	UM	750/817 (92%)	686 (92%)	64 (8%)	0	100	100
14	UN	197/899 (22%)	181 (92%)	16 (8%)	0	100	100
15	UO	489/513 (95%)	452 (92%)	37 (8%)	0	100	100
16	UP	58/214 (27%)	56 (97%)	2 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	UQ	810/896 (90%)	752 (93%)	58 (7%)	0	100	100
18	UR	473/594 (80%)	436 (92%)	37 (8%)	0	100	100
19	US	479/552 (87%)	450 (94%)	29 (6%)	0	100	100
20	UT	2265/2493 (91%)	2125 (94%)	136 (6%)	4 (0%)	47	79
21	UU	870/939 (93%)	821 (94%)	49 (6%)	0	100	100
22	UV	1071/1237 (87%)	1025 (96%)	46 (4%)	0	100	100
23	UX	163/189 (86%)	154 (94%)	9 (6%)	0	100	100
24	CA	238/327 (73%)	217 (91%)	21 (9%)	0	100	100
24	CB	224/327 (68%)	211 (94%)	13 (6%)	0	100	100
25	CD	376/504 (75%)	359 (96%)	16 (4%)	1 (0%)	41	74
26	CE	434/511 (85%)	404 (93%)	30 (7%)	0	100	100
27	CF	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
27	CG	119/126 (94%)	117 (98%)	2 (2%)	0	100	100
28	CH	461/573 (80%)	419 (91%)	41 (9%)	1 (0%)	47	79
29	CI	171/183 (93%)	161 (94%)	10 (6%)	0	100	100
30	CJ	252/290 (87%)	228 (90%)	24 (10%)	0	100	100
31	CK	214/593 (36%)	203 (95%)	11 (5%)	0	100	100
32	CL	796/1183 (67%)	751 (94%)	43 (5%)	2 (0%)	41	74
33	CM	358/367 (98%)	344 (96%)	14 (4%)	0	100	100
34	CN	221/297 (74%)	214 (97%)	7 (3%)	0	100	100
35	JD	793/1267 (63%)	726 (92%)	64 (8%)	3 (0%)	34	70
36	JF	212/252 (84%)	203 (96%)	9 (4%)	0	100	100
36	JG	226/252 (90%)	215 (95%)	11 (5%)	0	100	100
37	JH	257/483 (53%)	250 (97%)	7 (3%)	0	100	100
38	JI	263/1729 (15%)	252 (96%)	11 (4%)	0	100	100
39	JL	281/318 (88%)	269 (96%)	12 (4%)	0	100	100
40	JM	130/217 (60%)	118 (91%)	12 (9%)	0	100	100
41	JP	457/489 (94%)	423 (93%)	34 (7%)	0	100	100
42	Db	79/82 (96%)	71 (90%)	8 (10%)	0	100	100
43	JJ	195/274 (71%)	188 (96%)	7 (4%)	0	100	100
44	DA	236/255 (92%)	218 (92%)	18 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DE	244/261 (94%)	233 (96%)	10 (4%)	1 (0%)	34	70
46	DF	211/225 (94%)	191 (90%)	20 (10%)	0	100	100
47	DG	216/236 (92%)	204 (94%)	12 (6%)	0	100	100
48	DH	166/190 (87%)	159 (96%)	7 (4%)	0	100	100
49	DI	173/200 (86%)	169 (98%)	4 (2%)	0	100	100
50	DJ	183/197 (93%)	171 (93%)	12 (7%)	0	100	100
51	DL	138/156 (88%)	128 (93%)	10 (7%)	0	100	100
52	DN	148/151 (98%)	138 (93%)	10 (7%)	0	100	100
53	DO	125/137 (91%)	112 (90%)	13 (10%)	0	100	100
54	DQ	123/143 (86%)	112 (91%)	11 (9%)	0	100	100
55	DS	99/146 (68%)	93 (94%)	6 (6%)	0	100	100
56	DT	141/144 (98%)	127 (90%)	14 (10%)	0	100	100
57	DW	127/130 (98%)	112 (88%)	14 (11%)	1 (1%)	19	57
58	DX	141/145 (97%)	128 (91%)	12 (8%)	1 (1%)	22	60
59	DY	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
60	Dc	61/67 (91%)	58 (95%)	3 (5%)	0	100	100
All	All	23035/32037 (72%)	21501 (93%)	1497 (6%)	37 (0%)	50	79

5 of 37 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	UH	59	PRO
8	UH	61	PRO
8	UH	68	PRO
8	UH	235	PRO
8	UH	258	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	UA	695/812 (86%)	694 (100%)	1 (0%)	93	97
2	UB	382/732 (52%)	381 (100%)	1 (0%)	92	96
3	UC	74/538 (14%)	74 (100%)	0	100	100
4	UD	604/713 (85%)	596 (99%)	8 (1%)	69	82
5	UE	428/574 (75%)	426 (100%)	2 (0%)	88	94
6	UF	277/414 (67%)	276 (100%)	1 (0%)	91	95
7	UG	405/480 (84%)	404 (100%)	1 (0%)	93	97
8	UH	125/657 (19%)	123 (98%)	2 (2%)	62	79
9	UI	83/533 (16%)	82 (99%)	1 (1%)	71	84
10	UJ	1031/1633 (63%)	1026 (100%)	5 (0%)	88	94
11	UK	207/234 (88%)	205 (99%)	2 (1%)	76	86
12	UL	690/832 (83%)	689 (100%)	1 (0%)	93	97
13	UM	668/719 (93%)	663 (99%)	5 (1%)	84	91
14	UN	183/808 (23%)	182 (100%)	1 (0%)	88	94
15	UO	437/454 (96%)	437 (100%)	0	100	100
16	UP	57/196 (29%)	56 (98%)	1 (2%)	59	77
17	UQ	756/826 (92%)	753 (100%)	3 (0%)	91	95
18	UR	424/529 (80%)	423 (100%)	1 (0%)	93	97
19	US	332/506 (66%)	330 (99%)	2 (1%)	86	92
20	UT	2134/2307 (92%)	2126 (100%)	8 (0%)	91	95
21	UU	768/819 (94%)	765 (100%)	3 (0%)	91	95
22	UV	988/1125 (88%)	986 (100%)	2 (0%)	93	97
23	UX	148/169 (88%)	148 (100%)	0	100	100
24	CA	202/240 (84%)	201 (100%)	1 (0%)	88	94
24	CB	192/240 (80%)	192 (100%)	0	100	100
25	CD	326/435 (75%)	325 (100%)	1 (0%)	92	96
26	CE	352/433 (81%)	348 (99%)	4 (1%)	73	85
27	CF	100/104 (96%)	94 (94%)	6 (6%)	19	50
27	CG	100/104 (96%)	94 (94%)	6 (6%)	19	50
28	CH	407/503 (81%)	405 (100%)	2 (0%)	88	94
29	CI	165/172 (96%)	162 (98%)	3 (2%)	59	77
30	CJ	227/258 (88%)	223 (98%)	4 (2%)	59	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	CK	201/535 (38%)	201 (100%)	0	100	100
32	CL	710/1039 (68%)	698 (98%)	12 (2%)	60	78
33	CM	307/312 (98%)	307 (100%)	0	100	100
34	CN	209/274 (76%)	208 (100%)	1 (0%)	88	94
35	JD	724/1140 (64%)	712 (98%)	12 (2%)	60	78
36	JF	195/222 (88%)	193 (99%)	2 (1%)	76	86
36	JG	206/222 (93%)	205 (100%)	1 (0%)	88	94
39	JL	255/283 (90%)	255 (100%)	0	100	100
40	JM	125/200 (62%)	124 (99%)	1 (1%)	81	89
41	JP	416/443 (94%)	412 (99%)	4 (1%)	76	86
42	Db	70/71 (99%)	70 (100%)	0	100	100
43	JJ	174/238 (73%)	174 (100%)	0	100	100
44	DA	212/224 (95%)	211 (100%)	1 (0%)	88	94
45	DE	210/222 (95%)	209 (100%)	1 (0%)	88	94
46	DF	180/191 (94%)	180 (100%)	0	100	100
47	DG	187/201 (93%)	187 (100%)	0	100	100
48	DH	151/170 (89%)	151 (100%)	0	100	100
49	DI	142/161 (88%)	142 (100%)	0	100	100
50	DJ	158/166 (95%)	157 (99%)	1 (1%)	86	92
51	DL	125/137 (91%)	124 (99%)	1 (1%)	81	89
52	DN	127/128 (99%)	126 (99%)	1 (1%)	81	89
53	DO	90/105 (86%)	90 (100%)	0	100	100
54	DQ	104/119 (87%)	103 (99%)	1 (1%)	76	86
55	DS	96/129 (74%)	96 (100%)	0	100	100
56	DT	115/116 (99%)	114 (99%)	1 (1%)	78	88
57	DW	110/111 (99%)	109 (99%)	1 (1%)	78	88
58	DX	118/120 (98%)	118 (100%)	0	100	100
59	DY	112/113 (99%)	112 (100%)	0	100	100
60	Dc	56/60 (93%)	56 (100%)	0	100	100
All	All	19852/26551 (75%)	19733 (99%)	119 (1%)	86	92

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
27	CF	17	THR
41	JP	368	ASP
29	CI	5	LEU
41	JP	251	THR
57	DW	66	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 290 such sidechains are listed below:

Mol	Chain	Res	Type
33	CM	206	ASN
55	DS	104	ASN
35	JD	469	HIS
43	JJ	131	ASN
17	UQ	412	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
61	D2	76/81 (93%)	24 (31%)	0
62	D3	1388/1802 (77%)	377 (27%)	18 (1%)
63	D4	214/333 (64%)	60 (28%)	4 (1%)
All	All	1678/2216 (75%)	461 (27%)	22 (1%)

5 of 461 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
61	D2	6	A
61	D2	8	A
61	D2	11	A
61	D2	14	U
61	D2	15	G

5 of 22 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
62	D3	1620	C
62	D3	1745	G
62	D3	1706	C
63	D4	143	G
62	D3	912	U

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$
65	GTP	CL	2001	66	26,34,34	0.91	1 (3%)	32,54,54	1.58	5 (15%)

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
65	GTP	CL	2001	66	-	4/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
65	CL	2001	GTP	C6-N1	-2.41	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	CL	2001	GTP	PA-O3A-PB	-4.23	118.32	132.83
65	CL	2001	GTP	PB-O3B-PG	-4.21	118.39	132.83
65	CL	2001	GTP	C3'-C2'-C1'	2.80	105.19	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
65	CL	2001	GTP	C5-C6-N1	2.38	118.15	113.95
65	CL	2001	GTP	C8-N7-C5	2.29	107.35	102.99

There are no chirality outliers.

All (4) torsion outliers are listed below:

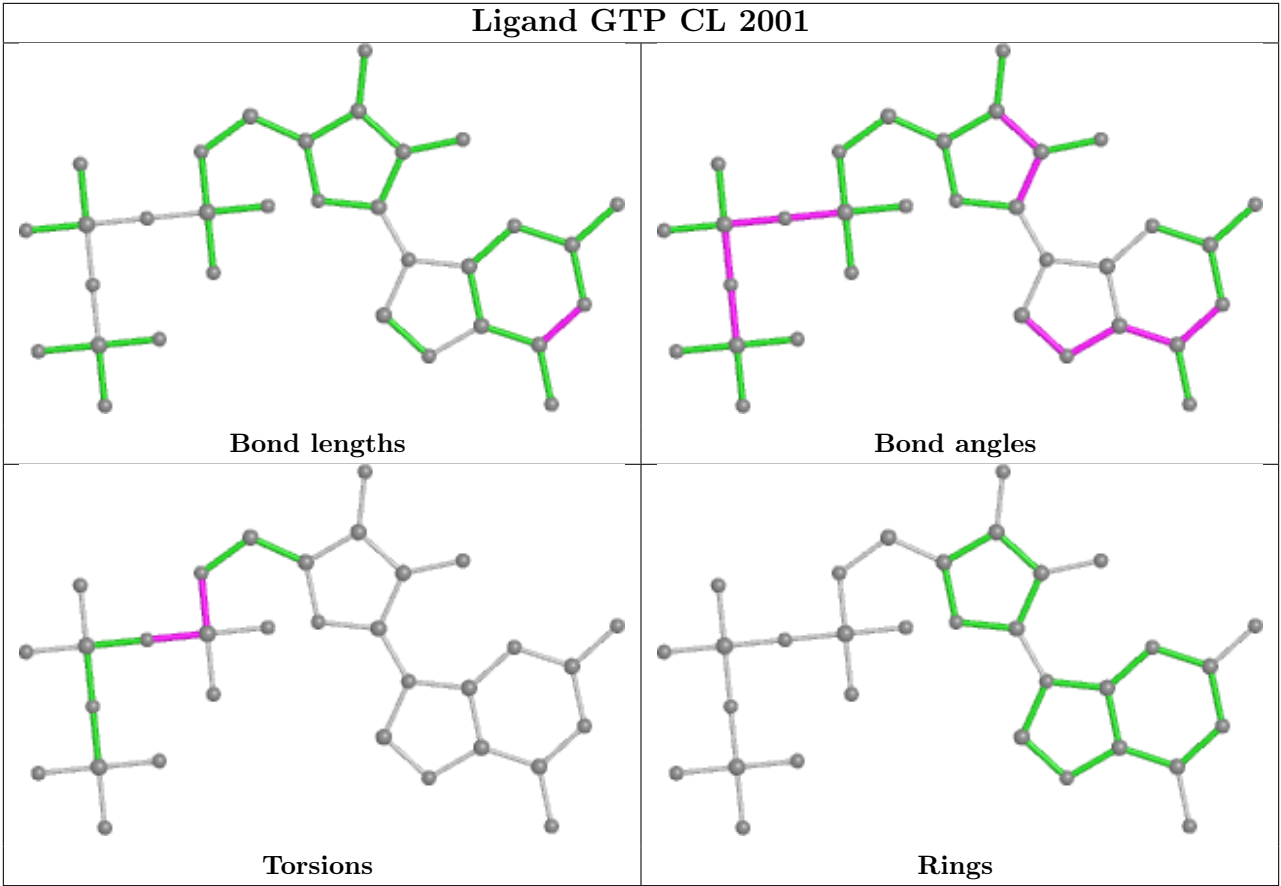
Mol	Chain	Res	Type	Atoms
65	CL	2001	GTP	C5'-O5'-PA-O3A
65	CL	2001	GTP	C5'-O5'-PA-O2A
65	CL	2001	GTP	PB-O3A-PA-O1A
65	CL	2001	GTP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
65	CL	2001	GTP	1	0

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 than 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.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
61	D2	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D2	92:C	O3'	281:G	P	62.59
1	D2	292:A	O3'	463:A	P	45.89
1	D2	70:A	O3'	80:A	P	19.69
1	D2	24:U	O3'	56:G	P	14.77

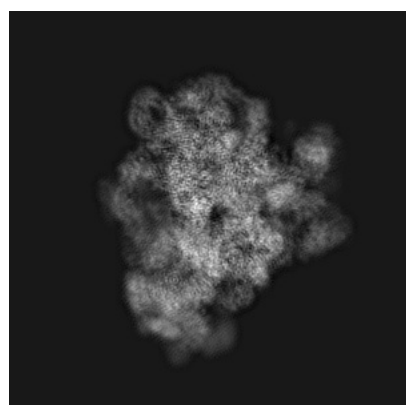
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11360. These allow visual inspection of the internal detail of the map and identification of artifacts.

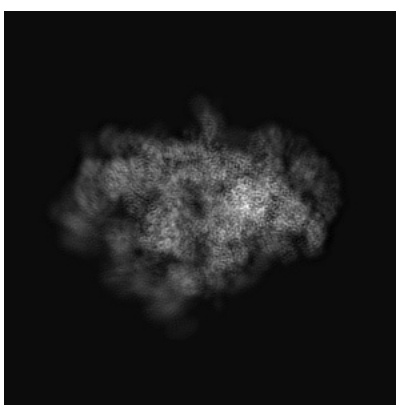
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

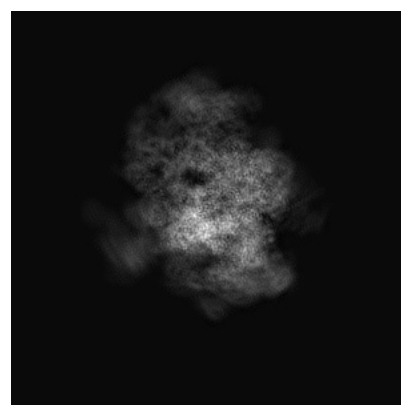
6.1.1 Primary map



X



Y

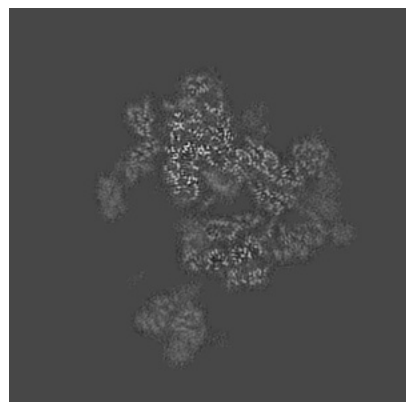


Z

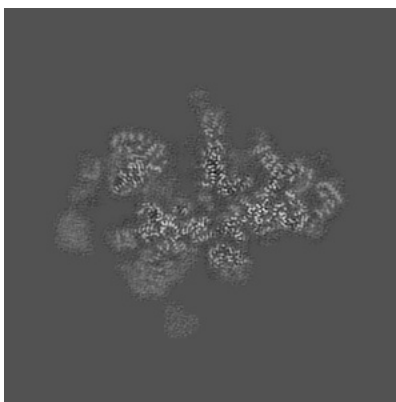
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

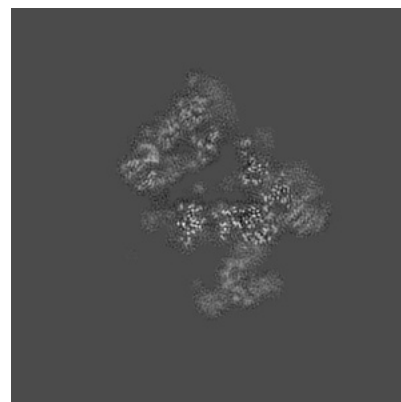
6.2.1 Primary map



X Index: 240



Y Index: 240

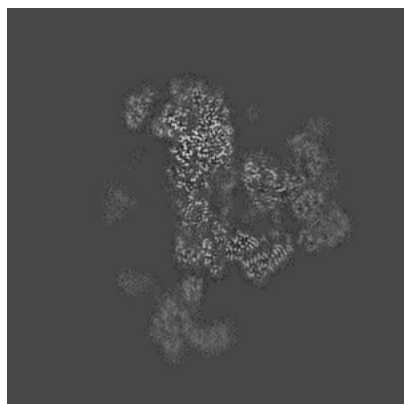


Z Index: 240

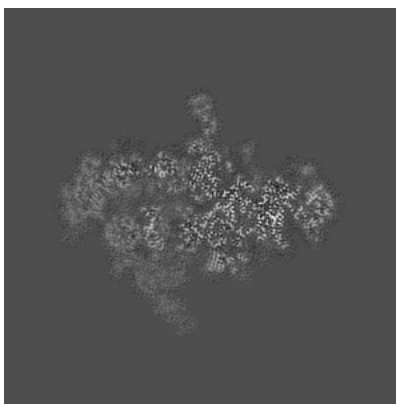
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

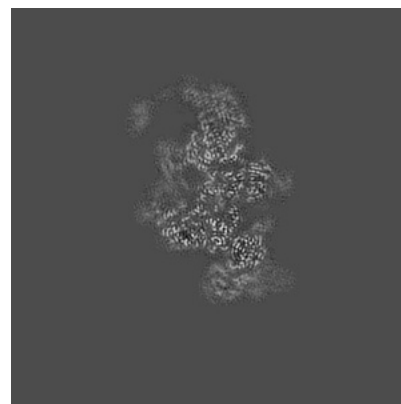
6.3.1 Primary map



X Index: 225



Y Index: 224

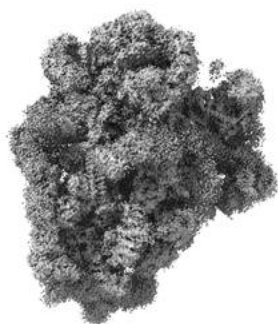


Z Index: 287

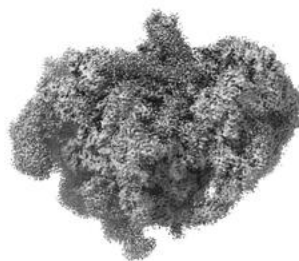
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

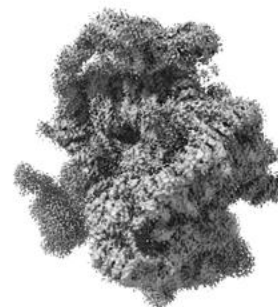
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

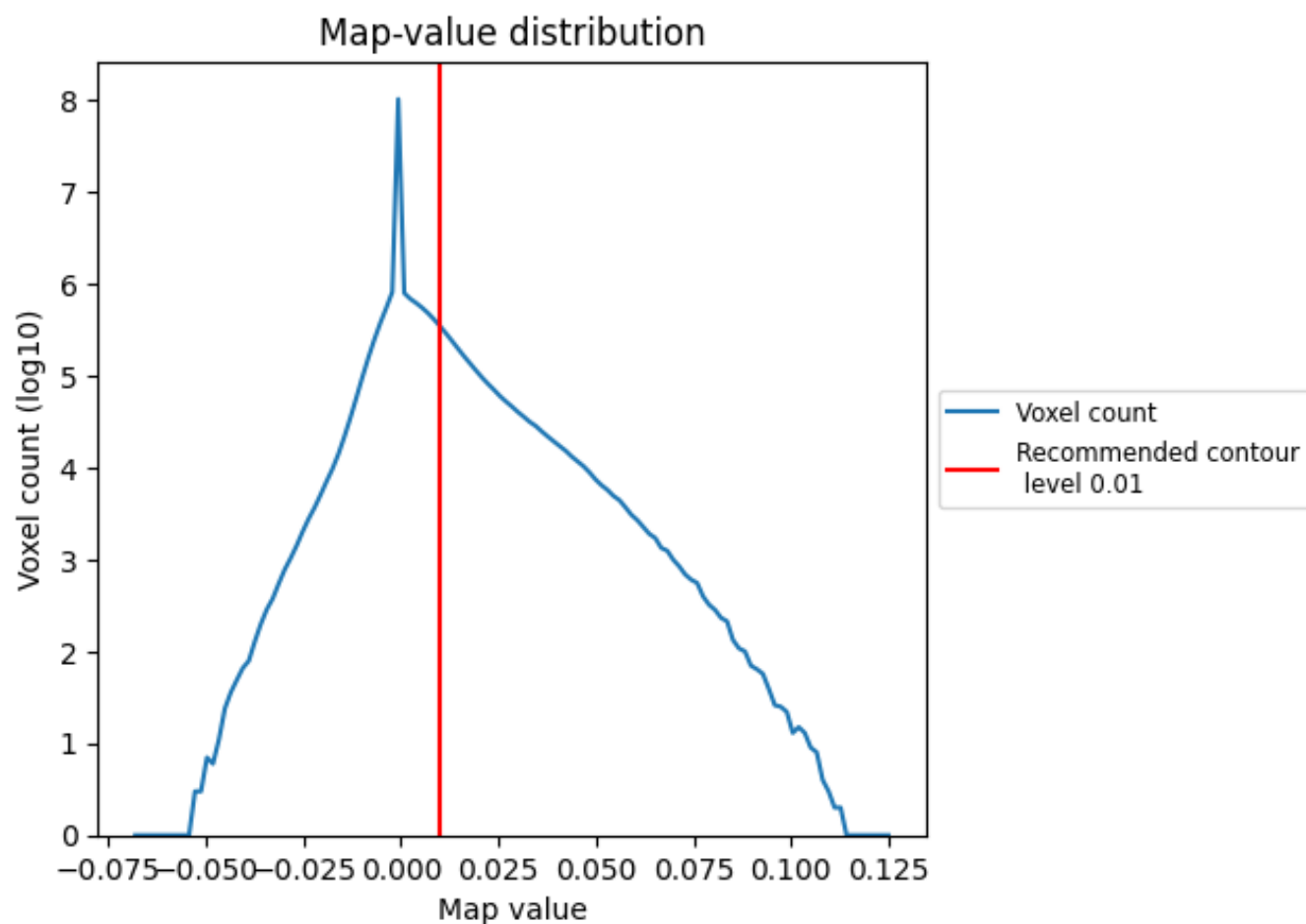
6.5 Mask visualisation

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

7 Map analysis [i](#)

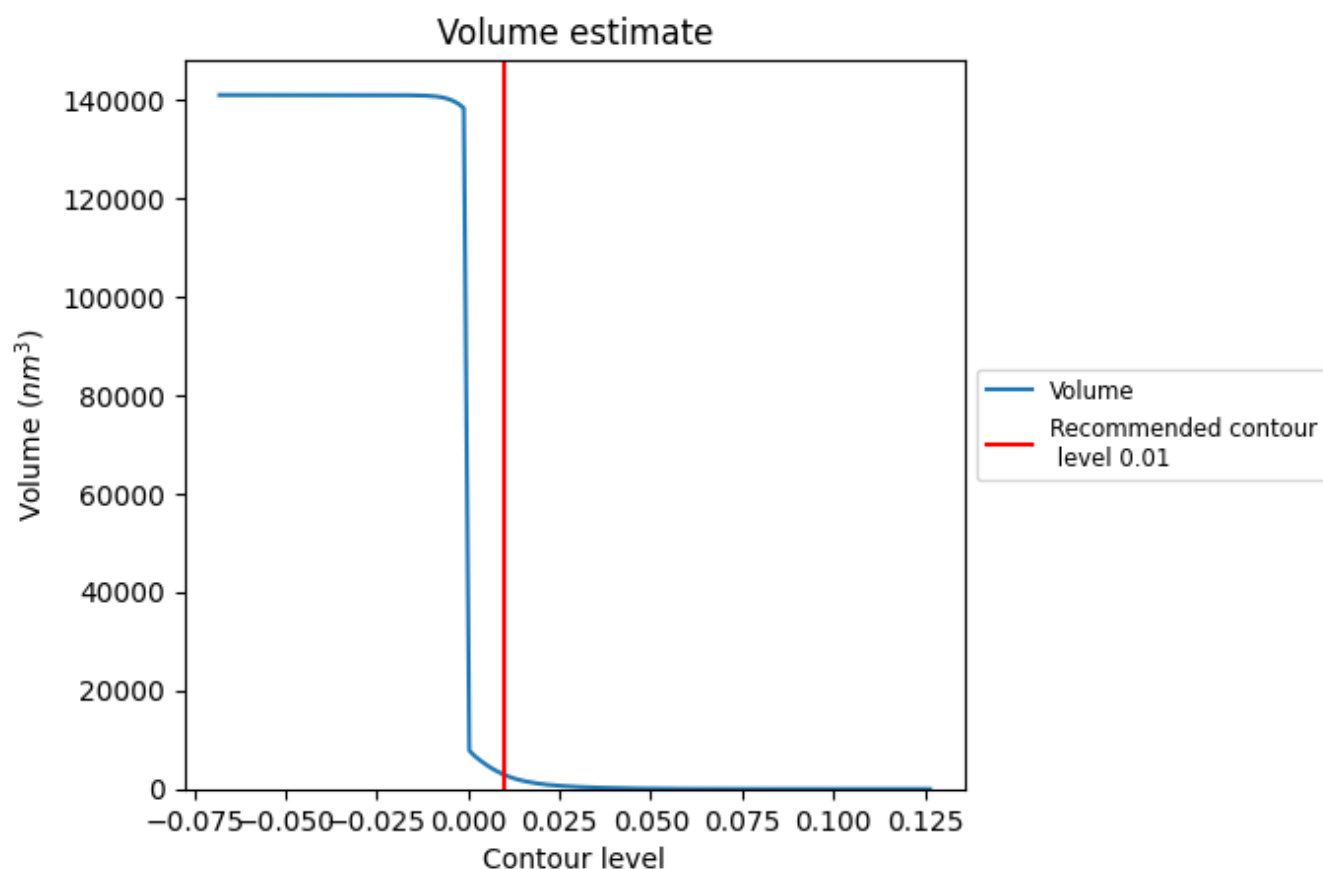
This section contains the results of statistical analysis of the map.

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.

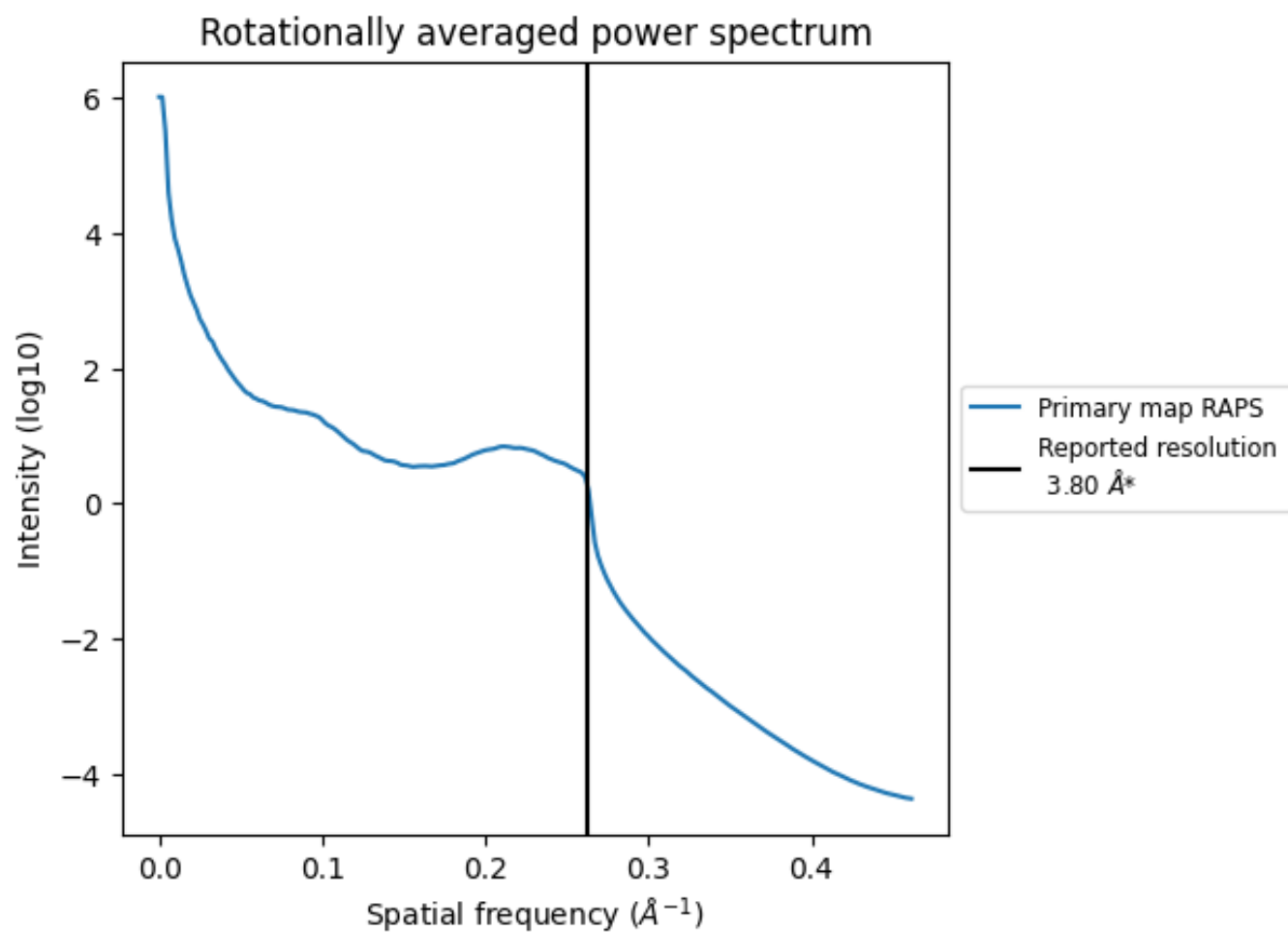
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2852 nm³; this corresponds to an approximate mass of 2576 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 ⓘ

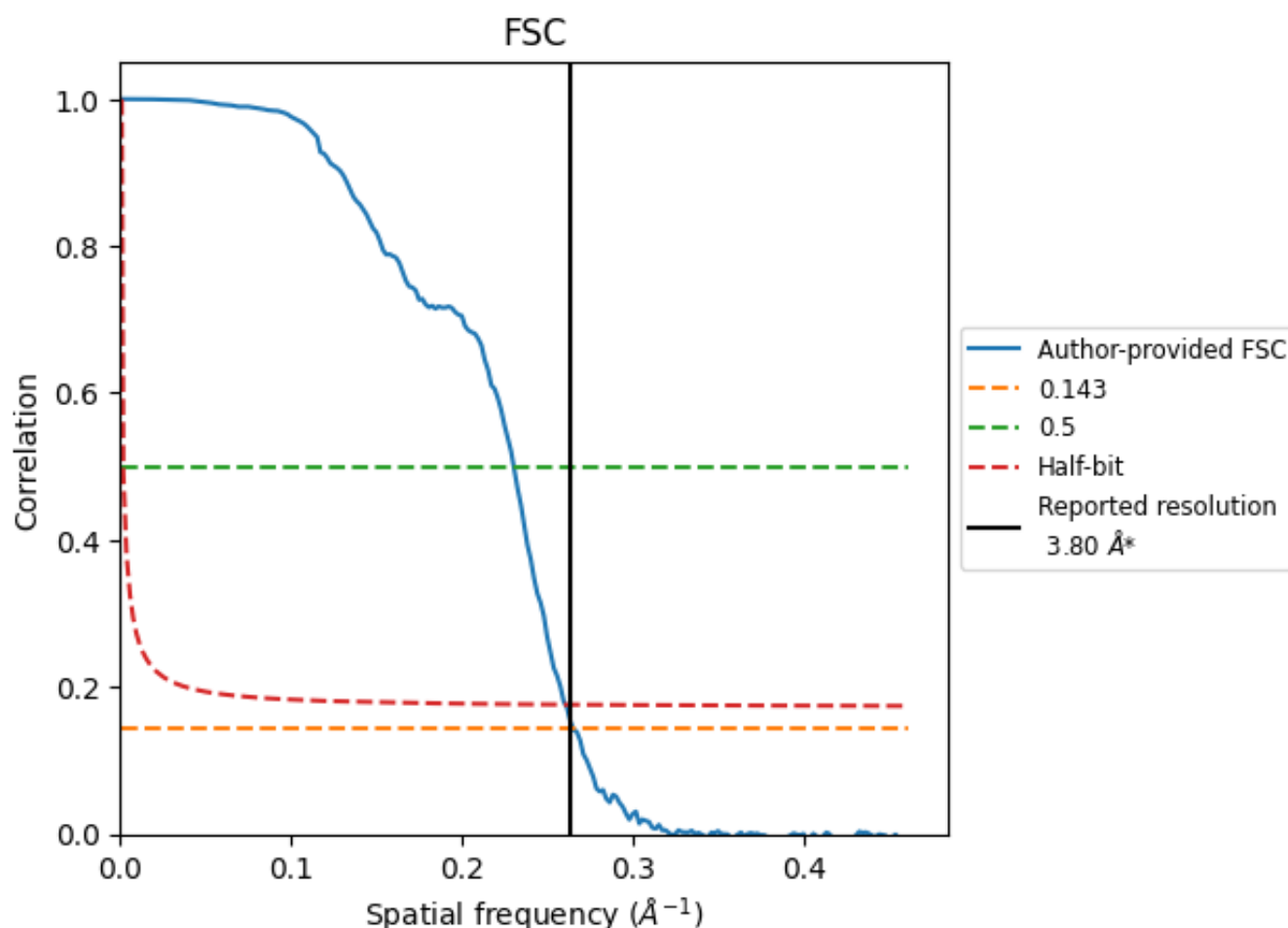


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

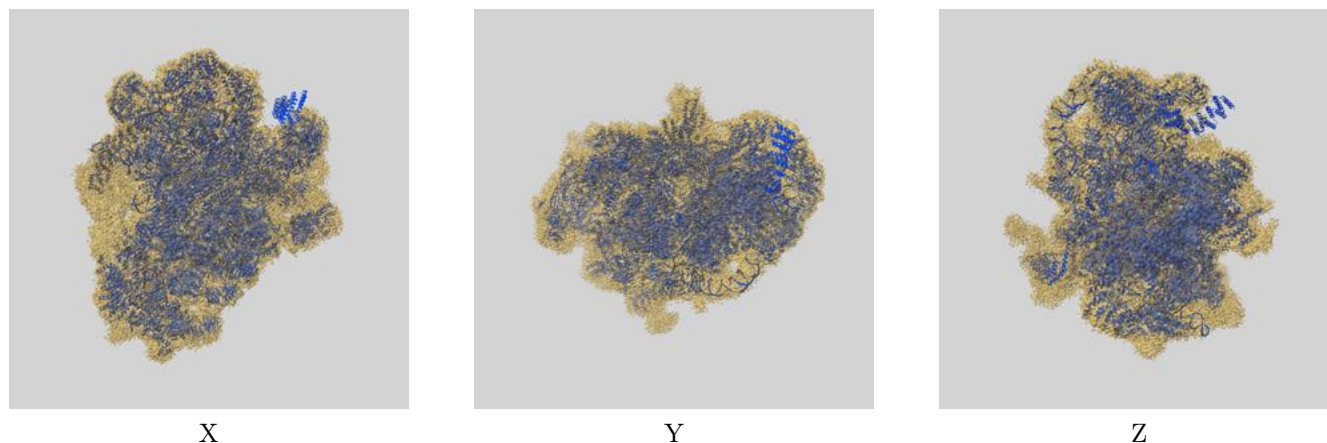
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.34	3.84
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

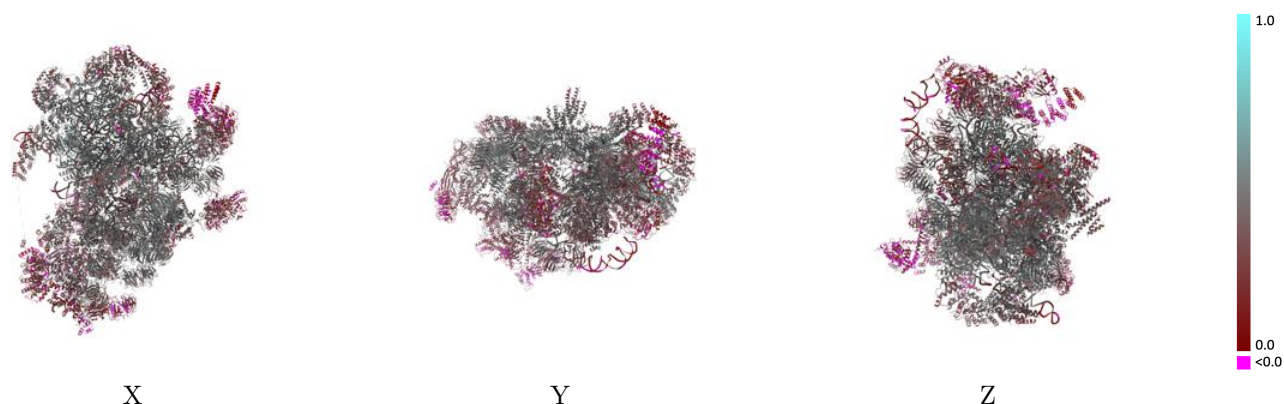
This section contains information regarding the fit between EMDB map EMD-11360 and PDB model 6ZQD. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



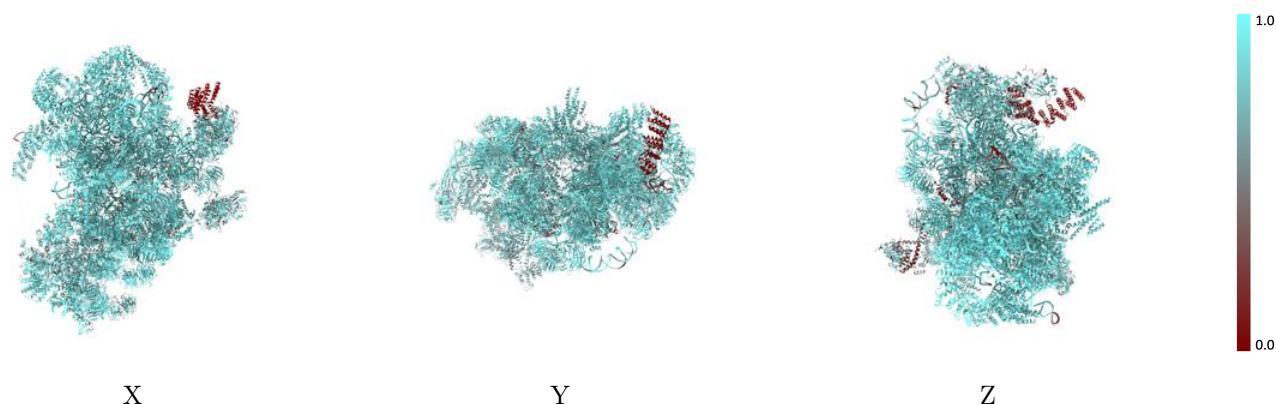
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



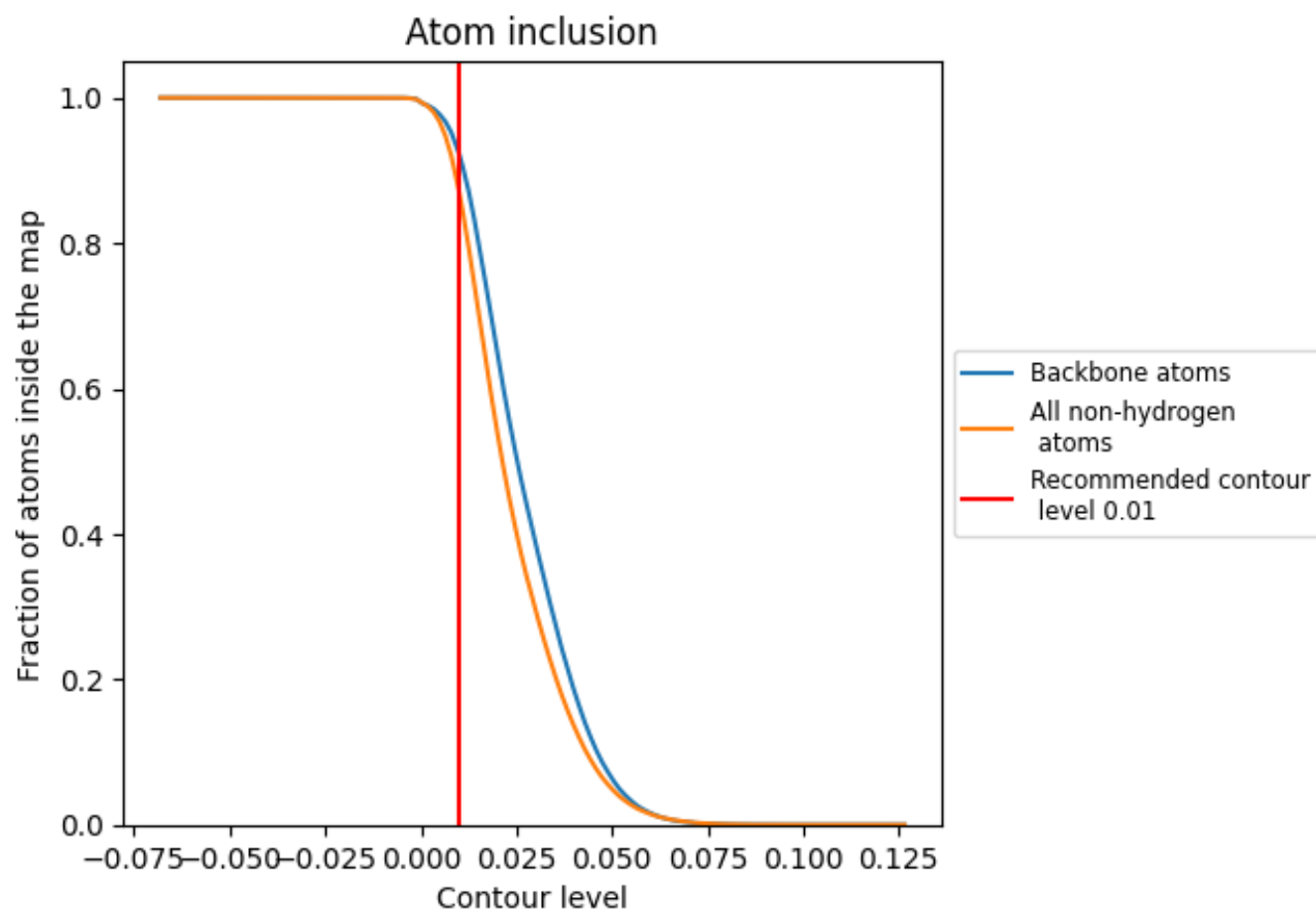
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

































































The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8706	 0.3870
CA	 0.9178	 0.5020
CB	 0.8965	 0.4430
CD	 0.9047	 0.4450
CE	 0.8637	 0.3960
CF	 0.9126	 0.4630
CG	 0.9170	 0.4750
CH	 0.9359	 0.4820
CI	 0.8233	 0.4020
CJ	 0.8630	 0.4600
CK	 0.8699	 0.4460
CL	 0.8990	 0.4660
CM	 0.9291	 0.4760
CN	 0.7518	 0.2680
D2	 0.8420	 0.2530
D3	 0.9418	 0.4040
D4	 0.8732	 0.3400
DA	 0.8839	 0.4580
DE	 0.9485	 0.5170
DF	 0.9105	 0.4710
DG	 0.9600	 0.4750
DH	 0.9060	 0.4330
DI	 0.9422	 0.4880
DJ	 0.9078	 0.5000
DL	 0.9536	 0.5110
DN	 0.9152	 0.4710
DO	 0.9204	 0.4600
DQ	 0.9358	 0.4940
DS	 0.8228	 0.3540
DT	 0.8779	 0.4290
DW	 0.9409	 0.5120
DX	 0.9035	 0.4850
DY	 0.9289	 0.5080
Db	 0.9369	 0.4970
Dc	 0.9161	 0.4830



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
JD	 0.6917	 0.2290
JF	 0.6593	 0.1780
JG	 0.7600	 0.2840
JH	 0.6170	 0.0740
JI	 0.0266	 0.0110
JJ	 0.8992	 0.4490
JL	 0.7644	 0.3440
JM	 0.8522	 0.4380
JP	 0.8949	 0.5000
UA	 0.9154	 0.4790
UB	 0.6444	 0.1960
UC	 0.8709	 0.4760
UD	 0.9008	 0.3780
UE	 0.8814	 0.3810
UF	 0.9151	 0.4150
UG	 0.8723	 0.4690
UH	 0.7858	 0.1730
UI	 0.8732	 0.2260
UJ	 0.8633	 0.3470
UK	 0.8602	 0.4230
UL	 0.9215	 0.4060
UM	 0.8862	 0.3680
UN	 0.8282	 0.4420
UO	 0.8630	 0.3290
UP	 0.7875	 0.3570
UQ	 0.8874	 0.3330
UR	 0.9064	 0.4530
US	 0.6876	 0.1740
UT	 0.9050	 0.3900
UU	 0.9187	 0.4570
UV	 0.7916	 0.2930
UX	 0.9140	 0.4930