Full wwPDB EM Validation Report

Aug 29, 2023 – 09:04 PM EDT

PDB ID	:	8EVP
EMDB ID	:	EMD-28632
Title	:	Hypopseudouridylated yeast 80S bound with Taura syndrome virus (TSV) internal ribosome entry site (IRES), Structure I
Authors	:	Zhao, Y.; Rai, J.; Li, H.
Deposited on	:	2022-10-20
Resolution	:	2.38 Å(reported)

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

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

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

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

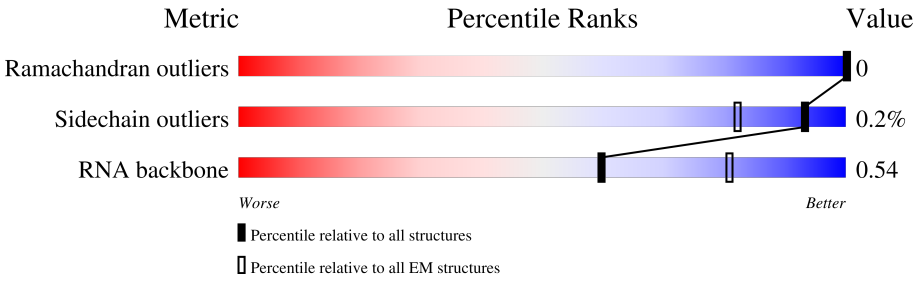
EMDB validation analysis	:	0.0.1.dev50
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.38 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	BA	252	81% 18%
2	BB	255	84% 16%
3	BC	254	85% 15%
4	BE	261	100%
5	BG	236	11% 96%
6	BH	190	13% 97%
7	BI	200	94% 6%
8	BJ	197	6% 93% 6%

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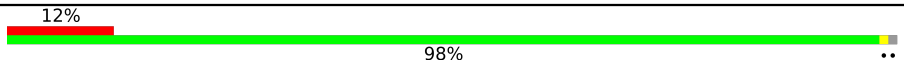
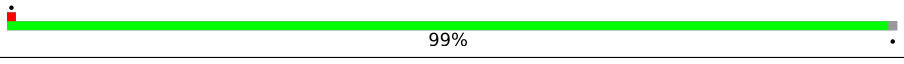
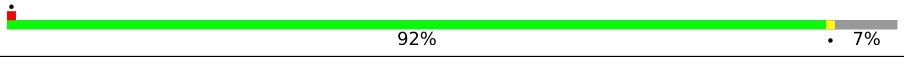
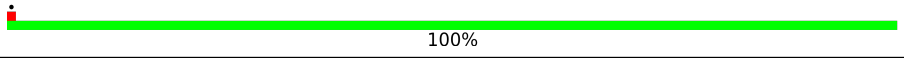
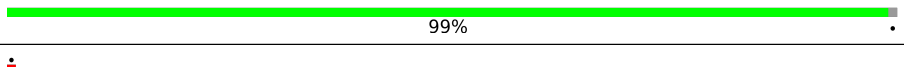
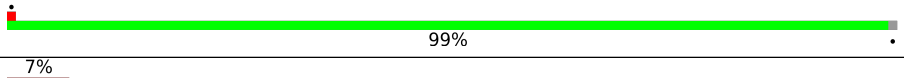
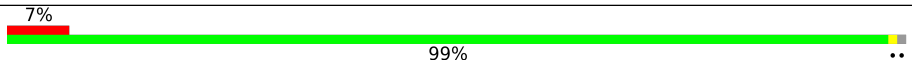
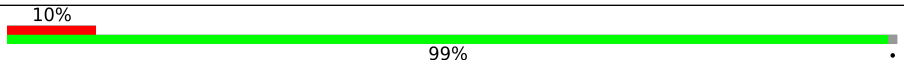
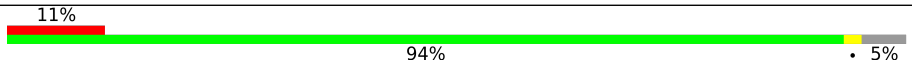
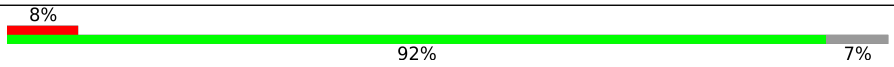
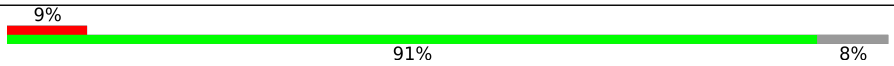
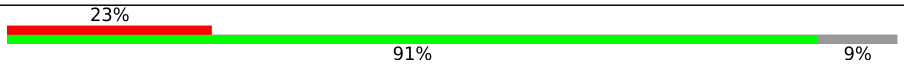
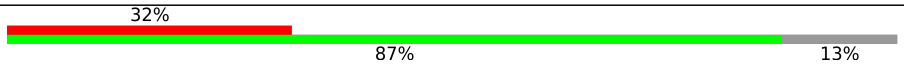
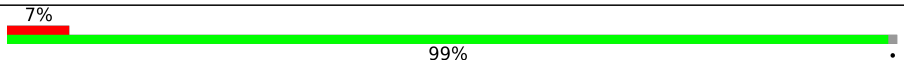
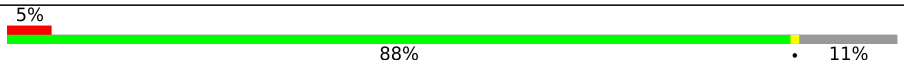
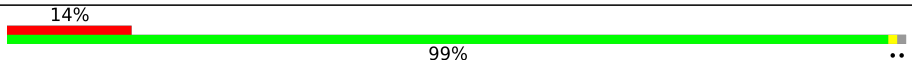
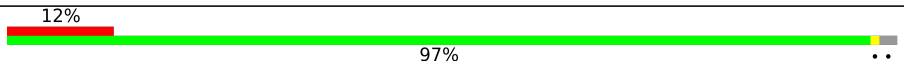
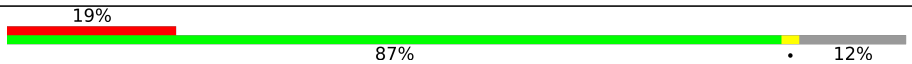
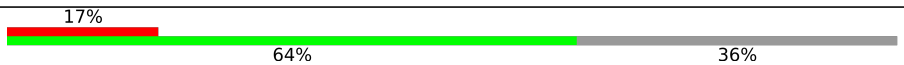
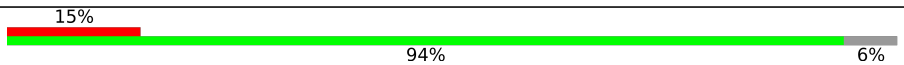
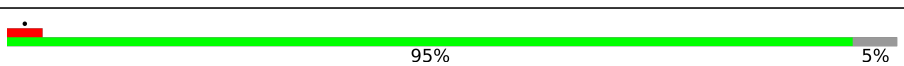
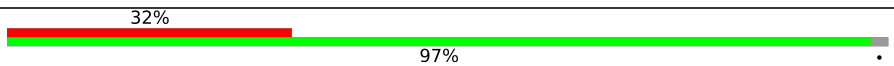
Mol	Chain	Length	Quality of chain
9	BL	156	
10	BN	151	
11	BO	137	
12	BV	87	
13	BW	130	
14	BX	145	
15	BY	135	
16	Ba	119	
17	Bb	82	
18	Be	63	
19	BD	240	
20	BF	225	
21	BK	105	
22	BP	142	
23	BQ	143	
24	BR	136	
25	BS	146	
26	BT	144	
27	BU	121	
28	BZ	108	
29	Bc	67	
30	Bd	56	
31	Bg	319	
32	Bf	152	
33	BM	143	

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Mol	Chain	Length	Quality of chain
34	B5	1798	8% 74% 24%
35	AA	254	97%
36	AB	387	99%
37	AC	362	99%
38	A1	3360	75% 19% 5%
39	A3	121	88% 12%
40	A4	158	82% 18%
41	AD	297	98%
42	AE	176	89% 11%
43	AF	244	91% 9%
44	AG	256	89% 10%
45	AH	191	98%
46	AI	221	93% 7%
47	AJ	174	11% 95%
48	AL	199	97%
49	AM	138	99%
50	AN	204	100%
51	AO	199	99%
52	AP	184	95% 5%
53	AQ	186	99%
54	AR	189	7% 99%
55	AS	178	96%
56	AT	160	99%
57	AU	121	83% 17%
58	AV	137	99%

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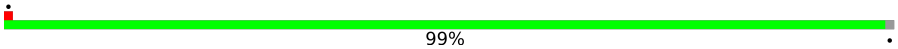
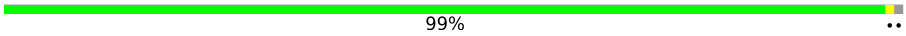
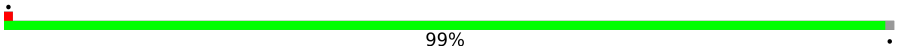
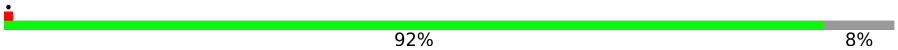
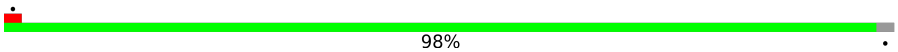
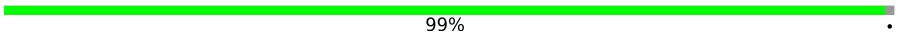
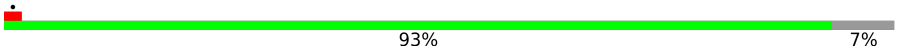
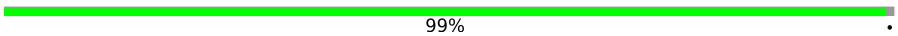
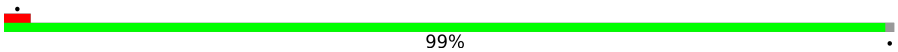
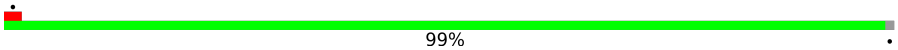
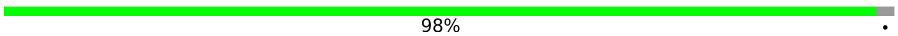
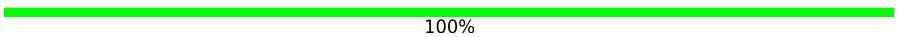
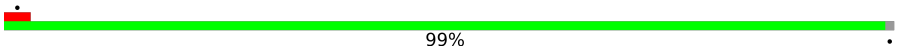
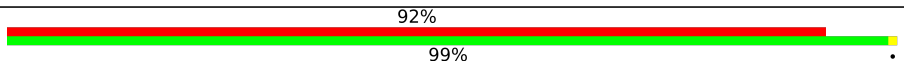
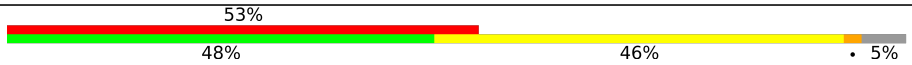
Mol	Chain	Length	Quality of chain
59	AW	155	
60	AX	142	
61	AY	127	
62	AZ	136	
63	Aa	149	
64	Ab	59	
65	Ac	105	
66	Ad	113	
67	Ae	130	
68	Af	107	
69	Ag	121	
70	Ah	120	
71	Ai	100	
72	Aj	88	
73	Ak	78	
74	Al	51	
75	Am	128	
76	An	25	
77	Ao	106	
78	Ap	92	
79	E	217	
80	EC	202	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	3AU	B5	1799	X	-	-	-

2 Entry composition

There are 82 unique types of molecules in this entry. The entry contains 205919 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 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	BA	206	1612	1034	285	291	2	0	0

- Molecule 2 is a protein called RPS1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BB	214	1709	1084	310	311	4	0	0

- Molecule 3 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	BC	217	1635	1047	289	297	2	0	0

- Molecule 4 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	BE	260	2068	1316	389	360	3	0	0

- Molecule 5 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	BG	226	1820	1142	350	325	3	0	0

- Molecule 6 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	BH	184	1481	951	265	265	0	0

- Molecule 7 is a protein called 40S ribosomal protein S8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BI	188	Total	C	N	O	S	0	0
			1489	925	298	264	2		

- Molecule 8 is a protein called 40S ribosomal protein S9-A.

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

- Molecule 9 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	BL	155	Total	C	N	O	S	0	0
			1244	798	235	208	3		

- Molecule 10 is a protein called 40S ribosomal protein S13.

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

- Molecule 11 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	BO	127	Total	C	N	O	S	0	0
			941	578	186	174	3		

- Molecule 12 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BV	87	Total	C	N	O	S	0	0
			684	420	125	137	2		

- Molecule 13 is a protein called RPS22A isoform 1.

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

- Molecule 14 is a protein called 40S ribosomal protein S23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	BX	144	Total	C	N	O	S	0	0
			1121	708	220	191	2		

- Molecule 15 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	BY	134	Total	C	N	O	0	0
			1073	676	208	189		

- Molecule 16 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Ba	97	Total	C	N	O	S	0	0
			769	475	160	129	5		

- Molecule 17 is a protein called 40S ribosomal protein S27-A.

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

- Molecule 18 is a protein called 40S ribosomal protein S30-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Be	60	Total	C	N	O	S	0	0
			475	299	98	77	1		

- Molecule 19 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	BD	223	Total	C	N	O	S	0	0
			1734	1101	313	314	6		

- Molecule 20 is a protein called Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	BF	206	Total	C	N	O	S	0	0
			1609	1007	300	299	3		

- Molecule 21 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	BK	96	Total	C	N	O	S	0	0
			817	529	133	153	2		

- Molecule 22 is a protein called RPS15 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BP	124	Total	C	N	O	S	0	0
			991	631	187	166	7		

- Molecule 23 is a protein called 40S ribosomal protein S16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	BQ	141	Total	C	N	O	0	0
			1105	708	203	194		

- Molecule 24 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BR	121	Total	C	N	O	S	0	0
			975	611	183	179	2		

- Molecule 25 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BS	145	Total	C	N	O	S	0	0
			1192	743	237	210	2		

- Molecule 26 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BT	141	Total	C	N	O	S	0	0
			1095	685	206	202	2		

- Molecule 27 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BU	107	Total	C	N	O	S	0	0
			855	539	156	159	1		

- Molecule 28 is a protein called RPS25A isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	BZ	69	Total	C	N	O	0	0
			558	357	103	98		

- Molecule 29 is a protein called RPS28A isoform 1.

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

- Molecule 30 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Bd	53	Total	C	N	O	S	0	0
			443	275	92	72	4		

- Molecule 31 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Bg	312	Total	C	N	O	S	0	0
			2401	1522	410	461	8		

- Molecule 32 is a protein called Ubiquitin-40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Bf	57	Total	C	N	O	S	0	0
			454	288	86	77	3		

- Molecule 33 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BM	121	Total	C	N	O	S	0	0
			913	574	162	175	2		

- Molecule 34 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B5	1782	Total	C	N	O	P	1	0
			38004	17005	6718	12499	1782		

- Molecule 35 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	AA	247	Total	C	N	O	S	0	0
			1878	1170	381	326	1		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	AB	386	Total	C	N	O	S	0	0
			3080	1955	584	533	8		

- Molecule 37 is a protein called RPL4A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	AC	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 38 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	A1	3198	Total	C	N	O	P	0	0
			68445	30596	12331	22320	3198		

- Molecule 39 is a RNA chain called 5s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	A3	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 40 is a RNA chain called 5.8 S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	A4	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 41 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AD	292	Total	C	N	O	S	0	0
			2341	1478	408	453	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AE	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 43 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AF	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 44 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AG	230	Total	C	N	O	S	0	0
			1798	1149	323	323	3		

- Molecule 45 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AH	190	Total	C	N	O	S	0	0
			1510	957	273	276	4		

- Molecule 46 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AI	205	Total	C	N	O	S	0	0
			1672	1063	316	288	5		

- Molecule 47 is a protein called RPL11A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AJ	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 48 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	AL	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 49 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AM	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 50 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	AN	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 51 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AO	197	Total	C	N	O	S	197	0
			1555	1003	289	262	1		

- Molecule 52 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	AP	175	Total	C	N	O	0	0
			1388	862	277	249		

- Molecule 53 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	AQ	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 54 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
54	AR	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 55 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AS	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 56 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 57 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	AU	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 58 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	AV	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 59 is a protein called RPL24A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	AW	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
60	AX	121	Total	C	N	O	S	0	0
			968	623	170	173	2		

- Molecule 61 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	AY	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 62 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	AZ	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 63 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	Aa	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 64 is a protein called RPL29 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	Ab	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 65 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	Ac	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 66 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	Ad	109	Total	C	N	O	S	0	0
			890	565	168	156	1		

- Molecule 67 is a protein called RPL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	Ae	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 68 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	Af	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 69 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	Ag	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 70 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	Ah	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 71 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	Ai	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 72 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	Aj	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 73 is a protein called RPL38 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	Ak	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 74 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	Al	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 75 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	Am	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 76 is a protein called 60S ribosomal protein L41-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	An	25	Total	C	N	O	S	0	0
			233	142	63	27	1		

- Molecule 77 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	Ao	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 78 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	Ap	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 79 is a protein called RPL1A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	E	217	Total	C	N	O	S	0	0
			1718	1097	299	312	10		

- Molecule 80 is a RNA chain called Internal ribosome entry site.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	EC	192	Total	C	N	O	P	0	0
			4090	1828	729	1341	192		

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
81	BE	1	Total	Mg	0
			1	1	
81	BN	1	Total	Mg	0
			1	1	
81	Ba	1	Total	Mg	0
			1	1	
81	B5	60	Total	Mg	0
			60	60	
81	AC	1	Total	Mg	0
			1	1	
81	A1	182	Total	Mg	0
			182	182	
81	A3	2	Total	Mg	0
			2	2	
81	A4	5	Total	Mg	0
			5	5	
81	AD	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms	AltConf
81	AL	1	Total Mg 1 1	0
81	AP	1	Total Mg 1 1	0

- Molecule 82 is ZINC ION (three-letter code: ZN) (formula: Zn).

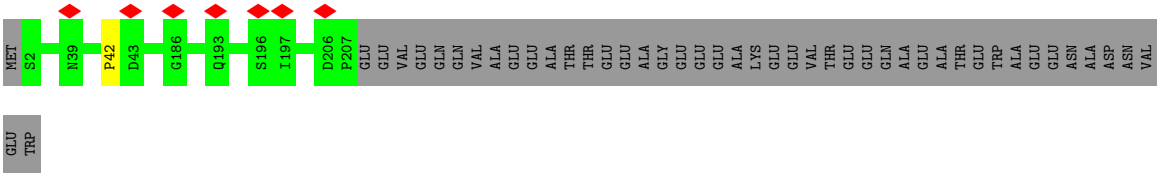
Mol	Chain	Residues	Atoms	AltConf
82	Ao	1	Total Zn 1 1	0

3 Residue-property plots (i)

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

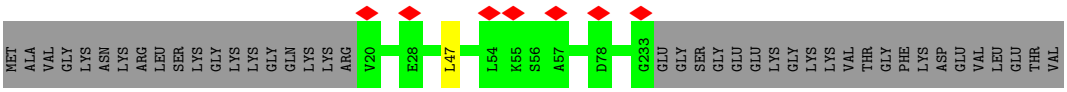
• Molecule 1: 40S ribosomal protein S0-A

Chain BA:



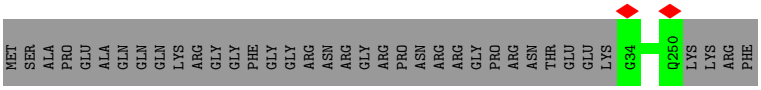
• Molecule 2: RPS1A isoform 1

Chain BB:



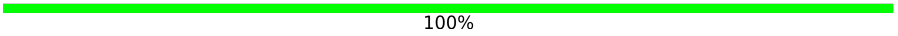
• Molecule 3: RPS2 isoform 1

Chain BC:



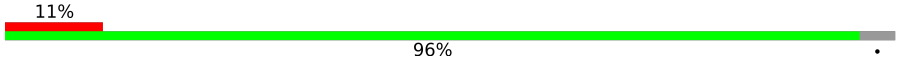
• Molecule 4: 40S ribosomal protein S4-A

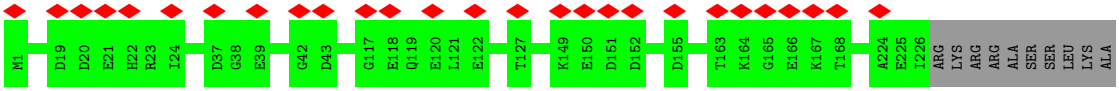
Chain BE:



• Molecule 5: 40S ribosomal protein S6-A

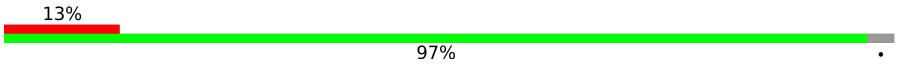
Chain BG:

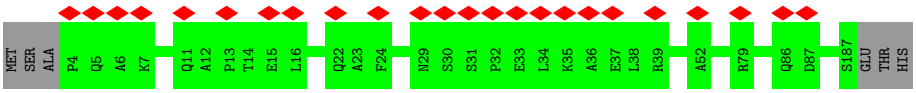




• Molecule 6: 40S ribosomal protein S7-A

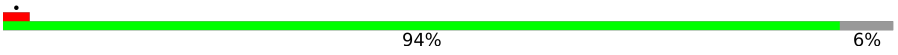
Chain BH:

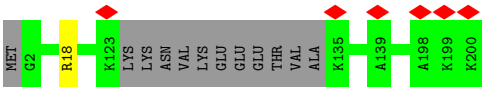




• Molecule 7: 40S ribosomal protein S8-A

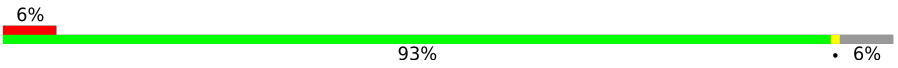
Chain BI:

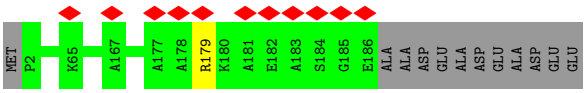




• Molecule 8: 40S ribosomal protein S9-A

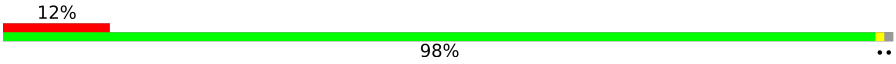
Chain BJ:

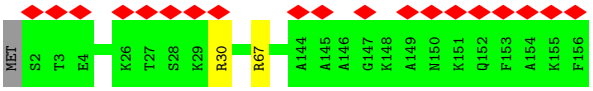




• Molecule 9: 40S ribosomal protein S11-A

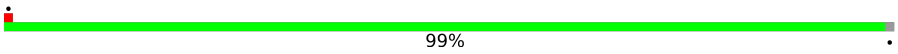
Chain BL:





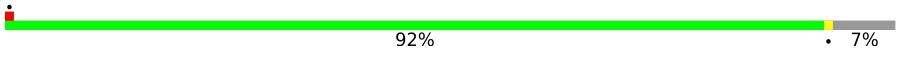
• Molecule 10: 40S ribosomal protein S13

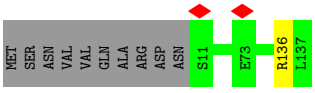
Chain BN:



• Molecule 11: 40S ribosomal protein S14-A

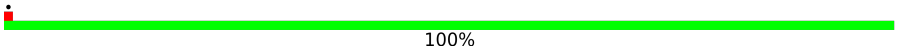
Chain BO:

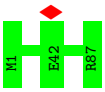




• Molecule 12: 40S ribosomal protein S21-A

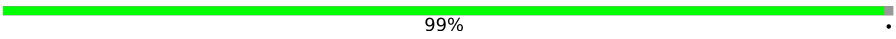
Chain BV:





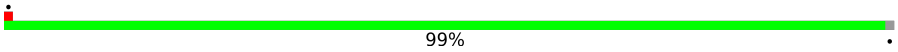
• Molecule 13: RPS22A isoform 1

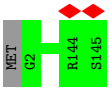
Chain BW:



• Molecule 14: 40S ribosomal protein S23-A

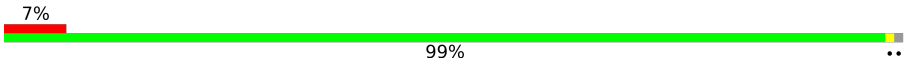
Chain BX:

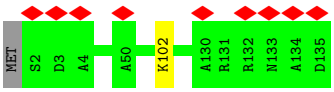




• Molecule 15: 40S ribosomal protein S24-A

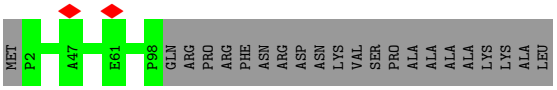
Chain BY:





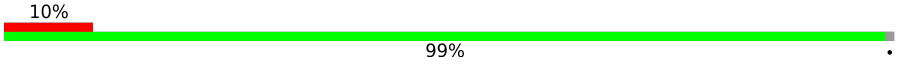
• Molecule 16: RPS26B isoform 1

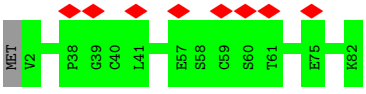
Chain Ba:



• Molecule 17: 40S ribosomal protein S27-A

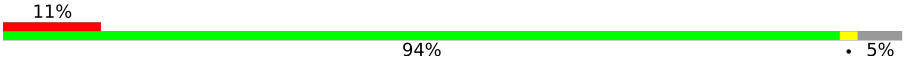
Chain Bb:

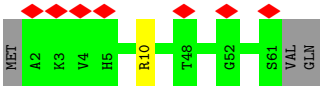




• Molecule 18: 40S ribosomal protein S30-A

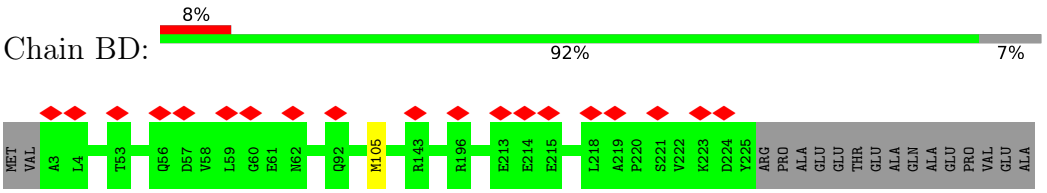
Chain Be:





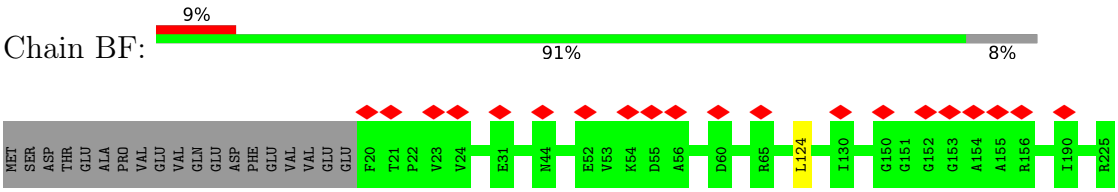
• Molecule 19: RPS3 isoform 1

Chain BD:



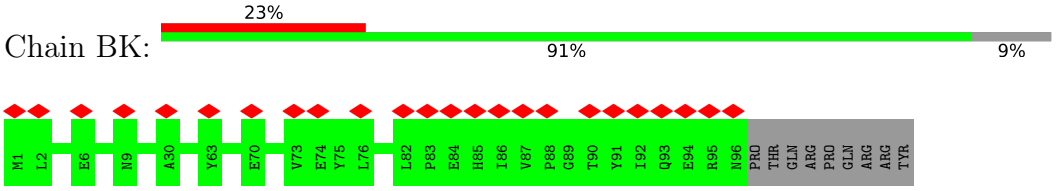
• Molecule 20: Rps5p

Chain BF:



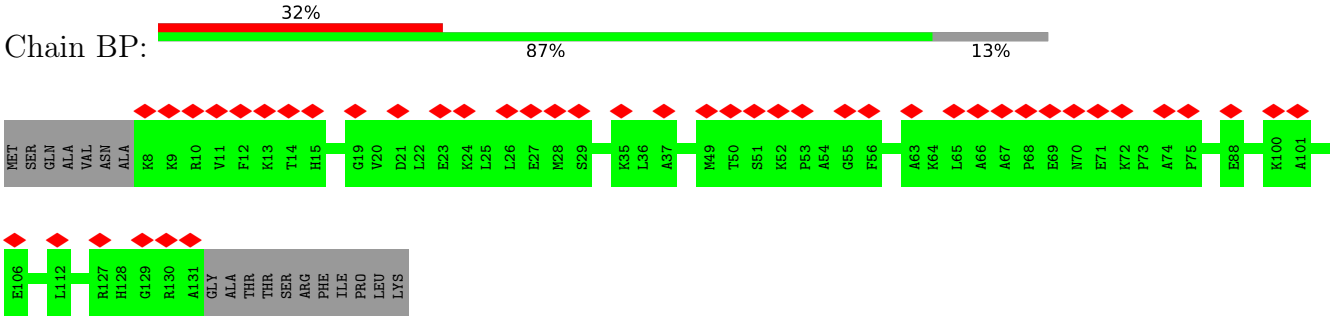
• Molecule 21: 40S ribosomal protein S10-A

Chain BK:



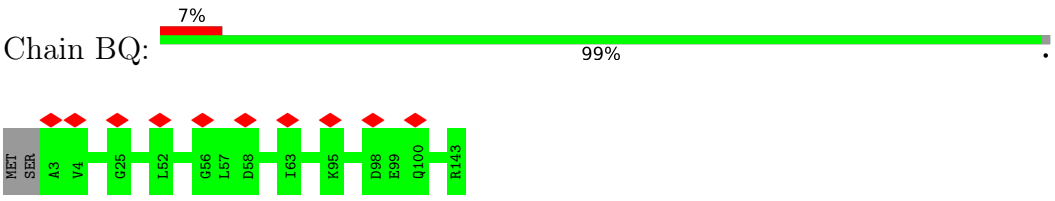
• Molecule 22: RPS15 isoform 1

Chain BP:



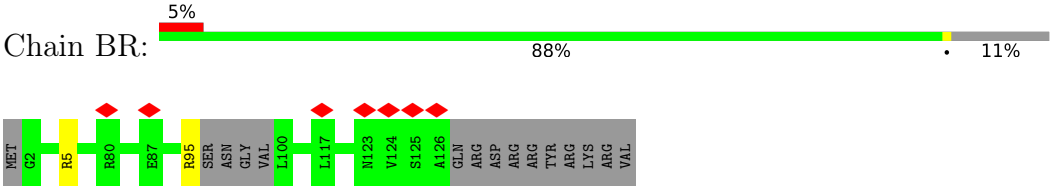
• Molecule 23: 40S ribosomal protein S16-A

Chain BQ:



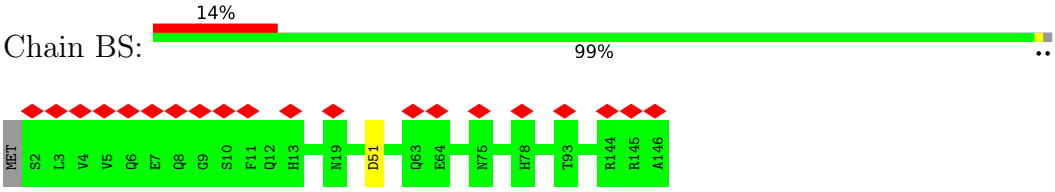
• Molecule 24: 40S ribosomal protein S17-A

Chain BR:



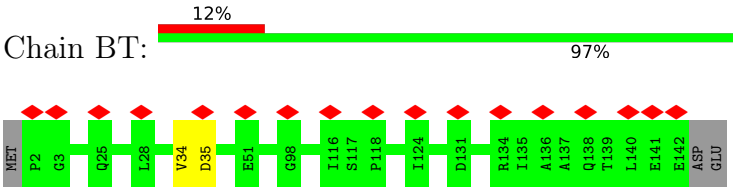
• Molecule 25: 40S ribosomal protein S18-A

Chain BS:



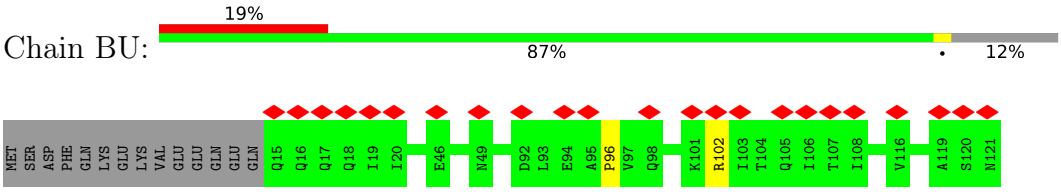
• Molecule 26: 40S ribosomal protein S19-A

Chain BT:



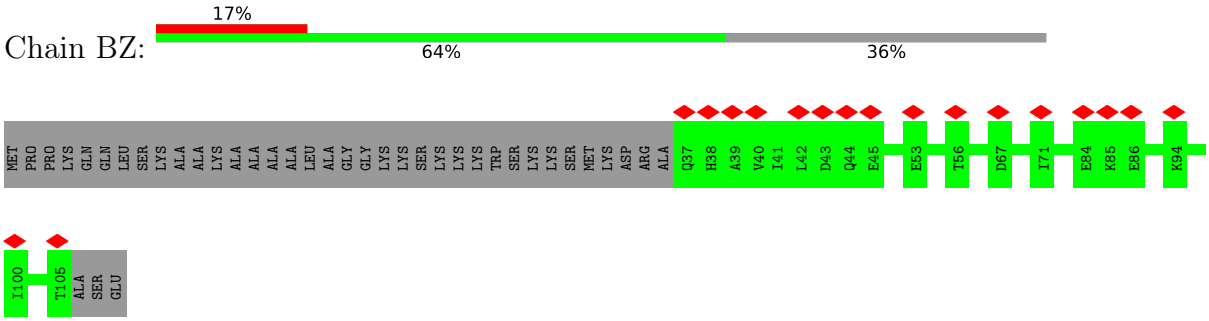
• Molecule 27: RPS20 isoform 1

Chain BU:



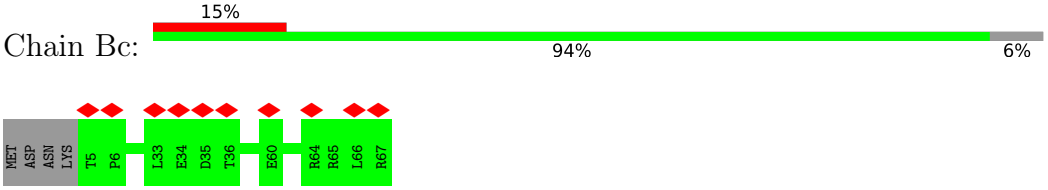
• Molecule 28: RPS25A isoform 1

Chain BZ:



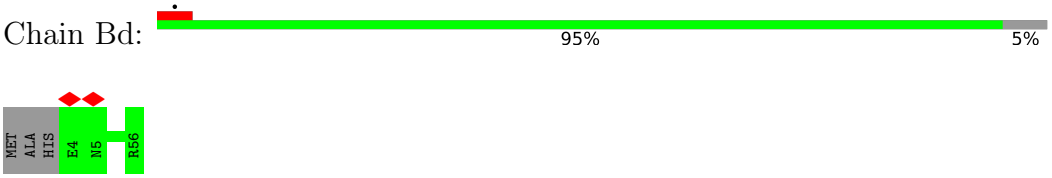
• Molecule 29: RPS28A isoform 1

Chain Bc:



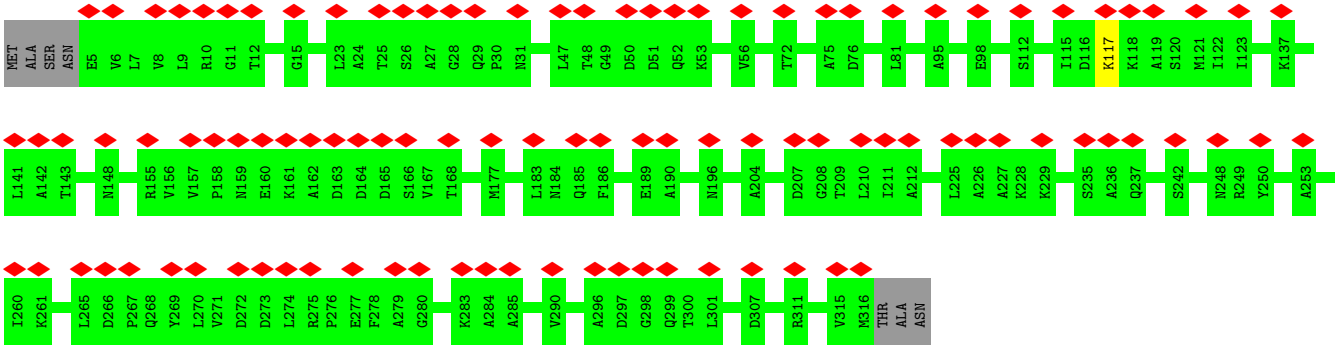
• Molecule 30: RPS29A isoform 1

Chain Bd:

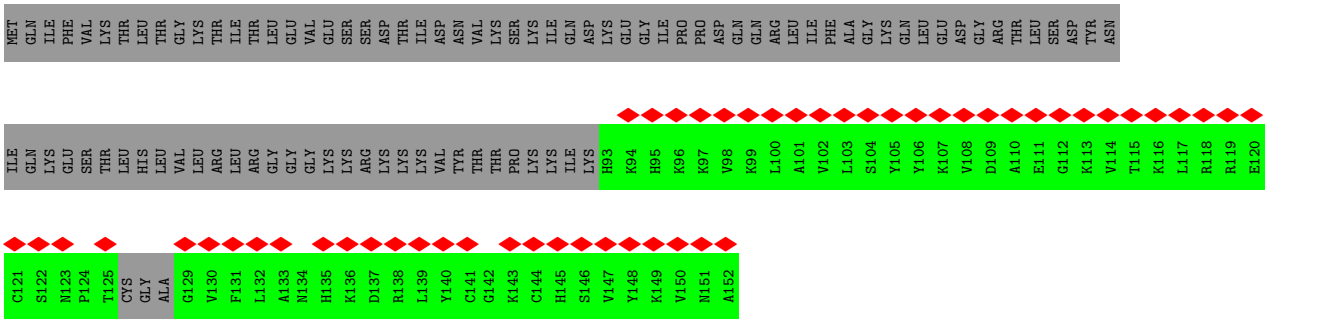


• Molecule 31: Guanine nucleotide-binding protein subunit beta-like protein

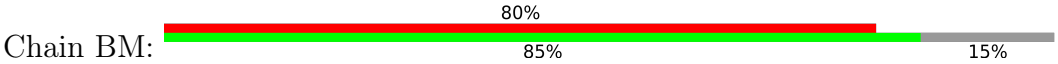
Chain Bg:

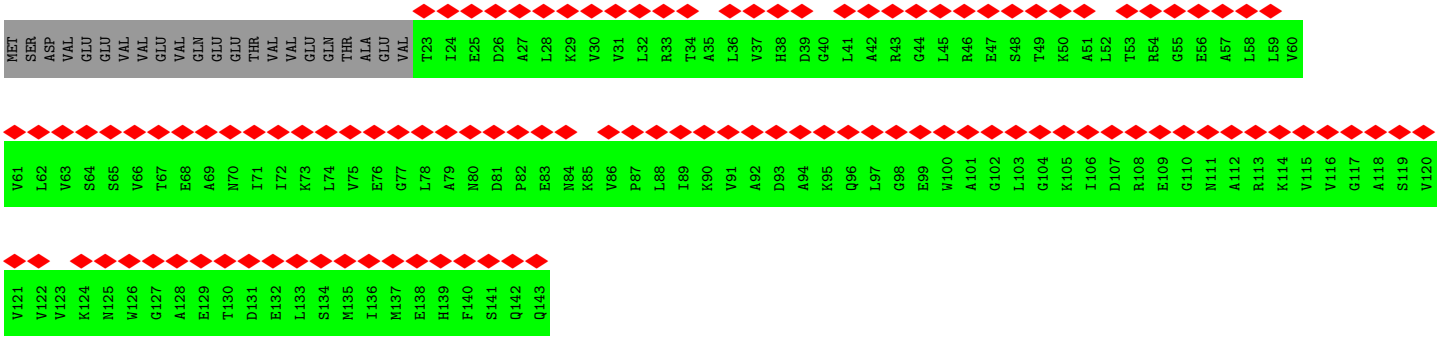


• Molecule 32: Ubiquitin-40S ribosomal protein S31

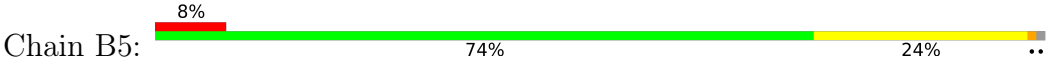


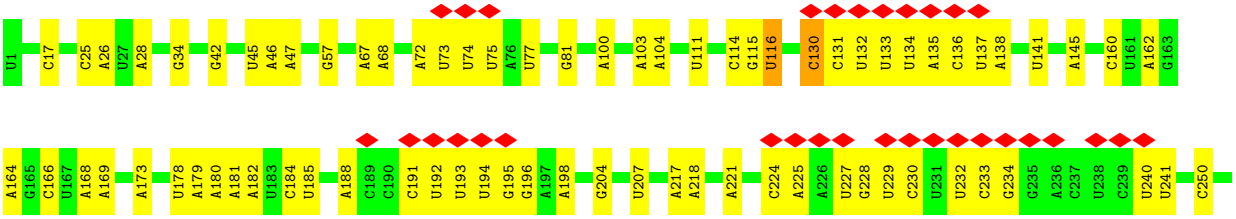
• Molecule 33: 40S ribosomal protein S12

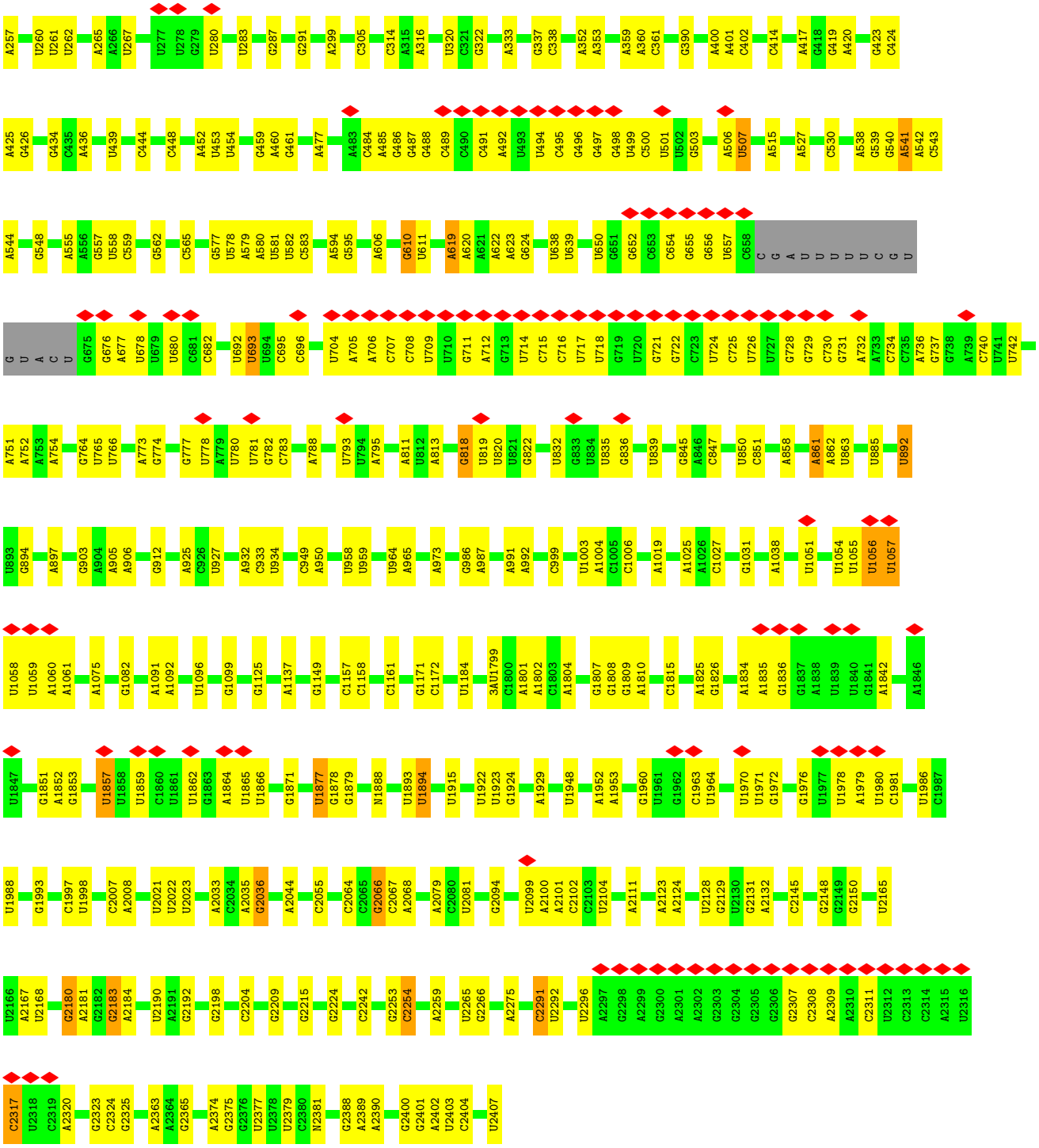




• Molecule 34: 18S rRNA

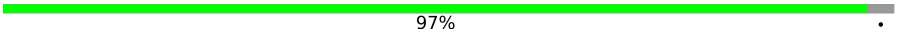






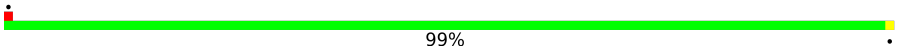
• Molecule 35: 60S ribosomal protein L2-A

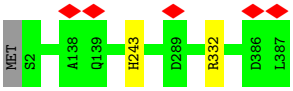
Chain AA:



• Molecule 36: 60S ribosomal protein L3

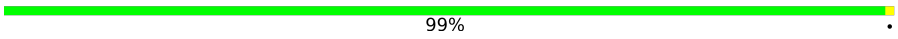
Chain AB:





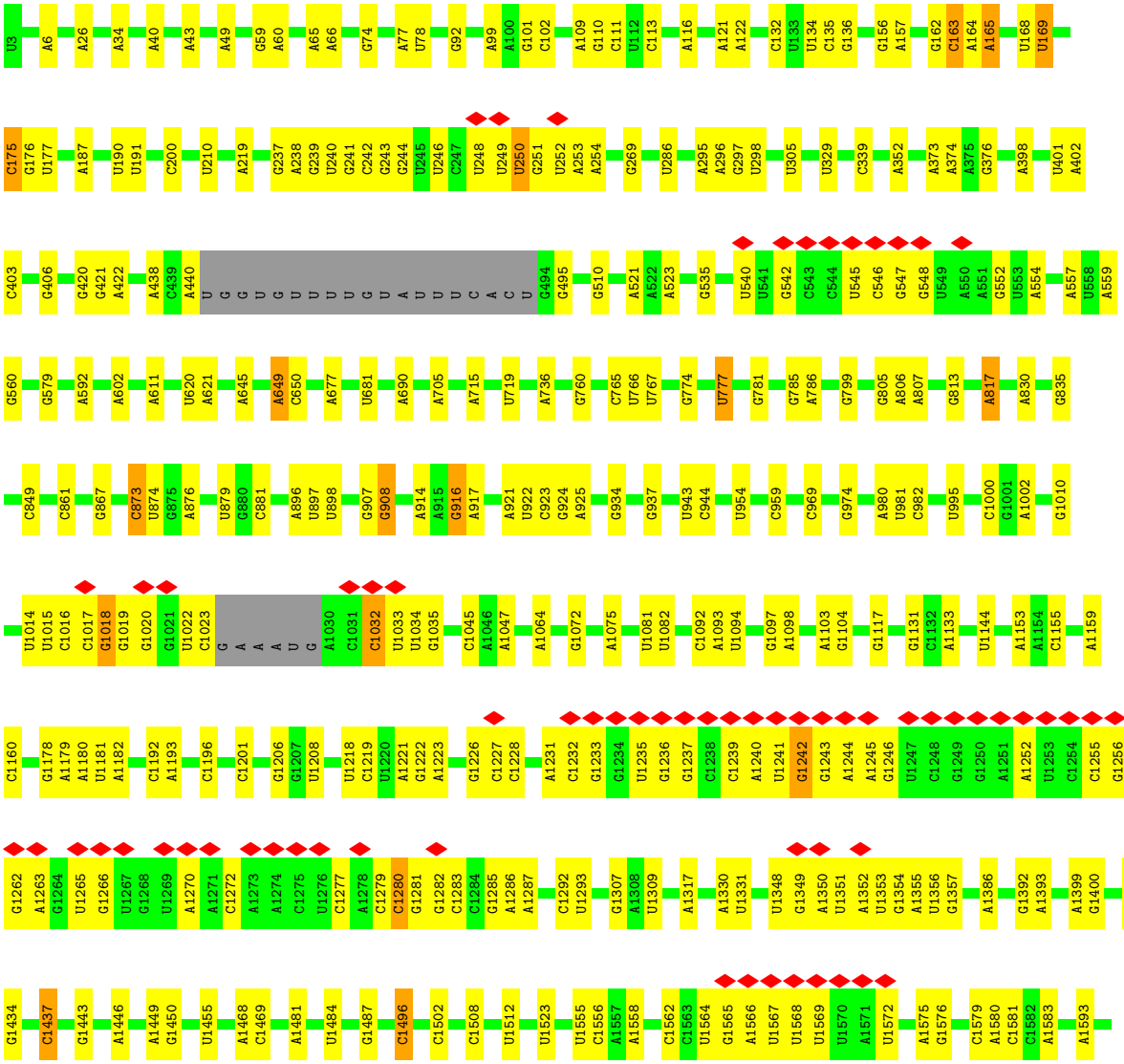
• Molecule 37: RPL4A isoform 1

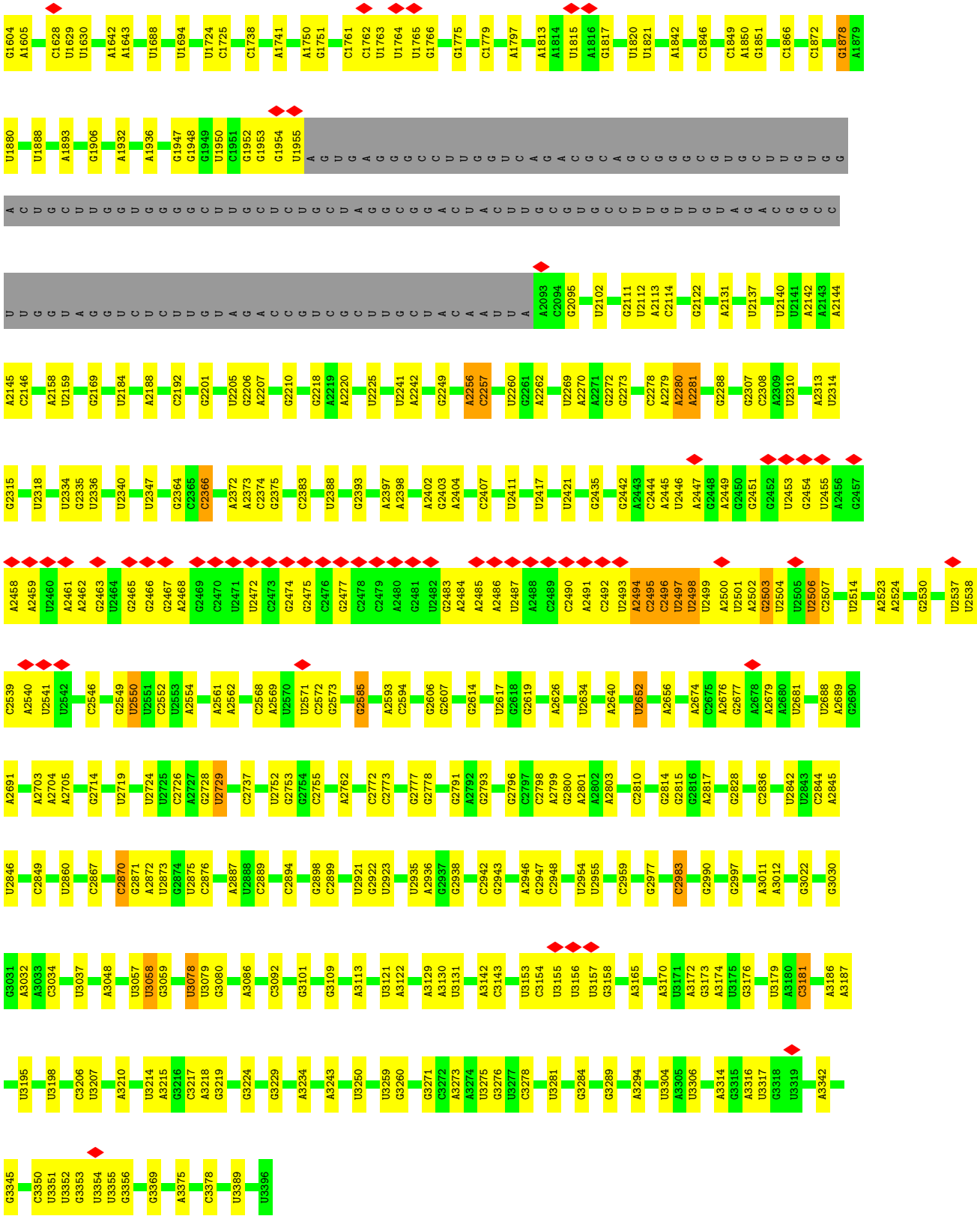
Chain AC:



• Molecule 38: 25S rRNA

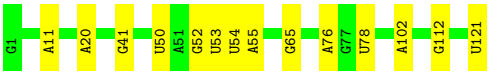
Chain A1:





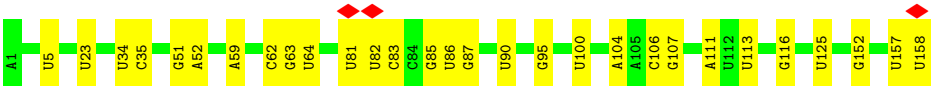
• Molecule 39: 5s rRNA

Chain A3:



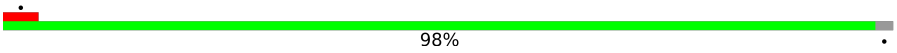
• Molecule 40: 5.8 S rRNA

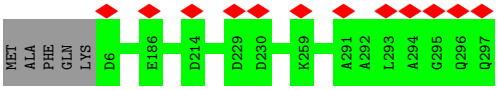
Chain A4:



• Molecule 41: RPL5 isoform 1

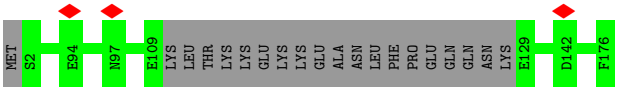
Chain AD:





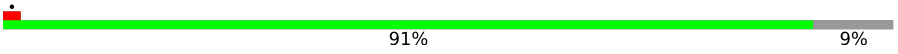
• Molecule 42: 60S ribosomal protein L6-A

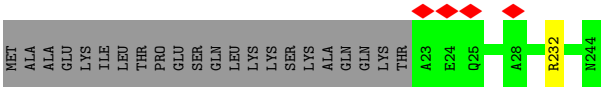
Chain AE:



• Molecule 43: 60S ribosomal protein L7-A

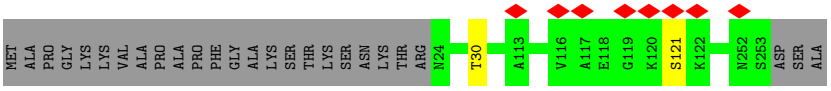
Chain AF:





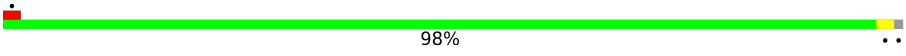
• Molecule 44: 60S ribosomal protein L8-A

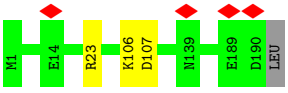
Chain AG:



• Molecule 45: 60S ribosomal protein L9-A

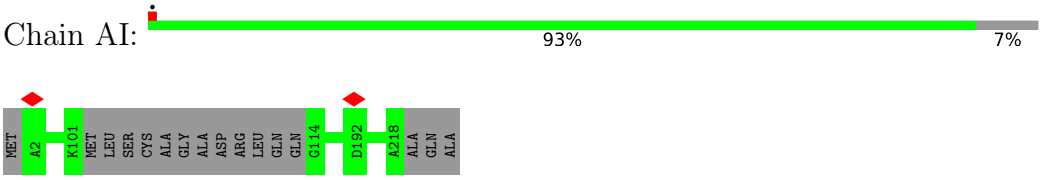
Chain AH:





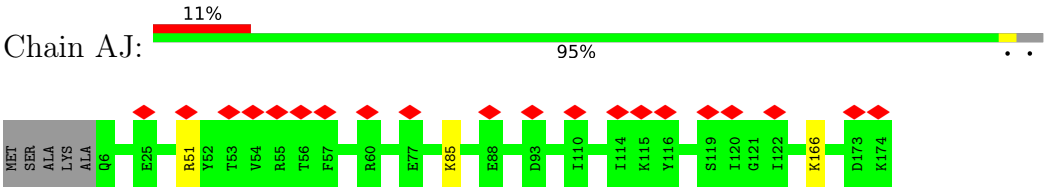
• Molecule 46: RPL10 isoform 1

Chain AI:



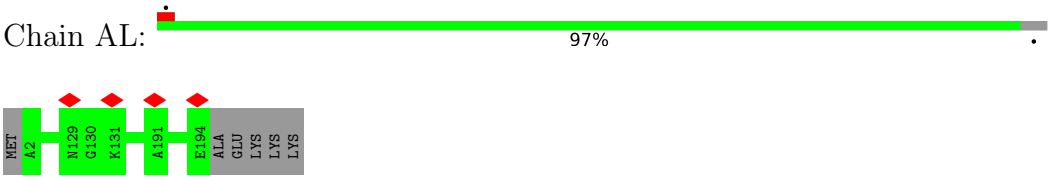
• Molecule 47: RPL11A isoform 1

Chain AJ:



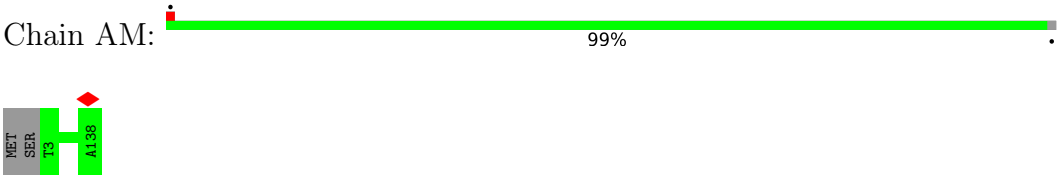
• Molecule 48: 60S ribosomal protein L13-A

Chain AL:



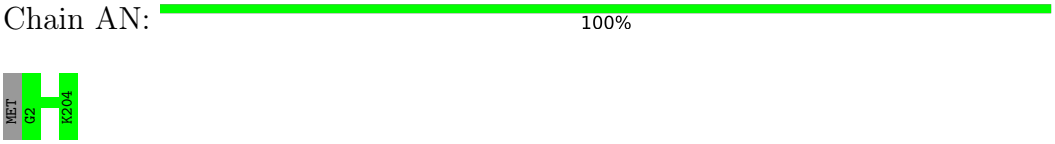
• Molecule 49: 60S ribosomal protein L14-A

Chain AM:



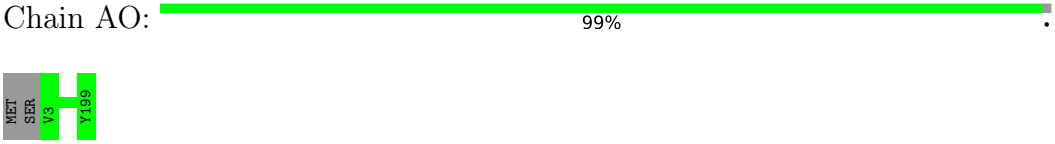
• Molecule 50: 60S ribosomal protein L15-A

Chain AN:



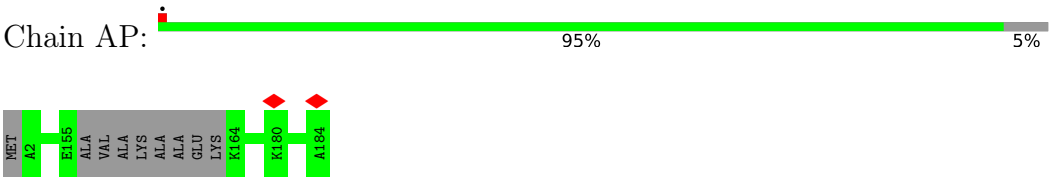
• Molecule 51: 60S ribosomal protein L16-A

Chain AO:



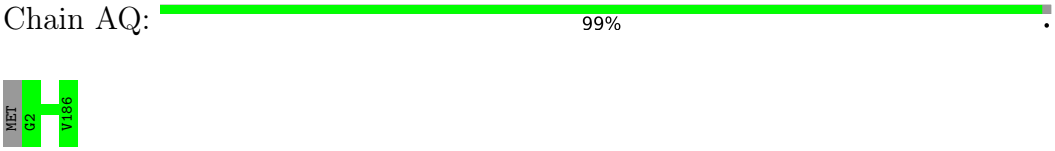
• Molecule 52: 60S ribosomal protein L17-A

Chain AP:



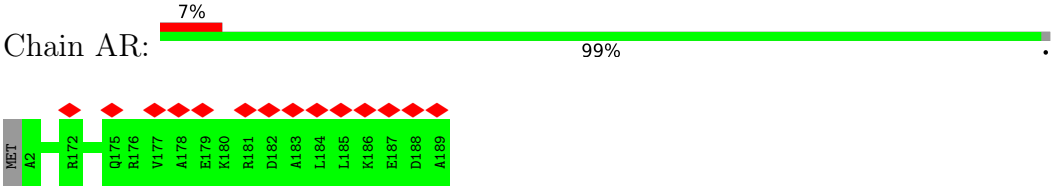
• Molecule 53: 60S ribosomal protein L18-A

Chain AQ:



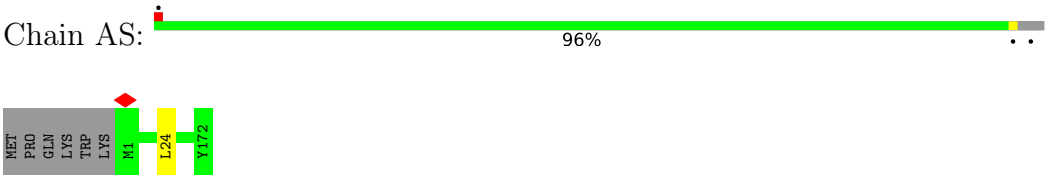
• Molecule 54: 60S ribosomal protein L19-A

Chain AR:



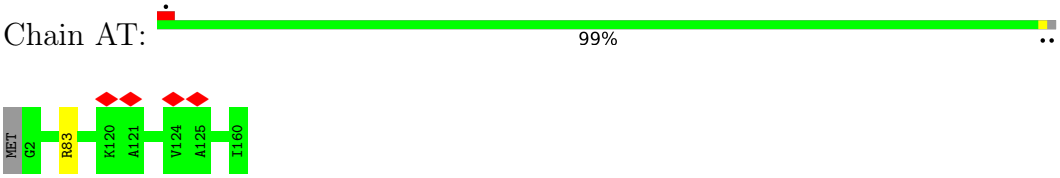
• Molecule 55: 60S ribosomal protein L20

Chain AS:



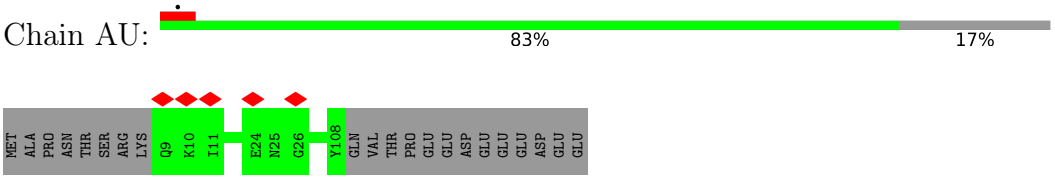
• Molecule 56: 60S ribosomal protein L21-A

Chain AT:



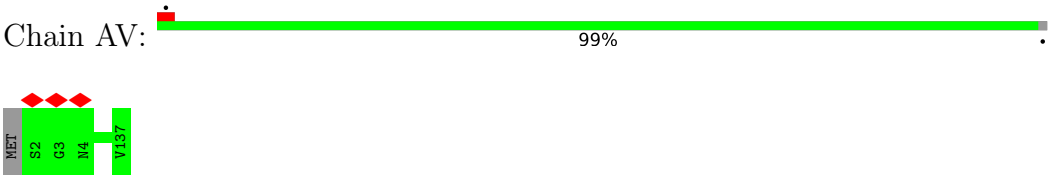
• Molecule 57: 60S ribosomal protein L22-A

Chain AU:



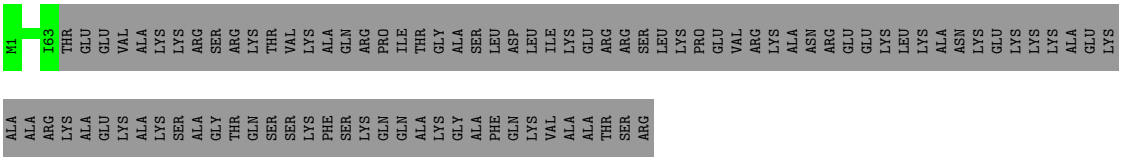
• Molecule 58: 60S ribosomal protein L23-A

Chain AV:



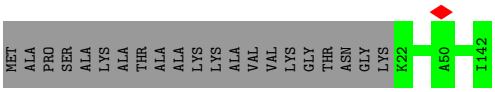
• Molecule 59: RPL24A isoform 1

Chain AW:



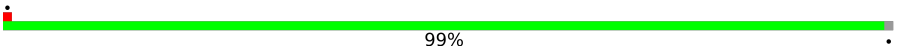
• Molecule 60: 60S ribosomal protein L25

Chain AX:



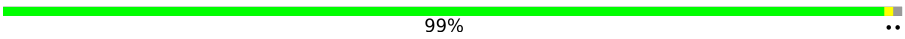
• Molecule 61: 60S ribosomal protein L26-A

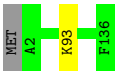
Chain AY:



• Molecule 62: 60S ribosomal protein L27-A

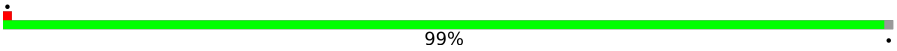
Chain AZ:

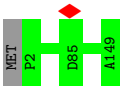




• Molecule 63: 60S ribosomal protein L28

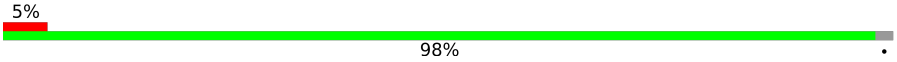
Chain Aa:

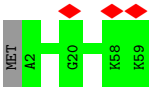




• Molecule 64: RPL29 isoform 1

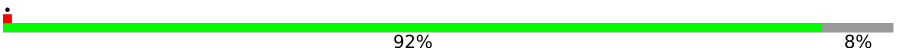
Chain Ab:

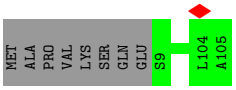




• Molecule 65: 60S ribosomal protein L30

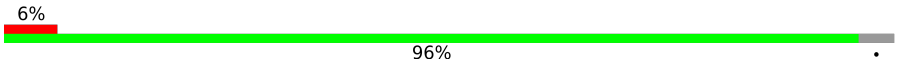
Chain Ac:

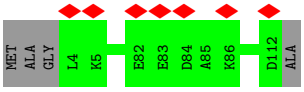




• Molecule 66: 60S ribosomal protein L31-A

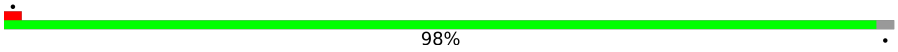
Chain Ad:

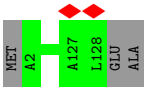




• Molecule 67: RPL32 isoform 1

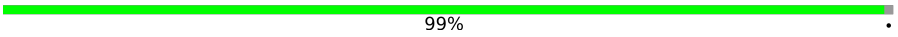
Chain Ae:





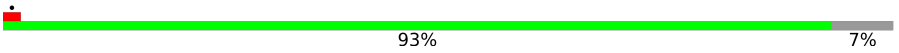
• Molecule 68: 60S ribosomal protein L33-A

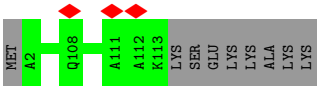
Chain Af:



• Molecule 69: 60S ribosomal protein L34-A

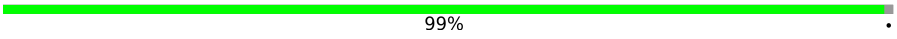
Chain Ag:





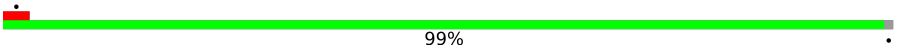
• Molecule 70: 60S ribosomal protein L35-A

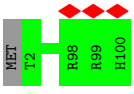
Chain Ah:



• Molecule 71: 60S ribosomal protein L36-A

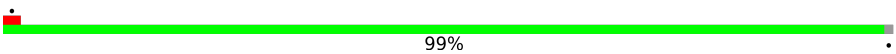
Chain Ai:

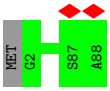




• Molecule 72: 60S ribosomal protein L37-A

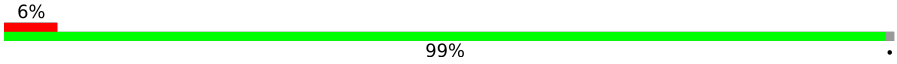
Chain Aj:

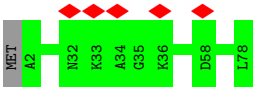




• Molecule 73: RPL38 isoform 1

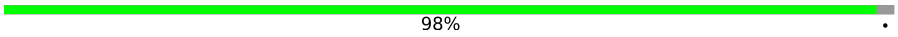
Chain Ak:





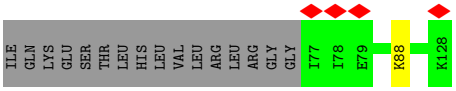
• Molecule 74: 60S ribosomal protein L39

Chain Al:



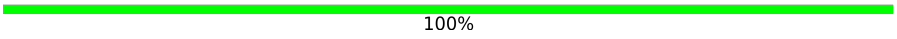
• Molecule 75: Ubiquitin-60S ribosomal protein L40

Chain Am:



• Molecule 76: 60S ribosomal protein L41-A

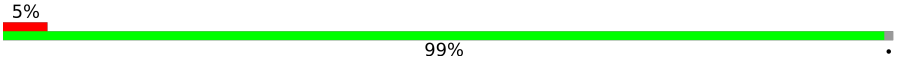
Chain An:

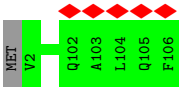


There are no outlier residues recorded for this chain.

• Molecule 77: 60S ribosomal protein L42-A

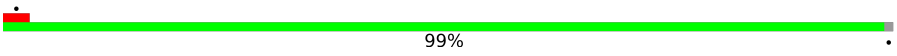
Chain Ao:

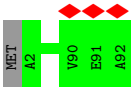




• Molecule 78: 60S ribosomal protein L43-A

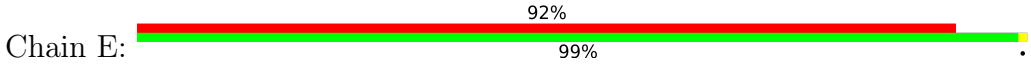
Chain Ap:

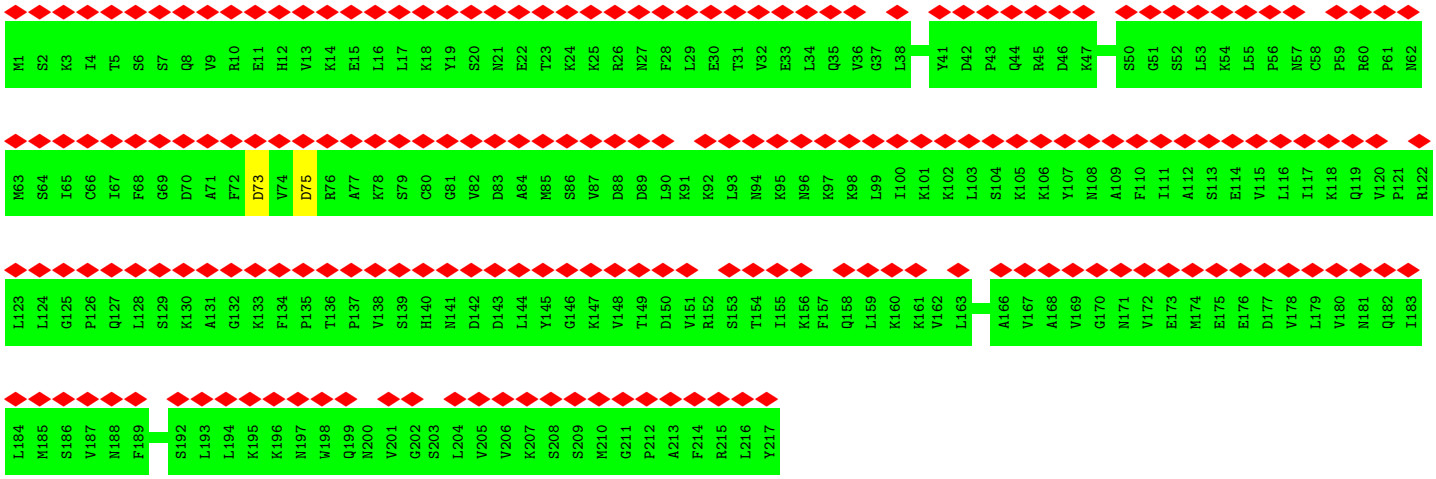




• Molecule 79: RPL1A isoform 1

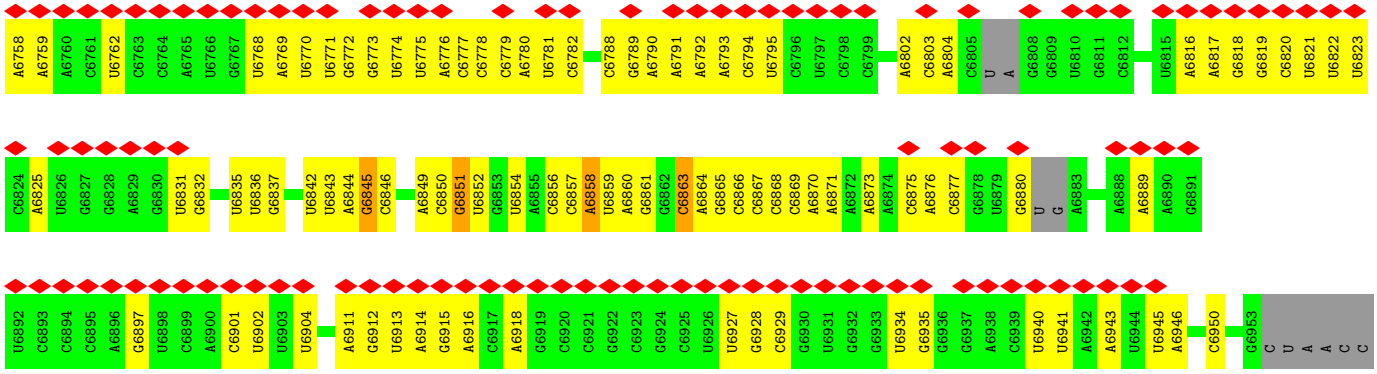
Chain E:





• Molecule 80: Internal ribosome entry site

Chain EC:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	112542	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	7.298	Depositor
Minimum map value	-3.391	Depositor
Average map value	0.017	Depositor
Map value standard deviation	0.255	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: UR3, HIC, 4AC, 3AU, MA6, ZN, OMG, MG, 1MA, OMC, A2M, 5MC, OMU, G7M

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	BA	0.29	0/1653	0.62	1/2261 (0.0%)
2	BB	0.28	0/1735	0.64	1/2335 (0.0%)
3	BC	0.28	0/1665	0.54	0/2263
4	BE	0.28	0/2109	0.60	0/2839
5	BG	0.26	0/1844	0.60	0/2464
6	BH	0.29	0/1506	0.61	0/2028
7	BI	0.28	0/1514	0.65	0/2021
8	BJ	0.26	0/1519	0.61	0/2035
9	BL	0.29	0/1272	0.56	0/1712
10	BN	0.28	0/1215	0.57	0/1638
11	BO	0.29	0/952	0.70	0/1279
12	BV	0.28	0/693	0.61	0/935
13	BW	0.27	0/1038	0.54	0/1395
14	BX	0.28	0/1139	0.60	0/1518
15	BY	0.27	0/1087	0.59	0/1449
16	Ba	0.28	0/782	0.68	0/1047
17	Bb	0.26	0/620	0.58	0/838
18	Be	0.25	0/483	0.62	0/643
19	BD	0.27	0/1759	0.61	1/2368 (0.0%)
20	BF	0.26	0/1629	0.59	0/2202
21	BK	0.29	0/837	0.59	0/1131
22	BP	0.28	0/1012	0.60	0/1356
23	BQ	0.28	0/1125	0.57	0/1510
24	BR	0.28	0/984	0.62	0/1318
25	BS	0.26	0/1211	0.63	1/1628 (0.1%)
26	BT	0.27	0/1113	0.68	2/1494 (0.1%)
27	BU	0.27	0/865	0.62	1/1169 (0.1%)
28	BZ	0.25	0/566	0.65	0/761
29	Bc	0.25	0/499	0.69	0/670
30	Bd	0.28	0/453	0.66	0/602
31	Bg	0.26	0/2454	0.60	0/3340
32	Bf	0.26	0/462	0.63	0/617

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	BM	0.25	0/921	0.61	0/1245
34	B5	0.32	0/41880	0.91	83/65248 (0.1%)
35	AA	0.29	0/1912	0.60	0/2569
36	AB	0.29	0/3138	0.58	0/4217
37	AC	0.29	0/2800	0.58	1/3790 (0.0%)
38	A1	0.39	0/75561	0.90	124/117806 (0.1%)
39	A3	0.32	0/2883	0.84	3/4491 (0.1%)
40	A4	0.38	0/3746	0.86	5/5832 (0.1%)
41	AD	0.27	0/2390	0.56	0/3225
42	AE	0.28	0/1260	0.57	0/1694
43	AF	0.29	0/1821	0.54	0/2451
44	AG	0.28	0/1830	0.55	0/2469
45	AH	0.28	0/1531	0.58	1/2062 (0.0%)
46	AI	0.27	0/1708	0.57	0/2290
47	AJ	0.28	0/1374	0.70	0/1842
48	AL	0.29	0/1568	0.61	0/2106
49	AM	0.27	0/1068	0.56	0/1438
50	AN	0.30	0/1757	0.61	0/2354
51	AO	0.28	0/1585	0.54	0/2128
52	AP	0.28	0/1410	0.57	0/1893
53	AQ	0.27	0/1465	0.58	0/1965
54	AR	0.26	0/1538	0.59	0/2050
55	AS	0.30	0/1481	0.59	1/1990 (0.1%)
56	AT	0.31	0/1300	0.60	0/1743
57	AU	0.28	0/812	0.56	0/1099
58	AV	0.29	0/1018	0.59	0/1369
59	AW	0.28	0/533	0.53	0/707
60	AX	0.31	0/983	0.56	0/1325
61	AY	0.29	0/1004	0.59	0/1341
62	AZ	0.28	0/1118	0.52	0/1497
63	Aa	0.29	0/1204	0.59	0/1612
64	Ab	0.24	0/473	0.53	0/629
65	Ac	0.30	0/751	0.55	0/1008
66	Ad	0.27	0/904	0.56	0/1213
67	Ae	0.26	0/1041	0.56	0/1394
68	Af	0.30	0/868	0.59	0/1168
69	Ag	0.32	0/890	0.62	0/1189
70	Ah	0.27	0/978	0.52	0/1301
71	Ai	0.29	0/778	0.61	0/1034
72	Aj	0.30	0/696	0.64	0/923
73	Ak	0.28	0/618	0.58	0/826
74	Al	0.26	0/443	0.68	0/588
75	Am	0.27	0/423	0.57	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	An	0.28	0/234	0.86	0/300
77	Ao	0.28	0/860	0.60	0/1136
78	Ap	0.28	0/701	0.62	0/934
79	E	0.27	0/1745	0.59	2/2342 (0.1%)
80	EC	0.32	1/4571 (0.0%)	0.96	14/7114 (0.2%)
All	All	0.33	1/219368 (0.0%)	0.80	241/322375 (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
20	BF	0	1
34	B5	1	0
43	AF	0	1
44	AG	0	2
47	AJ	0	1
All	All	1	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
80	EC	6758	A	OP3-P	-10.70	1.48	1.61

All (241) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	406	G	O4'-C1'-N9	9.55	115.84	108.20
38	A1	922	U	C2-N1-C1'	9.07	128.59	117.70
34	B5	1997	C	C2-N1-C1'	9.03	128.73	118.80
38	A1	2451	G	N7-C8-N9	8.95	117.57	113.10
38	A1	922	U	N1-C2-O2	8.37	128.66	122.80
38	A1	2225	U	C2-N1-C1'	8.26	127.61	117.70
38	A1	3034	C	C2-N1-C1'	8.21	127.83	118.80
38	A1	165	A	C8-N9-C4	-8.11	102.56	105.80
34	B5	964	U	C2-N1-C1'	7.97	127.27	117.70
80	EC	6868	C	N1-C2-O2	7.93	123.66	118.90
80	EC	6868	C	C2-N1-C1'	7.84	127.42	118.80
34	B5	581	U	C2-N1-C1'	7.78	127.04	117.70
34	B5	2066	G	N3-C4-C5	-7.78	124.71	128.60
38	A1	922	U	N3-C2-O2	-7.70	116.81	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	2451	G	C8-N9-C4	-7.66	103.34	106.40
38	A1	3181	C	N1-C2-O2	7.54	123.42	118.90
34	B5	453	U	N1-C2-O2	7.46	128.02	122.80
38	A1	2257	C	N1-C2-O2	7.45	123.37	118.90
40	A4	5	U	N3-C2-O2	-7.41	117.02	122.20
38	A1	163	C	C2-N1-C1'	7.40	126.94	118.80
38	A1	3181	C	C2-N1-C1'	7.38	126.92	118.80
34	B5	453	U	C2-N1-C1'	7.35	126.52	117.70
38	A1	2836	C	C2-N1-C1'	7.30	126.83	118.80
34	B5	1997	C	N1-C2-O2	7.26	123.26	118.90
38	A1	3034	C	N1-C2-O2	7.26	123.25	118.90
34	B5	581	U	N1-C2-O2	7.20	127.84	122.80
26	BT	34	VAL	C-N-CA	7.15	139.57	121.70
80	EC	6866	C	N1-C2-O2	7.13	123.18	118.90
37	AC	182	LEU	CA-CB-CG	7.11	131.64	115.30
38	A1	2846	U	C2-N1-C1'	7.09	126.21	117.70
38	A1	2652	U	N3-C2-O2	-7.07	117.25	122.20
80	EC	6851	G	P-O3'-C3'	7.06	128.18	119.70
34	B5	1894	U	N1-C2-O2	7.02	127.72	122.80
38	A1	2495	C	C2-N1-C1'	-6.99	111.11	118.80
38	A1	2836	C	N3-C2-O2	-6.99	117.01	121.90
38	A1	2497	U	P-O3'-C3'	6.99	128.09	119.70
34	B5	453	U	N3-C2-O2	-6.97	117.32	122.20
79	E	75	ASP	CB-CG-OD1	6.95	124.56	118.30
38	A1	1032	C	N1-C2-O2	6.92	123.05	118.90
40	A4	5	U	C2-N1-C1'	6.90	125.98	117.70
38	A1	2772	C	N1-C2-O2	6.89	123.04	118.90
38	A1	2495	C	C6-N1-C1'	6.88	129.06	120.80
34	B5	2066	G	C2-N3-C4	6.88	115.34	111.90
34	B5	1056	U	P-O3'-C3'	6.86	127.94	119.70
34	B5	863	U	C2-N1-C1'	6.83	125.90	117.70
34	B5	2168	U	C2-N1-C1'	6.82	125.89	117.70
38	A1	169	U	N3-C2-O2	-6.81	117.43	122.20
34	B5	1894	U	N3-C2-O2	-6.76	117.47	122.20
34	B5	1988	U	C2-N1-C1'	6.73	125.77	117.70
38	A1	2836	C	N1-C2-O2	6.72	122.94	118.90
34	B5	766	U	N3-C2-O2	-6.69	117.52	122.20
38	A1	2257	C	C2-N1-C1'	6.68	126.15	118.80
34	B5	766	U	C2-N1-C1'	6.67	125.71	117.70
34	B5	581	U	N3-C2-O2	-6.64	117.55	122.20
34	B5	1997	C	C6-N1-C2	-6.63	117.65	120.30
38	A1	1496	C	C2-N1-C1'	6.63	126.09	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	3058	U	C2-N1-C1'	6.61	125.63	117.70
34	B5	1915	U	C2-N1-C1'	6.58	125.60	117.70
38	A1	169	U	C2-N1-C1'	6.56	125.57	117.70
38	A1	169	U	N1-C2-O2	6.53	127.37	122.80
34	B5	2317	C	N1-C2-O2	6.49	122.80	118.90
38	A1	2899	C	C2-N1-C1'	6.47	125.92	118.80
38	A1	1280	C	C6-N1-C2	-6.47	117.71	120.30
38	A1	3034	C	N3-C2-O2	-6.45	117.39	121.90
34	B5	766	U	N1-C2-O2	6.42	127.29	122.80
34	B5	958	U	N1-C2-O2	6.41	127.29	122.80
38	A1	297	G	O4'-C1'-N9	6.41	113.33	108.20
34	B5	1894	U	C2-N1-C1'	6.40	125.38	117.70
34	B5	999	C	C2-N1-C1'	6.39	125.83	118.80
38	A1	1032	C	C2-N1-C1'	6.38	125.82	118.80
38	A1	250	U	N3-C2-O2	-6.36	117.75	122.20
34	B5	1915	U	N1-C2-O2	6.35	127.25	122.80
80	EC	6866	C	C2-N1-C1'	6.35	125.79	118.80
34	B5	863	U	N1-C2-O2	6.33	127.23	122.80
34	B5	863	U	N3-C2-O2	-6.30	117.79	122.20
34	B5	958	U	N3-C2-O2	-6.30	117.79	122.20
38	A1	2772	C	C2-N1-C1'	6.28	125.70	118.80
38	A1	250	U	N1-C2-O2	6.26	127.18	122.80
34	B5	2081	U	N1-C2-O2	6.24	127.17	122.80
38	A1	2225	U	C6-N1-C1'	-6.23	112.48	121.20
38	A1	2846	U	N3-C2-O2	-6.20	117.86	122.20
38	A1	3057	U	N3-C2-O2	-6.20	117.86	122.20
79	E	73	ASP	CB-CG-OD1	6.19	123.87	118.30
34	B5	1997	C	C5-C6-N1	6.19	124.09	121.00
38	A1	1604	G	C4-N9-C1'	6.18	134.54	126.50
38	A1	3181	C	N3-C2-O2	-6.18	117.58	121.90
34	B5	693	U	N3-C2-O2	-6.17	117.88	122.20
38	A1	835	G	O4'-C1'-N9	6.16	113.13	108.20
38	A1	922	U	C6-N1-C1'	-6.15	112.58	121.20
80	EC	6868	C	N3-C2-O2	-6.15	117.59	121.90
38	A1	954	U	C2-N1-C1'	6.13	125.05	117.70
34	B5	693	U	N1-C2-O2	6.10	127.07	122.80
38	A1	2846	U	N1-C2-O2	6.09	127.06	122.80
34	B5	2081	U	N3-C2-O2	-6.08	117.95	122.20
34	B5	583	C	C2-N1-C1'	6.05	125.45	118.80
38	A1	3317	U	C2-N1-C1'	6.03	124.94	117.70
26	BT	35	ASP	CB-CG-OD1	6.02	123.72	118.30
34	B5	2066	G	C8-N9-C4	-6.00	104.00	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B5	1997	C	C6-N1-C1'	-5.99	113.61	120.80
27	BU	96	PRO	N-CD-CG	-5.98	94.23	103.20
34	B5	2081	U	C2-N1-C1'	5.97	124.87	117.70
38	A1	3037	U	C2-N1-C1'	5.97	124.87	117.70
55	AS	24	LEU	CA-CB-CG	5.97	129.03	115.30
38	A1	102	C	N1-C2-O2	5.96	122.47	118.90
34	B5	610	G	N3-C4-C5	-5.93	125.63	128.60
34	B5	1988	U	N1-C2-O2	5.93	126.95	122.80
38	A1	3057	U	N1-C2-O2	5.93	126.95	122.80
38	A1	2257	C	N3-C2-O2	-5.92	117.76	121.90
34	B5	1997	C	N3-C2-O2	-5.90	117.77	121.90
38	A1	2652	U	N1-C2-O2	5.90	126.93	122.80
34	B5	1915	U	N3-C2-O2	-5.90	118.07	122.20
40	A4	100	U	C2-N1-C1'	5.88	124.75	117.70
25	BS	51	ASP	CB-CG-OD1	5.87	123.59	118.30
34	B5	2204	C	C2-N1-C1'	5.87	125.26	118.80
80	EC	6866	C	N3-C2-O2	-5.87	117.79	121.90
34	B5	861	A	P-O3'-C3'	5.86	126.73	119.70
34	B5	958	U	C2-N1-C1'	5.86	124.73	117.70
40	A4	5	U	N1-C2-O2	5.84	126.89	122.80
38	A1	2495	C	O4'-C1'-N1	5.83	112.87	108.20
34	B5	2168	U	N3-C2-O2	-5.82	118.13	122.20
38	A1	2444	C	C5-C6-N1	5.81	123.90	121.00
38	A1	3306	U	C2-N1-C1'	5.81	124.67	117.70
38	A1	1018	G	C4-N9-C1'	5.80	134.04	126.50
38	A1	873	C	P-O3'-C3'	5.80	126.66	119.70
34	B5	507	U	N1-C2-O2	5.78	126.85	122.80
38	A1	3037	U	N3-C2-O2	-5.78	118.15	122.20
38	A1	2836	C	C6-N1-C2	-5.77	117.99	120.30
38	A1	3034	C	C6-N1-C1'	-5.75	113.89	120.80
34	B5	583	C	N1-C2-O2	5.75	122.35	118.90
38	A1	1947	G	OP1-P-O3'	5.74	117.83	105.20
38	A1	2506	U	C2-N1-C1'	5.74	124.58	117.70
34	B5	850	U	O4'-C1'-N1	-5.73	103.61	108.20
34	B5	2317	C	N3-C2-O2	-5.73	117.89	121.90
38	A1	163	C	C5-C6-N1	5.73	123.86	121.00
34	B5	1988	U	N3-C2-O2	-5.72	118.19	122.20
40	A4	64	U	N3-C2-O2	-5.71	118.20	122.20
34	B5	610	G	C2-N3-C4	5.70	114.75	111.90
2	BB	47	LEU	CA-CB-CG	5.68	128.38	115.30
38	A1	2496	C	P-O3'-C3'	5.68	126.52	119.70
34	B5	964	U	N1-C2-O2	5.66	126.76	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	1018	G	N3-C4-N9	5.65	129.39	126.00
38	A1	1878	G	C4-N9-C1'	5.64	133.84	126.50
38	A1	2451	G	C6-C5-N7	-5.64	127.02	130.40
38	A1	1872	C	N1-C2-O2	5.63	122.28	118.90
38	A1	3317	U	N1-C2-O2	5.60	126.72	122.80
80	EC	6845	G	O5'-P-OP1	-5.60	100.66	105.70
80	EC	6868	C	C6-N1-C1'	-5.58	114.10	120.80
38	A1	163	C	C6-N1-C2	-5.58	118.07	120.30
34	B5	2168	U	N1-C2-O2	5.57	126.70	122.80
39	A3	50	U	C2-N1-C1'	5.57	124.38	117.70
38	A1	3214	U	C2-N1-C1'	5.57	124.38	117.70
34	B5	1054	U	C5-C6-N1	5.55	125.48	122.70
34	B5	1161	C	N1-C2-O2	5.55	122.23	118.90
34	B5	2066	G	N3-C4-N9	5.55	129.33	126.00
38	A1	1242	G	C4-N9-C1'	5.55	133.71	126.50
38	A1	3057	U	C2-N1-C1'	5.54	124.35	117.70
34	B5	2066	G	C4-N9-C1'	5.52	133.68	126.50
38	A1	78	U	N3-C2-O2	-5.52	118.34	122.20
39	A3	50	U	N1-C2-O2	5.50	126.65	122.80
38	A1	2451	G	C5-N7-C8	-5.49	101.55	104.30
34	B5	2183	G7M	O3'-P-O5'	5.49	114.43	104.00
38	A1	3306	U	N3-C2-O2	-5.49	118.36	122.20
34	B5	1857	U	C2-N1-C1'	5.48	124.28	117.70
38	A1	881	C	N1-C2-O2	5.48	122.19	118.90
38	A1	165	A	N7-C8-N9	5.48	116.54	113.80
38	A1	2366	C	C2-N1-C1'	5.48	124.82	118.80
38	A1	2497	U	OP1-P-O3'	5.48	117.25	105.20
38	A1	2983	C	C2-N1-C1'	5.46	124.81	118.80
38	A1	168	U	C2-N1-C1'	5.45	124.24	117.70
34	B5	507	U	N3-C2-O2	-5.45	118.39	122.20
38	A1	1694	U	N3-C2-O2	-5.42	118.40	122.20
80	EC	6858	A	P-O3'-C3'	5.42	126.21	119.70
34	B5	693	U	C2-N1-C1'	5.42	124.20	117.70
38	A1	113	C	C2-N1-C1'	5.39	124.73	118.80
34	B5	964	U	C6-N1-C1'	-5.39	113.66	121.20
34	B5	892	U	N3-C2-O2	-5.38	118.43	122.20
34	B5	2254	C	N1-C2-O2	5.38	122.13	118.90
39	A3	50	U	N3-C2-O2	-5.38	118.44	122.20
34	B5	184	C	C2-N1-C1'	5.38	124.71	118.80
34	B5	543	C	N1-C2-O2	5.37	122.12	118.90
38	A1	1032	C	N3-C2-O2	-5.37	118.14	121.90
19	BD	105	MET	CA-CB-CG	5.36	122.42	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	102	C	N3-C2-O2	-5.36	118.15	121.90
38	A1	175	C	N1-C2-O2	5.36	122.12	118.90
38	A1	2503	G	O4'-C1'-N9	5.36	112.48	108.20
38	A1	1242	G	N3-C4-C5	-5.35	125.92	128.60
34	B5	130	C	N1-C2-O2	5.35	122.11	118.90
34	B5	964	U	N3-C2-O2	-5.34	118.46	122.20
38	A1	954	U	N1-C2-O2	5.34	126.54	122.80
38	A1	2494	A	C8-N9-C4	-5.34	103.67	105.80
38	A1	2726	C	C2-N1-C1'	5.32	124.65	118.80
38	A1	954	U	N3-C2-O2	-5.32	118.48	122.20
34	B5	892	U	N1-C2-O2	5.28	126.50	122.80
38	A1	101	G	C8-N9-C1'	-5.25	120.17	127.00
34	B5	507	U	C2-N1-C1'	5.25	124.00	117.70
38	A1	3317	U	N3-C2-O2	-5.24	118.53	122.20
38	A1	777	U	N3-C2-O2	-5.23	118.54	122.20
80	EC	6846	C	C2-N1-C1'	5.23	124.56	118.80
38	A1	2498	U	C6-N1-C2	-5.22	117.87	121.00
38	A1	2225	U	N1-C2-O2	5.21	126.45	122.80
34	B5	2064	C	C2-N1-C1'	5.21	124.53	118.80
38	A1	2137	U	C2-N1-C1'	5.21	123.95	117.70
38	A1	2772	C	N3-C2-O2	-5.20	118.26	121.90
34	B5	818	G	P-O3'-C3'	5.20	125.94	119.70
38	A1	1018	G	C8-N9-C1'	-5.19	120.25	127.00
38	A1	2550	U	N3-C2-O2	-5.19	118.57	122.20
38	A1	3181	C	C6-N1-C1'	-5.18	114.58	120.80
38	A1	1604	G	C8-N9-C1'	-5.18	120.27	127.00
34	B5	116	U	N3-C2-O2	-5.17	118.58	122.20
34	B5	2291	C	O4'-C1'-N1	5.17	112.33	108.20
80	EC	6854	U	N3-C2-O2	-5.17	118.58	122.20
38	A1	1604	G	N3-C4-C5	-5.17	126.02	128.60
38	A1	2407	C	C5-C6-N1	5.17	123.58	121.00
38	A1	1694	U	C2-N1-C1'	5.16	123.89	117.70
1	BA	42	PRO	C-N-CA	5.16	134.59	121.70
34	B5	847	C	N3-C2-O2	-5.14	118.30	121.90
45	AH	107	ASP	CB-CG-OD1	5.14	122.92	118.30
34	B5	999	C	N1-C2-O2	5.13	121.98	118.90
38	A1	3078	U	C2-N1-C1'	5.13	123.85	117.70
34	B5	530	C	N1-C2-O2	5.12	121.97	118.90
38	A1	969	C	N1-C2-O2	5.11	121.97	118.90
38	A1	251	G	N3-C4-C5	-5.11	126.05	128.60
34	B5	581	U	C6-N1-C1'	-5.09	114.08	121.20
38	A1	2585	G	N3-C4-C5	-5.08	126.06	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	2550	U	C2-N1-C1'	5.08	123.79	117.70
38	A1	2617	U	N3-C2-O2	-5.07	118.65	122.20
38	A1	3034	C	C6-N1-C2	-5.07	118.27	120.30
38	A1	777	U	N1-C2-O2	5.07	126.35	122.80
38	A1	132	C	C2-N1-C1'	5.06	124.37	118.80
38	A1	1242	G	N3-C4-N9	5.06	129.04	126.00
80	EC	6863	C	P-O3'-C3'	5.06	125.77	119.70
34	B5	1057	U	O5'-P-OP2	-5.05	101.16	105.70
38	A1	1604	G	N3-C4-N9	5.05	129.03	126.00
38	A1	3048	A	O4'-C1'-N9	5.04	112.23	108.20
80	EC	6854	U	N1-C2-O2	5.04	126.33	122.80
34	B5	1161	C	C2-N1-C1'	5.03	124.33	118.80
38	A1	760	G	O4'-C1'-N9	5.02	112.22	108.20
38	A1	3058	U	N1-C2-O2	5.02	126.32	122.80
38	A1	2506	U	P-O3'-C3'	5.02	125.72	119.70
34	B5	933	C	C2-N1-C1'	5.02	124.32	118.80
38	A1	916	G	P-O3'-C3'	5.00	125.71	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	B5	1799	3AU	C12

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
43	AF	232	ARG	Peptide
44	AG	121	SER	Peptide
44	AG	30	THR	Peptide
47	AJ	166	LYS	Peptide
20	BF	124	LEU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BA	204/252 (81%)	186 (91%)	18 (9%)	0	100	100
2	BB	212/255 (83%)	185 (87%)	27 (13%)	0	100	100
3	BC	215/254 (85%)	206 (96%)	9 (4%)	0	100	100
4	BE	258/261 (99%)	244 (95%)	14 (5%)	0	100	100
5	BG	224/236 (95%)	215 (96%)	9 (4%)	0	100	100
6	BH	182/190 (96%)	170 (93%)	12 (7%)	0	100	100
7	BI	184/200 (92%)	168 (91%)	16 (9%)	0	100	100
8	BJ	183/197 (93%)	168 (92%)	15 (8%)	0	100	100
9	BL	153/156 (98%)	141 (92%)	12 (8%)	0	100	100
10	BN	148/151 (98%)	140 (95%)	8 (5%)	0	100	100
11	BO	125/137 (91%)	112 (90%)	13 (10%)	0	100	100
12	BV	85/87 (98%)	75 (88%)	10 (12%)	0	100	100
13	BW	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	BX	142/145 (98%)	131 (92%)	11 (8%)	0	100	100
15	BY	132/135 (98%)	124 (94%)	8 (6%)	0	100	100
16	Ba	95/119 (80%)	79 (83%)	16 (17%)	0	100	100
17	Bb	79/82 (96%)	67 (85%)	12 (15%)	0	100	100
18	Be	58/63 (92%)	53 (91%)	5 (9%)	0	100	100
19	BD	221/240 (92%)	209 (95%)	12 (5%)	0	100	100
20	BF	204/225 (91%)	191 (94%)	13 (6%)	0	100	100
21	BK	94/105 (90%)	83 (88%)	11 (12%)	0	100	100
22	BP	122/142 (86%)	111 (91%)	11 (9%)	0	100	100
23	BQ	139/143 (97%)	133 (96%)	6 (4%)	0	100	100
24	BR	117/136 (86%)	110 (94%)	7 (6%)	0	100	100
25	BS	143/146 (98%)	129 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BT	139/144 (96%)	127 (91%)	12 (9%)	0	100	100
27	BU	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
28	BZ	67/108 (62%)	62 (92%)	5 (8%)	0	100	100
29	Bc	61/67 (91%)	57 (93%)	4 (7%)	0	100	100
30	Bd	51/56 (91%)	50 (98%)	1 (2%)	0	100	100
31	Bg	310/319 (97%)	275 (89%)	35 (11%)	0	100	100
32	Bf	53/152 (35%)	39 (74%)	14 (26%)	0	100	100
33	BM	119/143 (83%)	95 (80%)	24 (20%)	0	100	100
35	AA	245/254 (96%)	232 (95%)	13 (5%)	0	100	100
36	AB	383/387 (99%)	367 (96%)	16 (4%)	0	100	100
37	AC	359/362 (99%)	335 (93%)	24 (7%)	0	100	100
41	AD	290/297 (98%)	276 (95%)	14 (5%)	0	100	100
42	AE	152/176 (86%)	141 (93%)	11 (7%)	0	100	100
43	AF	220/244 (90%)	213 (97%)	7 (3%)	0	100	100
44	AG	228/256 (89%)	212 (93%)	16 (7%)	0	100	100
45	AH	188/191 (98%)	172 (92%)	16 (8%)	0	100	100
46	AI	201/221 (91%)	191 (95%)	10 (5%)	0	100	100
47	AJ	167/174 (96%)	142 (85%)	25 (15%)	0	100	100
48	AL	191/199 (96%)	179 (94%)	12 (6%)	0	100	100
49	AM	134/138 (97%)	130 (97%)	4 (3%)	0	100	100
50	AN	201/204 (98%)	191 (95%)	10 (5%)	0	100	100
51	AO	195/199 (98%)	193 (99%)	2 (1%)	0	100	100
52	AP	171/184 (93%)	167 (98%)	4 (2%)	0	100	100
53	AQ	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
54	AR	186/189 (98%)	177 (95%)	9 (5%)	0	100	100
55	AS	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
56	AT	157/160 (98%)	149 (95%)	8 (5%)	0	100	100
57	AU	98/121 (81%)	94 (96%)	4 (4%)	0	100	100
58	AV	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
59	AW	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
60	AX	119/142 (84%)	115 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AY	124/127 (98%)	121 (98%)	3 (2%)	0	100	100
62	AZ	133/136 (98%)	128 (96%)	5 (4%)	0	100	100
63	Aa	146/149 (98%)	130 (89%)	16 (11%)	0	100	100
64	Ab	56/59 (95%)	48 (86%)	8 (14%)	0	100	100
65	Ac	95/105 (90%)	94 (99%)	1 (1%)	0	100	100
66	Ad	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
67	Ae	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
68	Af	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
69	Ag	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
70	Ah	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
71	Ai	97/100 (97%)	90 (93%)	7 (7%)	0	100	100
72	Aj	85/88 (97%)	82 (96%)	3 (4%)	0	100	100
73	Ak	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
74	Al	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
75	Am	50/128 (39%)	47 (94%)	3 (6%)	0	100	100
76	An	23/25 (92%)	23 (100%)	0	0	100	100
77	Ao	103/106 (97%)	94 (91%)	9 (9%)	0	100	100
78	Ap	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
79	E	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
All	All	11086/12103 (92%)	10364 (94%)	722 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BA	173/210 (82%)	173 (100%)	0	100	100
2	BB	191/224 (85%)	191 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	BC	176/205 (86%)	176 (100%)	0	100	100
4	BE	221/222 (100%)	221 (100%)	0	100	100
5	BG	193/201 (96%)	193 (100%)	0	100	100
6	BH	165/170 (97%)	165 (100%)	0	100	100
7	BI	150/161 (93%)	149 (99%)	1 (1%)	84	92
8	BJ	158/166 (95%)	157 (99%)	1 (1%)	86	93
9	BL	136/137 (99%)	134 (98%)	2 (2%)	65	79
10	BN	127/128 (99%)	127 (100%)	0	100	100
11	BO	96/105 (91%)	95 (99%)	1 (1%)	76	87
12	BV	74/74 (100%)	74 (100%)	0	100	100
13	BW	110/111 (99%)	110 (100%)	0	100	100
14	BX	119/120 (99%)	119 (100%)	0	100	100
15	BY	112/113 (99%)	111 (99%)	1 (1%)	78	89
16	Ba	83/100 (83%)	83 (100%)	0	100	100
17	Bb	70/71 (99%)	70 (100%)	0	100	100
18	Be	51/54 (94%)	50 (98%)	1 (2%)	55	72
19	BD	182/195 (93%)	182 (100%)	0	100	100
20	BF	173/191 (91%)	173 (100%)	0	100	100
21	BK	89/98 (91%)	89 (100%)	0	100	100
22	BP	104/118 (88%)	104 (100%)	0	100	100
23	BQ	117/119 (98%)	117 (100%)	0	100	100
24	BR	110/124 (89%)	108 (98%)	2 (2%)	59	75
25	BS	128/129 (99%)	128 (100%)	0	100	100
26	BT	113/116 (97%)	113 (100%)	0	100	100
27	BU	100/114 (88%)	99 (99%)	1 (1%)	76	87
28	BZ	61/89 (68%)	61 (100%)	0	100	100
29	Bc	56/60 (93%)	56 (100%)	0	100	100
30	Bd	47/49 (96%)	47 (100%)	0	100	100
31	Bg	256/262 (98%)	255 (100%)	1 (0%)	91	96
32	Bf	49/135 (36%)	49 (100%)	0	100	100
33	BM	98/119 (82%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	AA	189/196 (96%)	189 (100%)	0	100	100
36	AB	321/322 (100%)	320 (100%)	1 (0%)	92	97
37	AC	288/289 (100%)	287 (100%)	1 (0%)	92	97
41	AD	241/245 (98%)	241 (100%)	0	100	100
42	AE	134/153 (88%)	134 (100%)	0	100	100
43	AF	186/205 (91%)	186 (100%)	0	100	100
44	AG	189/208 (91%)	189 (100%)	0	100	100
45	AH	170/171 (99%)	168 (99%)	2 (1%)	71	84
46	AI	176/187 (94%)	176 (100%)	0	100	100
47	AJ	147/150 (98%)	145 (99%)	2 (1%)	67	81
48	AL	154/159 (97%)	154 (100%)	0	100	100
49	AM	107/109 (98%)	107 (100%)	0	100	100
50	AN	175/176 (99%)	175 (100%)	0	100	100
51	AO	160/162 (99%)	160 (100%)	0	100	100
52	AP	141/146 (97%)	141 (100%)	0	100	100
53	AQ	150/151 (99%)	150 (100%)	0	100	100
54	AR	153/154 (99%)	153 (100%)	0	100	100
55	AS	156/162 (96%)	156 (100%)	0	100	100
56	AT	136/137 (99%)	135 (99%)	1 (1%)	84	92
57	AU	87/107 (81%)	87 (100%)	0	100	100
58	AV	104/105 (99%)	104 (100%)	0	100	100
59	AW	55/129 (43%)	55 (100%)	0	100	100
60	AX	105/118 (89%)	105 (100%)	0	100	100
61	AY	109/110 (99%)	109 (100%)	0	100	100
62	AZ	115/116 (99%)	114 (99%)	1 (1%)	78	89
63	Aa	118/119 (99%)	118 (100%)	0	100	100
64	Ab	46/47 (98%)	46 (100%)	0	100	100
65	Ac	81/88 (92%)	81 (100%)	0	100	100
66	Ad	96/97 (99%)	96 (100%)	0	100	100
67	Ae	109/111 (98%)	109 (100%)	0	100	100
68	Af	90/91 (99%)	90 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
69	Ag	95/103 (92%)	95 (100%)	0	100 100
70	Ah	104/105 (99%)	104 (100%)	0	100 100
71	Ai	81/82 (99%)	81 (100%)	0	100 100
72	Aj	70/71 (99%)	70 (100%)	0	100 100
73	Ak	68/69 (99%)	68 (100%)	0	100 100
74	Al	45/46 (98%)	45 (100%)	0	100 100
75	Am	47/116 (40%)	46 (98%)	1 (2%)	53 70
76	An	23/23 (100%)	23 (100%)	0	100 100
77	Ao	90/91 (99%)	90 (100%)	0	100 100
78	Ap	71/72 (99%)	71 (100%)	0	100 100
79	E	198/198 (100%)	198 (100%)	0	100 100
All	All	9468/10186 (93%)	9448 (100%)	20 (0%)	93 97

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	BI	18	ARG
8	BJ	179	ARG
9	BL	30	ARG
9	BL	67	ARG
11	BO	136	ARG
15	BY	102	LYS
18	Be	10	ARG
24	BR	5	ARG
24	BR	95	ARG
27	BU	102	ARG
31	Bg	117	LYS
36	AB	332	ARG
37	AC	98	ARG
45	AH	23	ARG
45	AH	106	LYS
47	AJ	51	ARG
47	AJ	85	LYS
56	AT	83	ARG
62	AZ	93	LYS
75	Am	88	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100)

such sidechains are listed below:

Mol	Chain	Res	Type
1	BA	46	HIS
2	BB	183	GLN
3	BC	201	ASN
4	BE	197	HIS
4	BE	231	GLN
5	BG	34	GLN
5	BG	65	GLN
6	BH	5	GLN
7	BI	9	HIS
7	BI	32	GLN
7	BI	52	ASN
7	BI	138	ASN
8	BJ	38	ASN
8	BJ	110	GLN
10	BN	49	GLN
11	BO	12	GLN
11	BO	99	GLN
13	BW	15	ASN
13	BW	42	GLN
13	BW	56	HIS
13	BW	92	ASN
18	Be	17	GLN
19	BD	67	ASN
20	BF	34	GLN
20	BF	35	GLN
21	BK	62	GLN
22	BP	79	HIS
23	BQ	32	ASN
23	BQ	139	GLN
24	BR	31	ASN
24	BR	62	GLN
24	BR	74	GLN
25	BS	12	GLN
25	BS	74	GLN
25	BS	103	ASN
26	BT	77	ASN
26	BT	101	ASN
26	BT	106	GLN
26	BT	129	GLN
27	BU	44	ASN
30	Bd	41	GLN
31	Bg	101	GLN

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Mol	Chain	Res	Type
31	Bg	200	ASN
31	Bg	224	ASN
32	Bf	134	ASN
36	AB	68	HIS
36	AB	198	HIS
36	AB	279	ASN
36	AB	345	ASN
37	AC	58	HIS
37	AC	213	ASN
37	AC	296	GLN
41	AD	63	GLN
41	AD	264	GLN
42	AE	4	GLN
42	AE	167	ASN
43	AF	166	ASN
44	AG	38	GLN
44	AG	77	GLN
45	AH	157	ASN
46	AI	23	ASN
46	AI	51	HIS
46	AI	208	ASN
47	AJ	150	ASN
48	AL	19	GLN
49	AM	126	GLN
50	AN	117	ASN
50	AN	138	GLN
50	AN	194	GLN
51	AO	26[A]	GLN
51	AO	42[A]	ASN
52	AP	55	GLN
52	AP	92	GLN
52	AP	137	ASN
53	AQ	9	GLN
54	AR	7	GLN
55	AS	8	GLN
55	AS	89	ASN
56	AT	149	GLN
57	AU	87	ASN
60	AX	94	GLN
61	AY	42	GLN
61	AY	81	GLN
61	AY	98	ASN

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Mol	Chain	Res	Type
62	AZ	78	ASN
63	Aa	64	GLN
63	Aa	65	GLN
64	Ab	11	ASN
64	Ab	45	HIS
64	Ab	48	HIS
70	Ah	59	ASN
70	Ah	104	GLN
70	Ah	108	GLN
72	Aj	76	ASN
74	Al	4	GLN
77	Ao	23	HIS
77	Ao	102	GLN
79	E	12	HIS
79	E	108	ASN
79	E	127	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	B5	1775/1798 (98%)	402 (22%)	12 (0%)
38	A1	3194/3360 (95%)	605 (18%)	27 (0%)
39	A3	120/121 (99%)	12 (10%)	1 (0%)
40	A4	157/158 (99%)	26 (16%)	0
80	EC	189/202 (93%)	87 (46%)	11 (5%)
All	All	5435/5639 (96%)	1132 (20%)	51 (0%)

All (1132) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
34	B5	17	C
34	B5	25	C
34	B5	26	A
34	B5	34	G
34	B5	42	G
34	B5	45	U
34	B5	46	A
34	B5	47	A
34	B5	57	G
34	B5	67	A
34	B5	68	A

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Mol	Chain	Res	Type
34	B5	72	A
34	B5	73	U
34	B5	74	U
34	B5	75	U
34	B5	77	U
34	B5	81	G
34	B5	103	A
34	B5	104	A
34	B5	111	U
34	B5	114	C
34	B5	115	G
34	B5	116	U
34	B5	130	C
34	B5	131	C
34	B5	132	U
34	B5	133	U
34	B5	134	U
34	B5	135	A
34	B5	136	C
34	B5	137	U
34	B5	138	A
34	B5	141	U
34	B5	145	A
34	B5	160	C
34	B5	162	A
34	B5	164	A
34	B5	166	C
34	B5	168	A
34	B5	169	A
34	B5	173	A
34	B5	178	U
34	B5	179	A
34	B5	180	A
34	B5	181	A
34	B5	182	A
34	B5	185	U
34	B5	188	A
34	B5	191	C
34	B5	192	U
34	B5	193	U
34	B5	194	U
34	B5	195	G

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Mol	Chain	Res	Type
34	B5	196	G
34	B5	198	A
34	B5	204	G
34	B5	207	U
34	B5	217	A
34	B5	218	A
34	B5	221	A
34	B5	225	A
34	B5	227	U
34	B5	228	G
34	B5	229	U
34	B5	230	C
34	B5	232	U
34	B5	233	C
34	B5	234	G
34	B5	240	U
34	B5	241	U
34	B5	250	C
34	B5	257	A
34	B5	260	U
34	B5	261	U
34	B5	262	U
34	B5	265	A
34	B5	267	U
34	B5	280	U
34	B5	283	U
34	B5	287	G
34	B5	291	G
34	B5	299	A
34	B5	305	C
34	B5	314	C
34	B5	316	A
34	B5	320	U
34	B5	322	G
34	B5	333	A
34	B5	337	G
34	B5	338	C
34	B5	352	A
34	B5	353	A
34	B5	359	A
34	B5	360	A
34	B5	361	C

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Mol	Chain	Res	Type
34	B5	390	G
34	B5	400	A
34	B5	401	A
34	B5	402	C
34	B5	417	A
34	B5	419	G
34	B5	423	G
34	B5	424	C
34	B5	425	A
34	B5	426	G
34	B5	434	G
34	B5	439	U
34	B5	444	C
34	B5	448	C
34	B5	452	A
34	B5	454	U
34	B5	459	G
34	B5	460	A
34	B5	461	G
34	B5	477	A
34	B5	484	C
34	B5	485	A
34	B5	486	G
34	B5	487	G
34	B5	488	G
34	B5	489	C
34	B5	491	C
34	B5	492	A
34	B5	494	U
34	B5	495	C
34	B5	496	G
34	B5	497	G
34	B5	498	G
34	B5	499	U
34	B5	500	C
34	B5	501	U
34	B5	503	G
34	B5	506	A
34	B5	507	U
34	B5	515	A
34	B5	527	A
34	B5	538	A

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Mol	Chain	Res	Type
34	B5	539	G
34	B5	540	G
34	B5	541	A2M
34	B5	542	A
34	B5	544	A
34	B5	548	G
34	B5	555	A
34	B5	557	G
34	B5	558	U
34	B5	559	C
34	B5	565	C
34	B5	577	G
34	B5	579	A
34	B5	580	A
34	B5	582	U
34	B5	594	A
34	B5	595	G
34	B5	606	A
34	B5	610	G
34	B5	611	U
34	B5	619	A2M
34	B5	620	A
34	B5	622	A
34	B5	623	A
34	B5	624	G
34	B5	638	U
34	B5	639	U
34	B5	650	U
34	B5	652	G
34	B5	654	C
34	B5	655	G
34	B5	656	G
34	B5	657	U
34	B5	676	G
34	B5	677	A
34	B5	678	U
34	B5	680	U
34	B5	682	C
34	B5	692	U
34	B5	693	U
34	B5	695	C
34	B5	696	C

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Mol	Chain	Res	Type
34	B5	704	U
34	B5	705	A
34	B5	706	A
34	B5	707	C
34	B5	708	C
34	B5	709	U
34	B5	711	G
34	B5	712	A
34	B5	714	U
34	B5	715	C
34	B5	716	C
34	B5	717	U
34	B5	718	U
34	B5	721	G
34	B5	722	G
34	B5	724	U
34	B5	725	C
34	B5	726	U
34	B5	728	G
34	B5	729	G
34	B5	730	C
34	B5	731	G
34	B5	732	A
34	B5	734	C
34	B5	736	A
34	B5	737	G
34	B5	740	C
34	B5	742	U
34	B5	752	A
34	B5	754	A
34	B5	764	G
34	B5	765	U
34	B5	773	A
34	B5	774	G
34	B5	777	G
34	B5	778	U
34	B5	780	U
34	B5	781	U
34	B5	782	G
34	B5	783	C
34	B5	788	A
34	B5	793	U

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Mol	Chain	Res	Type
34	B5	811	A
34	B5	813	A
34	B5	819	U
34	B5	820	U
34	B5	822	G
34	B5	832	U
34	B5	835	U
34	B5	836	G
34	B5	839	U
34	B5	845	G
34	B5	851	C
34	B5	858	A
34	B5	862	A
34	B5	885	U
34	B5	892	U
34	B5	894	G
34	B5	897	A
34	B5	903	G
34	B5	905	A
34	B5	906	A
34	B5	912	G
34	B5	925	A
34	B5	927	U
34	B5	932	A
34	B5	934	U
34	B5	950	A
34	B5	959	U
34	B5	965	A
34	B5	986	G
34	B5	987	A
34	B5	991	A
34	B5	992	A
34	B5	1003	U
34	B5	1004	A
34	B5	1019	A
34	B5	1025	A
34	B5	1027	C
34	B5	1031	G
34	B5	1038	A
34	B5	1051	U
34	B5	1055	U
34	B5	1056	U

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Mol	Chain	Res	Type
34	B5	1057	U
34	B5	1058	U
34	B5	1059	U
34	B5	1060	A
34	B5	1061	A
34	B5	1075	A
34	B5	1082	G
34	B5	1091	A
34	B5	1092	A
34	B5	1096	U
34	B5	1099	G
34	B5	1137	A
34	B5	1149	G
34	B5	1157	C
34	B5	1158	C
34	B5	1171	G
34	B5	1172	C
34	B5	1184	U
34	B5	1801	A
34	B5	1802	A
34	B5	1804	A
34	B5	1807	G
34	B5	1808	G
34	B5	1809	G
34	B5	1810	A
34	B5	1815	C
34	B5	1825	A
34	B5	1826	G
34	B5	1834	A
34	B5	1835	A
34	B5	1836	G
34	B5	1842	A
34	B5	1851	G
34	B5	1852	A
34	B5	1853	G
34	B5	1857	U
34	B5	1859	U
34	B5	1862	U
34	B5	1864	A
34	B5	1865	U
34	B5	1866	U
34	B5	1871	G

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Mol	Chain	Res	Type
34	B5	1877	OMU
34	B5	1878	G
34	B5	1894	U
34	B5	1922	U
34	B5	1923	U
34	B5	1924	G
34	B5	1929	A
34	B5	1948	U
34	B5	1952	A
34	B5	1953	A
34	B5	1960	G
34	B5	1963	C
34	B5	1964	U
34	B5	1970	U
34	B5	1971	U
34	B5	1972	G
34	B5	1976	G
34	B5	1978	U
34	B5	1979	A
34	B5	1980	U
34	B5	1981	C
34	B5	1986	U
34	B5	1993	G
34	B5	1998	U
34	B5	2007	C
34	B5	2008	A
34	B5	2021	U
34	B5	2022	U
34	B5	2023	U
34	B5	2033	A
34	B5	2035	A
34	B5	2036	OMG
34	B5	2044	A
34	B5	2055	C
34	B5	2067	C
34	B5	2068	A
34	B5	2079	A
34	B5	2094	G
34	B5	2099	U
34	B5	2100	A
34	B5	2101	A
34	B5	2102	C

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Mol	Chain	Res	Type
34	B5	2104	U
34	B5	2111	A
34	B5	2123	A
34	B5	2124	A
34	B5	2128	U
34	B5	2129	G
34	B5	2131	G
34	B5	2132	A
34	B5	2145	C
34	B5	2148	G
34	B5	2150	G
34	B5	2165	U
34	B5	2167	A
34	B5	2180	OMG
34	B5	2181	A
34	B5	2183	G7M
34	B5	2184	A
34	B5	2190	U
34	B5	2192	G
34	B5	2198	G
34	B5	2209	G
34	B5	2215	G
34	B5	2224	G
34	B5	2242	C
34	B5	2253	G
34	B5	2254	C
34	B5	2259	A
34	B5	2265	U
34	B5	2266	G
34	B5	2275	A
34	B5	2291	C
34	B5	2292	U
34	B5	2296	U
34	B5	2307	G
34	B5	2308	C
34	B5	2309	A
34	B5	2311	C
34	B5	2317	C
34	B5	2320	A
34	B5	2323	G
34	B5	2324	C
34	B5	2325	G

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Mol	Chain	Res	Type
34	B5	2363	A
34	B5	2365	G
34	B5	2374	A
34	B5	2375	G
34	B5	2377	U
34	B5	2379	U
34	B5	2388	G
34	B5	2400	G
34	B5	2401	G
34	B5	2402	A
34	B5	2403	U
34	B5	2404	C
34	B5	2407	U
38	A1	6	A
38	A1	26	A
38	A1	34	A
38	A1	40	A
38	A1	43	A
38	A1	49	A
38	A1	59	G
38	A1	60	A
38	A1	65	A
38	A1	66	A
38	A1	74	G
38	A1	77	A
38	A1	92	G
38	A1	99	A
38	A1	109	A
38	A1	110	G
38	A1	111	C
38	A1	116	A
38	A1	121	A
38	A1	122	A
38	A1	134	U
38	A1	135	C
38	A1	136	G
38	A1	156	G
38	A1	157	A
38	A1	162	G
38	A1	163	C
38	A1	164	A
38	A1	165	A

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Mol	Chain	Res	Type
38	A1	169	U
38	A1	175	C
38	A1	176	G
38	A1	177	U
38	A1	187	A
38	A1	190	U
38	A1	191	U
38	A1	200	C
38	A1	210	U
38	A1	219	A
38	A1	237	G
38	A1	238	A
38	A1	239	G
38	A1	240	U
38	A1	241	G
38	A1	242	C
38	A1	243	G
38	A1	244	G
38	A1	246	U
38	A1	248	U
38	A1	249	U
38	A1	250	U
38	A1	252	U
38	A1	253	A
38	A1	254	A
38	A1	269	G
38	A1	286	U
38	A1	295	A
38	A1	296	A
38	A1	298	U
38	A1	305	U
38	A1	329	U
38	A1	339	C
38	A1	352	A
38	A1	373	A
38	A1	374	A
38	A1	376	G
38	A1	398	A
38	A1	401	U
38	A1	402	A
38	A1	403	C
38	A1	420	G

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Mol	Chain	Res	Type
38	A1	421	G
38	A1	422	A
38	A1	438	A
38	A1	440	A
38	A1	495	G
38	A1	510	G
38	A1	521	A
38	A1	523	A
38	A1	535	G
38	A1	540	U
38	A1	542	G
38	A1	545	U
38	A1	546	C
38	A1	547	G
38	A1	548	G
38	A1	552	G
38	A1	554	A
38	A1	557	A
38	A1	559	A
38	A1	560	G
38	A1	579	G
38	A1	592	A
38	A1	602	A
38	A1	611	A
38	A1	620	U
38	A1	621	A
38	A1	649	A2M
38	A1	677	A
38	A1	681	U
38	A1	690	A
38	A1	705	A
38	A1	715	A
38	A1	719	U
38	A1	736	A
38	A1	765	C
38	A1	766	U
38	A1	767	U
38	A1	774	G
38	A1	777	U
38	A1	781	G
38	A1	785	G
38	A1	786	A

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Mol	Chain	Res	Type
38	A1	799	G
38	A1	806	A
38	A1	813	G
38	A1	817	A2M
38	A1	830	A
38	A1	849	C
38	A1	861	C
38	A1	874	U
38	A1	879	U
38	A1	896	A
38	A1	897	U
38	A1	907	G
38	A1	908	OMG
38	A1	914	A
38	A1	916	G
38	A1	917	A
38	A1	921	A
38	A1	923	C
38	A1	924	G
38	A1	925	A
38	A1	934	G
38	A1	937	G
38	A1	943	U
38	A1	944	C
38	A1	959	C
38	A1	974	G
38	A1	980	A
38	A1	981	U
38	A1	982	C
38	A1	995	U
38	A1	1000	C
38	A1	1002	A
38	A1	1010	G
38	A1	1015	U
38	A1	1016	C
38	A1	1017	C
38	A1	1018	G
38	A1	1019	G
38	A1	1020	G
38	A1	1022	U
38	A1	1023	C
38	A1	1032	C

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Mol	Chain	Res	Type
38	A1	1033	U
38	A1	1034	U
38	A1	1035	G
38	A1	1045	C
38	A1	1047	A
38	A1	1064	A
38	A1	1072	G
38	A1	1075	A
38	A1	1081	U
38	A1	1082	U
38	A1	1093	A
38	A1	1094	U
38	A1	1097	G
38	A1	1098	A
38	A1	1103	A
38	A1	1104	G
38	A1	1117	G
38	A1	1131	G
38	A1	1144	U
38	A1	1153	A
38	A1	1155	C
38	A1	1159	A
38	A1	1160	C
38	A1	1178	G
38	A1	1179	A
38	A1	1180	A
38	A1	1181	U
38	A1	1182	A
38	A1	1192	C
38	A1	1193	A
38	A1	1196	C
38	A1	1201	C
38	A1	1206	G
38	A1	1208	U
38	A1	1219	C
38	A1	1221	A
38	A1	1222	G
38	A1	1223	A
38	A1	1226	G
38	A1	1227	C
38	A1	1228	C
38	A1	1231	A

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Mol	Chain	Res	Type
38	A1	1232	C
38	A1	1233	G
38	A1	1235	U
38	A1	1236	G
38	A1	1237	G
38	A1	1239	C
38	A1	1241	U
38	A1	1242	G
38	A1	1243	G
38	A1	1244	A
38	A1	1245	A
38	A1	1246	G
38	A1	1252	A
38	A1	1255	C
38	A1	1256	G
38	A1	1257	C
38	A1	1258	U
38	A1	1259	A
38	A1	1262	G
38	A1	1263	A
38	A1	1265	U
38	A1	1266	G
38	A1	1270	A
38	A1	1272	C
38	A1	1277	C
38	A1	1279	C
38	A1	1280	C
38	A1	1281	G
38	A1	1282	G
38	A1	1283	C
38	A1	1285	G
38	A1	1286	A
38	A1	1287	A
38	A1	1293	U
38	A1	1307	G
38	A1	1309	U
38	A1	1317	A
38	A1	1330	A
38	A1	1331	U
38	A1	1348	U
38	A1	1349	G
38	A1	1350	A

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Mol	Chain	Res	Type
38	A1	1351	U
38	A1	1352	A
38	A1	1353	U
38	A1	1354	G
38	A1	1355	A
38	A1	1356	U
38	A1	1357	G
38	A1	1386	A
38	A1	1392	G
38	A1	1393	A
38	A1	1399	A
38	A1	1400	G
38	A1	1419	A
38	A1	1434	G
38	A1	1437	OMC
38	A1	1443	G
38	A1	1446	A
38	A1	1455	U
38	A1	1468	A
38	A1	1469	C
38	A1	1481	A
38	A1	1484	U
38	A1	1487	G
38	A1	1496	C
38	A1	1502	C
38	A1	1508	C
38	A1	1512	U
38	A1	1523	U
38	A1	1555	U
38	A1	1556	C
38	A1	1558	A
38	A1	1562	C
38	A1	1564	U
38	A1	1565	G
38	A1	1566	A
38	A1	1567	U
38	A1	1568	U
38	A1	1569	U
38	A1	1572	U
38	A1	1575	A
38	A1	1576	G
38	A1	1579	C

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Mol	Chain	Res	Type
38	A1	1580	A
38	A1	1581	C
38	A1	1583	A
38	A1	1593	A
38	A1	1605	A
38	A1	1628	C
38	A1	1629	U
38	A1	1630	U
38	A1	1642	A
38	A1	1643	A
38	A1	1688	U
38	A1	1724	U
38	A1	1725	C
38	A1	1738	C
38	A1	1741	A
38	A1	1750	A
38	A1	1751	G
38	A1	1761	C
38	A1	1762	C
38	A1	1763	U
38	A1	1764	U
38	A1	1765	U
38	A1	1766	G
38	A1	1775	G
38	A1	1779	C
38	A1	1797	A
38	A1	1813	A
38	A1	1815	U
38	A1	1817	G
38	A1	1820	U
38	A1	1821	U
38	A1	1842	A
38	A1	1846	C
38	A1	1849	C
38	A1	1850	A
38	A1	1851	G
38	A1	1866	C
38	A1	1878	G
38	A1	1880	U
38	A1	1893	A
38	A1	1906	G
38	A1	1932	A

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Mol	Chain	Res	Type
38	A1	1936	A
38	A1	1948	G
38	A1	1950	U
38	A1	1952	G
38	A1	1953	G
38	A1	1954	G
38	A1	1955	U
38	A1	2095	G
38	A1	2102	U
38	A1	2111	G
38	A1	2112	U
38	A1	2113	A
38	A1	2114	C
38	A1	2122	G
38	A1	2131	A
38	A1	2140	U
38	A1	2144	A
38	A1	2145	A
38	A1	2146	C
38	A1	2158	A
38	A1	2159	U
38	A1	2169	G
38	A1	2184	U
38	A1	2188	A
38	A1	2192	C
38	A1	2201	G
38	A1	2205	U
38	A1	2206	G
38	A1	2207	A
38	A1	2210	G
38	A1	2218	G
38	A1	2242	A
38	A1	2249	G
38	A1	2256	A2M
38	A1	2257	C
38	A1	2260	U
38	A1	2262	A
38	A1	2269	U
38	A1	2270	A
38	A1	2272	G
38	A1	2273	G
38	A1	2279	A

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Mol	Chain	Res	Type
38	A1	2280	A2M
38	A1	2281	A2M
38	A1	2307	G
38	A1	2308	C
38	A1	2310	U
38	A1	2313	A
38	A1	2314	U
38	A1	2315	G
38	A1	2318	U
38	A1	2334	U
38	A1	2335	G
38	A1	2336	U
38	A1	2340	U
38	A1	2364	G
38	A1	2366	C
38	A1	2372	A
38	A1	2373	A
38	A1	2374	C
38	A1	2375	G
38	A1	2383	C
38	A1	2388	U
38	A1	2393	G
38	A1	2397	A
38	A1	2398	A
38	A1	2402	A
38	A1	2403	G
38	A1	2404	A
38	A1	2411	U
38	A1	2435	G
38	A1	2442	G
38	A1	2445	A
38	A1	2446	U
38	A1	2447	A
38	A1	2449	A
38	A1	2453	U
38	A1	2454	G
38	A1	2455	U
38	A1	2458	A
38	A1	2459	A
38	A1	2461	A
38	A1	2462	A
38	A1	2463	G

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Mol	Chain	Res	Type
38	A1	2465	G
38	A1	2467	G
38	A1	2468	A
38	A1	2472	U
38	A1	2474	G
38	A1	2475	G
38	A1	2477	G
38	A1	2483	G
38	A1	2484	A
38	A1	2485	A
38	A1	2486	A
38	A1	2487	U
38	A1	2490	C
38	A1	2491	A
38	A1	2492	C
38	A1	2493	U
38	A1	2494	A
38	A1	2495	C
38	A1	2496	C
38	A1	2497	U
38	A1	2498	U
38	A1	2499	U
38	A1	2500	A
38	A1	2501	U
38	A1	2502	A
38	A1	2503	G
38	A1	2504	U
38	A1	2506	U
38	A1	2507	C
38	A1	2514	U
38	A1	2523	A
38	A1	2524	A
38	A1	2530	G
38	A1	2537	U
38	A1	2538	U
38	A1	2539	C
38	A1	2540	A
38	A1	2541	U
38	A1	2546	C
38	A1	2549	G
38	A1	2550	U
38	A1	2552	C

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Mol	Chain	Res	Type
38	A1	2554	A
38	A1	2561	A
38	A1	2562	A
38	A1	2568	C
38	A1	2569	A
38	A1	2571	U
38	A1	2572	C
38	A1	2573	G
38	A1	2585	G
38	A1	2593	A
38	A1	2594	C
38	A1	2606	G
38	A1	2607	G
38	A1	2614	G
38	A1	2626	A
38	A1	2652	U
38	A1	2656	A
38	A1	2674	A
38	A1	2676	A
38	A1	2677	G
38	A1	2679	A
38	A1	2681	U
38	A1	2688	U
38	A1	2689	A
38	A1	2691	A
38	A1	2703	A
38	A1	2704	A
38	A1	2705	A
38	A1	2714	G
38	A1	2719	U
38	A1	2728	G
38	A1	2729	OMU
38	A1	2737	C
38	A1	2752	U
38	A1	2753	G
38	A1	2755	C
38	A1	2762	A
38	A1	2773	C
38	A1	2777	G
38	A1	2778	G
38	A1	2796	G
38	A1	2798	C

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Mol	Chain	Res	Type
38	A1	2799	A
38	A1	2800	G
38	A1	2801	A
38	A1	2803	A
38	A1	2810	C
38	A1	2814	G
38	A1	2817	A
38	A1	2828	G
38	A1	2842	U
38	A1	2844	C
38	A1	2845	A
38	A1	2849	C
38	A1	2860	U
38	A1	2867	C
38	A1	2871	G
38	A1	2872	A
38	A1	2873	U
38	A1	2875	U
38	A1	2876	C
38	A1	2887	A
38	A1	2889	C
38	A1	2894	C
38	A1	2898	G
38	A1	2923	U
38	A1	2935	U
38	A1	2936	A
38	A1	2938	G
38	A1	2942	C
38	A1	2943	G
38	A1	2947	G
38	A1	2954	U
38	A1	2955	U
38	A1	2977	G
38	A1	2983	C
38	A1	2990	G
38	A1	2997	G
38	A1	3011	A
38	A1	3012	A
38	A1	3022	G
38	A1	3030	G
38	A1	3032	A
38	A1	3058	U

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Mol	Chain	Res	Type
38	A1	3059	G
38	A1	3078	U
38	A1	3079	U
38	A1	3080	G
38	A1	3086	A
38	A1	3092	C
38	A1	3101	G
38	A1	3109	G
38	A1	3113	A
38	A1	3122	A
38	A1	3129	A
38	A1	3130	A
38	A1	3131	U
38	A1	3142	A
38	A1	3143	C
38	A1	3153	U
38	A1	3154	C
38	A1	3155	U
38	A1	3156	U
38	A1	3157	U
38	A1	3158	G
38	A1	3165	A
38	A1	3170	A
38	A1	3172	A
38	A1	3173	G
38	A1	3174	A
38	A1	3176	G
38	A1	3179	U
38	A1	3181	C
38	A1	3186	A
38	A1	3187	A
38	A1	3195	U
38	A1	3198	U
38	A1	3206	C
38	A1	3207	U
38	A1	3210	A
38	A1	3215	A
38	A1	3217	C
38	A1	3218	A
38	A1	3219	G
38	A1	3224	G
38	A1	3229	G

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Mol	Chain	Res	Type
38	A1	3234	A
38	A1	3243	A
38	A1	3250	U
38	A1	3259	U
38	A1	3260	G
38	A1	3271	G
38	A1	3273	A
38	A1	3275	U
38	A1	3276	G
38	A1	3278	C
38	A1	3281	U
38	A1	3284	G
38	A1	3289	G
38	A1	3294	A
38	A1	3304	U
38	A1	3314	A
38	A1	3316	A
38	A1	3342	A
38	A1	3345	G
38	A1	3350	C
38	A1	3351	U
38	A1	3352	U
38	A1	3353	G
38	A1	3354	U
38	A1	3355	U
38	A1	3356	G
38	A1	3369	G
38	A1	3375	A
38	A1	3378	C
38	A1	3389	U
39	A3	11	A
39	A3	20	A
39	A3	41	G
39	A3	53	U
39	A3	54	U
39	A3	55	A
39	A3	65	G
39	A3	76	A
39	A3	78	U
39	A3	102	A
39	A3	112	G
39	A3	121	U

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Mol	Chain	Res	Type
40	A4	23	U
40	A4	34	U
40	A4	35	C
40	A4	51	G
40	A4	52	A
40	A4	59	A
40	A4	62	C
40	A4	63	G
40	A4	81	U
40	A4	82	U
40	A4	83	C
40	A4	85	G
40	A4	86	U
40	A4	87	G
40	A4	90	U
40	A4	95	G
40	A4	104	A
40	A4	106	C
40	A4	107	G
40	A4	111	A
40	A4	113	U
40	A4	116	G
40	A4	125	U
40	A4	152	G
40	A4	157	U
40	A4	158	U
80	EC	6759	A
80	EC	6762	U
80	EC	6768	U
80	EC	6769	A
80	EC	6770	U
80	EC	6771	U
80	EC	6772	G
80	EC	6773	G
80	EC	6774	U
80	EC	6775	U
80	EC	6776	A
80	EC	6777	C
80	EC	6778	C
80	EC	6779	C
80	EC	6780	A
80	EC	6781	U

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Mol	Chain	Res	Type
80	EC	6782	C
80	EC	6788	C
80	EC	6789	G
80	EC	6790	A
80	EC	6791	A
80	EC	6792	A
80	EC	6793	A
80	EC	6794	C
80	EC	6795	U
80	EC	6802	A
80	EC	6803	C
80	EC	6804	A
80	EC	6816	A
80	EC	6817	A
80	EC	6818	G
80	EC	6819	G
80	EC	6820	C
80	EC	6821	U
80	EC	6822	U
80	EC	6823	U
80	EC	6825	A
80	EC	6831	U
80	EC	6832	G
80	EC	6835	U
80	EC	6836	U
80	EC	6837	G
80	EC	6842	U
80	EC	6843	U
80	EC	6844	A
80	EC	6845	G
80	EC	6849	A
80	EC	6850	C
80	EC	6851	G
80	EC	6852	U
80	EC	6856	C
80	EC	6858	A
80	EC	6859	U
80	EC	6860	A
80	EC	6861	G
80	EC	6863	C
80	EC	6864	A
80	EC	6865	G

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Mol	Chain	Res	Type
80	EC	6867	C
80	EC	6869	C
80	EC	6870	A
80	EC	6871	A
80	EC	6873	A
80	EC	6875	C
80	EC	6877	C
80	EC	6880	G
80	EC	6889	A
80	EC	6897	G
80	EC	6901	C
80	EC	6902	U
80	EC	6904	U
80	EC	6912	G
80	EC	6913	U
80	EC	6914	A
80	EC	6915	G
80	EC	6916	A
80	EC	6918	A
80	EC	6927	U
80	EC	6928	G
80	EC	6929	C
80	EC	6935	G
80	EC	6940	U
80	EC	6941	U
80	EC	6943	A
80	EC	6945	U
80	EC	6946	A
80	EC	6950	C

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
34	B5	224	C
34	B5	486	G
34	B5	751	A
34	B5	818	G
34	B5	861	A
34	B5	949	C
34	B5	1056	U
34	B5	1834	A
34	B5	1893	U

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Mol	Chain	Res	Type
34	B5	1952	A
34	B5	2066	G
34	B5	2253	G
38	A1	237	G
38	A1	238	A
38	A1	240	U
38	A1	242	C
38	A1	873	C
38	A1	916	G
38	A1	1014	U
38	A1	1092	C
38	A1	1218	U
38	A1	1236	G
38	A1	1240	A
38	A1	1292	C
38	A1	1354	G
38	A1	1568	U
38	A1	2241	U
38	A1	2466	G
38	A1	2496	C
38	A1	2497	U
38	A1	2498	U
38	A1	2499	U
38	A1	2501	U
38	A1	2503	G
38	A1	2504	U
38	A1	2506	U
38	A1	2870	5MC
38	A1	2954	U
38	A1	3121	U
39	A3	52	G
80	EC	6789	G
80	EC	6831	U
80	EC	6844	A
80	EC	6851	G
80	EC	6857	C
80	EC	6858	A
80	EC	6863	C
80	EC	6876	A
80	EC	6901	C
80	EC	6911	A
80	EC	6934	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
38	OMU	A1	2417	38	19,22,23	1.19	3 (15%)	26,31,34	1.69	5 (19%)
38	OMG	A1	2288	38	18,26,27	0.91	1 (5%)	19,38,41	1.05	2 (10%)
38	OMU	A1	2729	38	19,22,23	1.30	4 (21%)	26,31,34	1.74	7 (26%)
38	A2M	A1	2281	38	18,25,26	0.84	0	18,36,39	1.31	2 (11%)
38	OMG	A1	2791	38	18,26,27	0.94	1 (5%)	19,38,41	1.05	2 (10%)
34	A2M	B5	28	81,34	18,25,26	1.00	1 (5%)	18,36,39	1.20	2 (11%)
38	OMC	A1	663	38	19,22,23	0.81	0	26,31,34	0.79	0
38	OMU	A1	1888	38	19,22,23	1.24	3 (15%)	26,31,34	1.79	5 (19%)
38	1MA	A1	2142	38,81	16,25,26	1.45	2 (12%)	18,37,40	1.07	3 (16%)
38	A2M	A1	2256	80,38	18,25,26	1.02	1 (5%)	18,36,39	1.59	2 (11%)
34	MA6	B5	2389	34	19,26,27	0.94	1 (5%)	18,38,41	1.37	2 (11%)
34	A2M	B5	420	34	18,25,26	1.02	1 (5%)	18,36,39	1.21	2 (11%)
34	A2M	B5	541	34	18,25,26	1.03	1 (5%)	18,36,39	1.19	2 (11%)
34	OMG	B5	2180	34	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
38	OMG	A1	867	38	18,26,27	0.91	1 (5%)	19,38,41	1.14	2 (10%)
38	OMC	A1	2948	38	19,22,23	0.82	0	26,31,34	0.98	1 (3%)
38	A2M	A1	1133	38,81	18,25,26	1.00	1 (5%)	18,36,39	1.32	2 (11%)
34	3AU	B5	1799	34	24,28,29	0.97	0	33,40,43	2.27	4 (12%)
38	5MC	A1	2278	38,81	18,22,23	0.95	2 (11%)	26,32,35	1.23	3 (11%)
34	4AC	B5	2381	34	21,24,25	1.01	1 (4%)	29,34,37	1.90	7 (24%)
34	G7M	B5	2183	34	20,26,27	2.97	7 (35%)	17,39,42	1.51	4 (23%)
38	OMC	A1	1437	38,81	19,22,23	0.85	0	26,31,34	1.27	4 (15%)
38	OMC	A1	2337	38	19,22,23	0.80	0	26,31,34	0.77	0
34	OMC	B5	2247	34	19,22,23	0.78	0	26,31,34	0.75	0
38	OMG	A1	908	38	18,26,27	0.96	1 (5%)	19,38,41	1.13	2 (10%)
38	A2M	A1	807	38	18,25,26	0.98	1 (5%)	18,36,39	1.24	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	OMC	B5	1006	34	19,22,23	0.81	0	26,31,34	0.88	1 (3%)
38	OMU	A1	2921	38,81	19,22,23	1.21	3 (15%)	26,31,34	1.75	5 (19%)
38	5MC	A1	2870	38	18,22,23	0.97	2 (11%)	26,32,35	1.29	3 (11%)
34	OMU	B5	1877	34	19,22,23	1.25	4 (21%)	26,31,34	1.77	5 (19%)
38	OMG	A1	1450	38	18,26,27	0.91	1 (5%)	19,38,41	1.04	2 (10%)
34	OMG	B5	2036	34	18,26,27	0.94	1 (5%)	19,38,41	1.04	2 (10%)
34	A2M	B5	436	34	18,25,26	1.00	1 (5%)	18,36,39	1.25	2 (11%)
38	A2M	A1	2946	38,81	18,25,26	1.00	1 (5%)	18,36,39	1.36	2 (11%)
38	OMC	A1	650	38	19,22,23	0.80	0	26,31,34	0.81	1 (3%)
38	A2M	A1	2220	38	18,25,26	1.01	1 (5%)	18,36,39	1.15	2 (11%)
38	OMU	A1	2347	38	19,22,23	1.27	4 (21%)	26,31,34	1.74	5 (19%)
34	OMU	B5	578	34	19,22,23	1.19	2 (10%)	26,31,34	1.72	5 (19%)
38	OMG	A1	805	38	18,26,27	0.93	1 (5%)	19,38,41	1.12	2 (10%)
38	A2M	A1	2640	38	18,25,26	0.99	1 (5%)	18,36,39	1.20	2 (11%)
34	A2M	B5	619	81,34	18,25,26	0.95	1 (5%)	18,36,39	1.28	2 (11%)
38	OMG	A1	2793	38	18,26,27	0.94	1 (5%)	19,38,41	1.12	2 (10%)
38	OMU	A1	898	38	19,22,23	1.24	3 (15%)	26,31,34	1.71	4 (15%)
36	HIC	AB	243	36	8,11,12	1.64	2 (25%)	6,14,16	0.93	0
34	4AC	B5	1888	34	21,24,25	1.03	1 (4%)	29,34,37	1.06	4 (13%)
38	A2M	A1	2280	38	18,25,26	0.98	1 (5%)	18,36,39	1.36	2 (11%)
38	UR3	A1	2634	38	19,22,23	0.96	0	26,32,35	1.43	1 (3%)
34	OMC	B5	414	34	19,22,23	0.83	0	26,31,34	0.79	1 (3%)
38	A2M	A1	649	38	18,25,26	0.93	1 (5%)	18,36,39	1.20	2 (11%)
38	OMC	A1	2197	38	19,22,23	0.79	0	26,31,34	0.83	0
34	MA6	B5	2390	34	19,26,27	0.90	1 (5%)	18,38,41	1.35	2 (11%)
34	A2M	B5	795	34	18,25,26	1.03	1 (5%)	18,36,39	1.32	2 (11%)
38	OMU	A1	2421	38	19,22,23	1.21	3 (15%)	26,31,34	1.72	4 (15%)
38	OMG	A1	2922	38	18,26,27	0.93	1 (5%)	19,38,41	1.04	2 (10%)
38	OMG	A1	2619	38	18,26,27	0.93	1 (5%)	19,38,41	1.04	2 (10%)
38	A2M	A1	817	38,81	18,25,26	0.99	1 (5%)	18,36,39	1.31	2 (11%)
38	OMU	A1	2724	38	19,22,23	1.20	3 (15%)	26,31,34	1.72	5 (19%)
34	OMG	B5	1125	34	18,26,27	0.93	1 (5%)	19,38,41	1.09	2 (10%)
38	OMG	A1	2815	38	18,26,27	0.94	1 (5%)	19,38,41	1.04	2 (10%)
34	A2M	B5	973	34	18,25,26	0.95	1 (5%)	18,36,39	1.27	3 (16%)
38	1MA	A1	645	38,81	16,25,26	1.45	2 (12%)	18,37,40	1.09	3 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
38	A2M	A1	876	38	18,25,26	0.99	1 (5%)	18,36,39	1.21	2 (11%)
34	A2M	B5	100	81,34	18,25,26	1.03	1 (5%)	18,36,39	1.22	2 (11%)
38	OMC	A1	2959	38	19,22,23	0.84	0	26,31,34	0.81	1 (3%)
38	A2M	A1	1449	38,81	18,25,26	0.99	1 (5%)	18,36,39	1.25	2 (11%)
34	OMG	B5	1879	34	18,26,27	0.93	1 (5%)	19,38,41	1.03	2 (10%)
34	OMG	B5	562	34	18,26,27	0.91	1 (5%)	19,38,41	1.07	2 (10%)

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
38	OMU	A1	2417	38	-	0/9/27/28	0/2/2/2
38	OMG	A1	2288	38	-	0/5/27/28	0/3/3/3
38	OMU	A1	2729	38	-	3/9/27/28	0/2/2/2
38	A2M	A1	2281	38	-	1/5/27/28	0/3/3/3
38	OMG	A1	2791	38	-	1/5/27/28	0/3/3/3
34	A2M	B5	28	81,34	-	0/5/27/28	0/3/3/3
38	OMC	A1	663	38	-	1/9/27/28	0/2/2/2
38	OMU	A1	1888	38	-	0/9/27/28	0/2/2/2
38	1MA	A1	2142	38,81	-	0/3/25/26	0/3/3/3
38	A2M	A1	2256	80,38	-	1/5/27/28	0/3/3/3
34	MA6	B5	2389	34	-	0/7/29/30	0/3/3/3
34	A2M	B5	420	34	-	1/5/27/28	0/3/3/3
34	A2M	B5	541	34	-	3/5/27/28	0/3/3/3
34	OMG	B5	2180	34	-	3/5/27/28	0/3/3/3
38	OMG	A1	867	38	-	0/5/27/28	0/3/3/3
38	OMC	A1	2948	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	1133	38,81	-	0/5/27/28	0/3/3/3
34	3AU	B5	1799	34	1/1/7/7	2/16/34/35	0/2/2/2
38	5MC	A1	2278	38,81	-	0/7/25/26	0/2/2/2
34	4AC	B5	2381	34	-	4/11/29/30	0/2/2/2
34	G7M	B5	2183	34	-	0/3/25/26	0/3/3/3
38	OMC	A1	1437	38,81	-	3/9/27/28	0/2/2/2
38	OMC	A1	2337	38	-	0/9/27/28	0/2/2/2
34	OMC	B5	2247	34	-	0/9/27/28	0/2/2/2
38	OMG	A1	908	38	-	0/5/27/28	0/3/3/3
38	A2M	A1	807	38	-	0/5/27/28	0/3/3/3
34	OMC	B5	1006	34	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	OMU	A1	2921	38,81	-	0/9/27/28	0/2/2/2
38	5MC	A1	2870	38	-	4/7/25/26	0/2/2/2
34	OMU	B5	1877	34	-	5/9/27/28	0/2/2/2
38	OMG	A1	1450	38	-	0/5/27/28	0/3/3/3
34	OMG	B5	2036	34	-	3/5/27/28	0/3/3/3
34	A2M	B5	436	34	-	0/5/27/28	0/3/3/3
38	A2M	A1	2946	38,81	-	0/5/27/28	0/3/3/3
38	OMC	A1	650	38	-	1/9/27/28	0/2/2/2
38	A2M	A1	2220	38	-	1/5/27/28	0/3/3/3
38	OMU	A1	2347	38	-	2/9/27/28	0/2/2/2
34	OMU	B5	578	34	-	0/9/27/28	0/2/2/2
38	OMG	A1	805	38	-	1/5/27/28	0/3/3/3
38	A2M	A1	2640	38	-	0/5/27/28	0/3/3/3
34	A2M	B5	619	81,34	-	2/5/27/28	0/3/3/3
38	OMG	A1	2793	38	-	0/5/27/28	0/3/3/3
38	OMU	A1	898	38	-	0/9/27/28	0/2/2/2
36	HIC	AB	243	36	-	1/5/6/8	0/1/1/1
34	4AC	B5	1888	34	-	2/11/29/30	0/2/2/2
38	A2M	A1	2280	38	-	2/5/27/28	0/3/3/3
38	UR3	A1	2634	38	-	0/7/25/26	0/2/2/2
34	OMC	B5	414	34	-	1/9/27/28	0/2/2/2
38	A2M	A1	649	38	-	1/5/27/28	0/3/3/3
38	OMC	A1	2197	38	-	6/9/27/28	0/2/2/2
34	MA6	B5	2390	34	-	3/7/29/30	0/3/3/3
34	A2M	B5	795	34	-	0/5/27/28	0/3/3/3
38	OMU	A1	2421	38	-	1/9/27/28	0/2/2/2
38	OMG	A1	2922	38	-	0/5/27/28	0/3/3/3
38	OMG	A1	2619	38	-	3/5/27/28	0/3/3/3
38	A2M	A1	817	38,81	-	2/5/27/28	0/3/3/3
38	OMU	A1	2724	38	-	1/9/27/28	0/2/2/2
34	OMG	B5	1125	34	-	1/5/27/28	0/3/3/3
38	OMG	A1	2815	38	-	0/5/27/28	0/3/3/3
34	A2M	B5	973	34	-	0/5/27/28	0/3/3/3
38	1MA	A1	645	38,81	-	0/3/25/26	0/3/3/3
38	A2M	A1	876	38	-	1/5/27/28	0/3/3/3
34	A2M	B5	100	81,34	-	0/5/27/28	0/3/3/3
38	OMC	A1	2959	38	-	0/9/27/28	0/2/2/2
38	A2M	A1	1449	38,81	-	0/5/27/28	0/3/3/3
34	OMG	B5	1879	34	-	1/5/27/28	0/3/3/3
34	OMG	B5	562	34	-	0/5/27/28	0/3/3/3

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	B5	2183	G7M	C8-N7	7.03	1.45	1.33
34	B5	2183	G7M	C8-N9	6.96	1.45	1.33
34	B5	2183	G7M	C2'-C1'	-5.25	1.45	1.53
38	A1	2142	1MA	C2-N3	4.43	1.34	1.29
38	A1	645	1MA	C2-N3	4.36	1.34	1.29
34	B5	2183	G7M	C5-C4	3.80	1.46	1.39
36	AB	243	HIC	CD2-CG	3.47	1.41	1.36
34	B5	2183	G7M	C2'-C3'	-3.12	1.44	1.53
38	A1	2142	1MA	C6-N6	3.00	1.35	1.27
38	A1	645	1MA	C6-N6	2.98	1.35	1.27
38	A1	2870	5MC	C6-C5	2.92	1.39	1.34
38	A1	2729	OMU	C4-N3	-2.86	1.33	1.38
38	A1	898	OMU	C4-N3	-2.77	1.33	1.38
38	A1	2278	5MC	C6-C5	2.76	1.39	1.34
38	A1	2815	OMG	C6-N1	-2.76	1.33	1.37
38	A1	2921	OMU	C4-N3	-2.71	1.33	1.38
38	A1	2791	OMG	C6-N1	-2.70	1.33	1.37
38	A1	2347	OMU	C4-N3	-2.70	1.33	1.38
38	A1	2793	OMG	C6-N1	-2.70	1.33	1.37
38	A1	1888	OMU	C4-N3	-2.68	1.33	1.38
34	B5	1888	4AC	C4-N4	-2.67	1.35	1.39
38	A1	2417	OMU	C4-N3	-2.65	1.33	1.38
38	A1	908	OMG	C6-N1	-2.64	1.33	1.37
34	B5	1125	OMG	C6-N1	-2.64	1.33	1.37
38	A1	2619	OMG	C6-N1	-2.63	1.33	1.37
38	A1	2922	OMG	C6-N1	-2.61	1.34	1.37
38	A1	805	OMG	C6-N1	-2.59	1.34	1.37
38	A1	2288	OMG	C6-N1	-2.58	1.34	1.37
38	A1	1450	OMG	C6-N1	-2.58	1.34	1.37
38	A1	2421	OMU	C4-N3	-2.57	1.34	1.38
38	A1	2724	OMU	C4-N3	-2.56	1.34	1.38
34	B5	2036	OMG	C6-N1	-2.55	1.34	1.37
38	A1	867	OMG	C6-N1	-2.53	1.34	1.37
34	B5	562	OMG	C6-N1	-2.53	1.34	1.37
34	B5	541	A2M	C5-C4	2.51	1.47	1.40
34	B5	2389	MA6	C5-C4	2.49	1.47	1.40
34	B5	1877	OMU	C4-N3	-2.49	1.34	1.38
34	B5	2390	MA6	C5-C4	2.47	1.47	1.40
34	B5	578	OMU	C4-N3	-2.45	1.34	1.38
34	B5	1879	OMG	C6-N1	-2.45	1.34	1.37
34	B5	436	A2M	C5-C4	2.44	1.47	1.40
38	A1	2220	A2M	C5-C4	2.42	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2729	OMU	C2-N1	2.40	1.42	1.38
38	A1	876	A2M	C5-C4	2.40	1.47	1.40
34	B5	100	A2M	C5-C4	2.39	1.47	1.40
38	A1	2946	A2M	C5-C4	2.37	1.47	1.40
34	B5	420	A2M	C5-C4	2.36	1.47	1.40
34	B5	795	A2M	C5-C4	2.36	1.47	1.40
38	A1	2256	A2M	C5-C4	2.36	1.47	1.40
38	A1	807	A2M	C5-C4	2.35	1.47	1.40
38	A1	1449	A2M	C5-C4	2.34	1.47	1.40
34	B5	28	A2M	C5-C4	2.34	1.47	1.40
34	B5	619	A2M	C5-C4	2.34	1.47	1.40
38	A1	2280	A2M	C5-C4	2.33	1.47	1.40
34	B5	2381	4AC	C4-N4	-2.33	1.36	1.39
38	A1	2640	A2M	C5-C4	2.33	1.47	1.40
38	A1	1133	A2M	C5-C4	2.33	1.47	1.40
38	A1	1888	OMU	C2-N3	-2.32	1.33	1.38
34	B5	2180	OMG	C6-N1	-2.31	1.34	1.37
38	A1	2921	OMU	C2-N3	-2.30	1.33	1.38
38	A1	898	OMU	C2-N3	-2.28	1.33	1.38
34	B5	2183	G7M	C6-N1	-2.28	1.34	1.37
34	B5	973	A2M	C5-C4	2.27	1.46	1.40
38	A1	649	A2M	C5-C4	2.27	1.46	1.40
38	A1	817	A2M	C5-C4	2.25	1.46	1.40
34	B5	1877	OMU	C2-N1	2.25	1.42	1.38
38	A1	2421	OMU	C2-N3	-2.24	1.34	1.38
38	A1	2347	OMU	C2-N3	-2.24	1.34	1.38
34	B5	2183	G7M	O2'-C2'	-2.24	1.37	1.43
38	A1	2729	OMU	C2-N3	-2.22	1.34	1.38
38	A1	2347	OMU	C2-N1	2.21	1.42	1.38
38	A1	2417	OMU	C2-N3	-2.20	1.34	1.38
38	A1	2278	5MC	C6-N1	-2.19	1.34	1.38
38	A1	2724	OMU	C5-C4	-2.18	1.38	1.43
34	B5	1877	OMU	C2-N3	-2.17	1.34	1.38
34	B5	578	OMU	C2-N3	-2.16	1.34	1.38
38	A1	898	OMU	C5-C4	-2.16	1.38	1.43
38	A1	2417	OMU	C5-C4	-2.15	1.38	1.43
38	A1	2729	OMU	C5-C4	-2.15	1.38	1.43
38	A1	2870	5MC	C6-N1	-2.14	1.34	1.38
38	A1	2724	OMU	C2-N3	-2.14	1.34	1.38
34	B5	1877	OMU	C5-C4	-2.10	1.39	1.43
36	AB	243	HIC	CZ-NE2	-2.10	1.42	1.48
38	A1	2347	OMU	C5-C4	-2.09	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	A1	2921	OMU	C5-C4	-2.04	1.39	1.43
38	A1	1888	OMU	C5-C4	-2.04	1.39	1.43
38	A1	2421	OMU	C5-C4	-2.04	1.39	1.43

All (166) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	B5	1799	3AU	C11-C10-N3	10.74	132.13	112.00
34	B5	2381	4AC	N4-C4-N3	6.83	125.31	113.85
38	A1	2634	UR3	C4-N3-C2	-5.88	119.02	124.56
34	B5	1799	3AU	C4-N3-C2	-4.66	118.78	124.63
38	A1	1888	OMU	C4-N3-C2	-4.61	120.50	126.58
38	A1	2921	OMU	C4-N3-C2	-4.58	120.54	126.58
38	A1	2421	OMU	C4-N3-C2	-4.54	120.59	126.58
38	A1	898	OMU	C4-N3-C2	-4.44	120.72	126.58
34	B5	578	OMU	C4-N3-C2	-4.44	120.72	126.58
38	A1	1888	OMU	N3-C2-N1	4.39	120.72	114.89
38	A1	2724	OMU	C4-N3-C2	-4.38	120.80	126.58
38	A1	2921	OMU	N3-C2-N1	4.38	120.70	114.89
38	A1	898	OMU	N3-C2-N1	4.33	120.64	114.89
38	A1	2417	OMU	C4-N3-C2	-4.29	120.92	126.58
38	A1	2417	OMU	N3-C2-N1	4.24	120.52	114.89
38	A1	2729	OMU	N3-C2-N1	4.24	120.51	114.89
38	A1	2870	5MC	C5-C6-N1	-4.22	119.00	123.34
38	A1	2347	OMU	C4-N3-C2	-4.15	121.10	126.58
38	A1	2347	OMU	N3-C2-N1	4.11	120.34	114.89
34	B5	1877	OMU	C4-N3-C2	-4.09	121.18	126.58
38	A1	2421	OMU	N3-C2-N1	4.08	120.30	114.89
38	A1	2724	OMU	N3-C2-N1	4.02	120.22	114.89
34	B5	578	OMU	N3-C2-N1	3.99	120.18	114.89
34	B5	2389	MA6	C4-C5-N7	-3.96	105.28	109.40
38	A1	2729	OMU	C4-N3-C2	-3.95	121.38	126.58
34	B5	2381	4AC	C5-C4-N4	-3.90	116.14	122.92
34	B5	1877	OMU	N3-C2-N1	3.88	120.04	114.89
38	A1	2421	OMU	C5-C4-N3	3.77	120.47	114.84
34	B5	2390	MA6	C4-C5-N7	-3.71	105.53	109.40
38	A1	2921	OMU	C5-C4-N3	3.69	120.36	114.84
38	A1	898	OMU	C5-C4-N3	3.67	120.33	114.84
38	A1	2724	OMU	C5-C4-N3	3.63	120.28	114.84
34	B5	578	OMU	C5-C4-N3	3.54	120.14	114.84
38	A1	1888	OMU	C5-C4-N3	3.54	120.13	114.84
34	B5	2183	G7M	C3'-C2'-C1'	3.53	106.30	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	2417	OMU	C5-C4-N3	3.52	120.11	114.84
38	A1	1437	OMC	O2-C2-N3	-3.48	116.67	122.33
38	A1	2347	OMU	C5-C4-N3	3.48	120.05	114.84
38	A1	817	A2M	N3-C2-N1	-3.48	123.24	128.68
34	B5	1877	OMU	C1'-N1-C2	3.48	123.87	117.57
34	B5	1877	OMU	C5-C4-N3	3.45	120.00	114.84
34	B5	973	A2M	N3-C2-N1	-3.35	123.45	128.68
38	A1	2256	A2M	N3-C2-N1	-3.33	123.47	128.68
38	A1	2946	A2M	N3-C2-N1	-3.33	123.48	128.68
38	A1	2280	A2M	N3-C2-N1	-3.31	123.50	128.68
38	A1	2640	A2M	N3-C2-N1	-3.30	123.52	128.68
38	A1	2278	5MC	C5-C6-N1	-3.30	119.94	123.34
38	A1	876	A2M	N3-C2-N1	-3.30	123.52	128.68
38	A1	2347	OMU	C1'-N1-C2	3.30	123.55	117.57
34	B5	28	A2M	N3-C2-N1	-3.27	123.56	128.68
38	A1	2729	OMU	C5-C4-N3	3.25	119.71	114.84
34	B5	2389	MA6	N3-C2-N1	-3.25	123.59	128.68
34	B5	436	A2M	N3-C2-N1	-3.24	123.62	128.68
34	B5	795	A2M	N3-C2-N1	-3.23	123.62	128.68
34	B5	420	A2M	N3-C2-N1	-3.22	123.64	128.68
34	B5	2390	MA6	N3-C2-N1	-3.22	123.65	128.68
38	A1	1133	A2M	N3-C2-N1	-3.22	123.65	128.68
38	A1	1449	A2M	N3-C2-N1	-3.21	123.65	128.68
38	A1	1437	OMC	C1'-N1-C2	3.20	125.57	118.42
38	A1	2220	A2M	C4-C5-N7	-3.19	106.08	109.40
38	A1	649	A2M	N3-C2-N1	-3.19	123.70	128.68
34	B5	541	A2M	N3-C2-N1	-3.18	123.71	128.68
38	A1	2729	OMU	C1'-N1-C2	3.17	123.31	117.57
38	A1	2724	OMU	O4-C4-C5	-3.17	119.59	125.16
34	B5	619	A2M	N3-C2-N1	-3.16	123.74	128.68
38	A1	2281	A2M	N3-C2-N1	-3.16	123.74	128.68
34	B5	2381	4AC	C6-C5-C4	3.15	120.82	116.96
38	A1	2421	OMU	O4-C4-C5	-3.09	119.72	125.16
34	B5	2183	G7M	O3'-C3'-C4'	3.09	119.98	111.05
34	B5	100	A2M	N3-C2-N1	-3.09	123.86	128.68
34	B5	1799	3AU	C5-C4-N3	3.08	119.57	115.50
38	A1	2417	OMU	O4-C4-C5	-3.05	119.79	125.16
38	A1	2921	OMU	O4-C4-C5	-3.01	119.86	125.16
38	A1	898	OMU	O4-C4-C5	-3.01	119.87	125.16
34	B5	1877	OMU	O4-C4-C5	-3.00	119.88	125.16
38	A1	807	A2M	N3-C2-N1	-2.99	124.01	128.68
34	B5	578	OMU	O4-C4-C5	-2.95	119.97	125.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	2948	OMC	O2-C2-N3	-2.94	117.55	122.33
38	A1	2256	A2M	C4-C5-N7	-2.92	106.36	109.40
38	A1	2347	OMU	O4-C4-C5	-2.90	120.06	125.16
38	A1	2278	5MC	O2-C2-N3	-2.86	117.67	122.33
38	A1	2280	A2M	C4-C5-N7	-2.85	106.43	109.40
38	A1	1888	OMU	O4-C4-C5	-2.83	120.19	125.16
34	B5	795	A2M	C4-C5-N7	-2.82	106.46	109.40
34	B5	619	A2M	C4-C5-N7	-2.74	106.54	109.40
38	A1	2870	5MC	C5-C4-N3	-2.71	118.75	121.67
38	A1	1133	A2M	C4-C5-N7	-2.70	106.58	109.40
34	B5	28	A2M	C4-C5-N7	-2.69	106.60	109.40
38	A1	2729	OMU	O4-C4-C5	-2.67	120.47	125.16
34	B5	420	A2M	C4-C5-N7	-2.66	106.62	109.40
34	B5	1888	4AC	N4-C4-N3	2.62	118.25	113.85
34	B5	2183	G7M	CN7-N7-C8	-2.61	112.87	125.43
38	A1	807	A2M	C4-C5-N7	-2.55	106.74	109.40
34	B5	2381	4AC	C5-C4-N3	-2.54	118.50	122.59
38	A1	2946	A2M	C4-C5-N7	-2.52	106.77	109.40
38	A1	805	OMG	C8-N7-C5	2.50	107.76	102.99
34	B5	1888	4AC	C6-C5-C4	2.50	120.02	116.96
34	B5	1125	OMG	C8-N7-C5	2.49	107.74	102.99
34	B5	436	A2M	C4-C5-N7	-2.49	106.80	109.40
38	A1	2278	5MC	C5-C4-N3	-2.49	118.99	121.67
34	B5	973	A2M	C4-C5-N7	-2.48	106.81	109.40
38	A1	2793	OMG	C5-C6-N1	2.48	118.32	113.95
38	A1	2640	A2M	C4-C5-N7	-2.44	106.86	109.40
38	A1	876	A2M	C4-C5-N7	-2.44	106.86	109.40
34	B5	100	A2M	C4-C5-N7	-2.44	106.86	109.40
38	A1	817	A2M	C4-C5-N7	-2.42	106.87	109.40
34	B5	541	A2M	C4-C5-N7	-2.42	106.88	109.40
38	A1	867	OMG	C5-C6-N1	2.40	118.19	113.95
38	A1	649	A2M	C4-C5-N7	-2.39	106.91	109.40
38	A1	2815	OMG	C5-C6-N1	2.38	118.16	113.95
38	A1	2729	OMU	O2-C2-N3	-2.36	117.10	121.50
38	A1	908	OMG	C5-C6-N1	2.36	118.11	113.95
38	A1	867	OMG	C8-N7-C5	2.36	107.48	102.99
38	A1	2142	1MA	C5-C6-N1	2.36	117.41	113.90
34	B5	1799	3AU	C10-N3-C4	2.36	121.79	117.14
38	A1	2870	5MC	O2-C2-N3	-2.35	118.50	122.33
38	A1	2417	OMU	O2-C2-N1	-2.35	119.66	122.79
38	A1	1450	OMG	C5-C6-N1	2.35	118.10	113.95
38	A1	2791	OMG	C5-C6-N1	2.35	118.09	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	1449	A2M	C4-C5-N7	-2.34	106.96	109.40
38	A1	2619	OMG	C8-N7-C5	2.33	107.43	102.99
38	A1	805	OMG	C5-C6-N1	2.33	118.06	113.95
34	B5	1879	OMG	C8-N7-C5	2.32	107.41	102.99
34	B5	2180	OMG	C8-N7-C5	2.32	107.41	102.99
38	A1	650	OMC	O2-C2-N3	-2.32	118.56	122.33
38	A1	2791	OMG	C8-N7-C5	2.31	107.40	102.99
38	A1	645	1MA	C5-C6-N1	2.30	117.33	113.90
38	A1	2220	A2M	N3-C2-N1	-2.29	125.10	128.68
38	A1	2921	OMU	O2-C2-N1	-2.28	119.75	122.79
38	A1	2288	OMG	C5-C6-N1	2.28	117.98	113.95
38	A1	2922	OMG	C8-N7-C5	2.27	107.32	102.99
34	B5	1125	OMG	C5-C6-N1	2.27	117.96	113.95
38	A1	2815	OMG	C8-N7-C5	2.27	107.32	102.99
34	B5	2381	4AC	O2-C2-N3	-2.26	118.65	122.33
34	B5	2036	OMG	C5-C6-N1	2.26	117.94	113.95
38	A1	908	OMG	C8-N7-C5	2.25	107.28	102.99
38	A1	2619	OMG	C5-C6-N1	2.25	117.92	113.95
34	B5	1879	OMG	C5-C6-N1	2.25	117.92	113.95
34	B5	562	OMG	C8-N7-C5	2.25	107.27	102.99
38	A1	2793	OMG	C8-N7-C5	2.24	107.27	102.99
34	B5	2381	4AC	CM7-C7-N4	2.24	119.16	115.29
38	A1	1437	OMC	O2-C2-N1	2.23	123.50	118.89
38	A1	1450	OMG	C8-N7-C5	2.23	107.24	102.99
38	A1	2724	OMU	C1'-N1-C2	2.23	121.61	117.57
34	B5	2381	4AC	C1'-N1-C2	2.23	123.39	118.42
34	B5	2180	OMG	C5-C6-N1	2.22	117.87	113.95
34	B5	562	OMG	C5-C6-N1	2.21	117.86	113.95
34	B5	2036	OMG	C8-N7-C5	2.20	107.18	102.99
34	B5	1006	OMC	O2-C2-N3	-2.18	118.78	122.33
38	A1	2922	OMG	C5-C6-N1	2.18	117.80	113.95
38	A1	645	1MA	C8-N7-C5	2.16	107.10	102.99
34	B5	973	A2M	C2-N1-C6	2.15	122.44	118.75
34	B5	578	OMU	O2-C2-N1	-2.15	119.93	122.79
38	A1	2142	1MA	C8-N7-C5	2.14	107.08	102.99
38	A1	2288	OMG	C8-N7-C5	2.14	107.07	102.99
38	A1	645	1MA	N1-C2-N3	-2.14	123.53	126.02
38	A1	2729	OMU	C6-N1-C2	-2.13	118.27	120.99
34	B5	2183	G7M	O2'-C2'-C3'	2.12	118.67	111.82
38	A1	2281	A2M	C4-C5-N7	-2.08	107.23	109.40
34	B5	414	OMC	O2-C2-N3	-2.06	118.98	122.33
38	A1	1888	OMU	O2-C2-N1	-2.05	120.06	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	A1	2142	1MA	N1-C2-N3	-2.04	123.64	126.02
38	A1	1437	OMC	C1'-N1-C6	-2.03	116.42	120.84
34	B5	1888	4AC	C5-C4-N3	-2.02	119.34	122.59
38	A1	2959	OMC	O2-C2-N3	-2.02	119.04	122.33
34	B5	1888	4AC	O2-C2-N3	-2.01	119.06	122.33

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
34	B5	1799	3AU	C12

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	AB	243	HIC	CA-CB-CG-ND1
34	B5	414	OMC	C1'-C2'-O2'-CM2
34	B5	420	A2M	C1'-C2'-O2'-CM'
34	B5	541	A2M	O4'-C4'-C5'-O5'
34	B5	619	A2M	O4'-C4'-C5'-O5'
34	B5	1799	3AU	N40-C12-C13-O30
34	B5	1877	OMU	O4'-C4'-C5'-O5'
34	B5	1879	OMG	C1'-C2'-O2'-CM2
34	B5	1888	4AC	N3-C4-N4-C7
34	B5	1888	4AC	C5-C4-N4-C7
34	B5	2036	OMG	C1'-C2'-O2'-CM2
34	B5	2180	OMG	O4'-C4'-C5'-O5'
34	B5	2180	OMG	C1'-C2'-O2'-CM2
34	B5	2381	4AC	N3-C4-N4-C7
34	B5	2381	4AC	C5-C4-N4-C7
34	B5	2381	4AC	O7-C7-N4-C4
34	B5	2381	4AC	CM7-C7-N4-C4
34	B5	2390	MA6	O4'-C4'-C5'-O5'
38	A1	649	A2M	C1'-C2'-O2'-CM'
38	A1	650	OMC	C1'-C2'-O2'-CM2
38	A1	663	OMC	C1'-C2'-O2'-CM2
38	A1	876	A2M	C1'-C2'-O2'-CM'
38	A1	1437	OMC	C1'-C2'-O2'-CM2
38	A1	2197	OMC	C2'-C1'-N1-C2
38	A1	2197	OMC	C2'-C1'-N1-C6
38	A1	2220	A2M	C1'-C2'-O2'-CM'
38	A1	2619	OMG	C1'-C2'-O2'-CM2
38	A1	2724	OMU	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
38	A1	2729	OMU	C3'-C4'-C5'-O5'
38	A1	2791	OMG	C1'-C2'-O2'-CM2
38	A1	2948	OMC	C1'-C2'-O2'-CM2
34	B5	1877	OMU	C3'-C4'-C5'-O5'
34	B5	2036	OMG	O4'-C4'-C5'-O5'
34	B5	2390	MA6	C3'-C4'-C5'-O5'
38	A1	2197	OMC	O4'-C4'-C5'-O5'
38	A1	2280	A2M	C3'-C4'-C5'-O5'
34	B5	1799	3AU	N40-C12-C13-O31
34	B5	541	A2M	C3'-C4'-C5'-O5'
34	B5	619	A2M	C3'-C4'-C5'-O5'
34	B5	2180	OMG	C3'-C4'-C5'-O5'
38	A1	2280	A2M	O4'-C4'-C5'-O5'
38	A1	2729	OMU	O4'-C4'-C5'-O5'
38	A1	2870	5MC	C2'-C1'-N1-C6
38	A1	2347	OMU	C3'-C4'-C5'-O5'
38	A1	817	A2M	C4'-C5'-O5'-P
38	A1	2619	OMG	O4'-C4'-C5'-O5'
34	B5	1877	OMU	O4'-C1'-N1-C6
34	B5	1877	OMU	O4'-C1'-N1-C2
38	A1	2347	OMU	O4'-C4'-C5'-O5'
38	A1	2870	5MC	O4'-C1'-N1-C6
38	A1	2619	OMG	C3'-C4'-C5'-O5'
38	A1	2421	OMU	C1'-C2'-O2'-CM2
38	A1	2729	OMU	C4'-C5'-O5'-P
38	A1	2870	5MC	C2'-C1'-N1-C2
38	A1	805	OMG	C3'-C2'-O2'-CM2
38	A1	2197	OMC	O4'-C1'-N1-C6
34	B5	541	A2M	C4'-C5'-O5'-P
38	A1	2256	A2M	O4'-C4'-C5'-O5'
38	A1	2870	5MC	O4'-C1'-N1-C2
34	B5	2036	OMG	C4'-C5'-O5'-P
38	A1	2197	OMC	O4'-C1'-N1-C2
34	B5	1125	OMG	C3'-C4'-C5'-O5'
38	A1	2197	OMC	C3'-C4'-C5'-O5'
34	B5	1877	OMU	C4'-C5'-O5'-P
38	A1	817	A2M	O4'-C4'-C5'-O5'
38	A1	1437	OMC	O4'-C4'-C5'-O5'
38	A1	2281	A2M	O4'-C4'-C5'-O5'
38	A1	1437	OMC	C2'-C1'-N1-C2
34	B5	2390	MA6	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 257 ligands modelled in this entry, 257 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

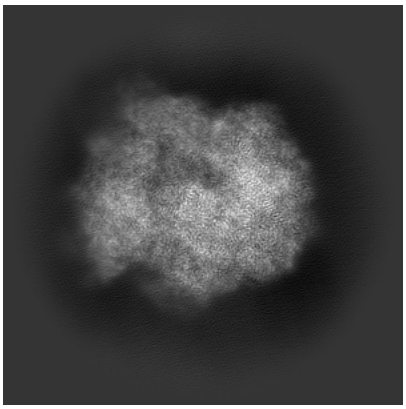
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28632. These allow visual inspection of the internal detail of the map and identification of artifacts.

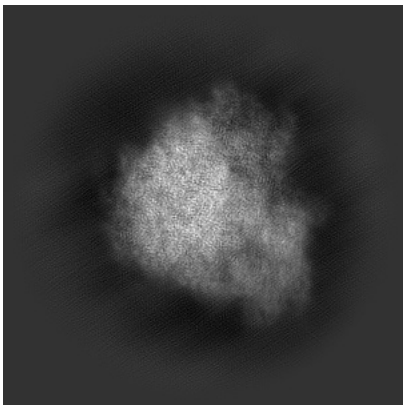
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

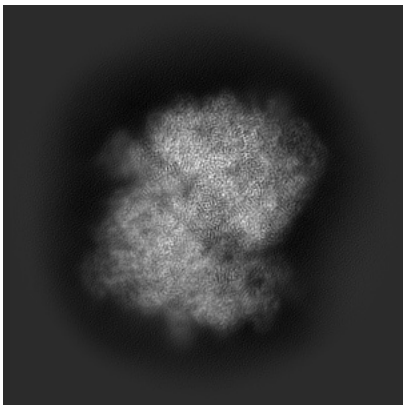
6.1.1 Primary map



X

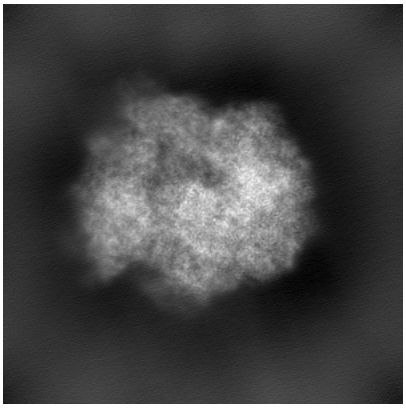


Y

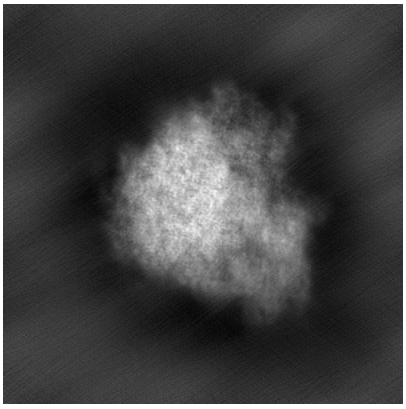


Z

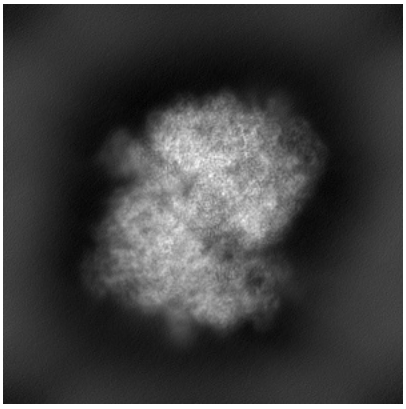
6.1.2 Raw map



X



Y

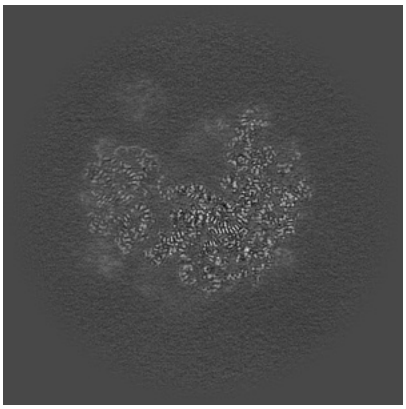


Z

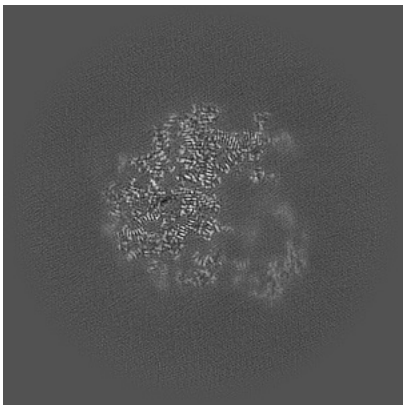
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

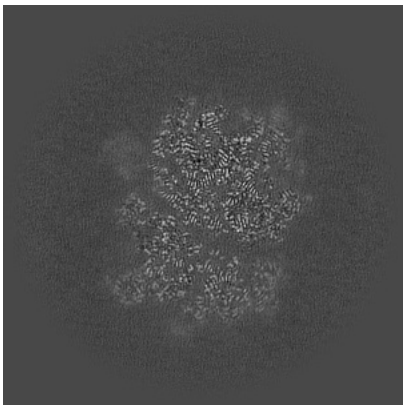
6.2.1 Primary map



X Index: 200

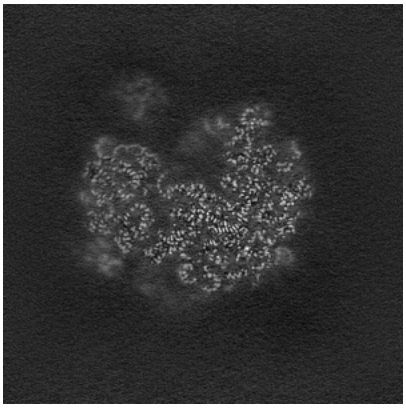


Y Index: 200

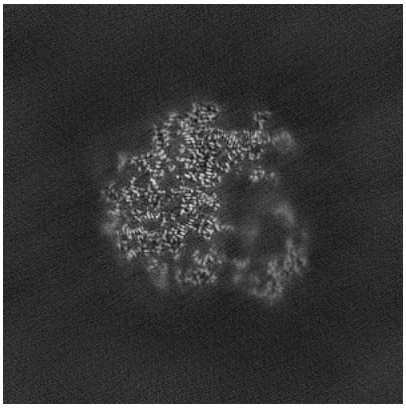


Z Index: 200

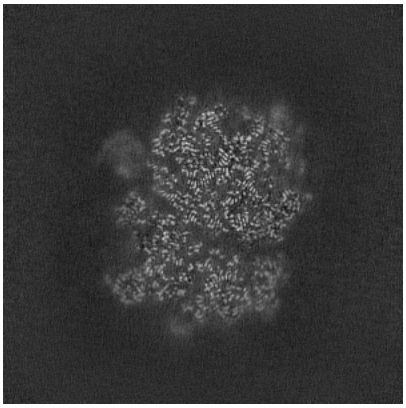
6.2.2 Raw map



X Index: 200



Y Index: 200

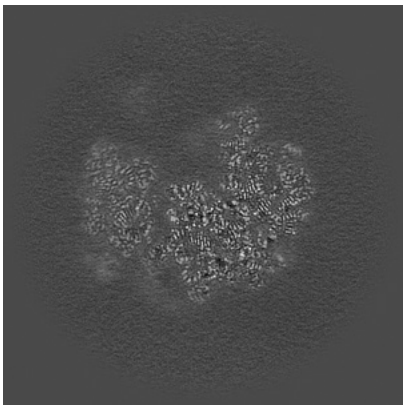


Z Index: 200

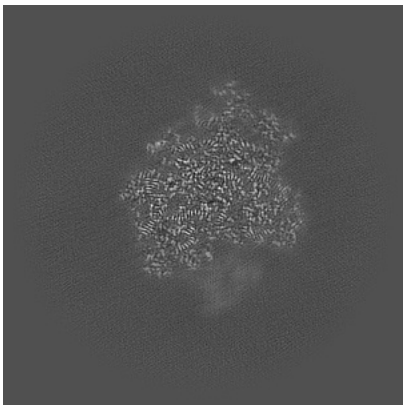
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

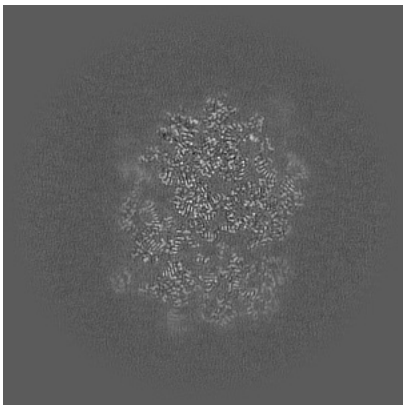
6.3.1 Primary map



X Index: 205

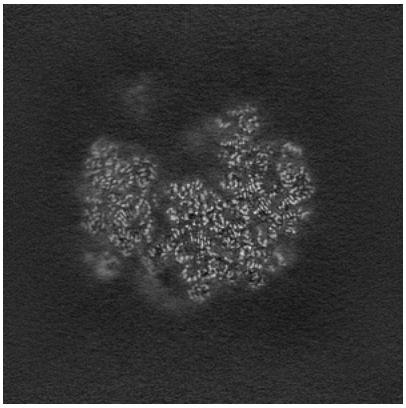


Y Index: 246

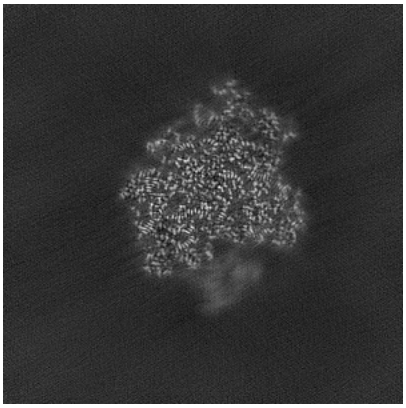


Z Index: 191

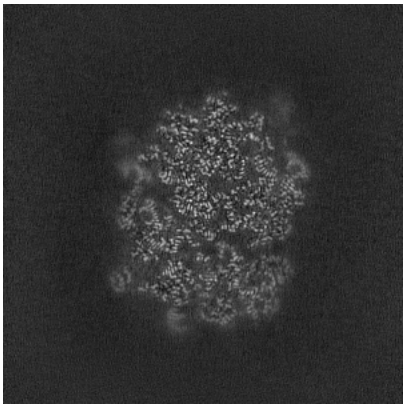
6.3.2 Raw map



X Index: 205



Y Index: 246

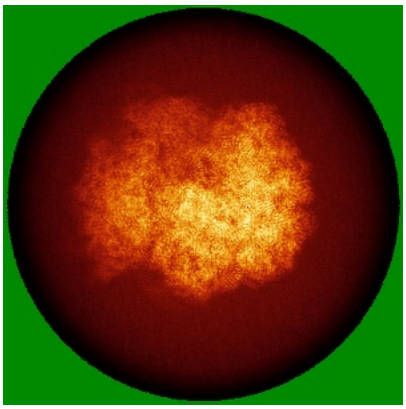


Z Index: 191

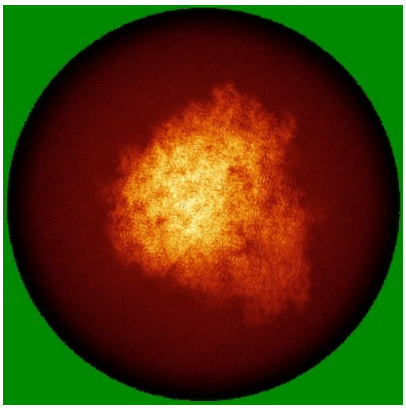
The images above show the largest variance slices of the map in three orthogonal directions.

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

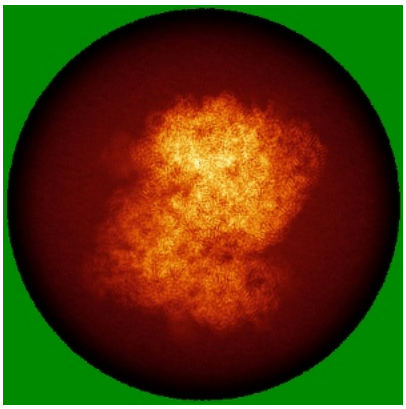
6.4.1 Primary map



X

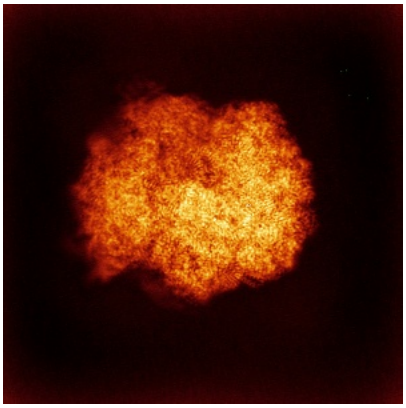


Y

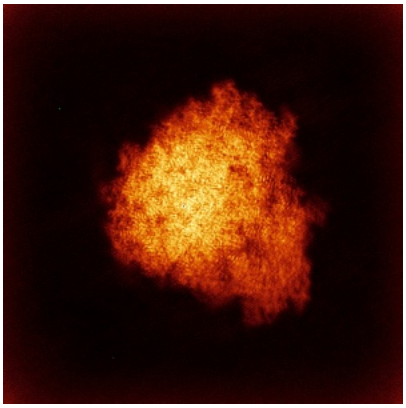


Z

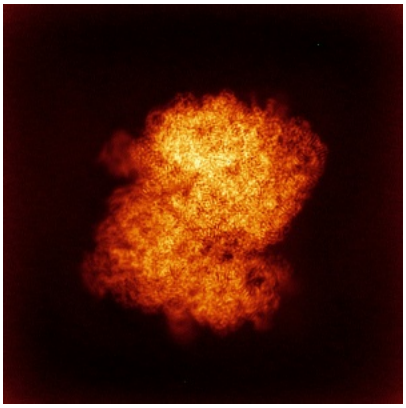
6.4.2 Raw map



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.

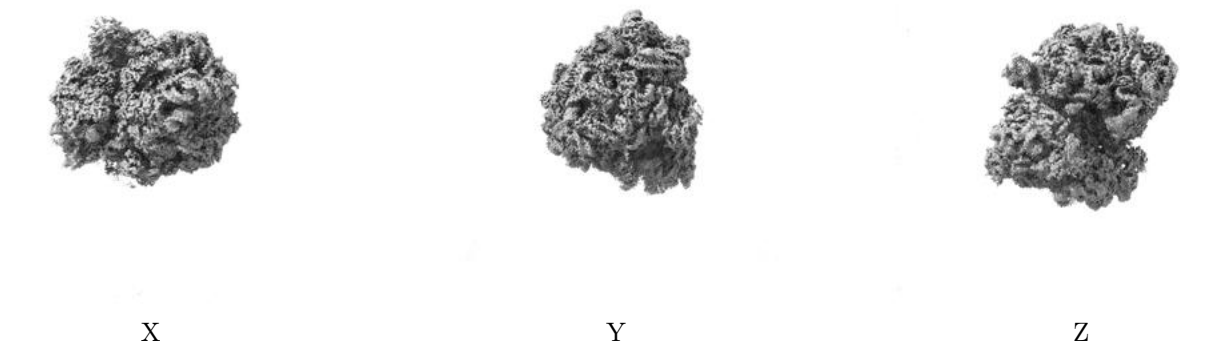
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

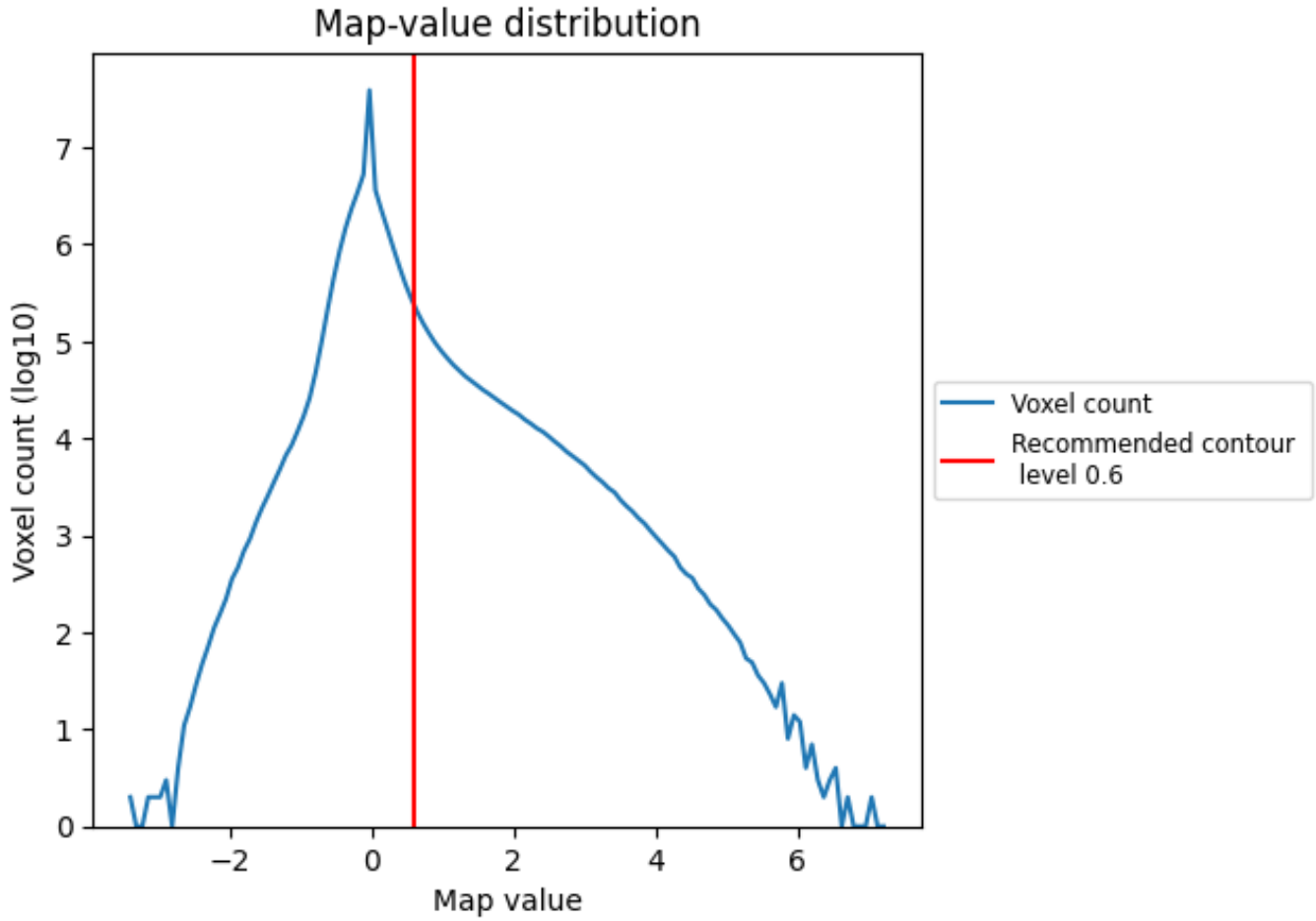
6.6 Mask visualisation (i)

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

7 Map analysis

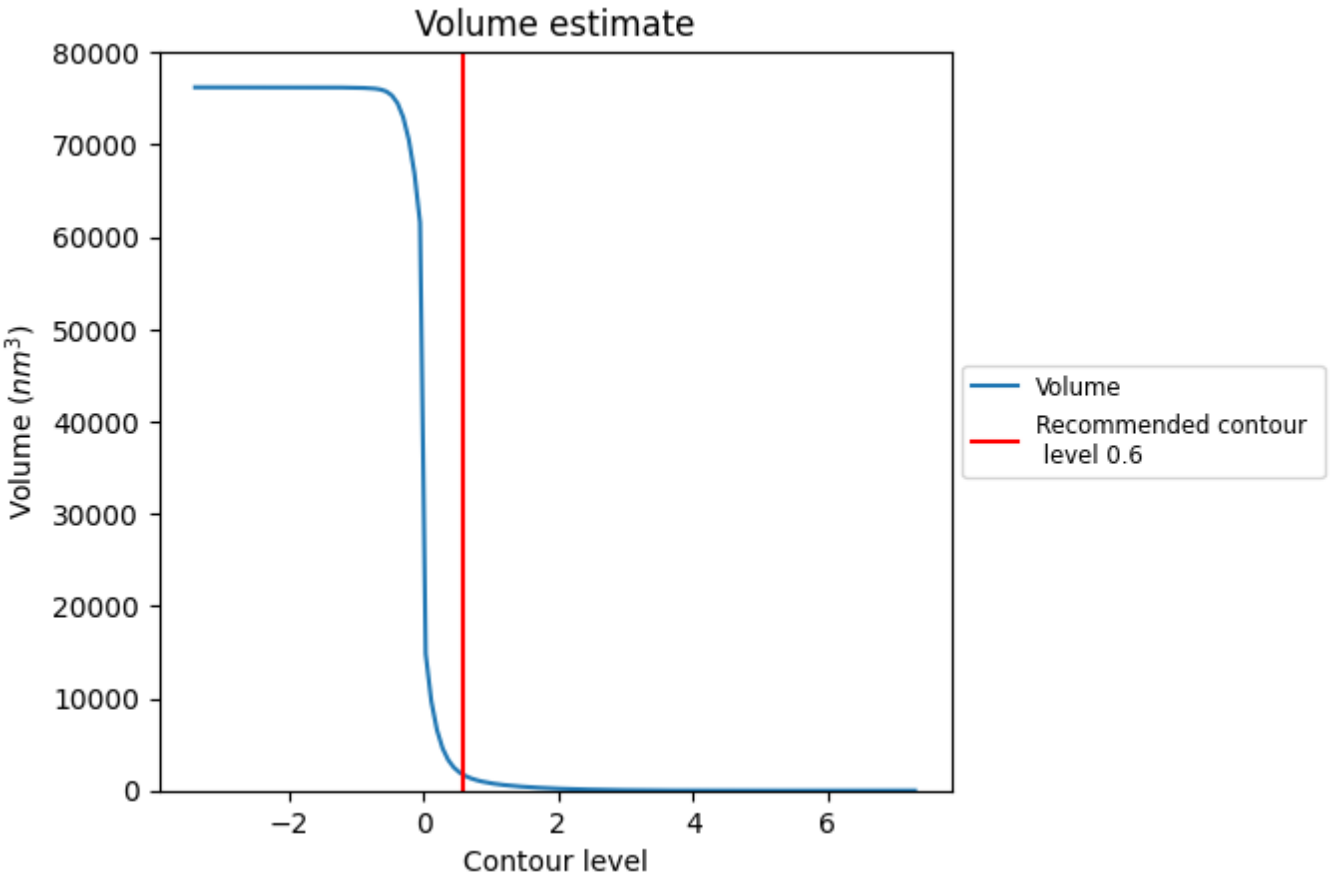
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

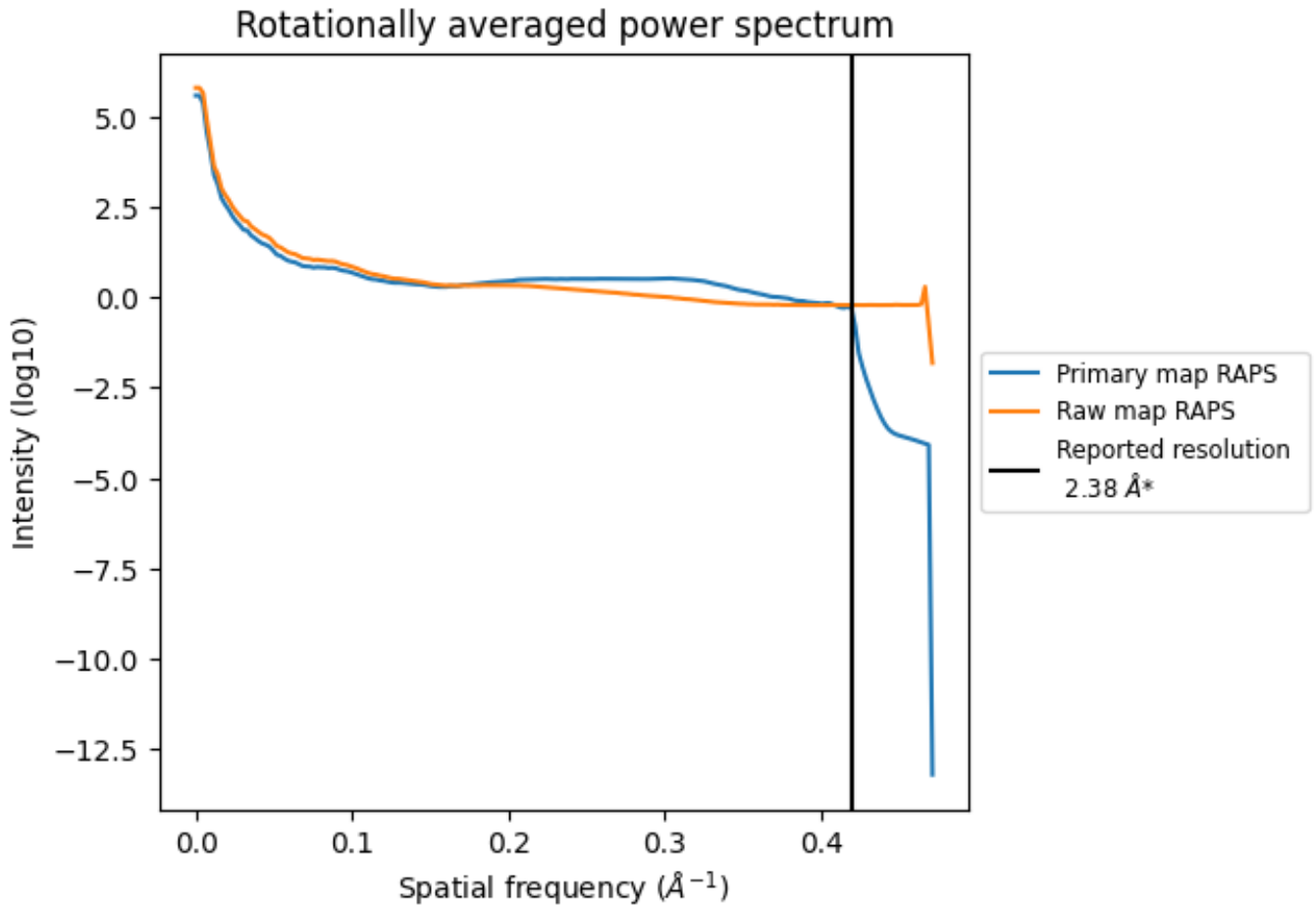
7.2 Volume estimate



The volume at the recommended contour level is 1679 nm^3; this corresponds to an approximate mass of 1517 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)

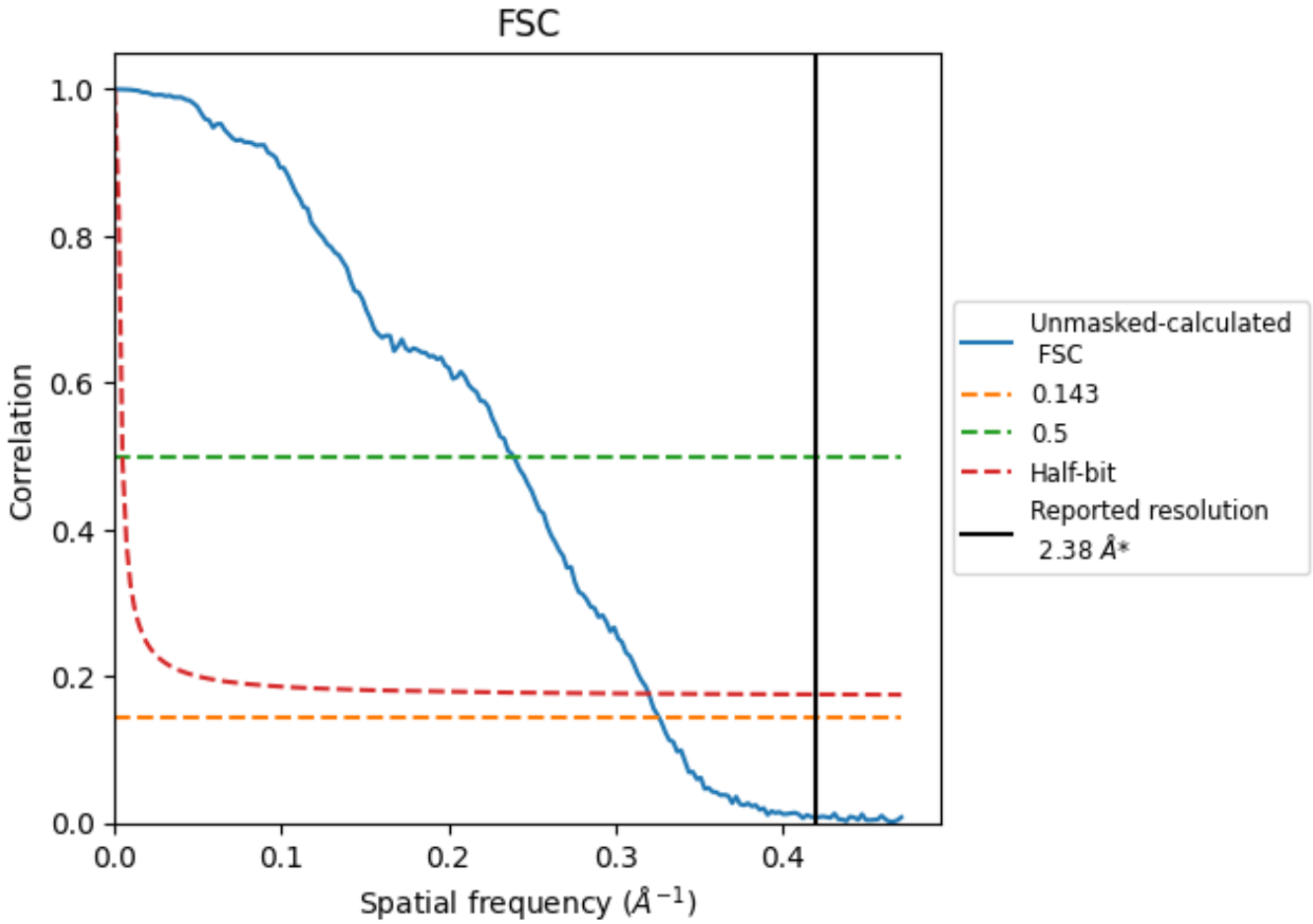


*Reported resolution corresponds to spatial frequency of 0.420 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.420 Å^{-1}

8.2 Resolution estimates (i)

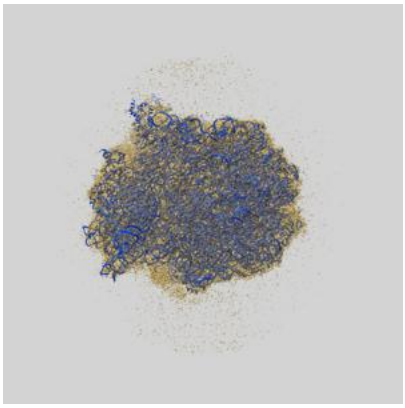
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.38	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.06	4.19	3.12

*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 3.06 differs from the reported value 2.38 by more than 10 %

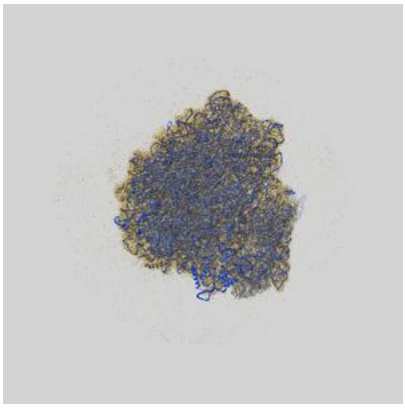
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28632 and PDB model 8EVP. Per-residue inclusion information can be found in section 3 on page 20.

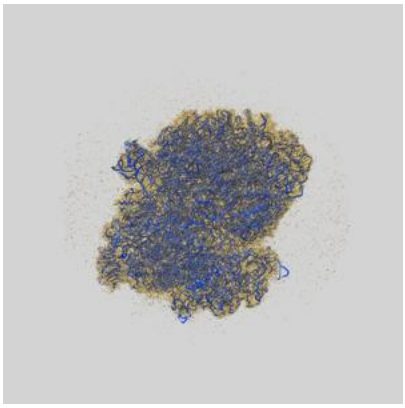
9.1 Map-model overlay



X



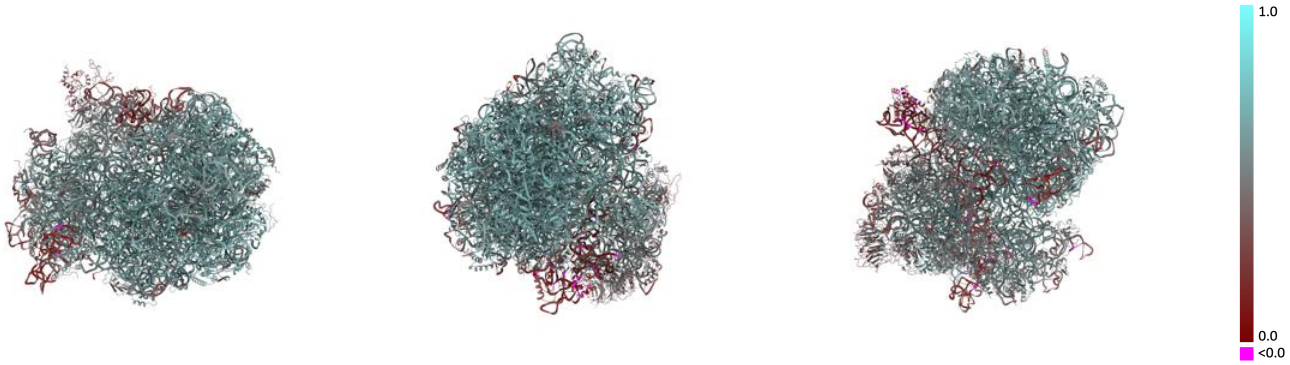
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

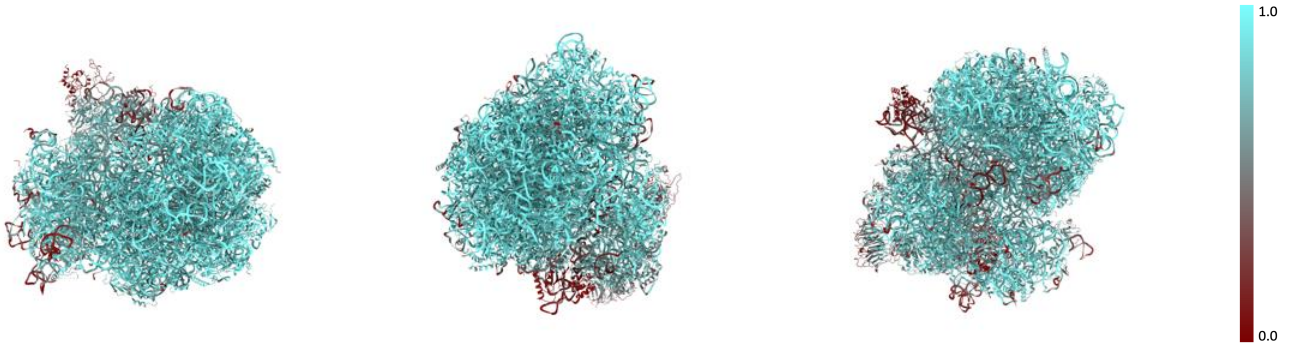
9.2 Q-score mapped to coordinate model (i)



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.

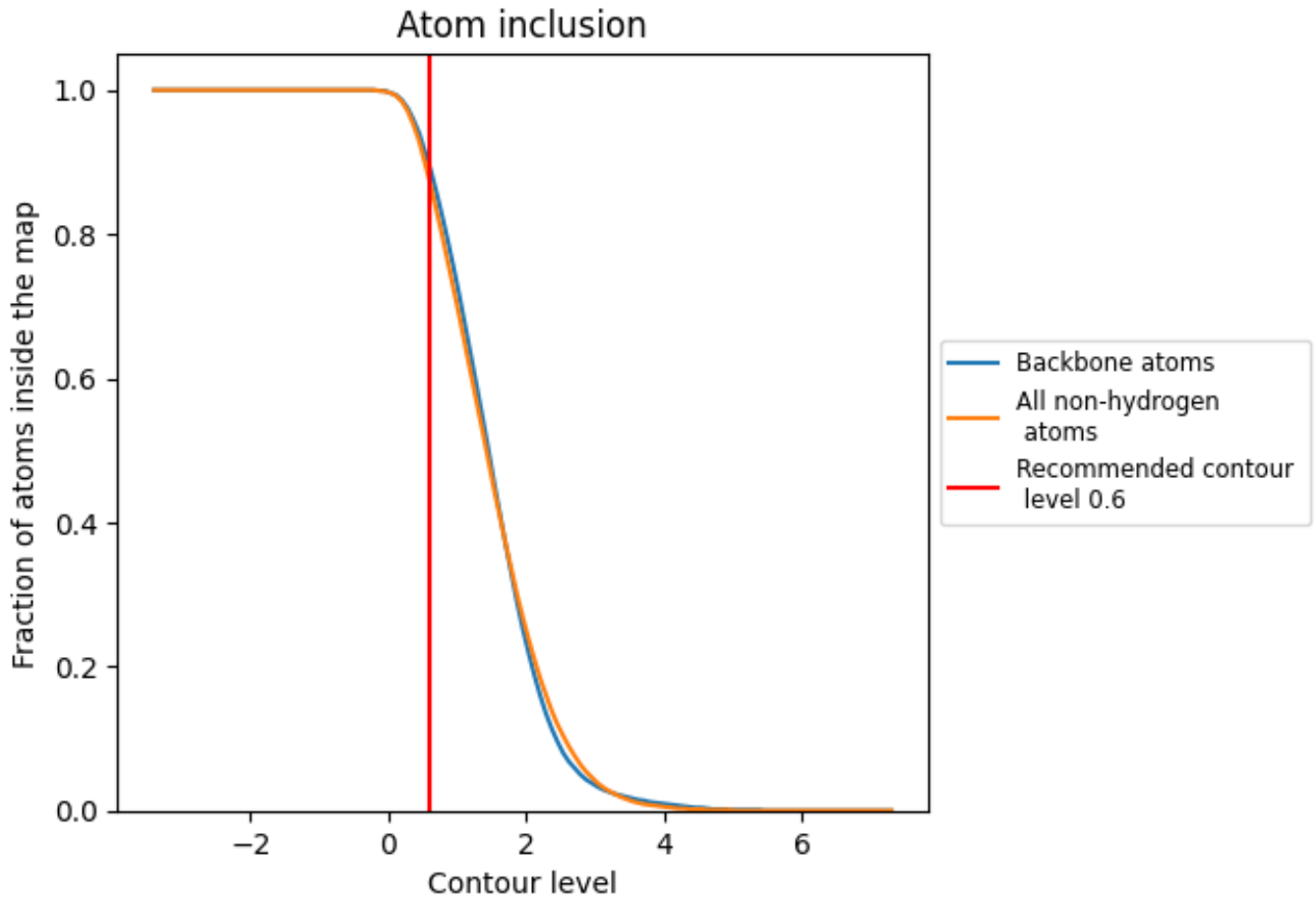
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8750	0.5650
A1	0.9390	0.6040
A3	0.9820	0.6100
A4	0.9730	0.6340
AA	0.9810	0.6660
AB	0.9490	0.6220
AC	0.9580	0.6390
AD	0.8710	0.5650
AE	0.8710	0.5700
AF	0.9500	0.6400
AG	0.8920	0.5810
AH	0.8940	0.5930
AI	0.9330	0.6150
AJ	0.7510	0.4710
AL	0.9310	0.6260
AM	0.9200	0.6030
AN	0.9870	0.6620
AO	0.9600	0.6330
AP	0.9500	0.6330
AQ	0.9820	0.6660
AR	0.8780	0.5910
AS	0.9350	0.6210
AT	0.9380	0.6160
AU	0.8310	0.5360
AV	0.9430	0.6340
AW	0.9600	0.6340
AX	0.9420	0.6240
AY	0.9230	0.6130
AZ	0.9360	0.6040
Aa	0.9560	0.6450
Ab	0.9270	0.6080
Ac	0.9430	0.6250
Ad	0.8840	0.5900
Ae	0.9620	0.6520
Af	0.9640	0.6410

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Chain	Atom inclusion	Q-score
Ag	0.9400	0.6180
Ah	0.9420	0.6230
Ai	0.9170	0.5930
Aj	0.9680	0.6580
Ak	0.7810	0.5550
Al	0.9780	0.6530
Am	0.8930	0.6150
An	0.9340	0.5920
Ao	0.9020	0.6070
Ap	0.9400	0.6370
B5	0.8700	0.5300
BA	0.8620	0.5530
BB	0.8560	0.5560
BC	0.9340	0.6080
BD	0.7480	0.4850
BE	0.9100	0.5800
BF	0.7220	0.4750
BG	0.7310	0.4860
BH	0.7250	0.4970
BI	0.8860	0.5880
BJ	0.8660	0.5570
BK	0.5850	0.3940
BL	0.8570	0.5810
BM	0.0820	0.2560
BN	0.9300	0.6100
BO	0.9000	0.5730
BP	0.5180	0.3960
BQ	0.7750	0.4850
BR	0.7780	0.4970
BS	0.6730	0.4460
BT	0.7490	0.4730
BU	0.6440	0.4400
BV	0.9080	0.5810
BW	0.9630	0.6390
BX	0.9150	0.6060
BY	0.7900	0.5040
BZ	0.6220	0.4250
Ba	0.9000	0.5700
Bb	0.8450	0.5610
Bc	0.6960	0.4810
Bd	0.8840	0.5350
Be	0.8000	0.5130

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Chain	Atom inclusion	Q-score
Bf	0.1190	0.2320
Bg	0.5440	0.4010
E	0.1450	0.1950
EC	0.3860	0.2180