Full wwPDB EM Validation Report ⓘ

Apr 25, 2023 – 03:22 pm BST

PDB ID	:	8BQD
EMDB ID	:	EMD-16182
Title	:	Yeast 80S ribosome in complex with Map1 (conformation 1)
Authors	:	Knorr, A.G.; Mackens-Kiani, T.; Musial, J.; Berninghausen, O.; Becker, T.; Beatrix, B.; Beckmann, R.
Deposited on	:	2022-11-21
Resolution	:	3.90 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:

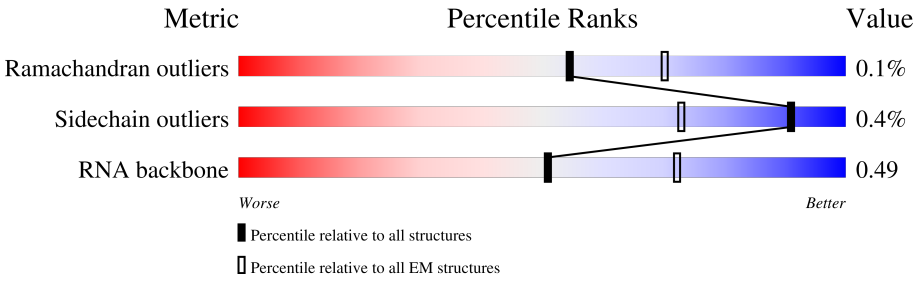
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	B	206	61% 100%
2	A	222	49% 100%
3	C	92	45% 100%
4	D	121	83% 98% .
5	E	142	38% 82% 18%
6	F	141	48% 99% .
7	G	125	45% 97% .
8	H	145	44% 99% .

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Mol	Chain	Length	Quality of chain
9	I	143	47% 99%
10	J	100	32% 99%
11	K	82	63% 99%
12	L	63	51% 98%
13	M	53	36% 98%
14	N	73	49% 99%
15	O	312	60% 100%
16	P	206	30% 100%
17	Q	232	37% 97%
18	R	216	18% 100%
19	S	258	22% 99%
20	T	228	19% 99%
21	U	184	30% 99%
22	V	200	9% 93% 6%
23	W	184	16% 99%
24	X	142	12% 99%
25	Y	150	17% 99%
26	Z	127	29% 98%
27	AA	233	7% 98%
28	BA	386	99%
29	AB	136	100%
30	BB	185	98%
31	AC	99	5% 100%
32	BC	109	7% 99%
33	2	1798	6% 66% 30%

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Mol	Chain	Length	Quality of chain
34	a	87	11% 100%
35	b	129	10% 98%
36	c	144	13% 98%
37	d	134	16% 99%
38	e	97	21% 100%
39	f	81	25% 100%
40	g	60	27% 100%
41	BQ	3395	72% 24%
42	BR	121	88% 12%
43	BS	158	78% 21%
44	AW	251	99%
45	BE	361	5% 98%
46	BI	294	7% 100%
47	BM	175	7% 95% 5%
48	BO	222	99%
49	AD	191	6% 99%
50	BD	218	16% 99%
51	AG	169	12% 99%
52	AJ	193	8% 98%
53	AM	136	100%
54	AQ	203	100%
55	AU	197	100%
56	AX	183	5% 100%
57	BF	188	11% 99%
58	BH	171	100%

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Mol	Chain	Length	Quality of chain
59	BJ	159	100%
60	BL	100	5% 100%
61	AE	126	43% 100%
62	AH	121	100%
63	AK	125	100%
64	AN	135	6% 99%
65	AR	148	97%
66	AV	58	9% 95% 5%
67	AY	96	6% 99%
68	BG	127	100%
69	BK	106	100%
70	BN	112	6% 99%
71	BP	119	6% 99%
72	AF	81	91% 7%
73	AI	77	8% 99%
74	AL	50	100%
75	AO	52	10% 94% 6%
76	AS	25	8% 96%
77	AP	103	5% 96%
78	AT	91	97%
79	x	387	92% 92% 5%
80	BT	217	92% 100%

2 Entry composition (i)

There are 81 unique types of molecules in this entry. The entry contains 205800 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 Rps5p.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	206	1605	1005	299	298	3	0	0

- Molecule 2 is a protein called RPS3 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A	222	1729	1098	312	313	6	0	0

- Molecule 3 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	92	752	487	122	141	2	0	0

- Molecule 4 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	121	875	551	153	169	2	0	0

- Molecule 5 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	117	916	583	171	155	7	0	0

- Molecule 6 is a protein called 40S ribosomal protein S16-A.

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

- Molecule 7 is a protein called 40S ribosomal protein S17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	121	Total	C	N	O	S	0	0
			948	596	179	171	2		

- Molecule 8 is a protein called 40S ribosomal protein S18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	145	Total	C	N	O	S	0	0
			1188	741	237	208	2		

- Molecule 9 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 10 is a protein called RPS20 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	100	Total	C	N	O	S	0	0
			797	506	144	146	1		

- Molecule 11 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	82	Total	C	N	O	0	0
			651	416	123	112		

- Molecule 12 is a protein called RPS28A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	63	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 13 is a protein called RPS29A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	53	Total	C	N	O	S	0	0
			442	274	92	72	4		

- Molecule 14 is a protein called 40S ribosomal protein S31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	73	Total	C	N	O	S	0	0
			556	352	105	95	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	97	ALA	LYS	conflict	UNP P05759

- Molecule 15 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	312	Total	C	N	O	S	0	0
			2383	1514	409	452	8		

- Molecule 16 is a protein called 40S ribosomal protein S0-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	206	Total	C	N	O	S	0	0
			1603	1030	284	287	2		

- Molecule 17 is a protein called 40S ribosomal protein S1-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	226	Total	C	N	O	S	0	0
			1798	1139	330	325	4		

- Molecule 18 is a protein called RPS2 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	216	Total	C	N	O	S	0	0
			1626	1042	287	295	2		

- Molecule 19 is a protein called 40S ribosomal protein S4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	258	Total	C	N	O	S	0	0
			2056	1308	387	358	3		

- Molecule 20 is a protein called 40S ribosomal protein S6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	228	Total	C	N	O	S	0	0
			1815	1138	351	323	3		

- Molecule 21 is a protein called 40S ribosomal protein S7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	184	Total	C	N	O	0	0
			1473	946	263	264		

- Molecule 22 is a protein called 40S ribosomal protein S8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	187	Total	C	N	O	S	0	0
			1476	916	295	263	2		

- Molecule 23 is a protein called 40S ribosomal protein S9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	184	Total	C	N	O	S	0	0
			1479	935	285	258	1		

- Molecule 24 is a protein called 40S ribosomal protein S11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	142	Total	C	N	O	S	0	0
			1142	733	217	189	3		

- Molecule 25 is a protein called 40S ribosomal protein S13.

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

- Molecule 26 is a protein called 40S ribosomal protein S14-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	127	Total	C	N	O	S	0	0
			923	568	185	167	3		

- Molecule 27 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	AA	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 29 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 30 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 31 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	AC	99	Total	C	N	O	S	0	0
			766	478	154	132	2		

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BC	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 33 is a RNA chain called 18S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	2	1771	Total	C	N	O	P	0	0
			37739	16872	6683	12413	1771		

- Molecule 34 is a protein called 40S ribosomal protein S21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	87	Total	C	N	O	S	0	0
			673	415	125	131	2		

- Molecule 35 is a protein called RPS22A isoform 1.

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

- Molecule 36 is a protein called 40S ribosomal protein S23-A.

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

- Molecule 37 is a protein called 40S ribosomal protein S24-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	d	134	Total	C	N	O	0	0
			1032	651	195	186		

- Molecule 38 is a protein called RPS26B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	97	Total	C	N	O	S	0	0
			765	473	160	127	5		

- Molecule 39 is a protein called 40S ribosomal protein S27-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	60	Total	C	N	O	S	0	0
			472	298	97	76	1		

- Molecule 41 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	3299	Total	C	N	O	P	0	0
			70544	31506	12682	23057	3299		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	?	-	G	deletion	GB 1262303
BQ	1962	A	G	conflict	GB 1262303

- Molecule 42 is a RNA chain called 5S rRNA.

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

- Molecule 43 is a RNA chain called 5.8S rRNA.

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

- Molecule 44 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AW	251	Total	C	N	O	S	0	0
			1899	1182	385	331	1		

- Molecule 45 is a protein called RPL4A isoform 1.

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

- Molecule 46 is a protein called RPL5 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BI	294	Total	C	N	O	S	0	0
			2351	1484	410	455	2		

- Molecule 47 is a protein called 60S ribosomal protein L6-B.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	BM	167	Total 1307	C 843	N 234	O 230	0	0

- Molecule 48 is a protein called 60S ribosomal protein L7-A.

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

- Molecule 49 is a protein called RPL9A isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	AD	191	Total 1508	C 957	N 274	O 273	S 4	0	0

- Molecule 50 is a protein called RPL10 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BD	218	Total 1764	C 1117	N 334	O 306	S 7	0	0

- Molecule 51 is a protein called RPL11B isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AG	169	Total 1346	C 843	N 252	O 247	S 4	0	0

- Molecule 52 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 53 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 54 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 55 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 56 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	AX	183	Total	C	N	O	0	0
			1416	879	284	253		

- Molecule 57 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	BF	188	Total	C	N	O	0	0
			1515	932	323	260		

- Molecule 58 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	BH	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 59 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	BJ	159	Total	C	N	O	S	0	0
			1272	802	245	221	4		

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

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

- Molecule 61 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	AE	126	Total	C	N	O	S	0	0
			836	525	165	145	1		

- Molecule 62 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	AH	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 63 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
63	AK	125	Total	C	N	O	0	0
			984	620	191	173		

- Molecule 64 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	AN	135	Total	C	N	O	0	0
			1080	701	199	180		

- Molecule 65 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	AR	148	Total	C	N	O	S	0	0
			1169	747	231	188	3		

- Molecule 66 is a protein called 60S ribosomal protein L29.

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

- Molecule 67 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AY	96	Total	C	N	O	S	0	0
			737	476	123	137	1		

- Molecule 68 is a protein called RPL32 isoform 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	BG	127	Total	C	N	O	S	0	0
			1017	644	205	167	1		

- Molecule 69 is a protein called 60S ribosomal protein L33-A.

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

- Molecule 70 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 71 is a protein called 60S ribosomal protein L35-A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
72	AF	81	Total	C	N	O	S	0	0
			645	393	141	106	5		

- Molecule 73 is a protein called RPL38 isoform 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
73	AI	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 60S ribosomal protein L40-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	AO	52	Total	C	N	O	S	0	0
			410	254	86	65	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
76	AS	25	Total	C	N	O	S	0	0
			229	139	62	27	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
77	AP	103	Total	C	N	O	S	0	0
			824	517	167	135	5		

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

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

- Molecule 79 is a protein called Methionine aminopeptidase 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	x	367	Total	C	N	O	S	0	0
			2899	1825	504	549	21		

- Molecule 80 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
80	BT	217	Total	C	N	O	0	0
			1075	641	217	217		

- Molecule 81 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
81	M	1	Total	Zn	0
			1	1	
81	N	1	Total	Zn	0
			1	1	
81	BN	1	Total	Zn	0
			1	1	

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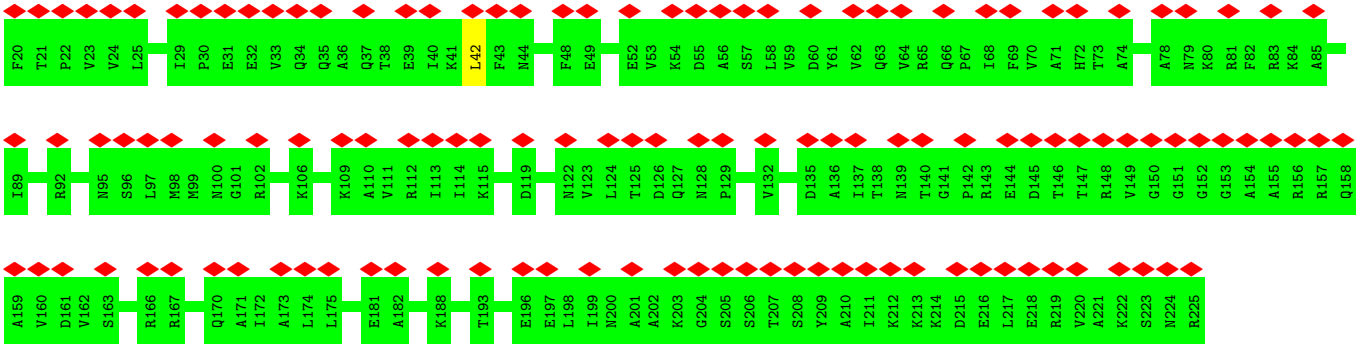
Mol	Chain	Residues	Atoms	AltConf
81	AF	1	Total Zn 1 1	0
81	AO	1	Total Zn 1 1	0
81	AP	1	Total Zn 1 1	0
81	AT	1	Total Zn 1 1	0

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.

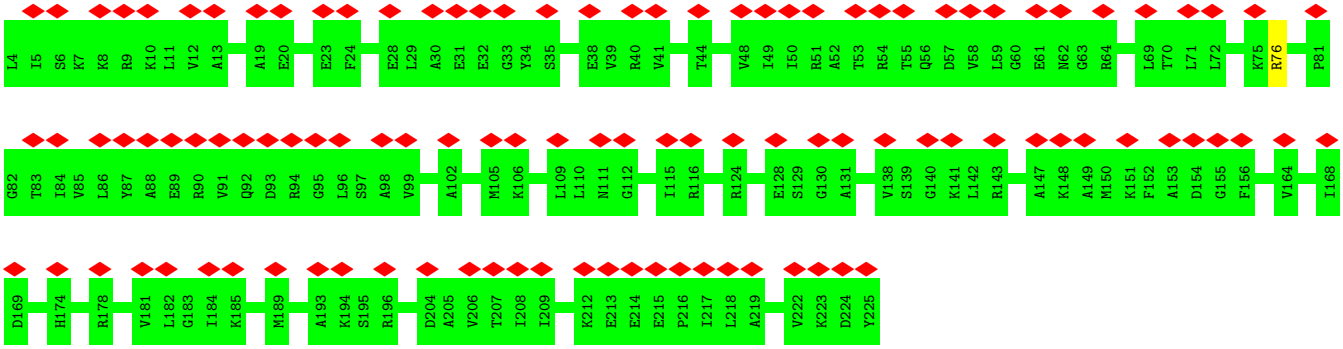
• Molecule 1: Rps5p

Chain B:



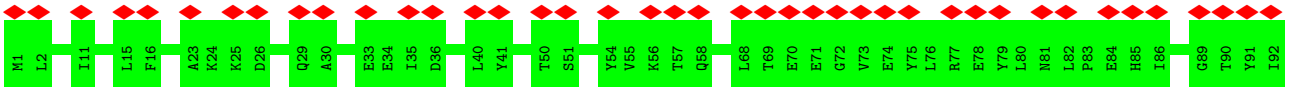
• Molecule 2: RPS3 isoform 1

Chain A:



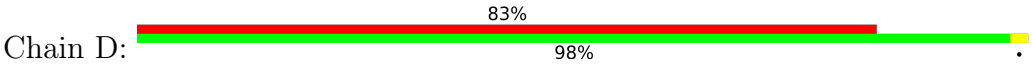
• Molecule 3: 40S ribosomal protein S10-A

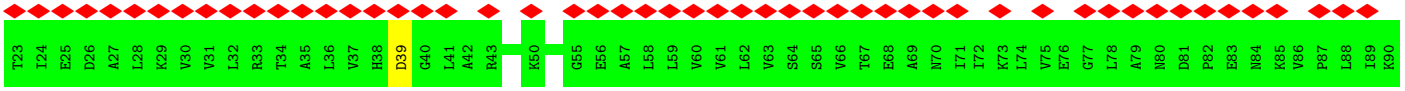
Chain C:

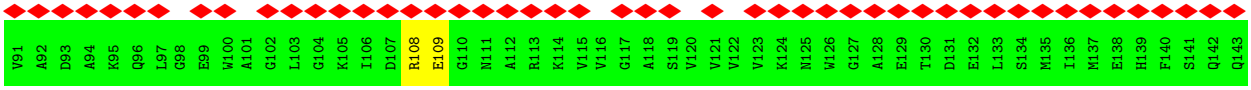


• Molecule 4: 40S ribosomal protein S12

Chain D:

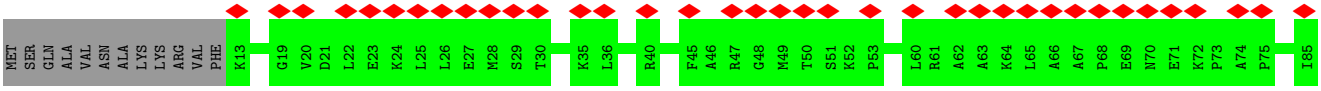


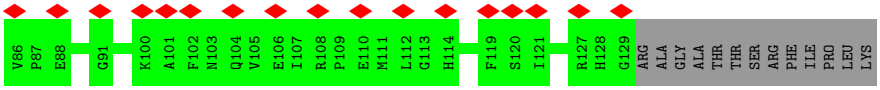




• Molecule 5: 40S ribosomal protein S15

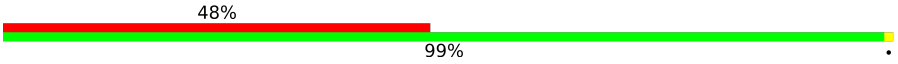
Chain E:

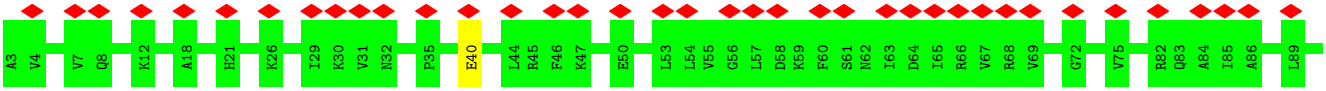


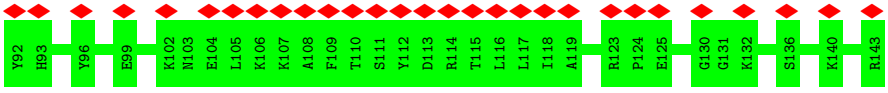


• Molecule 6: 40S ribosomal protein S16-A

Chain F:

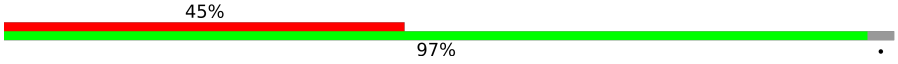


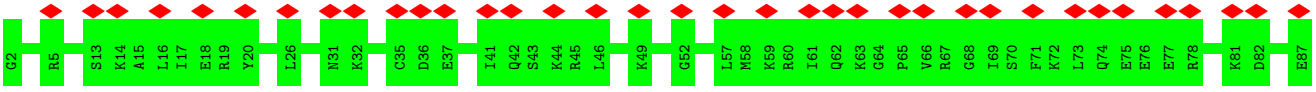


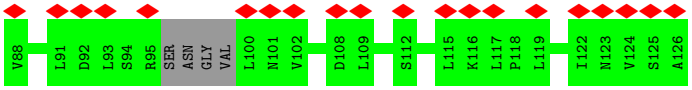


• Molecule 7: 40S ribosomal protein S17-A

Chain G:

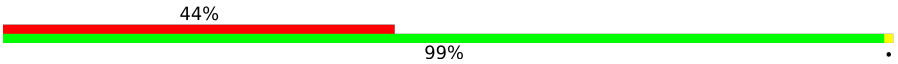


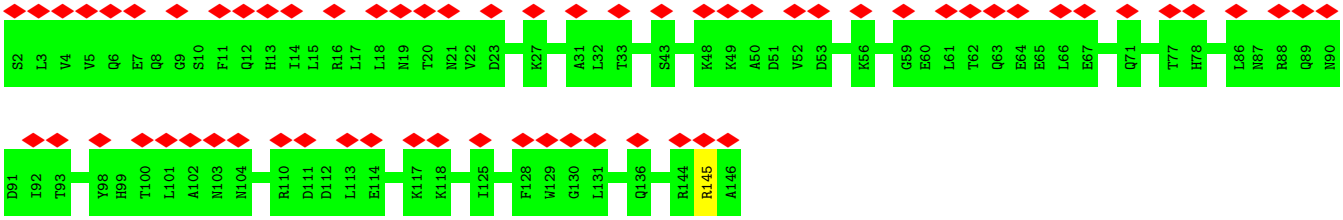




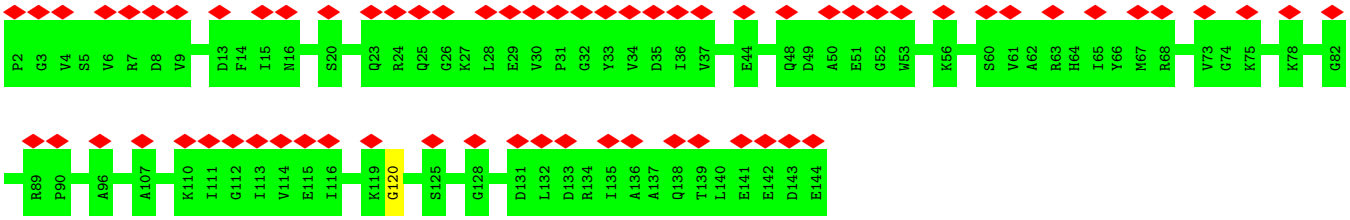
• Molecule 8: 40S ribosomal protein S18-A

Chain H:

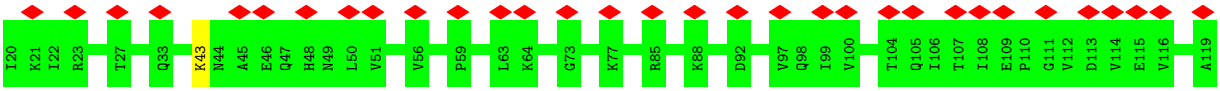




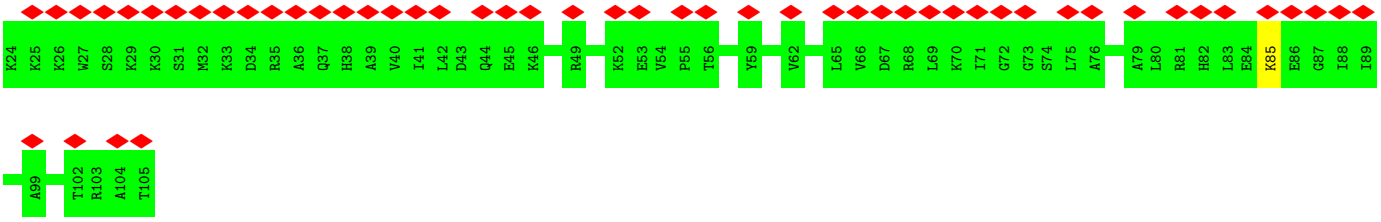
• Molecule 9: 40S ribosomal protein S19-A



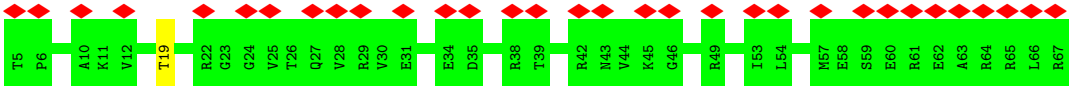
• Molecule 10: RPS20 isoform 1



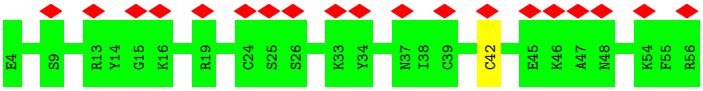
• Molecule 11: 40S ribosomal protein S25



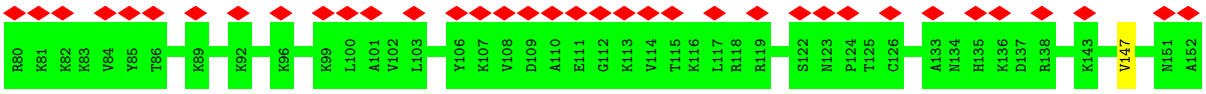
• Molecule 12: RPS28A isoform 1



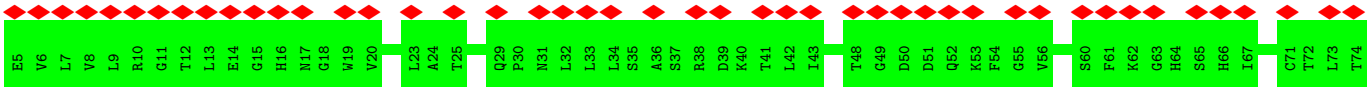
• Molecule 13: RPS29A isoform 1

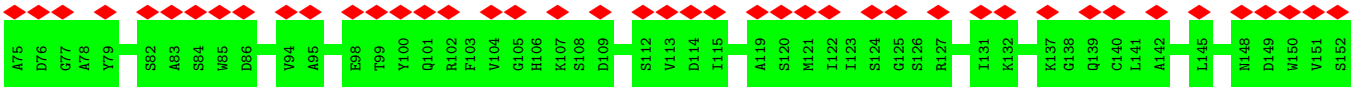


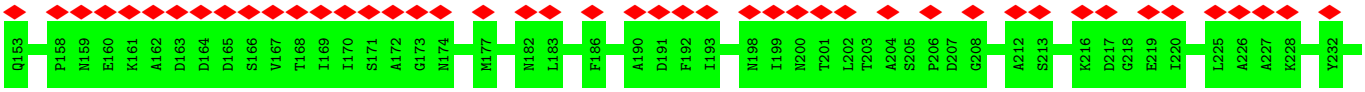
• Molecule 14: 40S ribosomal protein S31

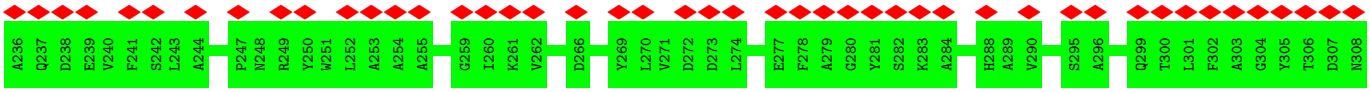


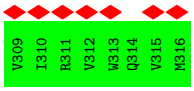
• Molecule 15: Guanine nucleotide-binding protein subunit beta-like protein



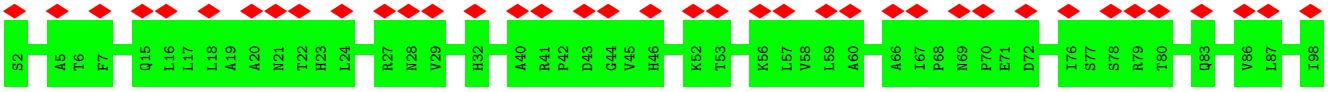


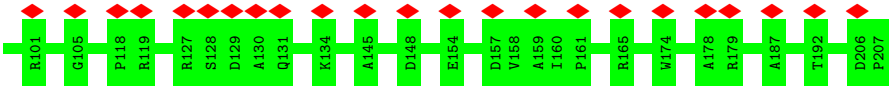




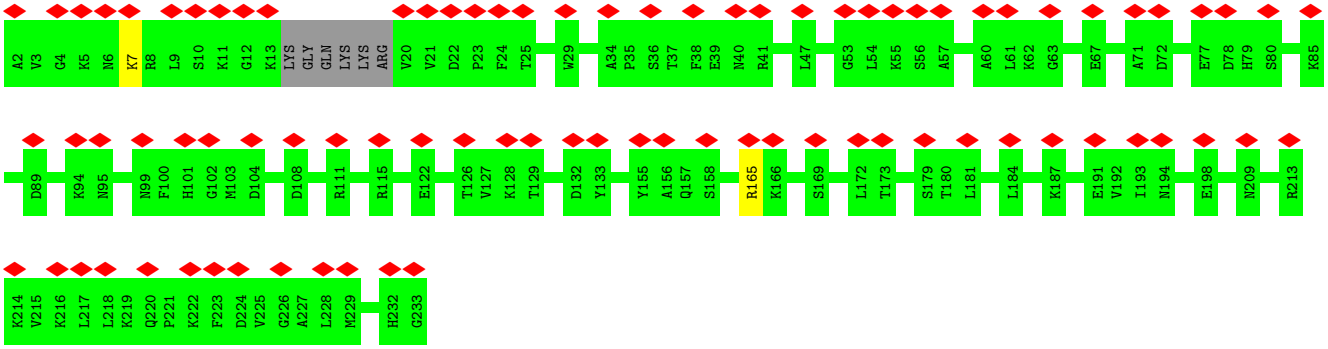


• Molecule 16: 40S ribosomal protein S0-A

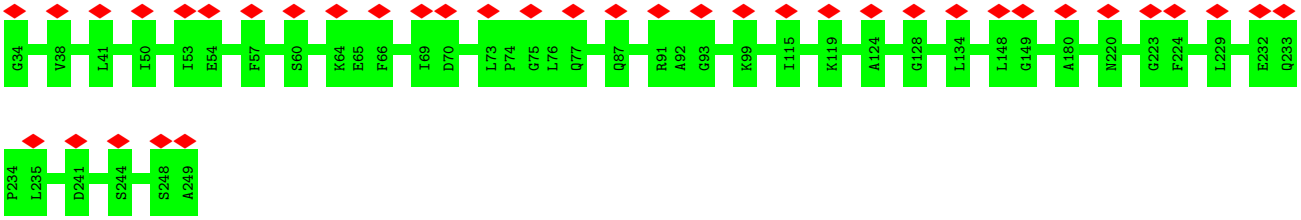




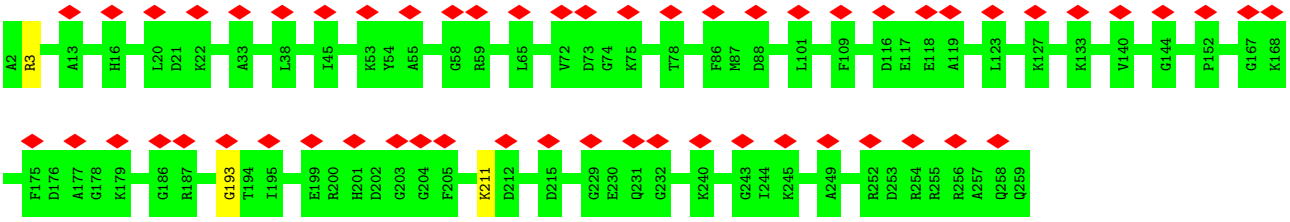
• Molecule 17: 40S ribosomal protein S1-A



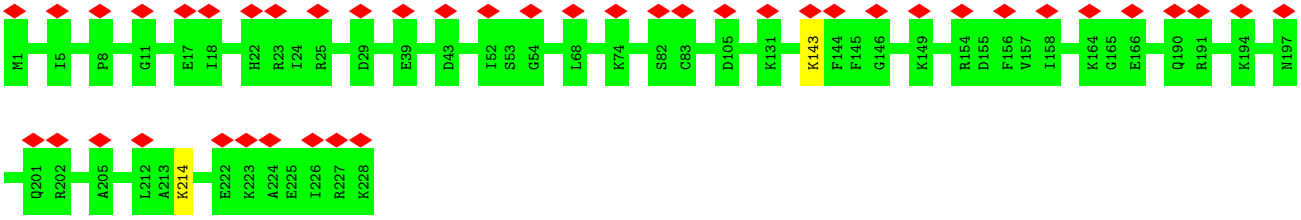
• Molecule 18: RPS2 isoform 1



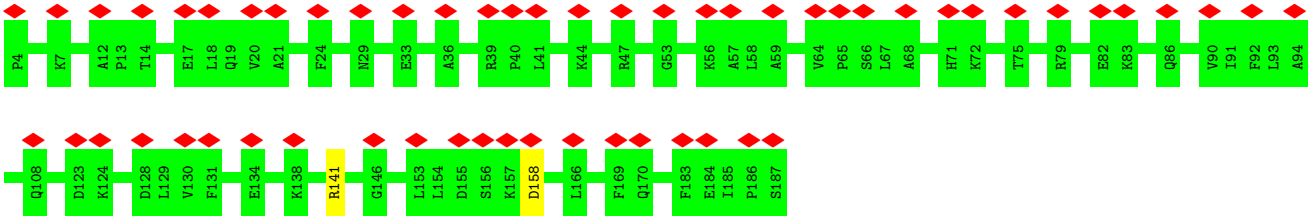
• Molecule 19: 40S ribosomal protein S4-A



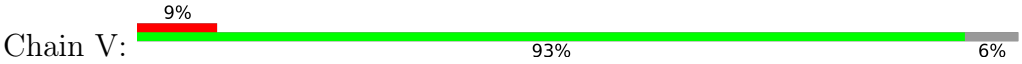
• Molecule 20: 40S ribosomal protein S6-A



• Molecule 21: 40S ribosomal protein S7-A



• Molecule 22: 40S ribosomal protein S8-B



• Molecule 23: 40S ribosomal protein S9-A

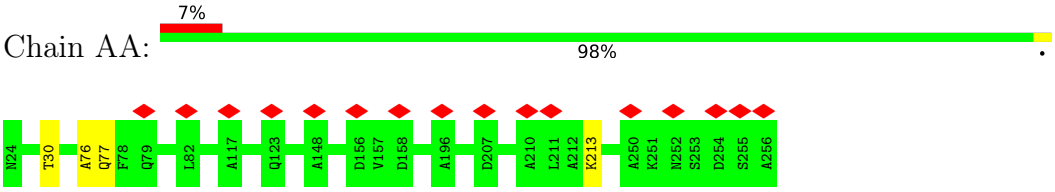
• Molecule 24: 40S ribosomal protein S11-A

• Molecule 25: 40S ribosomal protein S13

• Molecule 26: 40S ribosomal protein S14-B

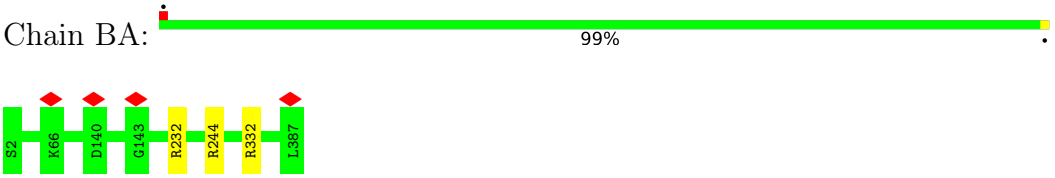
• Molecule 27: 60S ribosomal protein L8-A

Chain AA:



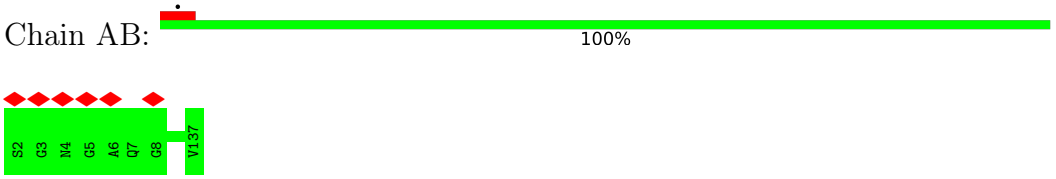
• Molecule 28: 60S ribosomal protein L3

Chain BA:



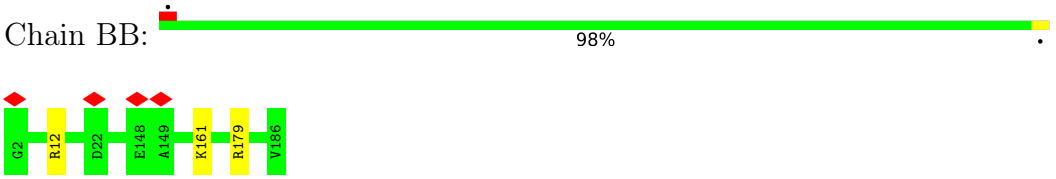
• Molecule 29: 60S ribosomal protein L23-A

Chain AB:



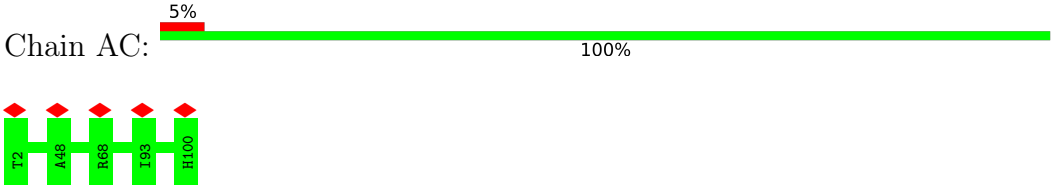
• Molecule 30: 60S ribosomal protein L18-A

Chain BB:



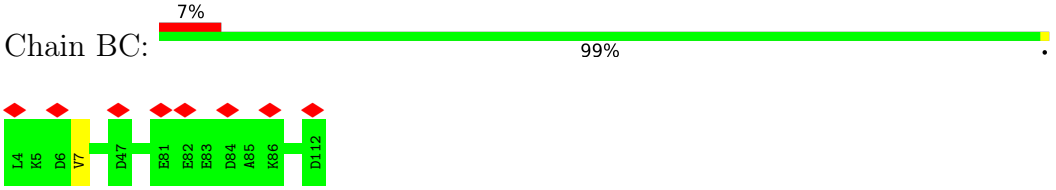
• Molecule 31: 60S ribosomal protein L36-A

Chain AC:



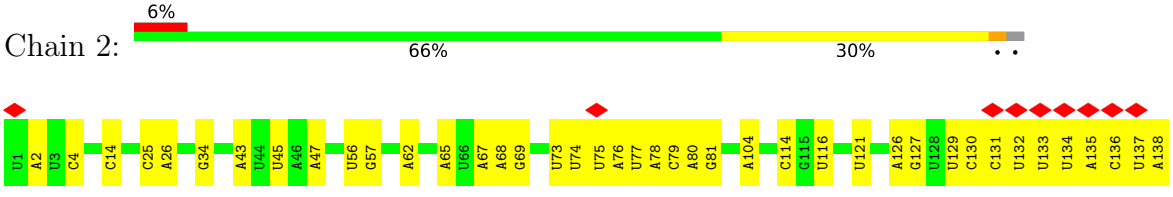
• Molecule 32: 60S ribosomal protein L31-A

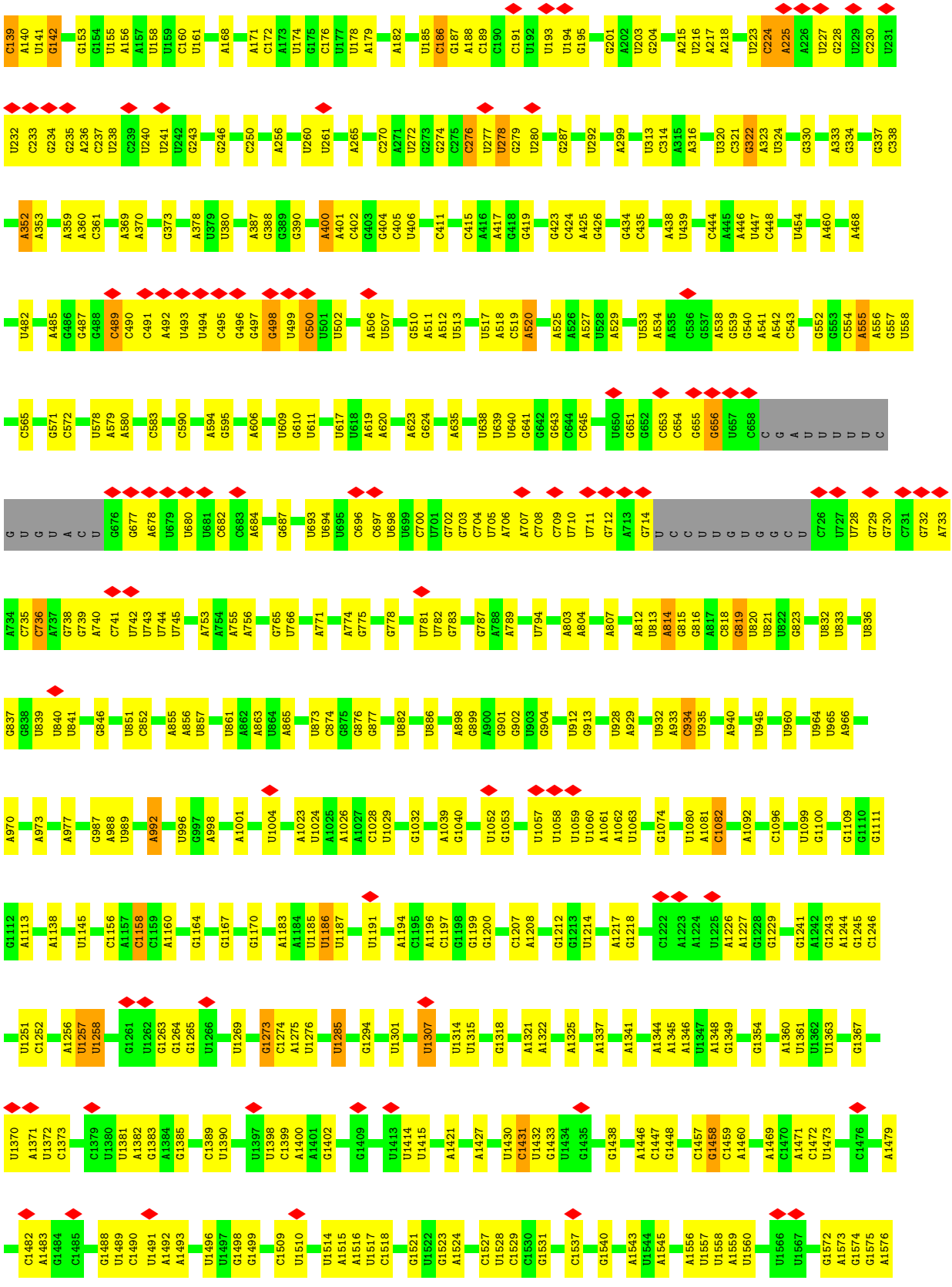
Chain BC:

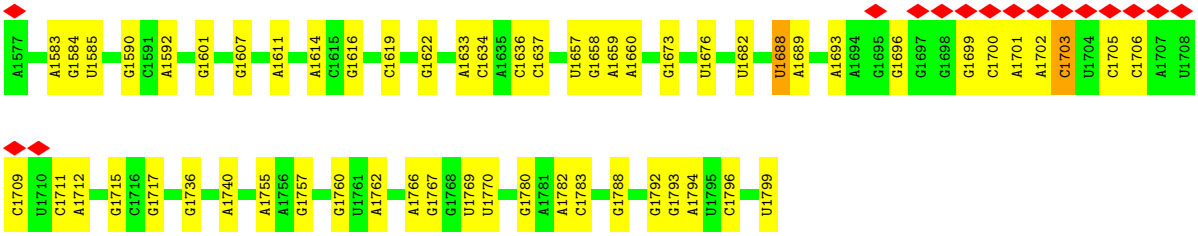


• Molecule 33: 18S rRNA

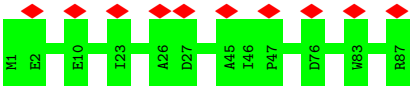
Chain 2:



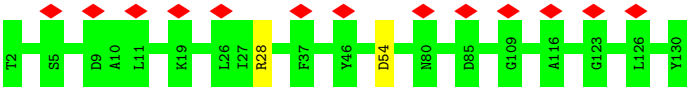




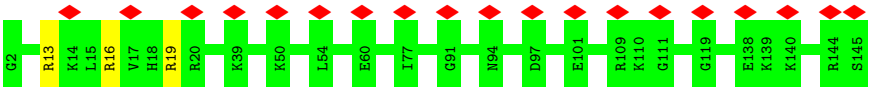
• Molecule 34: 40S ribosomal protein S21-A



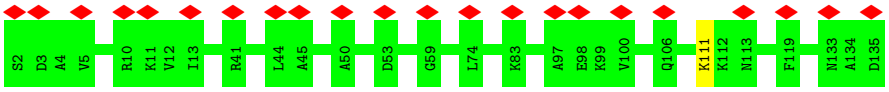
• Molecule 35: RPS22A isoform 1



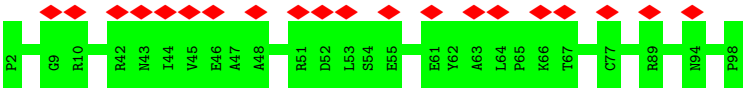
• Molecule 36: 40S ribosomal protein S23-A



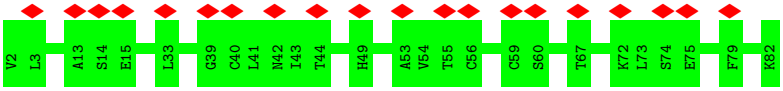
• Molecule 37: 40S ribosomal protein S24-A



• Molecule 38: RPS26B isoform 1

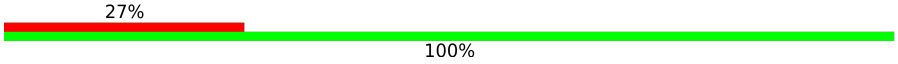


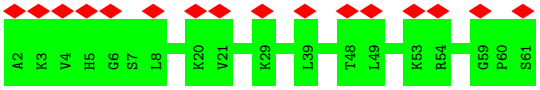
• Molecule 39: 40S ribosomal protein S27-A



• Molecule 40: 40S ribosomal protein S30-A

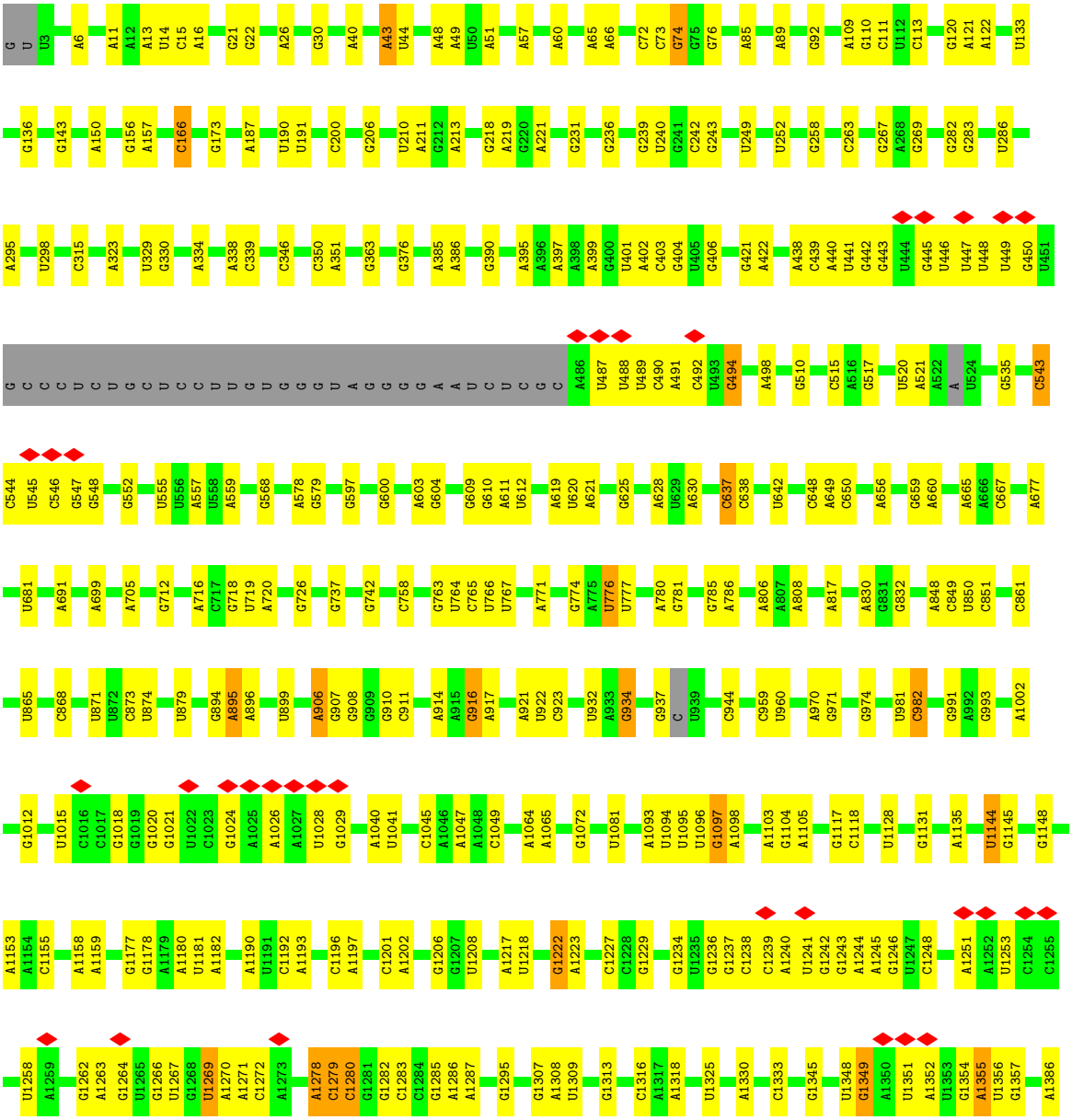
Chain g:

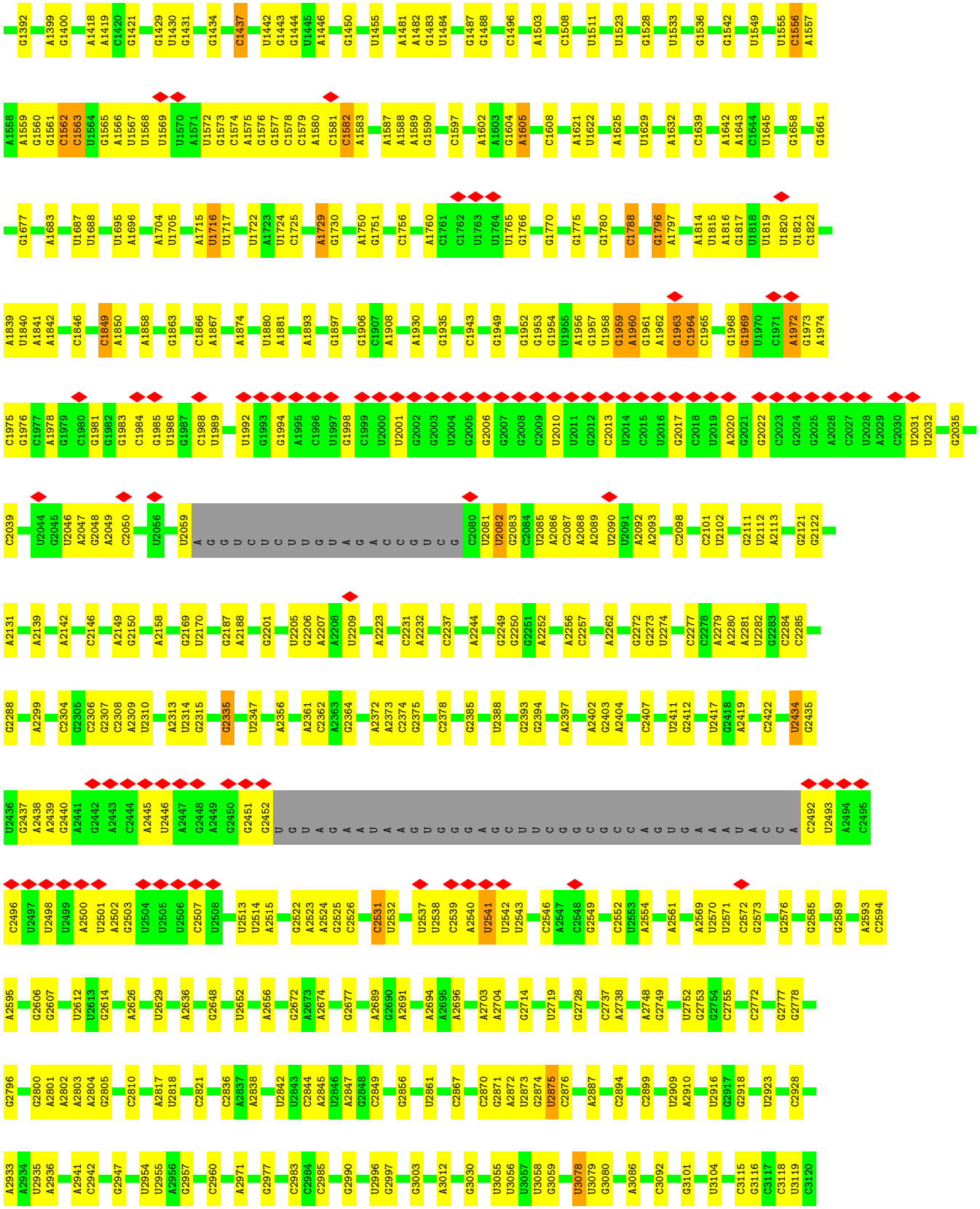


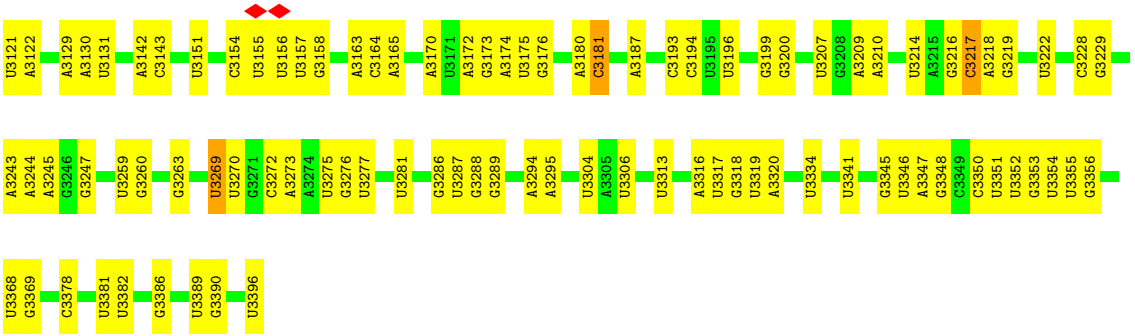


• Molecule 41: 25S rRNA

Chain BQ:

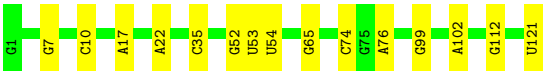






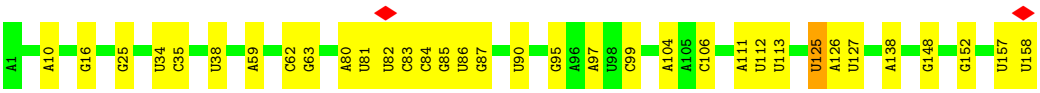
• Molecule 42: 5S rRNA

Chain BR:



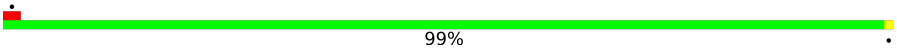
• Molecule 43: 5.8S rRNA

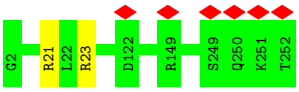
Chain BS:



• Molecule 44: 60S ribosomal protein L2-A

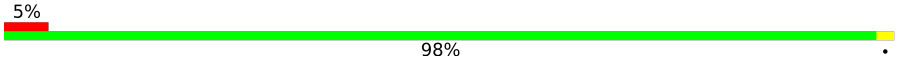
Chain AW:

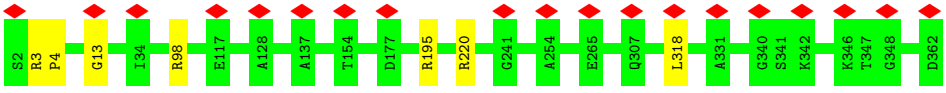




• Molecule 45: RPL4A isoform 1

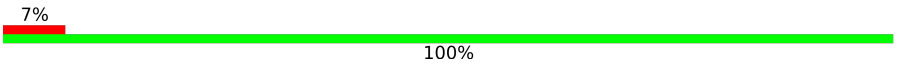
Chain BE:

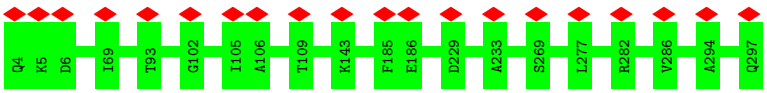




• Molecule 46: RPL5 isoform 1

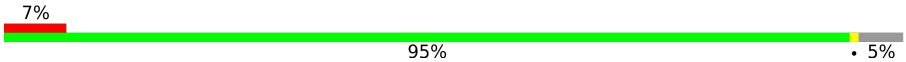
Chain BI:

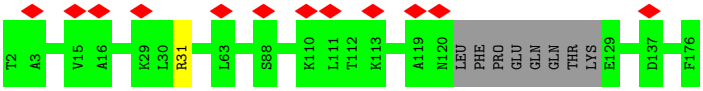




• Molecule 47: 60S ribosomal protein L6-B

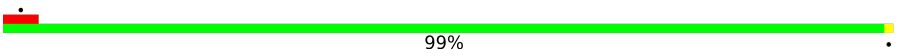
Chain BM:

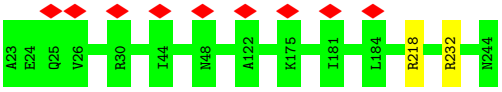




• Molecule 48: 60S ribosomal protein L7-A

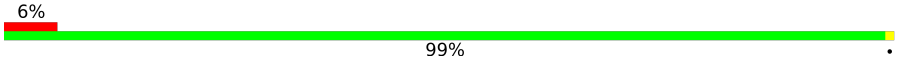
Chain BO:

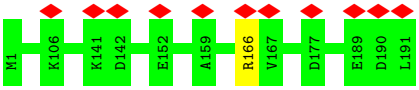




• Molecule 49: RPL9A isoform 1

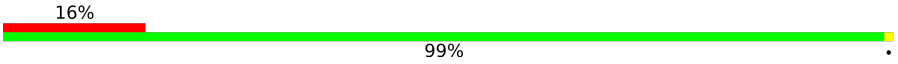
Chain AD:

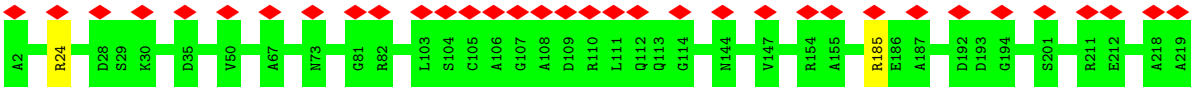




• Molecule 50: RPL10 isoform 1

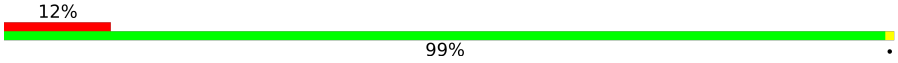
Chain BD:

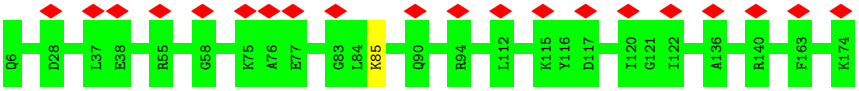




• Molecule 51: RPL11B isoform 1

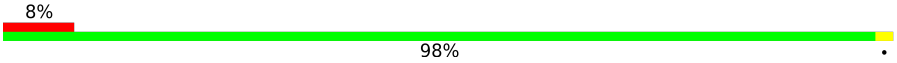
Chain AG:

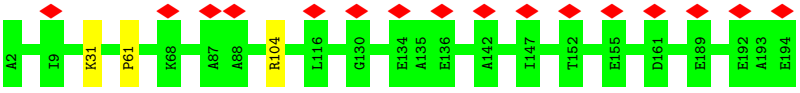




• Molecule 52: 60S ribosomal protein L13-A

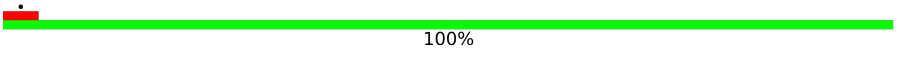
Chain AJ:

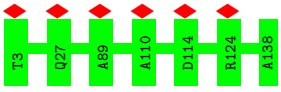




• Molecule 53: 60S ribosomal protein L14-A

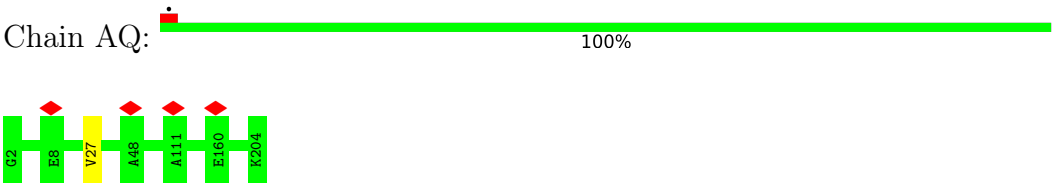
Chain AM:





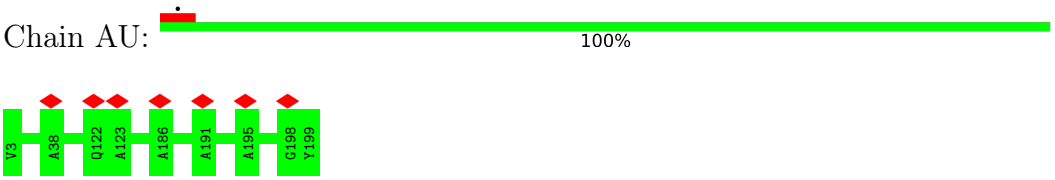
• Molecule 54: 60S ribosomal protein L15-A

Chain AQ:



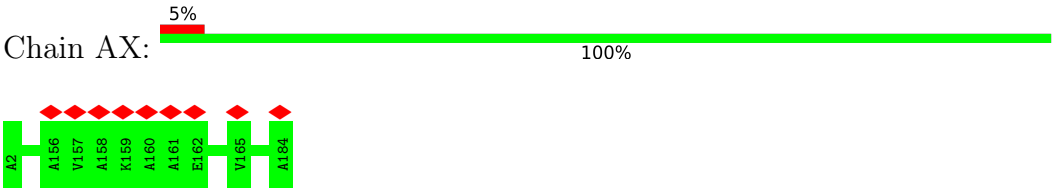
• Molecule 55: 60S ribosomal protein L16-A

Chain AU:



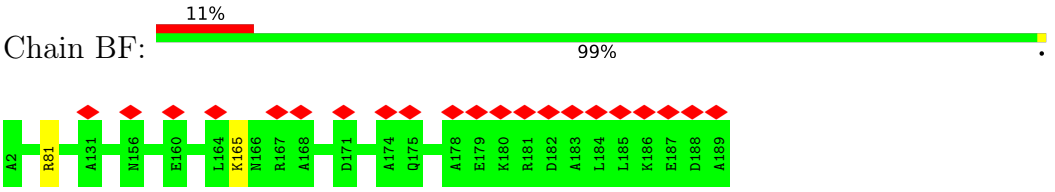
• Molecule 56: 60S ribosomal protein L17-A

Chain AX:



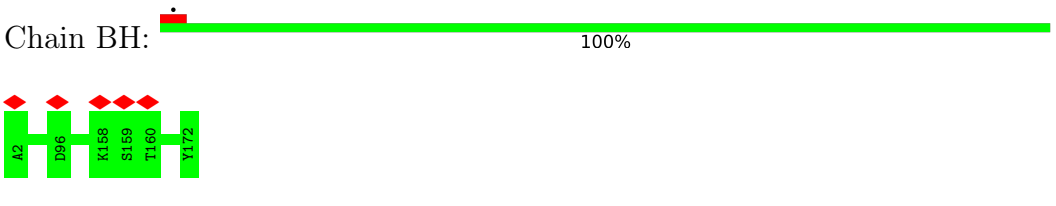
• Molecule 57: 60S ribosomal protein L19-A

Chain BF:



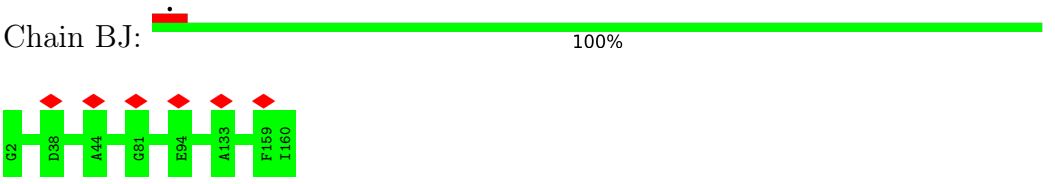
• Molecule 58: 60S ribosomal protein L20-A

Chain BH:



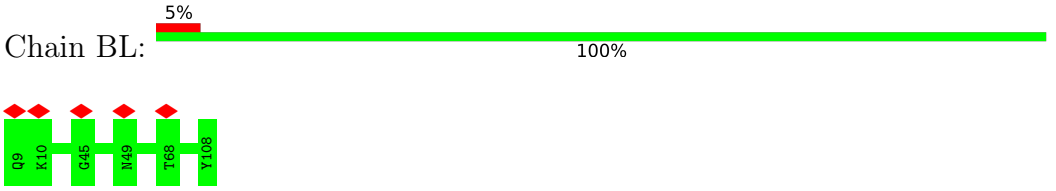
• Molecule 59: 60S ribosomal protein L21-A

Chain BJ:



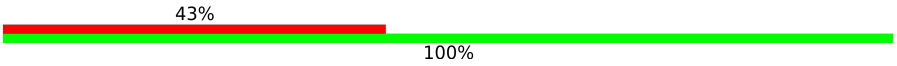
• Molecule 60: 60S ribosomal protein L22-A

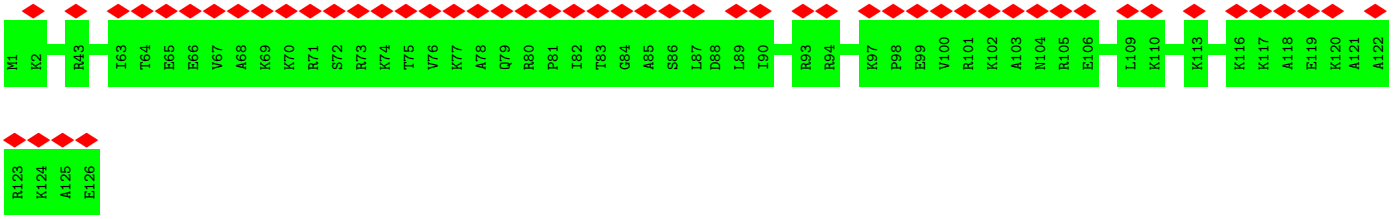
Chain BL:



• Molecule 61: 60S ribosomal protein L24-A

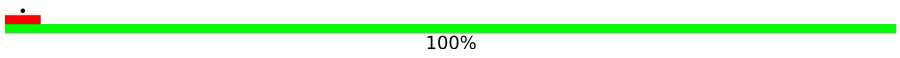
Chain AE:

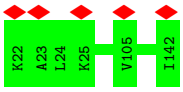




• Molecule 62: 60S ribosomal protein L25

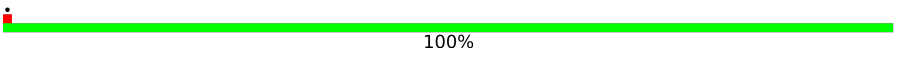
Chain AH:

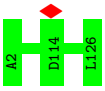




• Molecule 63: 60S ribosomal protein L26-A

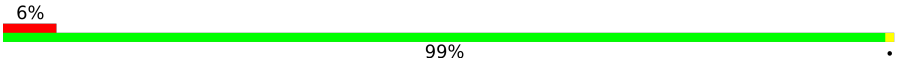
Chain AK:

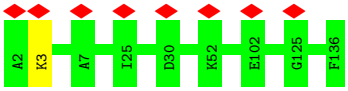




• Molecule 64: 60S ribosomal protein L27-A

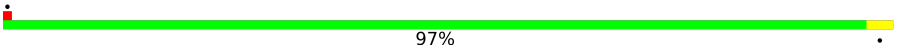
Chain AN:

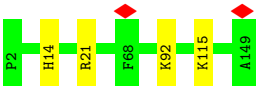




• Molecule 65: 60S ribosomal protein L28

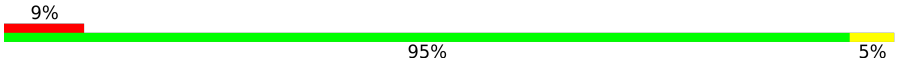
Chain AR:

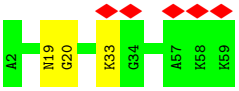




• Molecule 66: 60S ribosomal protein L29

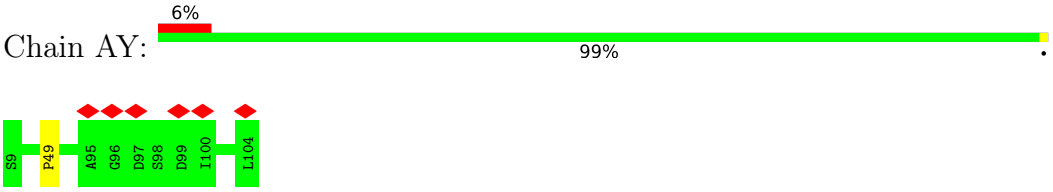
Chain AV:





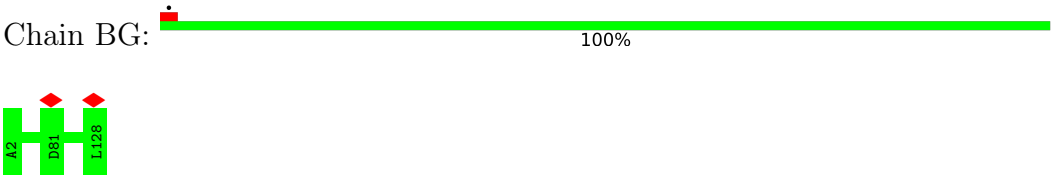
• Molecule 67: 60S ribosomal protein L30

Chain AY:



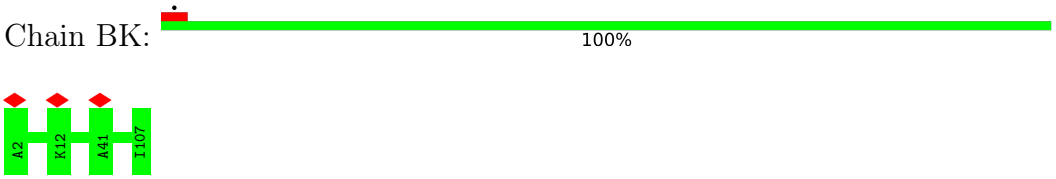
• Molecule 68: RPL32 isoform 1

Chain BG:



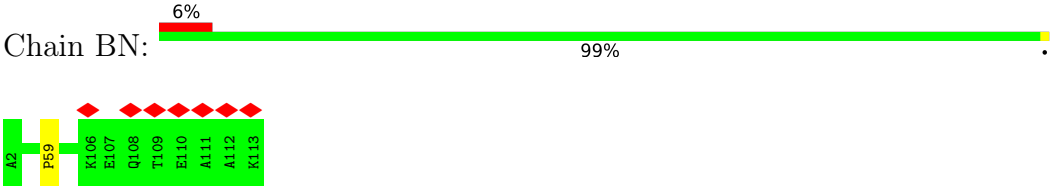
• Molecule 69: 60S ribosomal protein L33-A

Chain BK:



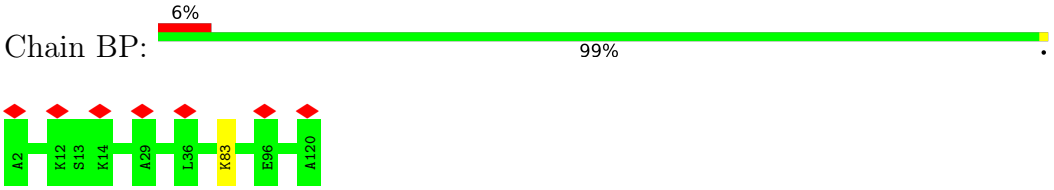
• Molecule 70: 60S ribosomal protein L34-A

Chain BN:



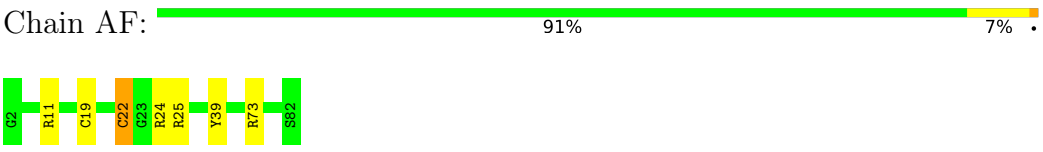
• Molecule 71: 60S ribosomal protein L35-A

Chain BP:



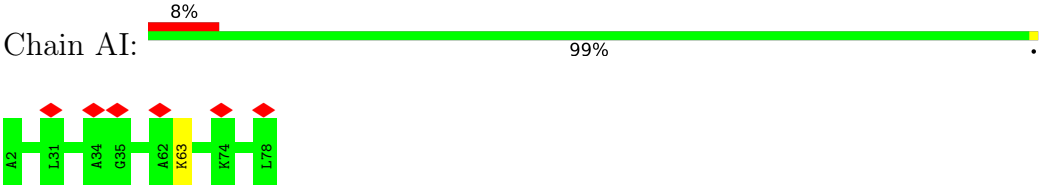
• Molecule 72: 60S ribosomal protein L37-A

Chain AF:



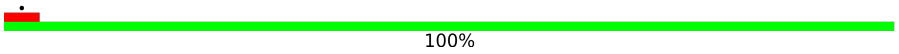
• Molecule 73: RPL38 isoform 1

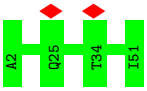
Chain AI:



• Molecule 74: 60S ribosomal protein L39

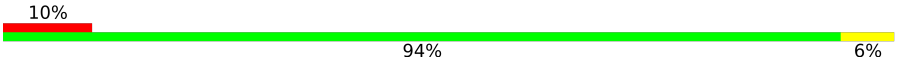
Chain AL:

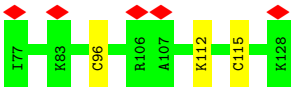




• Molecule 75: 60S ribosomal protein L40-A

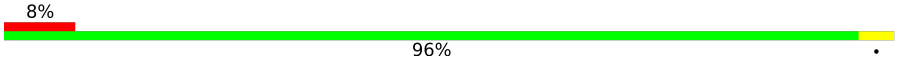
Chain AO:

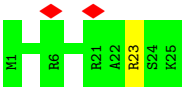




• Molecule 76: 60S ribosomal protein L41

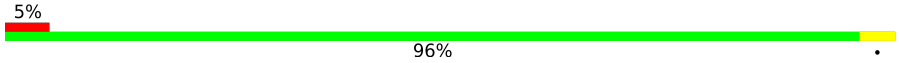
Chain AS:

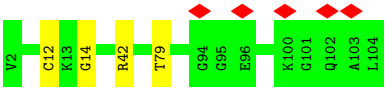




• Molecule 77: 60S ribosomal protein L42-A

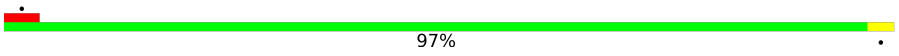
Chain AP:

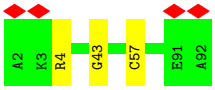




• Molecule 78: 60S ribosomal protein L43-A

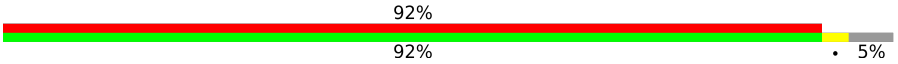
Chain AT:

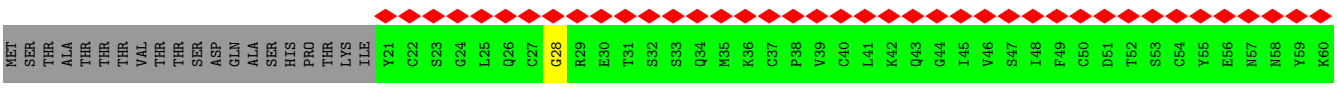


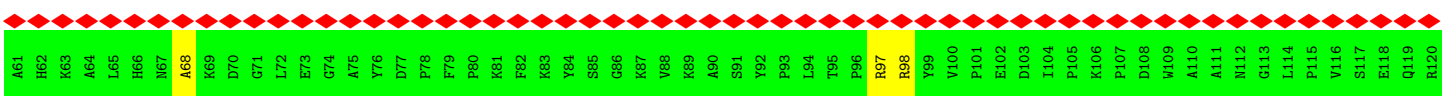


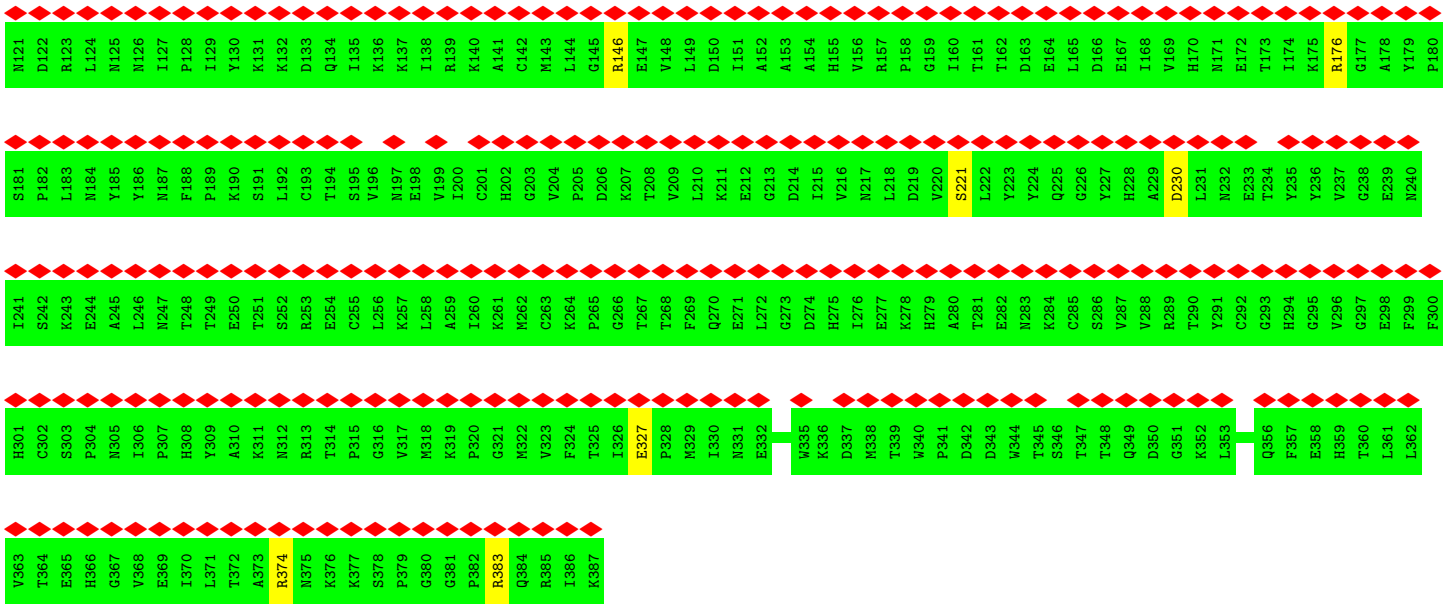
• Molecule 79: Methionine aminopeptidase 1

Chain x:



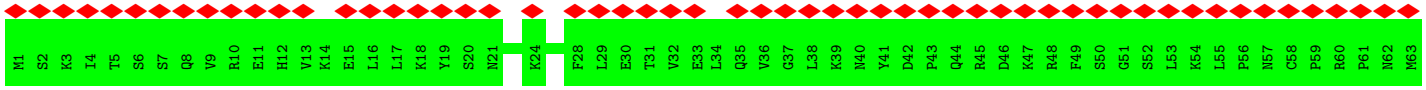


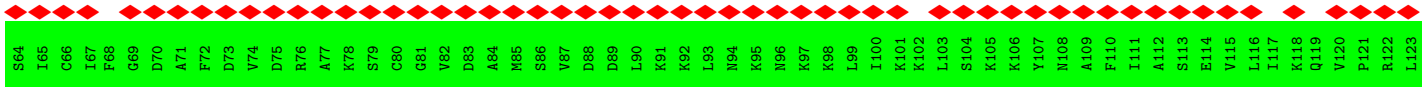


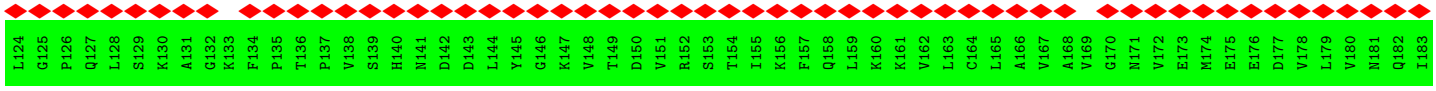


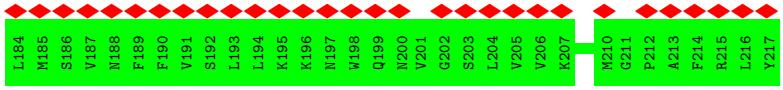
• Molecule 80: 60S ribosomal protein L1-A

Chain BT:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	11938	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 ($e^-/Å^2$)	56.16	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.094	Depositor
Minimum map value	-0.045	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.015	Depositor
Map size (Å)	455.28, 455.28, 455.28	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.084, 1.084, 1.084	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	B	0.34	0/1625	0.59	0/2197
2	A	0.38	0/1754	0.62	0/2361
3	C	0.36	0/769	0.54	0/1039
4	D	0.29	0/883	0.63	1/1199 (0.1%)
5	E	0.34	0/936	0.62	0/1259
6	F	0.41	0/1125	0.63	0/1510
7	G	0.35	0/957	0.58	0/1283
8	H	0.33	0/1207	0.59	0/1623
9	I	0.36	0/1130	0.61	0/1517
10	J	0.37	0/807	0.61	0/1091
11	K	0.32	0/661	0.62	0/888
12	L	0.37	0/493	0.73	0/663
13	M	0.43	0/452	0.64	0/600
14	N	0.33	0/567	0.66	0/764
15	O	0.32	0/2436	0.58	0/3318
16	P	0.36	0/1644	0.59	0/2249
17	Q	0.34	0/1823	0.66	1/2447 (0.0%)
18	R	0.44	0/1656	0.63	0/2251
19	S	0.38	0/2097	0.62	1/2823 (0.0%)
20	T	0.35	0/1839	0.65	0/2460
21	U	0.35	0/1498	0.68	2/2019 (0.1%)
22	V	0.42	0/1501	0.66	1/2006 (0.0%)
23	W	0.35	0/1504	0.67	0/2016
24	X	0.47	0/1168	0.62	0/1575
25	Y	0.42	0/1215	0.67	0/1638
26	Z	0.38	0/934	0.67	0/1257
27	AA	0.49	0/1836	0.58	0/2481
28	BA	0.61	0/3146	0.69	2/4228 (0.0%)
29	AB	0.59	0/1018	0.65	0/1369
30	BB	0.57	0/1465	0.73	2/1965 (0.1%)
31	AC	0.44	0/772	0.66	0/1026
32	BC	0.59	0/890	0.69	0/1196

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	2	0.71	0/42211	1.07	106/65773 (0.2%)
34	a	0.36	0/682	0.63	0/921
35	b	0.42	0/1038	0.64	1/1395 (0.1%)
36	c	0.47	0/1139	0.72	3/1518 (0.2%)
37	d	0.34	0/1046	0.58	0/1401
38	e	0.43	0/778	0.69	0/1042
39	f	0.33	0/620	0.63	0/838
40	g	0.35	0/480	0.67	0/639
41	BQ	1.05	1/78951 (0.0%)	1.13	232/123085 (0.2%)
42	BR	0.80	0/2883	1.01	0/4491
43	BS	1.08	0/3746	1.12	7/5832 (0.1%)
44	AW	0.68	0/1933	0.74	2/2598 (0.1%)
45	BE	0.60	0/2800	0.70	3/3790 (0.1%)
46	BI	0.45	0/2400	0.60	0/3239
47	BM	0.48	0/1329	0.66	2/1794 (0.1%)
48	BO	0.62	0/1821	0.65	1/2451 (0.0%)
49	AD	0.47	0/1529	0.62	1/2060 (0.0%)
50	BD	0.49	0/1801	0.68	1/2416 (0.0%)
51	AG	0.39	0/1367	0.62	0/1834
52	AJ	0.57	0/1568	0.71	0/2106
53	AM	0.46	0/1068	0.64	0/1438
54	AQ	0.74	0/1757	0.77	0/2354
55	AU	0.63	0/1585	0.67	0/2128
56	AX	0.65	0/1439	0.69	0/1938
57	BF	0.52	0/1532	0.65	0/2043
58	BH	0.57	0/1473	0.67	0/1980
59	BJ	0.59	0/1296	0.62	0/1739
60	BL	0.44	0/812	0.59	0/1099
61	AE	0.48	0/850	0.58	0/1152
62	AH	0.57	0/979	0.62	0/1321
63	AK	0.51	0/995	0.62	0/1329
64	AN	0.49	0/1106	0.60	0/1485
65	AR	0.65	0/1200	0.70	1/1607 (0.1%)
66	AV	0.49	0/473	0.67	0/629
67	AY	0.48	0/745	0.60	0/1001
68	BG	0.61	0/1038	0.69	0/1390
69	BK	0.72	0/868	0.72	0/1168
70	BN	0.62	0/890	0.75	0/1189
71	BP	0.51	0/978	0.67	0/1301
72	AF	0.76	1/660 (0.2%)	0.92	5/875 (0.6%)
73	AI	0.42	0/618	0.61	0/826
74	AL	0.66	0/443	0.78	0/588
75	AO	0.59	0/416	0.80	0/553

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
76	AS	0.50	0/230	0.96	1/296 (0.3%)
77	AP	0.67	0/836	0.81	4/1104 (0.4%)
78	AT	0.66	0/701	0.77	0/934
79	x	0.64	0/2970	0.92	7/4023 (0.2%)
80	BT	0.33	0/1074	0.67	0/1496
All	All	0.79	2/220962 (0.0%)	0.96	387/324527 (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
1	B	0	1
4	D	0	1
6	F	0	1
9	I	0	1
12	L	0	1
14	N	0	1
19	S	0	1
26	Z	0	1
27	AA	0	3
30	BB	0	1
32	BC	0	1
35	b	0	1
45	BE	0	3
48	BO	0	1
65	AR	0	2
66	AV	0	2
71	BP	0	1
All	All	0	23

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
72	AF	39	TYR	C-N	6.08	1.45	1.34
41	BQ	2031	U	O3'-P	5.87	1.68	1.61

All (387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	814	A	N1-C6-N6	-11.43	111.75	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	1699	G	C5-C6-O6	11.24	135.34	128.60
33	2	1699	G	N1-C6-O6	-10.37	113.68	119.90
41	BQ	1144	U	C5-C4-O4	-9.58	120.15	125.90
33	2	533	U	N3-C2-O2	-9.57	115.50	122.20
33	2	1703	C	N3-C4-N4	-9.54	111.32	118.00
33	2	1706	C	N3-C2-O2	-9.43	115.30	121.90
79	x	374	ARG	NE-CZ-NH1	9.28	124.94	120.30
41	BQ	1960	A	N9-C1'-C2'	-9.02	102.08	112.00
41	BQ	2737	C	N1-C2-O2	8.98	124.29	118.90
41	BQ	1562	C	N1-C2-O2	8.96	124.28	118.90
41	BQ	3348	G	C5-C6-O6	8.96	133.98	128.60
43	BS	125	U	C2-N1-C1'	8.94	128.42	117.70
33	2	934	C	C2-N1-C1'	8.91	128.60	118.80
41	BQ	74	G	C5-C6-O6	-8.85	123.29	128.60
41	BQ	2492	C	C2-N1-C1'	8.76	128.43	118.80
41	BQ	1563	C	N3-C2-O2	-8.75	115.78	121.90
41	BQ	637	C	C6-N1-C2	-8.73	116.81	120.30
33	2	520	A	N1-C6-N6	-8.71	113.37	118.60
41	BQ	2737	C	N3-C2-O2	-8.60	115.88	121.90
41	BQ	1974	A	N1-C6-N6	-8.52	113.49	118.60
41	BQ	2407	C	C6-N1-C2	-8.47	116.91	120.30
33	2	490	C	N3-C2-O2	-8.44	115.99	121.90
41	BQ	1280	C	N3-C2-O2	-8.38	116.03	121.90
41	BQ	3217	C	N1-C2-O2	8.37	123.92	118.90
33	2	736	C	N3-C2-O2	-8.34	116.06	121.90
41	BQ	1959	G	P-O3'-C3'	8.21	129.55	119.70
41	BQ	3193	C	N3-C2-O2	-7.99	116.31	121.90
41	BQ	1144	U	N3-C4-O4	7.94	124.96	119.40
33	2	1509	C	N3-C2-O2	-7.71	116.50	121.90
41	BQ	406	G	O4'-C1'-N9	7.69	114.35	108.20
33	2	276	C	N3-C2-O2	-7.59	116.58	121.90
33	2	292	U	C5-C4-O4	-7.59	121.34	125.90
33	2	1703	C	N3-C4-C5	7.56	124.92	121.90
79	x	146	ARG	NE-CZ-NH1	7.50	124.05	120.30
41	BQ	2407	C	C5-C6-N1	7.46	124.73	121.00
41	BQ	3200	G	N3-C4-N9	-7.39	121.56	126.00
41	BQ	3217	C	C2-N1-C1'	7.34	126.88	118.80
41	BQ	2492	C	N1-C2-O2	7.33	123.30	118.90
41	BQ	1968	G	N3-C2-N2	-7.28	114.81	119.90
41	BQ	2083	G	C5-C6-N1	7.23	115.11	111.50
41	BQ	1579	C	N3-C2-O2	-7.22	116.85	121.90
41	BQ	3348	G	N1-C6-O6	-7.18	115.59	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BQ	1788	C	N1-C2-O2	7.14	123.18	118.90
41	BQ	2046	U	N1-C2-N3	7.12	119.17	114.90
33	2	1431	C	N3-C4-N4	-7.11	113.03	118.00
41	BQ	1283	C	N3-C2-O2	-7.08	116.94	121.90
41	BQ	1562	C	N3-C2-O2	-7.08	116.95	121.90
41	BQ	1496	C	C6-N1-C2	-7.02	117.49	120.30
33	2	533	U	N1-C2-N3	7.01	119.11	114.90
33	2	583	C	C6-N1-C2	-6.99	117.50	120.30
41	BQ	1788	C	N3-C2-O2	-6.99	117.01	121.90
43	BS	125	U	N1-C2-O2	6.96	127.67	122.80
33	2	1706	C	N1-C2-O2	6.93	123.06	118.90
33	2	400	A	P-O3'-C3'	6.93	128.02	119.70
33	2	1186	U	C5-C4-O4	-6.91	121.75	125.90
41	BQ	3181	C	N1-C2-O2	6.88	123.03	118.90
41	BQ	922	U	C2-N1-C1'	6.84	125.90	117.70
41	BQ	3163	A	C5-C6-N6	-6.81	118.25	123.70
41	BQ	2304	C	N1-C2-O2	6.81	122.98	118.90
33	2	965	U	C2-N1-C1'	6.79	125.85	117.70
79	x	383	ARG	NE-CZ-NH1	6.79	123.69	120.30
33	2	1389	C	C2-N1-C1'	6.78	126.26	118.80
41	BQ	1978	A	C5-C6-N1	6.78	121.09	117.70
41	BQ	776	U	O4'-C1'-N1	6.76	113.61	108.20
41	BQ	2142	A	C5-C6-N6	-6.71	118.33	123.70
41	BQ	1974	A	C5-C6-N1	6.70	121.05	117.70
41	BQ	1968	G	N9-C4-C5	6.69	108.08	105.40
41	BQ	1222	G	O4'-C1'-N9	6.67	113.53	108.20
33	2	186	C	C2-N1-C1'	6.65	126.11	118.80
43	BS	125	U	N3-C2-O2	-6.65	117.55	122.20
41	BQ	628	A	C4-C5-N7	6.65	114.02	110.70
41	BQ	1969	G	C5'-C4'-O4'	6.63	117.06	109.10
41	BQ	1556	C	C6-N1-C2	-6.58	117.67	120.30
41	BQ	1563	C	C6-N1-C2	-6.54	117.69	120.30
41	BQ	2492	C	N3-C2-O2	-6.51	117.34	121.90
33	2	1688	U	C5-C4-O4	6.51	129.81	125.90
33	2	490	C	C6-N1-C2	-6.51	117.70	120.30
41	BQ	1972	A	C4-C5-C6	-6.49	113.75	117.00
33	2	1458	G	C4-N9-C1'	6.49	134.94	126.50
33	2	934	C	C6-N1-C1'	-6.48	113.02	120.80
41	BQ	776	U	C6-N1-C2	-6.42	117.15	121.00
41	BQ	3194	C	N3-C2-O2	-6.39	117.43	121.90
41	BQ	2738	A	N1-C2-N3	-6.39	126.11	129.30
41	BQ	1959	G	N3-C2-N2	-6.38	115.43	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	583	C	C2-N1-C1'	6.38	125.82	118.80
41	BQ	1968	G	C8-N9-C4	-6.37	103.85	106.40
41	BQ	1563	C	N1-C2-O2	6.36	122.71	118.90
41	BQ	2257	C	N1-C2-O2	6.34	122.70	118.90
65	AR	21	ARG	NE-CZ-NH2	-6.31	117.14	120.30
41	BQ	628	A	C5-C6-N6	-6.30	118.66	123.70
41	BQ	3164	C	N3-C2-O2	-6.30	117.49	121.90
41	BQ	2362	C	N1-C2-O2	6.29	122.67	118.90
33	2	1560	U	N3-C2-O2	-6.29	117.80	122.20
41	BQ	2082	U	N1-C2-N3	6.28	118.67	114.90
77	AP	12	CYS	CA-CB-SG	-6.27	102.71	114.00
41	BQ	982	C	N1-C2-O2	6.24	122.64	118.90
41	BQ	2492	C	C6-N1-C1'	-6.24	113.32	120.80
41	BQ	982	C	C6-N1-C2	-6.22	117.81	120.30
41	BQ	637	C	C5-C6-N1	6.17	124.08	121.00
41	BQ	3217	C	N3-C2-O2	-6.17	117.58	121.90
41	BQ	74	G	N1-C6-O6	6.16	123.60	119.90
41	BQ	2237	C	N3-C2-O2	-6.14	117.60	121.90
33	2	142	G	N3-C4-N9	-6.14	122.32	126.00
36	c	13	ARG	NE-CZ-NH1	6.12	123.36	120.30
33	2	498	G	C4-N9-C1'	-6.11	118.56	126.50
43	BS	125	U	C6-N1-C1'	-6.11	112.65	121.20
41	BQ	1577	G	N1-C6-O6	-6.10	116.24	119.90
41	BQ	3163	A	N1-C6-N6	6.10	122.26	118.60
33	2	1498	G	N3-C4-N9	6.09	129.65	126.00
41	BQ	628	A	N9-C4-C5	-6.09	103.36	105.80
41	BQ	1695	U	O4'-C1'-N1	6.08	113.07	108.20
41	BQ	659	G	C2-N3-C4	-6.08	108.86	111.90
33	2	555	A	N7-C8-N9	6.08	116.84	113.80
41	BQ	628	A	N1-C6-N6	6.06	122.23	118.60
41	BQ	3194	C	C6-N1-C2	-6.06	117.88	120.30
33	2	656	G	C4-N9-C1'	6.05	134.37	126.50
41	BQ	1496	C	C5-C6-N1	6.05	124.02	121.00
41	BQ	2612	U	N3-C4-O4	6.04	123.63	119.40
41	BQ	3269	U	N1-C2-O2	6.04	127.03	122.80
41	BQ	2417	U	N3-C4-O4	6.04	123.62	119.40
41	BQ	3217	C	C6-N1-C1'	-6.02	113.58	120.80
41	BQ	1965	C	N3-C4-C5	6.01	124.31	121.90
41	BQ	2304	C	N3-C2-O2	-6.01	117.69	121.90
41	BQ	2146	C	N1-C2-O2	6.01	122.50	118.90
41	BQ	1605	A	O4'-C1'-N9	6.00	113.00	108.20
41	BQ	1661	G	N3-C4-N9	5.99	129.59	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BQ	665	A	N7-C8-N9	5.98	116.79	113.80
41	BQ	1972	A	C5-C6-N1	5.98	120.69	117.70
41	BQ	2031	U	P-O3'-C3'	5.98	126.88	119.70
33	2	489	C	N1-C2-O2	5.97	122.48	118.90
33	2	874	C	N1-C2-O2	5.96	122.48	118.90
41	BQ	2870	C	N3-C2-O2	-5.96	117.73	121.90
33	2	861	U	C2-N1-C1'	5.96	124.85	117.70
41	BQ	3164	C	N1-C2-O2	5.96	122.47	118.90
41	BQ	1983	G	C8-N9-C4	-5.94	104.02	106.40
41	BQ	1496	C	C2-N1-C1'	5.92	125.31	118.80
45	BE	195	ARG	NE-CZ-NH2	-5.91	117.35	120.30
41	BQ	2090	U	O4'-C1'-N1	5.90	112.92	108.20
41	BQ	3200	G	C2-N3-C4	-5.89	108.95	111.90
41	BQ	1280	C	N1-C2-O2	5.89	122.43	118.90
41	BQ	2738	A	N9-C4-C5	-5.89	103.45	105.80
33	2	656	G	N3-C4-N9	5.88	129.53	126.00
41	BQ	72	C	N3-C2-O2	-5.86	117.80	121.90
33	2	874	C	C5-C6-N1	5.86	123.93	121.00
41	BQ	166	C	N3-C2-O2	-5.85	117.81	121.90
41	BQ	656	A	C5-N7-C8	-5.84	100.98	103.90
41	BQ	1349	G	N3-C4-C5	-5.84	125.68	128.60
72	AF	73	ARG	NE-CZ-NH1	5.83	123.22	120.30
41	BQ	911	C	C5-C4-N4	-5.82	116.12	120.20
41	BQ	1283	C	N1-C2-O2	5.82	122.39	118.90
33	2	1706	C	C6-N1-C2	-5.81	117.97	120.30
41	BQ	2085	U	O4'-C1'-N1	5.81	112.85	108.20
33	2	1307	U	C6-N1-C2	-5.80	117.52	121.00
41	BQ	1283	C	C6-N1-C2	-5.80	117.98	120.30
33	2	1258	U	N3-C2-O2	-5.80	118.14	122.20
41	BQ	2434	U	C2-N1-C1'	5.79	124.65	117.70
45	BE	195	ARG	NE-CZ-NH1	5.79	123.19	120.30
33	2	1257	U	N1-C2-O2	5.78	126.84	122.80
33	2	1158	C	C6-N1-C2	-5.77	117.99	120.30
33	2	1458	G	C8-N9-C1'	-5.77	119.50	127.00
41	BQ	2257	C	C2-N1-C1'	5.77	125.14	118.80
33	2	874	C	C2-N1-C1'	5.76	125.14	118.80
33	2	1257	U	N3-C2-O2	-5.75	118.17	122.20
41	BQ	1269	U	C2-N1-C1'	5.75	124.59	117.70
41	BQ	2870	C	N1-C2-O2	5.75	122.35	118.90
41	BQ	1496	C	N1-C2-O2	5.74	122.34	118.90
44	AW	21	ARG	NE-CZ-NH1	5.73	123.17	120.30
72	AF	25	ARG	NE-CZ-NH1	5.73	123.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BQ	166	C	N1-C2-O2	5.72	122.33	118.90
41	BQ	43	A	C8-N9-C4	-5.72	103.51	105.80
41	BQ	1155	C	C6-N1-C2	-5.70	118.02	120.30
41	BQ	2612	U	C5-C4-O4	-5.68	122.49	125.90
41	BQ	1135	A	N1-C6-N6	5.68	122.01	118.60
33	2	1145	U	C2-N1-C1'	5.68	124.52	117.70
33	2	224	C	P-O3'-C3'	5.67	126.50	119.70
41	BQ	2960	C	C5-C4-N4	-5.67	116.23	120.20
28	BA	232	ARG	NE-CZ-NH1	5.67	123.13	120.30
41	BQ	1333	C	N1-C2-O2	5.67	122.30	118.90
33	2	1258	U	N1-C2-O2	5.66	126.76	122.80
50	BD	24	ARG	NE-CZ-NH2	5.66	123.13	120.30
41	BQ	494	G	C5-C6-O6	5.65	131.99	128.60
41	BQ	2417	U	C5-C4-O4	-5.65	122.51	125.90
41	BQ	1562	C	C3'-C2'-C1'	5.65	106.02	101.50
33	2	160	C	C6-N1-C2	-5.64	118.04	120.30
33	2	322	G	P-O3'-C3'	5.64	126.47	119.70
33	2	656	G	C8-N9-C1'	-5.63	119.68	127.00
41	BQ	363	G	N3-C2-N2	-5.62	115.97	119.90
41	BQ	1796	G	C8-N9-C1'	5.62	134.30	127.00
33	2	1705	C	N1-C2-O2	5.61	122.27	118.90
41	BQ	1974	A	C4-C5-C6	-5.61	114.20	117.00
41	BQ	1716	U	P-O3'-C3'	5.60	126.42	119.70
77	AP	14	GLY	CA-C-O	-5.60	110.52	120.60
33	2	1307	U	N3-C2-O2	-5.60	118.28	122.20
33	2	500	C	N3-C2-O2	-5.60	117.98	121.90
33	2	590	C	C6-N1-C2	-5.60	118.06	120.30
41	BQ	1105	A	N9-C4-C5	-5.59	103.56	105.80
41	BQ	2378	C	C2-N1-C1'	5.58	124.94	118.80
30	BB	179	ARG	NE-CZ-NH2	-5.58	117.51	120.30
33	2	1509	C	N1-C2-O2	5.57	122.24	118.90
41	BQ	1349	G	N3-C4-N9	5.57	129.34	126.00
35	b	28	ARG	C-N-CD	-5.57	108.35	120.60
41	BQ	1964	C	C5'-C4'-O4'	5.57	115.78	109.10
33	2	405	C	N1-C2-O2	5.56	122.24	118.90
33	2	1082	C	C2-N1-C1'	5.55	124.91	118.80
41	BQ	895	A	C5-N7-C8	-5.55	101.13	103.90
41	BQ	1983	G	N7-C8-N9	5.55	115.87	113.10
33	2	352	A	C6-N1-C2	-5.54	115.28	118.60
41	BQ	3181	C	C2-N1-C1'	5.53	124.88	118.80
41	BQ	1349	G	C4-N9-C1'	5.53	133.69	126.50
41	BQ	1437	C	C6-N1-C2	-5.53	118.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BQ	1577	G	N1-C2-N2	-5.52	111.23	116.20
41	BQ	3269	U	N3-C2-O2	-5.52	118.34	122.20
33	2	552	G	C6-C5-N7	-5.51	127.09	130.40
43	BS	127	U	C2-N1-C1'	5.51	124.31	117.70
33	2	1499	G	N3-C4-N9	-5.51	122.70	126.00
41	BQ	548	G	N1-C6-O6	-5.51	116.60	119.90
33	2	590	C	N1-C2-O2	5.50	122.20	118.90
33	2	934	C	N1-C2-O2	5.50	122.20	118.90
41	BQ	982	C	C2-N1-C1'	5.49	124.84	118.80
33	2	1696	G	N1-C2-N2	-5.49	111.26	116.20
41	BQ	1444	G	C4-C5-N7	5.48	112.99	110.80
41	BQ	1135	A	C5-C6-N6	-5.48	119.32	123.70
41	BQ	2772	C	N1-C2-O2	5.47	122.18	118.90
33	2	874	C	C6-N1-C2	-5.46	118.11	120.30
41	BQ	2150	G	N1-C2-N2	-5.46	111.28	116.20
41	BQ	1796	G	N3-C4-N9	-5.45	122.73	126.00
41	BQ	242	C	N3-C2-O2	-5.45	118.09	121.90
33	2	735	C	N1-C2-O2	5.44	122.17	118.90
41	BQ	2098	C	N1-C2-O2	5.44	122.17	118.90
41	BQ	1097	G	P-O3'-C3'	5.44	126.23	119.70
79	x	176	ARG	NE-CZ-NH1	5.44	123.02	120.30
41	BQ	2875	U	C5-C6-N1	5.43	125.42	122.70
33	2	590	C	C2-N1-C1'	5.42	124.77	118.80
21	U	158	ASP	CB-CG-OD1	5.42	123.18	118.30
77	AP	79	THR	N-CA-C	-5.41	96.39	111.00
41	BQ	1796	G	C4-N9-C1'	-5.41	119.47	126.50
41	BQ	1661	G	C6-C5-N7	-5.40	127.16	130.40
43	BS	10	A	C6-C5-N7	-5.40	128.52	132.30
41	BQ	630	A	N9-C4-C5	-5.40	103.64	105.80
33	2	278	U	P-O3'-C3'	5.39	126.17	119.70
41	BQ	1578	C	N1-C2-O2	5.39	122.14	118.90
41	BQ	3181	C	N3-C2-O2	-5.39	118.12	121.90
47	BM	31	ARG	NE-CZ-NH1	5.39	123.00	120.30
41	BQ	1978	A	C4-C5-C6	-5.39	114.30	117.00
41	BQ	1985	G	N9-C1'-C2'	-5.39	106.07	112.00
41	BQ	2531	C	C6-N1-C2	-5.38	118.15	120.30
33	2	814	A	C5-C6-N1	5.38	120.39	117.70
41	BQ	2407	C	C2-N1-C1'	5.37	124.70	118.80
41	BQ	3193	C	N1-C2-O2	5.37	122.12	118.90
33	2	1498	G	C4-N9-C1'	5.36	133.47	126.50
41	BQ	1604	G	C4-N9-C1'	5.36	133.47	126.50
41	BQ	1625	A	N9-C4-C5	-5.36	103.66	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BQ	2378	C	C6-N1-C2	-5.36	118.16	120.30
33	2	819	G	P-O3'-C3'	5.34	126.11	119.70
33	2	352	A	C8-N9-C4	-5.34	103.67	105.80
79	x	97	ARG	NE-CZ-NH1	5.33	122.97	120.30
41	BQ	656	A	N7-C8-N9	5.33	116.47	113.80
41	BQ	1863	G	C2-N3-C4	-5.33	109.24	111.90
41	BQ	3317	U	C2-N1-C1'	5.33	124.09	117.70
41	BQ	910	G	C2-N3-C4	-5.33	109.24	111.90
41	BQ	2082	U	O4'-C1'-N1	5.32	112.45	108.20
41	BQ	543	C	N3-C2-O2	-5.32	118.18	121.90
33	2	498	G	C8-N9-C1'	5.32	133.91	127.00
41	BQ	2772	C	N3-C2-O2	-5.31	118.18	121.90
41	BQ	3194	C	C6-N1-C1'	5.31	127.17	120.80
41	BQ	3194	C	N1-C2-N3	5.31	122.92	119.20
41	BQ	1972	A	N1-C6-N6	-5.30	115.42	118.60
36	c	19	ARG	NE-CZ-NH2	5.30	122.95	120.30
33	2	498	G	N1-C6-O6	-5.30	116.72	119.90
41	BQ	1562	C	C2-N1-C1'	5.30	124.63	118.80
41	BQ	386	A	N1-C6-N6	5.30	121.78	118.60
41	BQ	1577	G	C5-C6-O6	5.29	131.78	128.60
41	BQ	1661	G	C4-N9-C1'	5.29	133.38	126.50
41	BQ	628	A	C5-N7-C8	-5.29	101.25	103.90
41	BQ	2909	U	C5-C4-O4	-5.29	122.73	125.90
41	BQ	3200	G	N3-C4-C5	5.29	131.24	128.60
41	BQ	363	G	N3-C4-N9	-5.28	122.83	126.00
41	BQ	2874	G	N3-C4-N9	-5.28	122.83	126.00
41	BQ	2492	C	C6-N1-C2	-5.27	118.19	120.30
41	BQ	3214	U	C2-N1-C1'	5.27	124.02	117.70
33	2	1527	C	C6-N1-C2	-5.25	118.20	120.30
41	BQ	895	A	C4-C5-N7	5.25	113.33	110.70
72	AF	11	ARG	NE-CZ-NH2	-5.25	117.67	120.30
33	2	126	A	N1-C6-N6	-5.25	115.45	118.60
41	BQ	2142	A	N9-C4-C5	-5.25	103.70	105.80
41	BQ	776	U	N1-C2-N3	5.24	118.05	114.90
33	2	1145	U	N3-C2-O2	-5.23	118.54	122.20
41	BQ	648	C	C5-C4-N4	-5.23	116.54	120.20
41	BQ	3078	U	P-O3'-C3'	5.23	125.97	119.70
41	BQ	1444	G	C6-C5-N7	-5.22	127.27	130.40
33	2	490	C	N1-C2-N3	5.22	122.86	119.20
79	x	98	ARG	NE-CZ-NH1	5.22	122.91	120.30
19	S	3	ARG	NE-CZ-NH1	5.22	122.91	120.30
22	V	8	ARG	NE-CZ-NH2	5.22	122.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	BS	10	A	N7-C8-N9	5.22	116.41	113.80
41	BQ	2836	C	N1-C2-O2	5.21	122.03	118.90
41	BQ	916	G	P-O3'-C3'	5.21	125.95	119.70
41	BQ	1582	C	OP1-P-O3'	5.21	116.66	105.20
33	2	1438	G	N1-C6-O6	-5.21	116.78	119.90
44	AW	23	ARG	NE-CZ-NH1	5.21	122.90	120.30
33	2	1273	G	P-O3'-C3'	5.21	125.95	119.70
33	2	186	C	C6-N1-C2	-5.20	118.22	120.30
41	BQ	2257	C	N3-C2-O2	-5.20	118.26	121.90
41	BQ	2378	C	N1-C2-O2	5.20	122.02	118.90
33	2	139	C	P-O3'-C3'	5.20	125.94	119.70
41	BQ	2356	A	C5-C6-N6	-5.20	119.54	123.70
41	BQ	1597	C	C5-C6-N1	5.20	123.60	121.00
41	BQ	1858	A	O4'-C1'-N9	5.20	112.36	108.20
33	2	814	A	C5-C6-N6	5.19	127.86	123.70
41	BQ	665	A	C5-N7-C8	-5.19	101.30	103.90
41	BQ	3306	U	C2-N1-C1'	5.19	123.93	117.70
41	BQ	2092	A	N9-C1'-C2'	-5.19	106.29	112.00
41	BQ	1949	G	O5'-P-OP2	-5.18	101.03	105.70
41	BQ	906	A	C5-C6-N6	-5.18	119.55	123.70
41	BQ	1278	A	O4'-C1'-N9	5.18	112.34	108.20
41	BQ	1562	C	P-O3'-C3'	5.18	125.92	119.70
33	2	1498	G	C8-N9-C1'	-5.18	120.27	127.00
41	BQ	1963	G	C4'-C3'-O3'	5.17	123.35	113.00
41	BQ	1975	C	N3-C2-O2	-5.17	118.28	121.90
41	BQ	1622	U	C5-C6-N1	5.17	125.29	122.70
41	BQ	1556	C	N3-C2-O2	-5.17	118.28	121.90
41	BQ	1849	C	C5-C4-N4	-5.17	116.58	120.20
41	BQ	16	A	N9-C4-C5	-5.17	103.73	105.80
41	BQ	1608	C	C6-N1-C2	-5.17	118.23	120.30
41	BQ	2985	C	C6-N1-C2	-5.16	118.23	120.30
72	AF	22	CYS	C-N-CA	5.16	133.13	122.30
41	BQ	72	C	N3-C4-N4	-5.16	114.39	118.00
33	2	142	G	C8-N9-C1'	5.16	133.70	127.00
41	BQ	1279	C	N1-C2-O2	5.16	121.99	118.90
48	BO	218	ARG	NE-CZ-NH1	5.16	122.88	120.30
41	BQ	2361	A	N1-C6-N6	5.15	121.69	118.60
33	2	1659	A	C5-C6-N6	-5.15	119.58	123.70
33	2	276	C	C6-N1-C2	-5.14	118.24	120.30
33	2	352	A	P-O3'-C3'	5.14	125.87	119.70
41	BQ	1974	A	C5'-C4'-O4'	5.14	115.27	109.10
41	BQ	1729	A	P-O3'-C3'	5.13	125.86	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	BQ	656	A	C4-C5-N7	5.13	113.27	110.70
33	2	736	C	N1-C2-O2	5.13	121.98	118.90
41	BQ	1561	G	O4'-C1'-N9	5.12	112.30	108.20
41	BQ	2378	C	C5-C4-N4	-5.12	116.62	120.20
79	x	327	GLU	OE1-CD-OE2	5.12	129.44	123.30
72	AF	24	ARG	NE-CZ-NH1	5.12	122.86	120.30
77	AP	42	ARG	NE-CZ-NH1	5.12	122.86	120.30
28	BA	244	ARG	NE-CZ-NH1	5.11	122.86	120.30
33	2	225	A	N9-C4-C5	-5.11	103.75	105.80
30	BB	179	ARG	NE-CZ-NH1	5.11	122.86	120.30
33	2	1285	U	N3-C4-O4	-5.11	115.82	119.40
33	2	736	C	C6-N1-C2	-5.11	118.26	120.30
41	BQ	2836	C	C2-N1-C1'	5.10	124.42	118.80
33	2	497	G	C8-N9-C4	-5.10	104.36	106.40
33	2	1307	U	C5-C6-N1	5.10	125.25	122.70
33	2	1389	C	C6-N1-C1'	-5.10	114.69	120.80
41	BQ	2977	G	C2-N3-C4	-5.09	109.35	111.90
21	U	141	ARG	NE-CZ-NH1	5.09	122.84	120.30
33	2	224	C	N3-C2-O2	-5.08	118.34	121.90
41	BQ	1960	A	C4'-C3'-O3'	5.08	123.17	113.00
41	BQ	1582	C	P-O3'-C3'	5.08	125.80	119.70
33	2	160	C	N3-C2-O2	-5.08	118.35	121.90
41	BQ	1135	A	N9-C4-C5	-5.08	103.77	105.80
41	BQ	2277	C	C5-C4-N4	-5.07	116.65	120.20
41	BQ	2541	U	P-O3'-C3'	5.06	125.77	119.70
41	BQ	1355	A	P-O3'-C3'	5.06	125.77	119.70
76	AS	23	ARG	NE-CZ-NH2	5.06	122.83	120.30
41	BQ	1959	G	N9-C1'-C2'	-5.06	106.44	112.00
41	BQ	1608	C	C2-N1-C1'	5.05	124.36	118.80
17	Q	165	ARG	NE-CZ-NH1	5.05	122.83	120.30
41	BQ	494	G	N1-C6-O6	-5.04	116.87	119.90
41	BQ	2335	G	O4'-C1'-N9	-5.04	104.17	108.20
41	BQ	2142	A	N1-C6-N6	5.04	121.62	118.60
33	2	160	C	N1-C2-O2	5.04	121.92	118.90
47	BM	31	ARG	NE-CZ-NH2	-5.04	117.78	120.30
49	AD	166	ARG	NE-CZ-NH1	5.03	122.81	120.30
4	D	39	ASP	CB-CG-OD1	5.03	122.82	118.30
36	c	16	ARG	NE-CZ-NH2	5.03	122.81	120.30
41	BQ	267	G	O4'-C1'-N9	-5.03	104.18	108.20
33	2	1696	G	N3-C2-N2	5.02	123.42	119.90
33	2	500	C	N1-C2-O2	5.02	121.91	118.90
33	2	656	G	N3-C4-C5	-5.02	126.09	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	2	992	A	C8-N9-C4	-5.01	103.79	105.80
33	2	533	U	C2-N3-C4	-5.01	123.99	127.00
41	BQ	934	G	C4-N9-C1'	5.01	133.01	126.50
41	BQ	970	A	N9-C4-C5	-5.01	103.80	105.80
45	BE	220	ARG	NE-CZ-NH1	5.01	122.80	120.30
33	2	1527	C	C2-N1-C1'	5.01	124.31	118.80
41	BQ	1964	C	O4'-C1'-N1	5.01	112.21	108.20
41	BQ	1280	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	AA	30	THR	Peptide
27	AA	76	ALA	Peptide
27	AA	77	GLN	Peptide
65	AR	115	LYS	Peptide
65	AR	14	HIS	Peptide
66	AV	19	ASN	Peptide
66	AV	20	GLY	Peptide
1	B	42	LEU	Peptide
30	BB	161	LYS	Peptide
32	BC	7	VAL	Peptide
45	BE	13	GLY	Peptide
45	BE	3	ARG	Peptide
45	BE	318	LEU	Peptide
48	BO	232	ARG	Peptide
71	BP	83	LYS	Peptide
4	D	108	ARG	Peptide
6	F	40	GLU	Peptide
9	I	120	GLY	Peptide
12	L	19	THR	Peptide
14	N	147	VAL	Peptide
19	S	193	GLY	Peptide
26	Z	90	ARG	Peptide
35	b	54	ASP	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	B	204/206 (99%)	190 (93%)	14 (7%)	0	100	100
2	A	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
3	C	90/92 (98%)	77 (86%)	13 (14%)	0	100	100
4	D	119/121 (98%)	89 (75%)	29 (24%)	1 (1%)	19	57
5	E	115/142 (81%)	100 (87%)	15 (13%)	0	100	100
6	F	139/141 (99%)	124 (89%)	15 (11%)	0	100	100
7	G	117/125 (94%)	111 (95%)	6 (5%)	0	100	100
8	H	143/145 (99%)	130 (91%)	13 (9%)	0	100	100
9	I	141/143 (99%)	128 (91%)	13 (9%)	0	100	100
10	J	98/100 (98%)	87 (89%)	11 (11%)	0	100	100
11	K	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
12	L	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
13	M	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
14	N	71/73 (97%)	48 (68%)	23 (32%)	0	100	100
15	O	310/312 (99%)	264 (85%)	46 (15%)	0	100	100
16	P	204/206 (99%)	181 (89%)	23 (11%)	0	100	100
17	Q	222/232 (96%)	196 (88%)	26 (12%)	0	100	100
18	R	214/216 (99%)	189 (88%)	25 (12%)	0	100	100
19	S	256/258 (99%)	224 (88%)	32 (12%)	0	100	100
20	T	226/228 (99%)	210 (93%)	16 (7%)	0	100	100
21	U	182/184 (99%)	158 (87%)	24 (13%)	0	100	100
22	V	183/200 (92%)	165 (90%)	18 (10%)	0	100	100
23	W	182/184 (99%)	161 (88%)	20 (11%)	1 (0%)	29	67
24	X	140/142 (99%)	125 (89%)	15 (11%)	0	100	100
25	Y	148/150 (99%)	131 (88%)	17 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	125/127 (98%)	108 (86%)	17 (14%)	0	100	100
27	AA	231/233 (99%)	209 (90%)	22 (10%)	0	100	100
28	BA	384/386 (100%)	354 (92%)	30 (8%)	0	100	100
29	AB	134/136 (98%)	127 (95%)	7 (5%)	0	100	100
30	BB	183/185 (99%)	170 (93%)	13 (7%)	0	100	100
31	AC	97/99 (98%)	91 (94%)	6 (6%)	0	100	100
32	BC	107/109 (98%)	92 (86%)	15 (14%)	0	100	100
34	a	85/87 (98%)	72 (85%)	13 (15%)	0	100	100
35	b	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
36	c	142/144 (99%)	122 (86%)	20 (14%)	0	100	100
37	d	132/134 (98%)	123 (93%)	9 (7%)	0	100	100
38	e	95/97 (98%)	85 (90%)	10 (10%)	0	100	100
39	f	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
40	g	58/60 (97%)	48 (83%)	10 (17%)	0	100	100
44	AW	249/251 (99%)	220 (88%)	29 (12%)	0	100	100
45	BE	359/361 (99%)	321 (89%)	37 (10%)	1 (0%)	41	75
46	BI	292/294 (99%)	268 (92%)	24 (8%)	0	100	100
47	BM	163/175 (93%)	146 (90%)	17 (10%)	0	100	100
48	BO	220/222 (99%)	205 (93%)	15 (7%)	0	100	100
49	AD	189/191 (99%)	172 (91%)	17 (9%)	0	100	100
50	BD	216/218 (99%)	188 (87%)	28 (13%)	0	100	100
51	AG	167/169 (99%)	155 (93%)	12 (7%)	0	100	100
52	AJ	191/193 (99%)	169 (88%)	21 (11%)	1 (0%)	29	67
53	AM	134/136 (98%)	120 (90%)	14 (10%)	0	100	100
54	AQ	201/203 (99%)	181 (90%)	20 (10%)	0	100	100
55	AU	195/197 (99%)	186 (95%)	9 (5%)	0	100	100
56	AX	181/183 (99%)	165 (91%)	16 (9%)	0	100	100
57	BF	186/188 (99%)	178 (96%)	8 (4%)	0	100	100
58	BH	169/171 (99%)	157 (93%)	12 (7%)	0	100	100
59	BJ	157/159 (99%)	142 (90%)	15 (10%)	0	100	100
60	BL	98/100 (98%)	93 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
61	AE	124/126 (98%)	106 (86%)	18 (14%)	0	100	100
62	AH	119/121 (98%)	109 (92%)	10 (8%)	0	100	100
63	AK	123/125 (98%)	116 (94%)	7 (6%)	0	100	100
64	AN	133/135 (98%)	117 (88%)	16 (12%)	0	100	100
65	AR	146/148 (99%)	128 (88%)	18 (12%)	0	100	100
66	AV	56/58 (97%)	47 (84%)	9 (16%)	0	100	100
67	AY	94/96 (98%)	89 (95%)	4 (4%)	1 (1%)	14	51
68	BG	125/127 (98%)	114 (91%)	11 (9%)	0	100	100
69	BK	104/106 (98%)	98 (94%)	6 (6%)	0	100	100
70	BN	110/112 (98%)	105 (96%)	5 (4%)	0	100	100
71	BP	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
72	AF	79/81 (98%)	72 (91%)	7 (9%)	0	100	100
73	AI	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
74	AL	48/50 (96%)	45 (94%)	3 (6%)	0	100	100
75	AO	50/52 (96%)	43 (86%)	7 (14%)	0	100	100
76	AS	23/25 (92%)	23 (100%)	0	0	100	100
77	AP	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
78	AT	89/91 (98%)	84 (94%)	4 (4%)	1 (1%)	14	51
79	x	365/387 (94%)	350 (96%)	13 (4%)	2 (0%)	29	67
80	BT	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
All	All	11558/11794 (98%)	10452 (90%)	1098 (10%)	8 (0%)	54	84

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	109	GLU
45	BE	4	PRO
79	x	68	ALA
52	AJ	61	PRO
67	AY	49	PRO
23	W	18	PRO
78	AT	43	GLY
79	x	28	GLY

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	B	172/173 (99%)	172 (100%)	0	100 100
2	A	182/182 (100%)	181 (100%)	1 (0%)	88 93
3	C	77/85 (91%)	77 (100%)	0	100 100
4	D	88/98 (90%)	88 (100%)	0	100 100
5	E	95/118 (80%)	95 (100%)	0	100 100
6	F	117/117 (100%)	117 (100%)	0	100 100
7	G	101/113 (89%)	101 (100%)	0	100 100
8	H	127/128 (99%)	126 (99%)	1 (1%)	81 89
9	I	115/115 (100%)	115 (100%)	0	100 100
10	J	93/93 (100%)	92 (99%)	1 (1%)	73 84
11	K	67/73 (92%)	66 (98%)	1 (2%)	65 80
12	L	55/56 (98%)	55 (100%)	0	100 100
13	M	47/47 (100%)	46 (98%)	1 (2%)	53 73
14	N	56/63 (89%)	56 (100%)	0	100 100
15	O	250/257 (97%)	250 (100%)	0	100 100
16	P	170/173 (98%)	170 (100%)	0	100 100
17	Q	200/205 (98%)	199 (100%)	1 (0%)	88 93
18	R	175/175 (100%)	175 (100%)	0	100 100
19	S	220/220 (100%)	219 (100%)	1 (0%)	88 93
20	T	189/195 (97%)	187 (99%)	2 (1%)	73 84
21	U	163/165 (99%)	163 (100%)	0	100 100
22	V	148/161 (92%)	148 (100%)	0	100 100
23	W	156/157 (99%)	155 (99%)	1 (1%)	86 91
24	X	126/127 (99%)	125 (99%)	1 (1%)	81 89
25	Y	127/127 (100%)	125 (98%)	2 (2%)	62 79
26	Z	90/96 (94%)	89 (99%)	1 (1%)	73 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	AA	187/191 (98%)	186 (100%)	1 (0%)	88 93
28	BA	318/322 (99%)	317 (100%)	1 (0%)	92 95
29	AB	104/104 (100%)	104 (100%)	0	100 100
30	BB	150/150 (100%)	149 (99%)	1 (1%)	84 90
31	AC	80/81 (99%)	80 (100%)	0	100 100
32	BC	92/96 (96%)	92 (100%)	0	100 100
34	a	71/74 (96%)	71 (100%)	0	100 100
35	b	110/110 (100%)	110 (100%)	0	100 100
36	c	119/119 (100%)	119 (100%)	0	100 100
37	d	102/112 (91%)	101 (99%)	1 (1%)	76 86
38	e	82/83 (99%)	82 (100%)	0	100 100
39	f	70/70 (100%)	70 (100%)	0	100 100
40	g	50/51 (98%)	50 (100%)	0	100 100
44	AW	190/193 (98%)	190 (100%)	0	100 100
45	BE	288/288 (100%)	287 (100%)	1 (0%)	92 95
46	BI	241/243 (99%)	241 (100%)	0	100 100
47	BM	139/154 (90%)	139 (100%)	0	100 100
48	BO	186/186 (100%)	186 (100%)	0	100 100
49	AD	168/171 (98%)	168 (100%)	0	100 100
50	BD	185/185 (100%)	184 (100%)	1 (0%)	88 93
51	AG	145/147 (99%)	144 (99%)	1 (1%)	84 90
52	AJ	154/154 (100%)	152 (99%)	2 (1%)	69 82
53	AM	107/107 (100%)	107 (100%)	0	100 100
54	AQ	175/175 (100%)	174 (99%)	1 (1%)	86 91
55	AU	160/160 (100%)	160 (100%)	0	100 100
56	AX	138/145 (95%)	138 (100%)	0	100 100
57	BF	152/153 (99%)	150 (99%)	2 (1%)	69 82
58	BH	155/155 (100%)	155 (100%)	0	100 100
59	BJ	135/136 (99%)	135 (100%)	0	100 100
60	BL	87/87 (100%)	87 (100%)	0	100 100
61	AE	56/108 (52%)	56 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
62	AH	104/105 (99%)	104 (100%)	0	100 100
63	AK	108/108 (100%)	108 (100%)	0	100 100
64	AN	112/115 (97%)	111 (99%)	1 (1%)	78 87
65	AR	117/118 (99%)	116 (99%)	1 (1%)	78 87
66	AV	46/46 (100%)	45 (98%)	1 (2%)	52 71
67	AY	81/81 (100%)	81 (100%)	0	100 100
68	BG	108/109 (99%)	108 (100%)	0	100 100
69	BK	90/90 (100%)	90 (100%)	0	100 100
70	BN	95/95 (100%)	94 (99%)	1 (1%)	73 84
71	BP	104/104 (100%)	104 (100%)	0	100 100
72	AF	67/67 (100%)	65 (97%)	2 (3%)	41 64
73	AI	68/68 (100%)	67 (98%)	1 (2%)	65 80
74	AL	45/45 (100%)	45 (100%)	0	100 100
75	AO	45/47 (96%)	42 (93%)	3 (7%)	16 46
76	AS	22/23 (96%)	22 (100%)	0	100 100
77	AP	87/88 (99%)	87 (100%)	0	100 100
78	AT	71/71 (100%)	69 (97%)	2 (3%)	43 66
79	x	322/340 (95%)	320 (99%)	2 (1%)	86 91
All	All	9494/9749 (97%)	9454 (100%)	40 (0%)	91 94

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	76	ARG
8	H	145	ARG
10	J	43	LYS
11	K	85	LYS
13	M	42	CYS
17	Q	7	LYS
19	S	211	LYS
20	T	143	LYS
20	T	214	LYS
23	W	149	ARG
24	X	67	ARG
25	Y	64	ARG
25	Y	76	LYS

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Mol	Chain	Res	Type
26	Z	136	ARG
27	AA	213	LYS
28	BA	332	ARG
30	BB	12	ARG
37	d	111	LYS
45	BE	98	ARG
50	BD	185	ARG
51	AG	85	LYS
52	AJ	31	LYS
52	AJ	104	ARG
54	AQ	27	VAL
57	BF	81	ARG
57	BF	165	LYS
64	AN	3	LYS
65	AR	92	LYS
66	AV	33	LYS
70	BN	59	PRO
72	AF	19	CYS
72	AF	22	CYS
73	AI	63	LYS
75	AO	96	CYS
75	AO	112	LYS
75	AO	115	CYS
78	AT	4	ARG
78	AT	57	CYS
79	x	221	SER
79	x	230	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	103	ASN
3	C	29	GLN
5	E	70	ASN
6	F	32	ASN
8	H	25	ASN
8	H	103	ASN
8	H	104	ASN
10	J	49	ASN
14	N	123	ASN
14	N	151	ASN
17	Q	177	GLN

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Mol	Chain	Res	Type
19	S	130	GLN
27	AA	240	ASN
28	BA	279	ASN
35	b	70	ASN
37	d	34	ASN
44	AW	97	ASN
44	AW	140	ASN
44	AW	144	ASN
44	AW	194	ASN
45	BE	48	GLN
49	AD	116	ASN
50	BD	55	ASN
52	AJ	19	GLN
54	AQ	57	GLN
56	AX	10	ASN
66	AV	43	HIS
70	BN	52	GLN
71	BP	16	GLN
77	AP	23	HIS
79	x	275	HIS
79	x	356	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	2	1768/1798 (98%)	536 (30%)	53 (2%)
41	BQ	3293/3395 (96%)	764 (23%)	53 (1%)
42	BR	120/121 (99%)	15 (12%)	1 (0%)
43	BS	157/158 (99%)	32 (20%)	3 (1%)
All	All	5338/5472 (97%)	1347 (25%)	110 (2%)

All (1347) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
33	2	2	A
33	2	4	C
33	2	14	C
33	2	25	C
33	2	26	A
33	2	34	G
33	2	43	A

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Mol	Chain	Res	Type
33	2	45	U
33	2	47	A
33	2	56	U
33	2	57	G
33	2	62	A
33	2	65	A
33	2	67	A
33	2	68	A
33	2	69	G
33	2	73	U
33	2	74	U
33	2	75	U
33	2	76	A
33	2	78	A
33	2	79	C
33	2	80	A
33	2	81	G
33	2	104	A
33	2	114	C
33	2	116	U
33	2	121	U
33	2	127	G
33	2	129	U
33	2	130	C
33	2	131	C
33	2	132	U
33	2	133	U
33	2	134	U
33	2	135	A
33	2	136	C
33	2	137	U
33	2	138	A
33	2	140	A
33	2	141	U
33	2	142	G
33	2	153	G
33	2	155	U
33	2	156	A
33	2	158	U
33	2	161	U
33	2	168	A
33	2	171	A

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Mol	Chain	Res	Type
33	2	172	C
33	2	174	U
33	2	176	C
33	2	178	U
33	2	179	A
33	2	182	A
33	2	185	U
33	2	186	C
33	2	187	G
33	2	188	A
33	2	189	C
33	2	191	C
33	2	193	U
33	2	194	U
33	2	195	G
33	2	201	G
33	2	203	U
33	2	204	G
33	2	216	U
33	2	217	A
33	2	218	A
33	2	223	U
33	2	224	C
33	2	225	A
33	2	227	U
33	2	228	G
33	2	230	C
33	2	232	U
33	2	233	C
33	2	234	G
33	2	235	G
33	2	236	A
33	2	238	U
33	2	240	U
33	2	241	U
33	2	243	G
33	2	246	G
33	2	250	C
33	2	256	A
33	2	260	U
33	2	261	U
33	2	265	A

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Mol	Chain	Res	Type
33	2	270	C
33	2	272	U
33	2	274	G
33	2	276	C
33	2	277	U
33	2	278	U
33	2	279	G
33	2	280	U
33	2	287	G
33	2	299	A
33	2	313	U
33	2	314	C
33	2	316	A
33	2	320	U
33	2	321	C
33	2	322	G
33	2	323	A
33	2	324	U
33	2	330	G
33	2	333	A
33	2	334	G
33	2	337	G
33	2	338	C
33	2	352	A
33	2	353	A
33	2	359	A
33	2	360	A
33	2	361	C
33	2	369	A
33	2	370	A
33	2	373	G
33	2	378	A
33	2	380	U
33	2	388	G
33	2	390	G
33	2	400	A
33	2	401	A
33	2	402	C
33	2	404	G
33	2	406	U
33	2	411	C
33	2	415	C

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Mol	Chain	Res	Type
33	2	417	A
33	2	419	G
33	2	423	G
33	2	424	C
33	2	425	A
33	2	426	G
33	2	434	G
33	2	435	C
33	2	438	A
33	2	439	U
33	2	444	C
33	2	446	A
33	2	447	U
33	2	448	C
33	2	454	U
33	2	460	A
33	2	468	A
33	2	482	U
33	2	485	A
33	2	487	G
33	2	489	C
33	2	491	C
33	2	492	A
33	2	493	U
33	2	494	U
33	2	495	C
33	2	496	G
33	2	498	G
33	2	499	U
33	2	500	C
33	2	502	U
33	2	506	A
33	2	507	U
33	2	510	G
33	2	511	A
33	2	512	A
33	2	513	U
33	2	517	U
33	2	518	A
33	2	519	C
33	2	520	A
33	2	525	A

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Mol	Chain	Res	Type
33	2	527	A
33	2	529	A
33	2	534	A
33	2	538	A
33	2	539	G
33	2	540	G
33	2	541	A
33	2	542	A
33	2	543	C
33	2	554	C
33	2	555	A
33	2	556	A
33	2	557	G
33	2	558	U
33	2	565	C
33	2	571	G
33	2	572	C
33	2	578	U
33	2	579	A
33	2	580	A
33	2	594	A
33	2	595	G
33	2	606	A
33	2	609	U
33	2	610	G
33	2	611	U
33	2	617	U
33	2	619	A
33	2	620	A
33	2	623	A
33	2	624	G
33	2	635	A
33	2	638	U
33	2	639	U
33	2	640	U
33	2	641	G
33	2	643	G
33	2	645	C
33	2	651	G
33	2	653	C
33	2	654	C
33	2	655	G

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Mol	Chain	Res	Type
33	2	656	G
33	2	677	G
33	2	678	A
33	2	680	U
33	2	682	C
33	2	684	A
33	2	687	G
33	2	693	U
33	2	694	U
33	2	696	C
33	2	697	C
33	2	698	U
33	2	700	C
33	2	702	G
33	2	703	G
33	2	704	C
33	2	705	U
33	2	706	A
33	2	707	A
33	2	708	C
33	2	709	C
33	2	710	U
33	2	711	U
33	2	712	G
33	2	714	G
33	2	728	U
33	2	729	G
33	2	730	G
33	2	732	G
33	2	733	A
33	2	736	C
33	2	738	G
33	2	739	G
33	2	741	C
33	2	742	U
33	2	743	U
33	2	744	U
33	2	745	U
33	2	753	A
33	2	755	A
33	2	756	A
33	2	765	G

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Mol	Chain	Res	Type
33	2	766	U
33	2	771	A
33	2	774	A
33	2	775	G
33	2	778	G
33	2	781	U
33	2	782	U
33	2	783	G
33	2	787	G
33	2	789	A
33	2	794	U
33	2	804	A
33	2	807	A
33	2	812	A
33	2	813	U
33	2	814	A
33	2	815	G
33	2	816	G
33	2	818	C
33	2	819	G
33	2	820	U
33	2	821	U
33	2	823	G
33	2	832	U
33	2	833	U
33	2	836	U
33	2	837	G
33	2	839	U
33	2	840	U
33	2	841	U
33	2	846	G
33	2	851	U
33	2	852	C
33	2	855	A
33	2	856	A
33	2	857	U
33	2	863	A
33	2	865	A
33	2	873	U
33	2	876	G
33	2	877	G
33	2	882	U

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Mol	Chain	Res	Type
33	2	886	U
33	2	898	A
33	2	899	G
33	2	901	G
33	2	902	G
33	2	904	G
33	2	912	U
33	2	913	G
33	2	929	A
33	2	932	U
33	2	933	A
33	2	934	C
33	2	935	U
33	2	940	A
33	2	945	U
33	2	960	U
33	2	964	U
33	2	966	A
33	2	970	A
33	2	973	A
33	2	977	A
33	2	988	A
33	2	989	U
33	2	992	A
33	2	996	U
33	2	998	A
33	2	1001	A
33	2	1004	U
33	2	1024	U
33	2	1026	A
33	2	1028	C
33	2	1029	U
33	2	1032	G
33	2	1039	A
33	2	1040	G
33	2	1052	U
33	2	1053	G
33	2	1057	U
33	2	1058	U
33	2	1059	U
33	2	1060	U
33	2	1061	A

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Mol	Chain	Res	Type
33	2	1062	A
33	2	1063	U
33	2	1074	G
33	2	1080	U
33	2	1081	A
33	2	1082	C
33	2	1092	A
33	2	1096	C
33	2	1099	U
33	2	1100	G
33	2	1109	G
33	2	1111	G
33	2	1113	A
33	2	1138	A
33	2	1156	C
33	2	1158	C
33	2	1160	A
33	2	1164	G
33	2	1167	G
33	2	1170	G
33	2	1183	A
33	2	1185	U
33	2	1186	U
33	2	1187	U
33	2	1191	U
33	2	1194	A
33	2	1196	A
33	2	1197	C
33	2	1199	G
33	2	1200	G
33	2	1208	A
33	2	1212	G
33	2	1214	U
33	2	1217	A
33	2	1218	G
33	2	1227	A
33	2	1229	G
33	2	1241	G
33	2	1243	G
33	2	1244	A
33	2	1245	G
33	2	1246	C

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Mol	Chain	Res	Type
33	2	1251	U
33	2	1252	C
33	2	1256	A
33	2	1257	U
33	2	1258	U
33	2	1263	G
33	2	1264	G
33	2	1265	G
33	2	1269	U
33	2	1273	G
33	2	1274	C
33	2	1275	A
33	2	1276	U
33	2	1285	U
33	2	1294	G
33	2	1301	U
33	2	1307	U
33	2	1314	U
33	2	1315	U
33	2	1318	G
33	2	1321	A
33	2	1322	A
33	2	1325	A
33	2	1337	A
33	2	1341	A
33	2	1344	A
33	2	1345	A
33	2	1346	A
33	2	1348	A
33	2	1349	G
33	2	1354	G
33	2	1360	A
33	2	1361	U
33	2	1363	U
33	2	1367	G
33	2	1370	U
33	2	1371	A
33	2	1372	U
33	2	1373	C
33	2	1381	U
33	2	1382	A
33	2	1383	G

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Mol	Chain	Res	Type
33	2	1385	G
33	2	1390	U
33	2	1398	U
33	2	1399	C
33	2	1400	A
33	2	1402	G
33	2	1414	U
33	2	1415	U
33	2	1421	A
33	2	1427	A
33	2	1431	C
33	2	1432	U
33	2	1433	G
33	2	1446	A
33	2	1447	C
33	2	1448	G
33	2	1457	C
33	2	1458	G
33	2	1459	C
33	2	1460	A
33	2	1469	A
33	2	1472	C
33	2	1473	U
33	2	1479	A
33	2	1482	C
33	2	1483	A
33	2	1488	G
33	2	1489	U
33	2	1490	C
33	2	1491	U
33	2	1492	A
33	2	1493	A
33	2	1496	U
33	2	1510	U
33	2	1514	U
33	2	1515	A
33	2	1516	A
33	2	1517	U
33	2	1518	C
33	2	1521	G
33	2	1523	G
33	2	1524	A

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Mol	Chain	Res	Type
33	2	1528	U
33	2	1529	C
33	2	1531	G
33	2	1537	C
33	2	1540	G
33	2	1543	A
33	2	1545	A
33	2	1556	A
33	2	1557	U
33	2	1558	U
33	2	1559	A
33	2	1572	G
33	2	1573	A
33	2	1574	G
33	2	1575	G
33	2	1576	A
33	2	1583	A
33	2	1584	G
33	2	1585	U
33	2	1590	G
33	2	1592	A
33	2	1601	G
33	2	1607	G
33	2	1611	A
33	2	1614	A
33	2	1616	G
33	2	1619	C
33	2	1622	G
33	2	1634	C
33	2	1637	C
33	2	1657	U
33	2	1658	G
33	2	1660	A
33	2	1673	G
33	2	1676	U
33	2	1682	U
33	2	1688	U
33	2	1689	A
33	2	1693	A
33	2	1700	C
33	2	1701	A
33	2	1702	A

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Mol	Chain	Res	Type
33	2	1703	C
33	2	1709	C
33	2	1711	C
33	2	1712	A
33	2	1715	G
33	2	1717	G
33	2	1736	G
33	2	1740	A
33	2	1755	A
33	2	1757	G
33	2	1760	G
33	2	1762	A
33	2	1766	A
33	2	1767	G
33	2	1769	U
33	2	1770	U
33	2	1780	G
33	2	1782	A
33	2	1783	C
33	2	1788	G
33	2	1792	G
33	2	1793	G
33	2	1794	A
33	2	1796	C
33	2	1799	U
41	BQ	6	A
41	BQ	11	A
41	BQ	14	U
41	BQ	15	C
41	BQ	21	G
41	BQ	22	G
41	BQ	26	A
41	BQ	30	G
41	BQ	40	A
41	BQ	43	A
41	BQ	44	U
41	BQ	48	A
41	BQ	49	A
41	BQ	51	A
41	BQ	57	A
41	BQ	60	A
41	BQ	65	A

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Mol	Chain	Res	Type
41	BQ	66	A
41	BQ	73	C
41	BQ	74	G
41	BQ	76	G
41	BQ	85	A
41	BQ	89	A
41	BQ	92	G
41	BQ	109	A
41	BQ	110	G
41	BQ	111	C
41	BQ	113	C
41	BQ	120	G
41	BQ	121	A
41	BQ	122	A
41	BQ	133	U
41	BQ	136	G
41	BQ	143	G
41	BQ	150	A
41	BQ	156	G
41	BQ	157	A
41	BQ	166	C
41	BQ	173	G
41	BQ	187	A
41	BQ	190	U
41	BQ	191	U
41	BQ	200	C
41	BQ	206	G
41	BQ	210	U
41	BQ	211	A
41	BQ	213	A
41	BQ	218	G
41	BQ	219	A
41	BQ	221	A
41	BQ	231	G
41	BQ	236	G
41	BQ	239	G
41	BQ	240	U
41	BQ	243	G
41	BQ	249	U
41	BQ	252	U
41	BQ	258	G
41	BQ	263	C

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Mol	Chain	Res	Type
41	BQ	269	G
41	BQ	282	G
41	BQ	283	G
41	BQ	286	U
41	BQ	295	A
41	BQ	298	U
41	BQ	315	C
41	BQ	323	A
41	BQ	329	U
41	BQ	330	G
41	BQ	334	A
41	BQ	338	A
41	BQ	339	C
41	BQ	346	C
41	BQ	350	C
41	BQ	351	A
41	BQ	376	G
41	BQ	385	A
41	BQ	390	G
41	BQ	395	A
41	BQ	397	A
41	BQ	399	A
41	BQ	401	U
41	BQ	402	A
41	BQ	403	C
41	BQ	404	G
41	BQ	421	G
41	BQ	422	A
41	BQ	438	A
41	BQ	440	A
41	BQ	441	U
41	BQ	442	G
41	BQ	443	G
41	BQ	445	G
41	BQ	446	U
41	BQ	447	U
41	BQ	448	U
41	BQ	449	U
41	BQ	450	G
41	BQ	487	U
41	BQ	488	U
41	BQ	489	U

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Mol	Chain	Res	Type
41	BQ	490	C
41	BQ	491	A
41	BQ	492	C
41	BQ	494	G
41	BQ	498	A
41	BQ	510	G
41	BQ	515	C
41	BQ	517	G
41	BQ	520	U
41	BQ	521	A
41	BQ	535	G
41	BQ	543	C
41	BQ	544	C
41	BQ	545	U
41	BQ	546	C
41	BQ	547	G
41	BQ	552	G
41	BQ	555	U
41	BQ	557	A
41	BQ	559	A
41	BQ	568	G
41	BQ	578	A
41	BQ	579	G
41	BQ	597	G
41	BQ	600	G
41	BQ	603	A
41	BQ	604	G
41	BQ	609	G
41	BQ	610	G
41	BQ	611	A
41	BQ	612	U
41	BQ	619	A
41	BQ	620	U
41	BQ	621	A
41	BQ	625	G
41	BQ	637	C
41	BQ	638	C
41	BQ	642	U
41	BQ	649	A
41	BQ	650	C
41	BQ	660	A
41	BQ	667	C

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Mol	Chain	Res	Type
41	BQ	677	A
41	BQ	681	U
41	BQ	691	A
41	BQ	699	A
41	BQ	705	A
41	BQ	712	G
41	BQ	716	A
41	BQ	718	G
41	BQ	719	U
41	BQ	720	A
41	BQ	726	G
41	BQ	737	G
41	BQ	742	G
41	BQ	758	C
41	BQ	763	G
41	BQ	764	U
41	BQ	765	C
41	BQ	766	U
41	BQ	767	U
41	BQ	771	A
41	BQ	774	G
41	BQ	776	U
41	BQ	777	U
41	BQ	780	A
41	BQ	781	G
41	BQ	785	G
41	BQ	786	A
41	BQ	806	A
41	BQ	808	A
41	BQ	817	A
41	BQ	830	A
41	BQ	832	G
41	BQ	848	A
41	BQ	849	C
41	BQ	850	U
41	BQ	851	C
41	BQ	861	C
41	BQ	865	U
41	BQ	868	C
41	BQ	871	U
41	BQ	874	U
41	BQ	879	U

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Mol	Chain	Res	Type
41	BQ	894	G
41	BQ	895	A
41	BQ	896	A
41	BQ	899	U
41	BQ	906	A
41	BQ	907	G
41	BQ	908	G
41	BQ	914	A
41	BQ	916	G
41	BQ	917	A
41	BQ	921	A
41	BQ	923	C
41	BQ	932	U
41	BQ	934	G
41	BQ	937	G
41	BQ	944	C
41	BQ	959	C
41	BQ	960	U
41	BQ	971	G
41	BQ	974	G
41	BQ	981	U
41	BQ	982	C
41	BQ	991	G
41	BQ	1002	A
41	BQ	1012	G
41	BQ	1015	U
41	BQ	1018	G
41	BQ	1020	G
41	BQ	1021	G
41	BQ	1024	G
41	BQ	1026	A
41	BQ	1028	U
41	BQ	1029	G
41	BQ	1040	A
41	BQ	1041	U
41	BQ	1045	C
41	BQ	1047	A
41	BQ	1049	C
41	BQ	1064	A
41	BQ	1065	A
41	BQ	1072	G
41	BQ	1081	U

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Mol	Chain	Res	Type
41	BQ	1093	A
41	BQ	1094	U
41	BQ	1095	U
41	BQ	1096	U
41	BQ	1097	G
41	BQ	1098	A
41	BQ	1103	A
41	BQ	1104	G
41	BQ	1117	G
41	BQ	1118	C
41	BQ	1128	U
41	BQ	1131	G
41	BQ	1144	U
41	BQ	1145	G
41	BQ	1148	G
41	BQ	1153	A
41	BQ	1158	A
41	BQ	1159	A
41	BQ	1177	G
41	BQ	1178	G
41	BQ	1180	A
41	BQ	1181	U
41	BQ	1182	A
41	BQ	1190	A
41	BQ	1192	C
41	BQ	1193	A
41	BQ	1196	C
41	BQ	1197	A
41	BQ	1201	C
41	BQ	1202	A
41	BQ	1206	G
41	BQ	1208	U
41	BQ	1217	A
41	BQ	1218	U
41	BQ	1222	G
41	BQ	1223	A
41	BQ	1227	C
41	BQ	1229	G
41	BQ	1234	G
41	BQ	1236	G
41	BQ	1237	G
41	BQ	1238	C

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Mol	Chain	Res	Type
41	BQ	1239	C
41	BQ	1240	A
41	BQ	1241	U
41	BQ	1242	G
41	BQ	1243	G
41	BQ	1244	A
41	BQ	1245	A
41	BQ	1246	G
41	BQ	1248	C
41	BQ	1251	A
41	BQ	1253	U
41	BQ	1258	U
41	BQ	1262	G
41	BQ	1263	A
41	BQ	1264	G
41	BQ	1266	G
41	BQ	1267	U
41	BQ	1269	U
41	BQ	1270	A
41	BQ	1271	A
41	BQ	1272	C
41	BQ	1278	A
41	BQ	1279	C
41	BQ	1280	C
41	BQ	1282	G
41	BQ	1285	G
41	BQ	1286	A
41	BQ	1287	A
41	BQ	1295	G
41	BQ	1307	G
41	BQ	1308	A
41	BQ	1309	U
41	BQ	1313	G
41	BQ	1316	C
41	BQ	1318	A
41	BQ	1325	U
41	BQ	1330	A
41	BQ	1345	G
41	BQ	1348	U
41	BQ	1349	G
41	BQ	1351	U
41	BQ	1352	A

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Mol	Chain	Res	Type
41	BQ	1354	G
41	BQ	1355	A
41	BQ	1356	U
41	BQ	1357	G
41	BQ	1386	A
41	BQ	1392	G
41	BQ	1399	A
41	BQ	1400	G
41	BQ	1418	A
41	BQ	1419	A
41	BQ	1421	G
41	BQ	1429	G
41	BQ	1430	U
41	BQ	1431	G
41	BQ	1434	G
41	BQ	1437	C
41	BQ	1442	U
41	BQ	1443	G
41	BQ	1446	A
41	BQ	1450	G
41	BQ	1455	U
41	BQ	1481	A
41	BQ	1482	A
41	BQ	1483	G
41	BQ	1484	U
41	BQ	1487	G
41	BQ	1488	G
41	BQ	1503	A
41	BQ	1508	C
41	BQ	1511	U
41	BQ	1523	U
41	BQ	1528	G
41	BQ	1533	U
41	BQ	1536	G
41	BQ	1542	G
41	BQ	1549	U
41	BQ	1555	U
41	BQ	1556	C
41	BQ	1557	A
41	BQ	1559	A
41	BQ	1560	G
41	BQ	1562	C

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Mol	Chain	Res	Type
41	BQ	1563	C
41	BQ	1565	G
41	BQ	1566	A
41	BQ	1567	U
41	BQ	1568	U
41	BQ	1569	U
41	BQ	1572	U
41	BQ	1573	G
41	BQ	1574	C
41	BQ	1575	A
41	BQ	1576	G
41	BQ	1580	A
41	BQ	1581	C
41	BQ	1582	C
41	BQ	1583	A
41	BQ	1587	A
41	BQ	1588	A
41	BQ	1589	A
41	BQ	1590	G
41	BQ	1602	A
41	BQ	1605	A
41	BQ	1621	A
41	BQ	1629	U
41	BQ	1632	A
41	BQ	1639	C
41	BQ	1642	A
41	BQ	1643	A
41	BQ	1645	U
41	BQ	1658	G
41	BQ	1677	G
41	BQ	1683	A
41	BQ	1687	U
41	BQ	1688	U
41	BQ	1696	A
41	BQ	1704	A
41	BQ	1705	U
41	BQ	1715	A
41	BQ	1716	U
41	BQ	1717	U
41	BQ	1722	U
41	BQ	1724	U
41	BQ	1725	C

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Mol	Chain	Res	Type
41	BQ	1729	A
41	BQ	1730	G
41	BQ	1750	A
41	BQ	1751	G
41	BQ	1756	C
41	BQ	1760	A
41	BQ	1765	U
41	BQ	1766	G
41	BQ	1770	G
41	BQ	1775	G
41	BQ	1780	G
41	BQ	1788	C
41	BQ	1796	G
41	BQ	1797	A
41	BQ	1814	A
41	BQ	1816	A
41	BQ	1817	G
41	BQ	1819	U
41	BQ	1820	U
41	BQ	1821	U
41	BQ	1822	C
41	BQ	1839	A
41	BQ	1840	U
41	BQ	1841	A
41	BQ	1842	A
41	BQ	1846	C
41	BQ	1849	C
41	BQ	1850	A
41	BQ	1866	C
41	BQ	1867	A
41	BQ	1874	A
41	BQ	1880	U
41	BQ	1881	A
41	BQ	1893	A
41	BQ	1897	G
41	BQ	1906	G
41	BQ	1908	A
41	BQ	1930	A
41	BQ	1935	G
41	BQ	1943	C
41	BQ	1952	G
41	BQ	1953	G

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Mol	Chain	Res	Type
41	BQ	1954	G
41	BQ	1956	A
41	BQ	1957	G
41	BQ	1958	U
41	BQ	1960	A
41	BQ	1961	G
41	BQ	1962	A
41	BQ	1963	G
41	BQ	1964	C
41	BQ	1969	G
41	BQ	1972	A
41	BQ	1973	G
41	BQ	1976	G
41	BQ	1981	G
41	BQ	1984	C
41	BQ	1986	U
41	BQ	1988	C
41	BQ	1989	U
41	BQ	1992	U
41	BQ	1994	G
41	BQ	1998	G
41	BQ	2001	U
41	BQ	2006	G
41	BQ	2010	U
41	BQ	2013	C
41	BQ	2017	G
41	BQ	2020	A
41	BQ	2022	G
41	BQ	2032	U
41	BQ	2035	G
41	BQ	2039	C
41	BQ	2047	A
41	BQ	2048	G
41	BQ	2049	A
41	BQ	2050	C
41	BQ	2059	U
41	BQ	2081	U
41	BQ	2082	U
41	BQ	2087	C
41	BQ	2088	A
41	BQ	2089	A
41	BQ	2093	A

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Mol	Chain	Res	Type
41	BQ	2101	C
41	BQ	2102	U
41	BQ	2111	G
41	BQ	2112	U
41	BQ	2113	A
41	BQ	2121	G
41	BQ	2122	G
41	BQ	2131	A
41	BQ	2139	A
41	BQ	2149	A
41	BQ	2158	A
41	BQ	2169	G
41	BQ	2170	U
41	BQ	2187	G
41	BQ	2188	A
41	BQ	2201	G
41	BQ	2205	U
41	BQ	2206	G
41	BQ	2207	A
41	BQ	2209	U
41	BQ	2223	A
41	BQ	2232	A
41	BQ	2244	A
41	BQ	2249	G
41	BQ	2250	G
41	BQ	2252	A
41	BQ	2256	A
41	BQ	2262	A
41	BQ	2272	G
41	BQ	2273	G
41	BQ	2274	U
41	BQ	2279	A
41	BQ	2280	A
41	BQ	2281	A
41	BQ	2282	U
41	BQ	2284	C
41	BQ	2285	C
41	BQ	2288	G
41	BQ	2299	A
41	BQ	2306	C
41	BQ	2307	G
41	BQ	2308	C

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Mol	Chain	Res	Type
41	BQ	2309	A
41	BQ	2310	U
41	BQ	2313	A
41	BQ	2314	U
41	BQ	2315	G
41	BQ	2335	G
41	BQ	2347	U
41	BQ	2364	G
41	BQ	2372	A
41	BQ	2373	A
41	BQ	2374	C
41	BQ	2375	G
41	BQ	2385	G
41	BQ	2388	U
41	BQ	2393	G
41	BQ	2394	G
41	BQ	2397	A
41	BQ	2402	A
41	BQ	2403	G
41	BQ	2404	A
41	BQ	2411	U
41	BQ	2412	G
41	BQ	2419	A
41	BQ	2422	C
41	BQ	2434	U
41	BQ	2435	G
41	BQ	2437	G
41	BQ	2438	A
41	BQ	2439	A
41	BQ	2440	G
41	BQ	2446	U
41	BQ	2451	G
41	BQ	2452	G
41	BQ	2493	U
41	BQ	2496	C
41	BQ	2498	U
41	BQ	2501	U
41	BQ	2502	A
41	BQ	2503	G
41	BQ	2507	C
41	BQ	2514	U
41	BQ	2515	A

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Mol	Chain	Res	Type
41	BQ	2522	G
41	BQ	2523	A
41	BQ	2524	A
41	BQ	2525	G
41	BQ	2526	C
41	BQ	2531	C
41	BQ	2532	U
41	BQ	2537	U
41	BQ	2538	U
41	BQ	2539	C
41	BQ	2540	A
41	BQ	2541	U
41	BQ	2542	U
41	BQ	2543	U
41	BQ	2546	C
41	BQ	2549	G
41	BQ	2552	C
41	BQ	2554	A
41	BQ	2561	A
41	BQ	2569	A
41	BQ	2570	U
41	BQ	2571	U
41	BQ	2572	C
41	BQ	2573	G
41	BQ	2576	G
41	BQ	2585	G
41	BQ	2589	G
41	BQ	2593	A
41	BQ	2594	C
41	BQ	2595	A
41	BQ	2606	G
41	BQ	2607	G
41	BQ	2614	G
41	BQ	2626	A
41	BQ	2629	U
41	BQ	2636	A
41	BQ	2648	G
41	BQ	2652	U
41	BQ	2656	A
41	BQ	2672	G
41	BQ	2674	A
41	BQ	2677	G

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Mol	Chain	Res	Type
41	BQ	2689	A
41	BQ	2691	A
41	BQ	2694	A
41	BQ	2696	A
41	BQ	2703	A
41	BQ	2704	A
41	BQ	2714	G
41	BQ	2719	U
41	BQ	2728	G
41	BQ	2748	A
41	BQ	2749	G
41	BQ	2752	U
41	BQ	2753	G
41	BQ	2755	C
41	BQ	2777	G
41	BQ	2778	G
41	BQ	2796	G
41	BQ	2800	G
41	BQ	2801	A
41	BQ	2802	A
41	BQ	2803	A
41	BQ	2804	A
41	BQ	2805	G
41	BQ	2810	C
41	BQ	2817	A
41	BQ	2818	U
41	BQ	2821	C
41	BQ	2838	A
41	BQ	2842	U
41	BQ	2844	C
41	BQ	2845	A
41	BQ	2847	A
41	BQ	2849	C
41	BQ	2856	G
41	BQ	2861	U
41	BQ	2867	C
41	BQ	2871	G
41	BQ	2872	A
41	BQ	2873	U
41	BQ	2875	U
41	BQ	2876	C
41	BQ	2887	A

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Mol	Chain	Res	Type
41	BQ	2894	C
41	BQ	2899	C
41	BQ	2910	A
41	BQ	2916	U
41	BQ	2918	G
41	BQ	2923	U
41	BQ	2928	C
41	BQ	2933	A
41	BQ	2935	U
41	BQ	2936	A
41	BQ	2941	A
41	BQ	2942	C
41	BQ	2947	G
41	BQ	2954	U
41	BQ	2955	U
41	BQ	2957	G
41	BQ	2971	A
41	BQ	2983	C
41	BQ	2990	G
41	BQ	2996	U
41	BQ	2997	G
41	BQ	3003	G
41	BQ	3012	A
41	BQ	3030	G
41	BQ	3055	U
41	BQ	3056	U
41	BQ	3058	U
41	BQ	3059	G
41	BQ	3078	U
41	BQ	3079	U
41	BQ	3080	G
41	BQ	3086	A
41	BQ	3092	C
41	BQ	3101	G
41	BQ	3104	U
41	BQ	3115	C
41	BQ	3116	G
41	BQ	3118	C
41	BQ	3119	U
41	BQ	3122	A
41	BQ	3129	A
41	BQ	3130	A

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Mol	Chain	Res	Type
41	BQ	3131	U
41	BQ	3142	A
41	BQ	3143	C
41	BQ	3151	U
41	BQ	3154	C
41	BQ	3155	U
41	BQ	3156	U
41	BQ	3157	U
41	BQ	3158	G
41	BQ	3165	A
41	BQ	3170	A
41	BQ	3172	A
41	BQ	3173	G
41	BQ	3174	A
41	BQ	3175	U
41	BQ	3176	G
41	BQ	3180	A
41	BQ	3181	C
41	BQ	3187	A
41	BQ	3196	U
41	BQ	3199	G
41	BQ	3207	U
41	BQ	3209	A
41	BQ	3210	A
41	BQ	3216	G
41	BQ	3217	C
41	BQ	3218	A
41	BQ	3219	G
41	BQ	3222	U
41	BQ	3229	G
41	BQ	3243	A
41	BQ	3244	A
41	BQ	3245	A
41	BQ	3247	G
41	BQ	3259	U
41	BQ	3260	G
41	BQ	3263	G
41	BQ	3270	U
41	BQ	3272	C
41	BQ	3273	A
41	BQ	3276	G
41	BQ	3277	U

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Mol	Chain	Res	Type
41	BQ	3281	U
41	BQ	3286	G
41	BQ	3287	U
41	BQ	3288	G
41	BQ	3289	G
41	BQ	3294	A
41	BQ	3295	A
41	BQ	3304	U
41	BQ	3313	U
41	BQ	3316	A
41	BQ	3318	G
41	BQ	3319	U
41	BQ	3320	A
41	BQ	3334	U
41	BQ	3341	U
41	BQ	3345	G
41	BQ	3346	U
41	BQ	3347	A
41	BQ	3351	U
41	BQ	3352	U
41	BQ	3353	G
41	BQ	3354	U
41	BQ	3355	U
41	BQ	3356	G
41	BQ	3368	U
41	BQ	3369	G
41	BQ	3378	C
41	BQ	3381	U
41	BQ	3382	U
41	BQ	3386	G
41	BQ	3389	U
41	BQ	3390	G
41	BQ	3396	U
42	BR	7	G
42	BR	10	C
42	BR	17	A
42	BR	22	A
42	BR	35	C
42	BR	52	G
42	BR	53	U
42	BR	54	U
42	BR	65	G

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Mol	Chain	Res	Type
42	BR	74	C
42	BR	76	A
42	BR	99	G
42	BR	102	A
42	BR	112	G
42	BR	121	U
43	BS	16	G
43	BS	25	G
43	BS	34	U
43	BS	35	C
43	BS	38	U
43	BS	59	A
43	BS	62	C
43	BS	63	G
43	BS	80	A
43	BS	81	U
43	BS	82	U
43	BS	83	C
43	BS	84	C
43	BS	85	G
43	BS	86	U
43	BS	87	G
43	BS	90	U
43	BS	95	G
43	BS	97	A
43	BS	99	C
43	BS	104	A
43	BS	106	C
43	BS	111	A
43	BS	112	U
43	BS	113	U
43	BS	125	U
43	BS	126	A
43	BS	138	A
43	BS	148	G
43	BS	152	G
43	BS	157	U
43	BS	158	U

All (110) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type

Mol	Chain	Res	Type
33	2	68	A
33	2	77	U
33	2	139	C
33	2	141	U
33	2	215	A
33	2	224	C
33	2	237	C
33	2	278	U
33	2	313	U
33	2	322	G
33	2	352	A
33	2	387	A
33	2	400	A
33	2	447	U
33	2	511	A
33	2	518	A
33	2	539	G
33	2	541	A
33	2	555	A
33	2	609	U
33	2	639	U
33	2	640	U
33	2	705	U
33	2	711	U
33	2	740	A
33	2	755	A
33	2	803	A
33	2	819	G
33	2	912	U
33	2	928	U
33	2	987	G
33	2	1023	A
33	2	1207	C
33	2	1226	A
33	2	1245	G
33	2	1251	U
33	2	1256	A
33	2	1273	G
33	2	1274	C
33	2	1314	U
33	2	1344	A

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Mol	Chain	Res	Type
33	2	1348	A
33	2	1382	A
33	2	1399	C
33	2	1430	U
33	2	1471	A
33	2	1556	A
33	2	1557	U
33	2	1573	A
33	2	1584	G
33	2	1633	A
33	2	1636	C
33	2	1700	C
41	BQ	13	A
41	BQ	282	G
41	BQ	439	C
41	BQ	637	C
41	BQ	763	G
41	BQ	849	C
41	BQ	873	C
41	BQ	896	A
41	BQ	916	G
41	BQ	993	G
41	BQ	1064	A
41	BQ	1097	G
41	BQ	1271	A
41	BQ	1307	G
41	BQ	1355	A
41	BQ	1562	C
41	BQ	1572	U
41	BQ	1582	C
41	BQ	1716	U
41	BQ	1729	A
41	BQ	1815	U
41	BQ	1820	U
41	BQ	1952	G
41	BQ	1953	G
41	BQ	1956	A
41	BQ	1957	G
41	BQ	1959	G
41	BQ	1961	G
41	BQ	1962	A
41	BQ	1963	G

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Mol	Chain	Res	Type
41	BQ	1964	C
41	BQ	2086	A
41	BQ	2112	U
41	BQ	2231	C
41	BQ	2445	A
41	BQ	2500	A
41	BQ	2501	U
41	BQ	2502	A
41	BQ	2513	U
41	BQ	2514	U
41	BQ	2525	G
41	BQ	2537	U
41	BQ	2538	U
41	BQ	2541	U
41	BQ	3055	U
41	BQ	3078	U
41	BQ	3121	U
41	BQ	3218	A
41	BQ	3228	C
41	BQ	3269	U
41	BQ	3275	U
41	BQ	3319	U
41	BQ	3350	C
42	BR	52	G
43	BS	82	U
43	BS	85	G
43	BS	125	U

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

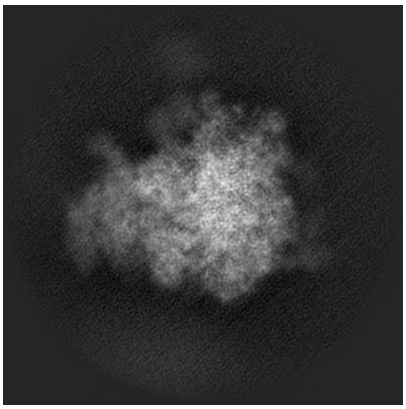
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-16182. These allow visual inspection of the internal detail of the map and identification of artifacts.

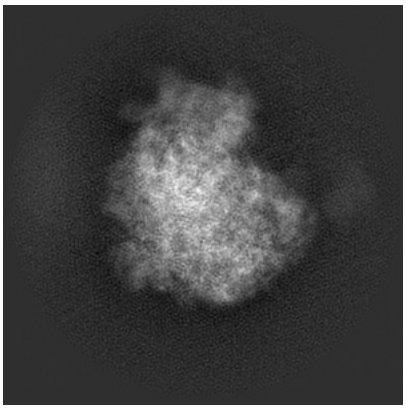
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

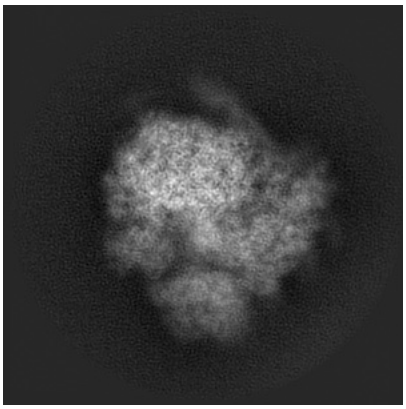
6.1.1 Primary map



X

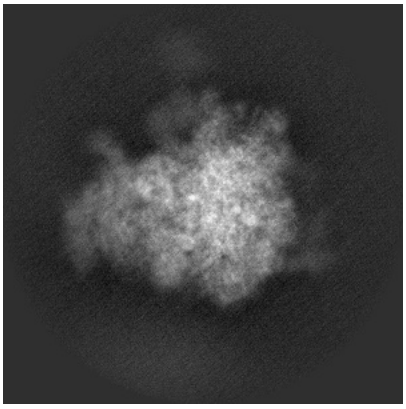


Y

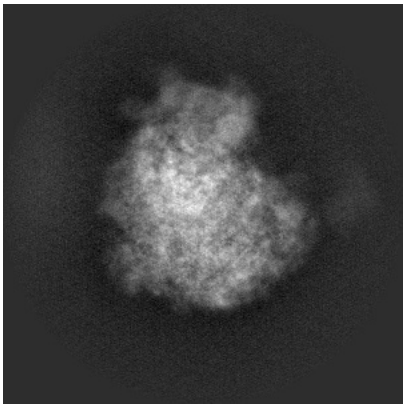


Z

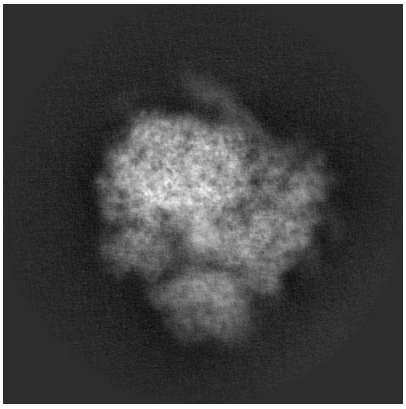
6.1.2 Raw map



X



Y

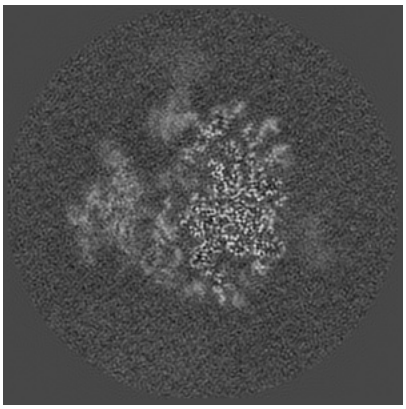


Z

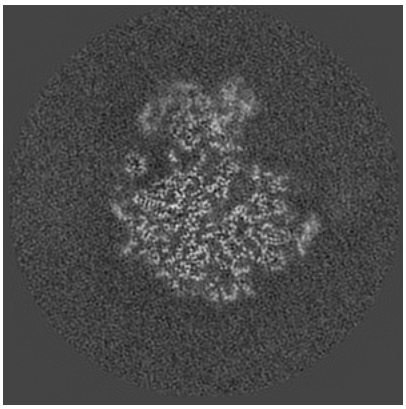
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

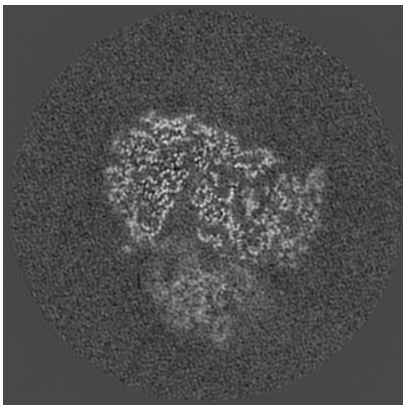
6.2.1 Primary map



X Index: 210

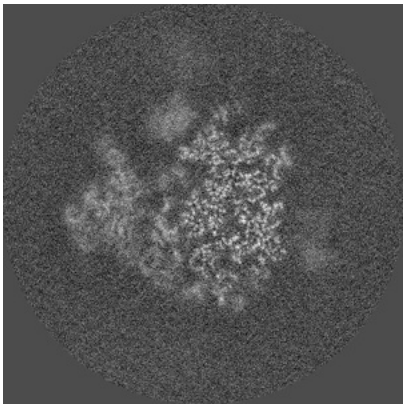


Y Index: 210

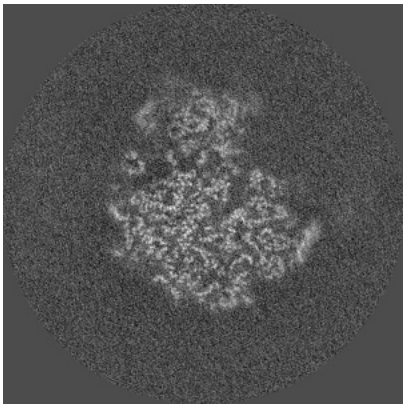


Z Index: 210

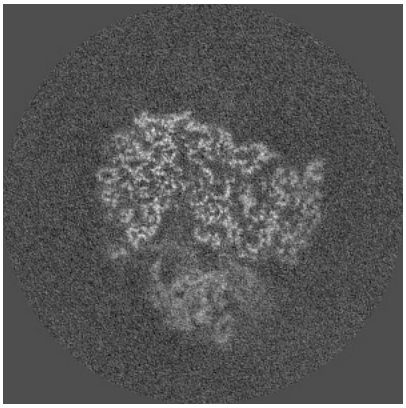
6.2.2 Raw map



X Index: 210



Y Index: 210

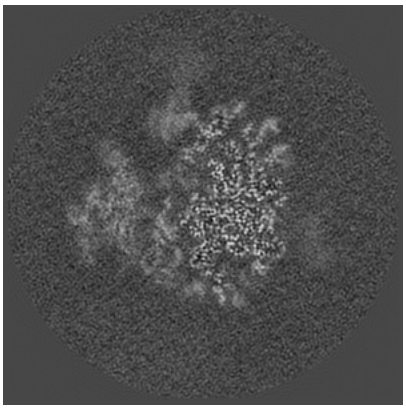


Z Index: 210

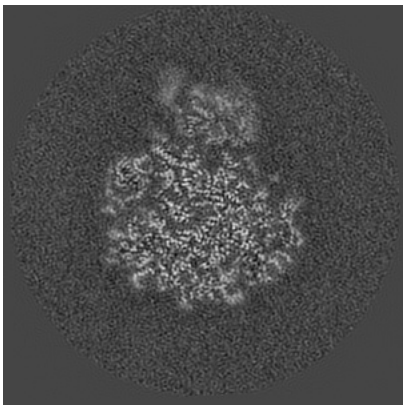
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

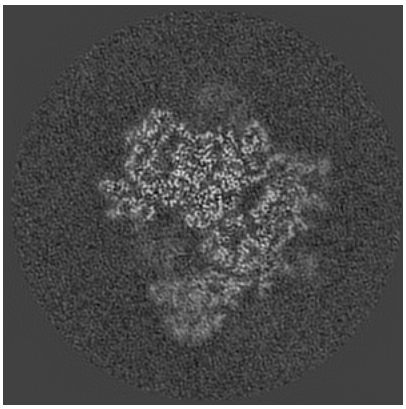
6.3.1 Primary map



X Index: 210

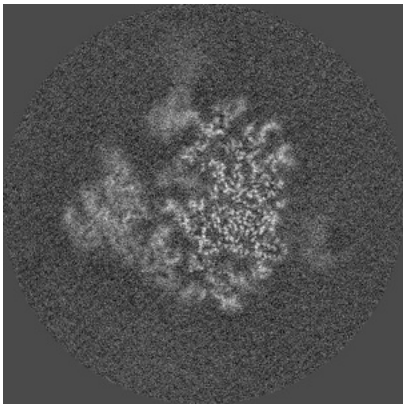


Y Index: 234

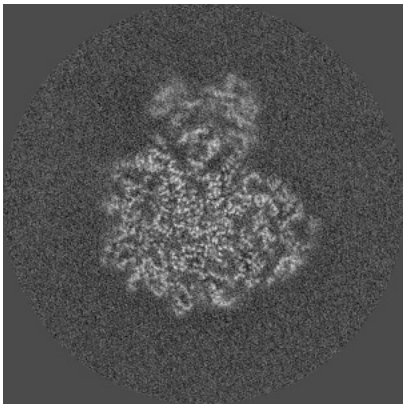


Z Index: 190

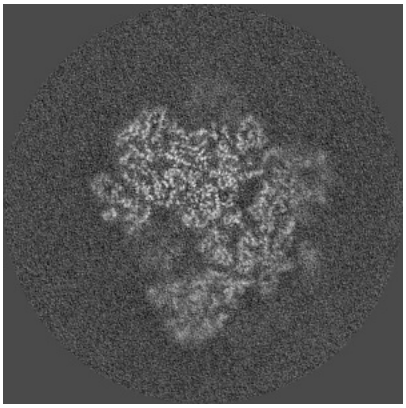
6.3.2 Raw map



X Index: 204



Y Index: 226

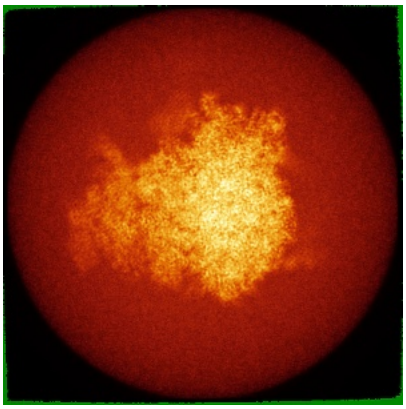


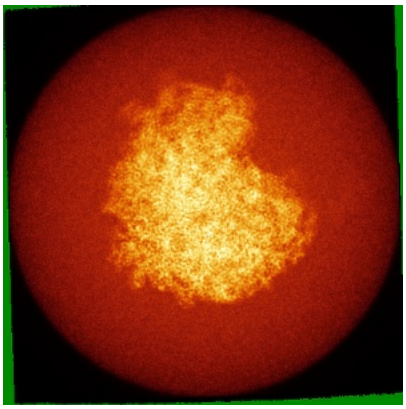
Z Index: 188

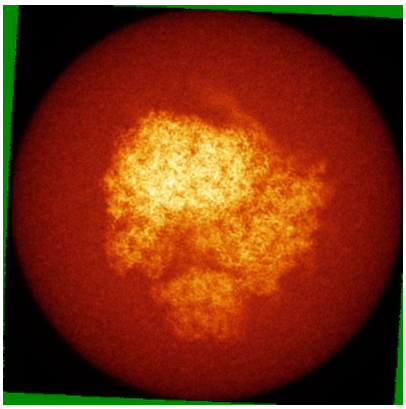
The images above show the largest variance slices of the map in three orthogonal directions.

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

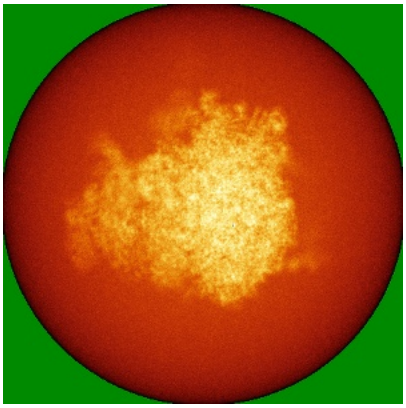
6.4.1 Primary map

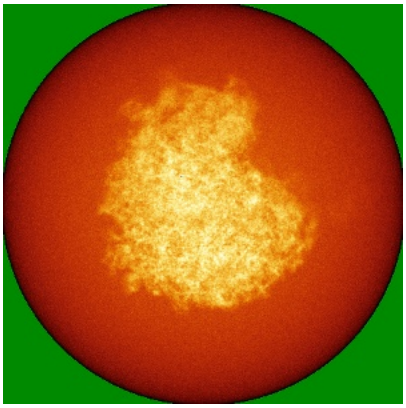

X

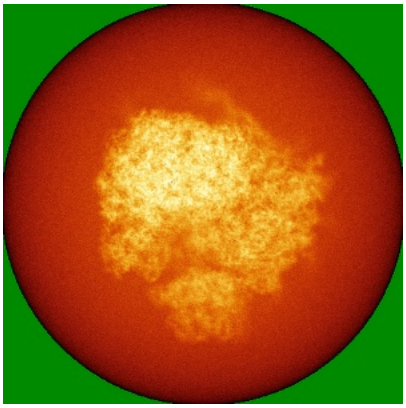

Y


Z

6.4.2 Raw map


X

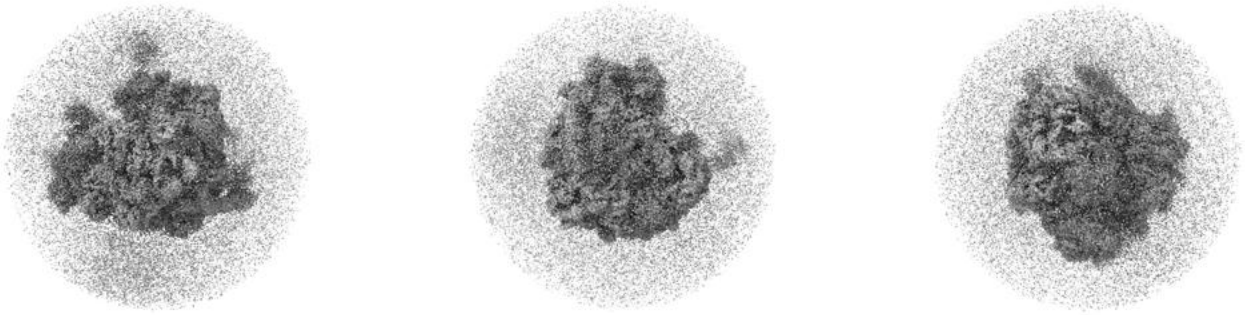

Y


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)

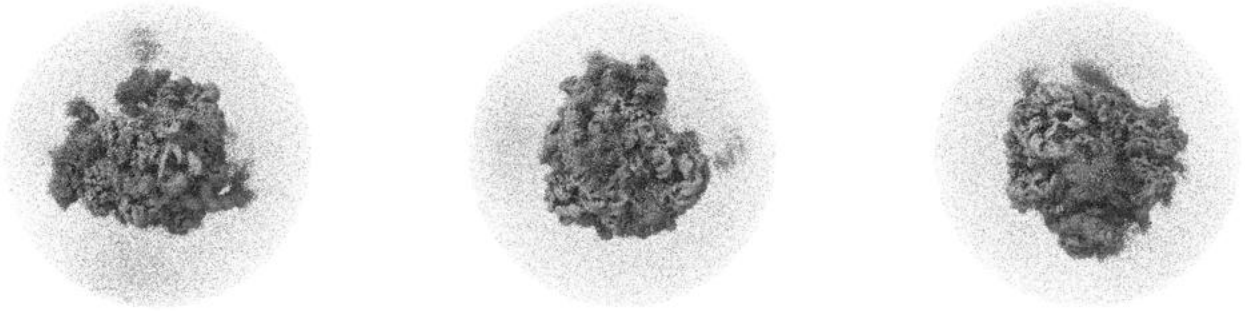
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.015. 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.

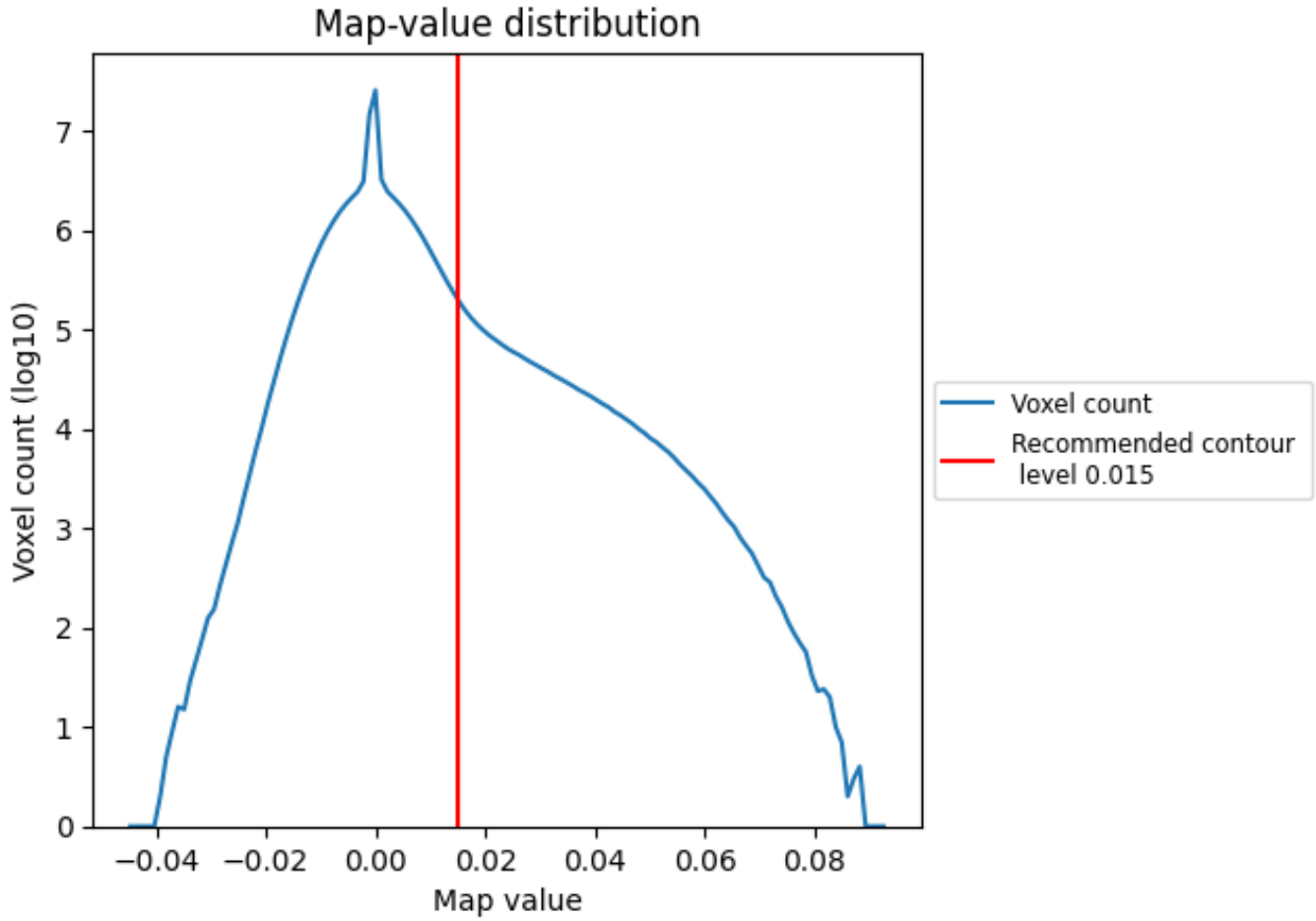
6.6 Mask visualisation (i)

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

7 Map analysis

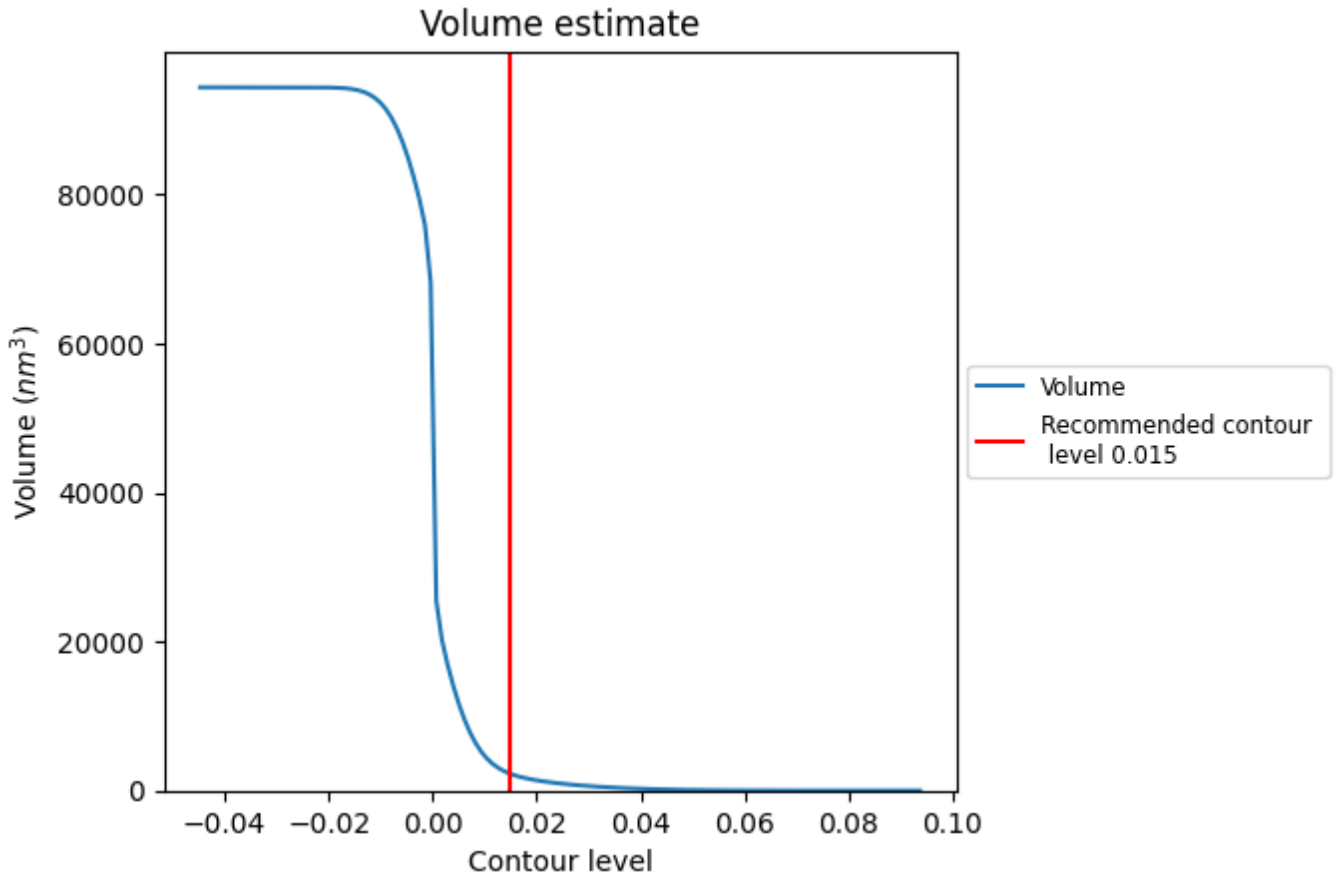
This section contains the results of statistical analysis of the map.

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.

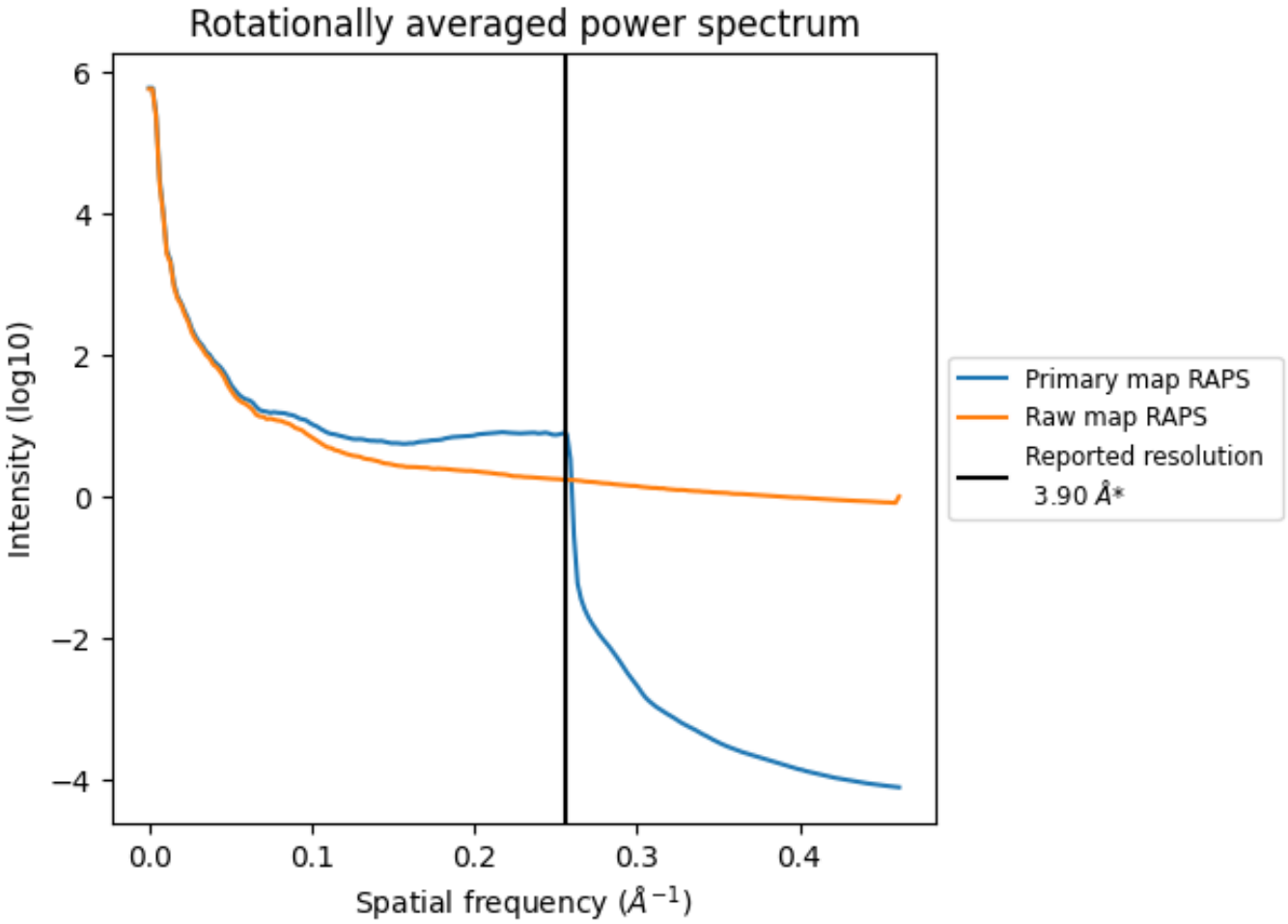
7.2 Volume estimate



The volume at the recommended contour level is 2238 nm^3; this corresponds to an approximate mass of 2022 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)

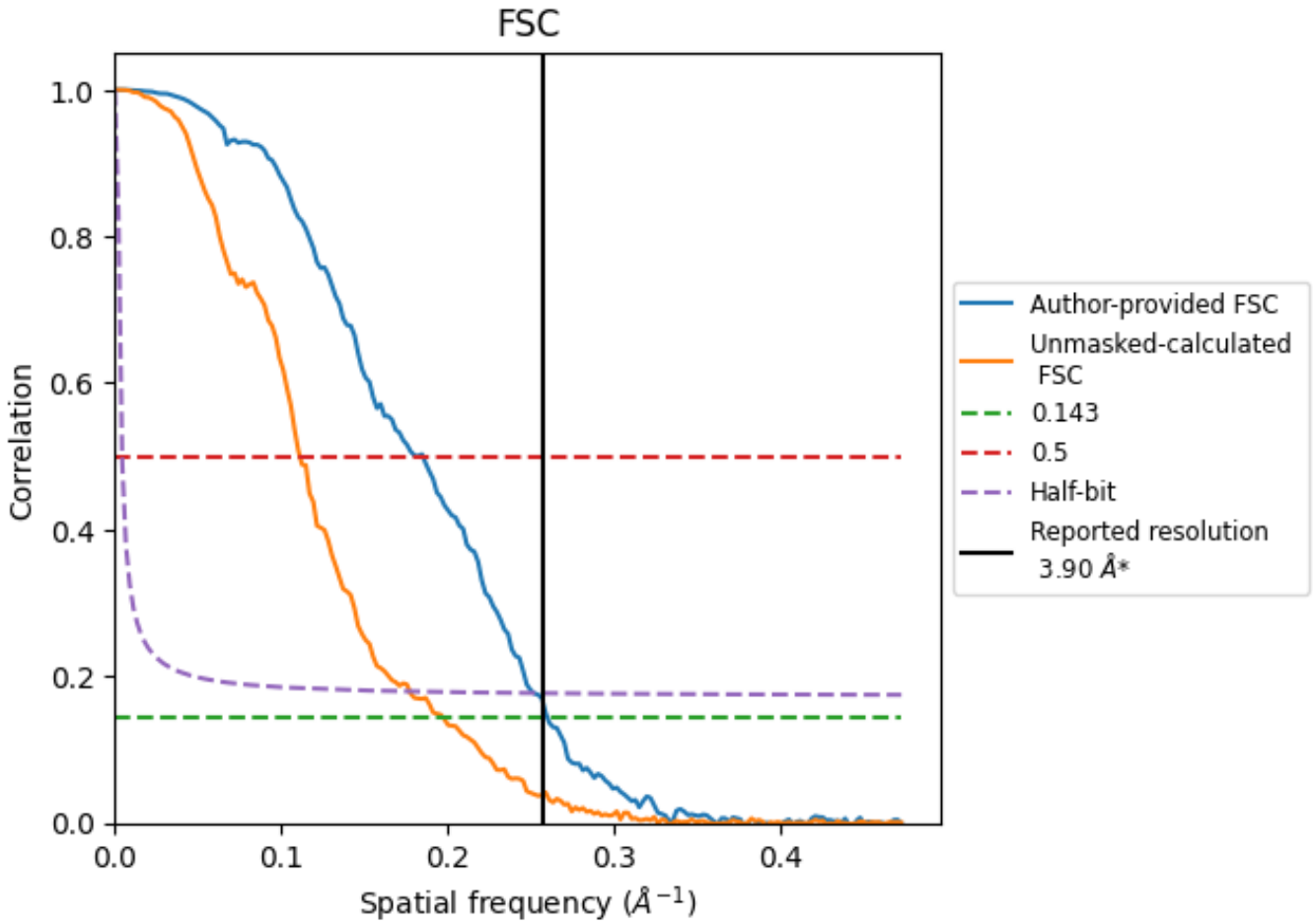


*Reported resolution corresponds to spatial frequency of 0.256 $Å^{-1}$

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 0.256 Å^{-1}

8.2 Resolution estimates (i)

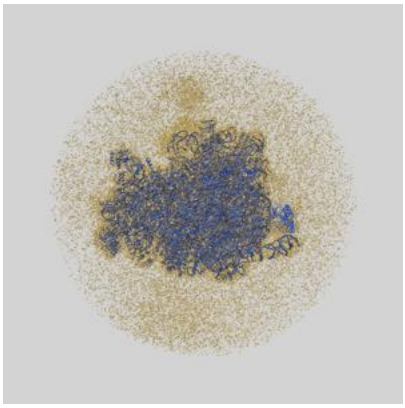
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	3.85	5.41	3.97
Unmasked-calculated*	5.07	9.00	5.65

*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 5.07 differs from the reported value 3.9 by more than 10 %

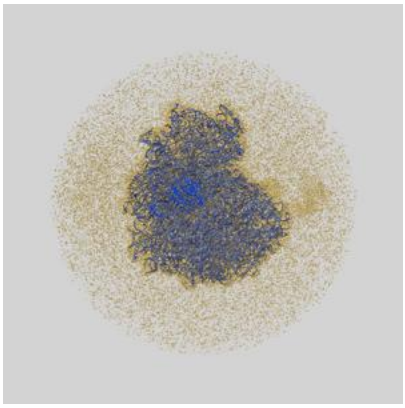
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-16182 and PDB model 8BQD. Per-residue inclusion information can be found in section 3 on page 19.

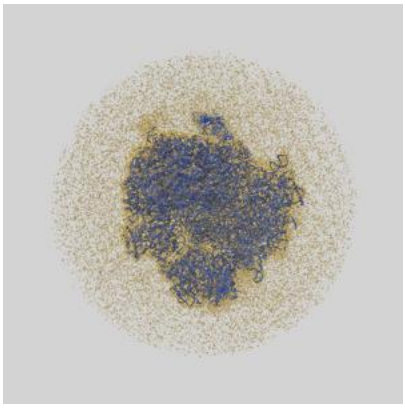
9.1 Map-model overlay



X



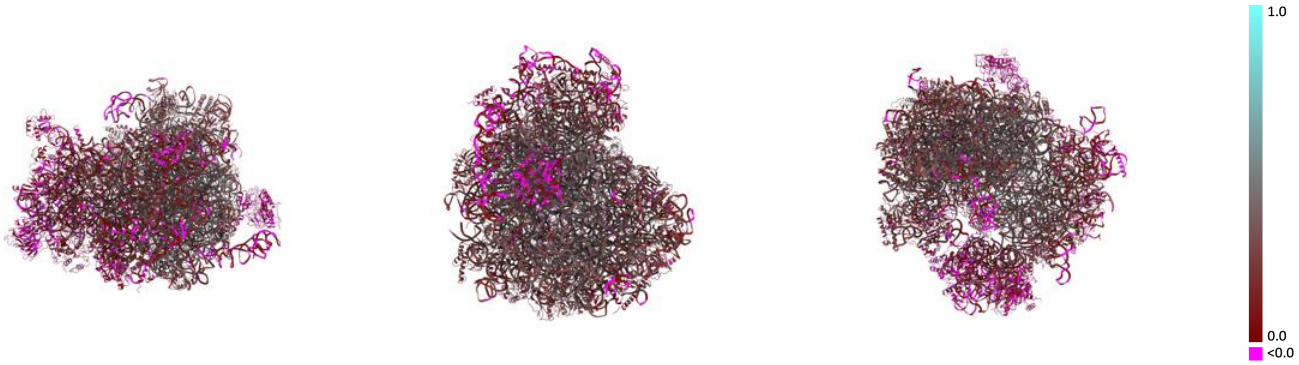
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.015 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.

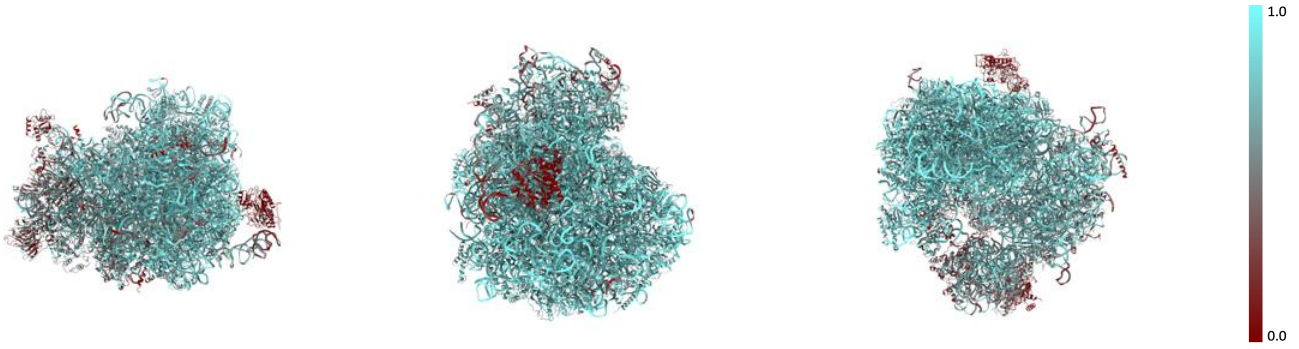
9.2 Q-score mapped to coordinate model (i)



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.

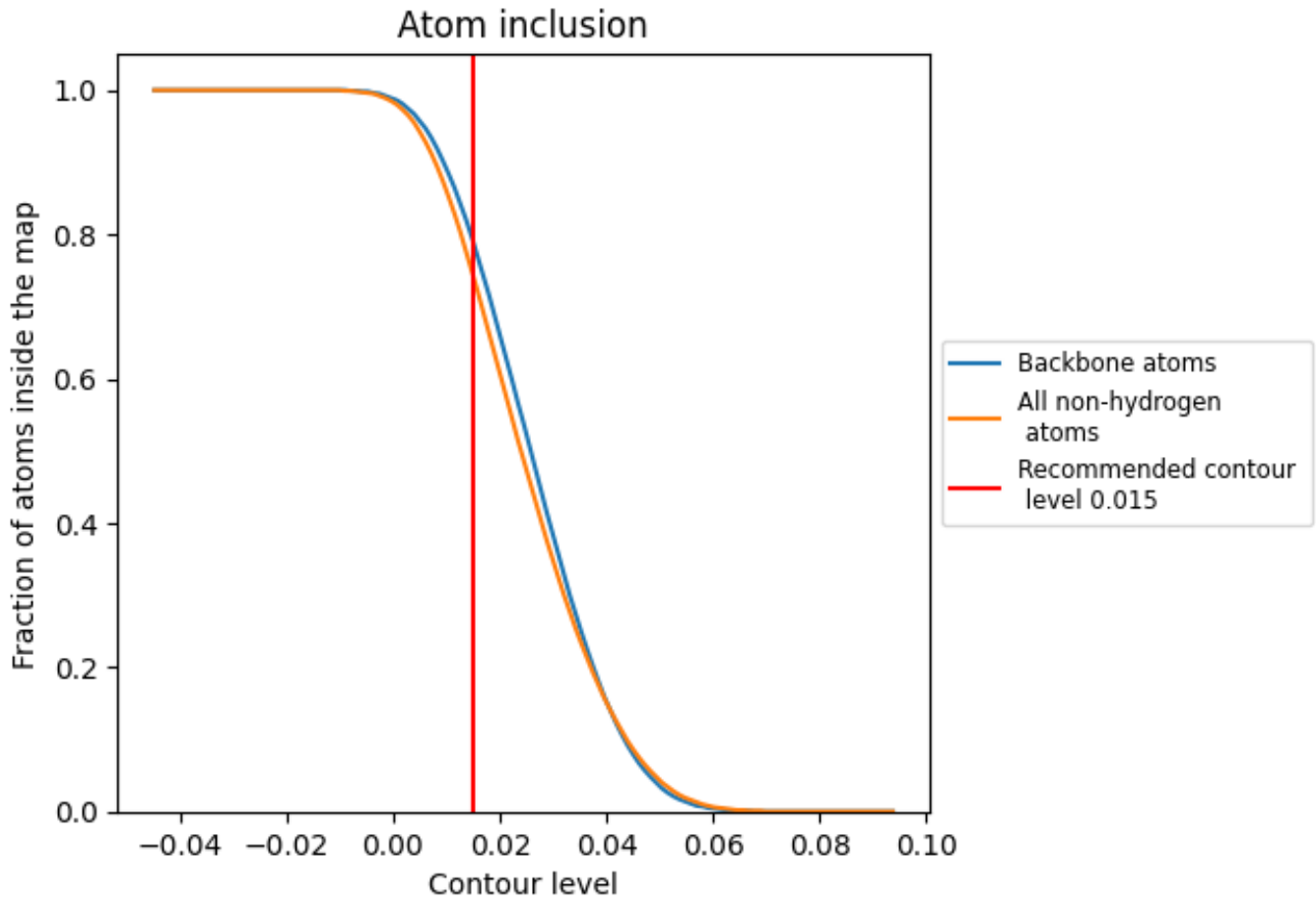
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.015).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 74% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7440	0.2600
2	0.7670	0.2040
A	0.4170	0.1210
AA	0.7120	0.2650
AB	0.7440	0.3750
AC	0.7150	0.2650
AD	0.7370	0.2810
AE	0.5680	0.2350
AF	0.8550	0.4080
AG	0.6770	0.2200
AH	0.7650	0.3430
AI	0.7110	0.3040
AJ	0.7340	0.2860
AK	0.7790	0.3130
AL	0.7710	0.3550
AM	0.7430	0.2710
AN	0.7090	0.2730
AO	0.7580	0.2840
AP	0.7490	0.3520
AQ	0.7820	0.3420
AR	0.7830	0.3310
AS	0.6730	0.2600
AT	0.7390	0.3600
AU	0.7610	0.3040
AV	0.7460	0.3250
AW	0.7810	0.3900
AX	0.7820	0.3600
AY	0.7450	0.3220
B	0.3660	0.0380
BA	0.7810	0.3370
BB	0.7730	0.3240
BC	0.7510	0.3530
BD	0.6430	0.2270
BE	0.7550	0.3080
BF	0.7290	0.3190

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Chain	Atom inclusion	Q-score
BG	0.7710	0.3430
BH	0.7690	0.3200
BI	0.7250	0.2450
BJ	0.7730	0.3330
BK	0.7540	0.3170
BL	0.7580	0.2960
BM	0.7000	0.2150
BN	0.7480	0.3660
BO	0.7620	0.3070
BP	0.7530	0.3070
BQ	0.8710	0.3260
BR	0.8930	0.2850
BS	0.9070	0.3440
BT	0.1430	0.0560
C	0.4820	0.1510
D	0.2020	0.0520
E	0.4730	0.1120
F	0.4410	0.0520
G	0.4540	0.0960
H	0.4500	0.0500
I	0.4700	0.0640
J	0.4920	0.0910
K	0.3460	0.0080
L	0.3950	0.0930
M	0.5280	0.1000
N	0.4170	0.0560
O	0.3390	0.0220
P	0.5450	0.1210
Q	0.5020	0.1420
R	0.6180	0.2140
S	0.6130	0.2080
T	0.6090	0.1620
U	0.5260	0.1190
V	0.6910	0.2410
W	0.6420	0.2120
X	0.6620	0.2750
Y	0.6630	0.2510
Z	0.5330	0.1600
a	0.6130	0.1810
b	0.6300	0.2330
c	0.6750	0.2970
d	0.6280	0.1720

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Chain	Atom inclusion	Q-score
e	0.5840	0.1750
f	0.5510	0.1600
g	0.5570	0.1940
x	0.0510	0.0080