wwPDB X-ray Structure Validation Summary Report (i)

Sep 14, 2023 – 09:57 AM EDT

PDB ID	:	4W29
Title	:	70S ribosome translocation intermediate containing elongation factor EFG/GDP/fusidic acid, mRNA, and tRNAs trapped in the AP/AP pe/E chimeric hybrid state.
Authors	:	Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on	:	2014-07-02
Resolution	:	3.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

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

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

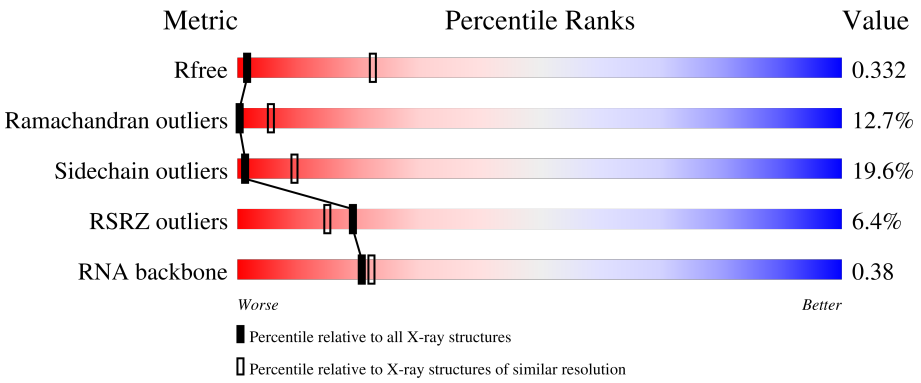
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AB	235	2%, 76%, 22%, •
1	CB	235	%, 75%, 23%, •
2	AC	207	43%, 72%, 27%, •
2	CC	207	39%, 75%, 24%, •

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Mol	Chain	Length	Quality of chain
3	AD	208	%, 71%, 27%
3	CD	208	75%, 24%
4	AE	151	10%, 80%, 19%
4	CE	151	6%, 78%, 19%
5	AF	101	76%, 23%
5	CF	101	79%, 20%
6	AG	155	5%, 86%, 14%
6	CG	155	4%, 83%, 15%
7	AH	138	78%, 22%
7	CH	138	76%, 22%
8	AI	127	2%, 83%, 17%
8	CI	127	%, 81%, 17%
9	AJ	99	37%, 72%, 27%
9	CJ	99	35%, 73%, 26%
10	AK	119	8%, 82%, 17%
10	CK	119	3%, 77%, 21%
11	AL	125	3%, 58%, 35%, 6%
11	CL	125	5%, 58%, 36%, 5%
12	AM	125	5%, 80%, 19%
12	CM	125	6%, 76%, 22%
13	AN	60	22%, 82%, 17%
13	CN	60	17%, 72%, 23%, 5%
14	AO	88	%, 80%, 18%
14	CO	88	85%, 13%
15	AP	84	8%, 85%, 15%

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Mol	Chain	Length	Quality of chain
15	CP	84	12% 76% 24%
16	AQ	100	80% 18%
16	CQ	100	2% 82% 16%
17	AR	70	6% 73% 24%
17	CR	70	4% 84% 16%
18	AS	79	% 70% 25% 5%
18	CS	79	6% 76% 24%
19	AT	99	5% 82% 16%
19	CT	99	16% 79% 19%
20	AY	687	3% 71% 23%
20	CY	687	3% 70% 24%
21	AA	1511	% 74% 24%
21	CA	1511	2% 71% 26%
22	AW	77	12% 42% 51% 8%
22	CW	77	9% 38% 52% 10%
23	AV	36	22% 19% 72% 8%
23	CV	36	44% 19% 64% 17%
24	AX	78	4% 50% 42% 8%
24	CX	78	3% 49% 42% 9%
25	BC	228	29% 58% 33% 8%
25	DC	228	21% 62% 32% 6%
26	BD	275	8% 74% 24%
26	DD	275	5% 74% 23%
27	BE	205	5% 74% 23%
27	DE	205	4% 69% 29%

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Mol	Chain	Length	Quality of chain
28	BF	208	11% 74% 21%
28	DF	208	15% 71% 27%
29	BG	181	12% 86% 14%
29	DG	181	14% 80% 18%
30	BH	167	4% 75% 25%
30	DH	167	5% 78% 22%
31	BJ	170	99%
31	DJ	170	98%
32	BK	140	5% 71% 26%
32	DK	140	5% 74% 22%
33	BN	139	40% 42% 40% 14%
33	DN	139	41% 43% 40% 12% 6%
34	BO	122	37% 75% 23%
34	DO	122	46% 77% 20%
35	BP	146	3% 66% 32%
35	DP	146	2% 71% 27%
36	BQ	141	3% 67% 28% 5%
36	DQ	141	6% 79% 21%
37	BR	117	74% 24%
37	DR	117	% 73% 25%
38	BS	99	20% 72% 23% 5%
38	DS	99	11% 66% 30%
39	BT	138	31% 66% 28% 5%
39	DT	138	25% 64% 30% 5%
40	BU	117	% 79% 21%

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Mol	Chain	Length	Quality of chain
40	DU	117	%, 80%, 18%
41	BV	101	5%, 68%, 24%, 8%
41	DV	101	5%, 74%, 23%
42	BW	113	3%, 78%, 21%
42	DW	113	4%, 73%, 23%
43	BX	93	4%, 75%, 23%
43	DX	93	2%, 70%, 27%
44	BY	107	9%, 64%, 31%, 5%
44	DY	107	6%, 71%, 25%
45	BZ	185	72%, 26%
45	DZ	185	2%, 72%, 25%
46	B0	84	18%, 87%, 12%
46	D0	84	5%, 79%, 21%
47	B1	93	22%, 63%, 26%, 6%
47	D1	93	29%, 61%, 30%, 8%
48	B2	71	79%, 20%
48	D2	71	3%, 83%, 15%
49	B3	60	2%, 85%, 13%
49	D3	60	83%, 17%
50	B4	35	31%, 66%, 31%
50	D4	35	23%, 63%, 34%
51	B5	59	69%, 27%
51	D5	59	3%, 69%, 29%
52	B6	50	28%, 60%, 30%, 8%
52	D6	50	26%, 50%, 42%, 8%

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Mol	Chain	Length	Quality of chain
53	B7	49	33% 80% 16%
53	D7	49	20% 76% 22%
54	B8	64	16% 70% 27%
54	D8	64	11% 66% 28% 6%
55	B9	37	3% 76% 24%
55	D9	37	84% 16%
56	Be	103	12% 86% 12%
56	De	103	9% 80% 19%
57	Bf	31	100%
57	Bg	31	100%
57	Df	31	100%
57	Dg	31	100%
58	Bh	30	100%
58	Dh	30	100%
59	BA	2879	% 71% 27%
59	DA	2879	% 71% 26%
60	BB	119	5% 67% 31%
60	DB	119	61% 38%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 312066 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	AB	235	1910	1218	342	345	5	0	0	0
1	CB	235	1910	1218	342	345	5	0	0	0

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	AC	207	1621	1022	315	283	1	0	0	0
2	CC	207	1621	1022	315	283	1	0	0	0

- Molecule 3 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AD	208	1703	1066	339	291	7	0	0	0
3	CD	208	1703	1066	339	291	7	0	0	0

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AE	151	1156	729	218	205	4	0	0	0
4	CE	151	1156	729	218	205	4	0	0	0

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AF	101	843	531	155	154	3	0	0	0
5	CF	101	843	531	155	154	3	0	0	0

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AG	155	1257	781	252	218	6	0	0	0
6	CG	155	1257	781	252	218	6	0	0	0

- Molecule 7 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AH	138	1116	705	215	193	3	0	0	0
7	CH	138	1116	705	215	193	3	0	0	0

- Molecule 8 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
8	AI	127	1010	639	197	174	0	0	0
8	CI	127	1010	639	197	174	0	0	0

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	AJ	99	802	504	157	140	1	0	0	0
9	CJ	99	802	504	157	140	1	0	0	0

- Molecule 10 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AK	119	885	549	168	165	3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	CK	119	885	549	168	165	3	0	0	0

- Molecule 11 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AL	125	976	614	196	165	1	0	0	0
11	CL	125	976	614	196	165	1	0	0	0

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AM	125	997	617	207	171	2	0	0	0
12	CM	125	997	617	207	171	2	0	0	0

- Molecule 13 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AN	60	492	312	104	72	4	0	0	0
13	CN	60	492	312	104	72	4	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
14	AO	88	734	459	147	126	2	0	0	0
14	CO	88	734	459	147	126	2	0	0	0

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AP	84	706	446	140	119	1	0	0	0
15	CP	84	706	446	140	119	1	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AQ	100	835	534	155	144	2	0	0	0
16	CQ	100	835	534	155	144	2	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	AR	70	574	367	112	95	0	0	0
17	CR	70	574	367	112	95	0	0	0

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
18	AS	79	634	405	115	112	2	0	0	0
18	CS	79	634	405	115	112	2	0	0	0

- Molecule 19 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AT	99	763	470	162	129	2	0	0	0
19	CT	99	763	470	162	129	2	0	0	0

- Molecule 20 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AY	661	5173	3288	884	983	18	0	0	0
20	CY	661	5173	3288	884	983	18	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	40	THR	HIS	conflict	UNP Q72I01

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Chain	Residue	Modelled	Actual	Comment	Reference
AY	129	LYS	HIS	conflict	UNP Q72I01
AY	226	ASN	HIS	conflict	UNP Q72I01
CY	40	THR	HIS	conflict	UNP Q72I01
CY	129	LYS	HIS	conflict	UNP Q72I01
CY	226	ASN	HIS	conflict	UNP Q72I01

- Molecule 21 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
21	AA	1511	32474	14455	6015	10494	1510	0	0	0
21	CA	1511	32474	14455	6015	10494	1510	0	0	0

- Molecule 22 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
22	AW	77	1635	732	291	536	76	0	0	0
22	CW	77	1635	732	291	536	76	0	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
23	AV	36	783	351	159	237	36	0	0	0
23	CV	36	781	352	159	235	35	0	0	0

- Molecule 24 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
24	AX	78	1629	730	293	531	75	0	0	0
24	CX	78	1629	730	293	531	75	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AX	77	VAL	-	expression tag	GB 1154835240

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Chain	Residue	Modelled	Actual	Comment	Reference
AX	78	ACE	-	expression tag	GB 1154835240
CX	77	VAL	-	expression tag	GB 1154835240
CX	78	ACE	-	expression tag	GB 1154835240

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	BC	228	1742	1101	319	319	3	0	0	0
25	DC	228	1742	1101	319	319	3	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	BD	275	2145	1353	428	361	3	0	0	0
26	DD	275	2145	1353	428	361	3	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	BE	205	1569	991	300	272	6	0	0	0
27	DE	205	1569	991	300	272	6	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	BF	208	1628	1037	304	284	3	0	0	0
28	DF	208	1628	1037	304	284	3	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	BG	181	1474	942	268	260	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	DG	181	1474	942	268	260	4	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	BH	167	1274	806	238	229	1	0	0	0
30	DH	167	1274	806	238	229	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein l10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
31	BJ	170	851	510	170	171	0	0	0
31	DJ	170	851	510	170	171	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	BK	140	1035	659	183	188	5	0	0	0
32	DK	140	1035	659	183	188	5	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	BN	139	1114	717	207	186	4	0	0	0
33	DN	139	1114	717	207	186	4	0	0	0

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
34	BO	122	933	588	171	170	4	0	0	0
34	DO	122	933	588	171	170	4	0	0	0

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
35	BP	146	1114	692	227	193	2	0	0	0
35	DP	146	1114	692	227	193	2	0	0	0

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
36	BQ	141	1122	715	212	188	7	0	0	0
36	DQ	141	1122	715	212	188	7	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BQ	32	TYR	PHE	conflict	UNP Q72I11
DQ	32	TYR	PHE	conflict	UNP Q72I11

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
37	BR	117	960	599	202	159	0	0	0
37	DR	117	960	599	202	159	0	0	0

- Molecule 38 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
38	BS	99	775	488	155	132	0	0	0
38	DS	99	775	488	155	132	0	0	0

- Molecule 39 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	BT	138	1147	713	235	198	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
39	DT	138	1147	713	235	198	1	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
40	BU	117	964	610	202	151	1	0	0	0
			Total	C	N	O	S			
40	DU	117	964	610	202	151	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
41	BV	101	779	501	142	135	1	0	0	0
			Total	C	N	O	S			
41	DV	101	779	501	142	135	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BW	113	900	566	177	155	2	0	0	0
			Total	C	N	O	S			
42	DW	113	900	566	177	155	2	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	BX	93	734	477	132	125	0	0	0
			Total	C	N	O			
43	DX	93	734	477	132	125	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	BY	107	818	524	155	134	5	0	0	0
			Total	C	N	O	S			
44	DY	107	818	524	155	134	5	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
45	BZ	185	1473	939	262	270	2	0	0	0
45	DZ	185	1473	939	262	270	2	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	B0	84	662	410	140	111	1	0	0	0
46	D0	84	662	410	140	111	1	0	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	B1	93	732	460	145	126	1	0	0	0
47	D1	93	732	460	145	126	1	0	0	0

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	B2	71	598	370	121	106	1	0	0	0
48	D2	71	598	370	121	106	1	0	0	0

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	B3	60	477	303	91	82	1	0	0	0
49	D3	60	477	303	91	82	1	0	0	0

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	B4	35	271	174	44	50	3	0	0	0
50	D4	35	271	174	44	50	3	0	0	0

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	B5	59	459	288	90	76	5	0	0	0
51	D5	59	459	288	90	76	5	0	0	0

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	B6	50	433	270	88	71	4	0	0	0
52	D6	50	433	270	88	71	4	0	0	0

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
53	B7	49	430	263	108	57	2	0	0	0
53	D7	49	430	263	108	57	2	0	0	0

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
54	B8	64	517	331	102	82	2	0	0	0
54	D8	64	517	331	102	82	2	0	0	0

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	B9	37	307	188	68	47	4	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
55	D9	37	307	188	68	47	4	0	0	0

- Molecule 56 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
56	Be	102	686	430	119	137	0	0	0
56	De	102	686	430	119	137	0	0	0

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Be	1	UNK	-	expression tag	UNP Q72GS2
Be	2	UNK	-	expression tag	UNP Q72GS2
Be	3	UNK	-	expression tag	UNP Q72GS2
Be	4	UNK	-	expression tag	UNP Q72GS2
Be	5	UNK	-	expression tag	UNP Q72GS2
Be	6	UNK	-	expression tag	UNP Q72GS2
Be	7	UNK	-	expression tag	UNP Q72GS2
Be	8	UNK	-	expression tag	UNP Q72GS2
Be	9	UNK	-	expression tag	UNP Q72GS2
Be	10	UNK	-	expression tag	UNP Q72GS2
Be	11	UNK	-	expression tag	UNP Q72GS2
Be	12	UNK	-	expression tag	UNP Q72GS2
Be	13	UNK	-	expression tag	UNP Q72GS2
Be	14	UNK	-	expression tag	UNP Q72GS2
Be	15	UNK	-	expression tag	UNP Q72GS2
Be	16	UNK	-	expression tag	UNP Q72GS2
Be	17	UNK	-	expression tag	UNP Q72GS2
Be	18	UNK	-	expression tag	UNP Q72GS2
Be	19	UNK	-	expression tag	UNP Q72GS2
Be	20	UNK	-	expression tag	UNP Q72GS2
Be	21	UNK	-	expression tag	UNP Q72GS2
Be	22	UNK	-	expression tag	UNP Q72GS2
Be	23	UNK	-	expression tag	UNP Q72GS2
Be	24	UNK	-	expression tag	UNP Q72GS2
Be	25	UNK	-	expression tag	UNP Q72GS2
Be	26	UNK	-	expression tag	UNP Q72GS2
Be	27	UNK	-	expression tag	UNP Q72GS2
Be	28	UNK	-	expression tag	UNP Q72GS2

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Chain	Residue	Modelled	Actual	Comment	Reference
Be	29	UNK	-	expression tag	UNP Q72GS2
Be	30	UNK	-	expression tag	UNP Q72GS2
Be	31	UNK	-	expression tag	UNP Q72GS2
De	1	UNK	-	expression tag	UNP Q72GS2
De	2	UNK	-	expression tag	UNP Q72GS2
De	3	UNK	-	expression tag	UNP Q72GS2
De	4	UNK	-	expression tag	UNP Q72GS2
De	5	UNK	-	expression tag	UNP Q72GS2
De	6	UNK	-	expression tag	UNP Q72GS2
De	7	UNK	-	expression tag	UNP Q72GS2
De	8	UNK	-	expression tag	UNP Q72GS2
De	9	UNK	-	expression tag	UNP Q72GS2
De	10	UNK	-	expression tag	UNP Q72GS2
De	11	UNK	-	expression tag	UNP Q72GS2
De	12	UNK	-	expression tag	UNP Q72GS2
De	13	UNK	-	expression tag	UNP Q72GS2
De	14	UNK	-	expression tag	UNP Q72GS2
De	15	UNK	-	expression tag	UNP Q72GS2
De	16	UNK	-	expression tag	UNP Q72GS2
De	17	UNK	-	expression tag	UNP Q72GS2
De	18	UNK	-	expression tag	UNP Q72GS2
De	19	UNK	-	expression tag	UNP Q72GS2
De	20	UNK	-	expression tag	UNP Q72GS2
De	21	UNK	-	expression tag	UNP Q72GS2
De	22	UNK	-	expression tag	UNP Q72GS2
De	23	UNK	-	expression tag	UNP Q72GS2
De	24	UNK	-	expression tag	UNP Q72GS2
De	25	UNK	-	expression tag	UNP Q72GS2
De	26	UNK	-	expression tag	UNP Q72GS2
De	27	UNK	-	expression tag	UNP Q72GS2
De	28	UNK	-	expression tag	UNP Q72GS2
De	29	UNK	-	expression tag	UNP Q72GS2
De	30	UNK	-	expression tag	UNP Q72GS2
De	31	UNK	-	expression tag	UNP Q72GS2

- Molecule 57 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
57	Bf	31	156	93	31	32	0	0	0
			Total	C	N	O			
57	Bg	31	156	93	31	32	0	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
57	Df	31	156	93	31	32	0	0	0
57	Dg	31	156	93	31	32	0	0	0

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
58	Bh	30	151	90	30	31	0	0	0
58	Dh	30	151	90	30	31	0	0	0

- Molecule 59 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
59	BA	2879	61997	27594	11582	19943	2878	0	0	0
59	DA	2879	61997	27594	11582	19943	2878	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

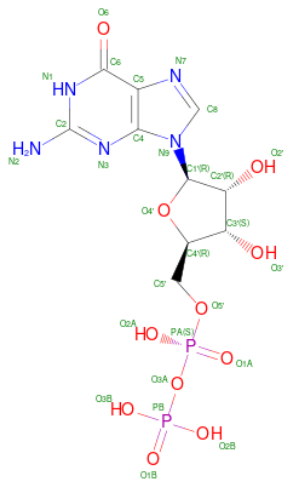
Chain	Residue	Modelled	Actual	Comment	Reference
BA	1141A	U	C	conflict	GB 46197919
BA	2825	U	G	conflict	GB 46197919
DA	1141A	U	C	conflict	GB 46197919
DA	2825	U	G	conflict	GB 46197919

- Molecule 60 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
60	BB	119	2551	1136	471	826	118	0	0	0
60	DB	119	2551	1136	471	826	118	0	0	0

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

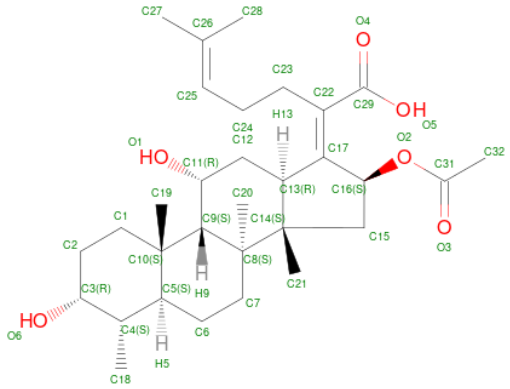
GDP



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
61	AY	1	28	10	5	11	2	0	0
			Total	C	N	O	P		
61	CY	1	28	10	5	11	2	0	0

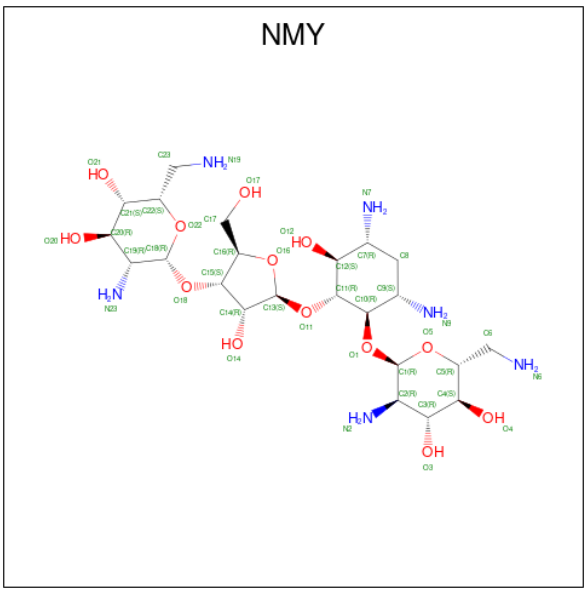
- Molecule 62 is FUSIDIC ACID (three-letter code: FUA) (formula: $C_{31}H_{48}O_6$).

FUA



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
62	AY	1	37	31	6	0	0
			Total	C	O		
62	CY	1	37	31	6	0	0

- Molecule 63 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
63	AA	1	42	23	6	13	0	0
			Total	C	N	O		
63	BA	1	42	23	6	13	0	0
			Total	C	N	O		
63	BA	1	42	23	6	13	0	0
			Total	C	N	O		
63	BA	1	42	23	6	13	0	0
			Total	C	N	O		
63	CA	1	42	23	6	13	0	0
			Total	C	N	O		
63	DA	1	42	23	6	13	0	0

- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

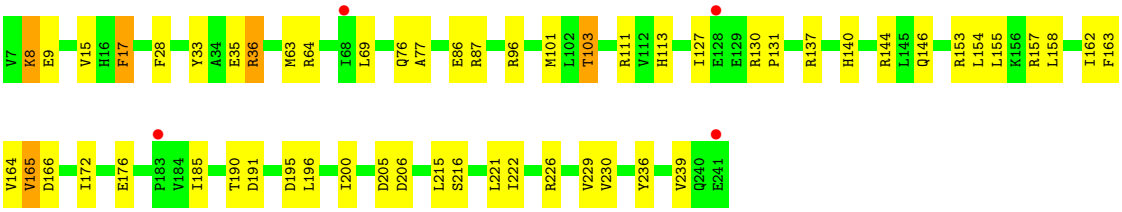
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
64	BA	1	1	1	0	0
			Total	Mg		
64	CY	1	1	1	0	0

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

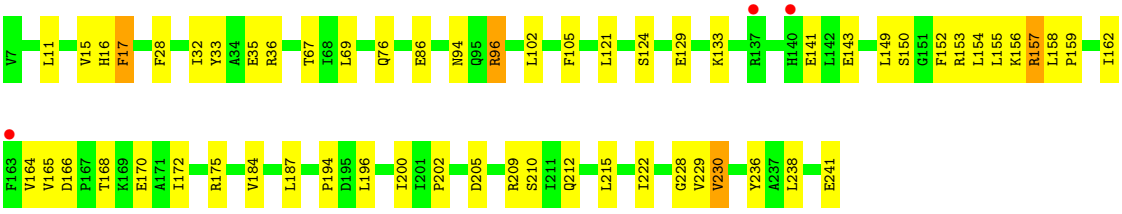
• Molecule 1: 30S ribosomal protein S2

Chain AB:



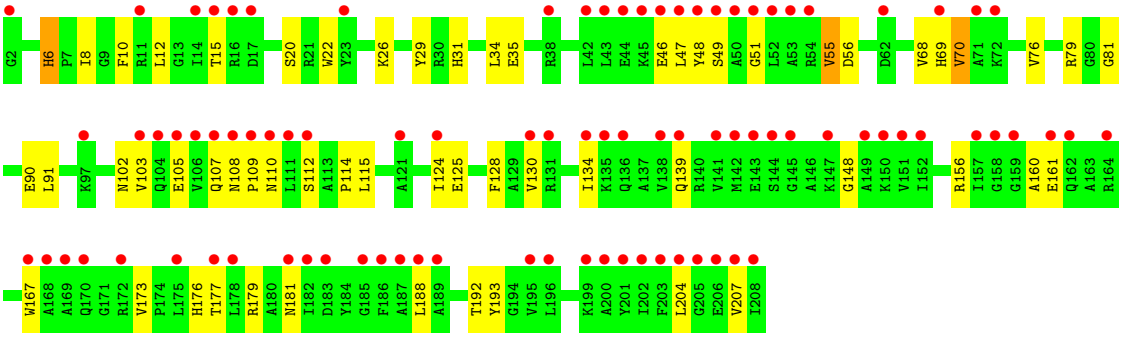
• Molecule 1: 30S ribosomal protein S2

Chain CB:



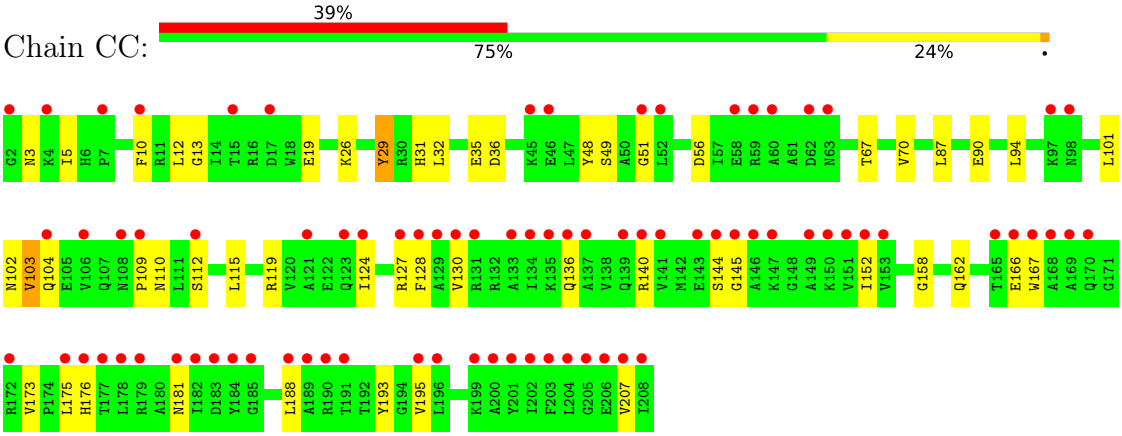
• Molecule 2: 30S ribosomal protein S3

Chain AC:



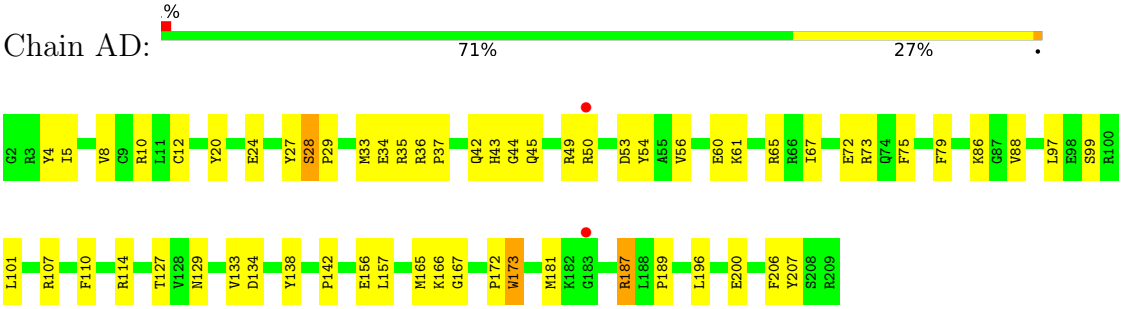
• Molecule 2: 30S ribosomal protein S3

Chain CC:



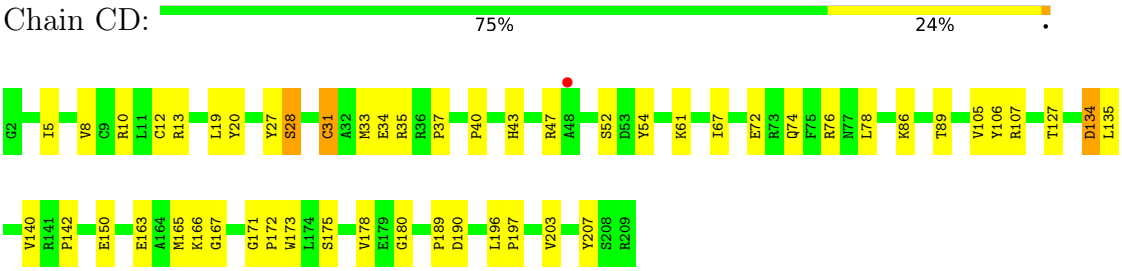
- Molecule 3: 30S ribosomal protein S4

Chain AD:



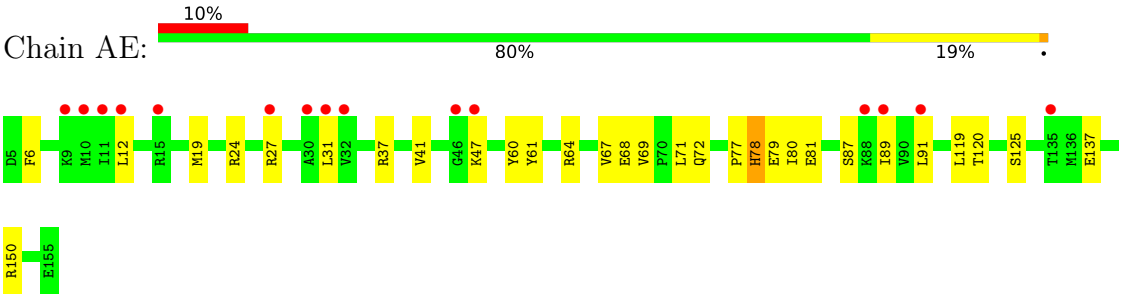
- Molecule 3: 30S ribosomal protein S4

Chain CD:



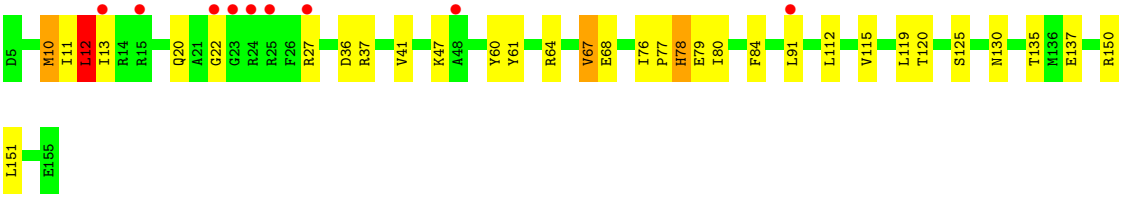
- Molecule 4: 30S ribosomal protein S5

Chain AE:



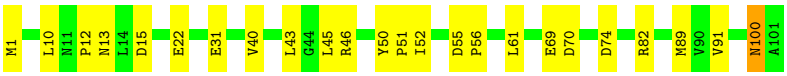
- Molecule 4: 30S ribosomal protein S5

Chain CE:



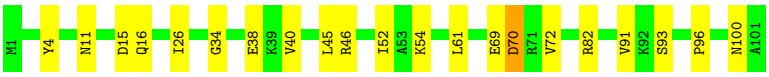
• Molecule 5: 30S ribosomal protein S6

Chain AF: 76% 23%



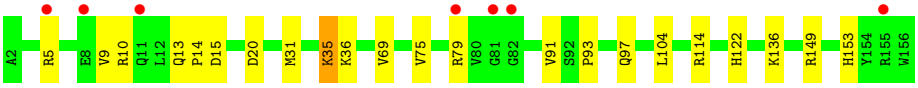
• Molecule 5: 30S ribosomal protein S6

Chain CF: 79% 20%



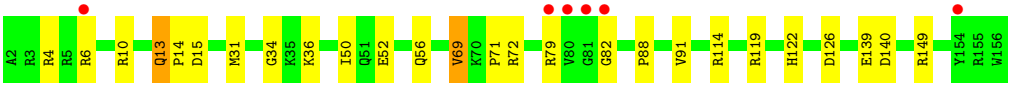
• Molecule 6: 30S ribosomal protein S7

Chain AG: 5% 86% 14%



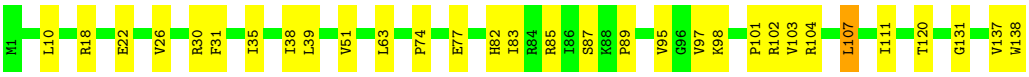
• Molecule 6: 30S ribosomal protein S7

Chain CG: 4% 83% 15%



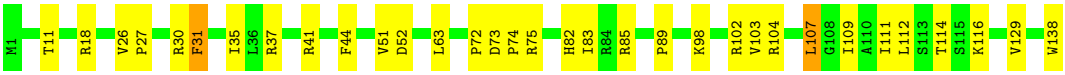
• Molecule 7: 30S ribosomal protein S8

Chain AH: 78% 22%



• Molecule 7: 30S ribosomal protein S8

Chain CH: 76% 22%



• Molecule 8: 30S ribosomal protein S9

Chain AI: 2% 83% 17%

E2 Q3 Y4 R10 K25 N29 E35 Q38 G39 L79 Y88 N89 P90 D91 Y92 R93 A94 K95 R104 D105 A106 R107 V108 V109 E110 K113 Y114 G115 K118 A119 S126 K127 R128

• Molecule 8: 30S ribosomal protein S9

Chain CI: % 81% 17%

E2 Q3 Y4 R10 G22 N23 G24 K25 E35 Y36 F37 Q38 V41 R42 L56 R66 L79 Y88 R93 A94 K95 L96 K97 R107 R111 Y114 G115 K118 R121 K127 R128

• Molecule 9: 30S ribosomal protein S10

Chain AJ: 37% 72% 27%

K3 I6 K7 L8 F11 D12 H13 K14 T15 L16 Q21 K22 I23 R29 A32 Q33 P37 L40 P41 T42 F47 T48 V49 I50 F54 K55 H56 K57 D58 S59 R60 E61 H62 F63 E64 L65 R66 T67 H68 N69 R70 L71 V72 D73 I74 I75 R79 K80 T81 I82

E83 Q84 L85 M86 T87 L88 D89 L90 P91 T92 G93 V94 E95 I96 E97 I98 K99 T100 V101

• Molecule 9: 30S ribosomal protein S10

Chain CJ: 35% 73% 26%

K3 I4 R5 I6 K7 L8 R9 G10 F11 D12 D17 A18 S19 A20 Q21 K22 E25 R29 A32 Q33 V34 S35 L40 F47 T48 V49 I50 P53 F54 K55 H56 K57 R60 E61 H62 F63 E64 N69 R70 L71 V72 D73 I74 I75 N78 R79 K80 T81 I82 E83

Q84 L85 M86 T87 L88 D89 G93 V94 E95 I96 E97 I98 K99 T100 V101

• Molecule 10: 30S ribosomal protein S11

Chain AK: 8% 82% 17%

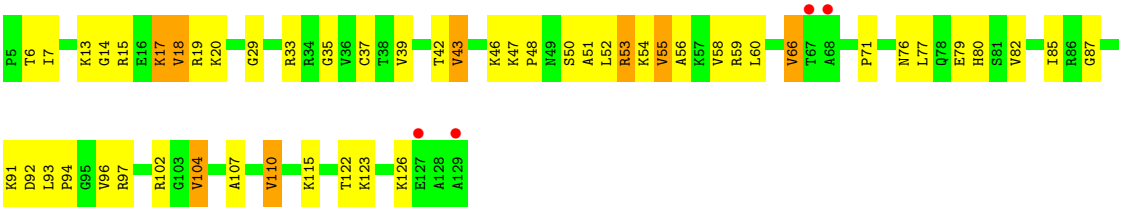
K11 R12 Q13 V14 R18 I21 T31 P35 D36 G37 N38 P39 I40 T41 W42 S43 S44 I48 G49 Y50 T57 K70 Q78 G88 G102 L103 Q104 I108 V109 D110 D111 T112 P113 G118 A128 S129

• Molecule 10: 30S ribosomal protein S11

Chain CK: 3% 77% 21%

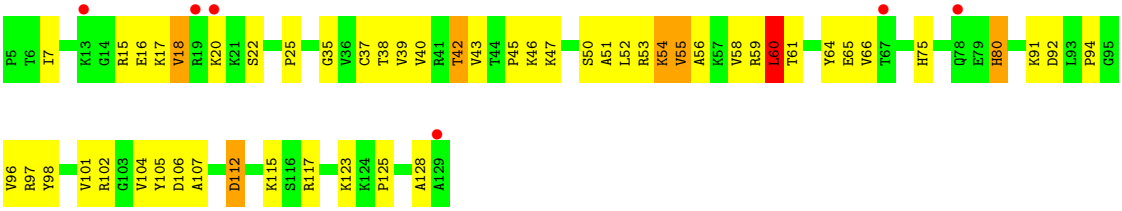
• Molecule 11: 30S ribosomal protein S12

Chain AL:



• Molecule 11: 30S ribosomal protein S12

Chain CL:



• Molecule 12: 30S ribosomal protein S13

Chain AM:

• Molecule 12: 30S ribosomal protein S13

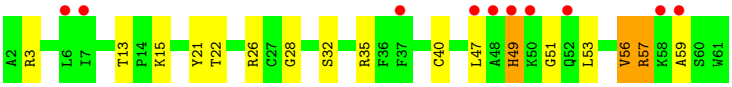
Chain CM:

• Molecule 13: 30S ribosomal protein S14 type Z

Chain AN:

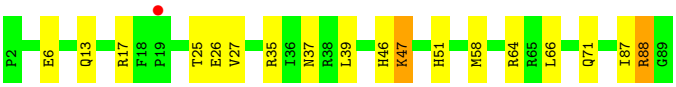
• Molecule 13: 30S ribosomal protein S14 type Z

Chain CN:



• Molecule 14: 30S ribosomal protein S15

Chain AO:

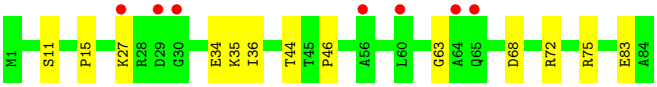


• Molecule 14: 30S ribosomal protein S15

Chain CO:

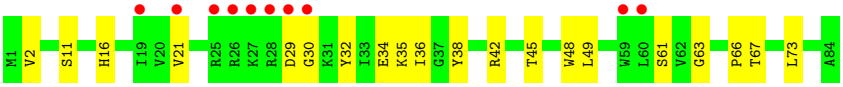
• Molecule 15: 30S ribosomal protein S16

Chain AP:



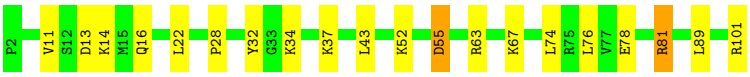
• Molecule 15: 30S ribosomal protein S16

Chain CP:



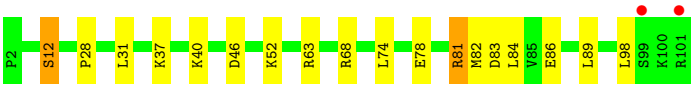
• Molecule 16: 30S ribosomal protein S17

Chain AQ:



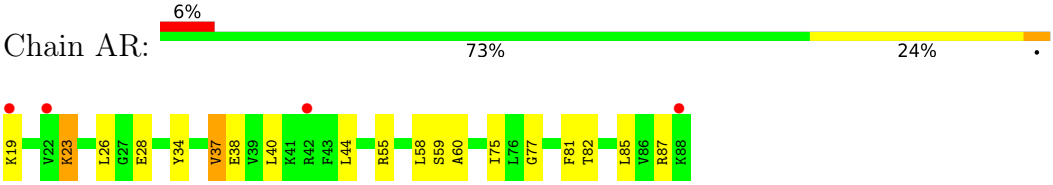
• Molecule 16: 30S ribosomal protein S17

Chain CQ:



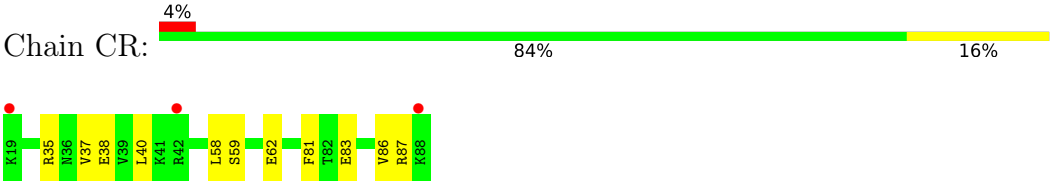
• Molecule 17: 30S ribosomal protein S18

Chain AR:



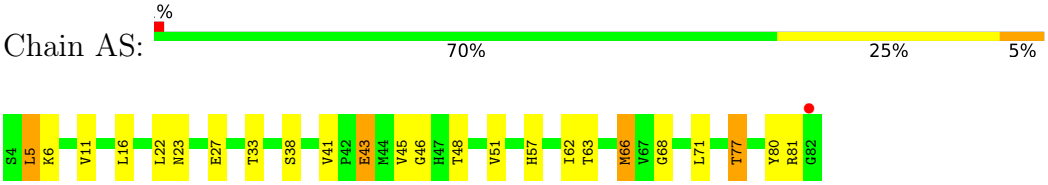
• Molecule 17: 30S ribosomal protein S18

Chain CR:



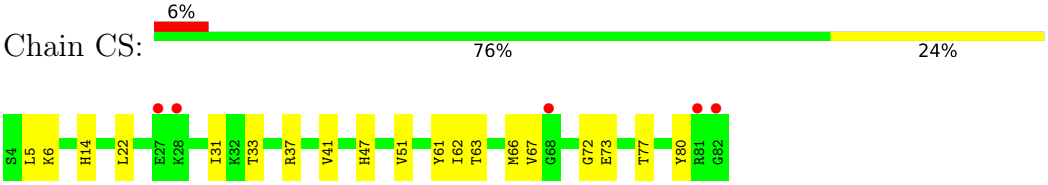
• Molecule 18: 30S ribosomal protein S19

Chain AS:



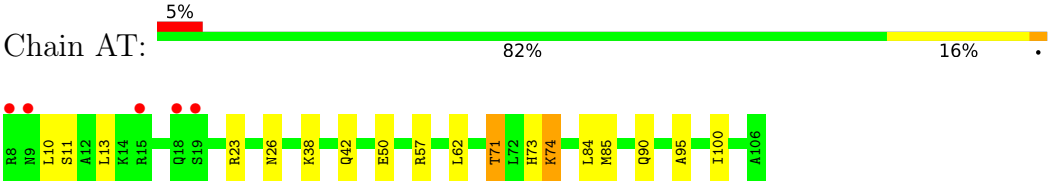
• Molecule 18: 30S ribosomal protein S19

Chain CS:



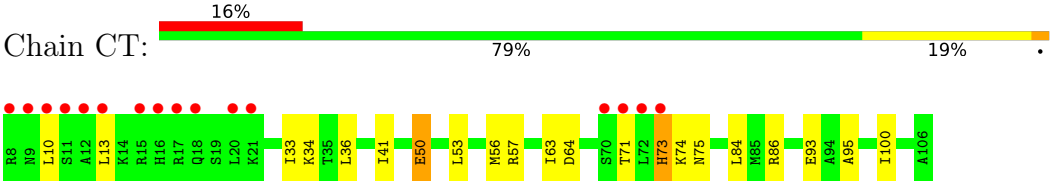
• Molecule 19: 30S ribosomal protein S20

Chain AT:



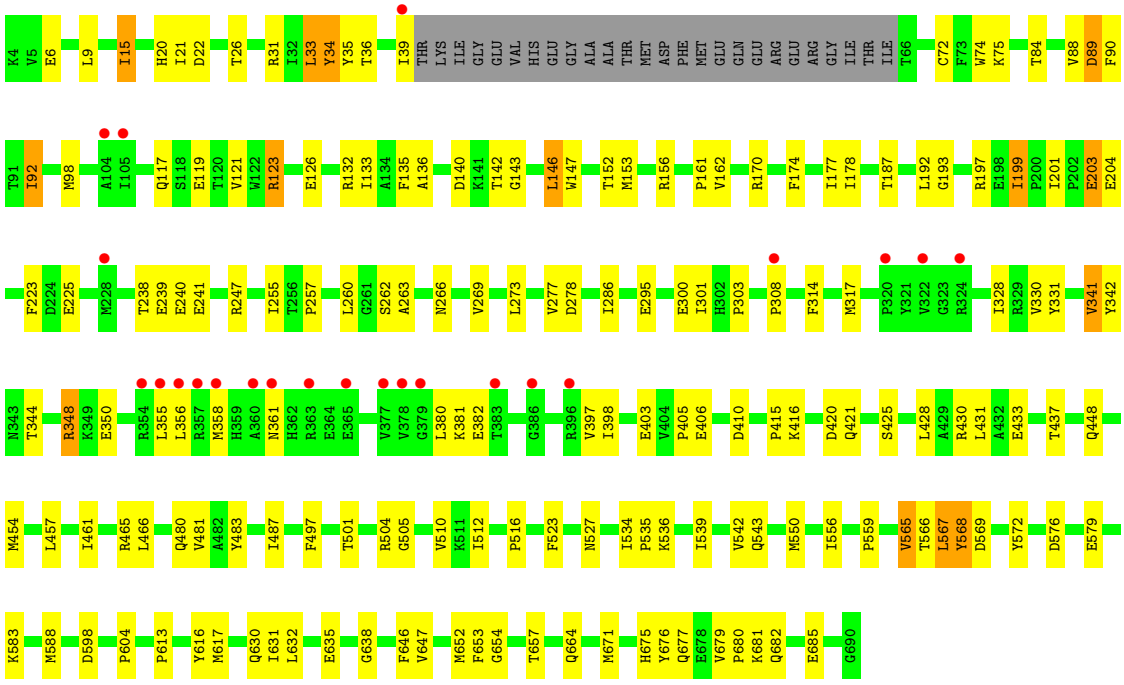
• Molecule 19: 30S ribosomal protein S20

Chain CT:



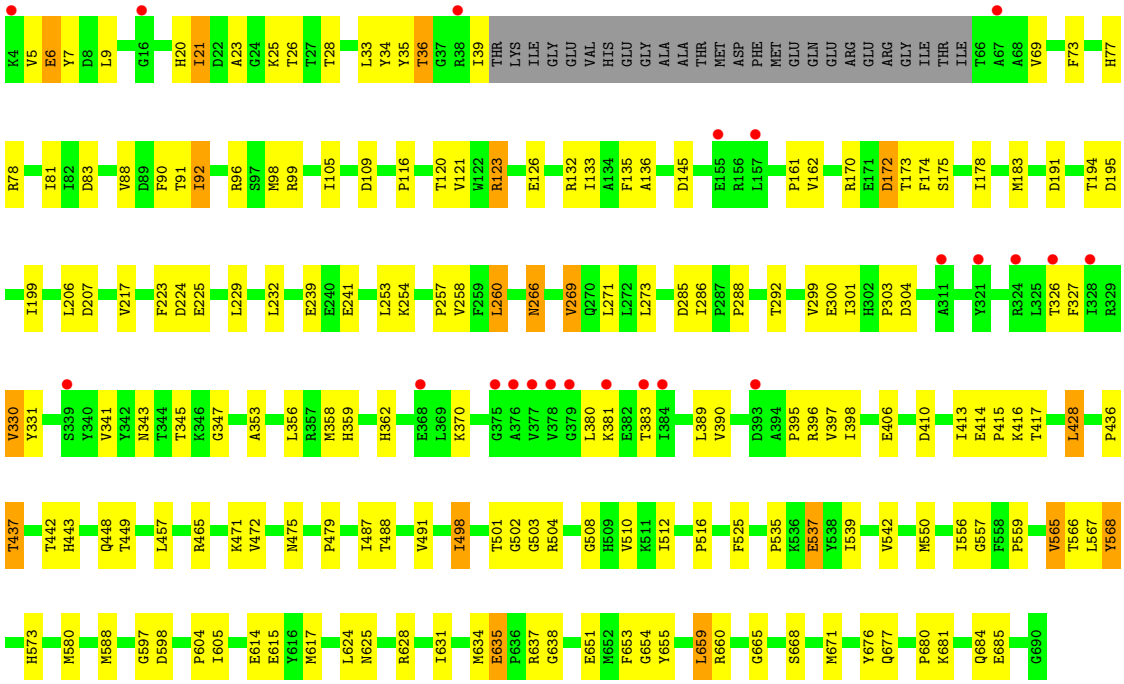
• Molecule 20: Elongation factor G

Chain AY:



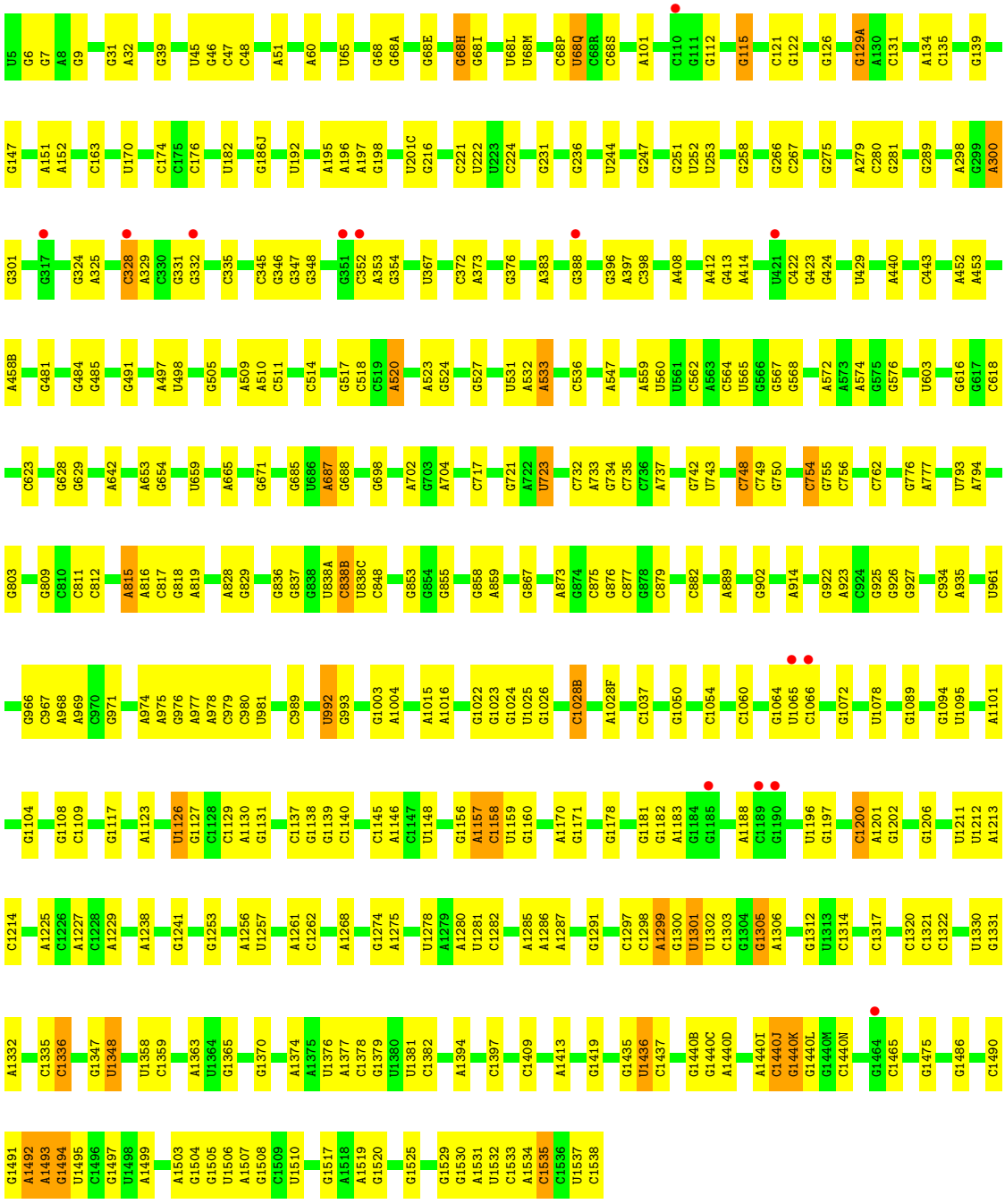
- Molecule 20: Elongation factor G

Chain CY:



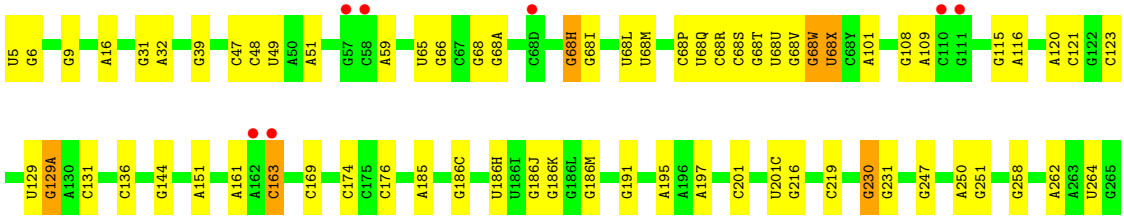
- Molecule 21: 16S Ribosomal RNA

Chain AA:



- Molecule 21: 16S Ribosomal RNA

Chain CA:



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G407 A412 G413 A414 U421 C422 G423 G424 U427 G428 U429 A430 U434 A440 A441 C442 C443 A452 A453 C454 C455 A478 G481 G485 A497 U498 A499 G500 C501 G505 C511 C514 G515 U516 G517 C518 C519 A520 G521 G524 C525 C526 G527 A532

A533 U534 A535 C536 A547 C555 A559 C562 G567 G568 A572 A573 A574 G575 G576 G585 C590 U591 C596 G597 U598 C599 C600 U603 A607 G616 G617 C618 U619 C620 G629 G638 U641 U652 A653 G661 A665 U669 G670 G671

A676 A687 G688 A702 G703 A704 A712 C717 G721 A722 U723 G734 C735 G741 C748 C749 C754 G755 C762 A766 A777 A781 A782 U89 U793 A794 C795 C796 C810 A815 A816 C817 G818 A819 A828 U838A C838B U838C C848 G853

G854 G855 A859 G867 U870 A873 G876 G885 G886 G887 G888 A889 G890 U891 A892 A900 A907 A908 A909 A914 A915 G916 G926 G927 G928 G929 C930 C936 G939 C940 G941 G942 U943 G944 G945 U950 A958 A959 U960 U961 A965 G966 C967 A968 A969

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G1419 G1422 U1436 C1439 G1440B G1440C A1440D G1440E A1440I C1440J G1440K C1440N A1440O C1465 C1484 G1487 G1491 A1492 A1493 G1494 G1497 A1502 A1503 G1504 G1505 U1506 A1507 G1508 G1517 A1518 A1519 G1520 G1525 G1526 C1527 U1528 G1529 G1530 A1531 U1532 C1533 A1534 C1535 C1536 U1537 C1538

- Molecule 22: tRNA

Chain AW:

G1 G2 C3 U4 A5 C6 G7 U8 A9 G10 A14 G15 U16 U17 G18 G19 U20 U20A A21 G22 A23 G24 C25 A26 C27 A28 U29 C30 A37 A38 U42 G43 G44 G45 G46 U47 C48 A49 C50 A51 G52 G53 U54 U55 C56 G57 A58 A59 U60 C61 C62 C63 G64 U68 A69 G70

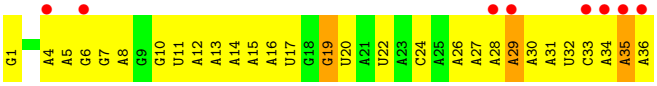
C71 C72 A73 C74 C75 A76

- Molecule 22: tRNA

Chain CW:

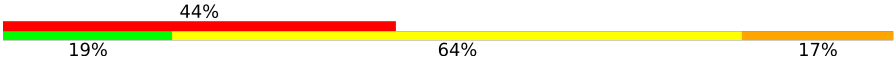
• Molecule 23: mRNA

Chain AV:



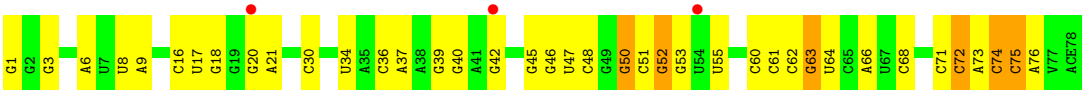
• Molecule 23: mRNA

Chain CV:



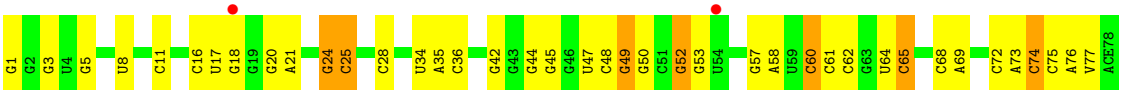
• Molecule 24: tRNA

Chain AX:



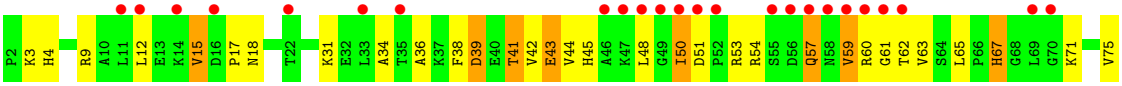
• Molecule 24: tRNA

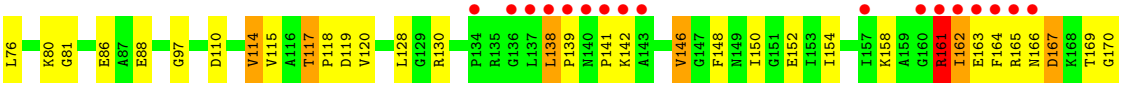
Chain CX:

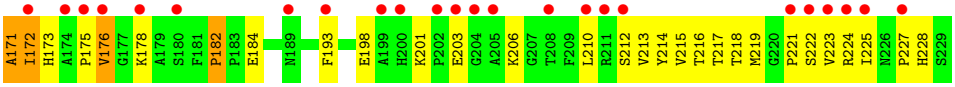


• Molecule 25: 50S ribosomal protein L1

Chain BC:

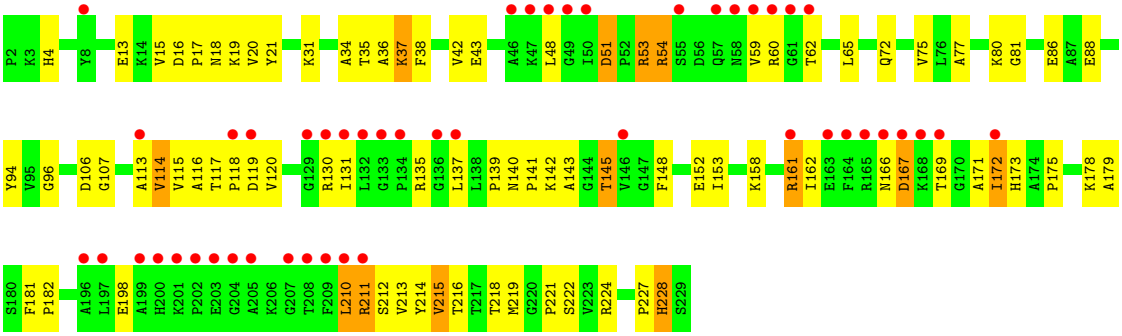






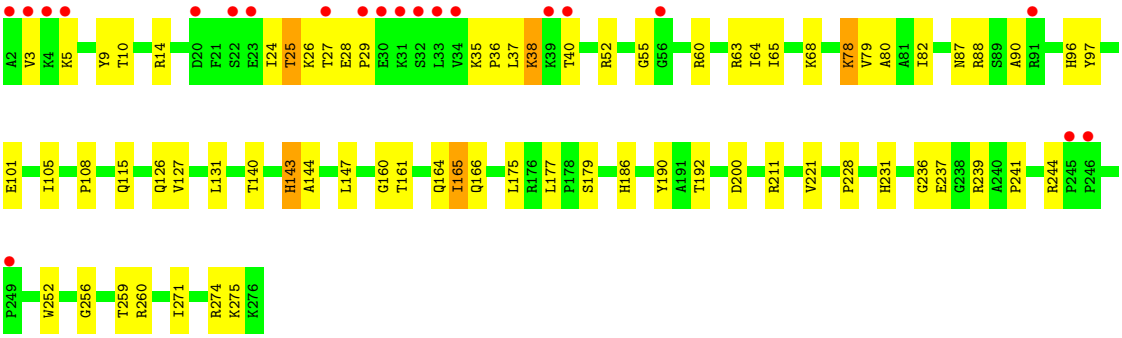
• Molecule 25: 50S ribosomal protein L1

Chain DC:



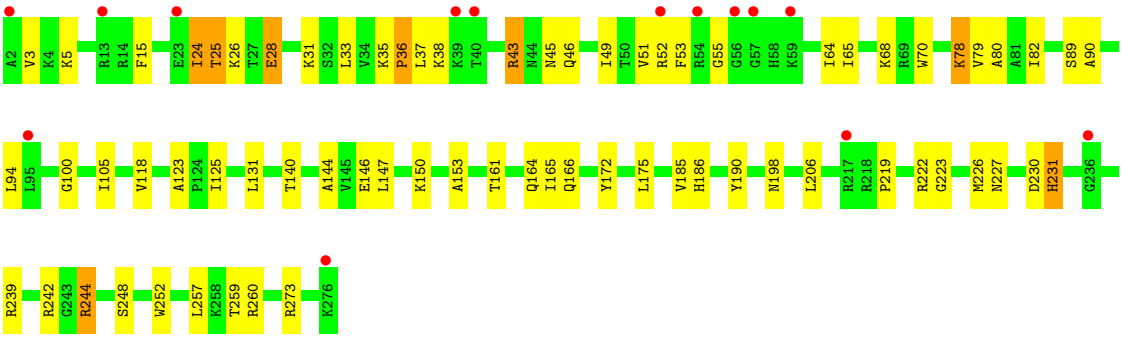
• Molecule 26: 50S ribosomal protein L2

Chain BD:



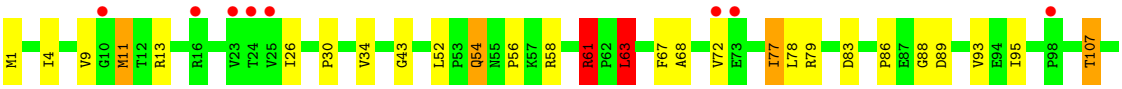
• Molecule 26: 50S ribosomal protein L2

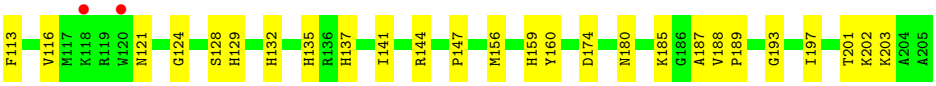
Chain DD:



• Molecule 27: 50S ribosomal protein L3

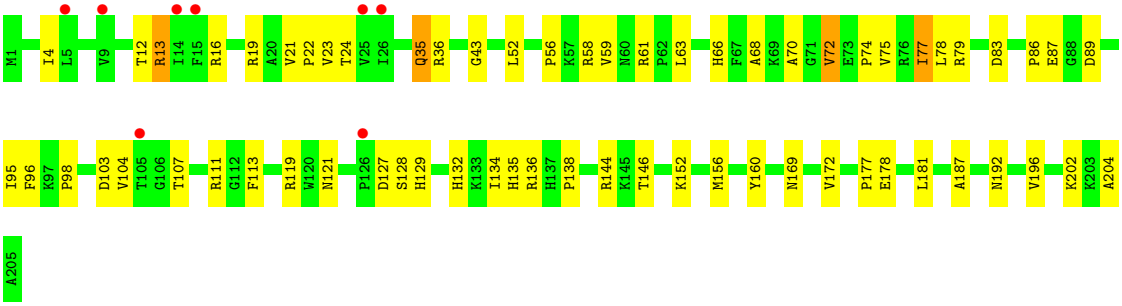
Chain BE:





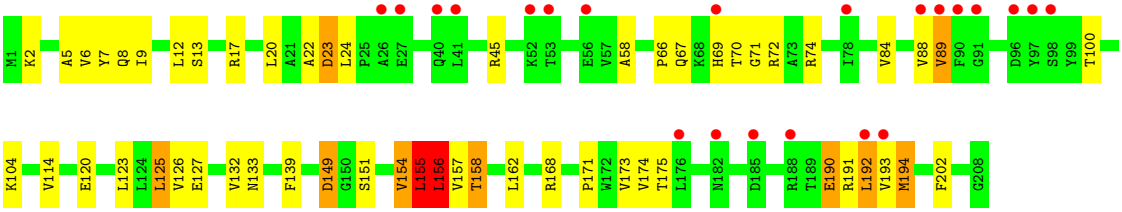
• Molecule 27: 50S ribosomal protein L3

Chain DE:



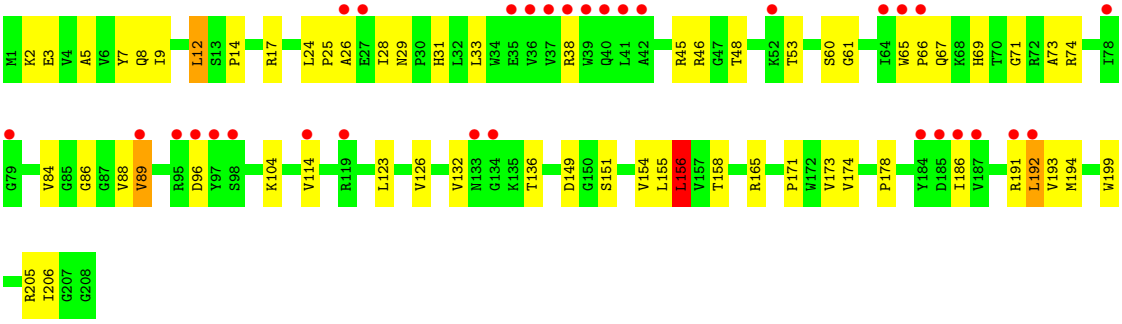
• Molecule 28: 50S ribosomal protein L4

Chain BF:



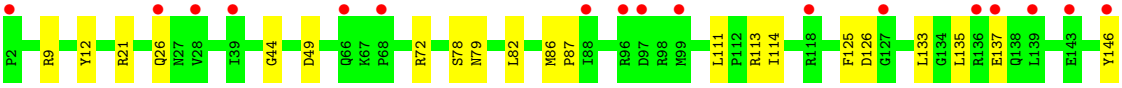
• Molecule 28: 50S ribosomal protein L4

Chain DF:



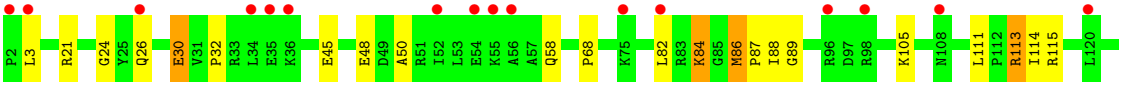
• Molecule 29: 50S ribosomal protein L5

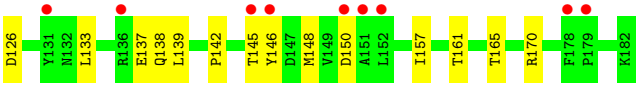
Chain BG:



• Molecule 29: 50S ribosomal protein L5

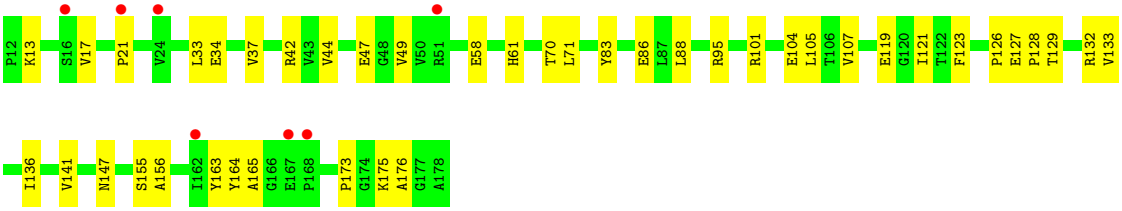
Chain DG:





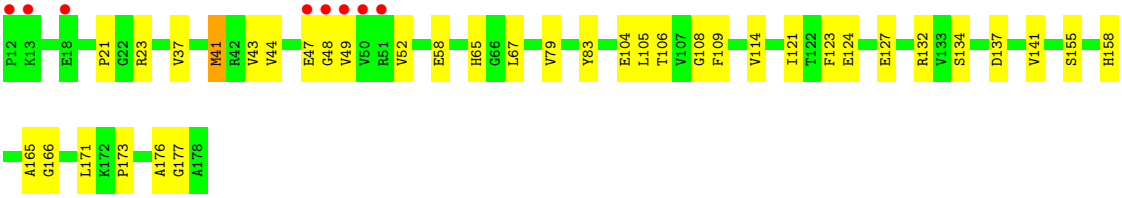
• Molecule 30: 50S ribosomal protein L6

Chain BH:



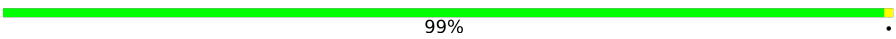
• Molecule 30: 50S ribosomal protein L6

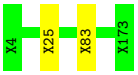
Chain DH:



• Molecule 31: 50S ribosomal protein l10

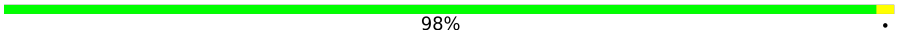
Chain BJ:

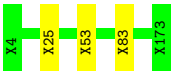




• Molecule 31: 50S ribosomal protein l10

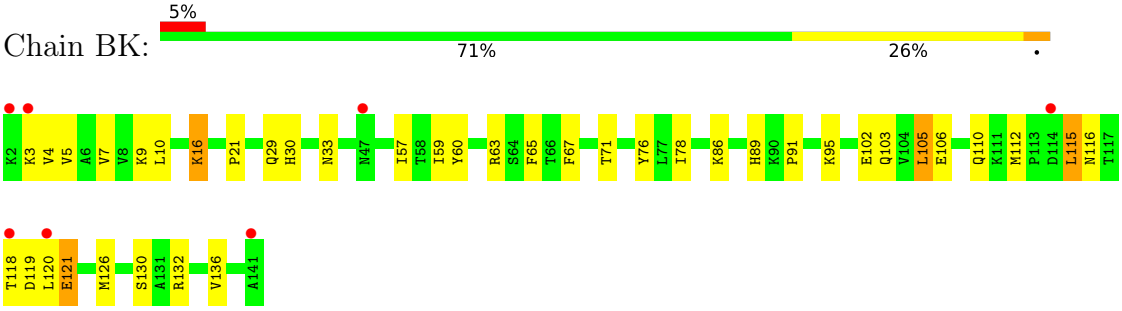
Chain DJ:





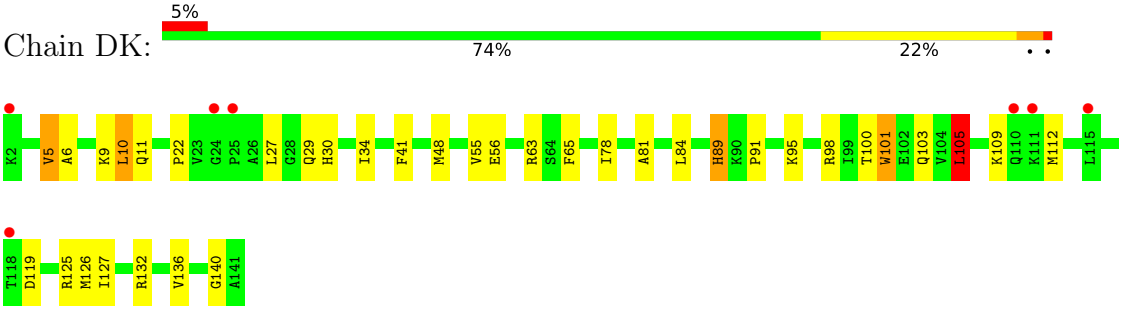
• Molecule 32: 50S ribosomal protein L11

Chain BK:



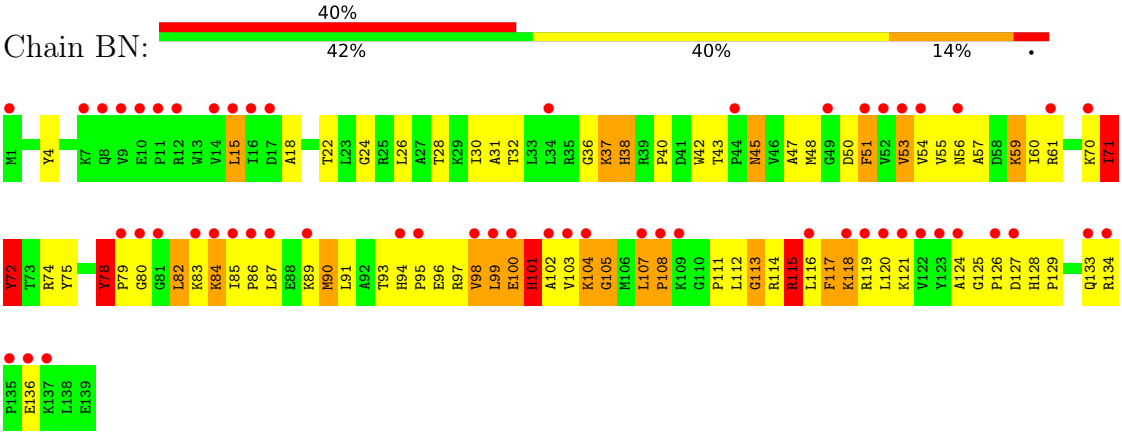
• Molecule 32: 50S ribosomal protein L11

Chain DK:



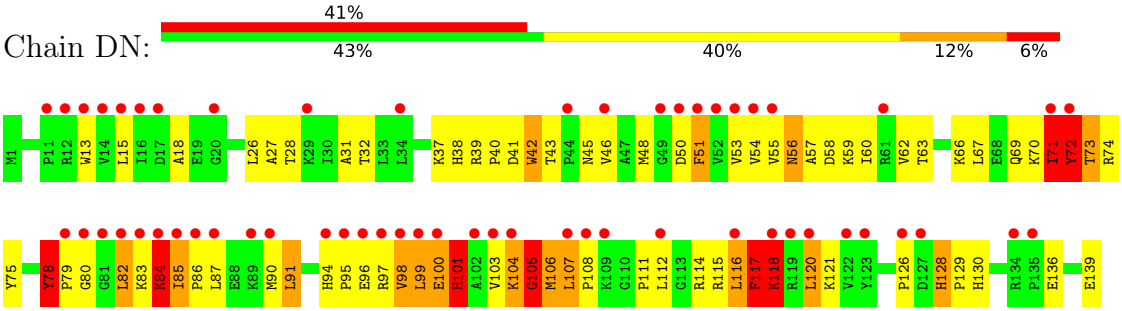
• Molecule 33: 50S ribosomal protein L13

Chain BN:



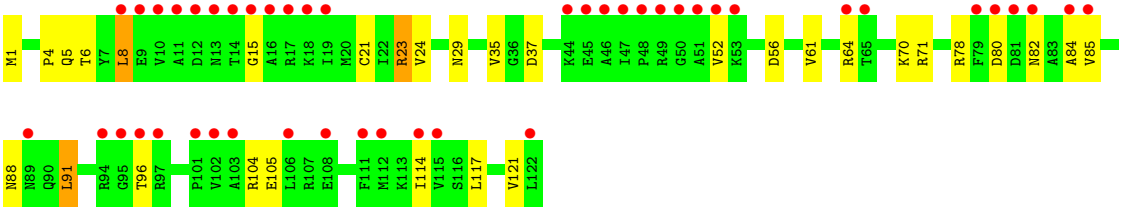
• Molecule 33: 50S ribosomal protein L13

Chain DN:



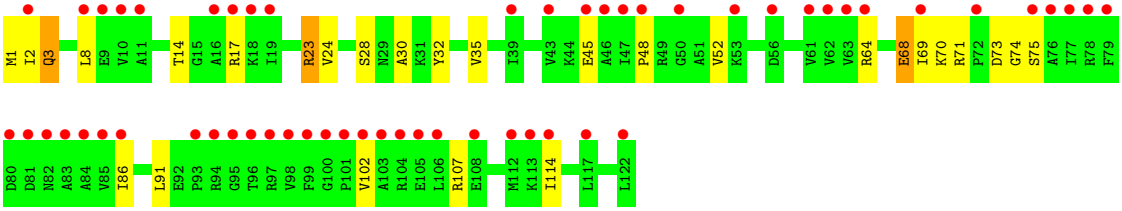
• Molecule 34: 50S ribosomal protein L14

Chain BO:



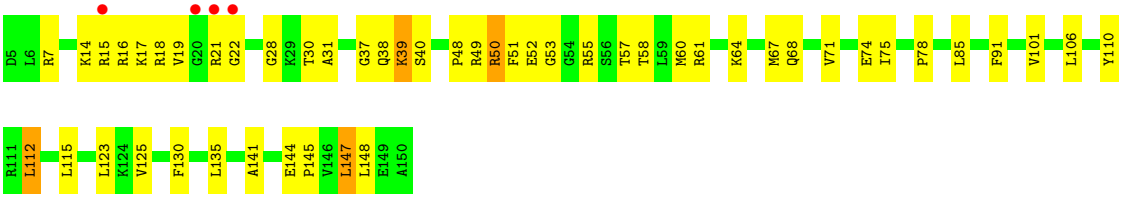
• Molecule 34: 50S ribosomal protein L14

Chain DO:



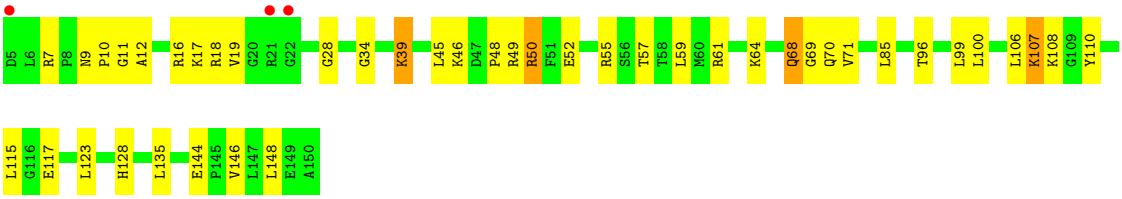
• Molecule 35: 50S ribosomal protein L15

Chain BP:



• Molecule 35: 50S ribosomal protein L15

Chain DP:



• Molecule 36: 50S ribosomal protein L16

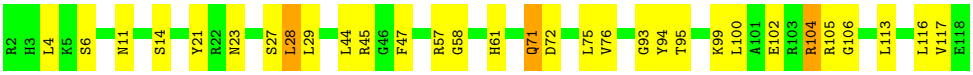
Chain BQ:

• Molecule 36: 50S ribosomal protein L16

Chain DQ:

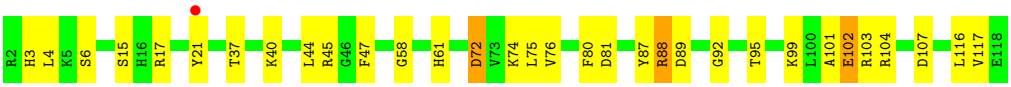
• Molecule 37: 50S ribosomal protein L17

Chain BR:



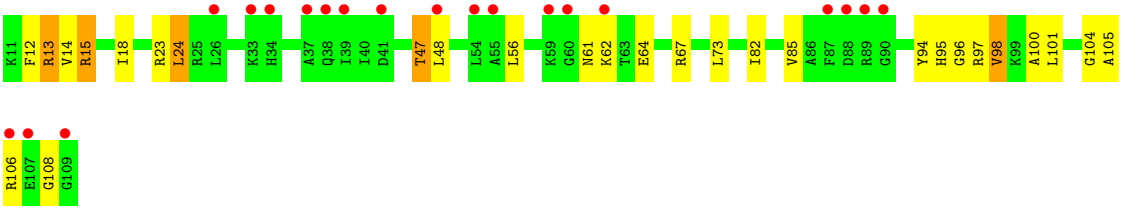
• Molecule 37: 50S ribosomal protein L17

Chain DR:



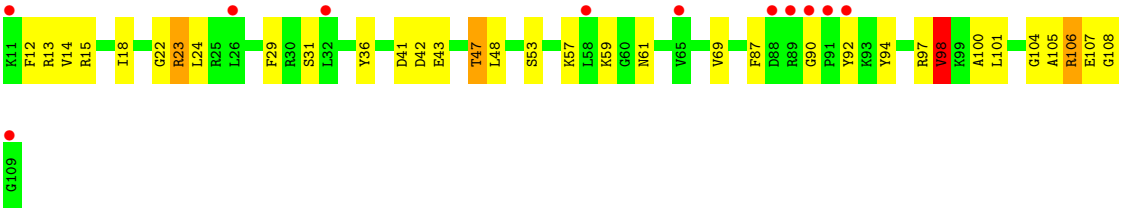
• Molecule 38: 50S ribosomal protein L18

Chain BS:



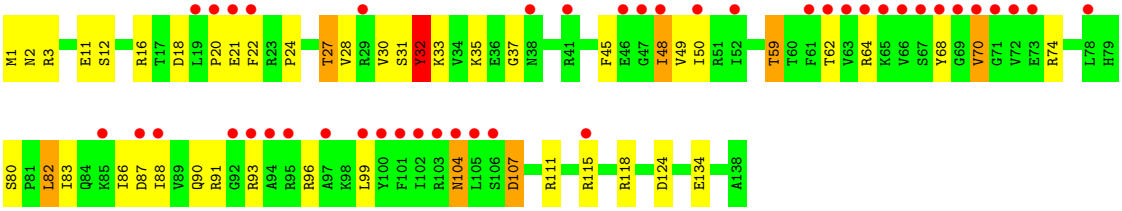
• Molecule 38: 50S ribosomal protein L18

Chain DS:



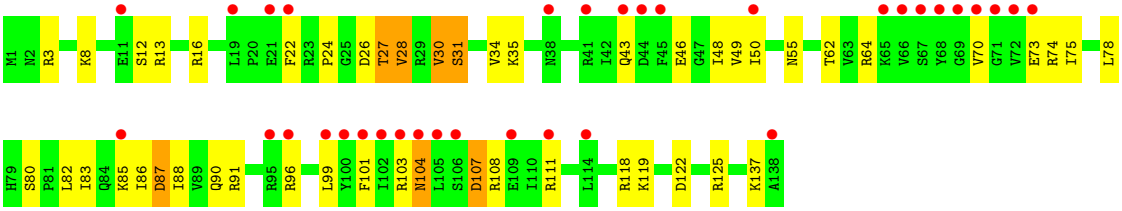
• Molecule 39: 50S ribosomal protein L19

Chain BT:



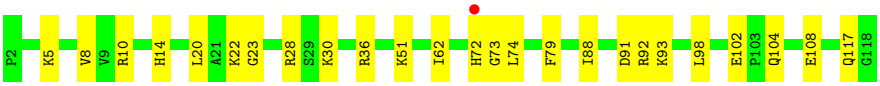
- Molecule 39: 50S ribosomal protein L19

Chain DT:



- Molecule 40: 50S ribosomal protein L20

Chain BU:

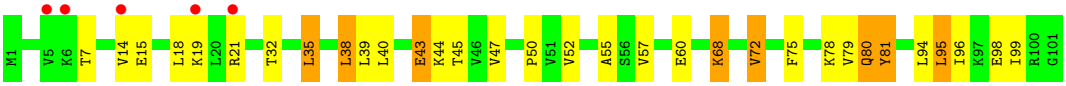


- Molecule 40: 50S ribosomal protein L20

Chain DU:

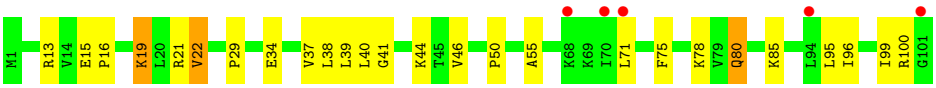
- Molecule 41: 50S ribosomal protein L21

Chain BV:



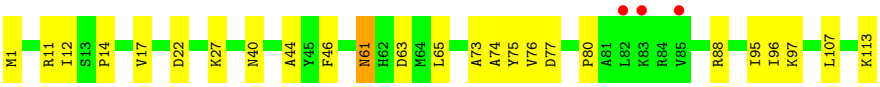
- Molecule 41: 50S ribosomal protein L21

Chain DV:



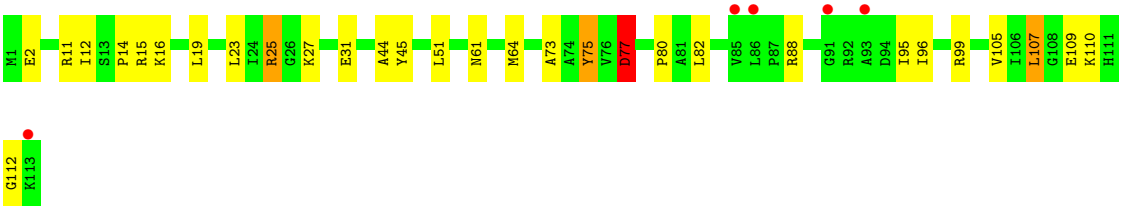
- Molecule 42: 50S ribosomal protein L22

Chain BW: 3% 78% 21%



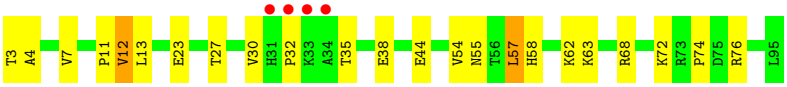
• Molecule 42: 50S ribosomal protein L22

Chain DW: 4% 73% 23%



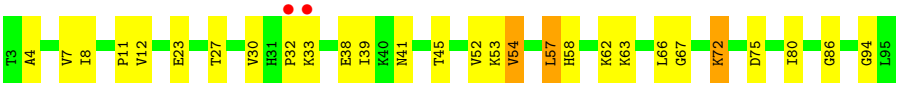
• Molecule 43: 50S ribosomal protein L23

Chain BX: 4% 75% 23%



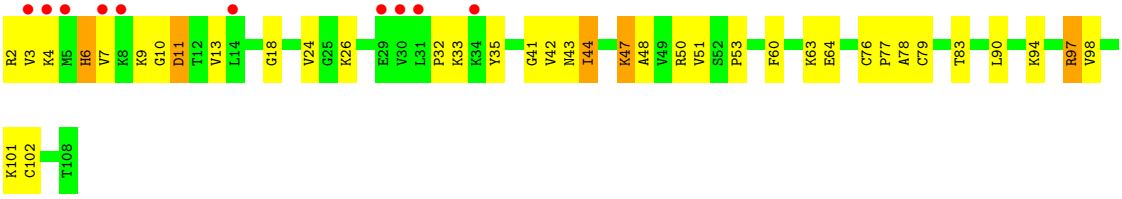
• Molecule 43: 50S ribosomal protein L23

Chain DX: 2% 70% 27%



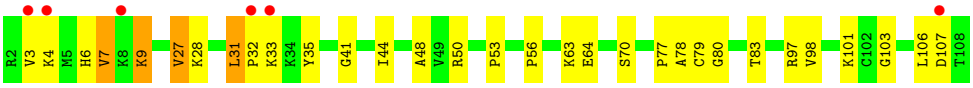
• Molecule 44: 50S ribosomal protein L24

Chain BY: 9% 64% 31% 5%



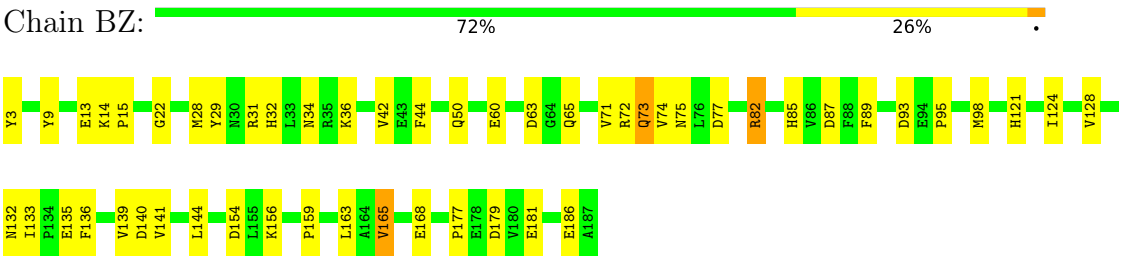
• Molecule 44: 50S ribosomal protein L24

Chain DY: 6% 71% 25%



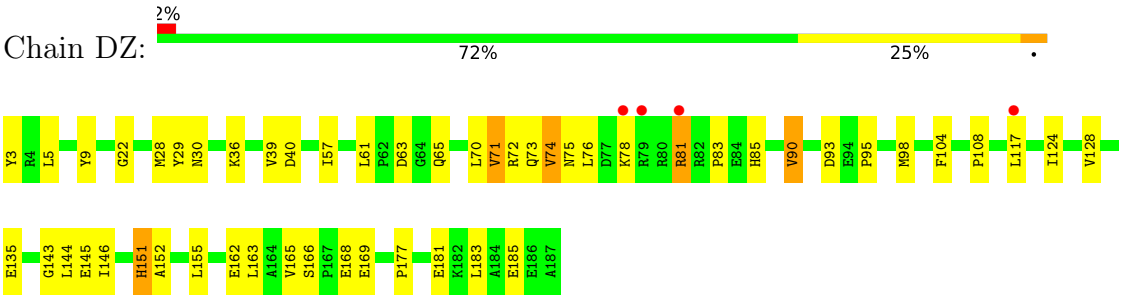
• Molecule 45: 50S ribosomal protein L25

Chain BZ:



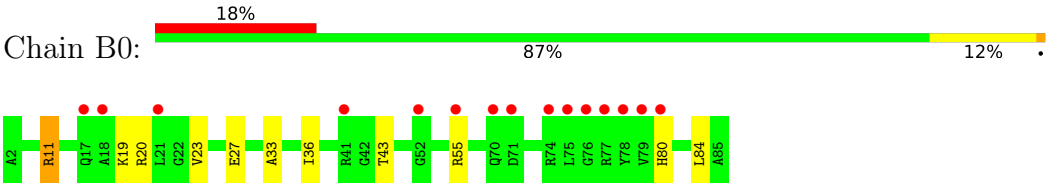
- Molecule 45: 50S ribosomal protein L25

Chain DZ:



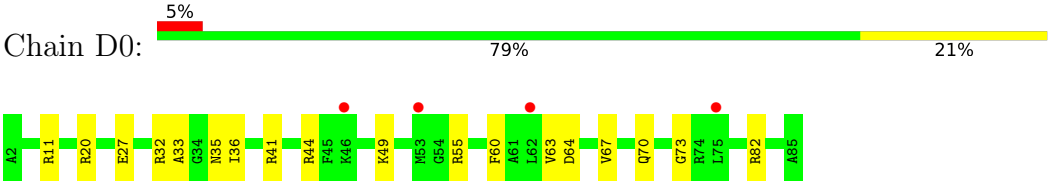
- Molecule 46: 50S ribosomal protein L27

Chain B0:



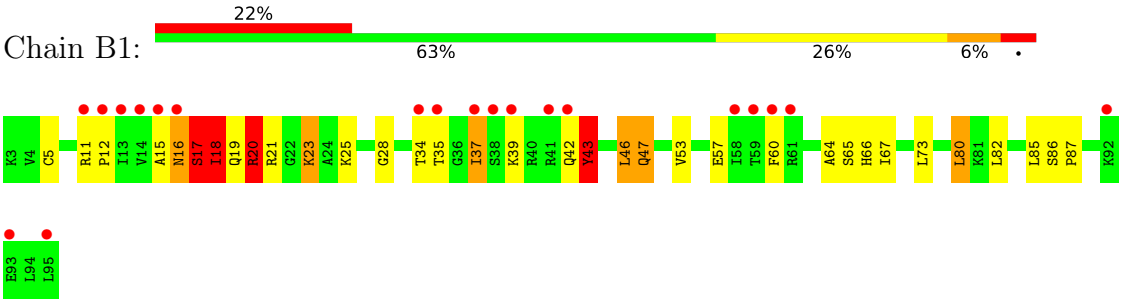
- Molecule 46: 50S ribosomal protein L27

Chain D0:



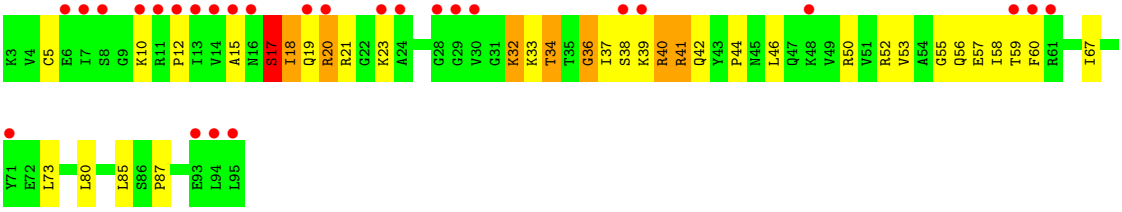
- Molecule 47: 50S ribosomal protein L28

Chain B1:



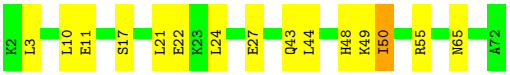
- Molecule 47: 50S ribosomal protein L28

Chain D1:



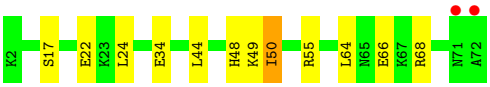
• Molecule 48: 50S ribosomal protein L29

Chain B2:



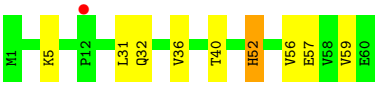
• Molecule 48: 50S ribosomal protein L29

Chain D2:



• Molecule 49: 50S ribosomal protein L30

Chain B3:

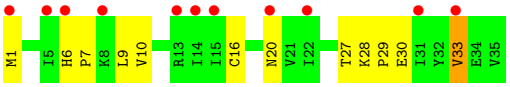


• Molecule 49: 50S ribosomal protein L30

Chain D3:

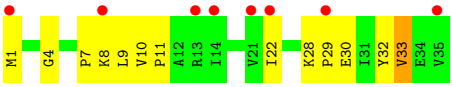
• Molecule 50: 50S ribosomal protein L31

Chain B4:



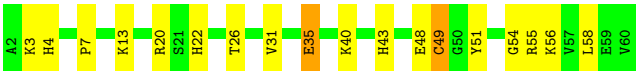
• Molecule 50: 50S ribosomal protein L31

Chain D4:



• Molecule 51: 50S ribosomal protein L32

Chain B5:



• Molecule 51: 50S ribosomal protein L32

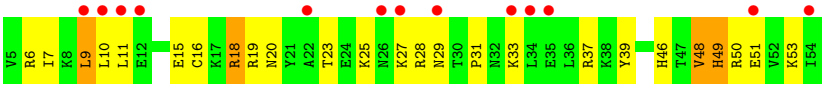
Chain D5:

• Molecule 52: 50S ribosomal protein L33

Chain B6:

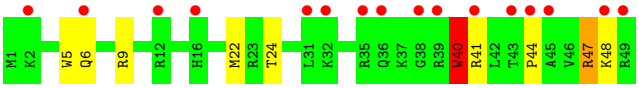
• Molecule 52: 50S ribosomal protein L33

Chain D6:



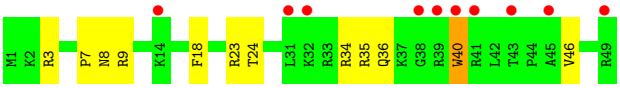
• Molecule 53: 50S ribosomal protein L34

Chain B7:



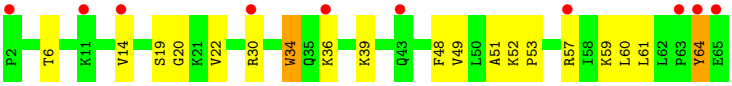
• Molecule 53: 50S ribosomal protein L34

Chain D7:



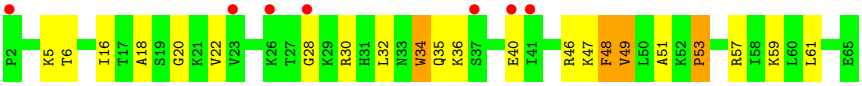
• Molecule 54: 50S ribosomal protein L35

Chain B8:



• Molecule 54: 50S ribosomal protein L35

Chain D8:

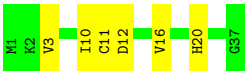


• Molecule 55: 50S ribosomal protein L36

Chain B9:

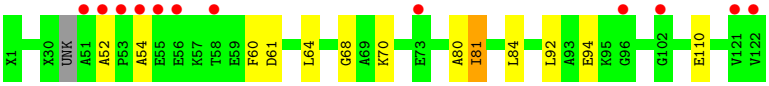
• Molecule 55: 50S ribosomal protein L36

Chain D9:



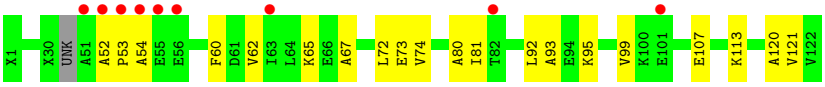
• Molecule 56: 50S ribosomal protein L7/L12

Chain Be:



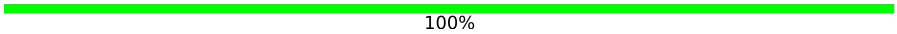
• Molecule 56: 50S ribosomal protein L7/L12

Chain De:



• Molecule 57: 50S ribosomal protein L7/L12

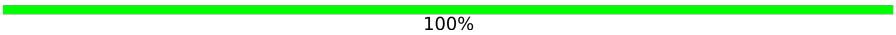
Chain Bf:



There are no outlier residues recorded for this chain.

• Molecule 57: 50S ribosomal protein L7/L12

Chain Bg:



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Df: 100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg: 100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh: 100%

There are no outlier residues recorded for this chain.

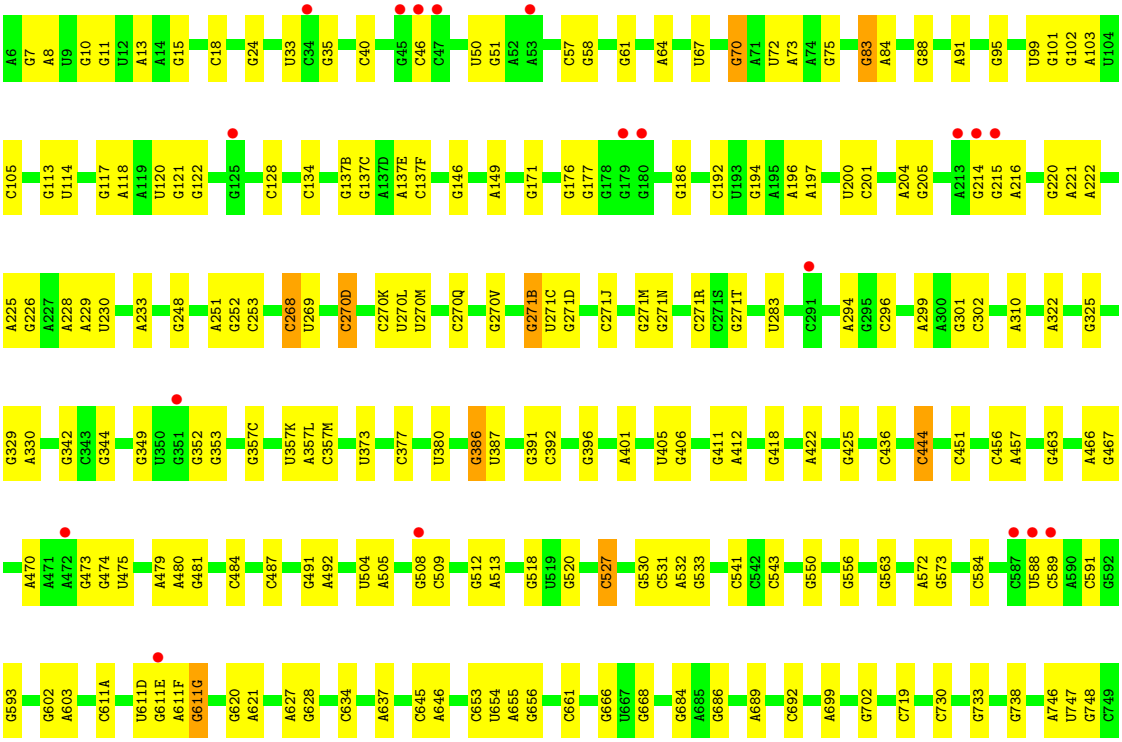
- Molecule 58: 50S ribosomal protein L7/L12

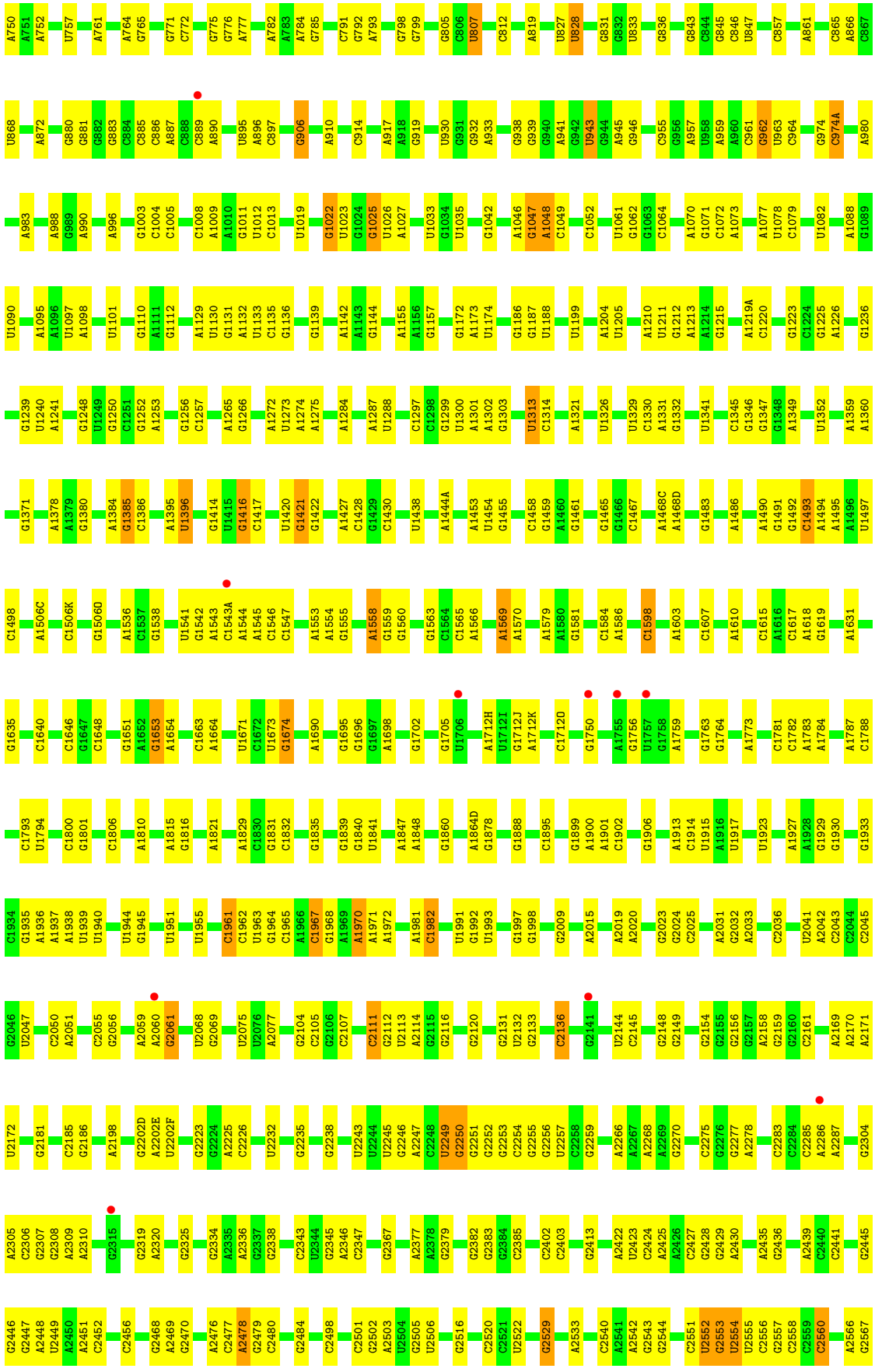
Chain Dh: 100%

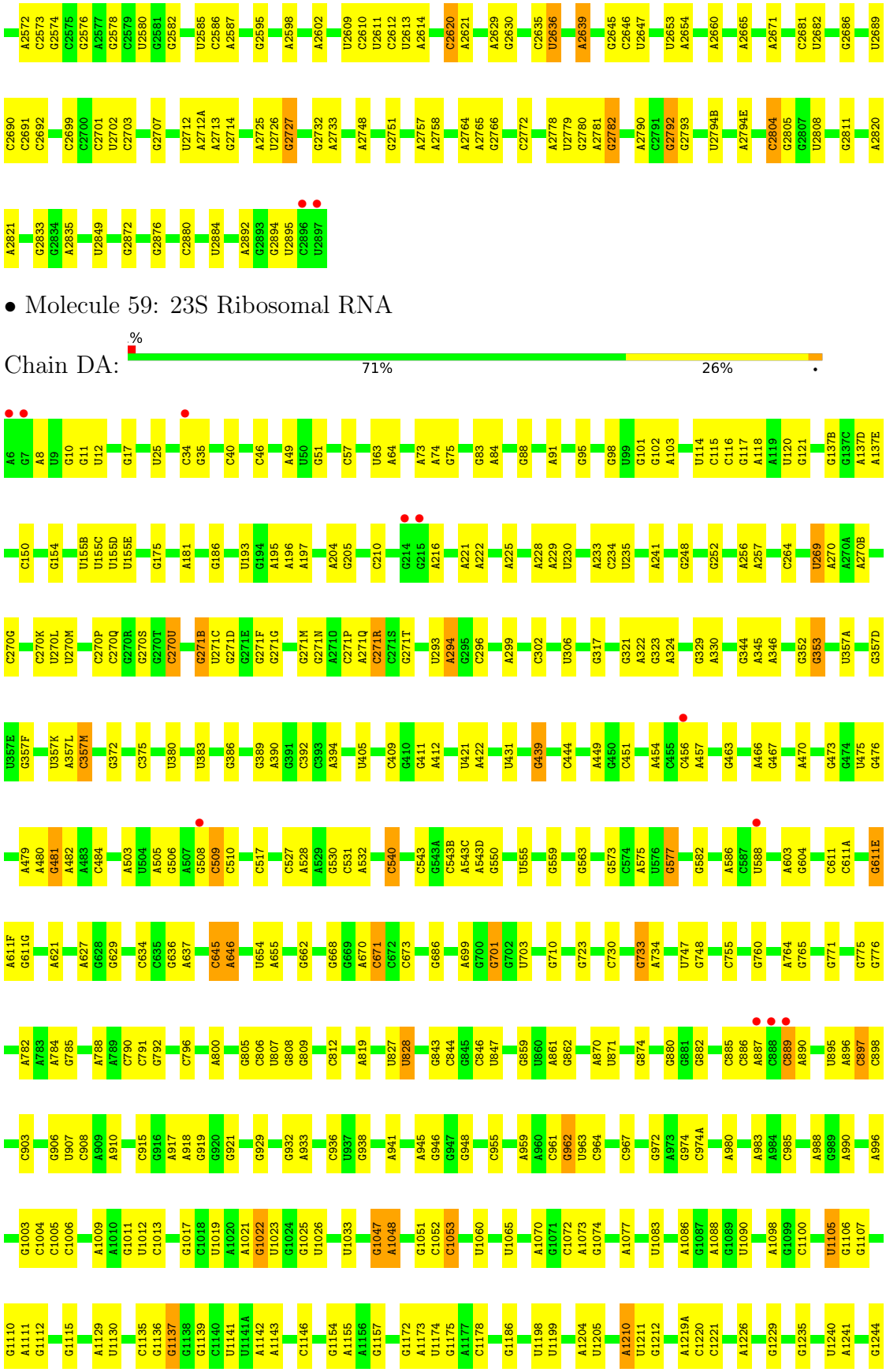
There are no outlier residues recorded for this chain.

- Molecule 59: 23S Ribosomal RNA

Chain BA: % 71% 27%

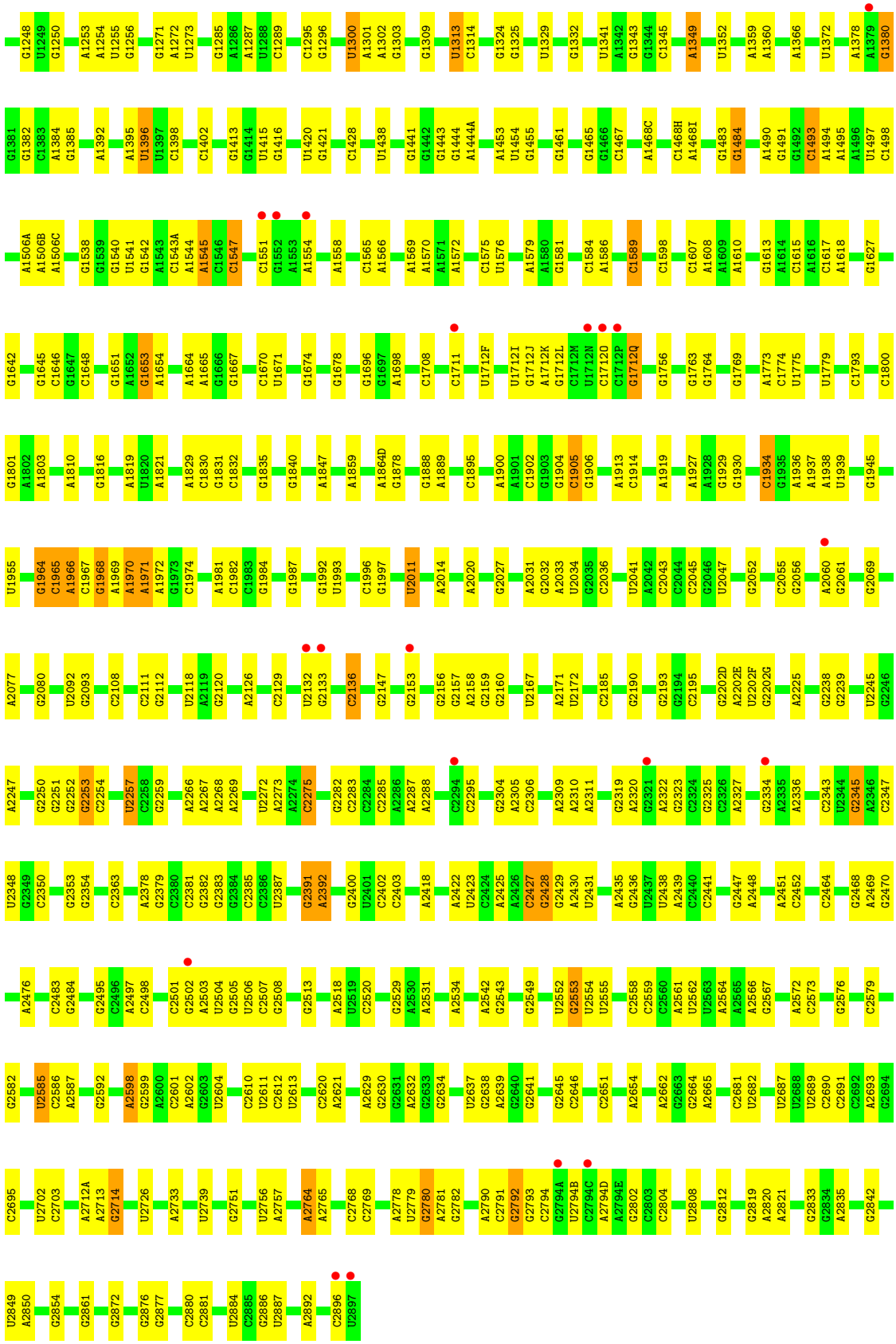



A750 A751 A752 U757 A761 A764 G765 G771 C772 G775 G776 A777 A782 A783 A784 G785 C791 G792 A793 G798 G799 G805 C806 U807 C812 A819 U827 U828 G831 G832 U833 G836 G843 C844 G845 C846 U847 C857 A861 C865 A866 C867
U868 A872 G880 G881 G882 G883 C884 C885 C886 A887 C888 C889 A890 U895 A896 C897 G906 A910 C914 A917 A918 G919 U930 G931 G932 A933 G938 G939 G940 A941 G942 U943 G944 A945 G946 C955 G956 A957 U958 A959 A960 C961 G962 U963 C964 G974 C974A A980
A983 A988 G989 A990 A996 G1003 C1004 C1005 C1008 A1009 A1010 G1011 U1012 C1013 U1019 G1022 U1023 G1024 G1025 U1026 A1027 U1033 G1034 U1035 G1042 A1046 G1047 A1048 C1049 C1052 U1061 G1062 G1063 C1064 A1070 G1071 C1072 A1073 A1077 U1078 C1079 U1082 A1088 G1089
U1090 A1095 A1096 U1097 A1098 U1101 G1110 A1111 G1112 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1139 A1142 A1143 G1144 A1155 A1156 G1157 G1172 A1173 U1174 G1186 U1187 U1188 U1199 A1204 U1205 A1210 U1211 G1212 A1213 A1214 G1215 A1219A C1220 G1223 C1224 G1225 A1226 G1236
G1239 U1240 A1241 G1248 U1249 G1250 C1251 G1252 A1253 G1256 C1257 A1265 G1266 A1272 U1273 A1274 A1275 A1284 A1287 U1288 C1297 C1298 G1299 U1300 A1301 A1302 G1303 U1313 C1314 A1321 U1326 U1329 C1330 A1331 G1332 U1341 C1345 G1346 G1347 G1348 A1349 U1352 A1359 A1360
G1371 A1378 A1379 G1380 A1384 G1385 C1386 A1395 U1396 G1414 U1415 G1416 C1417 U1420 G1421 G1422 A1427 C1428 G1429 C1430 U1438 A1444A A1453 U1454 G1455 C1458 G1459 A1460 G1461 G1465 G1466 C1467 A1468C A1468D G1483 A1486 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497
C1498 A1506C C1506K G1506D A1536 C1537 G1538 U1541 G1542 A1543 C1543A A1544 A1545 C1546 C1547 A1553 A1554 G1555 A1558 G1559 G1560 G1563 C1564 C1565 A1566 A1569 A1570 A1579 A1580 G1581 C1584 A1586 C1598 A1603 C1607 A1610 C1615 A1616 C1617 A1618 G1619 A1631
G1635 C1640 C1646 G1647 C1648 G1651 A1652 G1653 A1654 C1663 A1664 U1671 C1672 U1673 G1674 A1690 G1695 G1696 G1697 A1698 G1702 G1705 U1706 A1712H U1712I G1712J A1712K C1712O G1750 A1755 G1756 U1757 G1758 A1759 G1763 G1764 A1773 C1781 C1782 A1783 A1784 A1787 C1788
C1793 U1794 C1800 G1801 C1806 A1810 A1815 G1816 A1821 A1829 C1830 G1831 C1832 G1835 A1839 G1840 U1841 A1847 A1848 G1860 A1864D G1878 G1888 C1895 G1899 A1900 A1901 C1902 G1906 A1913 C1914 U1915 A1916 U1917 U1923 A1927 A1928 G1929 G1930 G1933
C1934 G1935 A1936 A1937 A1938 U1939 U1940 U1944 G1945 U1951 U1955 C1961 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 A1981 C1982 U1991 G1992 U1993 G1997 G1998 G2009 A2015 A2019 A2020 G2023 G2024 C2025 A2031 G2032 A2033 C2036 U2041 A2042 C2043 C2044 C2045
G2046 U2047 C2050 A2051 C2055 G2056 A2059 A2060 G2061 U2068 G2069 U2075 U2076 A2077 G2104 C2105 G2106 C2107 C2111 G2112 U2113 A2114 G2115 G2116 G2120 G2131 U2132 G2133 C2136 G2141 U2144 C2145 G2148 G2149 G2154 G2155 G2156 G2157 A2158 G2159 G2160 C2161 A2169 A2170 A2171
U2172 G2181 C2185 G2186 A2198 G2202D A2202E U2202F G2223 C2224 A2225 C2226 U2232 G2235 G2238 U2243 U2244 U2245 G2246 U2247 C2248 U2249 G2250 G2251 G2252 G2253 C2254 G2255 G2256 U2257 C2258 G2259 A2266 A2267 A2268 A2269 G2270 C2275 G2276 G2277 A2278 C2283 C2284 C2285 A2286 A2287 G2304
A2305 C2306 G2307 G2308 A2309 A2310 G2315 G2319 A2320 G2325 C2334 A2335 A2336 G2337 G2338 C2343 U2344 G2345 A2346 C2347 G2367 A2377 A2378 G2379 G2382 G2383 G2384 C2385 C2402 C2403 G2413 A2422 U2423 C2424 A2425 A2426 C2427 G2428 G2429 A2430 A2435 G2436 A2439 C2440 C2441 G2445
G2446 G2447 A2448 U2449 A2450 A2451 C2452 C2456 G2468 A2469 G2470 A2476 C2477 A2478 G2479 C2480 G2484 C2498 C2501 G2502 A2503 U2504 G2505 U2506 G2516 C2520 C2521 U2522 G2529 A2533 C2540 A2541 A2542 G2543 C2544 C2551 U2552 G2553 U2554 U2555 C2556 G2557 C2558 C2559 C2560 A2566 G2567



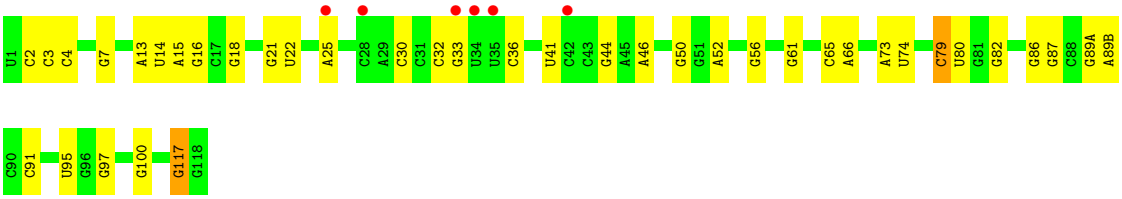
• Molecule 59: 23S Ribosomal RNA

Chain DA: % 71% 26% •



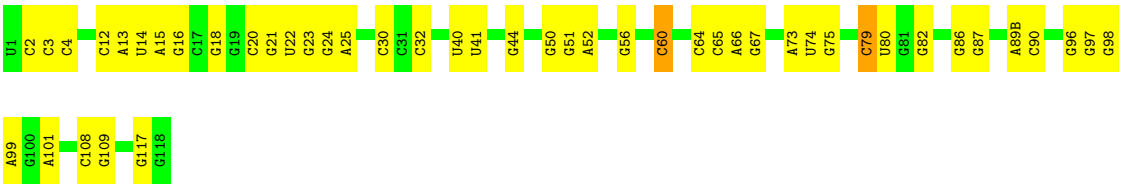
- Molecule 60: 5S Ribosomal RNA

Chain BB:



- Molecule 60: 5S Ribosomal RNA

Chain DB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	306.92Å 677.00Å 356.78Å 90.00° 89.90° 90.00°	Depositor
Resolution (Å)	49.98 – 3.80 127.40 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.98-3.80) 60.2 (127.40-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.295 , 0.331 0.302 , 0.332	Depositor DCC
R_{free} test set	8467 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , -101.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.17$, $< L^2 > = 0.05$	Xtriage
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	312066	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: MG, FUA, NMY, ACE, GDP

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	AB	0.41	0/1945	0.69	0/2621
1	CB	0.41	0/1945	0.69	1/2621 (0.0%)
2	AC	0.27	0/1645	0.55	0/2216
2	CC	0.29	0/1645	0.56	0/2216
3	AD	0.31	0/1733	0.59	0/2318
3	CD	0.29	0/1733	0.61	1/2318 (0.0%)
4	AE	0.30	0/1172	0.57	0/1576
4	CE	0.30	0/1172	0.61	1/1576 (0.1%)
5	AF	0.28	0/856	0.56	0/1154
5	CF	0.30	0/856	0.59	0/1154
6	AG	0.27	0/1276	0.51	0/1709
6	CG	0.28	0/1276	0.51	0/1709
7	AH	0.29	0/1136	0.60	0/1527
7	CH	0.28	0/1136	0.55	0/1527
8	AI	0.27	0/1029	0.56	0/1379
8	CI	0.27	0/1029	0.50	0/1379
9	AJ	0.27	0/815	0.54	0/1095
9	CJ	0.28	0/815	0.56	0/1095
10	AK	0.38	0/900	0.62	0/1213
10	CK	0.39	0/900	0.61	0/1213
11	AL	0.43	0/992	0.80	0/1327
11	CL	0.45	0/992	0.81	1/1327 (0.1%)
12	AM	0.27	0/1008	0.53	0/1347
12	CM	0.27	0/1008	0.58	0/1347
13	AN	0.29	0/501	0.51	0/664
13	CN	0.34	0/501	0.57	0/664
14	AO	0.34	0/745	0.61	0/992
14	CO	0.33	0/745	0.57	1/992 (0.1%)
15	AP	0.32	0/722	0.61	0/970
15	CP	0.32	0/722	0.60	0/970
16	AQ	0.35	0/848	0.67	1/1131 (0.1%)
16	CQ	0.36	0/848	0.68	0/1131

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AR	0.29	0/579	0.58	0/768
17	CR	0.29	0/579	0.57	0/768
18	AS	0.29	0/647	0.56	0/870
18	CS	0.26	0/647	0.53	0/870
19	AT	0.30	0/765	0.54	0/1007
19	CT	0.31	0/765	0.51	0/1007
20	AY	0.37	0/5270	0.66	1/7135 (0.0%)
20	CY	0.36	0/5270	0.67	3/7135 (0.0%)
21	AA	0.39	9/36351 (0.0%)	1.12	149/56736 (0.3%)
21	CA	0.42	6/36351 (0.0%)	1.17	239/56736 (0.4%)
22	AW	0.52	0/1827	1.42	41/2845 (1.4%)
22	CW	0.48	0/1827	1.36	23/2845 (0.8%)
23	AV	1.27	1/881 (0.1%)	1.42	12/1372 (0.9%)
23	CV	0.82	7/880 (0.8%)	2.11	42/1372 (3.1%)
24	AX	0.62	1/1815 (0.1%)	1.56	47/2826 (1.7%)
24	CX	0.60	3/1815 (0.2%)	1.54	43/2826 (1.5%)
25	BC	0.51	1/1774 (0.1%)	0.86	2/2391 (0.1%)
25	DC	0.51	0/1774	0.80	0/2391
26	BD	0.40	2/2195 (0.1%)	0.62	1/2955 (0.0%)
26	DD	0.31	0/2195	0.60	0/2955
27	BE	0.35	0/1602	0.69	2/2160 (0.1%)
27	DE	0.33	0/1602	0.67	0/2160
28	BF	0.39	0/1663	0.81	6/2249 (0.3%)
28	DF	0.38	0/1663	0.78	4/2249 (0.2%)
29	BG	0.27	0/1499	0.54	0/2016
29	DG	0.29	0/1499	0.58	0/2016
30	BH	0.28	0/1298	0.58	0/1751
30	DH	0.28	0/1298	0.55	0/1751
32	BK	0.28	0/1054	0.55	1/1427 (0.1%)
32	DK	0.31	0/1054	0.58	1/1427 (0.1%)
33	BN	0.81	3/1141 (0.3%)	1.39	16/1537 (1.0%)
33	DN	0.81	2/1141 (0.2%)	1.28	13/1537 (0.8%)
34	BO	0.32	0/943	0.63	2/1269 (0.2%)
34	DO	0.32	0/943	0.65	0/1269
35	BP	0.28	0/1131	0.64	2/1504 (0.1%)
35	DP	0.29	0/1131	0.63	0/1504
36	BQ	0.36	0/1143	0.67	0/1527
36	DQ	0.33	0/1143	0.63	0/1527
37	BR	0.33	0/974	0.64	1/1302 (0.1%)
37	DR	0.32	0/974	0.59	0/1302
38	BS	0.35	0/783	0.69	0/1041
38	DS	0.36	0/783	0.71	0/1041
39	BT	0.30	0/1161	0.63	0/1549

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
39	DT	0.30	0/1161	0.64	0/1549
40	BU	0.36	0/982	0.57	0/1306
40	DU	0.33	0/982	0.57	0/1306
41	BV	0.34	0/790	0.76	2/1057 (0.2%)
41	DV	0.31	0/790	0.65	1/1057 (0.1%)
42	BW	0.32	0/911	0.64	0/1220
42	DW	0.38	0/911	0.69	1/1220 (0.1%)
43	BX	0.28	0/748	0.56	1/1004 (0.1%)
43	DX	0.28	0/748	0.56	1/1004 (0.1%)
44	BY	0.28	0/831	0.54	0/1108
44	DY	0.27	0/831	0.57	1/1108 (0.1%)
45	BZ	0.28	0/1505	0.58	0/2042
45	DZ	0.29	0/1505	0.58	0/2042
46	B0	0.25	0/671	0.54	0/892
46	D0	0.25	0/671	0.50	0/892
47	B1	0.51	0/739	1.01	5/981 (0.5%)
47	D1	0.48	0/739	0.92	2/981 (0.2%)
48	B2	0.37	0/600	0.63	0/793
48	D2	0.34	0/600	0.65	0/793
49	B3	0.29	0/482	0.58	0/646
49	D3	0.26	0/482	0.58	0/646
50	B4	0.38	0/276	0.67	0/372
50	D4	0.37	0/276	0.68	0/372
51	B5	0.28	0/473	0.57	0/639
51	D5	0.32	0/473	0.62	0/639
52	B6	0.30	0/440	0.82	3/586 (0.5%)
52	D6	0.31	0/440	0.68	0/586
53	B7	1.14	6/438 (1.4%)	1.51	7/575 (1.2%)
53	D7	0.29	0/438	0.55	0/575
54	B8	0.31	0/525	0.58	0/691
54	D8	0.30	0/525	0.61	0/691
55	B9	0.28	0/310	0.55	0/407
55	D9	0.32	0/310	0.57	0/407
56	Be	0.25	0/538	0.53	0/715
56	De	0.27	0/538	0.51	0/715
59	BA	0.38	1/69437 (0.0%)	1.11	247/108401 (0.2%)
59	DA	0.40	2/69437 (0.0%)	1.14	333/108401 (0.3%)
60	BB	0.43	0/2853	1.28	29/4451 (0.7%)
60	DB	0.48	0/2853	1.34	49/4451 (1.1%)
All	All	0.40	44/334735 (0.0%)	1.04	1339/498724 (0.3%)

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	AB	0	1
3	CD	0	1
10	AK	0	1
10	CK	0	1
15	AP	0	1
15	CP	0	1
20	AY	0	2
25	BC	0	6
25	DC	0	5
26	BD	0	1
26	DD	0	1
27	BE	0	1
28	BF	0	4
28	DF	0	2
29	DG	0	1
31	BJ	0	2
31	DJ	0	3
33	BN	0	17
33	DN	0	15
34	BO	0	1
34	DO	0	1
36	BQ	0	1
38	BS	0	1
38	DS	0	1
39	BT	0	1
39	DT	0	1
42	BW	0	1
42	DW	0	2
45	BZ	0	1
45	DZ	0	1
47	B1	0	4
47	D1	0	3
53	B7	0	1
All	All	0	86

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AV	1	G	P-O5'	35.77	1.95	1.59
53	B7	40	TRP	CD2-CE2	-12.82	1.25	1.41
21	AA	1126	U	C2-O2	-9.80	1.13	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	CA	1126	U	C2-O2	-9.32	1.14	1.22
53	B7	40	TRP	CE3-CZ3	8.92	1.53	1.38

The worst 5 of 1339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	AV	1	G	O5'-P-OP2	24.05	139.56	110.70
23	CV	10	G	N1-C6-O6	-22.12	106.63	119.90
21	AA	1126	U	N1-C2-N3	18.77	126.16	114.90
53	B7	40	TRP	CE2-CD2-CG	18.75	122.30	107.30
21	CA	1126	U	N1-C2-N3	18.50	126.00	114.90

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide
10	AK	43	SER	Peptide
15	AP	34	GLU	Peptide
20	AY	34	TYR	Peptide
20	AY	630	GLN	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 X-ray entries followed by that with respect to entries of similar resolution.

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	AB	233/235 (99%)	168 (72%)	45 (19%)	20 (9%)	1 12
1	CB	233/235 (99%)	171 (73%)	45 (19%)	17 (7%)	1 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	205/207 (99%)	137 (67%)	39 (19%)	29 (14%)	0	4
2	CC	205/207 (99%)	150 (73%)	35 (17%)	20 (10%)	0	10
3	AD	206/208 (99%)	140 (68%)	41 (20%)	25 (12%)	0	6
3	CD	206/208 (99%)	152 (74%)	33 (16%)	21 (10%)	0	9
4	AE	149/151 (99%)	122 (82%)	20 (13%)	7 (5%)	2	24
4	CE	149/151 (99%)	115 (77%)	24 (16%)	10 (7%)	1	19
5	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1	14
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	1	12
6	AG	153/155 (99%)	123 (80%)	22 (14%)	8 (5%)	2	23
6	CG	153/155 (99%)	118 (77%)	23 (15%)	12 (8%)	1	15
7	AH	136/138 (99%)	102 (75%)	23 (17%)	11 (8%)	1	14
7	CH	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1	16
8	AI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	24
8	CI	125/127 (98%)	98 (78%)	21 (17%)	6 (5%)	2	24
9	AJ	97/99 (98%)	71 (73%)	15 (16%)	11 (11%)	0	7
9	CJ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	17
10	AK	117/119 (98%)	83 (71%)	21 (18%)	13 (11%)	0	7
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	4
11	AL	123/125 (98%)	41 (33%)	44 (36%)	38 (31%)	0	0
11	CL	123/125 (98%)	49 (40%)	37 (30%)	37 (30%)	0	0
12	AM	123/125 (98%)	94 (76%)	19 (15%)	10 (8%)	1	14
12	CM	123/125 (98%)	95 (77%)	17 (14%)	11 (9%)	1	12
13	AN	58/60 (97%)	38 (66%)	17 (29%)	3 (5%)	2	23
13	CN	58/60 (97%)	35 (60%)	14 (24%)	9 (16%)	0	4
14	AO	86/88 (98%)	72 (84%)	12 (14%)	2 (2%)	6	38
14	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	31
15	AP	82/84 (98%)	58 (71%)	16 (20%)	8 (10%)	0	10
15	CP	82/84 (98%)	62 (76%)	13 (16%)	7 (8%)	1	12
16	AQ	98/100 (98%)	70 (71%)	22 (22%)	6 (6%)	1	20
16	CQ	98/100 (98%)	76 (78%)	16 (16%)	6 (6%)	1	20
17	AR	68/70 (97%)	50 (74%)	9 (13%)	9 (13%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	CR	68/70 (97%)	56 (82%)	8 (12%)	4 (6%)	1	21
18	AS	77/79 (98%)	43 (56%)	23 (30%)	11 (14%)	0	4
18	CS	77/79 (98%)	47 (61%)	27 (35%)	3 (4%)	3	28
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	1	13
19	CT	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	2	23
20	AY	657/687 (96%)	407 (62%)	174 (26%)	76 (12%)	0	6
20	CY	657/687 (96%)	437 (66%)	135 (20%)	85 (13%)	0	5
25	BC	226/228 (99%)	107 (47%)	63 (28%)	56 (25%)	0	1
25	DC	226/228 (99%)	114 (50%)	52 (23%)	60 (26%)	0	0
26	BD	273/275 (99%)	174 (64%)	60 (22%)	39 (14%)	0	4
26	DD	273/275 (99%)	180 (66%)	59 (22%)	34 (12%)	0	6
27	BE	203/205 (99%)	134 (66%)	41 (20%)	28 (14%)	0	4
27	DE	203/205 (99%)	124 (61%)	49 (24%)	30 (15%)	0	4
28	BF	206/208 (99%)	139 (68%)	43 (21%)	24 (12%)	0	6
28	DF	206/208 (99%)	127 (62%)	51 (25%)	28 (14%)	0	4
29	BG	179/181 (99%)	131 (73%)	37 (21%)	11 (6%)	1	20
29	DG	179/181 (99%)	127 (71%)	37 (21%)	15 (8%)	1	13
30	BH	165/167 (99%)	117 (71%)	31 (19%)	17 (10%)	0	9
30	DH	165/167 (99%)	116 (70%)	30 (18%)	19 (12%)	0	7
32	BK	138/140 (99%)	91 (66%)	32 (23%)	15 (11%)	0	8
32	DK	138/140 (99%)	77 (56%)	44 (32%)	17 (12%)	0	6
33	BN	137/139 (99%)	52 (38%)	32 (23%)	53 (39%)	0	0
33	DN	137/139 (99%)	55 (40%)	28 (20%)	54 (39%)	0	0
34	BO	120/122 (98%)	89 (74%)	21 (18%)	10 (8%)	1	13
34	DO	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	0	9
35	BP	144/146 (99%)	84 (58%)	36 (25%)	24 (17%)	0	3
35	DP	144/146 (99%)	82 (57%)	39 (27%)	23 (16%)	0	3
36	BQ	139/141 (99%)	84 (60%)	35 (25%)	20 (14%)	0	4
36	DQ	139/141 (99%)	94 (68%)	34 (24%)	11 (8%)	1	14
37	BR	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	5
37	DR	115/117 (98%)	80 (70%)	22 (19%)	13 (11%)	0	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BS	97/99 (98%)	52 (54%)	26 (27%)	19 (20%)	0	2
38	DS	97/99 (98%)	51 (53%)	27 (28%)	19 (20%)	0	2
39	BT	136/138 (99%)	81 (60%)	27 (20%)	28 (21%)	0	2
39	DT	136/138 (99%)	79 (58%)	31 (23%)	26 (19%)	0	2
40	BU	115/117 (98%)	88 (76%)	17 (15%)	10 (9%)	1	12
40	DU	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	17
41	BV	99/101 (98%)	56 (57%)	28 (28%)	15 (15%)	0	4
41	DV	99/101 (98%)	64 (65%)	21 (21%)	14 (14%)	0	4
42	BW	111/113 (98%)	74 (67%)	25 (22%)	12 (11%)	0	8
42	DW	111/113 (98%)	76 (68%)	23 (21%)	12 (11%)	0	8
43	BX	91/93 (98%)	71 (78%)	13 (14%)	7 (8%)	1	15
43	DX	91/93 (98%)	67 (74%)	10 (11%)	14 (15%)	0	4
44	BY	105/107 (98%)	54 (51%)	31 (30%)	20 (19%)	0	2
44	DY	105/107 (98%)	59 (56%)	26 (25%)	20 (19%)	0	2
45	BZ	183/185 (99%)	121 (66%)	43 (24%)	19 (10%)	0	9
45	DZ	183/185 (99%)	109 (60%)	45 (25%)	29 (16%)	0	3
46	B0	82/84 (98%)	63 (77%)	14 (17%)	5 (6%)	1	20
46	D0	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	1	20
47	B1	91/93 (98%)	48 (53%)	24 (26%)	19 (21%)	0	1
47	D1	91/93 (98%)	52 (57%)	20 (22%)	19 (21%)	0	1
48	B2	69/71 (97%)	51 (74%)	12 (17%)	6 (9%)	1	12
48	D2	69/71 (97%)	53 (77%)	12 (17%)	4 (6%)	1	21
49	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	31
49	D3	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	2	23
50	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	4
50	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	4
51	B5	57/59 (97%)	36 (63%)	14 (25%)	7 (12%)	0	6
51	D5	57/59 (97%)	38 (67%)	6 (10%)	13 (23%)	0	1
52	B6	48/50 (96%)	24 (50%)	15 (31%)	9 (19%)	0	2
52	D6	48/50 (96%)	20 (42%)	17 (35%)	11 (23%)	0	1
53	B7	47/49 (96%)	33 (70%)	11 (23%)	3 (6%)	1	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
53	D7	47/49 (96%)	26 (55%)	14 (30%)	7 (15%)	0 4
54	B8	62/64 (97%)	34 (55%)	16 (26%)	12 (19%)	0 2
54	D8	62/64 (97%)	35 (56%)	13 (21%)	14 (23%)	0 1
55	B9	35/37 (95%)	29 (83%)	5 (14%)	1 (3%)	4 34
55	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	1 12
56	Be	70/103 (68%)	39 (56%)	23 (33%)	8 (11%)	0 7
56	De	70/103 (68%)	40 (57%)	17 (24%)	13 (19%)	0 2
All	All	13246/13568 (98%)	8764 (66%)	2800 (21%)	1682 (13%)	0 5

5 of 1682 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	76	GLN
1	AB	190	THR
2	AC	12	LEU
2	AC	110	ASN
2	AC	130	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	AB	203/203 (100%)	163 (80%)	40 (20%)	1 9
1	CB	203/203 (100%)	158 (78%)	45 (22%)	1 6
2	AC	161/161 (100%)	129 (80%)	32 (20%)	1 9
2	CC	161/161 (100%)	128 (80%)	33 (20%)	1 8
3	AD	180/180 (100%)	142 (79%)	38 (21%)	1 8
3	CD	180/180 (100%)	148 (82%)	32 (18%)	2 12
4	AE	116/116 (100%)	92 (79%)	24 (21%)	1 8
4	CE	116/116 (100%)	89 (77%)	27 (23%)	1 5
5	AF	90/90 (100%)	73 (81%)	17 (19%)	1 10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	CF	90/90 (100%)	77 (86%)	13 (14%)	3	20
6	AG	126/126 (100%)	111 (88%)	15 (12%)	5	26
6	CG	126/126 (100%)	110 (87%)	16 (13%)	4	23
7	AH	119/119 (100%)	98 (82%)	21 (18%)	2	13
7	CH	119/119 (100%)	94 (79%)	25 (21%)	1	8
8	AI	98/98 (100%)	83 (85%)	15 (15%)	2	17
8	CI	98/98 (100%)	78 (80%)	20 (20%)	1	8
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	9
9	CJ	89/89 (100%)	68 (76%)	21 (24%)	1	5
10	AK	90/90 (100%)	80 (89%)	10 (11%)	6	29
10	CK	90/90 (100%)	79 (88%)	11 (12%)	5	25
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	7
11	CL	104/104 (100%)	82 (79%)	22 (21%)	1	7
12	AM	100/100 (100%)	84 (84%)	16 (16%)	2	16
12	CM	100/100 (100%)	79 (79%)	21 (21%)	1	8
13	AN	49/49 (100%)	40 (82%)	9 (18%)	1	11
13	CN	49/49 (100%)	38 (78%)	11 (22%)	1	6
14	AO	79/79 (100%)	61 (77%)	18 (23%)	1	6
14	CO	79/79 (100%)	68 (86%)	11 (14%)	3	21
15	AP	72/72 (100%)	68 (94%)	4 (6%)	21	52
15	CP	72/72 (100%)	60 (83%)	12 (17%)	2	15
16	AQ	95/95 (100%)	80 (84%)	15 (16%)	2	17
16	CQ	95/95 (100%)	81 (85%)	14 (15%)	3	19
17	AR	61/61 (100%)	49 (80%)	12 (20%)	1	9
17	CR	61/61 (100%)	54 (88%)	7 (12%)	5	27
18	AS	69/69 (100%)	52 (75%)	17 (25%)	0	5
18	CS	69/69 (100%)	53 (77%)	16 (23%)	1	6
19	AT	76/76 (100%)	64 (84%)	12 (16%)	2	17
19	CT	76/76 (100%)	58 (76%)	18 (24%)	1	5
20	AY	558/579 (96%)	450 (81%)	108 (19%)	1	9
20	CY	558/579 (96%)	446 (80%)	112 (20%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BC	180/180 (100%)	130 (72%)	50 (28%)	0	3
25	DC	180/180 (100%)	146 (81%)	34 (19%)	1	10
26	BD	217/217 (100%)	182 (84%)	35 (16%)	2	16
26	DD	217/217 (100%)	173 (80%)	44 (20%)	1	8
27	BE	165/165 (100%)	134 (81%)	31 (19%)	1	10
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	6
28	BF	165/165 (100%)	129 (78%)	36 (22%)	1	7
28	DF	165/165 (100%)	132 (80%)	33 (20%)	1	9
29	BG	155/155 (100%)	140 (90%)	15 (10%)	8	33
29	DG	155/155 (100%)	131 (84%)	24 (16%)	2	17
30	BH	136/136 (100%)	111 (82%)	25 (18%)	1	11
30	DH	136/136 (100%)	117 (86%)	19 (14%)	3	21
32	BK	105/105 (100%)	77 (73%)	28 (27%)	0	3
32	DK	105/105 (100%)	81 (77%)	24 (23%)	1	6
33	BN	118/118 (100%)	88 (75%)	30 (25%)	0	4
33	DN	118/118 (100%)	84 (71%)	34 (29%)	0	2
34	BO	100/100 (100%)	79 (79%)	21 (21%)	1	8
34	DO	100/100 (100%)	82 (82%)	18 (18%)	1	12
35	BP	112/112 (100%)	84 (75%)	28 (25%)	0	4
35	DP	112/112 (100%)	88 (79%)	24 (21%)	1	7
36	BQ	111/111 (100%)	78 (70%)	33 (30%)	0	2
36	DQ	111/111 (100%)	91 (82%)	20 (18%)	1	12
37	BR	100/100 (100%)	82 (82%)	18 (18%)	1	12
37	DR	100/100 (100%)	78 (78%)	22 (22%)	1	7
38	BS	77/77 (100%)	64 (83%)	13 (17%)	2	14
38	DS	77/77 (100%)	58 (75%)	19 (25%)	0	5
39	BT	120/120 (100%)	93 (78%)	27 (22%)	1	6
39	DT	120/120 (100%)	91 (76%)	29 (24%)	0	5
40	BU	93/93 (100%)	78 (84%)	15 (16%)	2	16
40	DU	93/93 (100%)	76 (82%)	17 (18%)	1	11
41	BV	82/82 (100%)	59 (72%)	23 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DV	82/82 (100%)	68 (83%)	14 (17%)	2	14
42	BW	92/92 (100%)	79 (86%)	13 (14%)	3	21
42	DW	92/92 (100%)	72 (78%)	20 (22%)	1	7
43	BX	75/75 (100%)	58 (77%)	17 (23%)	1	6
43	DX	75/75 (100%)	59 (79%)	16 (21%)	1	7
44	BY	88/88 (100%)	65 (74%)	23 (26%)	0	4
44	DY	88/88 (100%)	74 (84%)	14 (16%)	2	16
45	BZ	162/162 (100%)	127 (78%)	35 (22%)	1	7
45	DZ	162/162 (100%)	135 (83%)	27 (17%)	2	15
46	B0	66/66 (100%)	59 (89%)	7 (11%)	6	30
46	D0	66/66 (100%)	53 (80%)	13 (20%)	1	9
47	B1	78/78 (100%)	56 (72%)	22 (28%)	0	2
47	D1	78/78 (100%)	57 (73%)	21 (27%)	0	3
48	B2	66/66 (100%)	56 (85%)	10 (15%)	3	18
48	D2	66/66 (100%)	57 (86%)	9 (14%)	3	22
49	B3	52/52 (100%)	44 (85%)	8 (15%)	2	17
49	D3	52/52 (100%)	45 (86%)	7 (14%)	4	22
50	B4	31/31 (100%)	23 (74%)	8 (26%)	0	4
50	D4	31/31 (100%)	22 (71%)	9 (29%)	0	2
51	B5	51/51 (100%)	38 (74%)	13 (26%)	0	4
51	D5	51/51 (100%)	45 (88%)	6 (12%)	5	26
52	B6	49/49 (100%)	35 (71%)	14 (29%)	0	2
52	D6	49/49 (100%)	31 (63%)	18 (37%)	0	0
53	B7	42/42 (100%)	35 (83%)	7 (17%)	2	15
53	D7	42/42 (100%)	36 (86%)	6 (14%)	3	20
54	B8	54/54 (100%)	45 (83%)	9 (17%)	2	15
54	D8	54/54 (100%)	42 (78%)	12 (22%)	1	6
55	B9	34/34 (100%)	26 (76%)	8 (24%)	1	5
55	D9	34/34 (100%)	31 (91%)	3 (9%)	10	38
56	Be	54/54 (100%)	48 (89%)	6 (11%)	6	29
56	De	54/54 (100%)	47 (87%)	7 (13%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	11130/11172 (100%)	8951 (80%)	2179 (20%)	1 9

5 of 2179 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	DP	50	ARG
37	DR	89	ASP
35	DP	39	LYS
46	D0	82	ARG
36	BQ	66	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
28	DF	75	HIS
42	DW	102	HIS
29	DG	138	GLN
34	DO	29	ASN
45	DZ	75	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1510/1511 (99%)	358 (23%)	16 (1%)
21	CA	1511/1511 (100%)	377 (24%)	16 (1%)
22	AW	76/77 (98%)	37 (48%)	1 (1%)
22	CW	76/77 (98%)	42 (55%)	2 (2%)
23	AV	35/36 (97%)	24 (68%)	9 (25%)
23	CV	35/36 (97%)	27 (77%)	7 (20%)
24	AX	75/78 (96%)	29 (38%)	1 (1%)
24	CX	75/78 (96%)	30 (40%)	0
59	BA	2878/2879 (99%)	748 (25%)	28 (0%)
59	DA	2878/2879 (99%)	715 (24%)	29 (1%)
60	BB	118/119 (99%)	27 (22%)	0
60	DB	118/119 (99%)	32 (27%)	0
All	All	9385/9400 (99%)	2446 (26%)	109 (1%)

5 of 2446 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	6	G
21	AA	7	G
21	AA	9	G
21	AA	31	G
21	AA	32	A

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	CA	115	G
23	CV	14	A
59	DA	2422	A
21	CA	328	C
21	CA	1200	C

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 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
63	NMY	BA	2903	-	45,45,45	0.60	0	63,67,67	0.97	4 (6%)
63	NMY	AA	1601	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
63	NMY	BA	2904	-	45,45,45	0.59	0	63,67,67	0.97	4 (6%)
61	GDP	CY	701	-	24,30,30	1.30	3 (12%)	30,47,47	1.69	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
63	NMY	CA	1601	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
63	NMY	DA	2901	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
63	NMY	BA	2902	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
62	FUA	CY	702	-	39,40,40	1.67	7 (17%)	49,64,64	1.52	6 (12%)
62	FUA	AY	702	-	39,40,40	1.67	7 (17%)	49,64,64	1.52	6 (12%)
61	GDP	AY	701	-	24,30,30	1.37	4 (16%)	30,47,47	1.76	8 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
63	NMY	BA	2903	-	-	12/18/94/94	0/4/4/4
63	NMY	AA	1601	-	-	12/18/94/94	0/4/4/4
63	NMY	BA	2904	-	-	12/18/94/94	0/4/4/4
61	GDP	CY	701	-	-	5/12/32/32	0/3/3/3
63	NMY	CA	1601	-	-	12/18/94/94	0/4/4/4
63	NMY	DA	2901	-	-	12/18/94/94	0/4/4/4
63	NMY	BA	2902	-	-	12/18/94/94	0/4/4/4
62	FUA	CY	702	-	-	6/15/92/92	0/4/4/4
62	FUA	AY	702	-	-	6/15/92/92	0/4/4/4
61	GDP	AY	701	-	-	3/12/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CY	702	FUA	C23-C22	-4.39	1.39	1.51
62	AY	702	FUA	C23-C22	-4.33	1.40	1.51
62	AY	702	FUA	C23-C24	-4.28	1.39	1.53
62	CY	702	FUA	C23-C24	-4.26	1.39	1.53
61	AY	701	GDP	C5-C6	-4.22	1.38	1.47

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	CY	702	FUA	C13-C12-C11	-4.32	105.84	111.90
62	AY	702	FUA	C13-C12-C11	-4.31	105.87	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
62	AY	702	FUA	C16-O2-C31	-3.90	111.13	117.06
62	CY	702	FUA	C16-O2-C31	-3.88	111.16	117.06
61	CY	701	GDP	C2-N1-C6	-3.85	118.01	125.10

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

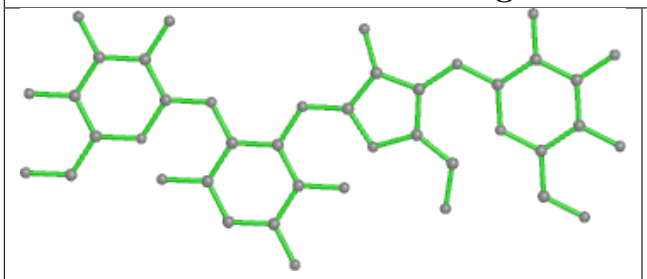
Mol	Chain	Res	Type	Atoms
61	AY	701	GDP	PA-O3A-PB-O3B
61	CY	701	GDP	C5'-O5'-PA-O3A
61	CY	701	GDP	C5'-O5'-PA-O1A
61	CY	701	GDP	C5'-O5'-PA-O2A
61	CY	701	GDP	O4'-C4'-C5'-O5'

There are no ring outliers.

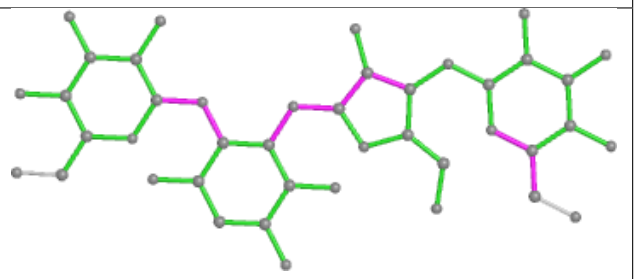
No monomer is involved in short contacts.

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

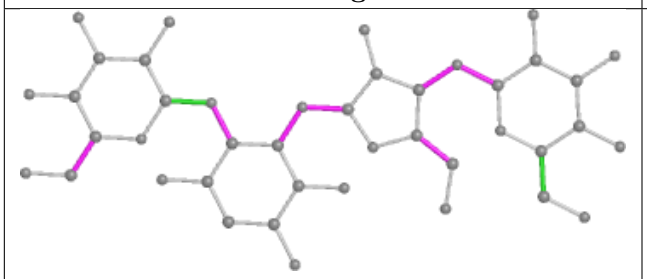
Ligand NMY BA 2903



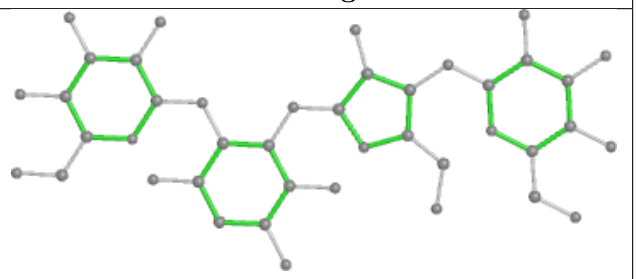
Bond lengths



Bond angles

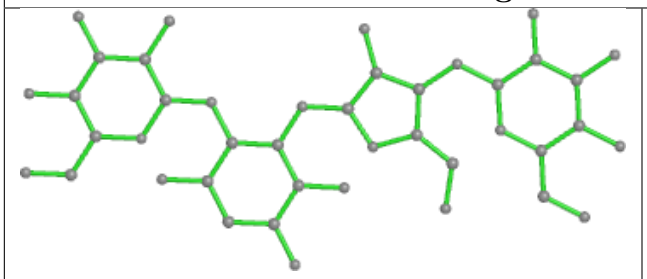


Torsions

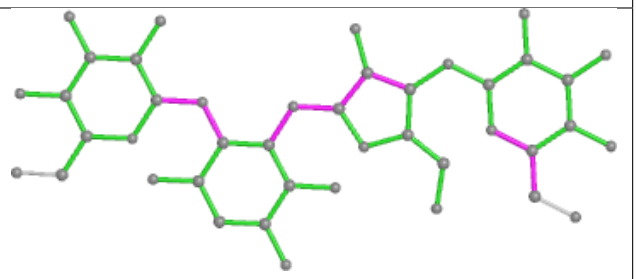


Rings

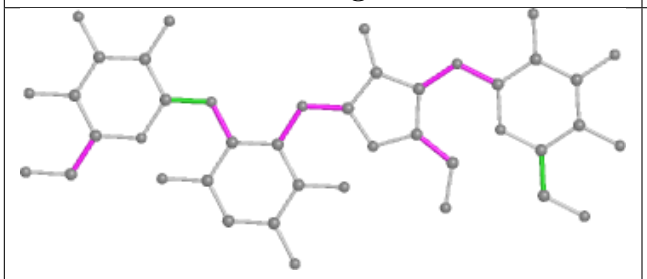
Ligand NMY AA 1601



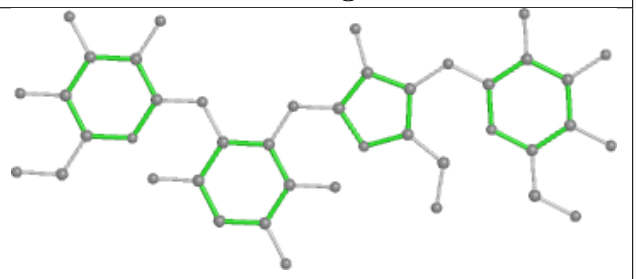
Bond lengths



Bond angles

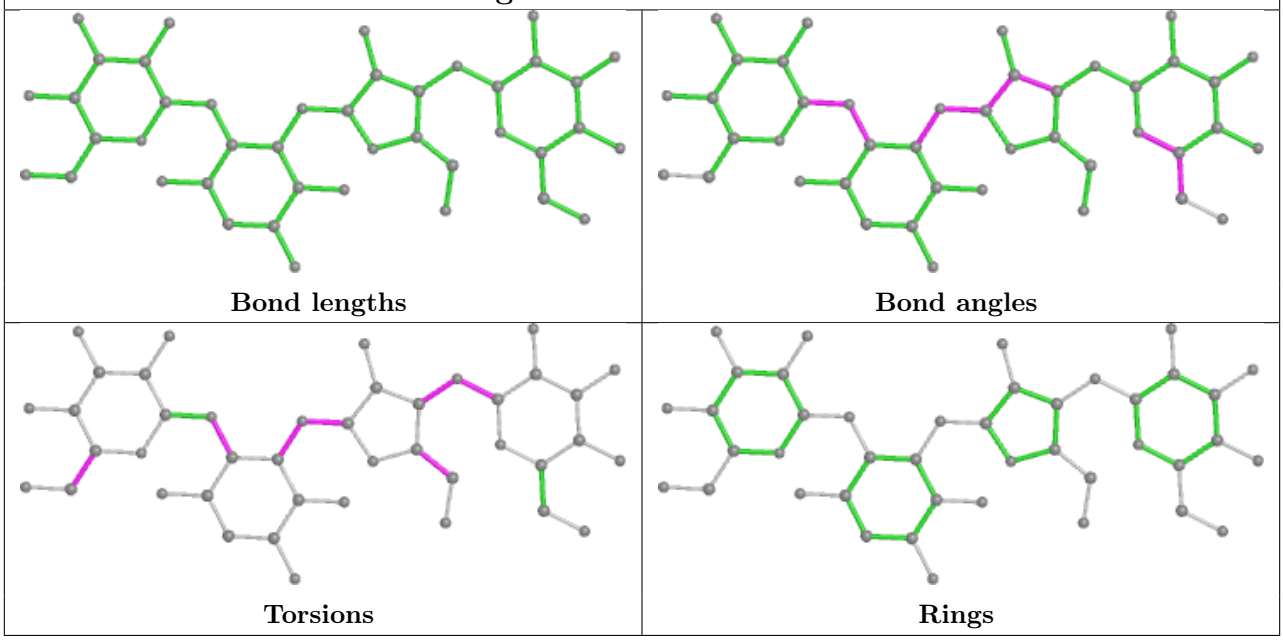


Torsions

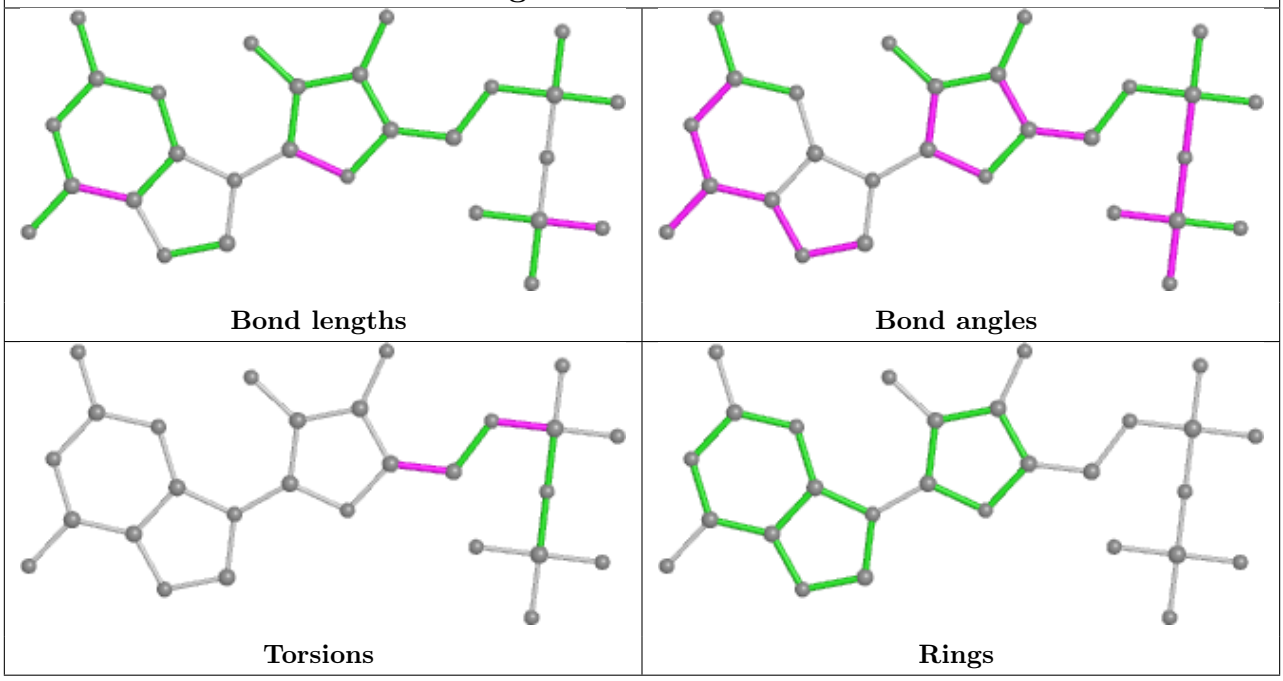


Rings

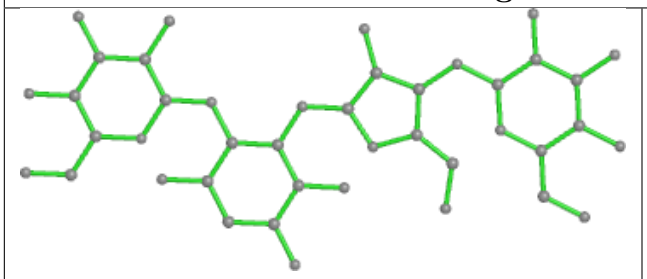
Ligand NMY BA 2904



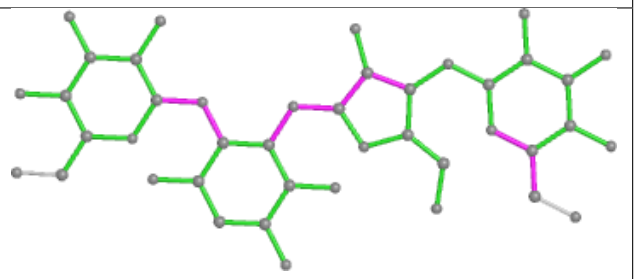
Ligand GDP CY 701



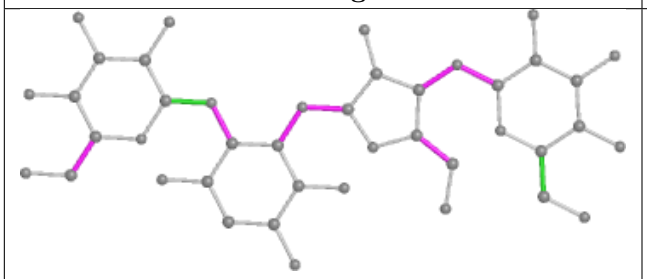
Ligand NMY CA 1601



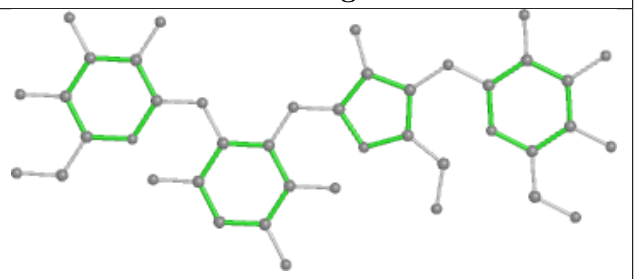
Bond lengths



Bond angles

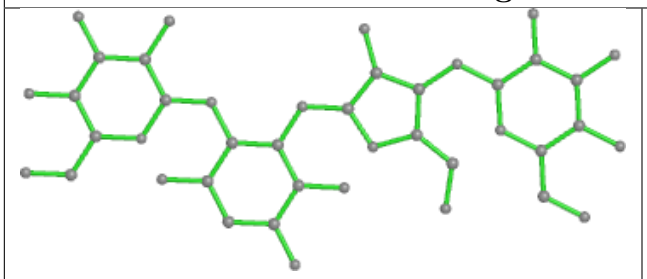


Torsions

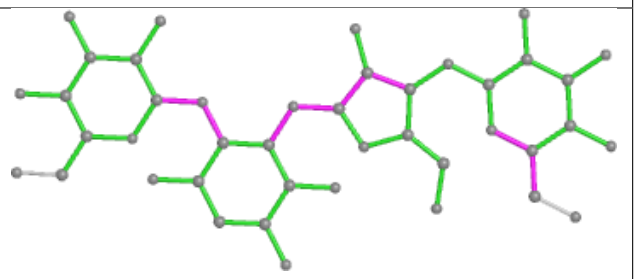


Rings

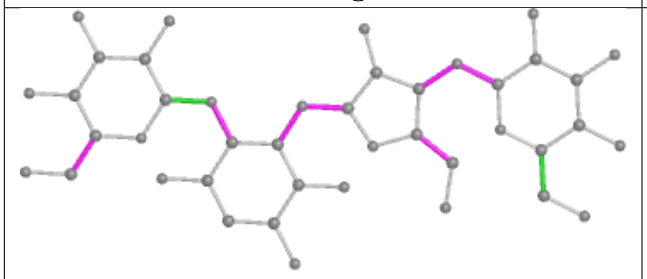
Ligand NMY DA 2901



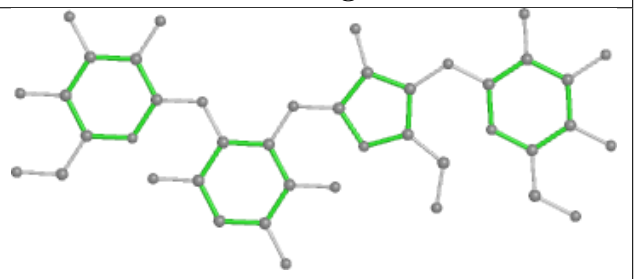
Bond lengths



Bond angles

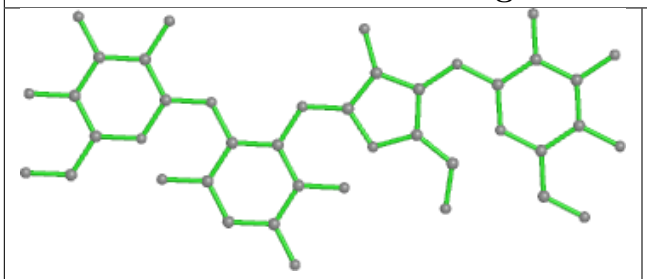


Torsions

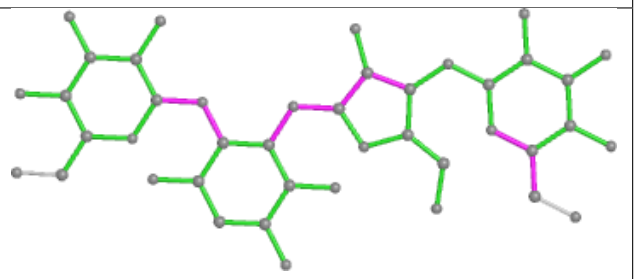


Rings

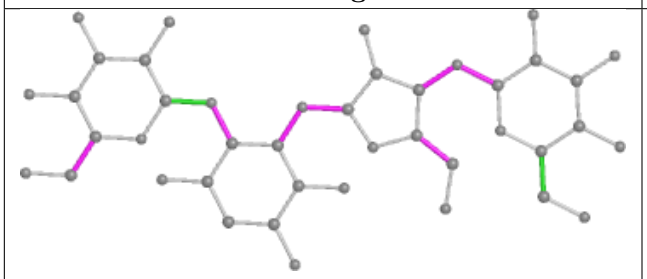
Ligand NMY BA 2902



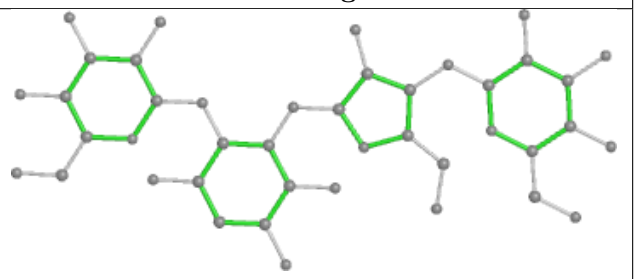
Bond lengths



Bond angles

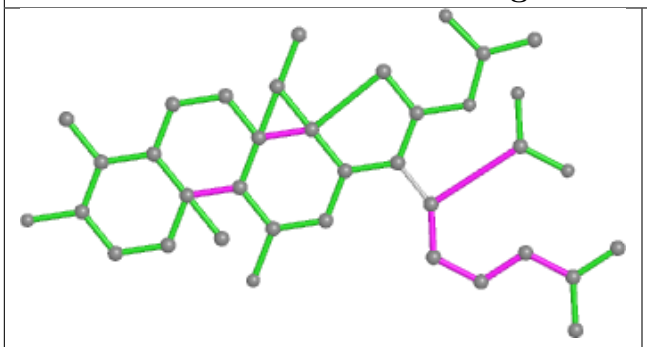


Torsions

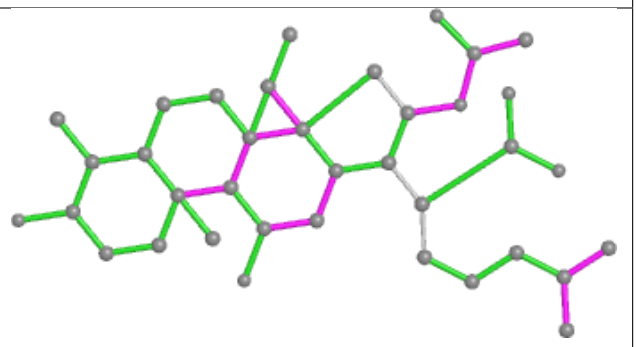


Rings

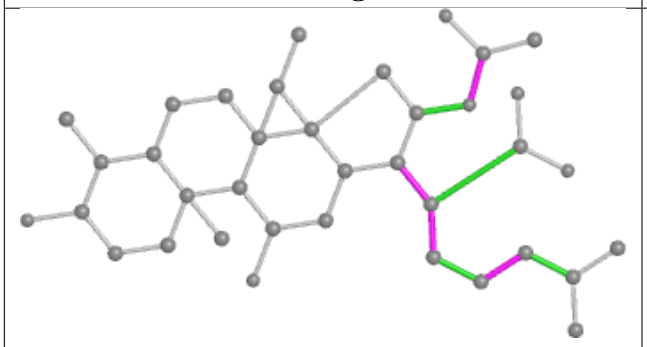
Ligand FUA CY 702



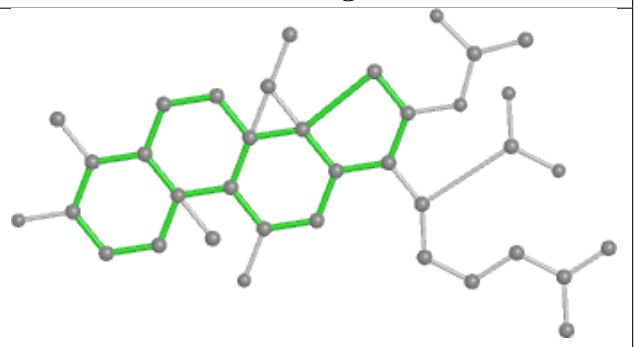
Bond lengths



Bond angles

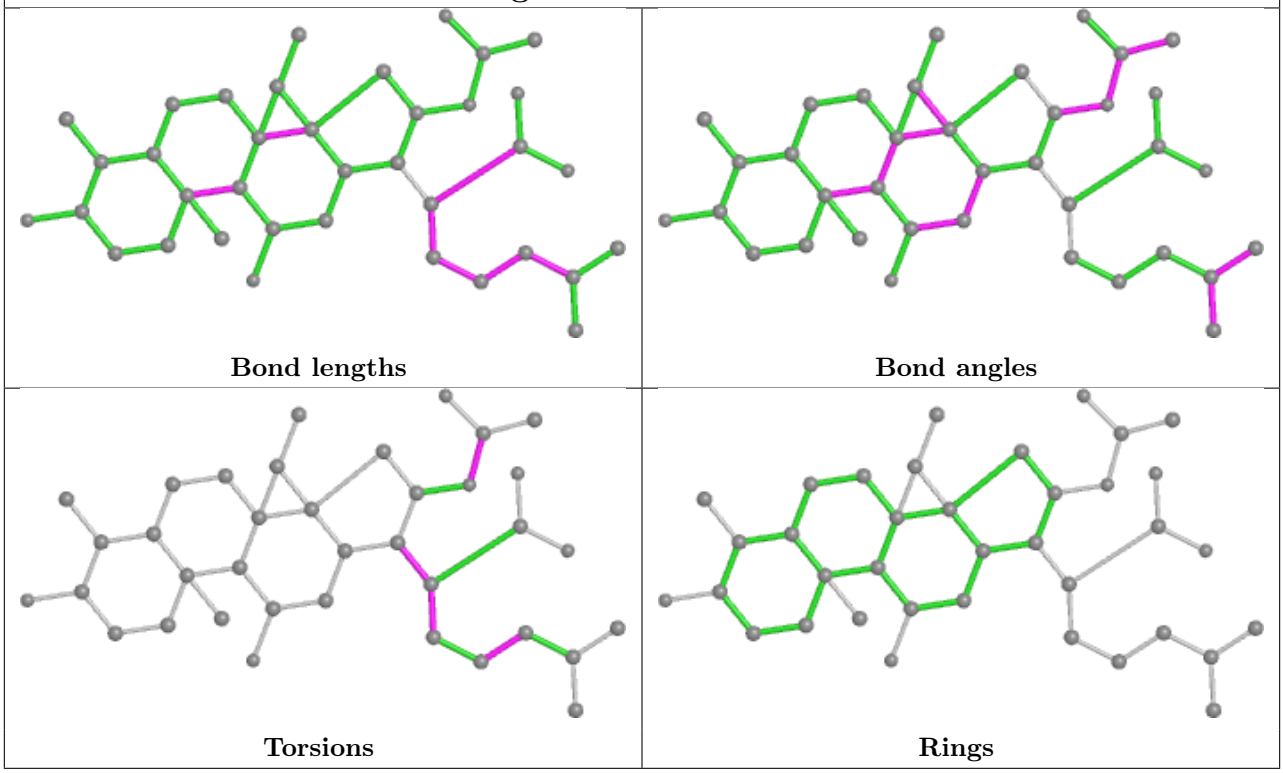


Torsions

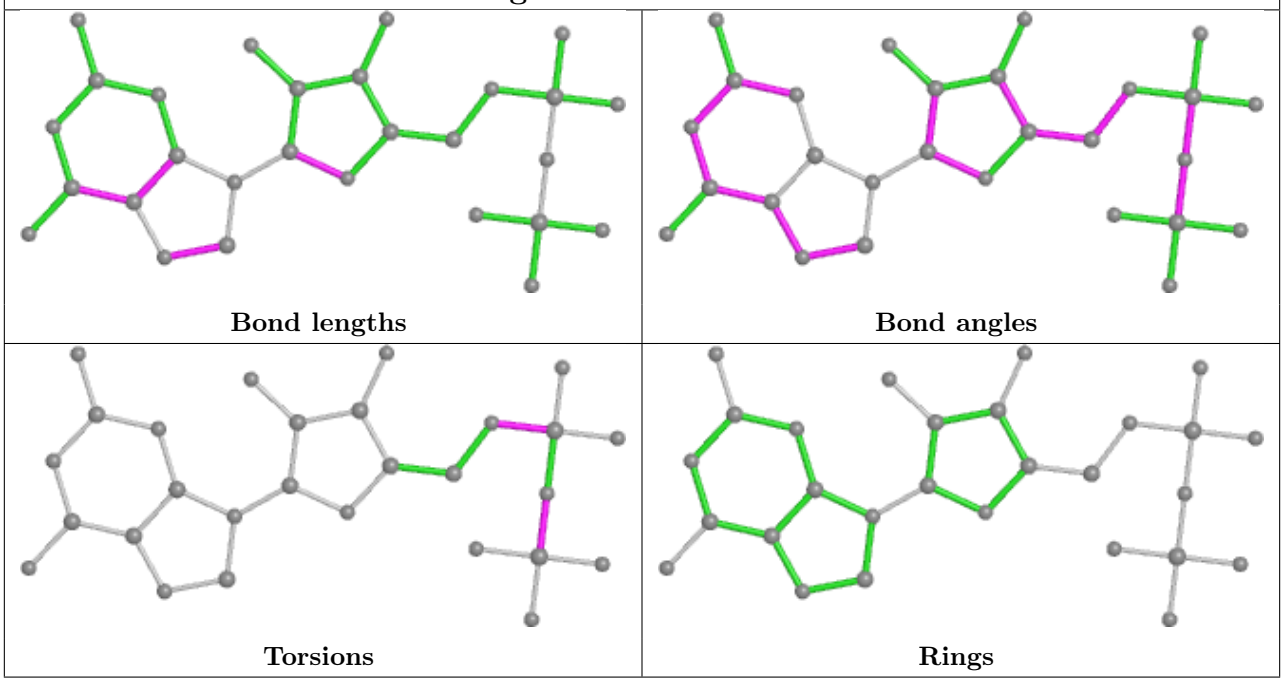


Rings

Ligand FUA AY 702



Ligand GDP AY 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	CX	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CX	76:A	O3'	77:VAL	N	3.06

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AB	235/235 (100%)	-0.33	4 (1%)	70	62	17, 55, 103, 129	0
1	CB	235/235 (100%)	-0.09	3 (1%)	77	70	17, 63, 111, 140	0
2	AC	207/207 (100%)	1.77	89 (42%)	0	0	18, 52, 99, 118	0
2	CC	207/207 (100%)	1.85	81 (39%)	0	0	15, 58, 99, 132	0
3	AD	208/208 (100%)	-0.46	2 (0%)	82	76	14, 59, 107, 137	0
3	CD	208/208 (100%)	-0.32	1 (0%)	91	87	20, 52, 102, 136	0
4	AE	151/151 (100%)	0.08	15 (9%)	7	6	26, 62, 96, 129	0
4	CE	151/151 (100%)	-0.05	9 (5%)	21	17	19, 56, 99, 143	0
5	AF	101/101 (100%)	-0.60	0	100	100	22, 57, 111, 128	0
5	CF	101/101 (100%)	-0.65	0	100	100	19, 56, 106, 128	0
6	AG	155/155 (100%)	-0.28	7 (4%)	33	28	26, 78, 122, 150	0
6	CG	155/155 (100%)	-0.32	6 (3%)	39	32	38, 85, 120, 147	0
7	AH	138/138 (100%)	-0.75	0	100	100	16, 43, 87, 109	0
7	CH	138/138 (100%)	-0.63	0	100	100	10, 49, 86, 102	0
8	AI	127/127 (100%)	-0.59	3 (2%)	59	50	30, 64, 101, 127	0
8	CI	127/127 (100%)	-0.59	1 (0%)	86	81	9, 77, 108, 134	0
9	AJ	99/99 (100%)	1.69	37 (37%)	0	0	34, 64, 104, 146	0
9	CJ	99/99 (100%)	1.63	35 (35%)	0	0	22, 57, 107, 115	0
10	AK	119/119 (100%)	0.03	10 (8%)	11	9	13, 74, 139, 160	0
10	CK	119/119 (100%)	-0.03	3 (2%)	57	49	21, 71, 125, 161	0
11	AL	125/125 (100%)	-0.27	4 (3%)	47	38	15, 73, 145, 164	0
11	CL	125/125 (100%)	0.00	6 (4%)	30	26	27, 85, 148, 170	0
12	AM	125/125 (100%)	0.06	6 (4%)	30	26	43, 86, 129, 159	0
12	CM	125/125 (100%)	-0.10	8 (6%)	19	15	27, 63, 103, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	AN	60/60 (100%)	1.04	13 (21%) 0 1	33, 70, 116, 128	0
13	CN	60/60 (100%)	0.81	10 (16%) 1 2	30, 58, 105, 128	0
14	AO	88/88 (100%)	-0.36	1 (1%) 80 74	26, 53, 99, 110	0
14	CO	88/88 (100%)	-0.42	0 100 100	8, 44, 84, 109	0
15	AP	84/84 (100%)	0.40	7 (8%) 11 9	33, 71, 110, 143	0
15	CP	84/84 (100%)	0.45	10 (11%) 4 5	39, 69, 111, 165	0
16	AQ	100/100 (100%)	-0.52	0 100 100	27, 62, 107, 131	0
16	CQ	100/100 (100%)	-0.34	2 (2%) 65 58	22, 66, 120, 135	0
17	AR	70/70 (100%)	-0.30	4 (5%) 23 19	19, 61, 102, 130	0
17	CR	70/70 (100%)	-0.29	3 (4%) 35 30	24, 56, 100, 125	0
18	AS	79/79 (100%)	-0.49	1 (1%) 77 70	17, 69, 111, 124	0
18	CS	79/79 (100%)	-0.13	5 (6%) 20 15	28, 65, 108, 130	0
19	AT	99/99 (100%)	-0.17	5 (5%) 28 24	17, 51, 85, 128	0
19	CT	99/99 (100%)	0.52	16 (16%) 1 2	26, 69, 110, 139	0
20	AY	661/687 (96%)	-0.44	23 (3%) 44 36	19, 64, 113, 178	0
20	CY	661/687 (96%)	-0.36	22 (3%) 46 38	11, 66, 108, 152	0
21	AA	1511/1511 (100%)	-0.46	14 (0%) 84 79	10, 90, 161, 248	0
21	CA	1511/1511 (100%)	-0.47	28 (1%) 66 59	10, 88, 160, 242	0
22	AW	77/77 (100%)	-0.15	9 (11%) 4 5	15, 71, 130, 150	0
22	CW	77/77 (100%)	0.09	7 (9%) 9 7	30, 88, 145, 178	0
23	AV	36/36 (100%)	1.73	8 (22%) 0 0	32, 89, 137, 186	0
23	CV	36/36 (100%)	3.53	16 (44%) 0 0	23, 139, 232, 237	0
24	AX	77/78 (98%)	-0.49	3 (3%) 39 32	3, 65, 233, 320	0
24	CX	77/78 (98%)	-0.36	2 (2%) 56 47	37, 123, 185, 285	0
25	BC	228/228 (100%)	1.24	65 (28%) 0 0	54, 104, 139, 159	0
25	DC	228/228 (100%)	0.75	48 (21%) 1 1	37, 90, 130, 169	0
26	BD	275/275 (100%)	-0.08	21 (7%) 13 11	10, 61, 103, 125	0
26	DD	275/275 (100%)	-0.03	14 (5%) 28 24	16, 57, 100, 127	0
27	BE	205/205 (100%)	0.16	10 (4%) 29 25	21, 60, 107, 131	0
27	DE	205/205 (100%)	0.15	8 (3%) 39 32	22, 57, 97, 142	0
28	BF	208/208 (100%)	0.37	22 (10%) 6 5	20, 67, 108, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
28	DF	208/208 (100%)	0.58	31 (14%)	2	2	23, 75, 120, 140	0
29	BG	181/181 (100%)	0.77	22 (12%)	4	4	28, 69, 113, 148	0
29	DG	181/181 (100%)	0.67	25 (13%)	2	3	25, 71, 113, 148	0
30	BH	167/167 (100%)	0.00	7 (4%)	36	30	29, 65, 108, 121	0
30	DH	167/167 (100%)	-0.01	8 (4%)	30	26	24, 59, 100, 132	0
31	BJ	0/170	-	-			-	-
31	DJ	0/170	-	-			-	-
32	BK	140/140 (100%)	-0.28	7 (5%)	28	25	32, 71, 114, 126	0
32	DK	140/140 (100%)	-0.08	7 (5%)	28	25	34, 77, 113, 138	0
33	BN	139/139 (100%)	2.00	56 (40%)	0	0	23, 105, 298, 334	0
33	DN	139/139 (100%)	2.07	57 (41%)	0	0	16, 116, 252, 312	0
34	BO	122/122 (100%)	1.65	45 (36%)	0	0	12, 50, 93, 111	0
34	DO	122/122 (100%)	2.17	56 (45%)	0	0	28, 59, 103, 132	0
35	BP	146/146 (100%)	-0.51	4 (2%)	54	45	25, 63, 106, 123	0
35	DP	146/146 (100%)	-0.45	3 (2%)	63	55	25, 67, 104, 131	0
36	BQ	141/141 (100%)	-0.35	4 (2%)	53	43	5, 54, 93, 109	0
36	DQ	141/141 (100%)	0.02	8 (5%)	23	19	27, 70, 113, 141	0
37	BR	117/117 (100%)	-0.62	0	100	100	29, 65, 116, 145	0
37	DR	117/117 (100%)	-0.71	1 (0%)	84	79	27, 62, 97, 126	0
38	BS	99/99 (100%)	1.00	20 (20%)	1	1	14, 70, 108, 117	0
38	DS	99/99 (100%)	0.78	11 (11%)	5	5	19, 52, 96, 120	0
39	BT	138/138 (100%)	1.23	43 (31%)	0	0	16, 59, 101, 123	0
39	DT	138/138 (100%)	1.14	34 (24%)	0	0	15, 51, 109, 140	0
40	BU	117/117 (100%)	-0.48	1 (0%)	84	79	20, 56, 96, 121	0
40	DU	117/117 (100%)	-0.45	1 (0%)	84	79	13, 53, 94, 142	0
41	BV	101/101 (100%)	0.22	5 (4%)	28	25	21, 66, 108, 127	0
41	DV	101/101 (100%)	0.13	5 (4%)	28	25	15, 65, 101, 126	0
42	BW	113/113 (100%)	-0.42	3 (2%)	54	45	13, 54, 99, 111	0
42	DW	113/113 (100%)	-0.35	5 (4%)	34	29	15, 64, 116, 148	0
43	BX	93/93 (100%)	-0.25	4 (4%)	35	30	20, 54, 96, 115	0
43	DX	93/93 (100%)	-0.34	2 (2%)	62	54	13, 45, 87, 126	0
44	BY	107/107 (100%)	0.31	10 (9%)	8	7	29, 58, 109, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	DY	107/107 (100%)	0.10	6 (5%) 24 20	25, 62, 97, 138	0
45	BZ	185/185 (100%)	-0.34	0 100 100	17, 58, 97, 113	0
45	DZ	185/185 (100%)	-0.22	4 (2%) 62 54	33, 64, 101, 138	0
46	B0	84/84 (100%)	0.60	15 (17%) 1 1	26, 75, 117, 131	0
46	D0	84/84 (100%)	0.06	4 (4%) 30 26	19, 65, 108, 116	0
47	B1	93/93 (100%)	1.11	20 (21%) 0 1	21, 84, 140, 156	0
47	D1	93/93 (100%)	1.41	27 (29%) 0 0	31, 103, 148, 181	0
48	B2	71/71 (100%)	-0.72	0 100 100	23, 55, 95, 116	0
48	D2	71/71 (100%)	-0.44	2 (2%) 53 43	35, 61, 103, 118	0
49	B3	60/60 (100%)	-0.50	1 (1%) 70 62	29, 60, 99, 112	0
49	D3	60/60 (100%)	-0.39	0 100 100	36, 68, 94, 110	0
50	B4	35/35 (100%)	1.49	11 (31%) 0 0	26, 71, 110, 122	0
50	D4	35/35 (100%)	1.26	8 (22%) 0 0	64, 109, 144, 185	0
51	B5	59/59 (100%)	-0.69	0 100 100	24, 63, 106, 123	0
51	D5	59/59 (100%)	-0.64	2 (3%) 45 37	31, 68, 113, 138	0
52	B6	50/50 (100%)	1.20	14 (28%) 0 0	13, 57, 107, 154	0
52	D6	50/50 (100%)	0.96	13 (26%) 0 0	26, 65, 120, 154	0
53	B7	49/49 (100%)	1.24	16 (32%) 0 0	46, 91, 136, 164	0
53	D7	49/49 (100%)	0.91	10 (20%) 1 1	51, 73, 109, 134	0
54	B8	64/64 (100%)	1.05	10 (15%) 2 2	26, 58, 109, 132	0
54	D8	64/64 (100%)	0.61	7 (10%) 5 5	30, 64, 104, 118	0
55	B9	37/37 (100%)	-0.34	1 (2%) 54 45	39, 64, 109, 116	0
55	D9	37/37 (100%)	-0.62	0 100 100	34, 65, 116, 134	0
56	Be	72/103 (69%)	0.63	12 (16%) 1 2	15, 49, 122, 163	0
56	De	72/103 (69%)	0.69	9 (12%) 3 4	14, 57, 118, 157	0
57	Bf	0/31	-	-	-	-
57	Bg	0/31	-	-	-	-
57	Df	0/31	-	-	-	-
57	Dg	0/31	-	-	-	-
58	Bh	0/30	-	-	-	-
58	Dh	0/30	-	-	-	-
59	BA	2879/2879 (100%)	-0.49	31 (1%) 80 74	11, 89, 164, 284	0
59	DA	2879/2879 (100%)	-0.49	31 (1%) 80 74	9, 88, 171, 274	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
60	BB	119/119 (100%)	-0.37	6 (5%) 28 25	18, 80, 158, 172	0
60	DB	119/119 (100%)	-0.36	0 100 100	30, 88, 150, 175	0
All	All	22852/23492 (97%)	-0.09	1472 (6%) 19 15	3, 73, 146, 334	0

The worst 5 of 1472 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	CV	36	A	21.2
23	CV	34	A	20.9
23	CV	35	A	18.6
23	AV	35	A	18.0
23	AV	34	A	13.7

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
64	MG	CY	703	1/1	0.74	0.18	6,6,6,6	0
64	MG	BA	2901	1/1	0.75	0.12	2,2,2,2	0
63	NMY	BA	2904	42/42	0.79	0.26	42,50,59,62	42
61	GDP	AY	701	28/28	0.80	0.24	179,183,185,185	0
62	FUA	AY	702	37/37	0.81	0.69	198,199,200,201	0
63	NMY	DA	2901	42/42	0.81	0.24	31,42,51,53	42
62	FUA	CY	702	37/37	0.82	0.89	194,196,197,197	0
63	NMY	BA	2902	42/42	0.82	0.22	14,24,43,44	42
63	NMY	AA	1601	42/42	0.87	0.31	16,27,36,38	42
63	NMY	BA	2903	42/42	0.87	0.28	18,29,38,41	42

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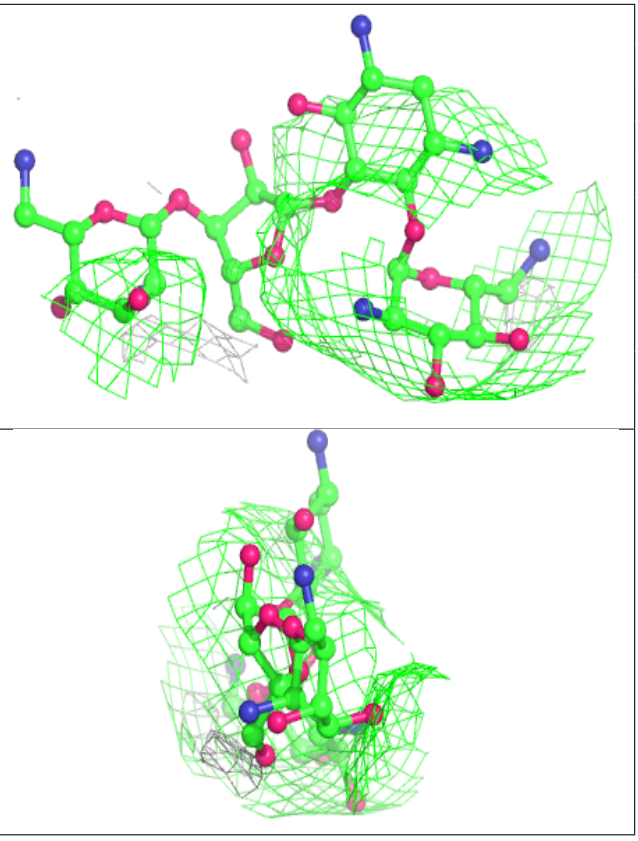
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
61	GDP	CY	701	28/28	0.88	0.14	104,108,109,110	0
63	NMY	CA	1601	42/42	0.90	0.23	14,25,34,37	42

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

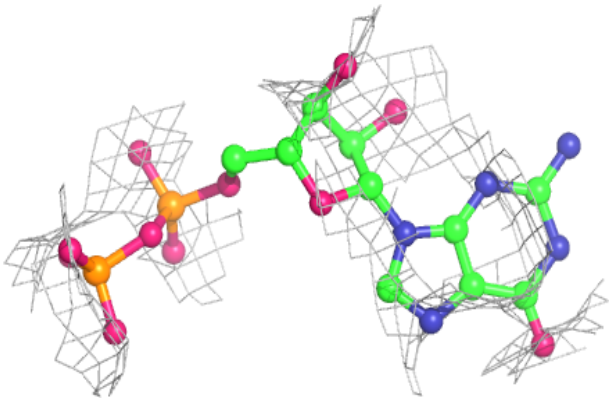
Electron density around NMY BA 2904:

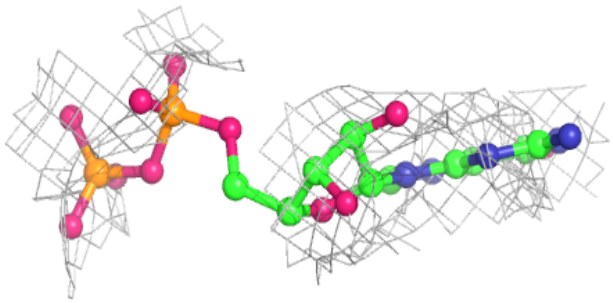
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

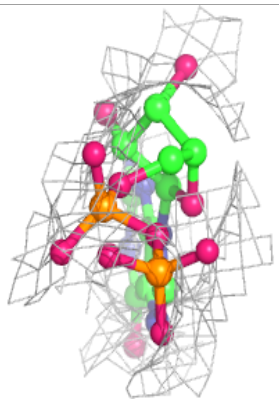


Electron density around GDP AY 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

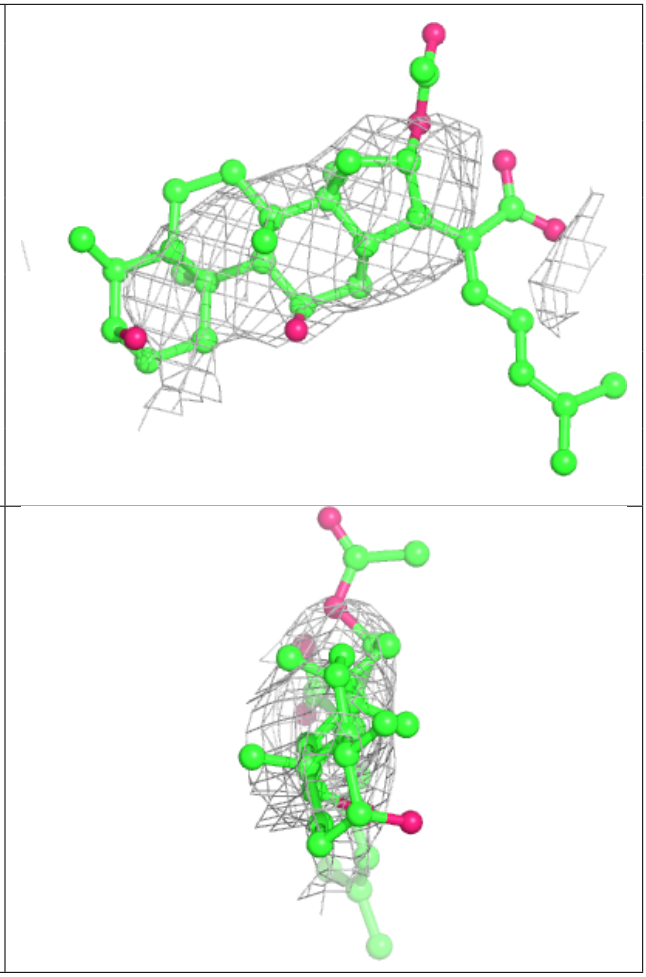






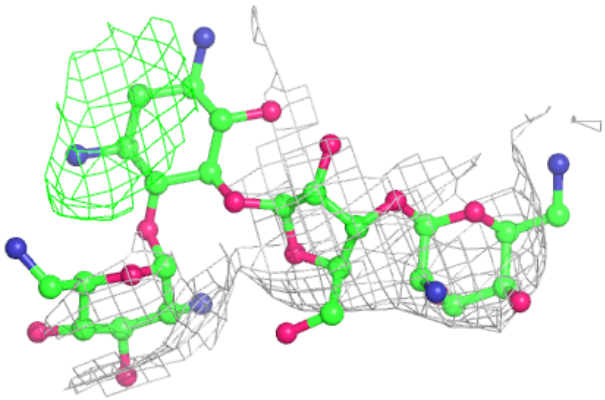
Electron density around FUA AY 702:

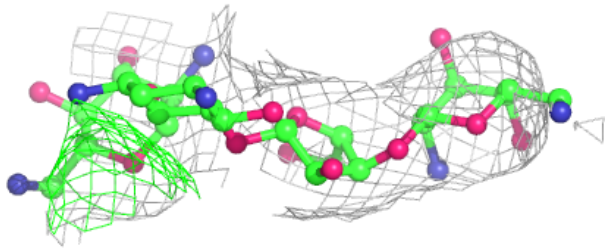
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

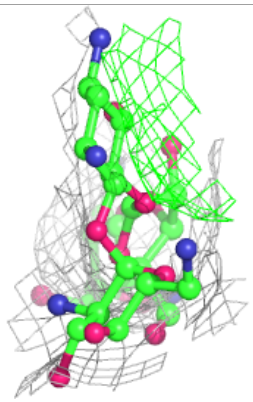


Electron density around NMY DA 2901:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

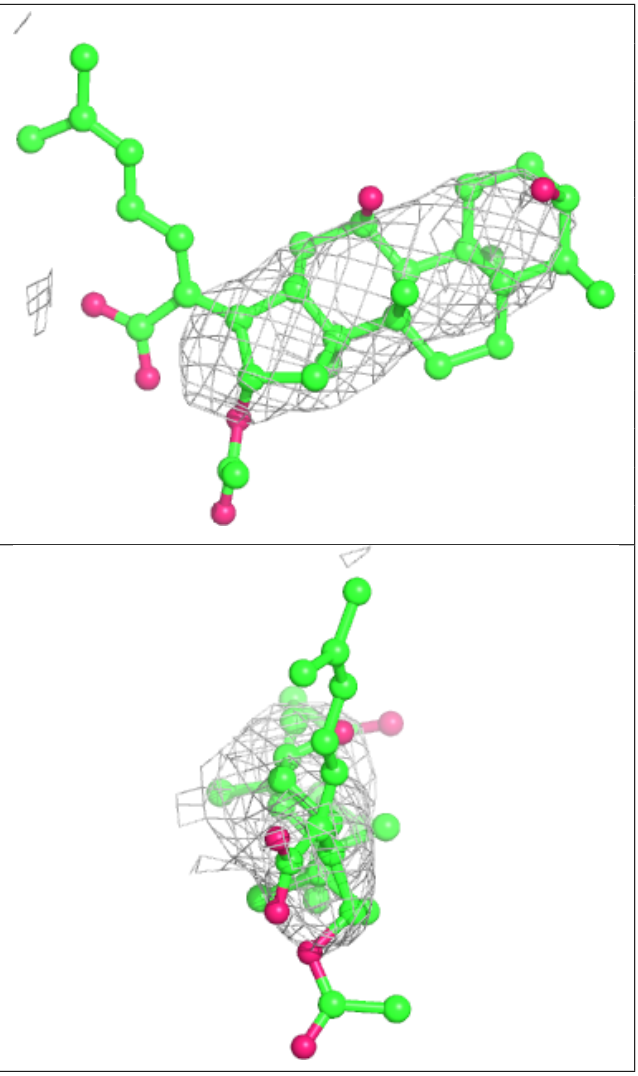






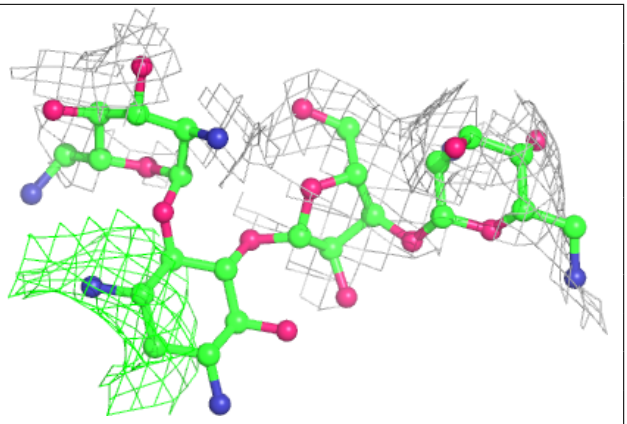
Electron density around FUA CY 702:

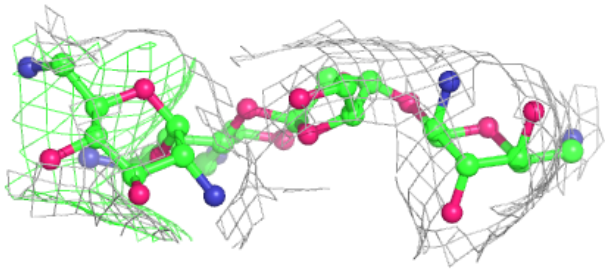
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

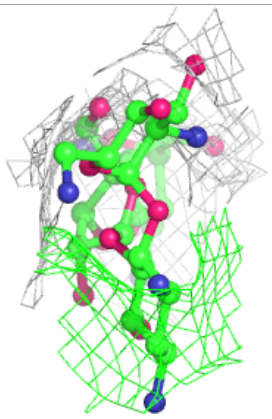


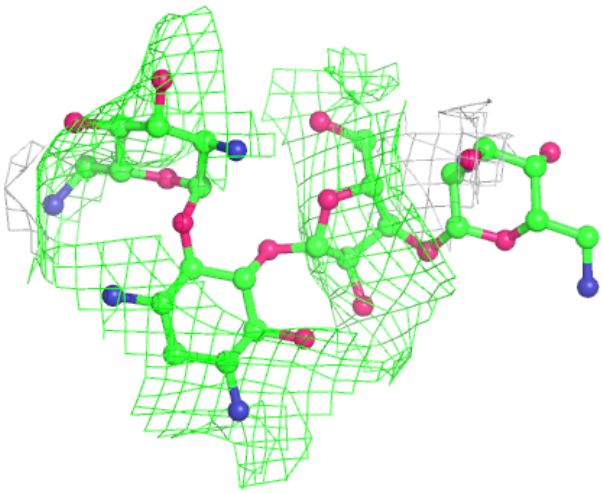
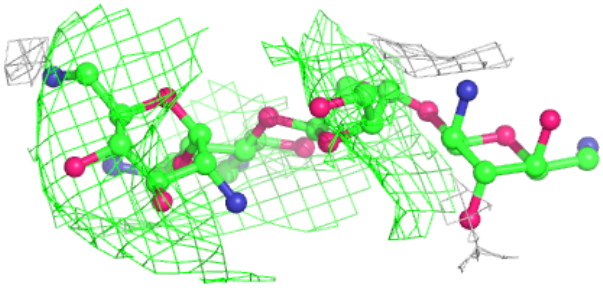
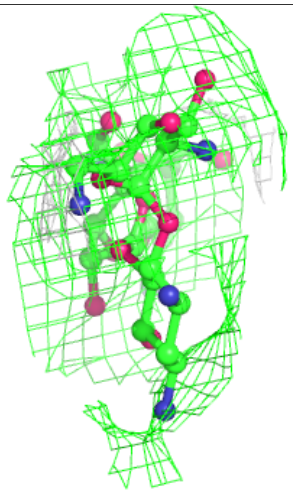
Electron density around NMY BA 2902:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



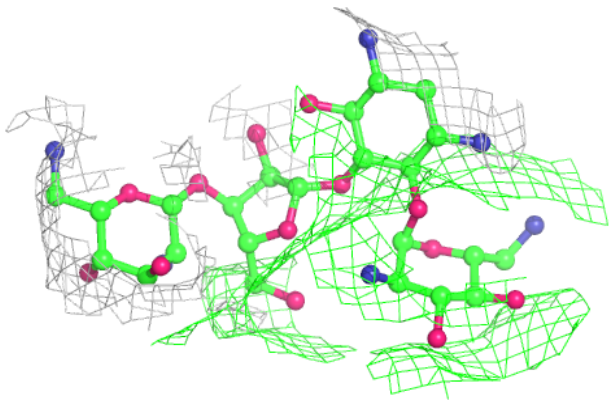


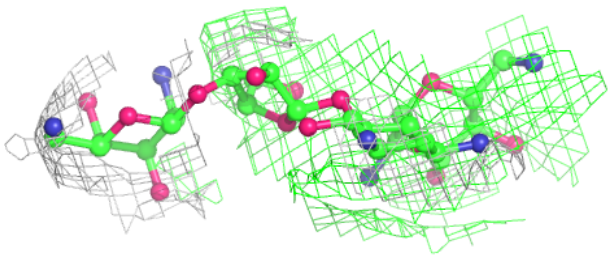


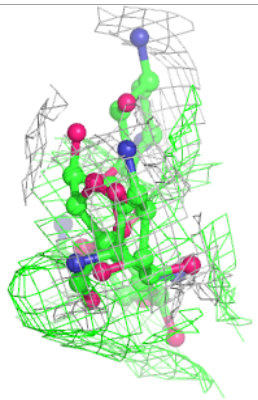
Electron density around NMY AA 1601: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

Electron density around NMY BA 2903:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

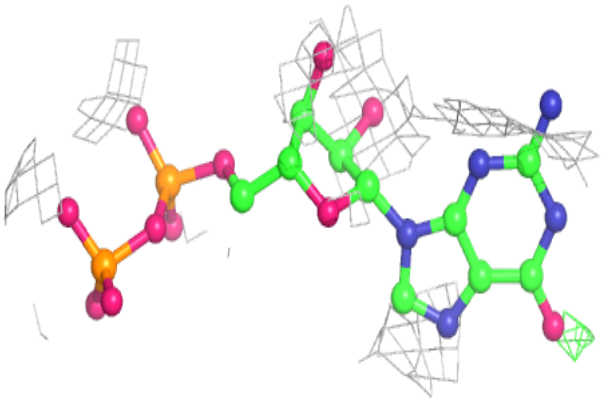


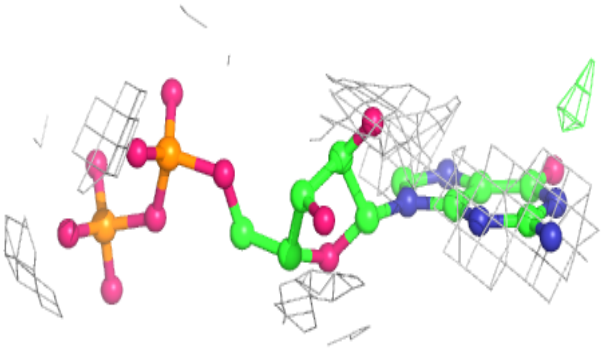


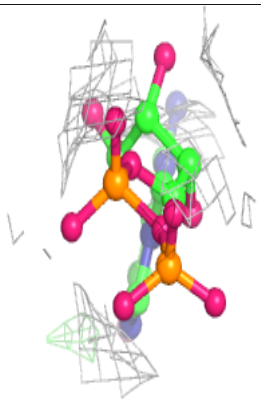


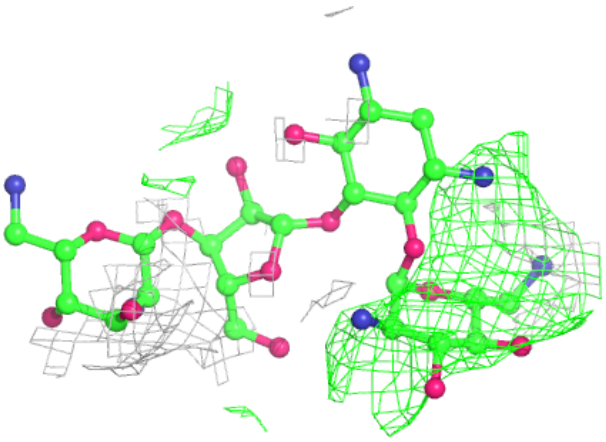
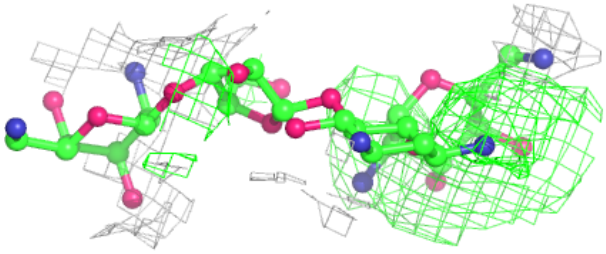
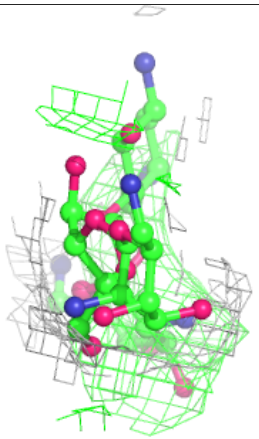
Electron density around GDP CY 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







Electron density around NMY CA 1601: $2mF_o$-DF_c (at 0.7 rmsd) in gray mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)	
	

6.5 Other polymers (i)

There are no such residues in this entry.