



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 09:07 AM UTC

PDB ID : 4W29 / pdb_00004w29
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

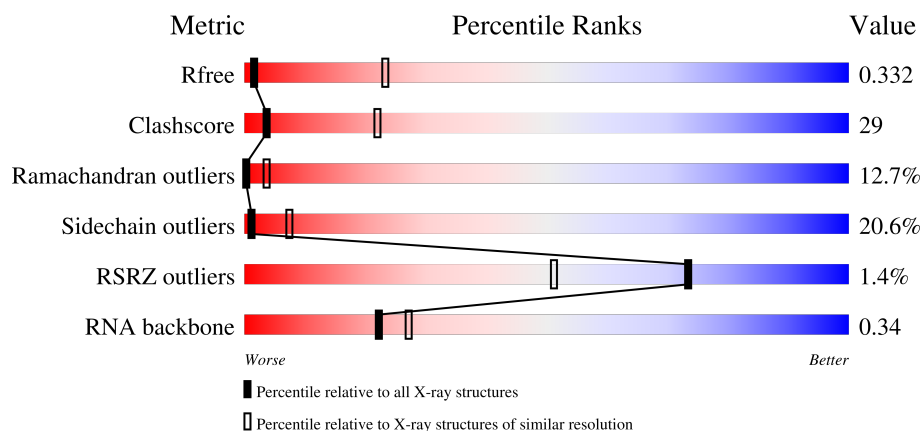
1 Overall quality at a glance

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.



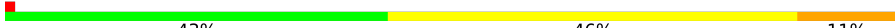
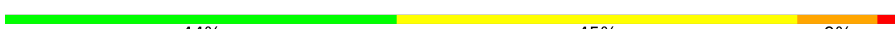
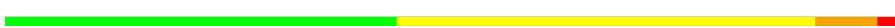
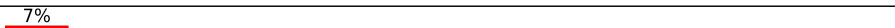
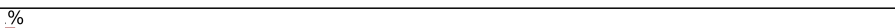
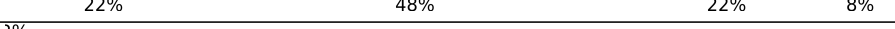
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)
RNA backbone	3983	1007 (4.50-3.10)

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 $\leq 5\%$. 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	40% 43% 14% •
1	CB	235	37% 46% 14% •
2	AC	207	36% 48% 15% •

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Mol	Chain	Length	Quality of chain
2	CC	207	
3	AD	208	
3	CD	208	
4	AE	151	
4	CE	151	
5	AF	101	
5	CF	101	
6	AG	155	
6	CG	155	
7	AH	138	
7	CH	138	
8	AI	127	
8	CI	127	
9	AJ	99	
9	CJ	99	
10	AK	119	
10	CK	119	
11	AL	125	
11	CL	125	
12	AM	125	
12	CM	125	
13	AN	60	
13	CN	60	
14	AO	88	
14	CO	88	

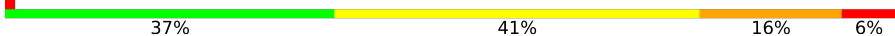
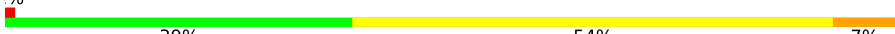
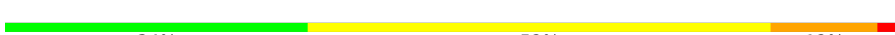
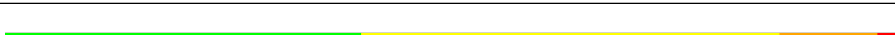
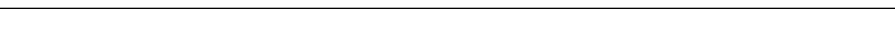
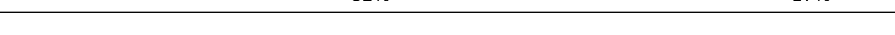
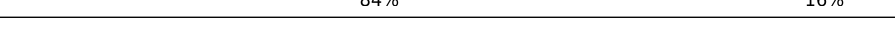
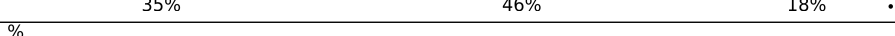
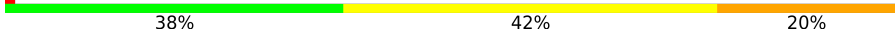
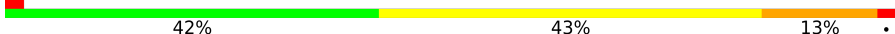
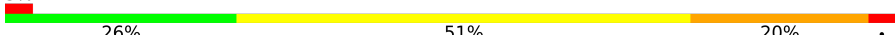
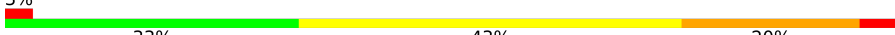
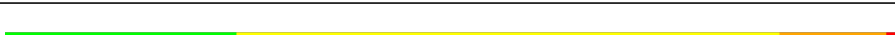
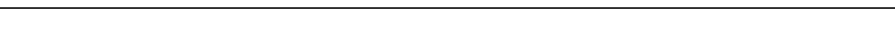
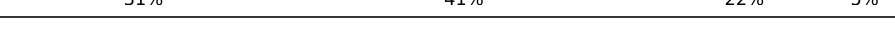
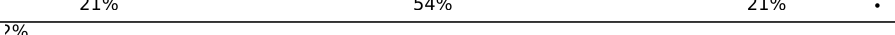
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Mol	Chain	Length	Quality of chain
15	AP	84	
15	CP	84	
16	AQ	100	
16	CQ	100	
17	AR	70	
17	CR	70	
18	AS	79	
18	CS	79	
19	AT	99	
19	CT	99	
20	AY	687	
20	CY	687	
21	AA	1511	
21	CA	1511	
22	AW	77	
22	CW	77	
23	AV	36	
23	CV	36	
24	AX	78	
24	CX	78	
25	BC	228	
25	DC	228	
26	BD	275	
26	DD	275	
27	BE	205	

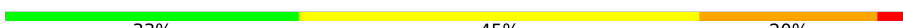
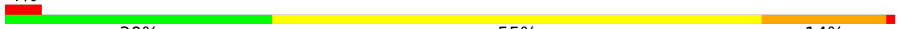
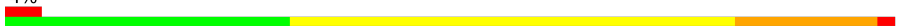
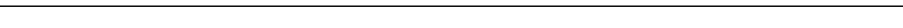
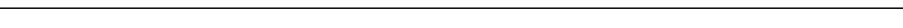
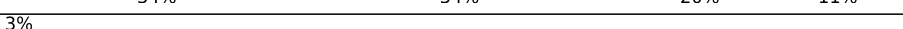
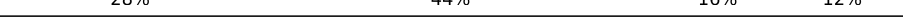
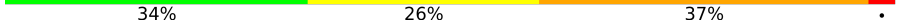
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Mol	Chain	Length	Quality of chain
27	DE	205	
28	BF	208	
28	DF	208	
29	BG	181	
29	DG	181	
30	BH	167	
30	DH	167	
31	BJ	170	
31	DJ	170	
32	BK	140	
32	DK	140	
33	BN	139	
33	DN	139	
34	BO	122	
34	DO	122	
35	BP	146	
35	DP	146	
36	BQ	141	
36	DQ	141	
37	BR	117	
37	DR	117	
38	BS	99	
38	DS	99	
39	BT	138	
39	DT	138	

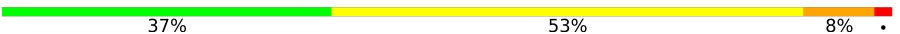
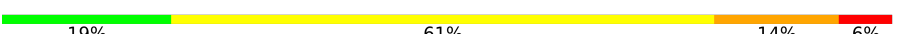
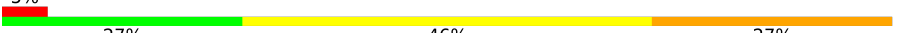
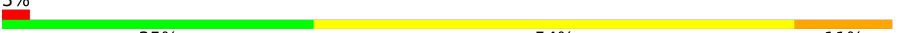
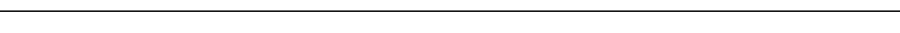
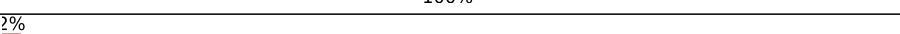
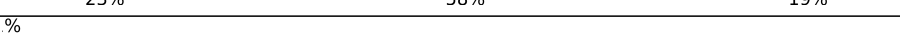
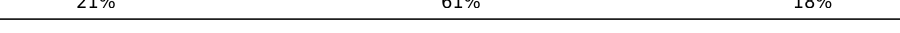
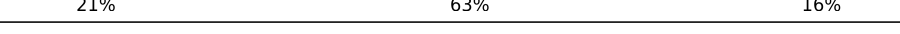
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Mol	Chain	Length	Quality of chain
40	BU	117	
40	DU	117	
41	BV	101	
41	DV	101	
42	BW	113	
42	DW	113	
43	BX	93	
43	DX	93	
44	BY	107	
44	DY	107	
45	BZ	185	
45	DZ	185	
46	B0	84	
46	D0	84	
47	B1	93	
47	D1	93	
48	B2	71	
48	D2	71	
49	B3	60	
49	D3	60	
50	B4	35	
50	D4	35	
51	B5	59	
51	D5	59	
52	B6	50	

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Mol	Chain	Length	Quality of chain
52	D6	50	
53	B7	49	
53	D7	49	
54	B8	64	
54	D8	64	
55	B9	37	
55	D9	37	
56	Be	103	
56	De	103	
57	Bf	31	
57	Bg	31	
57	Df	31	
57	Dg	31	
58	Bh	30	
58	Dh	30	
59	BA	2879	
59	DA	2879	
60	BB	119	
60	DB	119	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
61	GDP	CY	701	-	-	X	-
62	FUA	AY	702	-	-	X	-
63	NMY	AA	1601	-	-	X	-
63	NMY	BA	2904	-	-	X	-
63	NMY	CA	1601	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
63	NMY	DA	2901	-	-	X	-

2 Entry composition

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
1	AB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			
1	CB	235	Total	C	N	O	S	0	0	0
			1910	1218	342	345	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 20 is a protein called Elongation factor G.

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

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
21	AA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			
21	CA	1511	Total	C	N	O	P	0	0	0
			32474	14455	6015	10494	1510			

- Molecule 22 is a RNA chain called tRNA.

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

- Molecule 23 is a RNA chain called mRNA.

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

- Molecule 24 is a RNA chain called tRNA.

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

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
25	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
25	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
37	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
37	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
57	Bf	31	Total	C	N	O	0	0	0
			156	93	31	32			
57	Bg	31	Total	C	N	O	0	0	0
			156	93	31	32			

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

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

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

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

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

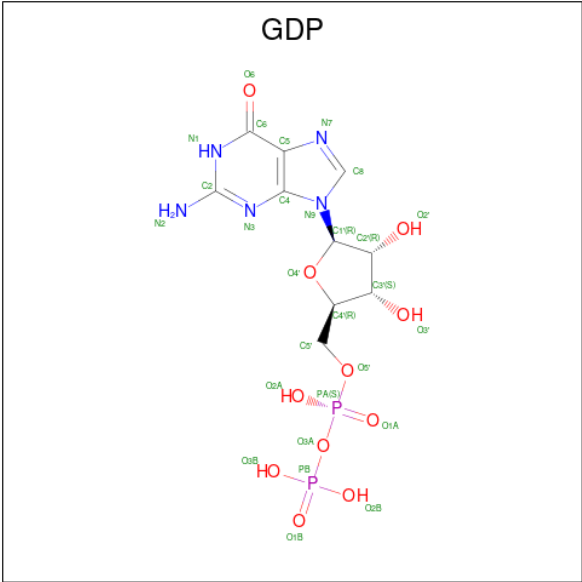
There are 4 discrepancies between the modelled and reference sequences:

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.

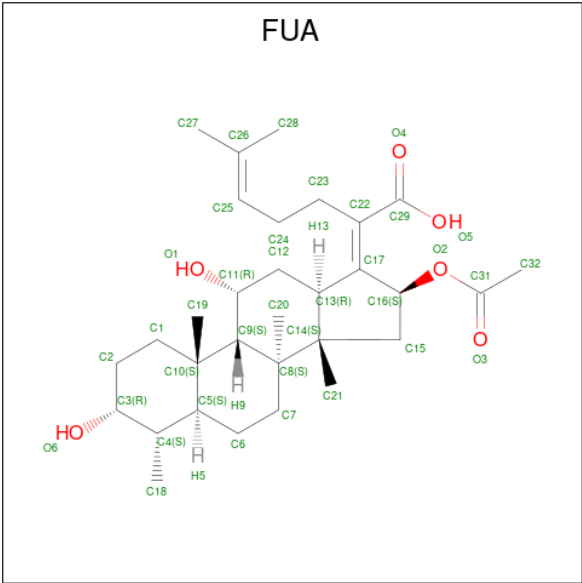
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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

- Molecule 62 is FUSIDIC ACID (CCD ID: FUA) (formula: C₃₁H₄₈O₆).



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

-
- The chemical structure of NMY is a complex pentasaccharide. It consists of five sugar rings linked by various glycosidic bonds. The structure is highly branched and contains several functional groups, including amino groups (NH₂) and hydroxyl groups (OH). The atoms are labeled with their respective element symbols and indices, such as C1, C2, C3, C4, C5, O1, O2, N1, N2, etc. The structure is shown in a 3D representation with wedged and dashed bonds to indicate stereochemistry.

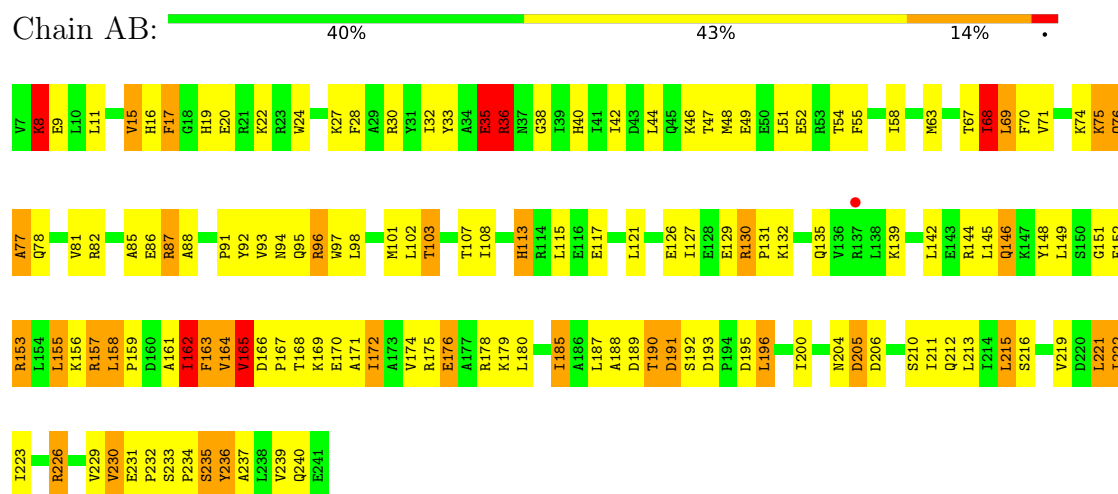
- Molecule 64 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

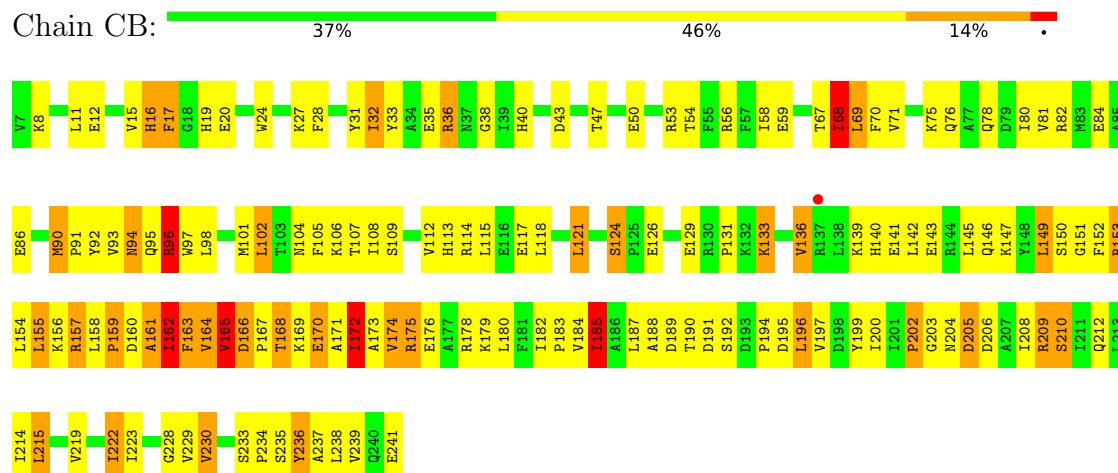
3 Residue-property plots

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

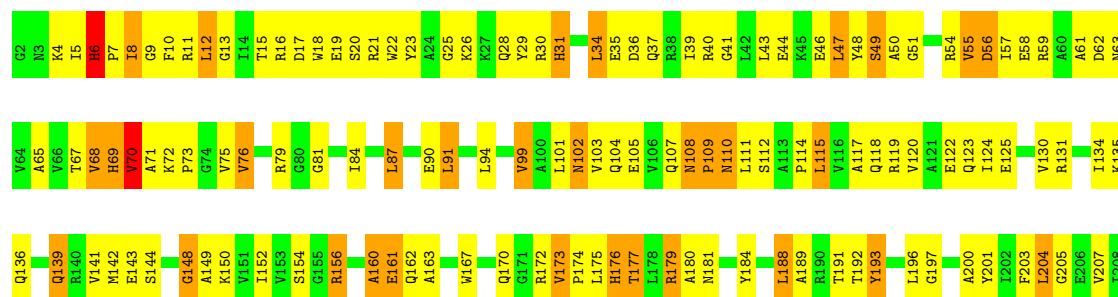


• Molecule 1: 30S ribosomal protein S2



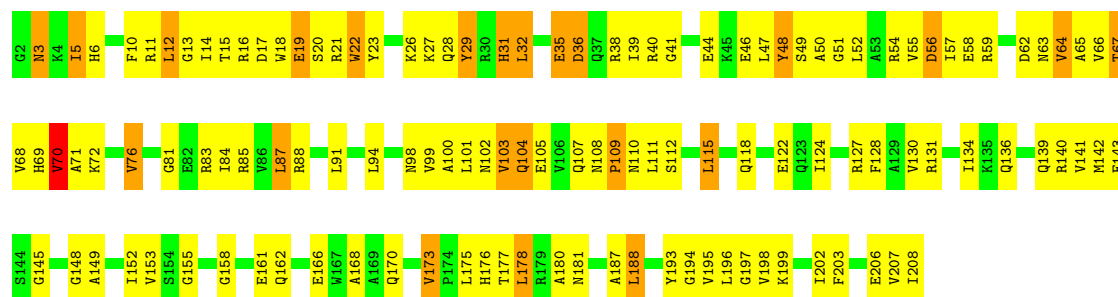
• Molecule 2: 30S ribosomal protein S3





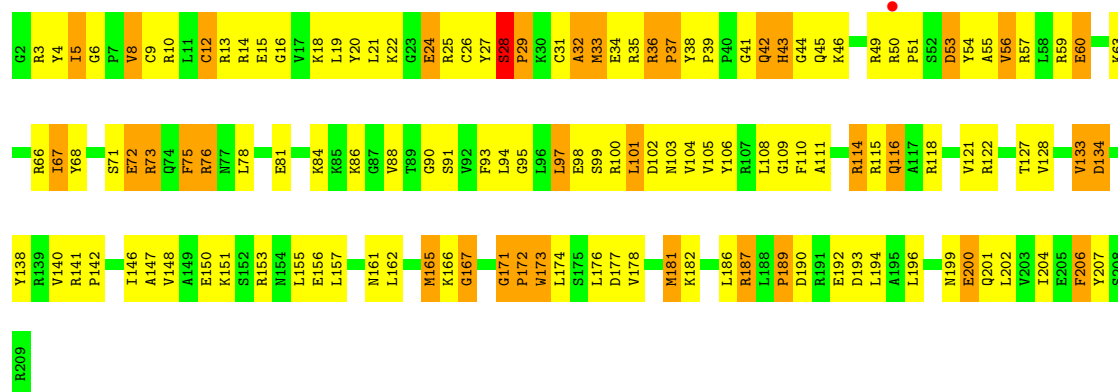
• Molecule 2: 30S ribosomal protein S3

Chain CC: 40% 49% 11%



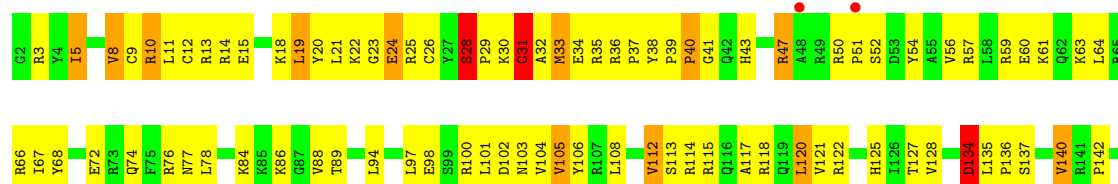
• Molecule 3: 30S ribosomal protein S4

Chain AD: 36% 47% 17%



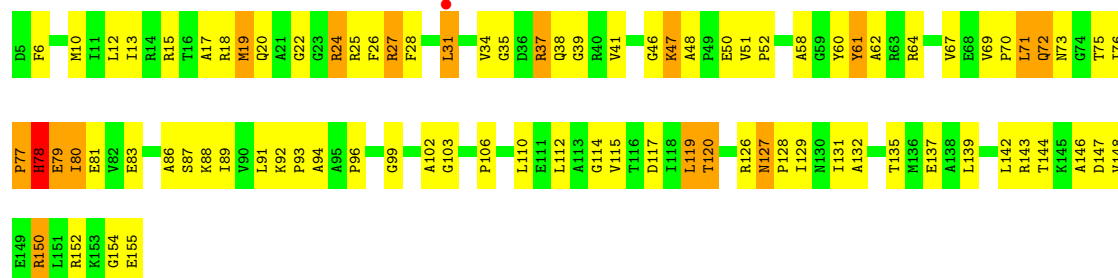
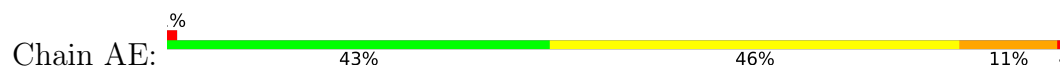
• Molecule 3: 30S ribosomal protein S4

Chain CD: 39% 48% 12%

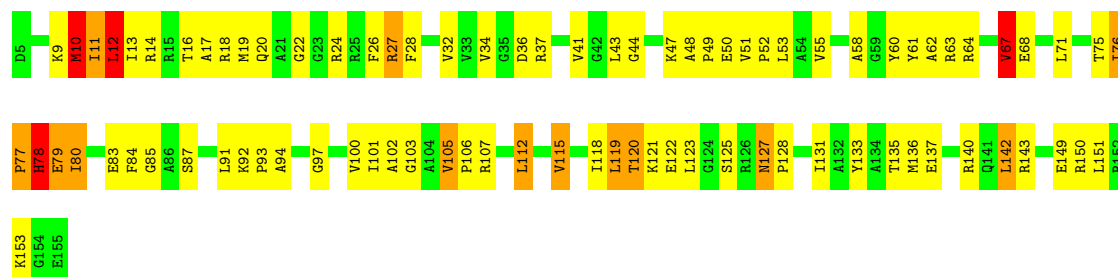




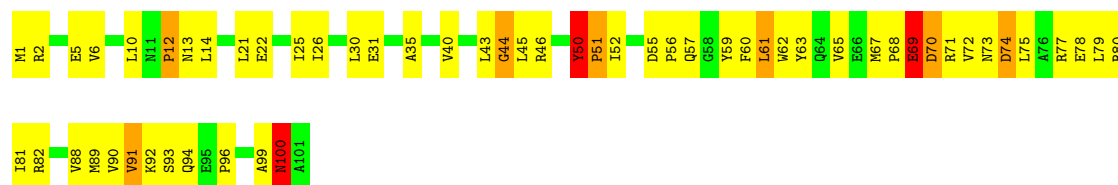
• Molecule 4: 30S ribosomal protein S5



• Molecule 4: 30S ribosomal protein S5



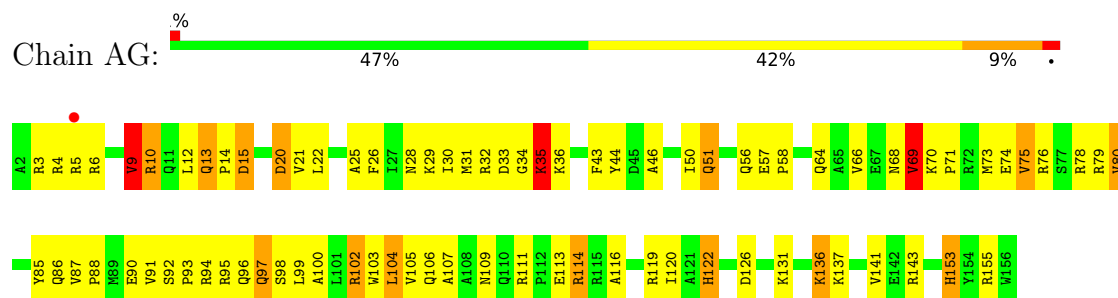
• Molecule 5: 30S ribosomal protein S6



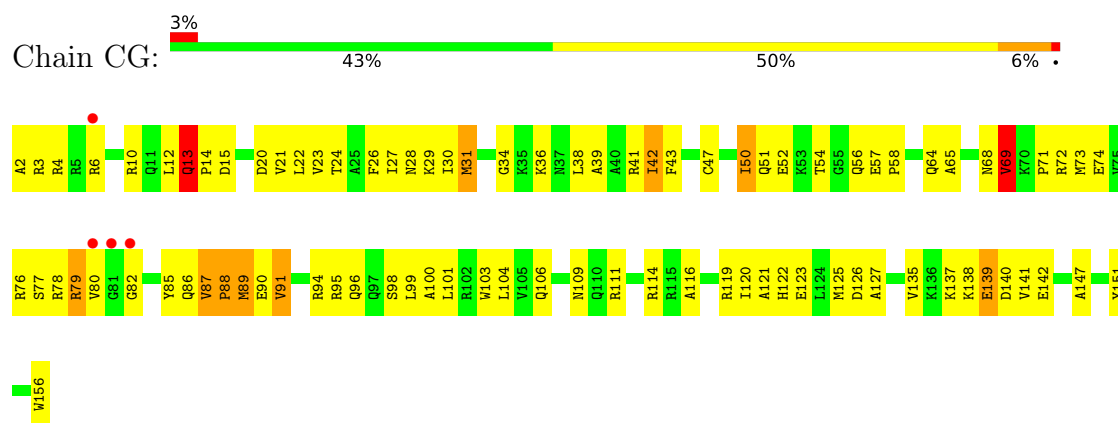
• Molecule 5: 30S ribosomal protein S6



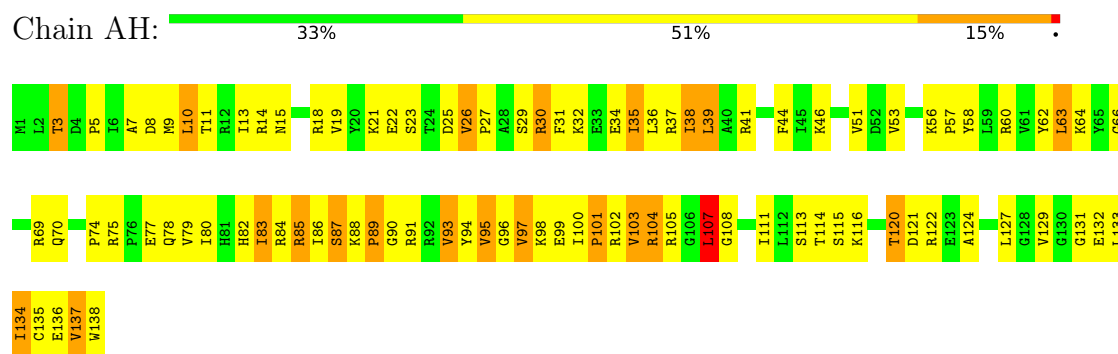
- Molecule 6: 30S ribosomal protein S7



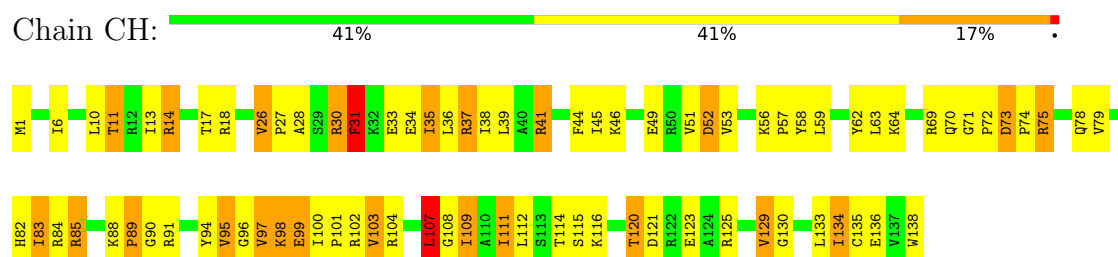
- Molecule 6: 30S ribosomal protein S7



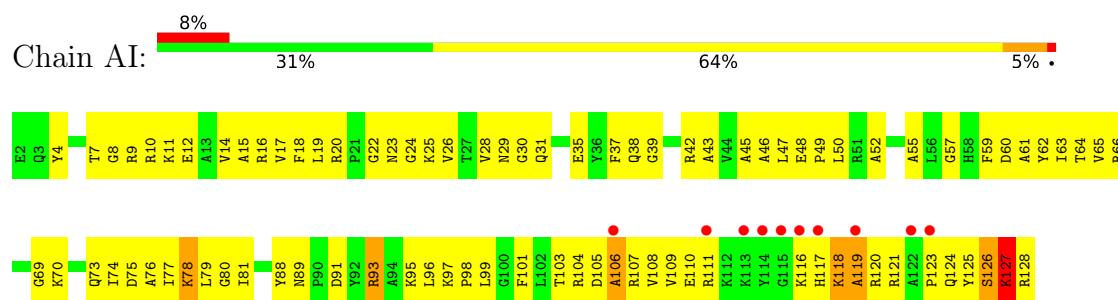
- Molecule 7: 30S ribosomal protein S8



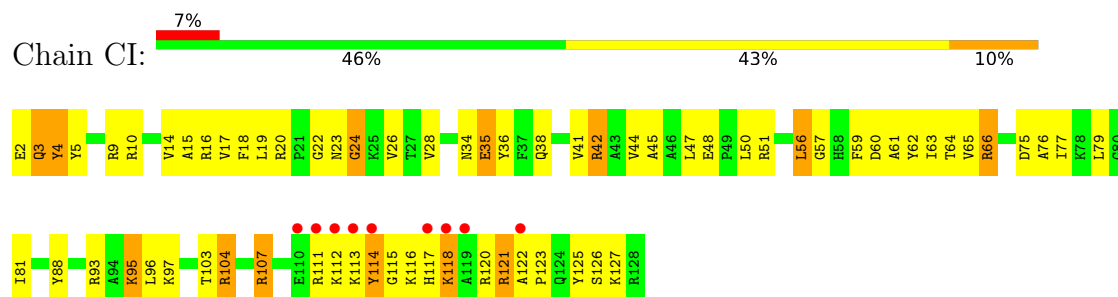
- Molecule 7: 30S ribosomal protein S8



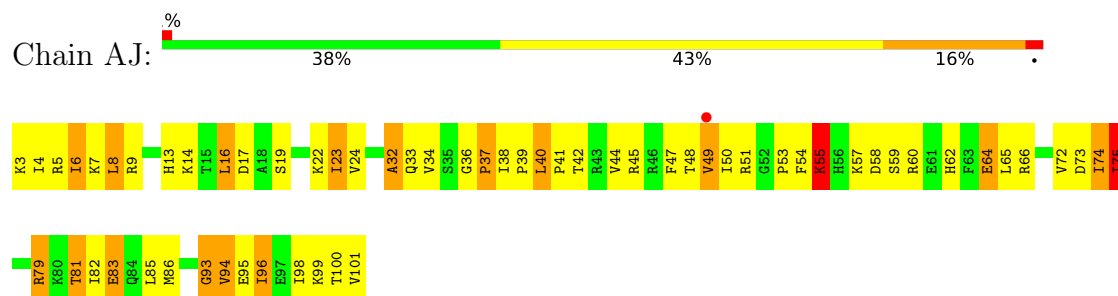
- Molecule 8: 30S ribosomal protein S9



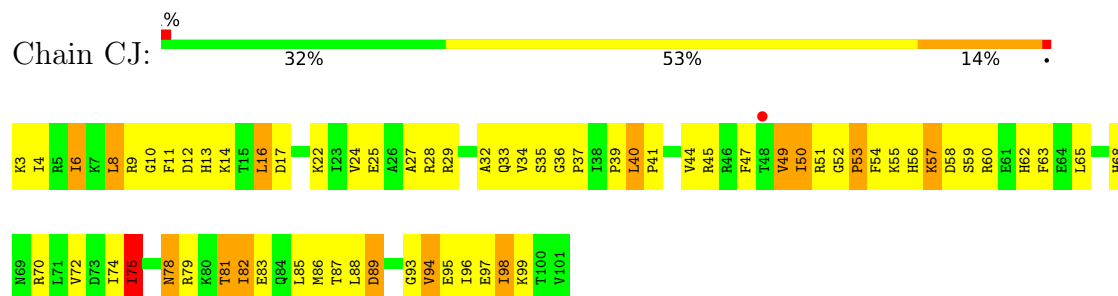
• Molecule 8: 30S ribosomal protein S9



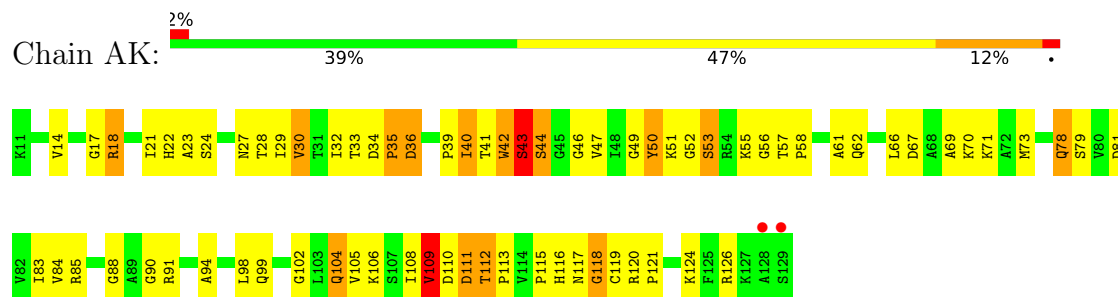
• Molecule 9: 30S ribosomal protein S10



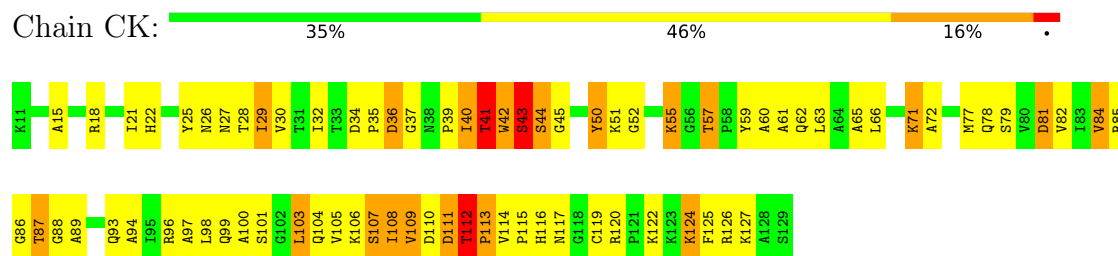
• Molecule 9: 30S ribosomal protein S10



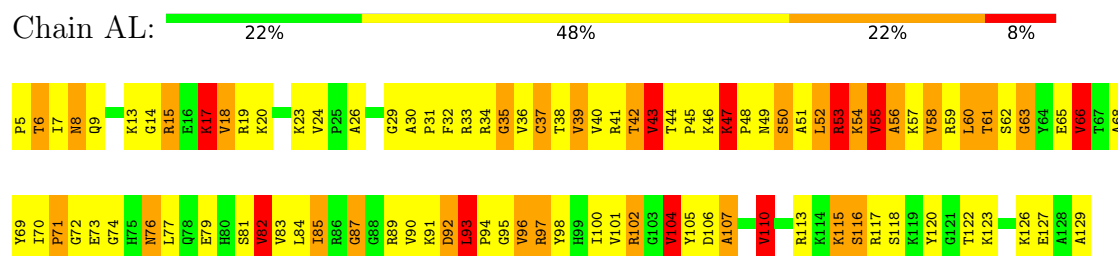
• Molecule 10: 30S ribosomal protein S11



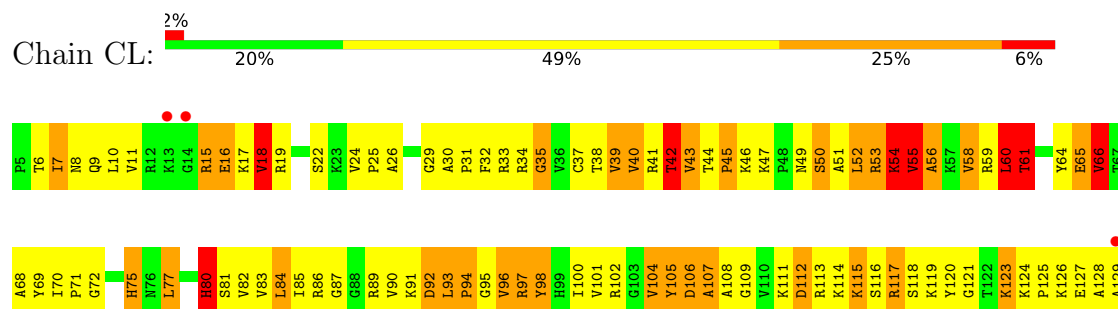
- Molecule 10: 30S ribosomal protein S11



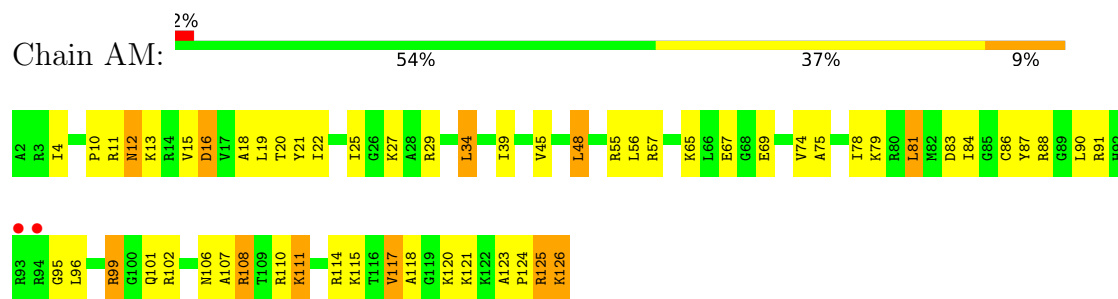
- Molecule 11: 30S ribosomal protein S12



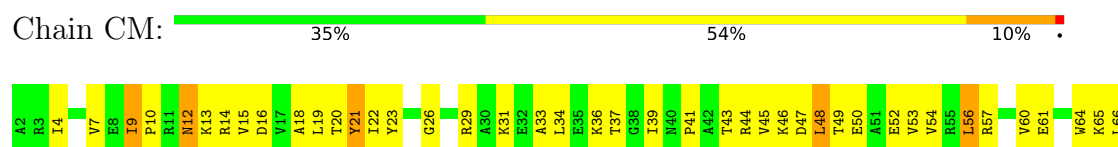
- Molecule 11: 30S ribosomal protein S12



- Molecule 12: 30S ribosomal protein S13



- Molecule 12: 30S ribosomal protein S13





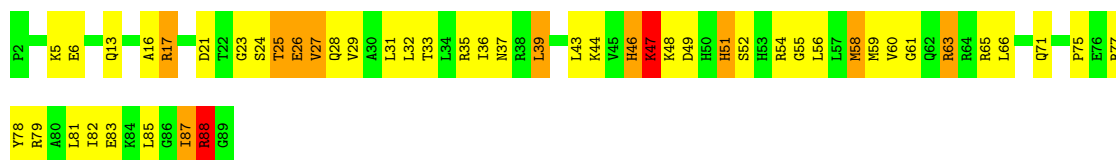
- Molecule 13: 30S ribosomal protein S14 type Z



- Molecule 13: 30S ribosomal protein S14 type Z



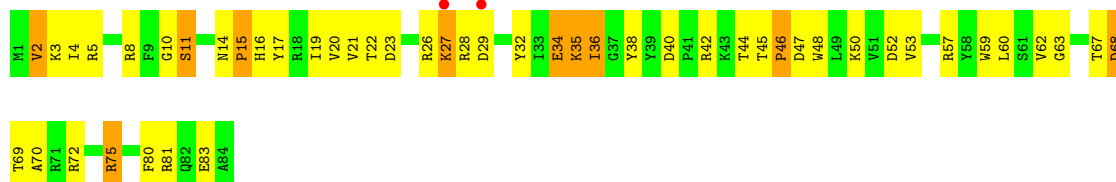
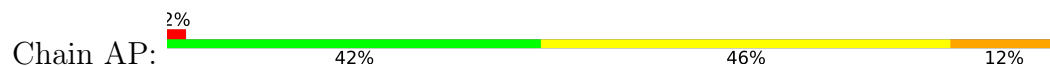
- Molecule 14: 30S ribosomal protein S15



- Molecule 14: 30S ribosomal protein S15

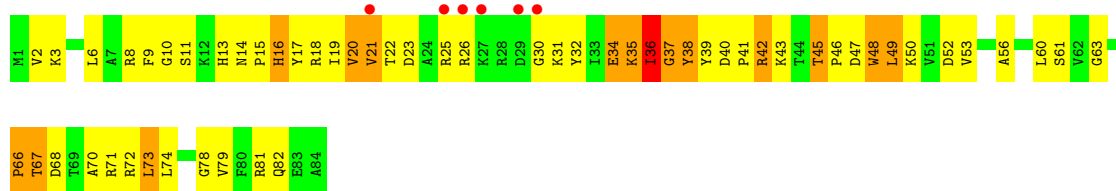


- Molecule 15: 30S ribosomal protein S16

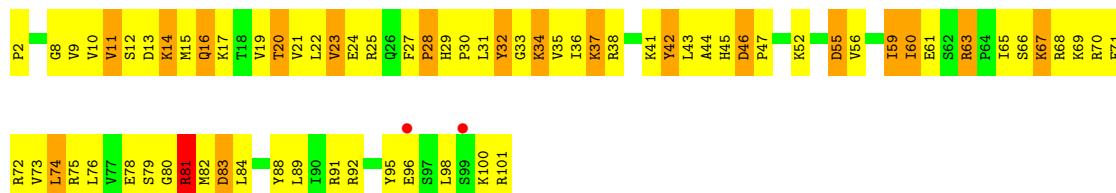
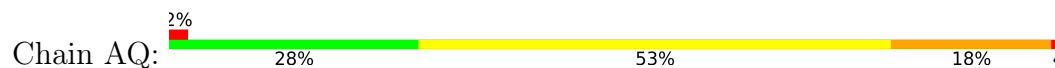


- Molecule 15: 30S ribosomal protein S16

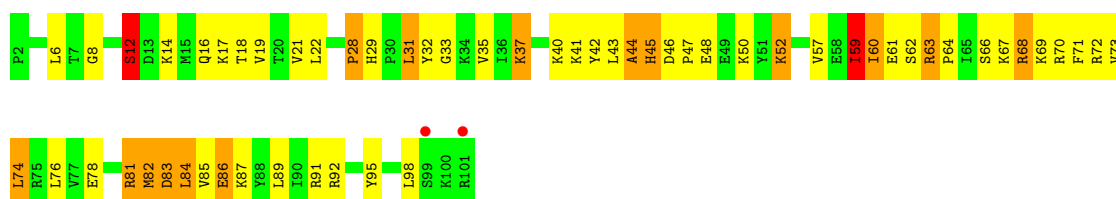




• Molecule 16: 30S ribosomal protein S17



• Molecule 16: 30S ribosomal protein S17



• Molecule 17: 30S ribosomal protein S18

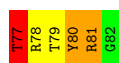


• Molecule 17: 30S ribosomal protein S18



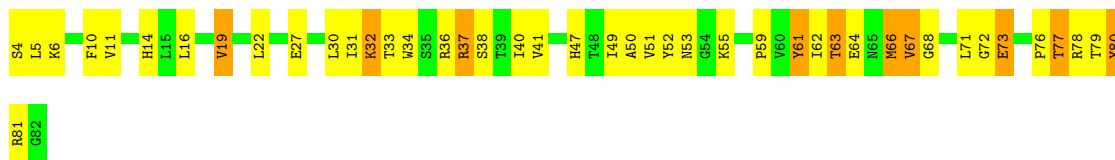
• Molecule 18: 30S ribosomal protein S19





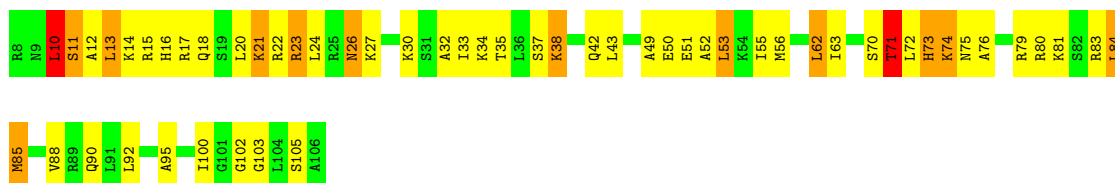
• Molecule 18: 30S ribosomal protein S19

Chain CS: 44% 43% 13%



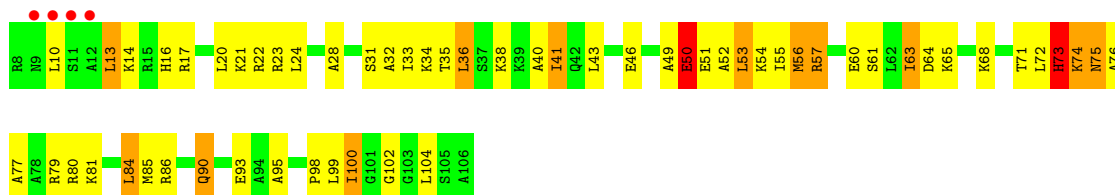
• Molecule 19: 30S ribosomal protein S20

Chain AT: 44% 41% 12% •



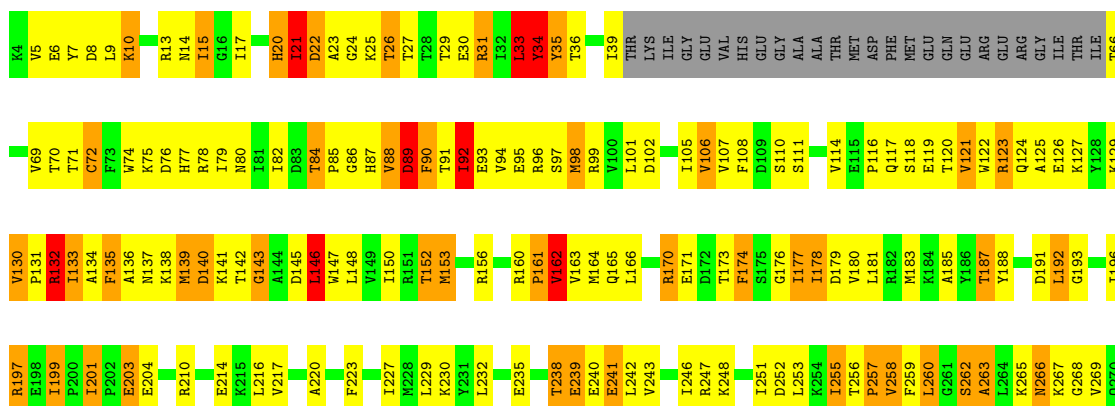
• Molecule 19: 30S ribosomal protein S20

Chain CT: 4% 41% 44% 12% •



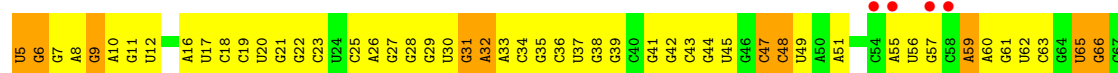
• Molecule 20: Elongation factor G

Chain AY: 2% 34% 44% 16% • •

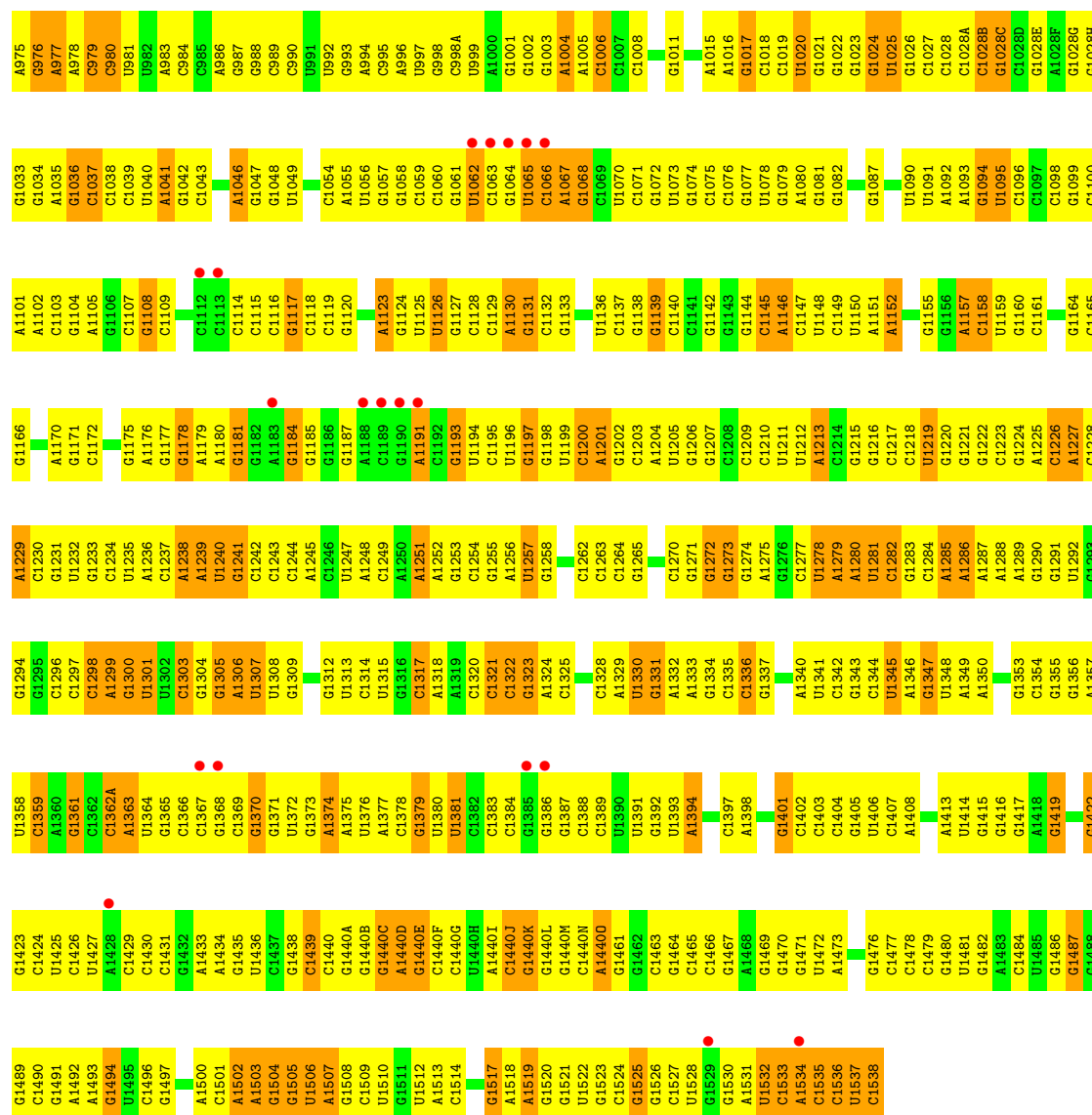






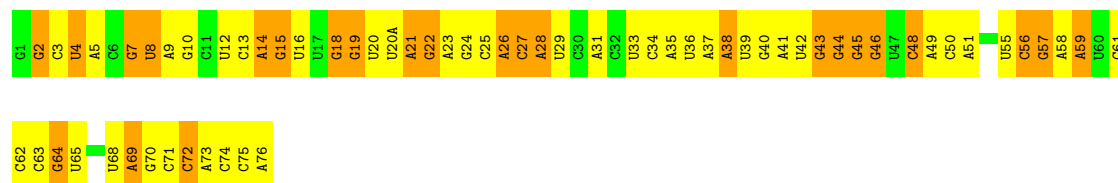


A915	G852	G786	G724	G595	A533	C457	C390	A327	G265	G1860	G138	G68
G916	G853	A787	G725	C596	U534	C458	G391	C328	G266	U186P	G139	G68A
G917	G854	U788		G597	A535		G392	C329	G267	G191	A140	G68B
A918	G855	U789	A728	U598	C536	A458E	A393	A330	C268	G192	A141	C68C
A919	C856	G790	A729	C599	G537	G474		G332	C269	C194	G142	C68D
U920	C857	G791	G730	C600	G538	G475	G396	G333	A270	A195	A143	G68E
U921	G858	A792	G731	C601	A539	G476	A397	G334	C271	A196	G144	
G922	A859	U793	G732	A602	G540	G477	C398	C335	A272	A197	G145	G68H
A923	A860	A794	A733	U603	G541	A478	G399	C336	A273	G198	G146	G68I
G924	G861		G734	G604	G542	C479	C400	C337			G147	G68J
G925			C735	U605	C543	A480	C401	C338			G148	U68K
G926			G736	G606	G544	G481	C402	A338			A149	U68L
G927	A864		A737	A607	C545	A482	C403	C339			G150	U68M
G928			G738	A608	G546	C483	U404	U340	A279		A151	U68N
G929	G867		G739	A609	A547	G484	U405	C341	C280		A152	A880
G930	G868		U740	G610	G548	G485	G406	A282	G216		C153	C68P
G931	U870		G741	A611	C549	U486	C407	C283	C218		C154	U68Q
G932	U871		G742	G612	G550	U487	A408	G284	C219		G155	C68R
G933	A872		U743	U551	C488	C488	C409	G285	G220		G156	C68S
G934	A873		G744	U552	C489	C489	C410	G286	C221		G157	G68T
A935	G874		G745	A553	G490		C411	U287	U222			U68U
G936	C875		A746	C554	A495		U412	A288	U223		A160	G68V
A937	G876		G747	G555	G492		C413	G289	C224		A161	G68W
A938	C877		C748	C556	G493		C414	G290	C225		A162	U68X
G939	G878		G749	G557	U494		A414	C291	G226		G163	C68Y
G940	C879		G750	G558			C419	A353			U164	A101
G941	G880		U751	A559	A497		U420	G354	U229		C165	G102
G942	C881		G752	U560	U498		U421	G293	G230		G166	C103
U943	C882		A753	C561	A499		C422	A356	G231		G167	G104
G944	C883		G754	C562	G500		C423	G295	G232		G168	G105
G945	U884		G755	U563	C501		G424	U358	G233		C169	C106
A946	G885		G756	C564	G502		C425	U359	C234			G107
G947	G886		U757	U565			C426	A360	C235		A172	G108
G948	C887		G758	G566	G505		U427	A361	G236		U173	A109
A949	G888		A759	G567	G506		C428	G362	C237		C174	C110
U950	A889			G568			U429	A363	G238		G175	G111
G951	G890		G762	G571	A509		A430	A364	G239		G176	G112
U952	U891		G763	A572	A510		A431	U365	C240		C177	G113
G953	C892		G764	A573	C511		A432	C366	A243			U114
G954	G893		G765	A574	U512		C433	U367	G306		G181	A116
U955	C894		A766	G575	C513		U434	U368	U244		U182	
U956			G767	G576	C514		C435	C369	C245		G183	A120
U957	G897		A768		G515		U436	G370	A246		G184	C121
A958	G898		G769	G579	U516		G437	G371	G309		A185	G122
A959	C899		C770	U641	G517		G438	C372	G310		C186	C123
U960	A900			A642	C518		A440	A373	A250		C186A	G124
U961	A901		G707	G643	C519		A441	A374	G251		C186B	U125
G962	G902		C708	G644	A520		C442	U375	U252		C186C	G126
G963	G903		G709	G645	C443		C443		U253		G186D	
A964	C904		G710	U646	C522		G444		G254		C186E	
A965	U905			G647	A523		G445		G255		C186F	U129
G966	G906		A775	A648	G524		G446		U256		C186G	G129A
G967	A907		G778	G649	C525		A448		G257		C186H	A130
A968	A908		C779	G650	C526		C449		G258		U186I	C131
A969	A909		G780	C651	G527		A382		C320		G186J	G132
G970	C910		A781	U652	G528		A383		A321		U186K	U133
G971	U911		A782	A653	G529		G384		G260		G186L	A134
G972	C912		G783	G530	G530		A452		U261		C186M	C135
G973	A913		A784	U531	C455		A453		A262		G186N	C136
A974	A914		G785	G532	A532		C456		U264		U186N	C137



• Molecule 22: tRNA

Chain AW: 17% 51% 32%



• Molecule 22: tRNA

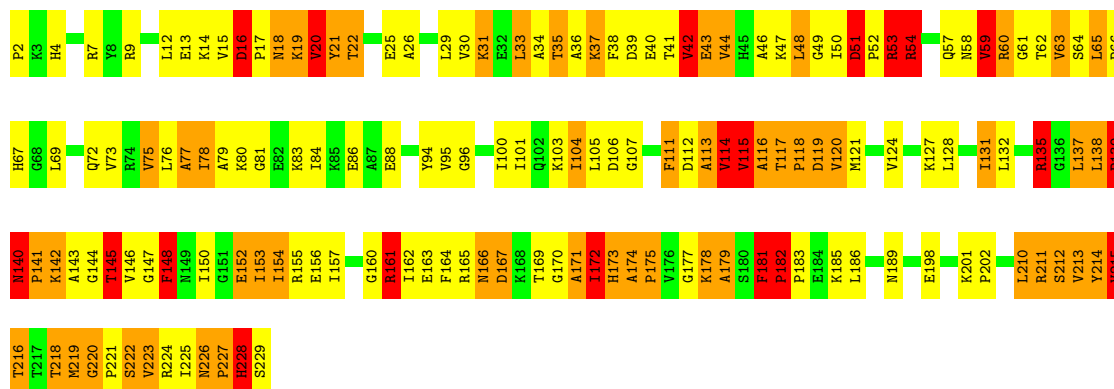
Chain CW: 16% 47% 38%





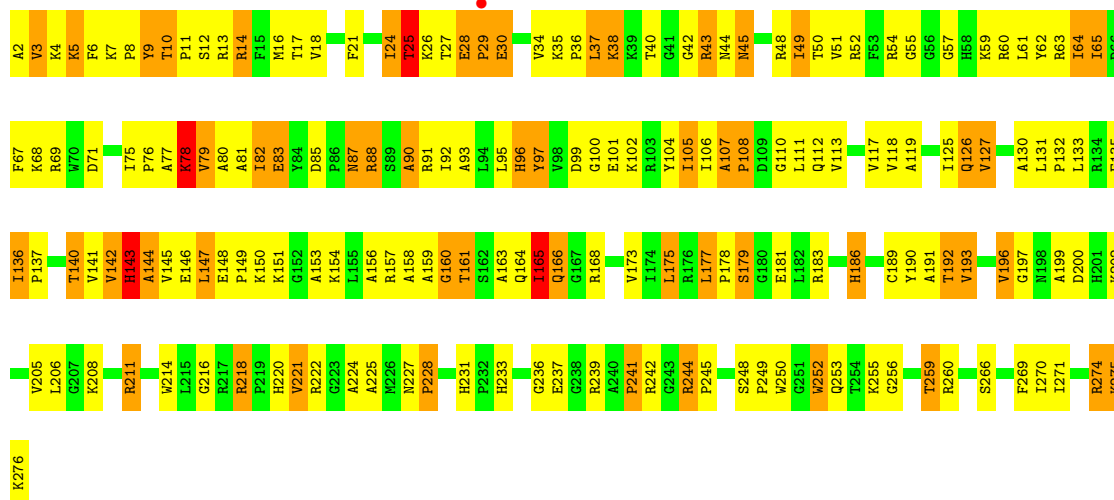
• Molecule 25: 50S ribosomal protein L1

Chain DC: 31% 37% 24% 9%



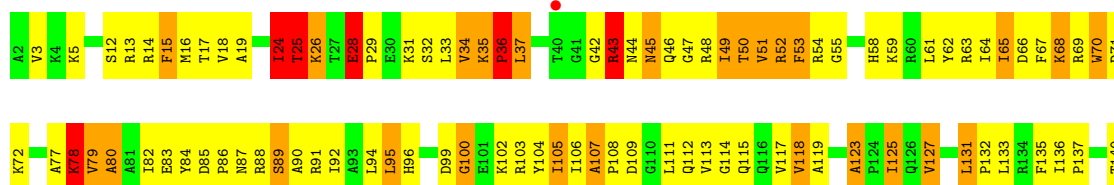
• Molecule 26: 50S ribosomal protein L2

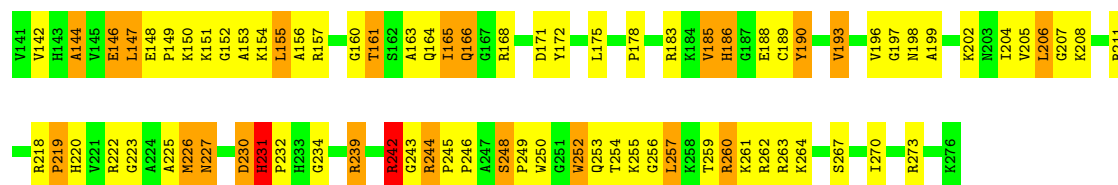
Chain BD: 35% 44% 20%



• Molecule 26: 50S ribosomal protein L2

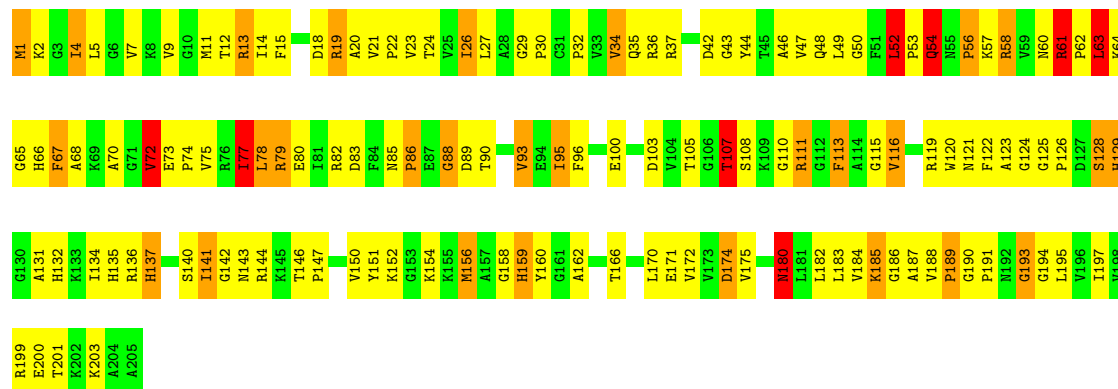
Chain DD: 36% 43% 17%





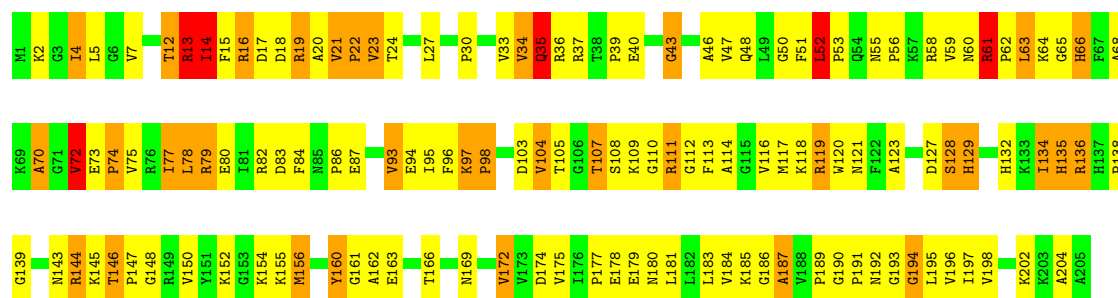
• Molecule 27: 50S ribosomal protein L3

Chain BE: 34% 49% 14% .



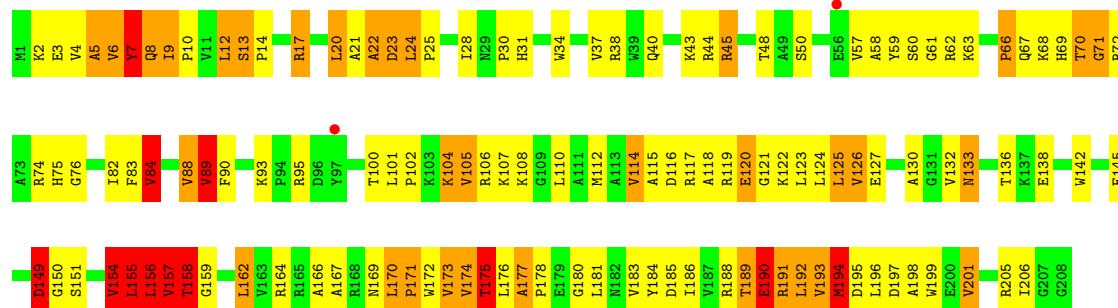
• Molecule 27: 50S ribosomal protein L3

Chain DE: 34% 46% 17% .



• Molecule 28: 50S ribosomal protein L4

Chain BF: 37% 41% 16% 6%



Chain DF:

Chain BG:

Item	Chain BG
P2	39%
L3	39%
D4	39%
L7	39%
K8	39%
Y12	39%
E13	39%
E14	39%
V15	39%
R16	39%
P17	39%
E18	39%
L19	39%
L20	39%
R21	39%
Y25	39%
Q26	39%
W29	39%
E30	39%
V31	39%
P32	39%
R33	39%
L34	39%
E35	39%
V37	39%
V38	39%
L39	39%
N40	39%
Q41	39%
G42	39%
L43	39%
G44	39%
E45	39%
A46	39%
K47	39%
E48	39%
D49	39%
A50	39%
R51	39%
K55	39%
A56	39%
A57	39%
Q58	39%
E59	39%
L60	7%
A61	39%
L62	39%
L63	39%
T64	39%
K67	39%
P68	39%
A69	39%
V70	39%
T71	39%
R72	39%
A73	39%
K74	39%
S75	39%
S76	39%
I77	39%
S78	39%
N79	39%
F80	39%
K81	39%
L82	39%
R83	39%
G85	39%
R84	39%
M86	39%
P87	39%
T88	39%
G89	39%
L90	39%
R91	39%
L94	39%
R95	39%
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W100	39%
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F102	39%
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R113	39%
L114	39%
F125	39%
D126	39%
G127	39%
R128	39%
G129	39%
N130	39%
Y131	39%
N132	39%
L133	39%
G134	39%
L135	39%
R136	39%
E137	39%
Q138	39%
L139	39%
P140	39%
Y146	39%
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A163	39%
D166	39%
E167	39%
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A169	39%
R170	39%
L173	39%
E174	39%
L175	39%
L176	39%
G177	39%
F178	39%
P179	39%
F180	39%
R181	39%
K182	39%

Chain DG: 34% 52% 12%

Category	Item	Value
Green	P2	1
	L3	1
	D4	1
	L7	1
	K8	1
	K9	1
	K10	1
	Y11	1
	V15	1
	R16	1
	P17	1
	E18	1
	L19	1
	I20	1
	R21	1
	G24	1
	G25	1
	Q26	1
	N27	1
	V28	1
V29	1	
Yellow	E30	1
	P31	1
	P32	1
	R33	1
	L34	1
	E35	1
	K36	1
	V37	1
	V38	1
	L39	1
	N40	1
	Q41	1
	G42	1
	L43	1
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	E45	1
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	K47	1
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	A69	1
	V70	1
	T71	1
	R72	1
	A73	1
	K74	1
	K75	1
	R76	1
	S77	1
	I77	1
	F80	1
	K81	1
	L82	1
	R83	1
	K84	1
	G85	1
	K86	1
	P87	1
	I88	1
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R115	1	
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R128	1	
G129	1	
N130	1	
Y131	1	
N132	1	
L133	1	
E137	1	
Q138	1	
L139	1	
Yellow	L140	1
	P141	1
	E142	1
	E143	1
	L144	1
	T145	1
	Y146	1
	M148	1
	V149	1
	D150	1
	R153	1
	G154	1
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	D156	1
	I157	1
	A158	1
V159	1	
V160	1	
T161	1	
T165	1	
D166	1	
R170	1	
L173	1	
E174	1	
L175	1	
L176	1	
G177	1	
F178	1	
P179	1	
F180	1	
R181	1	
K182	1	

Chain BH:



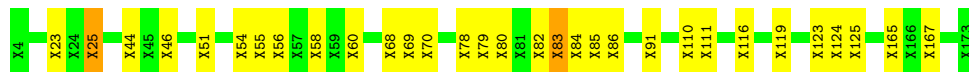
- Molecule 30: 50S ribosomal protein L6

Chain DH: 40% 47% 11%



- Molecule 31: 50S ribosomal protein I10

Chain BJ: 82% 17%



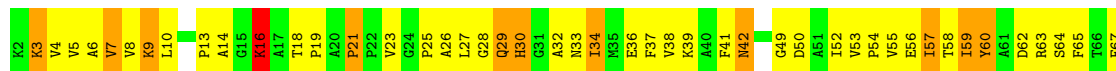
- Molecule 31: 50S ribosomal protein I10

Chain DJ: 84% 16%



- Molecule 32: 50S ribosomal protein L11

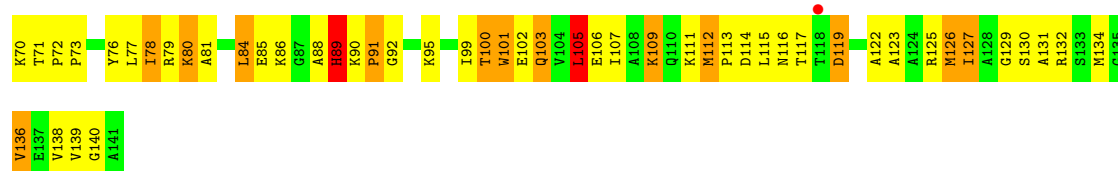
Chain BK: 35% 46% 18%



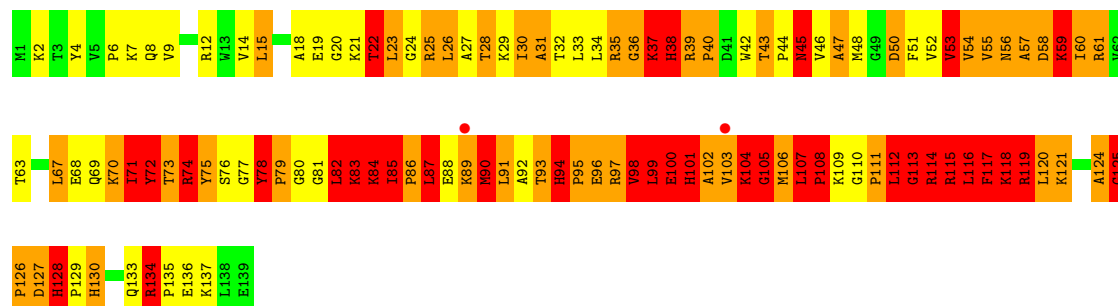
- Molecule 32: 50S ribosomal protein L11

Chain DK: 36% 46% 16%

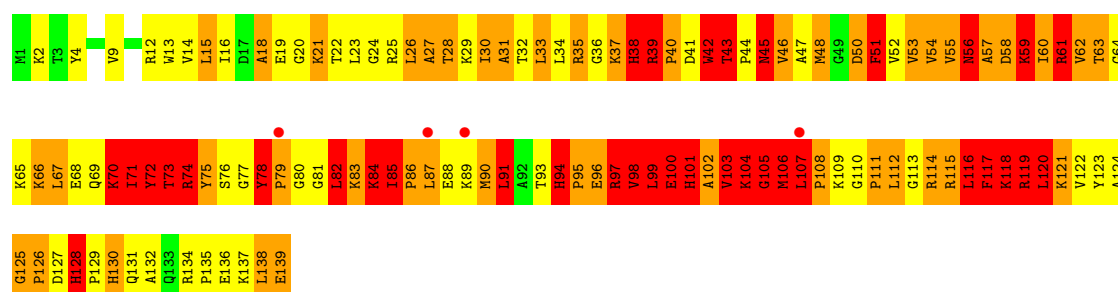




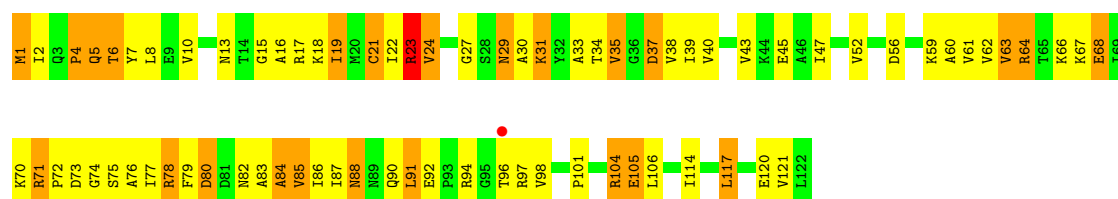
• Molecule 33: 50S ribosomal protein L13



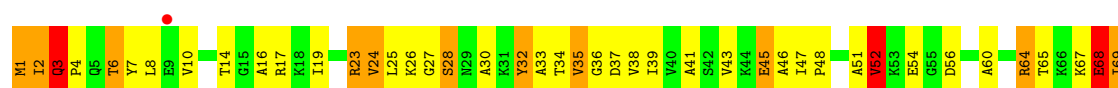
• Molecule 33: 50S ribosomal protein L13



• Molecule 34: 50S ribosomal protein L14

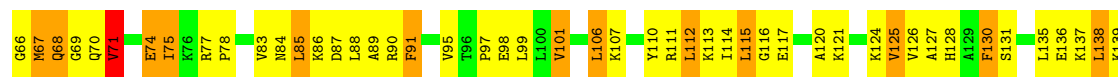


• Molecule 34: 50S ribosomal protein L14

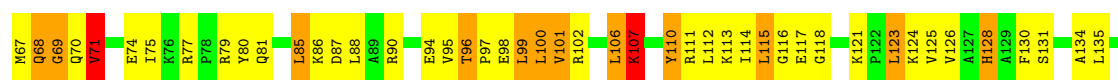




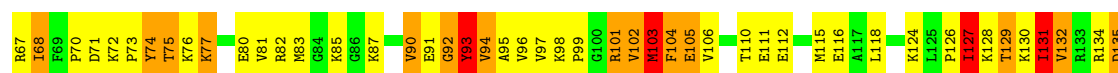
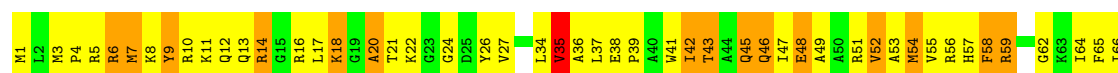
• Molecule 35: 50S ribosomal protein L15



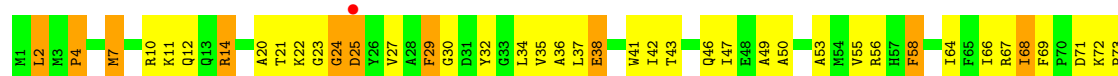
• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L16

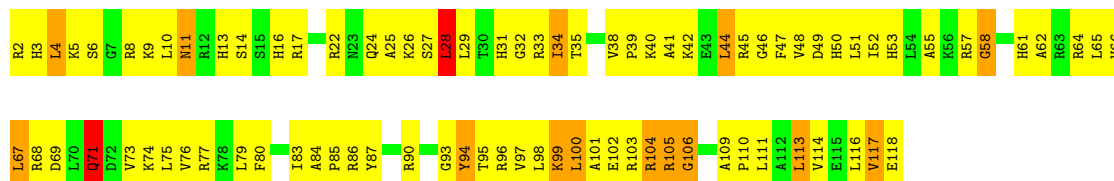


• Molecule 36: 50S ribosomal protein L16

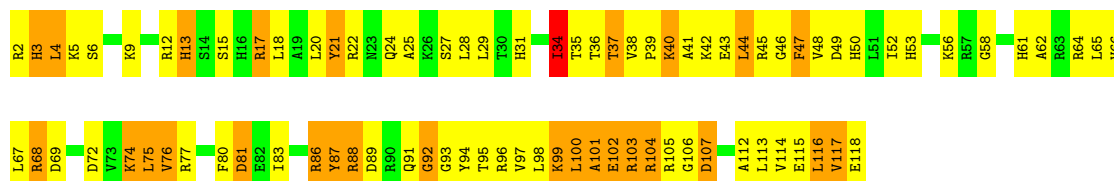




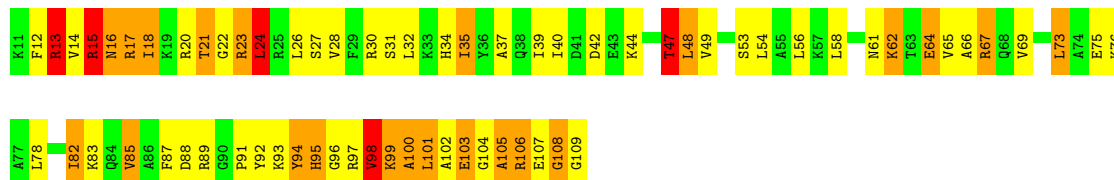
- Molecule 37: 50S ribosomal protein L17



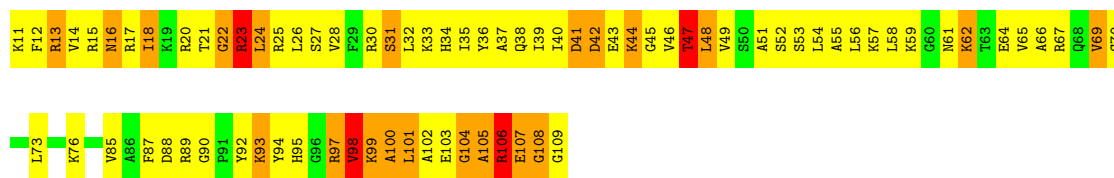
- Molecule 37: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L18

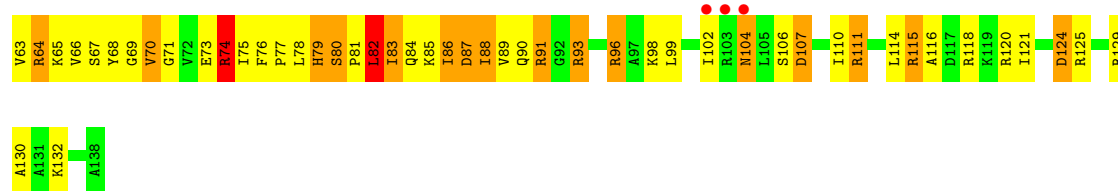


- Molecule 38: 50S ribosomal protein L18

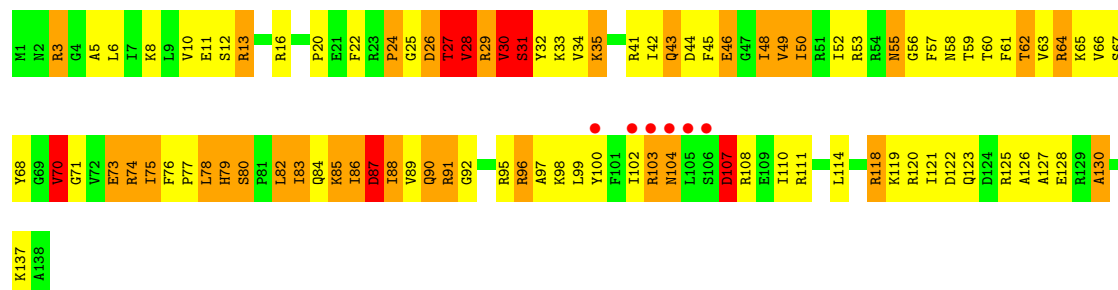


- Molecule 39: 50S ribosomal protein L19

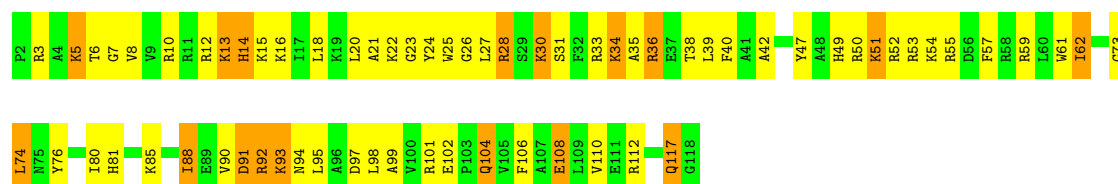




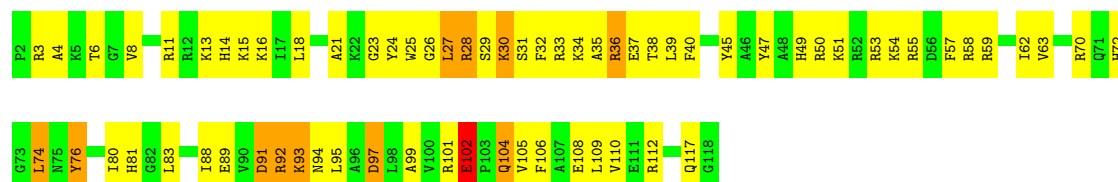
• Molecule 39: 50S ribosomal protein L19



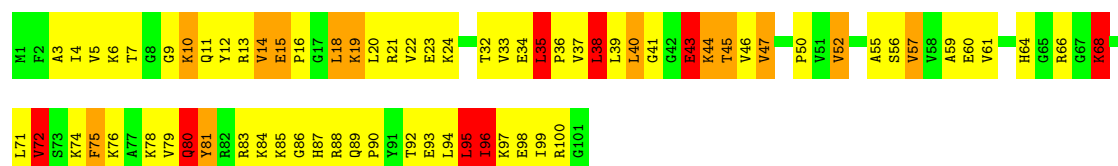
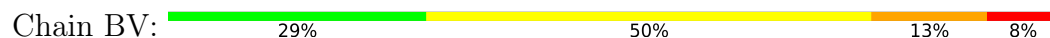
• Molecule 40: 50S ribosomal protein L20



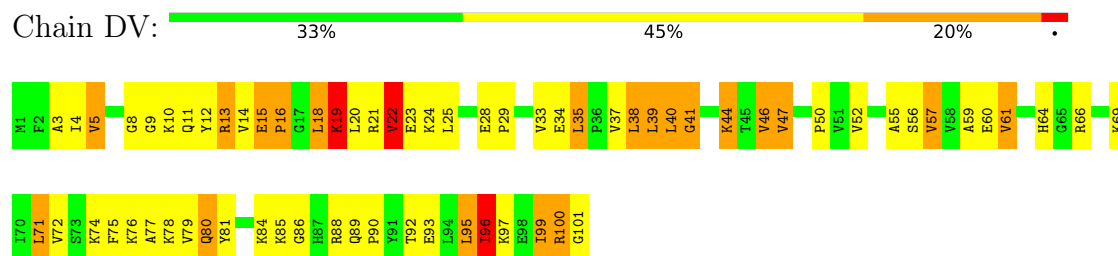
• Molecule 40: 50S ribosomal protein L20



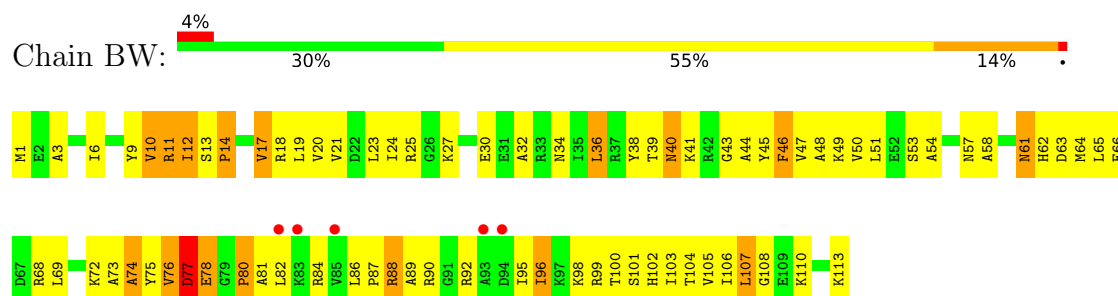
• Molecule 41: 50S ribosomal protein L21



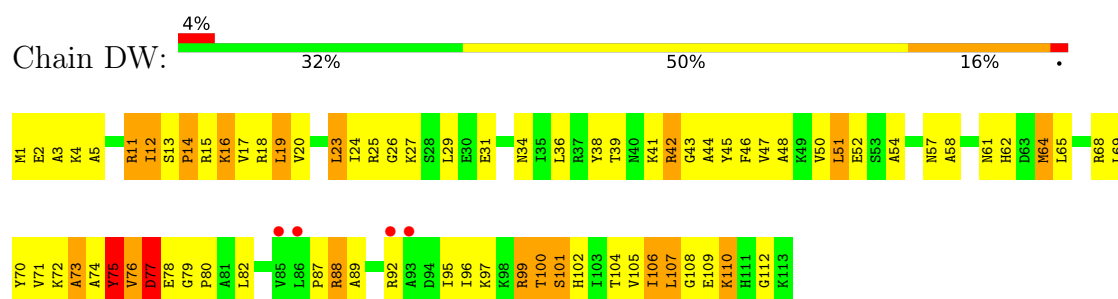
- Molecule 41: 50S ribosomal protein L21



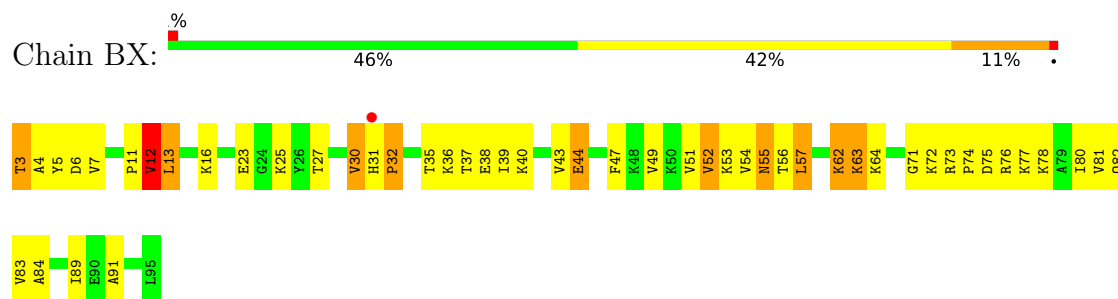
- Molecule 42: 50S ribosomal protein L22



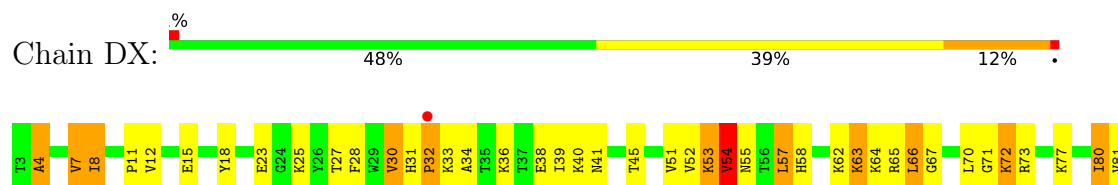
- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23

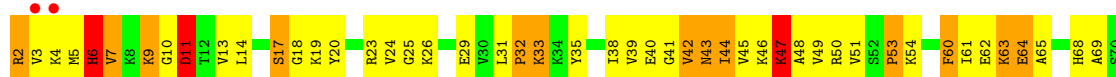


- Molecule 43: 50S ribosomal protein L23

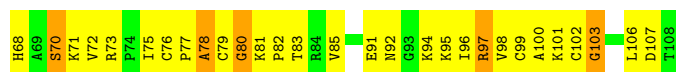
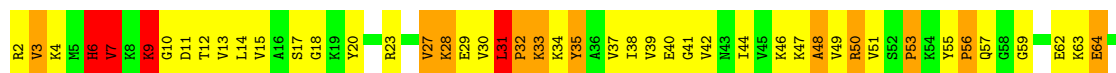




- Molecule 44: 50S ribosomal protein L24



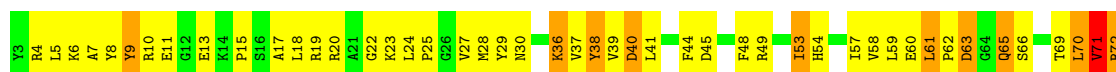
- Molecule 44: 50S ribosomal protein L24



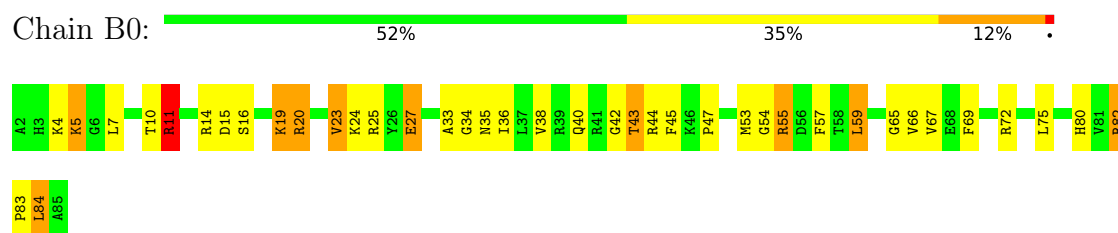
- Molecule 45: 50S ribosomal protein L25



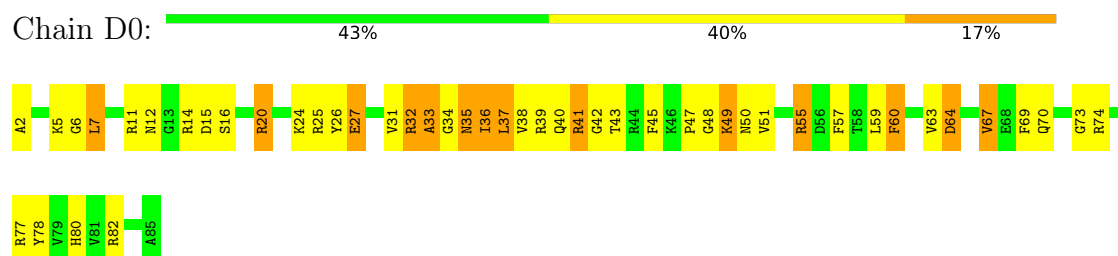
- Molecule 45: 50S ribosomal protein L25



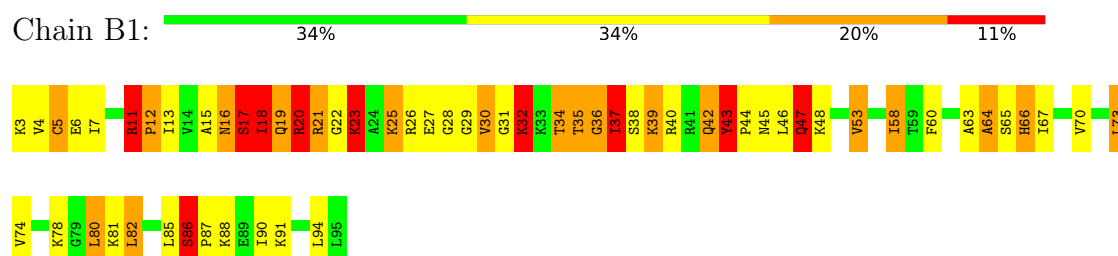
• Molecule 46: 50S ribosomal protein L27



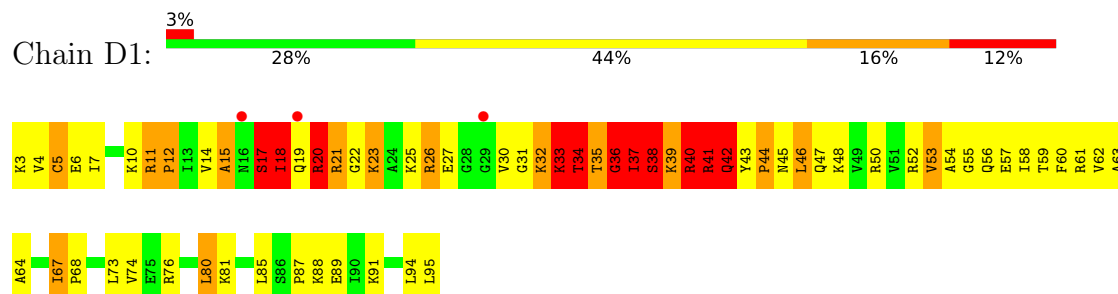
• Molecule 46: 50S ribosomal protein L27



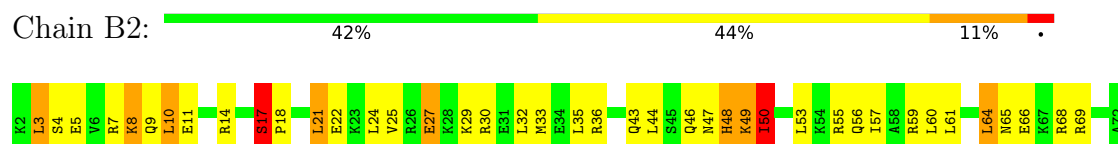
• Molecule 47: 50S ribosomal protein L28



• Molecule 47: 50S ribosomal protein L28

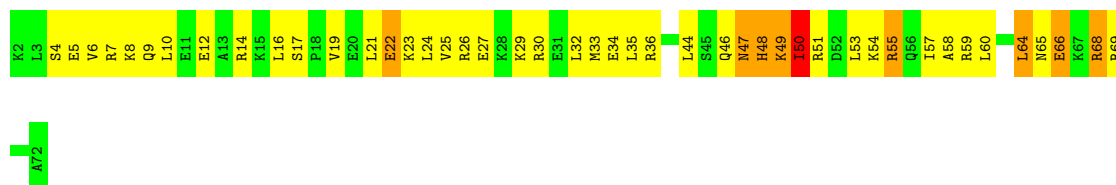


• Molecule 48: 50S ribosomal protein L29



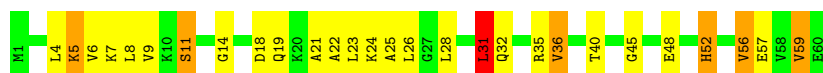
• Molecule 48: 50S ribosomal protein L29

Chain D2: 37% 51% 11% .



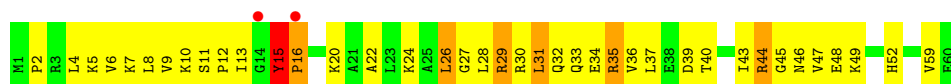
- Molecule 49: 50S ribosomal protein L30

Chain B3: 53% 35% 10% .



- Molecule 49: 50S ribosomal protein L30

Chain D3: 3% 35% 53% 10% .



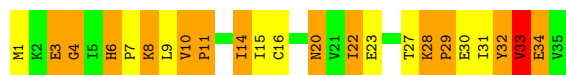
- Molecule 50: 50S ribosomal protein L31

Chain B4: 49% 29% 14% 9% .



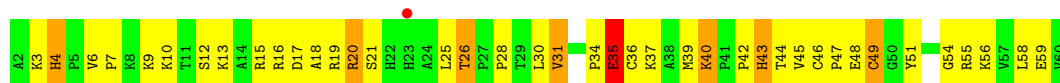
- Molecule 50: 50S ribosomal protein L31

Chain D4: 34% 26% 37% .



- Molecule 51: 50S ribosomal protein L32

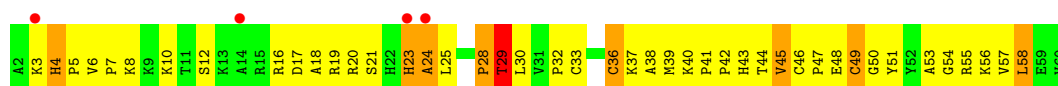
Chain B5: 2% 32% 54% 12% .



- Molecule 51: 50S ribosomal protein L32

Chain D5: 7% 25% 59% 14% .

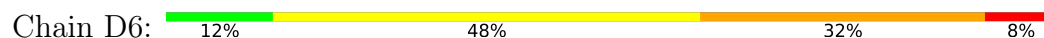




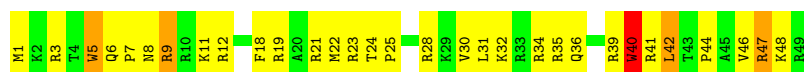
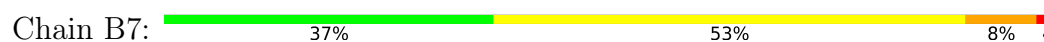
- Molecule 52: 50S ribosomal protein L33



- Molecule 52: 50S ribosomal protein L33



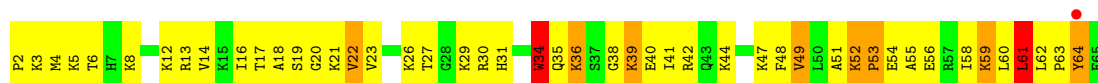
- Molecule 53: 50S ribosomal protein L34



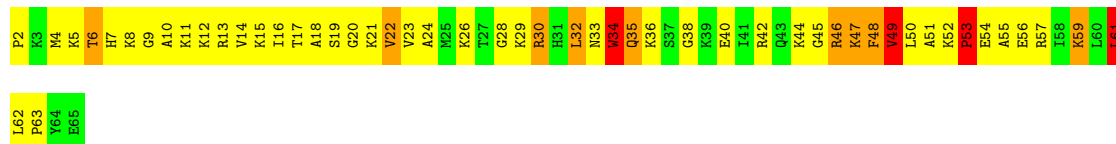
- Molecule 53: 50S ribosomal protein L34



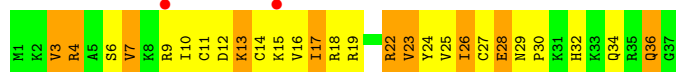
- Molecule 54: 50S ribosomal protein L35



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



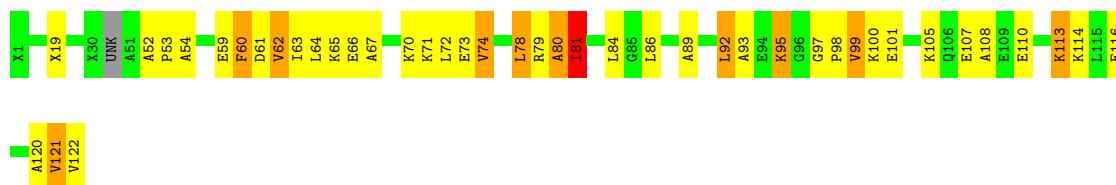
- Molecule 55: 50S ribosomal protein L36



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 56: 50S ribosomal protein L7/L12



- Molecule 57: 50S ribosomal protein L7/L12



There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

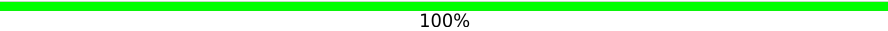


There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12



- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg:  100%

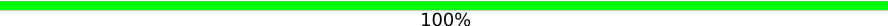
There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh:  93% 7%

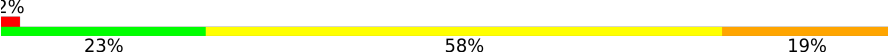


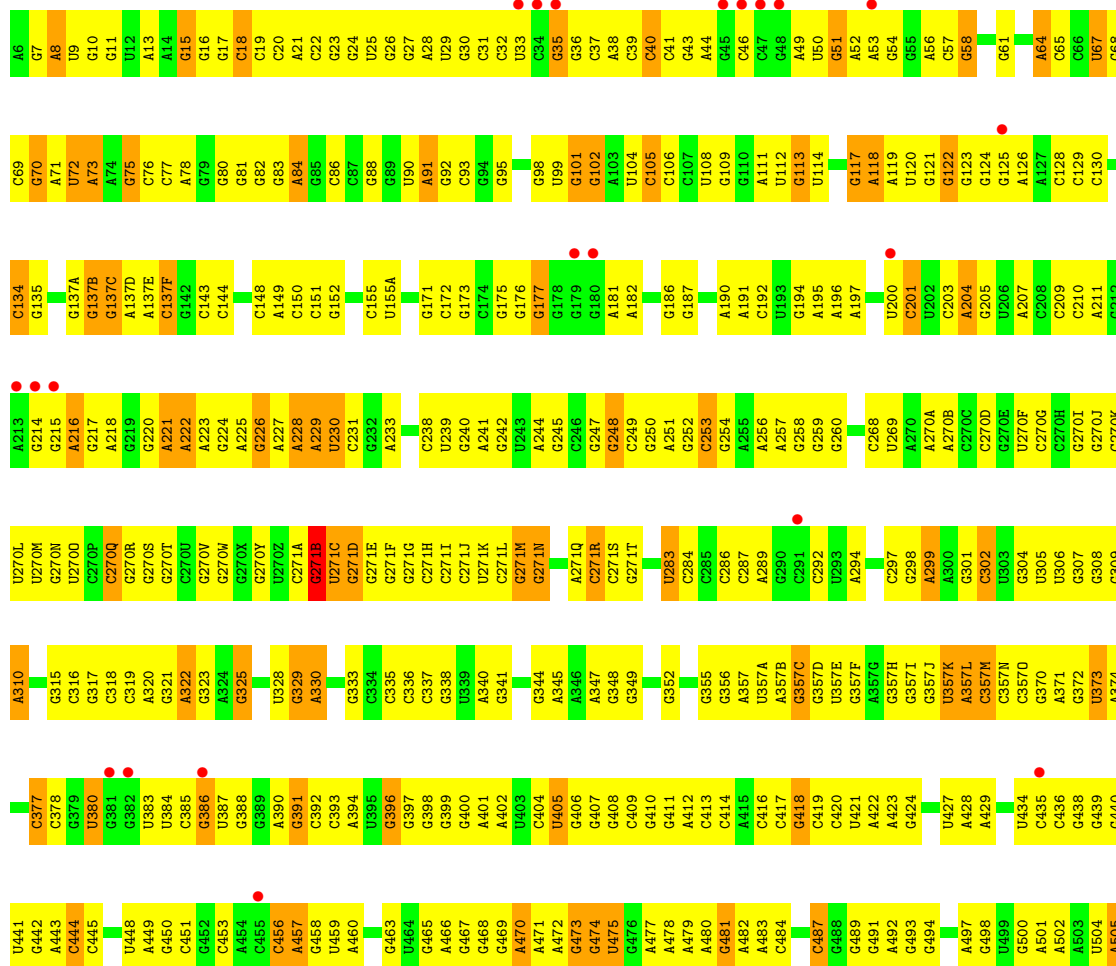
- Molecule 58: 50S ribosomal protein L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

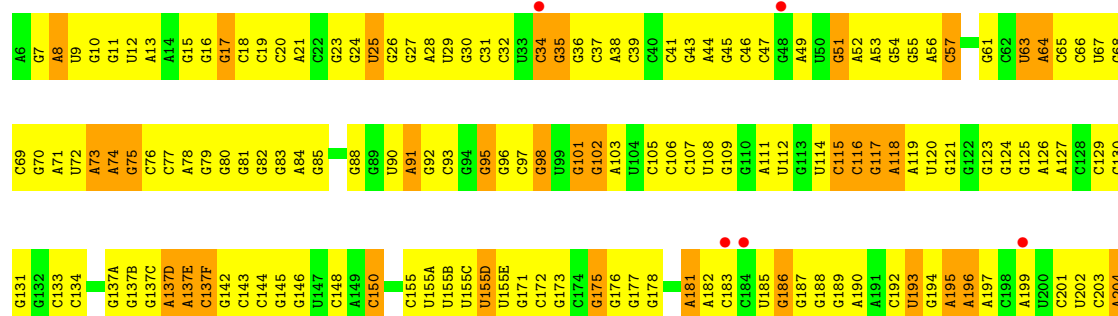
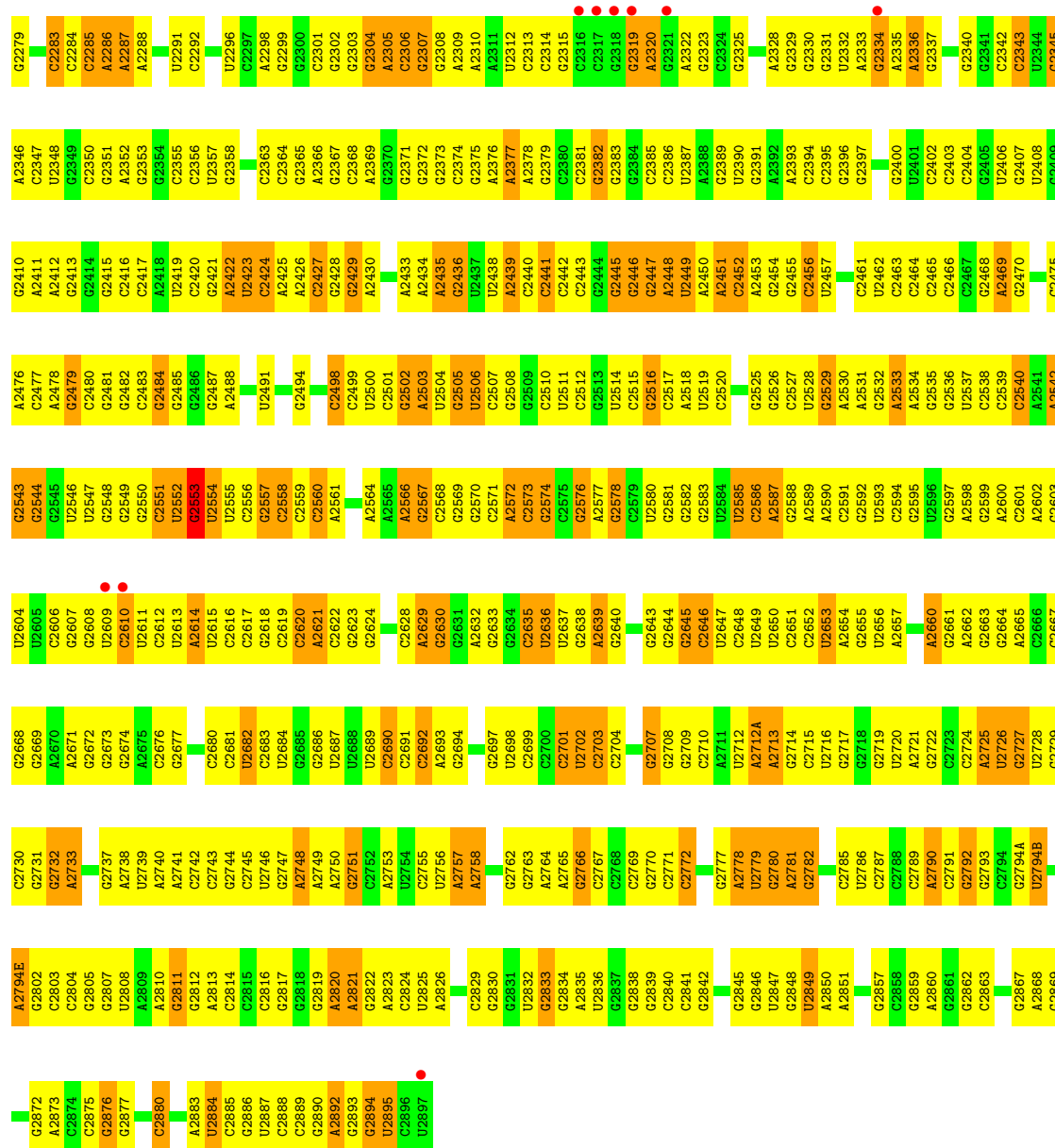
- Molecule 59: 23S Ribosomal RNA

Chain BA:  23% 58% 19%



U1385	A1272	A1204	C1140	A1077	G1011	C949	C884	A820	C758	G696	A632	G573	G506
A1386	U1273	U1205	U1141	U1078	U1012	G952	C885	A821	G759	C697	A633	C574	A507
G1338	A1274	G1206	U1141A	C1079	C1013	A953	C886	U826	G760	A699	C634	U576	G508
G1339	A1275	C1207	A1142	C1080	G1016	C988	A887	U827	A761	G698	C635	U577	C509
U1340	G1276	G1208	A1143	U1081	G1017	C989	C888	U828	G762	G701	A637	A578	C510
U1341	A1277	G1209	G1144	U1082	C1018	C956	A890	A829	A764	G702	G638	C579	U511
A1342	A1278	A1210	G1145	U1083	U1019	A957	C892	G830	G765	G703	G639	G580	G512
G1343	G1279	U1211	C1146	A1084	A1020	U958	C892	U831	G766	G704	G640	C581	A514
G1344	G1280	A1212	G1149	A1085	A1021	A959	C894	G832	G767	G705	G641	G582	A515
G1345	A1281	A1213	U1282	G1087	G1022	A960	C895	G833	G768	A706	G642	G583	C516
G1346	G1283	G1215	G1151	A1088	U1023	C961	A896	C834	G769	G707	A644	C584	C517
A1284	A1284	G1216	C1152	G1089	G1024	G962	C897	A835	G770	G708	A645	G585	G518
G1285	G1285	C1153	C1153	U1090	G1025	U963	C898	G836	G771	U709	A646	A586	U519
A1286	A1286	G1154	G1154	G1091	U1026	G964	A899	C837	G772	G710	G647	G587	G520
A1287	A1287	A1155	A1155	C1102	A1027	C965	A900	C838	G773	G712	G648	U588	G521
U1288	U1288	C1220	C1220	A1103	A1028	G966	A901	U839	A774	G713	G649	C589	G522
C1289	C1289	C1221	G1156	A1095	A1029	C967	A902	C840	G775	G714	C650	A590	C523
C1290	C1290	G1225	C1158	A1096	G1030	C968	C903	A841	G776	U714	G651	C591	U524
C1291	C1291	A1226	U1159	U1097	G1031	G969	C904	G842	A777	G715	U652	G592	U525
U1292	U1292	G1227	G1160	A1098	A1032	C970	U905	G843	G778	A716	C653	G593	A526
C1293	C1293	G1228	G1161	C1101	U1033	C971	G906	C844	U779	U654	G655	U594	C527
U1294	U1294	G1229	G1162	G972	G1034	G972	U906	G845	G780	A718	G656	C595	A528
C1295	C1295	G1163	G1163	A973	U1035	A973	A910	C846	A781	C719	G657	C596	A529
U1234	U1234	G1164	G1164	G974	G1042	G974	A911	U847	A782	G720	U657	U597	G530
G1235	G1235	U1165	U1165	C974A	C1043	C974A	C912	C848	A783	G721	G658	G598	C531
G1236	G1236	C1166	C1166	G975	G1044	G975	U913	A849	A784	A722	C659	G599	A532
A1301	A1301	U1237	U1167	U1105	A1045	U978	C914	C850	G785	G723	G660	G600	G533
A1302	A1302	G1168	G1168	G978	A1046	G979	C915	U851	G786	U724	C661	C601	U534
C1303	C1303	U1108	U1108	A800	A1047	G980	C916	G852	U787	G732	G662	G602	C535
G1304	G1304	G1171	G1171	A801	G1048	A801	A917	G853	A788	A727	G663	A603	A536
C1305	C1305	G1172	G1172	A811	A1049	A811	A918	G854	A789	G728	C664	G604	C537
C1306	C1306	U1173	U1173	C982	C1049	C982	G919	C857	C790	G729	C665	C605	G538
U1307	U1307	G1174	G1174	A983	A1050	A983	G920	U858	G791	C730	G666	U606	G539
A1308	A1308	G1175	G1175	A984	G1051	A984	U922	G859	G792	G731	G667	U607	C540
G1309	G1309	A1177	A1177	C985	C1052	C985	U923	U860	A793	G733	G668	A608	C541
G1310	G1310	C1178	C1178	C986	G1053	C986	C924	G861	G794	A734	G669	A609	C542
C1311	C1311	C1179	C1179	G987	A1054	G987	C925	G862	C797	A735	A670	C610	A543D
U1312	U1312	G1248	C1180	A988	G1055	A988	G926	G863	G798	C736	C671	C611	G550
U1313	U1313	U1249	C1181	G989	G1056	G989	A926	A863	G799	C737	C672	C611A	G551
C1314	C1314	A1182	A1182	A990	A1057	A990	G928	G864	G800	G738	G674	U611C	G553
G1315	G1315	C1251	G1183	C991	G1058	C991	G929	C865	A801	G739	A675	U611D	U554
U1316	U1316	G1252	G1184	C1121	G1059	C992	U930	A866	G802	U740	A676	G611E	U555
A1317	A1317	A1253	C1185	G993	U1060	G993	G931	C867	U803	G741	G677	A611F	G556
C1318	C1318	G1186	G1186	U996	U1061	U996	G932	U868	U804	G742	G681	G611G	U557
A1321	A1321	U1285	U1187	G997	G1062	G997	A933	G869	G805	G745	C682	G617	G558
U1322	U1322	G1256	U1188	C998	G1063	C998	C936	U870	C906	A804	C683	G620	C560
G1323	G1323	C1257	A1189	U999	C1064	U999	U937	A872	U807	A746	G684	A621	G561
G1324	G1324	G1259	G1190	A1128	U1065	U999	G938	G873	U810	G747	A685	G622	U562
G1325	G1325	G1260	G1193	A1129	U1066	A1001	G939	G874	U811	G748	G686	G623	G563
U1326	U1326	U1194	G1194	U1130	G1068	G1002	G940	G875	U812	C749	U688	G624	U564
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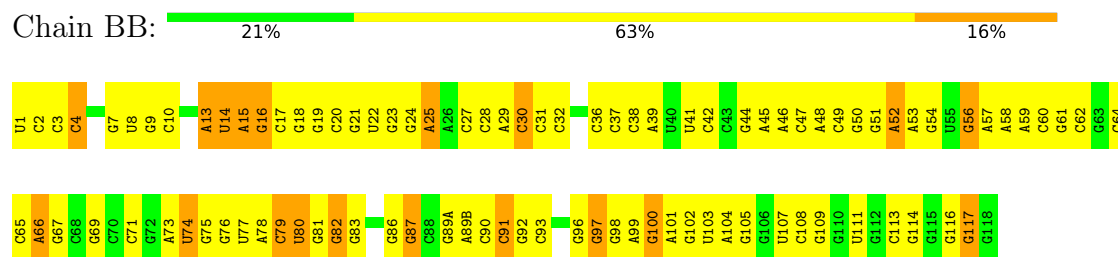


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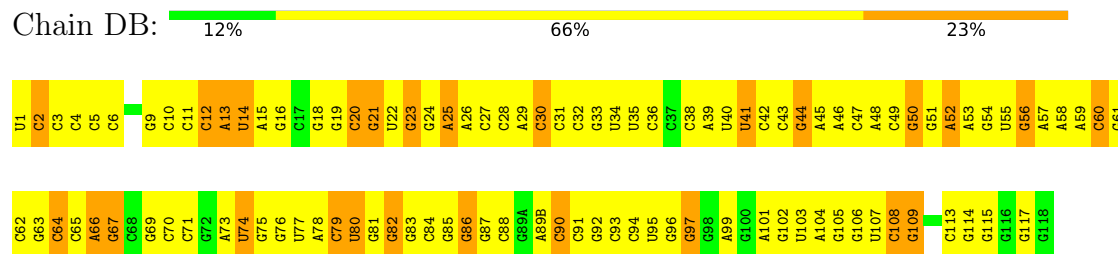
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C1934	G1860	G1861	C1796	G1712B	G1847	A1590	G1506K		A1384	G1256	C1196	C1135
A1936	G1861		U1797	G1712C	G1848	G1581	G1506L		C1385	C1257	G1198	G1137
A1937	G1862		U1798	G1712D	G1849	A1592	G1506M		C1386	C1258	U1199	G1136
A1938	G1863		U1799	G1712E	G1850	A1593	G1506N		C1387	C1259	C1200	G1133
A1939	G1864		U1800	G1712F	G1851	C1584	G1506O		C1388	G1260	G1139	G1140
A1940	G1864B		G1801	G1712G	A1852	A1586	G1525		G1389	C1261	C1202	U1141A
C1941	A1864C		A1802	A1712H	G1853	A1587	G1526		A1392	U1262	G1203	U1141
C1942	A1864D		A1803	G1712I	A1854	C1588	G1527		A1393	U1263	A1204	A1142
C1943	G1878		A1804	G1712J	A1855	C1589	G1528		U1394	G1264	U1205	A1143
C1944	C1879		U1805	G1712K	G1856	U1590	A1529		A1395	G1265	G1207	G1144
C1945	G1880		C1806	G1712L	C1857		G1530		U1396	U1267	C1208	C1145
C1946	C1881		G1807	U1712M	U1859	G1594			U1397	A1268	G1209	
C1947	G1882		C1808	G1712N	G1860	G1595	C1533		A1269	G1270	A1210	G1149
C1948	G1883		A1809	G1712O	A1596	A1597	G1534		C1398	C1271	G1212	C1150
	A1884		G1810	G1712P	A1597	U1598	U1535		C1399	G1272	A1213	C1151
	C1885		C1811	G1712Q	G1661		G1536		G1401	U1273	A1214	C1152
	C1886		A1812		C1662	C1599	U1541		G1402	A1274	G1215	C1153
	C1887		A1813		U1608	G1600	G1542		C1403	G1275	G1216	A1155
	C1888		G1814		A1609	U1602	A1543		U1341	A1276	A1217	G1156
	A1889		A1815		G1610	G1603	C1543A		A1342	G1277	G1218	C1157
	A1890		C1816		G1611	A1603	A1544		G1343	A1278	A1219	C1158
	G1891		A1817		C1612	U1607	A1545		G1344	G1279	G1220	U1159
	U1955		U1818		G1613	A1608	A1546		G1345	G1280	G1221	G1160
	C1892		A1819		C1614	U1609	A1547		G1346	G1281	C1222	C1161
	C1893		U1820		G1615	A1610	C1548		G1347	G1282	G1223	G1164
	C1894		A1821		U1616	G1611	A1549		G1348	U1283	G1224	U1165
	G1896		G1812		C1617	C1612	C1550		A1349	A1284	A1225	A1166
			A1813		G1618	G1613	C1551		U1352	G1285	G1226	U1167
			G1814		C1619	A1614	G1552		U1353	A1286	G1227	G1168
			A1815		U1620	C1615	A1553		U1354	U1287	G1228	G1169
			C1816		G1621	C1616	A1554		A1355	U1288	G1229	G1170
			G1817		A1617	C1617	G1555		A1356	G1289	G1230	G1171
			U1818		C1618	A1618	A1556		A1357	C1290	G1231	G1172
			A1819		U1619	G1619	A1557		A1358	C1291	G1232	A1173
			U1820		G1620	G1620	A1558		A1359	U1294	G1233	U1174
			A1821		G1621	G1621	A1559		A1360	C1295	U1234	U1175
			G1822		C1622	G1622	G1560		A1361	G1296	G1235	A1177
			C1823		U1623	G1623	G1561		A1362	C1297		C1178
			A1824		G1624	G1624	A1562		A1363	U1300	G1238	C1179
			G1825		C1625	G1625	G1563		A1364	A1301	G1239	C1180
			A1826		U1626	U1626	G1564		A1365	A1302	U1240	C1181
			C1827		G1627	G1627	C1565		A1366	A1303	A1241	A1182
			U1828		C1628	C1628	A1566		A1367	G1304	G1243	G1183
			G1829		U1629	G1629	A1567		A1368	A1304	G1244	C1184
			A1830		G1630	G1630	A1568		A1369	G1305	G1245	C1185
			G1831		C1631	C1631	A1569		A1370	G1306	A1246	G1186
			C1832		U1632	U1632	A1570		A1371	G1307	U1247	G1187
			A1833		G1633	G1633	A1571		A1372	A1307	U1248	U1188
			U1834		C1634	C1634	A1572		A1373	A1308	G1249	C1189
			G1835		U1635	U1635	C1573		A1374	G1309	G1250	G1190
			C1836		G1636	G1636	A1574		A1375	G1310	C1251	G1191
			A1837		C1637	C1637	A1575		A1376	G1311	G1192	U1195
			U1838		U1638	U1638	A1576		A1377	G1312	A1253	G1193
			G1839		C1639	C1639	A1577		A1378	C1314		
			A1840		U1640	U1640	C1578		A1379	G1315		
			C1841		G1641	G1641	A1579		A1380	U1316		
			U1842		C1642	C1642	A1580		A1381	G1317		
			G1843		U1643	U1643	A1581		A1382	G1318		
			A1844		C1644	C1644	A1582		A1383	G1319		
			C1845		U1645	U1645	A1583		A1384	G1320		
			G1846		G1646	G1646	A1584		A1385	G1321		
			A1847		C1647	C1647	A1585		A1386	G1322		
			U1848		U1648	U1648	A1586		A1387	G1323		
			C1849		G1649	G1649	A1587		A1388	G1324		
			A1850		C1650	C1650	A1588		A1389	G1325		
			G1851		U1651	U1651	A1589		A1390	G1326		
			U1852		C1652	C1652	A1590		A1391	G1327		
			A1853		U1653	U1653	A1591		A1392	G1328		
			C1854		G1654	G1654	A1592		A1393	G1329		
			U1855		C1655	C1655	A1593		A1394	G1330		
			G1856		U1656	U1656	A1594		A1395	G1331		
			A1857		G1657	G1657	A1595		A1396	G1332		
			U1858		C1658	C1658	A1596		A1397	G1333		
			C1859		U1659	U1659	A1597		A1398	G1334		
			A1860		G1660	G1660	A1598		A1399	G1335		
			G1861		C1661	C1661	A1599		A1400	G1336		
			U1862		U1662	U1662	A1600		A1401	G1337		
			A1863		G1663	G1663	A1601		A1402	G1338		
			C1864		U1664	U1664	A1602		A1403	G1339		
			U1865		C1665	C1665	A1603		A1404	G1340		
			G1866		U1666	U1666	A1604		A1405	G1341		
			A1867		G1667	G1667	A1605		A1406	G1342		
			U1868		C1668	C1668	A1606		A1407	G1343		
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			A1870		G1670	G1670	A1608		A1409	G1345		
			U1871		C1671	C1671	A1609		A1410	G1346		
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			A1873		C1673	C1673	A1611		A1412	G1348		
			U1874		G1674	G1674	A1612		A1413	G1349		
			C1875		U1675	U1675	A1613		A1414	G1350		
			A1876		G1676	G1676	A1614		A1415	G1351		
			U1877		C1677	C1677	A1615		A1416	G1352		
			G1878		U1678	U1678	A1616		A1417	G1353		
			A1879		C1679	C1679	A1617		U1420	G1354		
			U1880		U1680	U1680	A1618		A1421	G1355		
			C1881		G1681	G1681	A1619		A1422	G1356		
			A1882		C1682	C1682	A1620		A1423	G1357		
			U1883		U1683	U1683	A1621		A1424	G1358		
			G1884		G1684	G1684	A1622		A1425	G1359		
			A1885		C1685	C1685	A1623		A1426	G1360		
			U1886		U1686	U1686	A1624		A1427	G1361		
			C1887		G1687	G1687	A1625		A1428	G1362		
			A1888		C1688	C1688	A1626		A1429	G1363		
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			C1890		G1690	G1690	A1628		A1431	G1365		
			A1891		C1691	C1691	A1629		A1432	A1306		
			U1892		U1692	U1692	A1630		A1433	A1307		
			C1893		G1693	G1693	A1631		A1434	A1308		
			A1894		C1694	C1694	A1632		A1435	G1309		
			U1895		U1695	U1695	A1633		A1436	G1310		
			C1896		G1696	G1696	A1634		A1437	G1311		
			A1897		C1697	C1697	A1635		A1438	G1312		
			U1898		U1698	U1698	A1636		A1439	U1313		
			C1899		G1699	G1699	A1637		A1440	G1314		
			A1900		C1700	C1700	A1638		A1441	C1314		
			U1901		U1701	U1701	A1639		A1442	G1315		
			C1902		G1702	G1702	A1640		A1443	U1316		
			A1903		C1703	C1703	A1641		A1444	G1317		
			U1904		U1704	U1704	A1642		A1445	A1253		
			C1905		G1705	G1705	A1643					
			A1906		C1706	C1706	A1644					
			U1907		U1707	U1707	A1645					
			C1908		G1708	G1708	A1646					
			A1909		C1709	C1709	A1647					
			U1910		U1710	U1710	A1648					
			C1911		G1711	G1711	A1649					
			A1912		C1712	C1712	A1650					
			U1913		U1713	U1713	A1651					
			C1914		G1714	G1714	A1652					
			A1915		C1715	C17						

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G2848	C2785	U2720	G2853	G2588	G2526	U2457	C2395	A2333	A2266	G2192	G2126	G1998
U2849	C2786	A2721	A2854	A2589	G2526	C2457	C2396	G2334	A2267	G2193	C2064	C2065
A2850	C2787	C2722	C2850	A2590	G2527	C2457	C2397	A2335	A2268	C2194	C2066	G2002
G2851	C2788	C2723	G2859	G2591	U2528	C2463	U2398	A2336	A2269	C2195	G2069	
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C2853	A2790	A2725	G2661	U2593	A2530	C2465	G2400	G2340	G2271	U2132	C2071	C2006
G2854	C2791	U2726	A2662	G2594	A2531	C2466	U2401	U2341	C2200	G2133	A2071	C2007
C2855	C2792	C2727	G2663	G2595	G2532	C2467	C2402	G2342	A2273	A2134	C2072	C2008
G2856	G2793	U2728	G2664	C2596	A2533	G2468	C2403	C2342	C2202	A2135	C2073	G2009
U2857	C2794	C2729	G2665	A2598	A2534	A2469	C2404	G2343	C2275	U2202A	U2074	G2010
G2858	G2794A	C2730	G2666	G2599	G2535	G2470	C2405	U2344	G2276	C2137	U2075	G2011
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G2862	A2794E	A2735	A2670	U2604	C2539	C2475	G2409	U2348	C2282	U2202F	U2079	A2014
C2863	G2802	G2736	G2665	U2605	C2540	A2476	G2410	G2349	G2283	G2202G	G2080	A2015
G2864	C2803	G2737	G2666	C2606	A2541	C2477	A2411	C2350	C2284	G2202H	C2081	U2016
C2865	C2804	U2738	G2674	G2607	A2542	A2478	A2412	G2351	C2285	G2221	U2144	U2017
G2867	G2805	U2739	G2675	G2608	G2543	G2479	G2413	A2352	C2286	G2222	G2083	G2018
A2868	C2807	A2740	G2678	U2609	G2544	C2480	G2414	G2353	A2287	G2223	C2084	A2019
C2869	A2741	C2742	A2679	G2610	G2545	G2481	G2415	C2354	A2288	G2224	C2085	A2020
C2870	C2743	C2743	C2681	U2611	U2546	G2482	C2416	C2355	A2289	C2225	U2086	C2021
C2871	A2810	G2744	U2682	U2612	G2547	G2483	C2417	C2356	G2290	A2226	G2087	U2022
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C2876	C2815	A2748	G2687	G2617	U2552	G2489	A2422	A2361	C2294	U2232	U2092	G2027
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A2882	G2818	G2751	U2689	G2622	U2555	G2492	A2425	C2364	C2301	G2235	C2095	A2031
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U2887	G2822	U2756	C2694	C2629	C2560	C2499	A2430	A2369	C2306	G2161	U2099	G2035
C2888	C2823	U2757	U2696	A2629	A2561	U2500	U2431	C2372	G2307	G2242	G2101	C2036
C2889	U2824	A2757	G2697	G2630	U2562	C2501	A2432	G2373	C2308	U2102	U2102	G2037
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G2900	C2834	U2706	G2706	A2639	A2572	C2511	C2442	G2382	G2253	C2177	G2112	U2047
A2905	C2835	C2707	G2707	G2640	C2573	U2512	C2443	G2383	G2254	C2178	U2113	G2048
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G2908	C2838	C2710	C2710	G2643	G2576	U2515	G2446	C2386	U2257	G2181	G2115	
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G2910	C2840	C2777	A2712A	G2645	G2578	U2516	G2447	C2388	C2259	C2183	A2119	C2056
C2911	A2841	U2778	C2713	C2646	C2579	C2517	A2448	A2389	C2260	G2184	G2120	C2055
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C2915	G2845	G2717	U2717	U2650	U2585	C2521	C2452	A2392	G2330	C2263	G2124	A2062
G2916	C2846	C2718	C2718	C2651	C2586	U2522	A2453	A2393	C2331	C2264	G2125	A2063

- Molecule 60: 5S Ribosomal RNA



• Molecule 60: 5S Ribosomal RNA



4 Data and refinement statistics

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 49.98 – 3.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.98-3.80) 60.1 (49.98-3.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.05 (at 3.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.295 , 0.331 0.303 , 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)	0.11 , 0.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.17$, $\langle L^2 \rangle = 0.05$	Xtriage
Estimated twinning fraction	0.340 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FUA, ACE, MG, GDP, NMY

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	0.58	1/1945 (0.1%)	1.07	11/2621 (0.4%)
1	CB	0.60	3/1945 (0.2%)	1.09	21/2621 (0.8%)
2	AC	0.37	0/1645	0.86	1/2216 (0.0%)
2	CC	0.41	0/1645	0.90	2/2216 (0.1%)
3	AD	0.39	0/1733	0.96	6/2318 (0.3%)
3	CD	0.40	0/1733	0.98	7/2318 (0.3%)
4	AE	0.43	0/1172	0.92	4/1576 (0.3%)
4	CE	0.44	0/1172	1.00	6/1576 (0.4%)
5	AF	0.37	0/856	0.88	3/1154 (0.3%)
5	CF	0.44	0/856	0.90	1/1154 (0.1%)
6	AG	0.36	0/1276	0.88	3/1709 (0.2%)
6	CG	0.39	0/1276	0.89	2/1709 (0.1%)
7	AH	0.40	0/1136	0.91	2/1527 (0.1%)
7	CH	0.37	0/1136	0.86	0/1527
8	AI	0.34	0/1029	0.89	0/1379
8	CI	0.36	0/1029	0.84	0/1379
9	AJ	0.38	0/815	0.89	0/1095
9	CJ	0.43	0/815	0.97	0/1095
10	AK	0.56	0/900	0.99	4/1213 (0.3%)
10	CK	0.57	0/900	0.95	2/1213 (0.2%)
11	AL	0.63	0/992	1.17	9/1327 (0.7%)
11	CL	0.64	0/992	1.16	5/1327 (0.4%)
12	AM	0.37	0/1008	0.90	1/1347 (0.1%)
12	CM	0.37	0/1008	0.92	1/1347 (0.1%)
13	AN	0.36	0/501	0.87	1/664 (0.2%)
13	CN	0.38	0/501	0.84	0/664
14	AO	0.44	0/745	0.96	0/992
14	CO	0.43	0/745	0.86	0/992
15	AP	0.46	0/722	0.99	1/970 (0.1%)
15	CP	0.44	0/722	0.99	2/970 (0.2%)
16	AQ	0.45	0/848	1.10	7/1131 (0.6%)
16	CQ	0.48	0/848	1.11	8/1131 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.37	0/579	0.91	3/768 (0.4%)
17	CR	0.42	0/579	0.96	1/768 (0.1%)
18	AS	0.39	0/647	0.86	0/870
18	CS	0.35	0/647	0.84	2/870 (0.2%)
19	AT	0.41	0/765	0.84	0/1007
19	CT	0.40	0/765	0.81	0/1007
20	AY	0.53	1/5270 (0.0%)	1.08	24/7135 (0.3%)
20	CY	0.52	1/5270 (0.0%)	1.07	36/7135 (0.5%)
21	AA	0.20	0/36351	0.45	2/56736 (0.0%)
21	CA	0.21	0/36351	0.46	0/56736
22	AW	0.25	0/1827	0.54	0/2845
22	CW	0.23	0/1827	0.51	0/2845
23	AV	0.84	1/881 (0.1%)	0.81	2/1372 (0.1%)
23	CV	0.38	0/880	0.85	0/1372
24	AX	0.29	0/1815	0.55	0/2826
24	CX	0.29	0/1815	0.57	0/2826
25	BC	0.69	1/1774 (0.1%)	1.40	38/2391 (1.6%)
25	DC	0.73	2/1774 (0.1%)	1.30	25/2391 (1.0%)
26	BD	0.70	5/2195 (0.2%)	1.03	11/2955 (0.4%)
26	DD	0.43	0/2195	1.02	8/2955 (0.3%)
27	BE	0.50	0/1602	1.05	6/2160 (0.3%)
27	DE	0.48	0/1602	1.07	8/2160 (0.4%)
28	BF	0.56	1/1663 (0.1%)	1.27	17/2249 (0.8%)
28	DF	0.53	0/1663	1.18	22/2249 (1.0%)
29	BG	0.37	0/1499	0.88	1/2016 (0.0%)
29	DG	0.39	0/1499	0.97	8/2016 (0.4%)
30	BH	0.40	0/1298	1.03	7/1751 (0.4%)
30	DH	0.39	0/1298	0.94	2/1751 (0.1%)
32	BK	0.43	0/1054	0.95	2/1427 (0.1%)
32	DK	0.48	0/1054	1.00	5/1427 (0.4%)
33	BN	1.26	13/1141 (1.1%)	1.89	48/1537 (3.1%)
33	DN	1.24	7/1141 (0.6%)	1.76	42/1537 (2.7%)
34	BO	0.46	0/943	1.04	3/1269 (0.2%)
34	DO	0.47	0/943	1.05	6/1269 (0.5%)
35	BP	0.40	0/1131	0.98	4/1504 (0.3%)
35	DP	0.41	0/1131	0.94	5/1504 (0.3%)
36	BQ	0.48	0/1143	1.06	3/1527 (0.2%)
36	DQ	0.44	0/1143	1.05	5/1527 (0.3%)
37	BR	0.45	0/974	0.94	0/1302
37	DR	0.42	0/974	0.90	3/1302 (0.2%)
38	BS	0.53	0/783	1.05	4/1041 (0.4%)
38	DS	0.54	0/783	1.11	2/1041 (0.2%)
39	BT	0.43	0/1161	0.99	6/1549 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DT	0.43	0/1161	0.95	3/1549 (0.2%)
40	BU	0.45	0/982	0.91	0/1306
40	DU	0.42	0/982	0.89	3/1306 (0.2%)
41	BV	0.49	0/790	1.07	5/1057 (0.5%)
41	DV	0.47	0/790	1.01	3/1057 (0.3%)
42	BW	0.45	0/911	1.02	4/1220 (0.3%)
42	DW	0.53	0/911	1.04	6/1220 (0.5%)
43	BX	0.37	0/748	0.87	0/1004
43	DX	0.36	0/748	0.85	0/1004
44	BY	0.40	0/831	0.94	2/1108 (0.2%)
44	DY	0.37	0/831	0.86	2/1108 (0.2%)
45	BZ	0.41	0/1505	0.97	2/2042 (0.1%)
45	DZ	0.43	0/1505	0.99	7/2042 (0.3%)
46	B0	0.32	0/671	0.93	3/892 (0.3%)
46	D0	0.35	0/671	0.87	2/892 (0.2%)
47	B1	0.86	5/739 (0.7%)	1.59	17/981 (1.7%)
47	D1	0.67	1/739 (0.1%)	1.40	12/981 (1.2%)
48	B2	0.45	0/600	0.93	2/793 (0.3%)
48	D2	0.44	0/600	1.00	1/793 (0.1%)
49	B3	0.48	0/482	0.99	2/646 (0.3%)
49	D3	0.38	0/482	1.02	2/646 (0.3%)
50	B4	0.63	0/276	1.18	4/372 (1.1%)
50	D4	0.58	0/276	1.25	6/372 (1.6%)
51	B5	0.47	0/473	1.05	2/639 (0.3%)
51	D5	0.51	0/473	1.04	2/639 (0.3%)
52	B6	0.43	0/440	1.12	2/586 (0.3%)
52	D6	0.43	0/440	0.94	0/586
53	B7	1.06	4/438 (0.9%)	1.45	8/575 (1.4%)
53	D7	0.37	0/438	0.94	1/575 (0.2%)
54	B8	0.44	0/525	0.89	0/691
54	D8	0.41	0/525	0.96	1/691 (0.1%)
55	B9	0.37	0/310	0.90	0/407
55	D9	0.39	0/310	0.92	0/407
56	Be	0.35	0/538	0.90	0/715
56	De	0.34	0/538	0.95	2/715 (0.3%)
59	BA	0.20	0/69437	0.45	6/108401 (0.0%)
59	DA	0.21	0/69437	0.46	3/108401 (0.0%)
60	BB	0.21	0/2853	0.47	0/4451
60	DB	0.23	0/2853	0.47	0/4451
All	All	0.34	46/334735 (0.0%)	0.68	586/498724 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	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 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AV	1	G	P-O5'	23.85	1.95	1.59
26	BD	143	HIS	CE1-NE2	-14.66	1.17	1.32
26	BD	143	HIS	CG-ND1	-14.65	1.22	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	BN	101	HIS	CA-C	-12.69	1.35	1.52
33	DN	117	PHE	CA-C	-12.48	1.36	1.52

The worst 5 of 586 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	DF	156	LEU	N-CA-C	-15.91	89.07	110.55
28	BF	193	VAL	N-CA-C	-15.72	87.60	109.45
28	BF	156	LEU	N-CA-C	-15.25	88.48	110.59
47	B1	19	GLN	N-CA-C	-13.97	93.25	112.94
28	DF	193	VAL	N-CA-C	-13.66	87.53	109.12

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1910	0	1957	125	0
1	CB	1910	0	1957	116	0
2	AC	1621	0	1688	92	0
2	CC	1621	0	1688	86	0
3	AD	1703	0	1767	113	0
3	CD	1703	0	1767	97	0
4	AE	1156	0	1213	57	0
4	CE	1156	0	1213	57	0
5	AF	843	0	857	34	0
5	CF	843	0	857	51	0
6	AG	1257	0	1296	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	CG	1257	0	1296	61	0
7	AH	1116	0	1177	79	0
7	CH	1116	0	1177	80	0
8	AI	1010	0	1037	67	0
8	CI	1010	0	1037	61	0
9	AJ	802	0	849	49	0
9	CJ	802	0	849	56	0
10	AK	885	0	904	62	0
10	CK	885	0	904	64	0
11	AL	976	0	1062	110	0
11	CL	976	0	1062	105	0
12	AM	997	0	1072	36	0
12	CM	997	0	1072	68	0
13	AN	492	0	533	36	0
13	CN	492	0	533	39	0
14	AO	734	0	771	50	0
14	CO	734	0	771	32	0
15	AP	706	0	725	45	0
15	CP	706	0	725	46	0
16	AQ	835	0	904	71	0
16	CQ	835	0	904	63	0
17	AR	574	0	644	34	0
17	CR	574	0	644	35	0
18	AS	634	0	655	41	0
18	CS	634	0	655	31	0
19	AT	763	0	861	53	0
19	CT	763	0	861	45	0
20	AY	5173	0	5239	348	0
20	CY	5173	0	5239	342	0
21	AA	32474	0	16393	1213	0
21	CA	32474	0	16392	1576	0
22	AW	1635	0	831	83	0
22	CW	1635	0	831	86	0
23	AV	783	0	391	43	0
23	CV	781	0	393	74	0
24	AX	1629	0	832	76	0
24	CX	1629	0	832	93	0
25	BC	1742	0	1798	163	0
25	DC	1742	0	1798	133	0
26	BD	2145	0	2234	179	0
26	DD	2145	0	2234	161	0
27	BE	1569	0	1634	136	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	DE	1569	0	1634	125	0
28	BF	1628	0	1680	159	0
28	DF	1628	0	1680	134	0
29	BG	1474	0	1535	83	0
29	DG	1474	0	1535	104	0
30	BH	1274	0	1342	69	0
30	DH	1274	0	1342	77	0
31	BJ	851	0	207	26	0
31	DJ	851	0	207	18	0
32	BK	1035	0	1082	66	0
32	DK	1035	0	1082	77	0
33	BN	1114	0	1185	290	0
33	DN	1114	0	1185	320	0
34	BO	933	0	996	73	0
34	DO	933	0	996	64	0
35	BP	1114	0	1187	109	0
35	DP	1114	0	1187	113	0
36	BQ	1122	0	1179	97	0
36	DQ	1122	0	1179	88	0
37	BR	960	0	1021	87	0
37	DR	960	0	1021	85	0
38	BS	775	0	835	77	0
38	DS	775	0	835	86	0
39	BT	1147	0	1207	94	0
39	DT	1147	0	1207	95	0
40	BU	964	0	1022	79	0
40	DU	964	0	1022	70	0
41	BV	779	0	852	70	0
41	DV	779	0	852	56	0
42	BW	900	0	964	76	0
42	DW	900	0	964	58	0
43	BX	734	0	789	33	0
43	DX	734	0	789	28	0
44	BY	818	0	908	56	0
44	DY	818	0	908	62	0
45	BZ	1473	0	1497	85	0
45	DZ	1473	0	1497	80	0
46	B0	662	0	688	33	0
46	D0	662	0	688	49	0
47	B1	732	0	808	57	0
47	D1	732	0	808	67	0
48	B2	598	0	653	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	D2	598	0	653	56	0
49	B3	477	0	529	24	0
49	D3	477	0	529	29	0
50	B4	271	0	284	11	0
50	D4	271	0	284	23	0
51	B5	459	0	480	29	0
51	D5	459	0	480	36	0
52	B6	433	0	461	34	0
52	D6	433	0	461	47	0
53	B7	430	0	480	31	0
53	D7	430	0	480	33	0
54	B8	517	0	582	47	0
54	D8	517	0	582	48	0
55	B9	307	0	338	30	0
55	D9	307	0	338	26	0
56	Be	686	0	620	21	0
56	De	686	0	621	24	0
57	Bf	156	0	47	0	0
57	Bg	156	0	47	0	0
57	Df	156	0	48	2	0
57	Dg	156	0	46	0	0
58	Bh	151	0	41	1	0
58	Dh	151	0	48	0	0
59	BA	61997	0	31250	2491	0
59	DA	61997	0	31250	2834	0
60	BB	2551	0	1295	143	0
60	DB	2551	0	1295	162	0
61	AY	28	0	12	8	0
61	CY	28	0	12	14	0
62	AY	37	0	47	21	0
62	CY	37	0	47	14	0
63	AA	42	0	46	27	0
63	BA	126	0	138	60	0
63	CA	42	0	46	34	0
63	DA	42	0	46	23	0
64	BA	1	0	0	0	0
64	CY	1	0	0	0	0
All	All	312066	0	215233	15158	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 15158 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:DN:114:ARG:HH21	59:DA:527:C:C1'	1.22	1.51
24:CX:75:C:N4	59:DA:2553:G:H1	1.11	1.47
59:DA:2681:C:N4	59:DA:2725:A:H62	1.09	1.47
33:DN:114:ARG:NH2	59:DA:527:C:H1'	1.12	1.44
21:CA:1538:C:C2	23:CV:7:G:N2	1.88	1.41

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	0	9
1	CB	233/235 (99%)	171 (73%)	45 (19%)	17 (7%)	1	11
2	AC	205/207 (99%)	137 (67%)	39 (19%)	29 (14%)	0	3
2	CC	205/207 (99%)	150 (73%)	35 (17%)	20 (10%)	0	7
3	AD	206/208 (99%)	140 (68%)	41 (20%)	25 (12%)	0	4
3	CD	206/208 (99%)	152 (74%)	33 (16%)	21 (10%)	0	7
4	AE	149/151 (99%)	122 (82%)	20 (13%)	7 (5%)	2	18
4	CE	149/151 (99%)	115 (77%)	24 (16%)	10 (7%)	1	13
5	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1	10
5	CF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	0	8
6	AG	153/155 (99%)	123 (80%)	22 (14%)	8 (5%)	1	17
6	CG	153/155 (99%)	118 (77%)	23 (15%)	12 (8%)	1	11
7	AH	136/138 (99%)	102 (75%)	23 (17%)	11 (8%)	1	10
7	CH	136/138 (99%)	96 (71%)	30 (22%)	10 (7%)	1	11
8	AI	125/127 (98%)	97 (78%)	22 (18%)	6 (5%)	2	17
8	CI	125/127 (98%)	98 (78%)	21 (17%)	6 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AJ	97/99 (98%)	71 (73%)	15 (16%)	11 (11%)	0	5
9	CJ	97/99 (98%)	74 (76%)	16 (16%)	7 (7%)	1	12
10	AK	117/119 (98%)	83 (71%)	21 (18%)	13 (11%)	0	5
10	CK	117/119 (98%)	79 (68%)	21 (18%)	17 (14%)	0	2
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	10
12	CM	123/125 (98%)	95 (77%)	17 (14%)	11 (9%)	0	9
13	AN	58/60 (97%)	38 (66%)	17 (29%)	3 (5%)	1	17
13	CN	58/60 (97%)	35 (60%)	14 (24%)	9 (16%)	0	2
14	AO	86/88 (98%)	72 (84%)	12 (14%)	2 (2%)	5	30
14	CO	86/88 (98%)	65 (76%)	18 (21%)	3 (4%)	3	23
15	AP	82/84 (98%)	58 (71%)	16 (20%)	8 (10%)	0	7
15	CP	82/84 (98%)	62 (76%)	13 (16%)	7 (8%)	0	9
16	AQ	98/100 (98%)	70 (71%)	22 (22%)	6 (6%)	1	14
16	CQ	98/100 (98%)	76 (78%)	16 (16%)	6 (6%)	1	14
17	AR	68/70 (97%)	50 (74%)	9 (13%)	9 (13%)	0	3
17	CR	68/70 (97%)	56 (82%)	8 (12%)	4 (6%)	1	15
18	AS	77/79 (98%)	43 (56%)	23 (30%)	11 (14%)	0	3
18	CS	77/79 (98%)	47 (61%)	27 (35%)	3 (4%)	2	20
19	AT	97/99 (98%)	72 (74%)	17 (18%)	8 (8%)	0	10
19	CT	97/99 (98%)	82 (84%)	10 (10%)	5 (5%)	1	17
20	AY	657/687 (96%)	407 (62%)	174 (26%)	76 (12%)	0	4
20	CY	657/687 (96%)	437 (66%)	135 (20%)	85 (13%)	0	3
25	BC	226/228 (99%)	107 (47%)	63 (28%)	56 (25%)	0	0
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	3
26	DD	273/275 (99%)	180 (66%)	59 (22%)	34 (12%)	0	4
27	BE	203/205 (99%)	134 (66%)	41 (20%)	28 (14%)	0	3
27	DE	203/205 (99%)	124 (61%)	49 (24%)	30 (15%)	0	2
28	BF	206/208 (99%)	139 (68%)	43 (21%)	24 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	DF	206/208 (99%)	127 (62%)	51 (25%)	28 (14%)	0	3
29	BG	179/181 (99%)	131 (73%)	37 (21%)	11 (6%)	1	14
29	DG	179/181 (99%)	127 (71%)	37 (21%)	15 (8%)	0	9
30	BH	165/167 (99%)	117 (71%)	31 (19%)	17 (10%)	0	6
30	DH	165/167 (99%)	116 (70%)	30 (18%)	19 (12%)	0	4
32	BK	138/140 (99%)	91 (66%)	32 (23%)	15 (11%)	0	5
32	DK	138/140 (99%)	77 (56%)	44 (32%)	17 (12%)	0	4
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%)	0	9
34	DO	120/122 (98%)	86 (72%)	22 (18%)	12 (10%)	0	7
35	BP	144/146 (99%)	84 (58%)	36 (25%)	24 (17%)	0	2
35	DP	144/146 (99%)	82 (57%)	39 (27%)	23 (16%)	0	2
36	BQ	139/141 (99%)	84 (60%)	35 (25%)	20 (14%)	0	3
36	DQ	139/141 (99%)	94 (68%)	34 (24%)	11 (8%)	1	10
37	BR	115/117 (98%)	80 (70%)	20 (17%)	15 (13%)	0	3
37	DR	115/117 (98%)	80 (70%)	22 (19%)	13 (11%)	0	5
38	BS	97/99 (98%)	52 (54%)	26 (27%)	19 (20%)	0	1
38	DS	97/99 (98%)	51 (53%)	27 (28%)	19 (20%)	0	1
39	BT	136/138 (99%)	81 (60%)	27 (20%)	28 (21%)	0	1
39	DT	136/138 (99%)	79 (58%)	31 (23%)	26 (19%)	0	1
40	BU	115/117 (98%)	88 (76%)	17 (15%)	10 (9%)	0	9
40	DU	115/117 (98%)	90 (78%)	17 (15%)	8 (7%)	1	12
41	BV	99/101 (98%)	56 (57%)	28 (28%)	15 (15%)	0	2
41	DV	99/101 (98%)	64 (65%)	21 (21%)	14 (14%)	0	3
42	BW	111/113 (98%)	74 (67%)	25 (22%)	12 (11%)	0	5
42	DW	111/113 (98%)	76 (68%)	23 (21%)	12 (11%)	0	5
43	BX	91/93 (98%)	71 (78%)	13 (14%)	7 (8%)	1	11
43	DX	91/93 (98%)	67 (74%)	10 (11%)	14 (15%)	0	2
44	BY	105/107 (98%)	54 (51%)	31 (30%)	20 (19%)	0	1
44	DY	105/107 (98%)	59 (56%)	26 (25%)	20 (19%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	BZ	183/185 (99%)	121 (66%)	43 (24%)	19 (10%)	0	6
45	DZ	183/185 (99%)	109 (60%)	45 (25%)	29 (16%)	0	2
46	B0	82/84 (98%)	63 (77%)	14 (17%)	5 (6%)	1	14
46	D0	82/84 (98%)	59 (72%)	18 (22%)	5 (6%)	1	14
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%)	0	9
48	D2	69/71 (97%)	53 (77%)	12 (17%)	4 (6%)	1	15
49	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	23
49	D3	58/60 (97%)	47 (81%)	8 (14%)	3 (5%)	1	17
50	B4	33/35 (94%)	15 (46%)	13 (39%)	5 (15%)	0	2
50	D4	33/35 (94%)	17 (52%)	11 (33%)	5 (15%)	0	2
51	B5	57/59 (97%)	36 (63%)	14 (25%)	7 (12%)	0	4
51	D5	57/59 (97%)	38 (67%)	6 (10%)	13 (23%)	0	0
52	B6	48/50 (96%)	24 (50%)	15 (31%)	9 (19%)	0	1
52	D6	48/50 (96%)	20 (42%)	17 (35%)	11 (23%)	0	0
53	B7	47/49 (96%)	33 (70%)	11 (23%)	3 (6%)	1	14
53	D7	47/49 (96%)	26 (55%)	14 (30%)	7 (15%)	0	2
54	B8	62/64 (97%)	34 (55%)	16 (26%)	12 (19%)	0	1
54	D8	62/64 (97%)	35 (56%)	13 (21%)	14 (23%)	0	0
55	B9	35/37 (95%)	29 (83%)	5 (14%)	1 (3%)	3	25
55	D9	35/37 (95%)	25 (71%)	7 (20%)	3 (9%)	0	9
56	Be	70/103 (68%)	39 (56%)	23 (33%)	8 (11%)	0	5
56	De	70/103 (68%)	40 (57%)	17 (24%)	13 (19%)	0	1
All	All	13246/13568 (98%)	8764 (66%)	2800 (21%)	1682 (13%)	0	4

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 ⓘ

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%)	168 (83%)	35 (17%)	2	13
1	CB	203/203 (100%)	156 (77%)	47 (23%)	1	5
2	AC	161/161 (100%)	130 (81%)	31 (19%)	1	9
2	CC	161/161 (100%)	125 (78%)	36 (22%)	1	5
3	AD	180/180 (100%)	146 (81%)	34 (19%)	1	10
3	CD	180/180 (100%)	150 (83%)	30 (17%)	2	13
4	AE	116/116 (100%)	93 (80%)	23 (20%)	1	8
4	CE	116/116 (100%)	90 (78%)	26 (22%)	1	5
5	AF	90/90 (100%)	74 (82%)	16 (18%)	2	12
5	CF	90/90 (100%)	75 (83%)	15 (17%)	2	13
6	AG	126/126 (100%)	107 (85%)	19 (15%)	3	16
6	CG	126/126 (100%)	110 (87%)	16 (13%)	4	21
7	AH	119/119 (100%)	99 (83%)	20 (17%)	2	13
7	CH	119/119 (100%)	89 (75%)	30 (25%)	0	3
8	AI	98/98 (100%)	81 (83%)	17 (17%)	2	12
8	CI	98/98 (100%)	77 (79%)	21 (21%)	1	6
9	AJ	89/89 (100%)	71 (80%)	18 (20%)	1	8
9	CJ	89/89 (100%)	68 (76%)	21 (24%)	1	5
10	AK	90/90 (100%)	79 (88%)	11 (12%)	5	21
10	CK	90/90 (100%)	74 (82%)	16 (18%)	2	12
11	AL	104/104 (100%)	82 (79%)	22 (21%)	1	6
11	CL	104/104 (100%)	80 (77%)	24 (23%)	1	5
12	AM	100/100 (100%)	83 (83%)	17 (17%)	2	13
12	CM	100/100 (100%)	78 (78%)	22 (22%)	1	5
13	AN	49/49 (100%)	39 (80%)	10 (20%)	1	7
13	CN	49/49 (100%)	36 (74%)	13 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	79/79 (100%)	59 (75%)	20 (25%)	0	3
14	CO	79/79 (100%)	70 (89%)	9 (11%)	5	23
15	AP	72/72 (100%)	68 (94%)	4 (6%)	19	45
15	CP	72/72 (100%)	60 (83%)	12 (17%)	2	13
16	AQ	95/95 (100%)	76 (80%)	19 (20%)	1	8
16	CQ	95/95 (100%)	79 (83%)	16 (17%)	2	13
17	AR	61/61 (100%)	47 (77%)	14 (23%)	1	5
17	CR	61/61 (100%)	53 (87%)	8 (13%)	4	20
18	AS	69/69 (100%)	52 (75%)	17 (25%)	1	4
18	CS	69/69 (100%)	48 (70%)	21 (30%)	0	1
19	AT	76/76 (100%)	61 (80%)	15 (20%)	1	8
19	CT	76/76 (100%)	57 (75%)	19 (25%)	0	4
20	AY	558/579 (96%)	446 (80%)	112 (20%)	1	8
20	CY	558/579 (96%)	440 (79%)	118 (21%)	1	6
25	BC	180/180 (100%)	128 (71%)	52 (29%)	0	2
25	DC	180/180 (100%)	140 (78%)	40 (22%)	1	5
26	BD	217/217 (100%)	176 (81%)	41 (19%)	1	10
26	DD	217/217 (100%)	169 (78%)	48 (22%)	1	6
27	BE	165/165 (100%)	134 (81%)	31 (19%)	1	10
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	5
28	BF	165/165 (100%)	128 (78%)	37 (22%)	1	5
28	DF	165/165 (100%)	130 (79%)	35 (21%)	1	6
29	BG	155/155 (100%)	139 (90%)	16 (10%)	7	27
29	DG	155/155 (100%)	129 (83%)	26 (17%)	2	13
30	BH	136/136 (100%)	110 (81%)	26 (19%)	1	9
30	DH	136/136 (100%)	116 (85%)	20 (15%)	3	17
32	BK	105/105 (100%)	78 (74%)	27 (26%)	0	3
32	DK	105/105 (100%)	80 (76%)	25 (24%)	1	5
33	BN	118/118 (100%)	83 (70%)	35 (30%)	0	2
33	DN	118/118 (100%)	76 (64%)	42 (36%)	0	0
34	BO	100/100 (100%)	76 (76%)	24 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	DO	100/100 (100%)	83 (83%)	17 (17%)	2	13
35	BP	112/112 (100%)	87 (78%)	25 (22%)	1	5
35	DP	112/112 (100%)	87 (78%)	25 (22%)	1	5
36	BQ	111/111 (100%)	77 (69%)	34 (31%)	0	1
36	DQ	111/111 (100%)	93 (84%)	18 (16%)	2	14
37	BR	100/100 (100%)	83 (83%)	17 (17%)	2	13
37	DR	100/100 (100%)	75 (75%)	25 (25%)	0	4
38	BS	77/77 (100%)	63 (82%)	14 (18%)	2	12
38	DS	77/77 (100%)	58 (75%)	19 (25%)	1	4
39	BT	120/120 (100%)	93 (78%)	27 (22%)	1	5
39	DT	120/120 (100%)	91 (76%)	29 (24%)	1	4
40	BU	93/93 (100%)	78 (84%)	15 (16%)	2	14
40	DU	93/93 (100%)	75 (81%)	18 (19%)	1	9
41	BV	82/82 (100%)	59 (72%)	23 (28%)	0	2
41	DV	82/82 (100%)	61 (74%)	21 (26%)	0	3
42	BW	92/92 (100%)	79 (86%)	13 (14%)	3	18
42	DW	92/92 (100%)	69 (75%)	23 (25%)	0	4
43	BX	75/75 (100%)	59 (79%)	16 (21%)	1	6
43	DX	75/75 (100%)	58 (77%)	17 (23%)	1	5
44	BY	88/88 (100%)	61 (69%)	27 (31%)	0	1
44	DY	88/88 (100%)	73 (83%)	15 (17%)	2	13
45	BZ	162/162 (100%)	131 (81%)	31 (19%)	1	9
45	DZ	162/162 (100%)	132 (82%)	30 (18%)	1	11
46	B0	66/66 (100%)	55 (83%)	11 (17%)	2	13
46	D0	66/66 (100%)	51 (77%)	15 (23%)	1	5
47	B1	78/78 (100%)	54 (69%)	24 (31%)	0	1
47	D1	78/78 (100%)	57 (73%)	21 (27%)	0	3
48	B2	66/66 (100%)	54 (82%)	12 (18%)	2	12
48	D2	66/66 (100%)	57 (86%)	9 (14%)	3	18
49	B3	52/52 (100%)	45 (86%)	7 (14%)	4	19
49	D3	52/52 (100%)	45 (86%)	7 (14%)	4	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	B4	31/31 (100%)	22 (71%)	9 (29%)	0	2
50	D4	31/31 (100%)	22 (71%)	9 (29%)	0	2
51	B5	51/51 (100%)	39 (76%)	12 (24%)	1	5
51	D5	51/51 (100%)	46 (90%)	5 (10%)	7	29
52	B6	49/49 (100%)	34 (69%)	15 (31%)	0	1
52	D6	49/49 (100%)	30 (61%)	19 (39%)	0	0
53	B7	42/42 (100%)	35 (83%)	7 (17%)	2	13
53	D7	42/42 (100%)	35 (83%)	7 (17%)	2	13
54	B8	54/54 (100%)	46 (85%)	8 (15%)	3	16
54	D8	54/54 (100%)	44 (82%)	10 (18%)	1	11
55	B9	34/34 (100%)	25 (74%)	9 (26%)	0	3
55	D9	34/34 (100%)	31 (91%)	3 (9%)	9	33
56	Be	54/54 (100%)	44 (82%)	10 (18%)	1	11
56	De	54/54 (100%)	45 (83%)	9 (17%)	2	13
All	All	11130/11172 (100%)	8836 (79%)	2294 (21%)	1	7

5 of 2294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	DH	116	GLU
56	De	99	VAL
33	DN	87	LEU
30	DH	106	THR
41	DV	28	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 126 such sidechains are listed below:

Mol	Chain	Res	Type
1	CB	40	HIS
38	DS	61	ASN
9	CJ	69	ASN
34	DO	88	ASN
43	DX	55	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%)	28 (80%)	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%)	717 (24%)	29 (1%)
60	BB	118/119 (99%)	27 (22%)	0
60	DB	118/119 (99%)	32 (27%)	0
All	All	9385/9400 (99%)	2449 (26%)	109 (1%)

5 of 2449 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 oligosaccharides in this entry.

5.6 Ligand geometry

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	2902	-	43,45,45	0.56	0	62,67,67	0.97	4 (6%)
61	GDP	AY	701	-	29,30,30	1.15	3 (10%)	45,47,47	1.97	14 (31%)
63	NMY	AA	1601	-	43,45,45	0.56	0	62,67,67	0.97	4 (6%)
62	FUA	CY	702	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	8 (16%)
63	NMY	BA	2904	-	43,45,45	0.56	0	62,67,67	0.97	4 (6%)
61	GDP	CY	701	-	29,30,30	1.14	3 (10%)	45,47,47	1.98	12 (26%)
62	FUA	AY	702	-	39,40,40	1.70	7 (17%)	50,64,64	1.70	7 (14%)
63	NMY	BA	2903	-	43,45,45	0.57	0	62,67,67	0.97	4 (6%)
63	NMY	CA	1601	-	43,45,45	0.56	0	62,67,67	0.97	4 (6%)
63	NMY	DA	2901	-	43,45,45	0.56	0	62,67,67	0.97	4 (6%)

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	2902	-	-	12/18/94/94	0/4/4/4
61	GDP	AY	701	-	-	2/16/32/32	0/3/3/3
63	NMY	AA	1601	-	-	12/18/94/94	0/4/4/4
62	FUA	CY	702	-	-	7/16/92/92	0/4/4/4
63	NMY	BA	2904	-	-	12/18/94/94	0/4/4/4
61	GDP	CY	701	-	-	5/16/32/32	0/3/3/3
62	FUA	AY	702	-	-	7/16/92/92	0/4/4/4
63	NMY	BA	2903	-	-	12/18/94/94	0/4/4/4
63	NMY	CA	1601	-	-	12/18/94/94	0/4/4/4
63	NMY	DA	2901	-	-	12/18/94/94	0/4/4/4

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CY	702	FUA	C23-C22	-4.44	1.39	1.51
62	AY	702	FUA	C23-C22	-4.38	1.40	1.51
62	AY	702	FUA	C23-C24	-4.36	1.39	1.53
62	CY	702	FUA	C23-C24	-4.34	1.39	1.53
62	CY	702	FUA	C29-C22	4.22	1.53	1.47

The worst 5 of 65 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	GDP	C2-N3-C4	5.86	122.40	112.30
61	CY	701	GDP	C5-C4-N3	-5.54	119.56	128.39
62	CY	702	FUA	C24-C23-C22	5.33	124.08	112.72
62	AY	702	FUA	C24-C23-C22	5.32	124.05	112.72
61	AY	701	GDP	C2-N3-C4	4.96	120.84	112.30

There are no chirality outliers.

5 of 93 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'

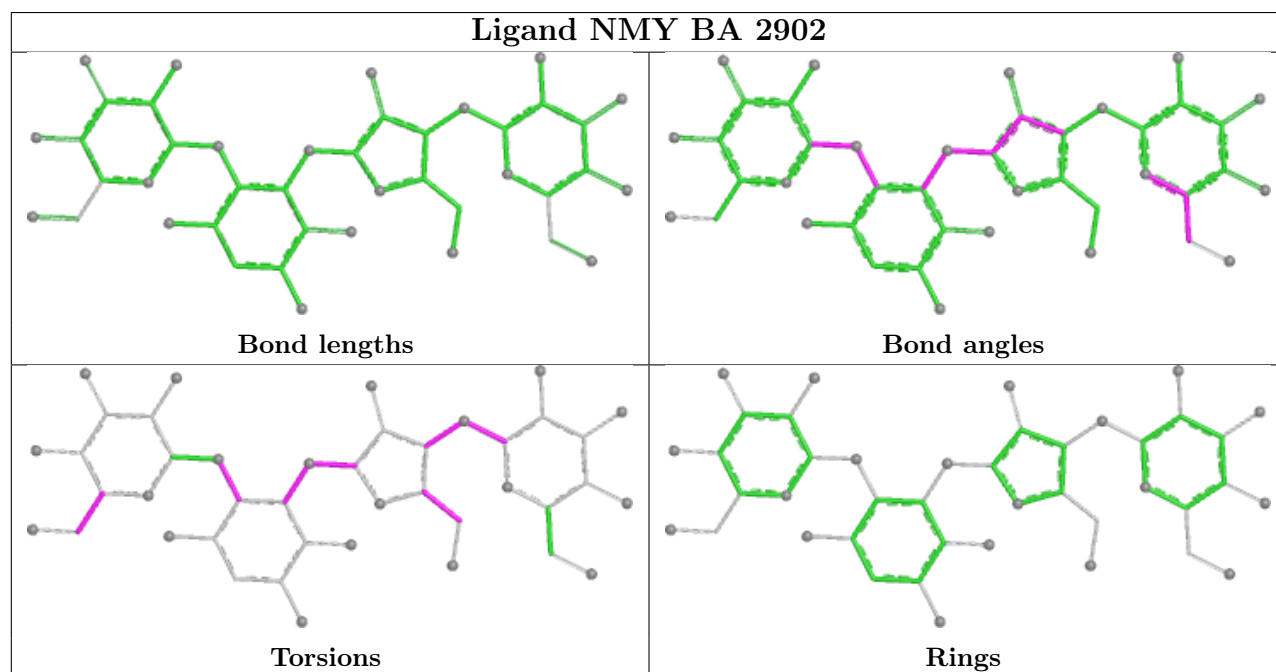
There are no ring outliers.

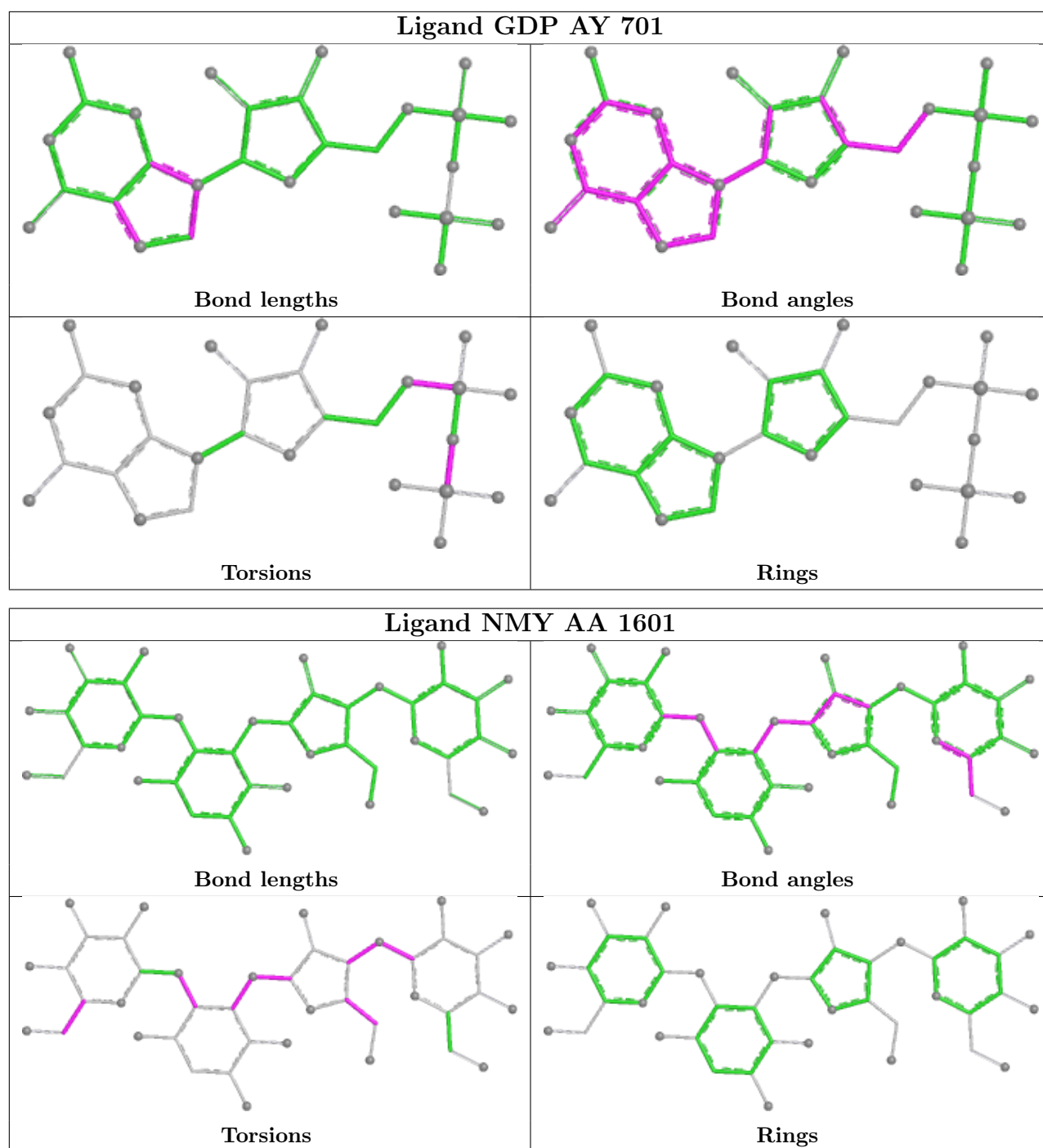
10 monomers are involved in 200 short contacts:

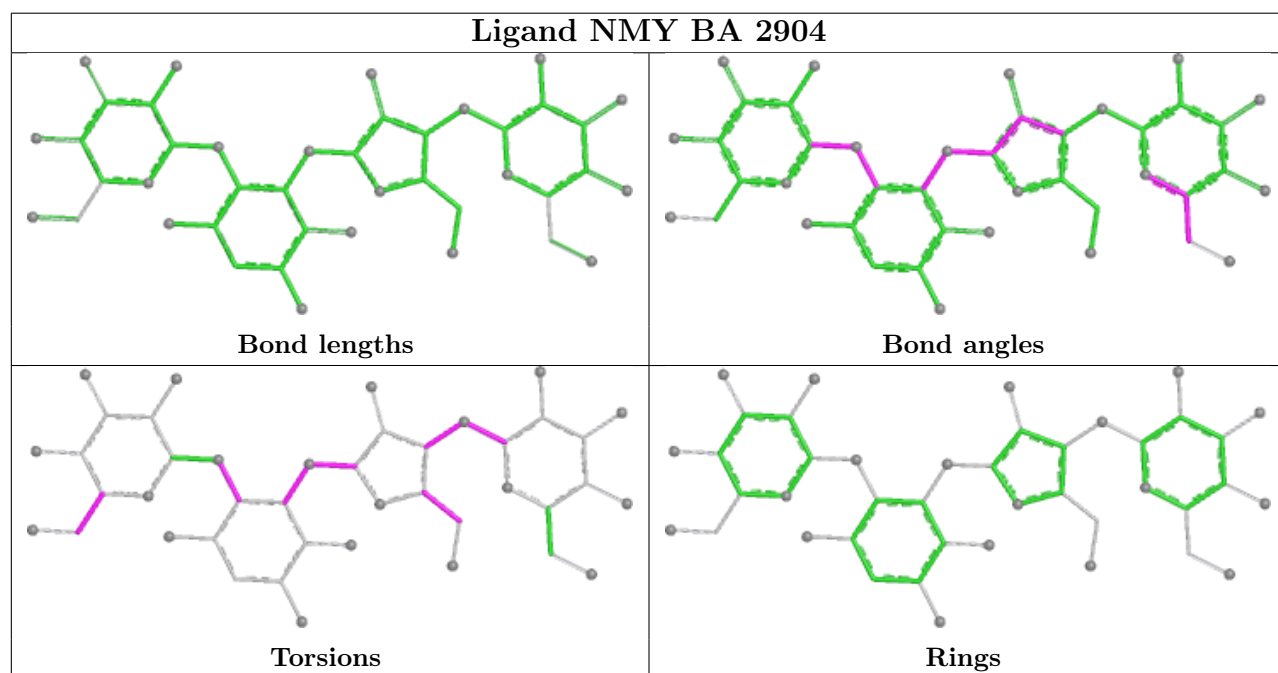
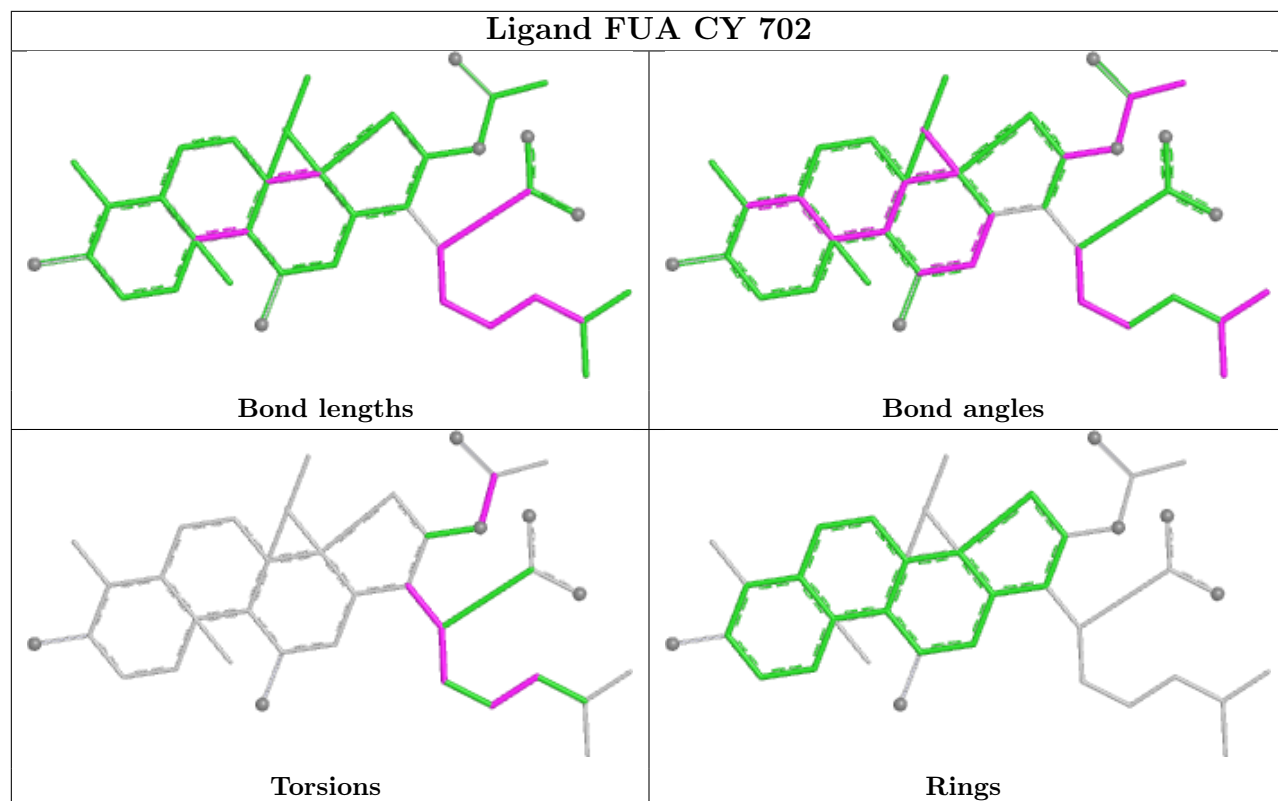
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	BA	2902	NMY	13	0
61	AY	701	GDP	8	0
63	AA	1601	NMY	27	0
62	CY	702	FUA	14	0
63	BA	2904	NMY	32	0
61	CY	701	GDP	14	0
62	AY	702	FUA	21	0
63	BA	2903	NMY	15	0
63	CA	1601	NMY	34	0
63	DA	2901	NMY	23	0

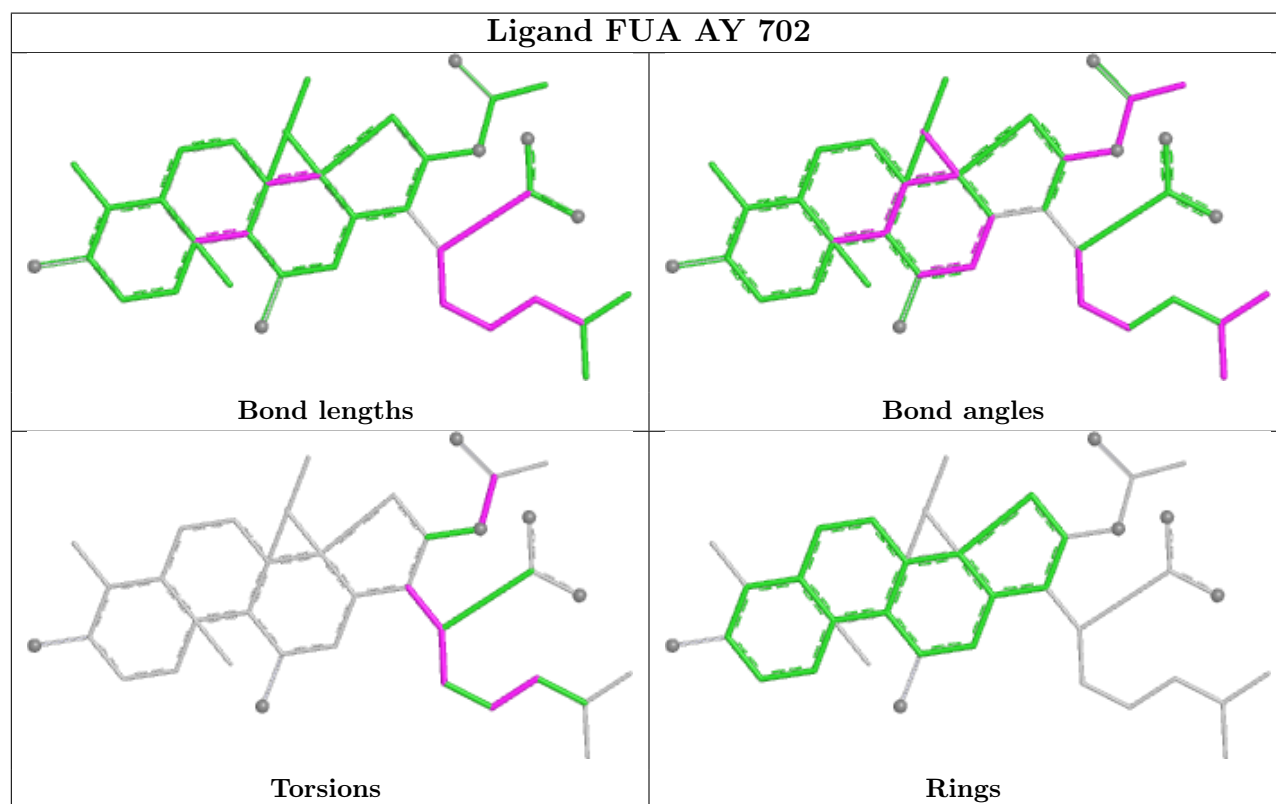
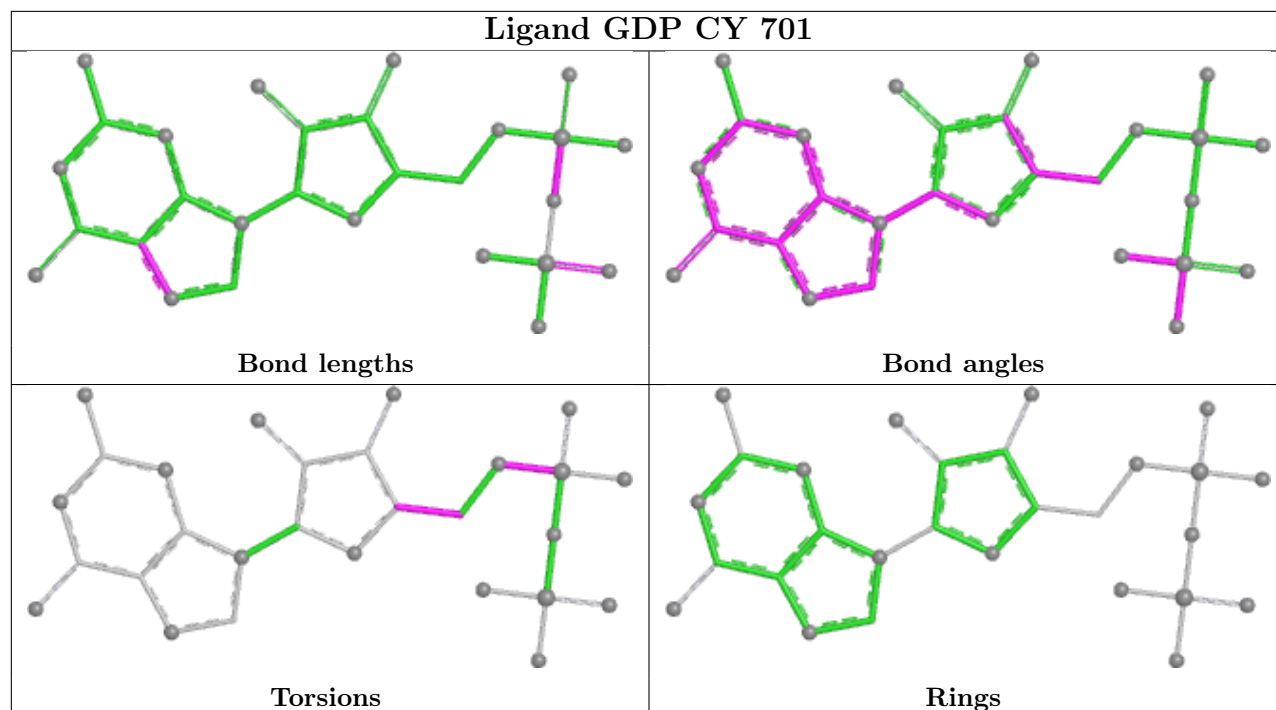
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

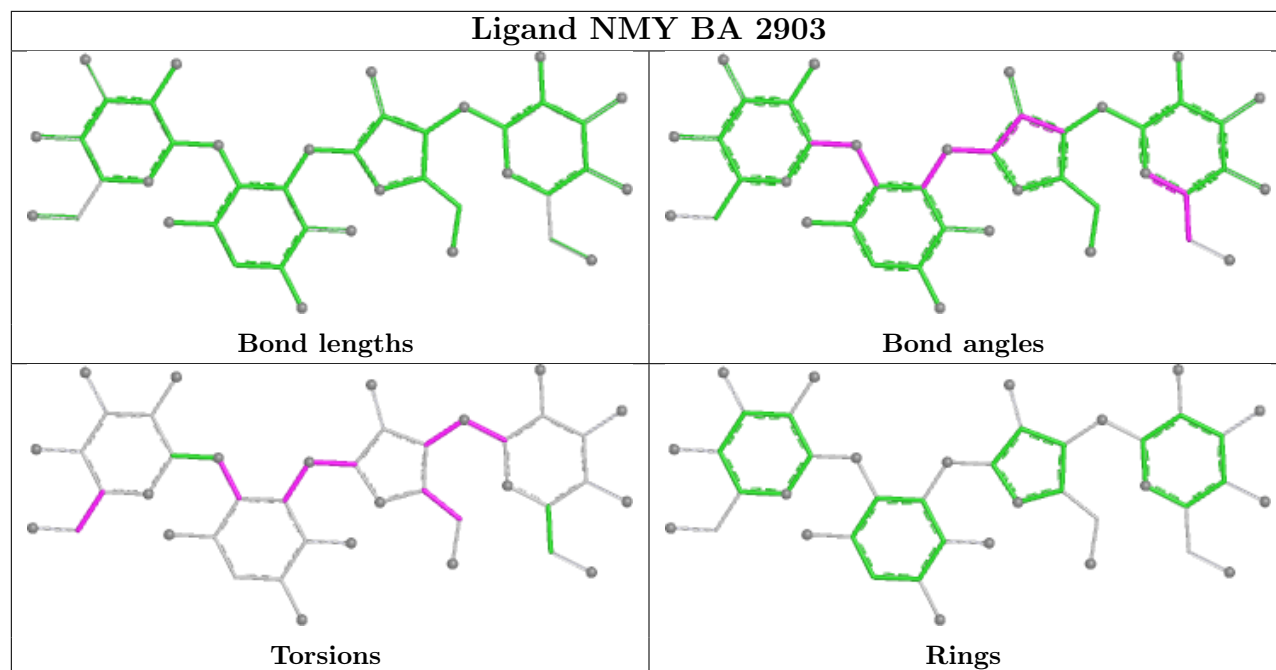




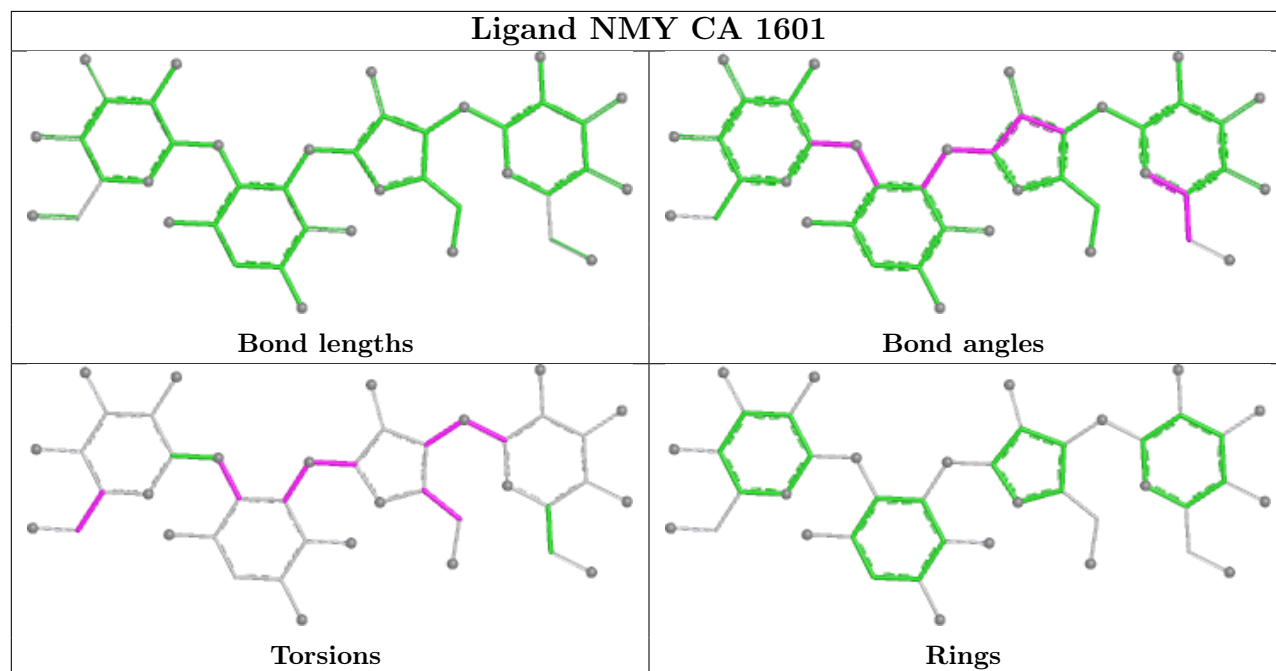


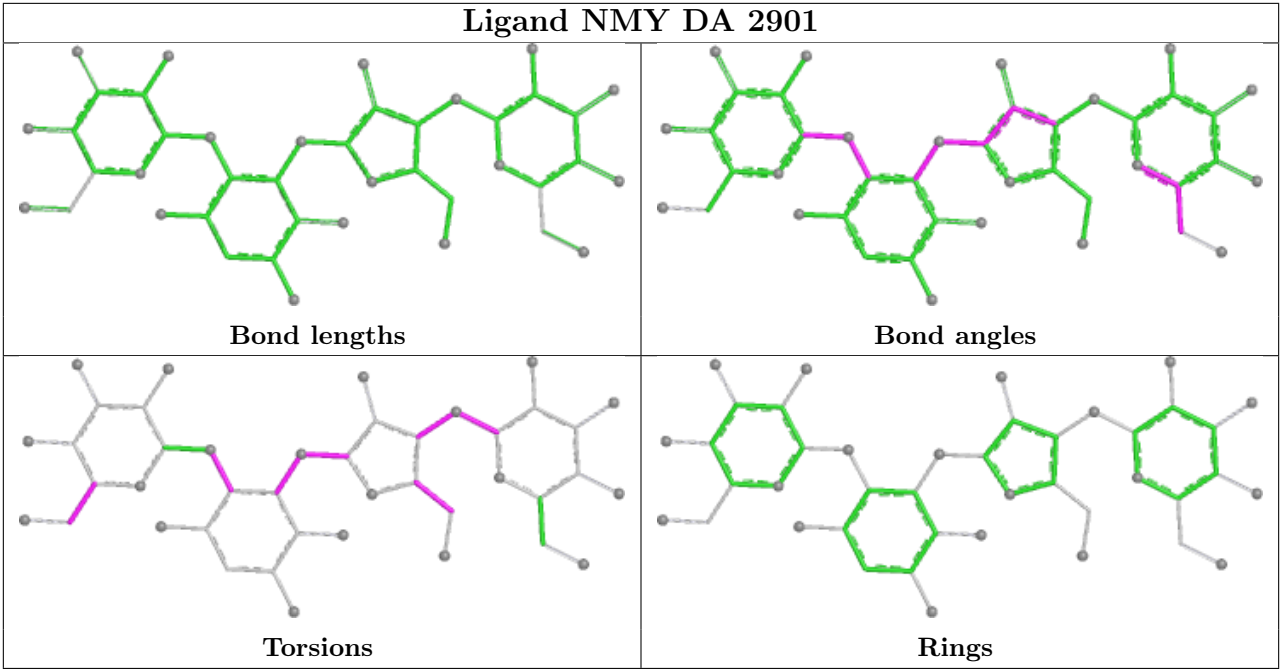


Ligand NMY BA 2903



Ligand NMY CA 1601





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-1.24	1 (0%) 88 74	17, 55, 103, 129	0
1	CB	235/235 (100%)	-1.24	1 (0%) 88 74	17, 63, 111, 140	0
2	AC	207/207 (100%)	-1.22	0 100 100	18, 52, 99, 118	0
2	CC	207/207 (100%)	-1.11	0 100 100	15, 58, 99, 132	0
3	AD	208/208 (100%)	-1.22	1 (0%) 87 71	14, 59, 107, 137	0
3	CD	208/208 (100%)	-1.16	2 (0%) 79 58	20, 52, 102, 136	0
4	AE	151/151 (100%)	-0.81	1 (0%) 84 65	26, 62, 96, 129	0
4	CE	151/151 (100%)	-0.91	0 100 100	19, 56, 99, 143	0
5	AF	101/101 (100%)	-1.35	0 100 100	22, 57, 111, 128	0
5	CF	101/101 (100%)	-1.42	0 100 100	19, 56, 106, 128	0
6	AG	155/155 (100%)	-1.24	1 (0%) 85 68	26, 78, 122, 150	0
6	CG	155/155 (100%)	-1.01	4 (2%) 57 39	38, 85, 120, 147	0
7	AH	138/138 (100%)	-1.28	0 100 100	16, 43, 87, 109	0
7	CH	138/138 (100%)	-1.23	0 100 100	10, 49, 86, 102	0
8	AI	127/127 (100%)	-0.82	10 (7%) 18 17	30, 64, 101, 127	0
8	CI	127/127 (100%)	-0.69	9 (7%) 22 19	9, 77, 108, 134	0
9	AJ	99/99 (100%)	-1.15	1 (1%) 79 58	34, 64, 104, 146	0
9	CJ	99/99 (100%)	-1.19	1 (1%) 79 58	22, 57, 107, 115	0
10	AK	119/119 (100%)	-0.98	2 (1%) 69 47	13, 74, 139, 160	0
10	CK	119/119 (100%)	-1.03	0 100 100	21, 71, 125, 161	0
11	AL	125/125 (100%)	-0.98	0 100 100	15, 73, 145, 164	0
11	CL	125/125 (100%)	-0.85	3 (2%) 59 41	27, 85, 148, 170	0
12	AM	125/125 (100%)	-0.91	2 (1%) 70 48	43, 86, 129, 159	0
12	CM	125/125 (100%)	-1.02	0 100 100	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%)	-1.02	0	100	100	33, 70, 116, 128	0
13	CN	60/60 (100%)	-0.93	0	100	100	30, 58, 105, 128	0
14	AO	88/88 (100%)	-1.35	0	100	100	26, 53, 99, 110	0
14	CO	88/88 (100%)	-1.42	0	100	100	8, 44, 84, 109	0
15	AP	84/84 (100%)	-0.96	2 (2%)	59	41	33, 71, 110, 143	0
15	CP	84/84 (100%)	-0.62	6 (7%)	22	19	39, 69, 111, 165	0
16	AQ	100/100 (100%)	-0.89	2 (2%)	65	44	27, 62, 107, 131	0
16	CQ	100/100 (100%)	-0.97	2 (2%)	65	44	22, 66, 120, 135	0
17	AR	70/70 (100%)	-1.21	0	100	100	19, 61, 102, 130	0
17	CR	70/70 (100%)	-1.20	0	100	100	24, 56, 100, 125	0
18	AS	79/79 (100%)	-1.24	0	100	100	17, 69, 111, 124	0
18	CS	79/79 (100%)	-1.18	0	100	100	28, 65, 108, 130	0
19	AT	99/99 (100%)	-0.95	0	100	100	17, 51, 85, 128	0
19	CT	99/99 (100%)	-0.71	4 (4%)	42	30	26, 69, 110, 139	0
20	AY	661/687 (96%)	-1.05	13 (1%)	65	44	19, 64, 113, 178	0
20	CY	661/687 (96%)	-1.09	4 (0%)	85	68	11, 66, 108, 152	0
21	AA	1511/1511 (100%)	-1.22	32 (2%)	63	44	10, 90, 161, 248	0
21	CA	1511/1511 (100%)	-1.25	40 (2%)	57	39	10, 88, 160, 242	0
22	AW	77/77 (100%)	-1.52	0	100	100	15, 71, 130, 150	0
22	CW	77/77 (100%)	-1.64	0	100	100	30, 88, 145, 178	0
23	AV	36/36 (100%)	-0.94	0	100	100	32, 89, 137, 186	0
23	CV	36/36 (100%)	-0.36	2 (5%)	30	23	23, 139, 232, 237	0
24	AX	77/78 (98%)	-1.37	0	100	100	3, 65, 233, 320	0
24	CX	77/78 (98%)	-1.10	1 (1%)	75	53	37, 123, 185, 285	0
25	BC	228/228 (100%)	-1.00	1 (0%)	88	74	54, 104, 139, 159	0
25	DC	228/228 (100%)	-1.07	0	100	100	37, 90, 130, 169	0
26	BD	275/275 (100%)	-0.80	1 (0%)	88	74	10, 61, 103, 125	0
26	DD	275/275 (100%)	-0.93	1 (0%)	88	74	16, 57, 100, 127	0
27	BE	205/205 (100%)	-1.09	0	100	100	21, 60, 107, 131	0
27	DE	205/205 (100%)	-1.11	0	100	100	22, 57, 97, 142	0
28	BF	208/208 (100%)	-1.03	2 (0%)	79	58	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%)	-1.03	2 (0%) 79 58	23, 75, 120, 140	0
29	BG	181/181 (100%)	-1.46	1 (0%) 85 68	28, 69, 113, 148	0
29	DG	181/181 (100%)	-1.50	0 100 100	25, 71, 113, 148	0
30	BH	167/167 (100%)	-1.26	2 (1%) 76 54	29, 65, 108, 121	0
30	DH	167/167 (100%)	-1.39	0 100 100	24, 59, 100, 132	0
31	BJ	0/170	-	-	-	-
31	DJ	0/170	-	-	-	-
32	BK	140/140 (100%)	-1.28	0 100 100	32, 71, 114, 126	0
32	DK	140/140 (100%)	-1.14	1 (0%) 84 65	34, 77, 113, 138	0
33	BN	139/139 (100%)	-0.70	2 (1%) 73 51	23, 105, 298, 334	0
33	DN	139/139 (100%)	-0.69	4 (2%) 53 37	16, 116, 252, 312	0
34	BO	122/122 (100%)	-0.51	1 (0%) 82 62	12, 50, 93, 111	0
34	DO	122/122 (100%)	-0.60	3 (2%) 58 40	28, 59, 103, 132	0
35	BP	146/146 (100%)	-0.78	5 (3%) 48 33	25, 63, 106, 123	0
35	DP	146/146 (100%)	-0.67	4 (2%) 56 38	25, 67, 104, 131	0
36	BQ	141/141 (100%)	-1.06	0 100 100	5, 54, 93, 109	0
36	DQ	141/141 (100%)	-0.83	3 (2%) 63 44	27, 70, 113, 141	0
37	BR	117/117 (100%)	-0.97	0 100 100	29, 65, 116, 145	0
37	DR	117/117 (100%)	-1.05	0 100 100	27, 62, 97, 126	0
38	BS	99/99 (100%)	-1.38	0 100 100	14, 70, 108, 117	0
38	DS	99/99 (100%)	-1.25	0 100 100	19, 52, 96, 120	0
39	BT	138/138 (100%)	-0.90	3 (2%) 62 44	16, 59, 101, 123	0
39	DT	138/138 (100%)	-0.88	6 (4%) 40 28	15, 51, 109, 140	0
40	BU	117/117 (100%)	-1.17	0 100 100	20, 56, 96, 121	0
40	DU	117/117 (100%)	-1.21	0 100 100	13, 53, 94, 142	0
41	BV	101/101 (100%)	-1.19	0 100 100	21, 66, 108, 127	0
41	DV	101/101 (100%)	-1.23	0 100 100	15, 65, 101, 126	0
42	BW	113/113 (100%)	-0.93	5 (4%) 39 28	13, 54, 99, 111	0
42	DW	113/113 (100%)	-0.97	4 (3%) 47 33	15, 64, 116, 148	0
43	BX	93/93 (100%)	-1.09	1 (1%) 78 56	20, 54, 96, 115	0
43	DX	93/93 (100%)	-1.02	1 (1%) 78 56	13, 45, 87, 126	0
44	BY	107/107 (100%)	-0.91	2 (1%) 66 45	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%)	-1.17	0	100	100	25, 62, 97, 138	0
45	BZ	185/185 (100%)	-1.39	0	100	100	17, 58, 97, 113	0
45	DZ	185/185 (100%)	-1.36	0	100	100	33, 64, 101, 138	0
46	B0	84/84 (100%)	-0.63	0	100	100	26, 75, 117, 131	0
46	D0	84/84 (100%)	-0.86	0	100	100	19, 65, 108, 116	0
47	B1	93/93 (100%)	-0.77	0	100	100	21, 84, 140, 156	0
47	D1	93/93 (100%)	-0.71	3 (3%)	50	35	31, 103, 148, 181	0
48	B2	71/71 (100%)	-1.54	0	100	100	23, 55, 95, 116	0
48	D2	71/71 (100%)	-1.46	0	100	100	35, 61, 103, 118	0
49	B3	60/60 (100%)	-1.28	0	100	100	29, 60, 99, 112	0
49	D3	60/60 (100%)	-0.92	2 (3%)	49	34	36, 68, 94, 110	0
50	B4	35/35 (100%)	-1.37	0	100	100	26, 71, 110, 122	0
50	D4	35/35 (100%)	-1.46	0	100	100	64, 109, 144, 185	0
51	B5	59/59 (100%)	-0.73	1 (1%)	69	47	24, 63, 106, 123	0
51	D5	59/59 (100%)	-0.48	4 (6%)	23	20	31, 68, 113, 138	0
52	B6	50/50 (100%)	-1.01	0	100	100	13, 57, 107, 154	0
52	D6	50/50 (100%)	-1.01	0	100	100	26, 65, 120, 154	0
53	B7	49/49 (100%)	-0.87	0	100	100	46, 91, 136, 164	0
53	D7	49/49 (100%)	-0.95	0	100	100	51, 73, 109, 134	0
54	B8	64/64 (100%)	-0.74	1 (1%)	70	48	26, 58, 109, 132	0
54	D8	64/64 (100%)	-0.66	0	100	100	30, 64, 104, 118	0
55	B9	37/37 (100%)	-0.76	2 (5%)	31	24	39, 64, 109, 116	0
55	D9	37/37 (100%)	-0.56	1 (2%)	56	38	34, 65, 116, 134	0
56	Be	72/103 (69%)	-1.37	0	100	100	15, 49, 122, 163	0
56	De	72/103 (69%)	-1.34	0	100	100	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%)	-1.24	64 (2%)	62	44	11, 89, 164, 284	0
59	DA	2879/2879 (100%)	-1.26	38 (1%)	75	53	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%)	-1.63	0	100	100	18, 80, 158, 172	0
60	DB	119/119 (100%)	-1.59	0	100	100	30, 88, 150, 175	0
All	All	22852/23492 (97%)	-1.14	318 (1%)	73	51	3, 73, 146, 334	0

The worst 5 of 318 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
59	BA	34	C	10.6
59	BA	180	G	9.2
21	AA	388	G	9.0
21	AA	1529	G	7.5
59	BA	47	C	7.3

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 oligosaccharides 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
63	NMY	BA	2902	42/42	0.96	0.07	14,24,43,44	42
63	NMY	BA	2904	42/42	0.97	0.04	42,50,59,62	42
63	NMY	DA	2901	42/42	0.97	0.10	31,42,51,53	42
61	GDP	AY	701	28/28	0.98	0.04	179,183,185,185	0
63	NMY	BA	2903	42/42	0.98	0.05	18,29,38,41	42
62	FUA	AY	702	37/37	0.98	0.06	198,199,200,201	0
62	FUA	CY	702	37/37	0.98	0.07	194,196,197,197	0
61	GDP	CY	701	28/28	0.99	0.02	104,108,109,110	0
63	NMY	CA	1601	42/42	0.99	0.04	14,25,34,37	42
63	NMY	AA	1601	42/42	0.99	0.04	16,27,36,38	42

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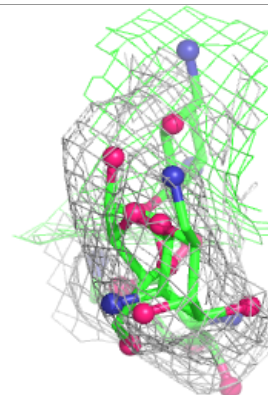
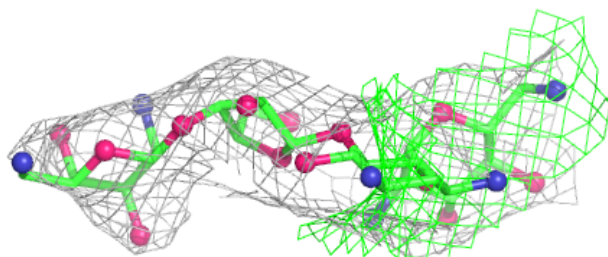
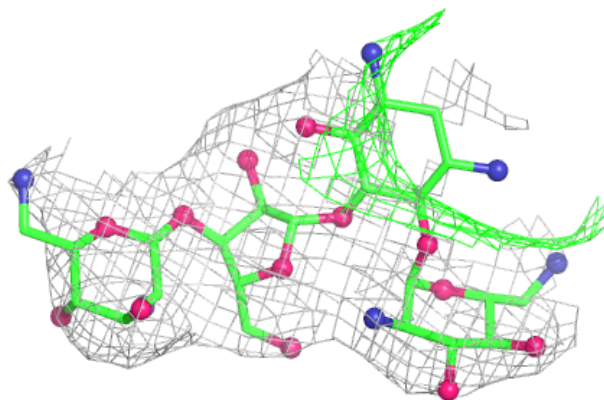
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
64	MG	CY	703	1/1	0.99	0.06	6,6,6,6	0
64	MG	BA	2901	1/1	1.00	0.07	2,2,2,2	0

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.

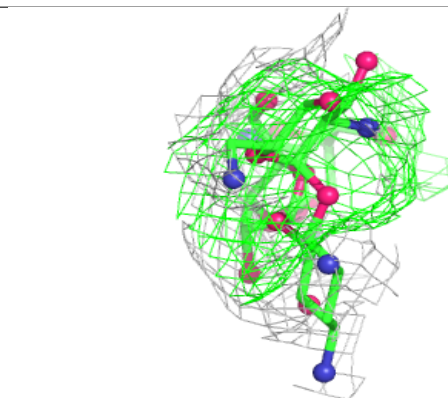
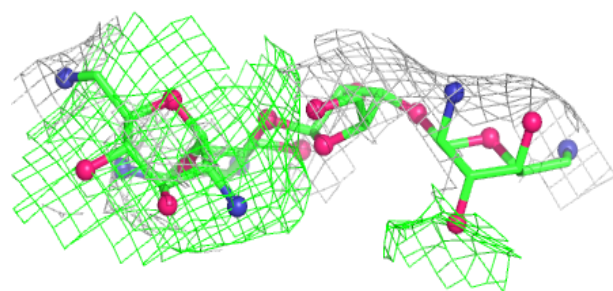
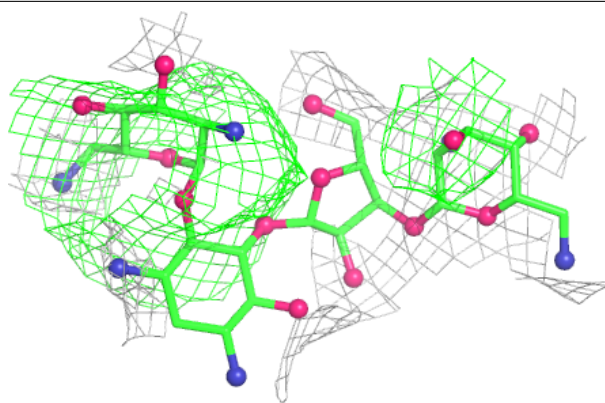
Electron density around NMY BA 2902:

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

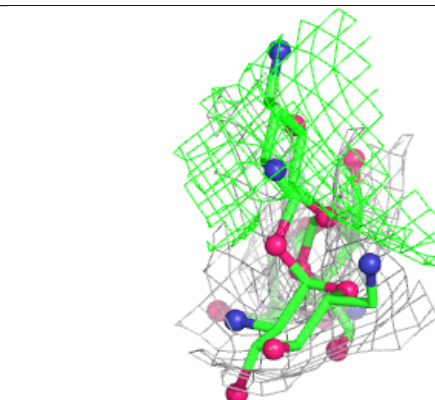
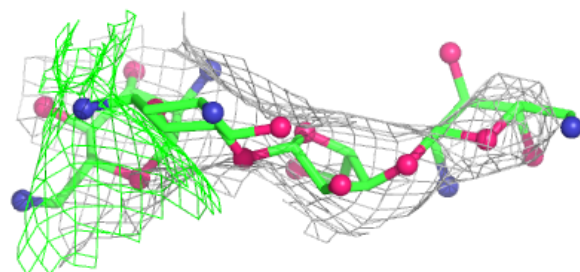
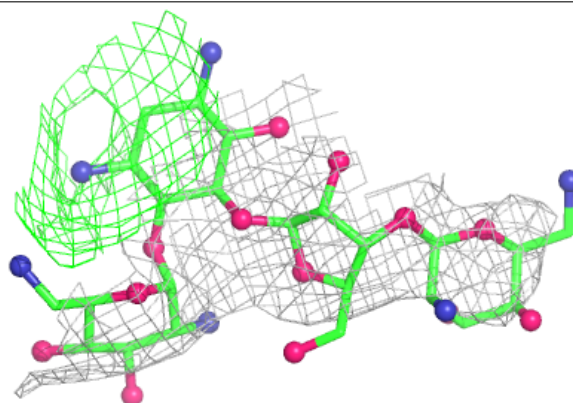


Electron density around NMY BA 2904:

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

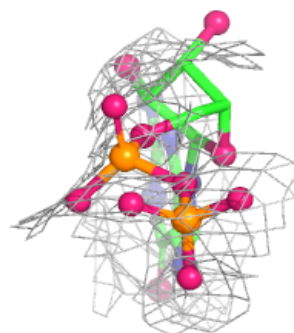
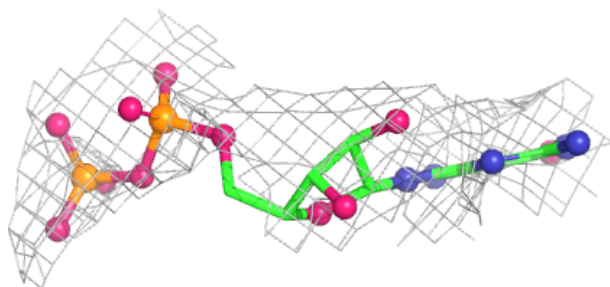
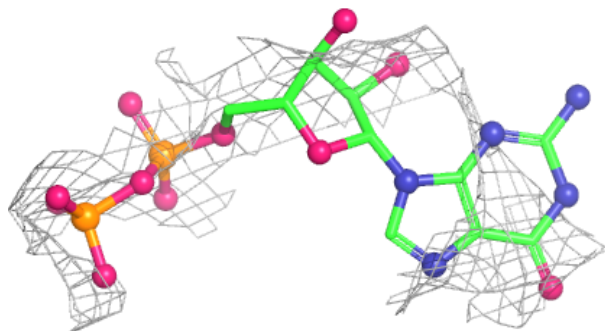
**Electron density around NMY DA 2901:**

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

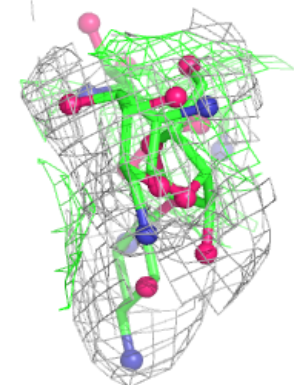
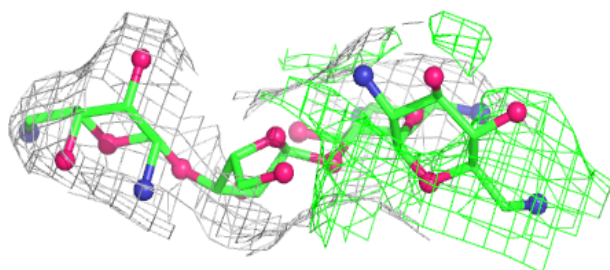
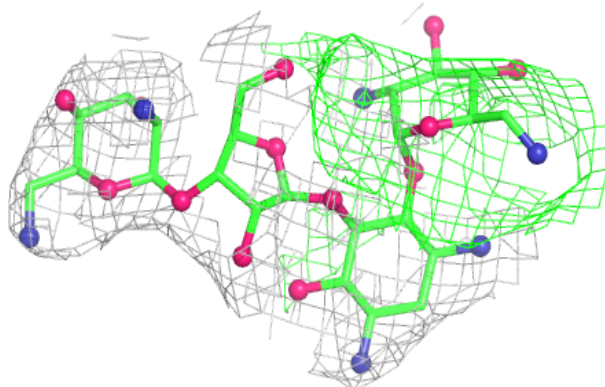


Electron density around GDP AY 701:

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

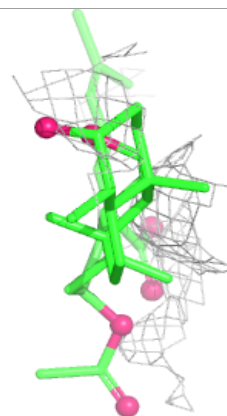
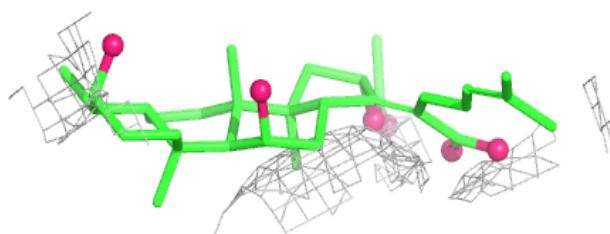
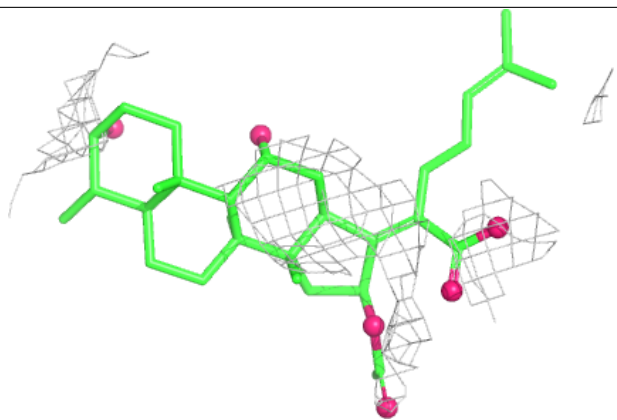
**Electron density around NMY BA 2903:**

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



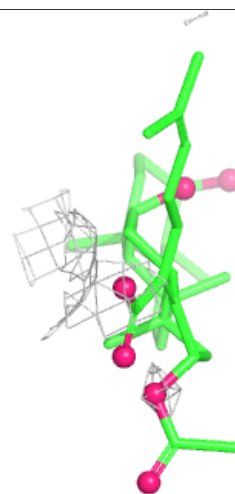
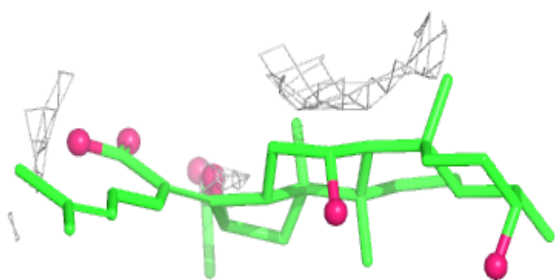
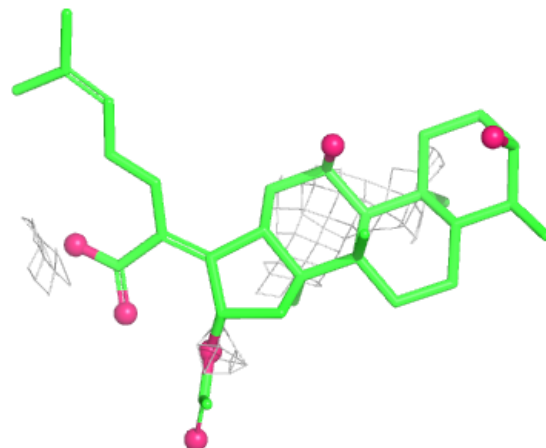
Electron density around FUA AY 702:

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



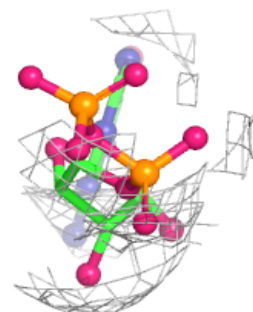
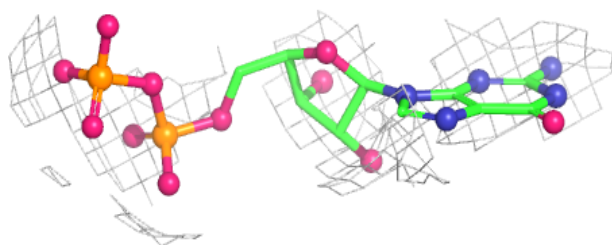
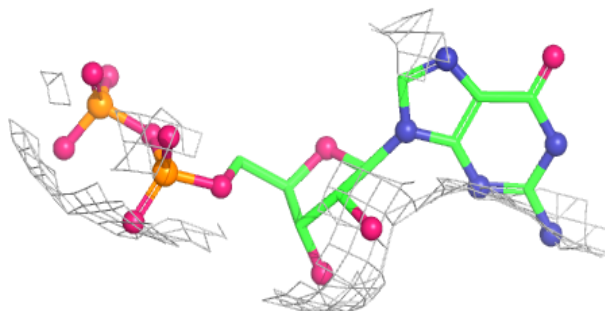
Electron density around FUA CY 702:

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

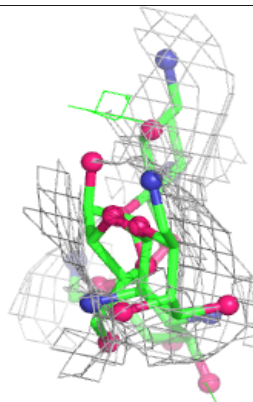
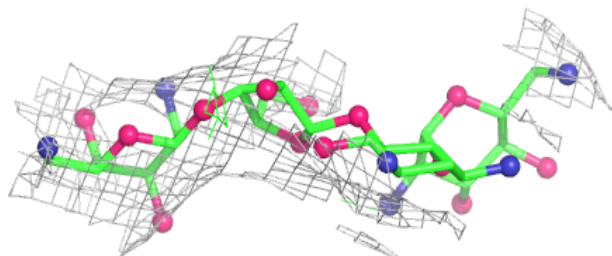
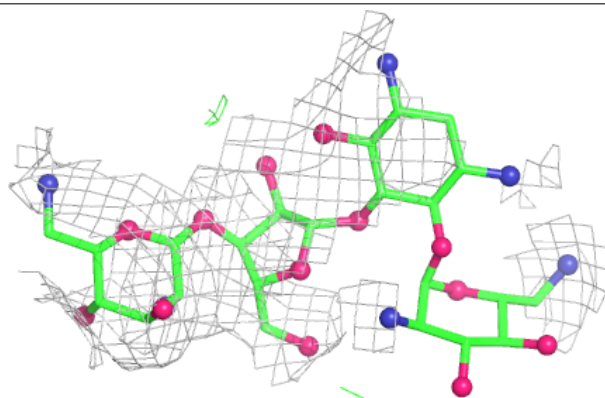


Electron density around GDP CY 701:

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

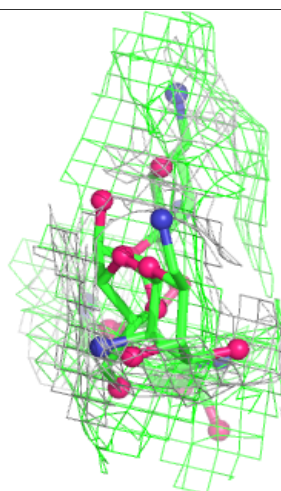
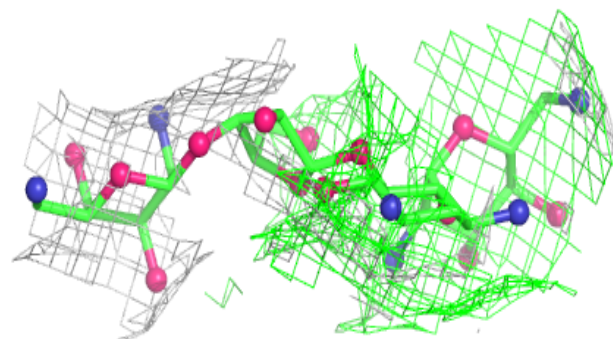
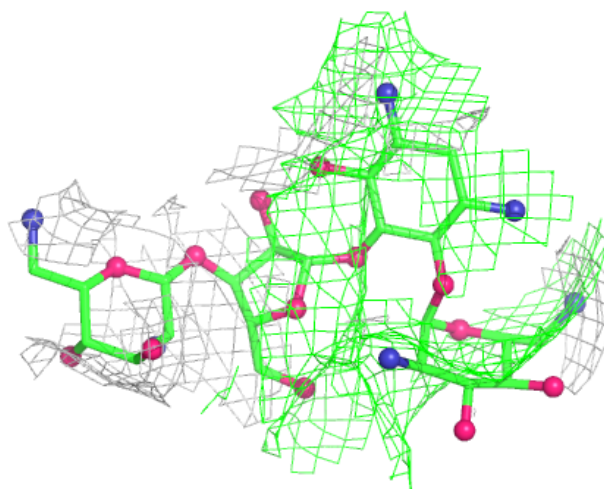
**Electron density around NMY CA 1601:**

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.