



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 19, 2020 – 04:57 AM BST

PDB ID : 4W29  
Title : 70S ribosome translocation intermediate containing elongation factor EFG/GDP/fusidic acid, mRNA, and tRNAs trapped in the AP/AP<sup>pe</sup>/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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

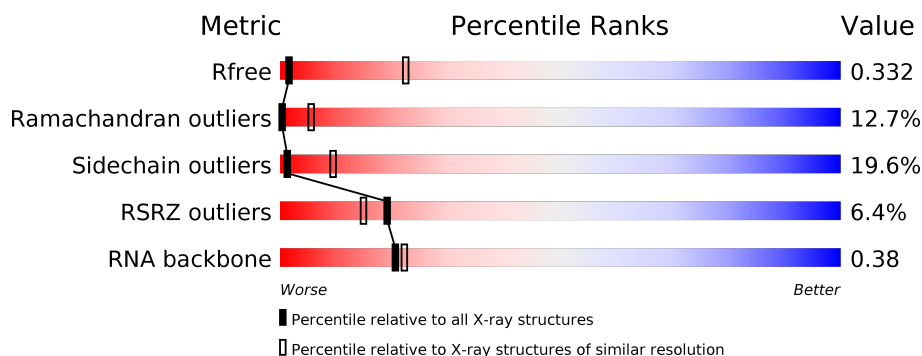
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1212 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	<div> <div>2%</div> <div>76%</div> <div>22%</div> <div>.</div> </div>
1	CB	235	<div> <div>%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
2	AC	207	<div> <div>43%</div> <div>72%</div> <div>27%</div> <div>.</div> </div>
2	CC	207	<div> <div>39%</div> <div>75%</div> <div>24%</div> <div>.</div> </div>
3	AD	208	<div> <div>%</div> <div>71%</div> <div>27%</div> <div>.</div> </div>
3	CD	208	<div> <div>75%</div> <div>24%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
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	
15	AP	84	
15	CP	84	
16	AQ	100	

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Mol	Chain	Length	Quality of chain
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	
27	DE	205	
28	BF	208	
28	DF	208	

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Mol	Chain	Length	Quality of chain
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	
40	BU	117	
40	DU	117	
41	BV	101	

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Mol	Chain	Length	Quality of chain
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	
52	D6	50	
53	B7	49	
53	D7	49	

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Mol	Chain	Length	Quality of chain
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	

## 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			

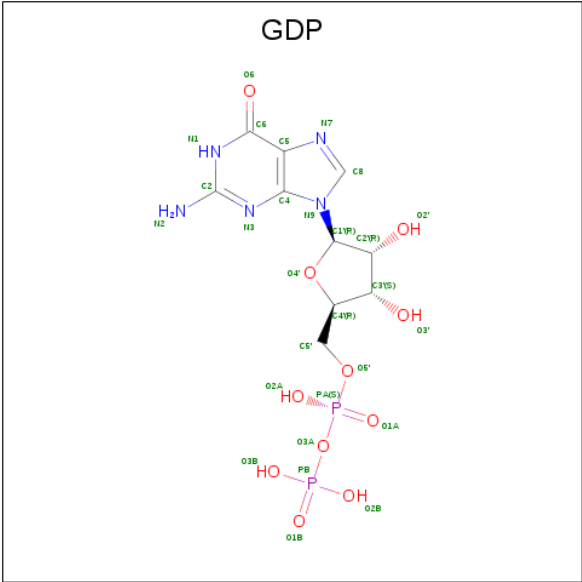
There are 4 discrepancies between the modelled and reference sequences:

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.

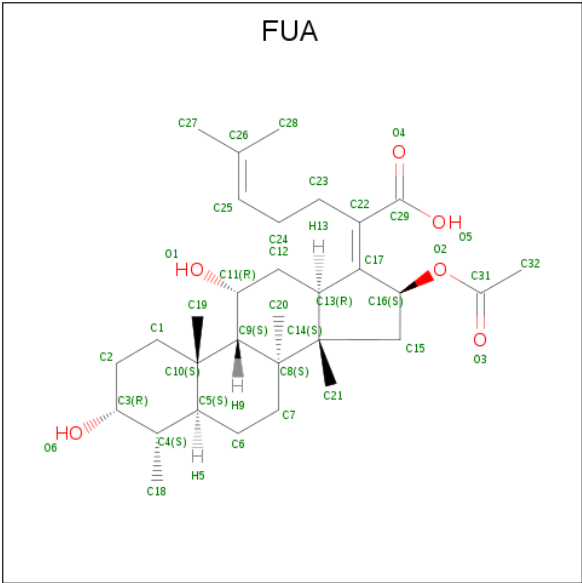
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
60	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).

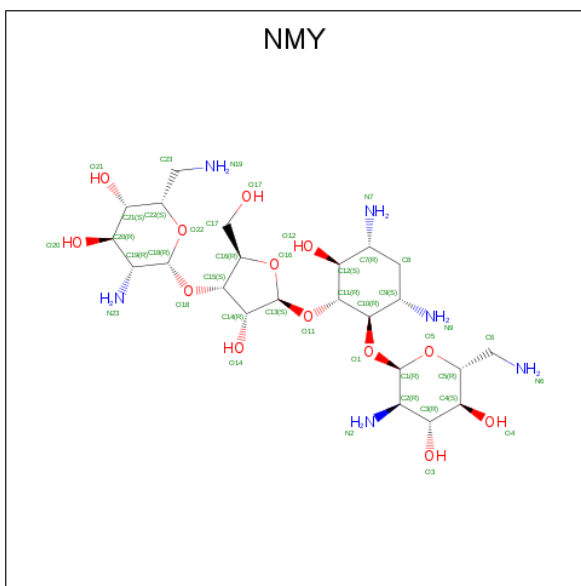


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
61	AY	1	Total 28	C 10	N 5	O 11	P 2	0	0
61	CY	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 62 is FUSIDIC ACID (three-letter code: FUA) (formula: C<sub>31</sub>H<sub>48</sub>O<sub>6</sub>).



- Molecule 63 is NEOMYCIN (three-letter code: NMY) (formula:  $\text{C}_{23}\text{H}_{46}\text{N}_6\text{O}_{13}$ ).



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

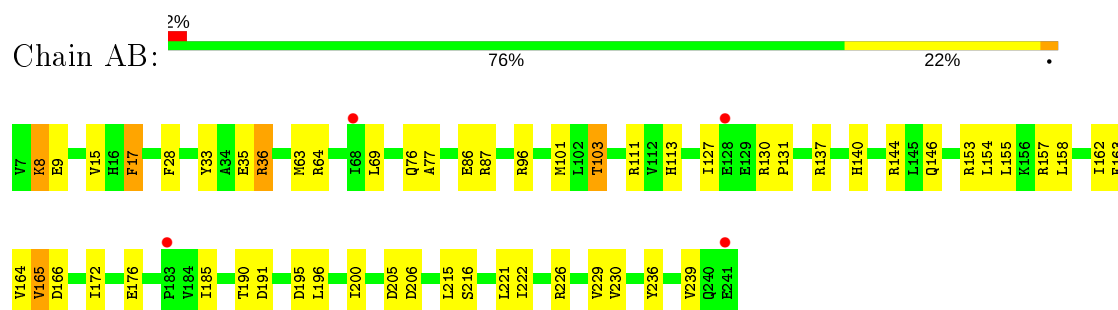
- Molecule 64 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

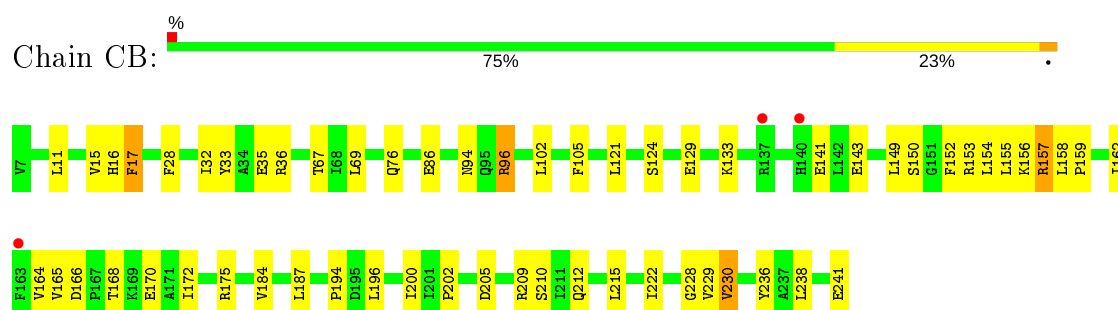
### 3 Residue-property plots [i](#)

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

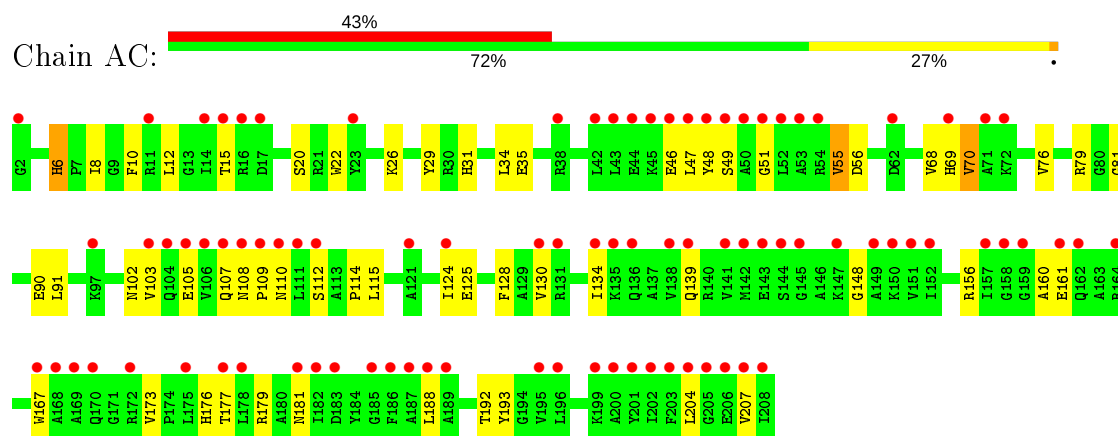
- Molecule 1: 30S ribosomal protein S2



- Molecule 1: 30S ribosomal protein S2

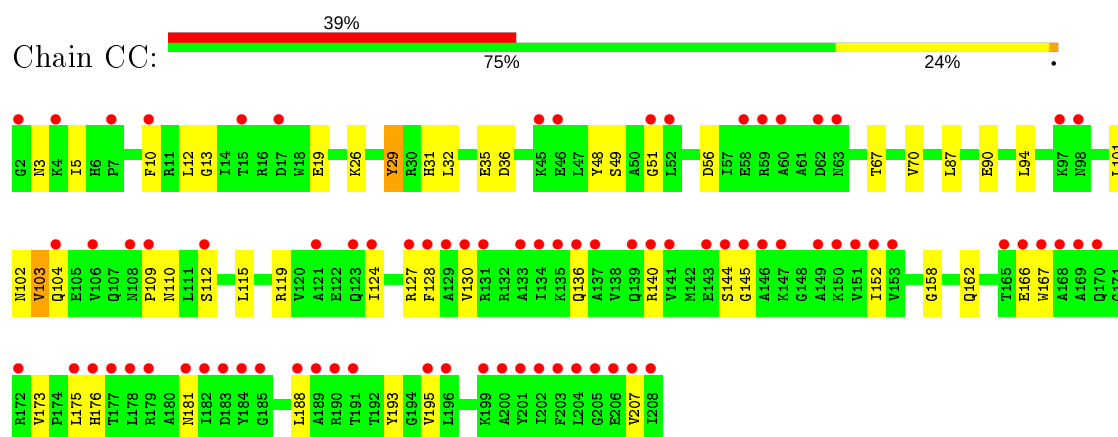


- Molecule 2: 30S ribosomal protein S3

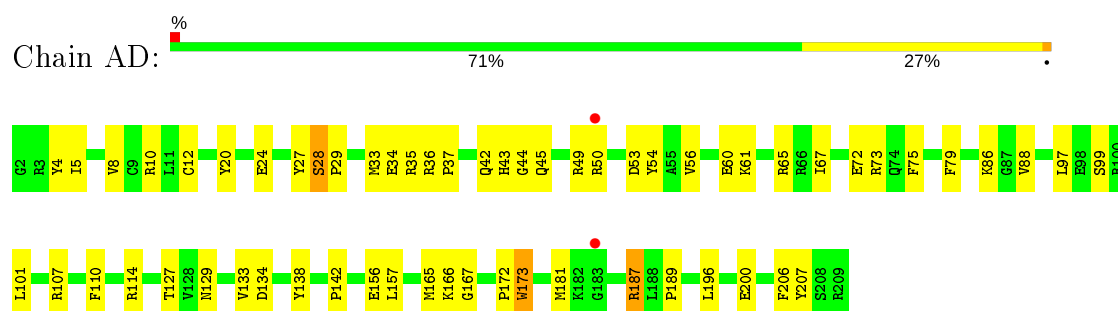


- Molecule 2: 30S ribosomal protein S3

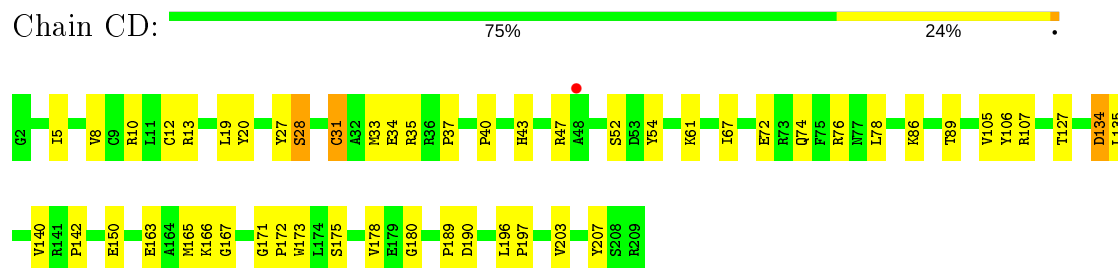




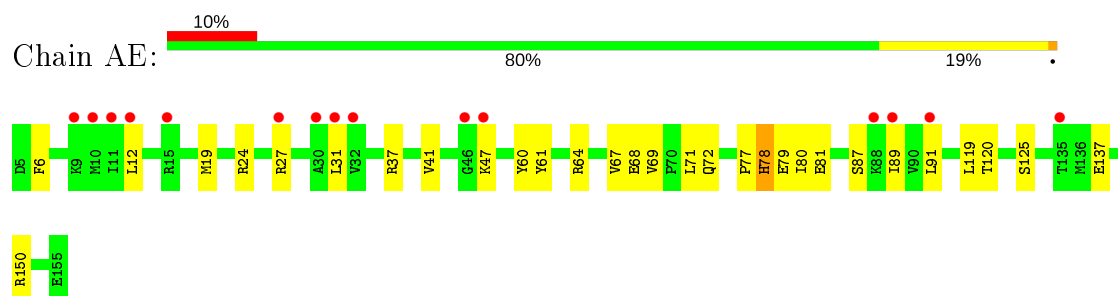
- Molecule 3: 30S ribosomal protein S4



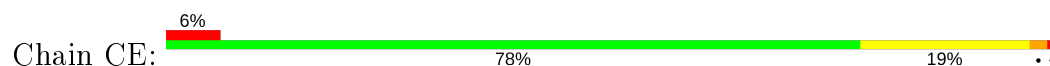
- Molecule 3: 30S ribosomal protein S4

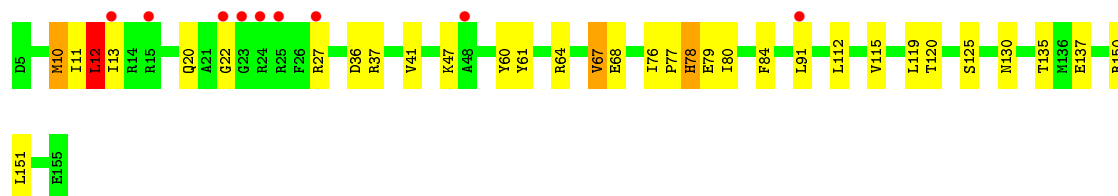


- Molecule 4: 30S ribosomal protein S5



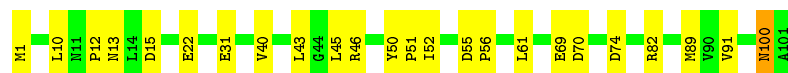
- Molecule 4: 30S ribosomal protein S5





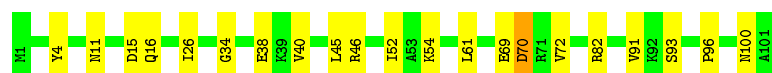
- Molecule 5: 30S ribosomal protein S6

Chain AF: 76% 23%



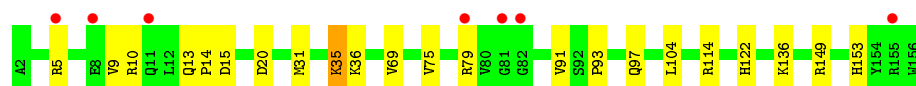
- Molecule 5: 30S ribosomal protein S6

Chain CF: 79% 20%



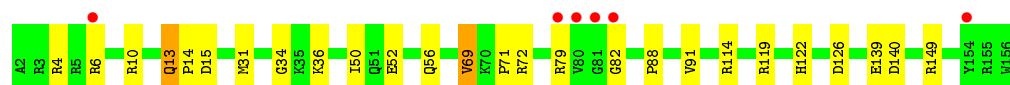
- Molecule 6: 30S ribosomal protein S7

Chain AG: 5% 86% 14%



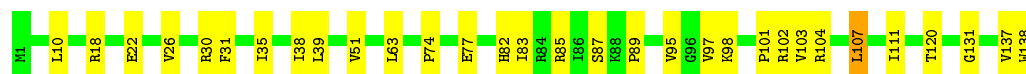
- Molecule 6: 30S ribosomal protein S7

Chain CG: 4% 83% 15%



- Molecule 7: 30S ribosomal protein S8

Chain AH: 78% 22%

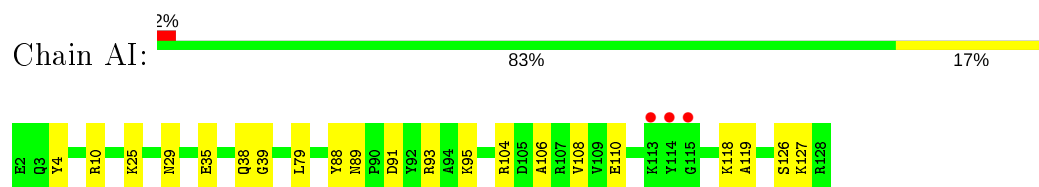


- Molecule 7: 30S ribosomal protein S8

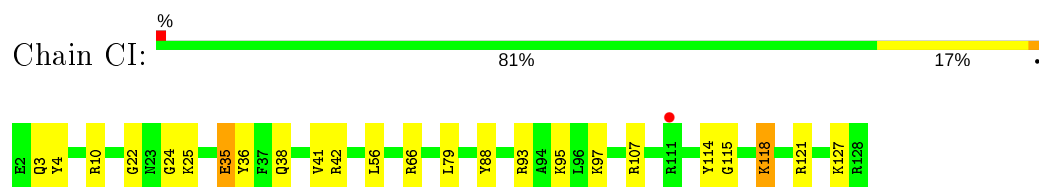
Chain CH: 76% 22%



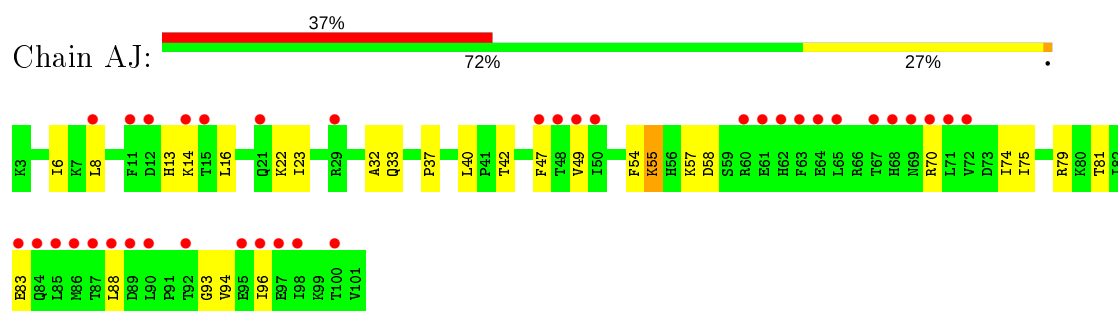
- Molecule 8: 30S ribosomal protein S9



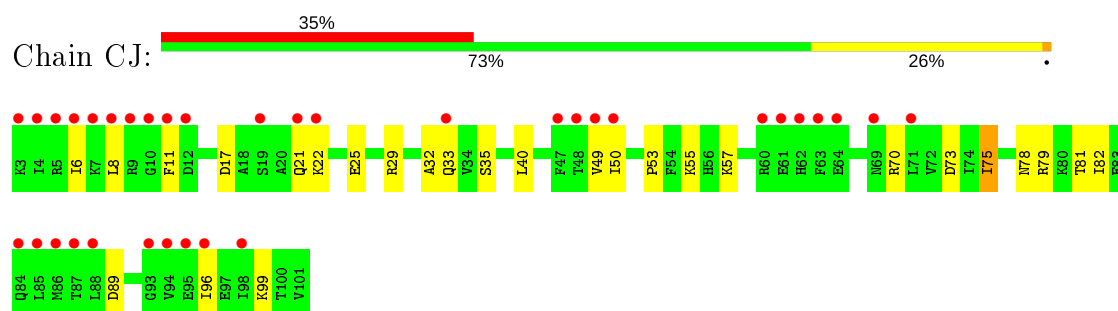
- Molecule 8: 30S ribosomal protein S9



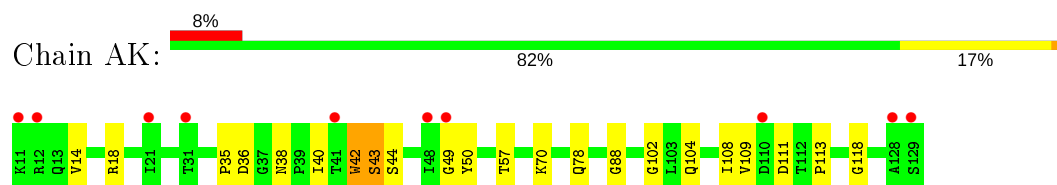
- Molecule 9: 30S ribosomal protein S10



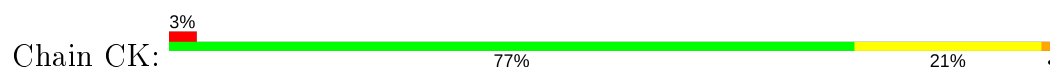
- Molecule 9: 30S ribosomal protein S10



- Molecule 10: 30S ribosomal protein S11



- Molecule 10: 30S ribosomal protein S11

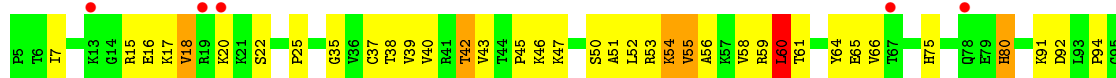




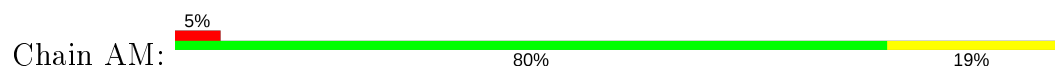
- Molecule 11: 30S ribosomal protein S12



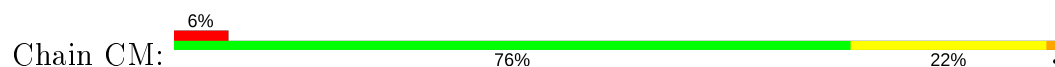
- Molecule 11: 30S ribosomal protein S12



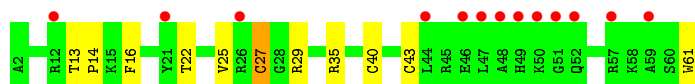
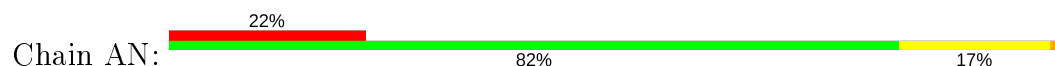
- Molecule 12: 30S ribosomal protein S13



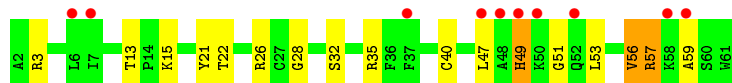
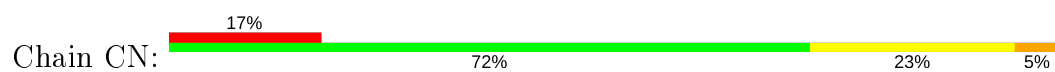
- Molecule 12: 30S ribosomal protein S13



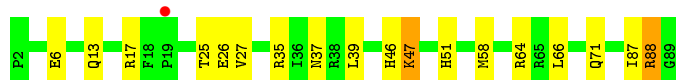
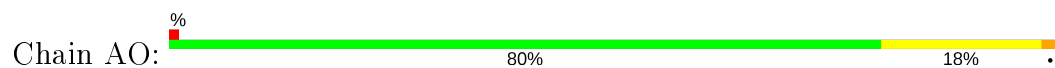
- Molecule 13: 30S ribosomal protein S14 type Z



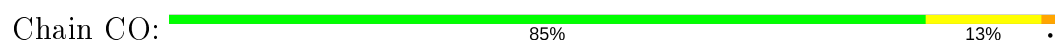
- Molecule 13: 30S ribosomal protein S14 type Z



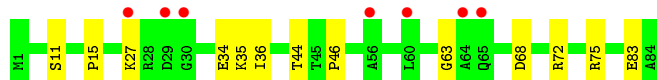
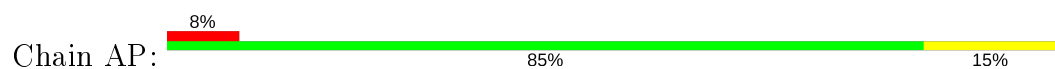
- Molecule 14: 30S ribosomal protein S15



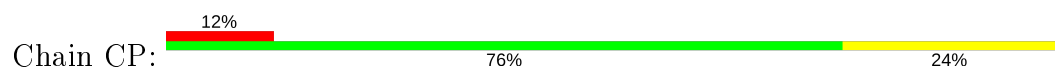
- Molecule 14: 30S ribosomal protein S15



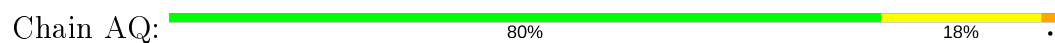
- Molecule 15: 30S ribosomal protein S16



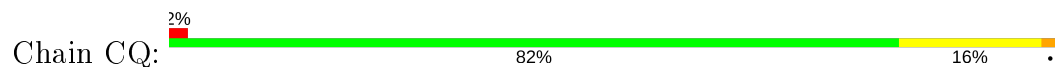
- Molecule 15: 30S ribosomal protein S16



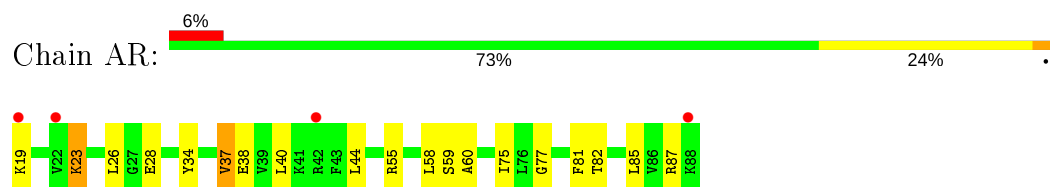
- Molecule 16: 30S ribosomal protein S17



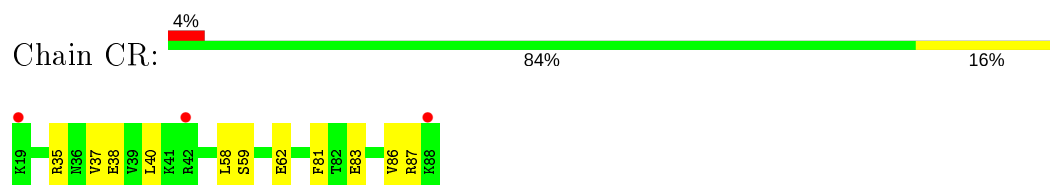
- Molecule 16: 30S ribosomal protein S17



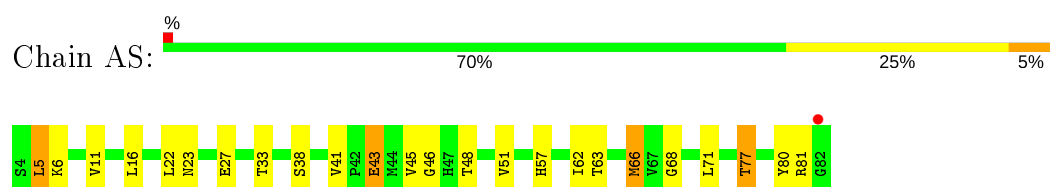
## • Molecule 17: 30S ribosomal protein S18



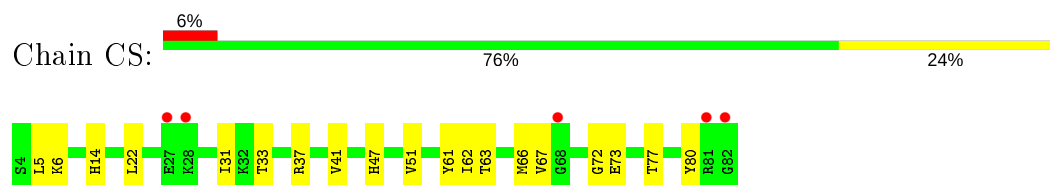
## • Molecule 17: 30S ribosomal protein S18



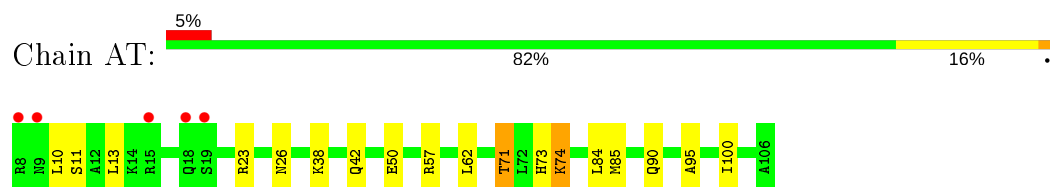
## • Molecule 18: 30S ribosomal protein S19



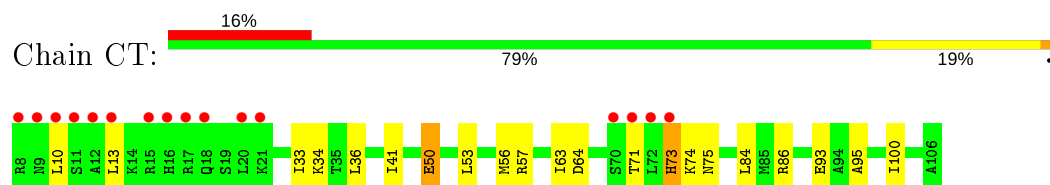
## • Molecule 18: 30S ribosomal protein S19



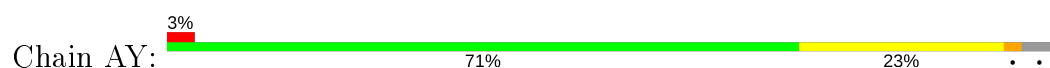
## • Molecule 19: 30S ribosomal protein S20

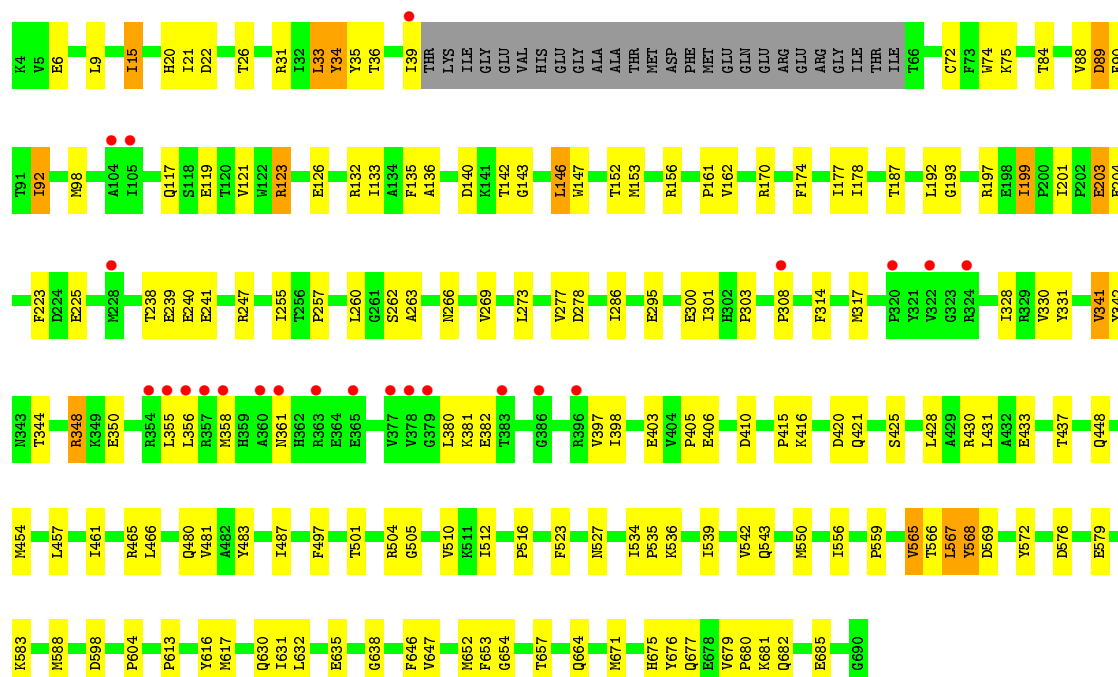


## • Molecule 19: 30S ribosomal protein S20

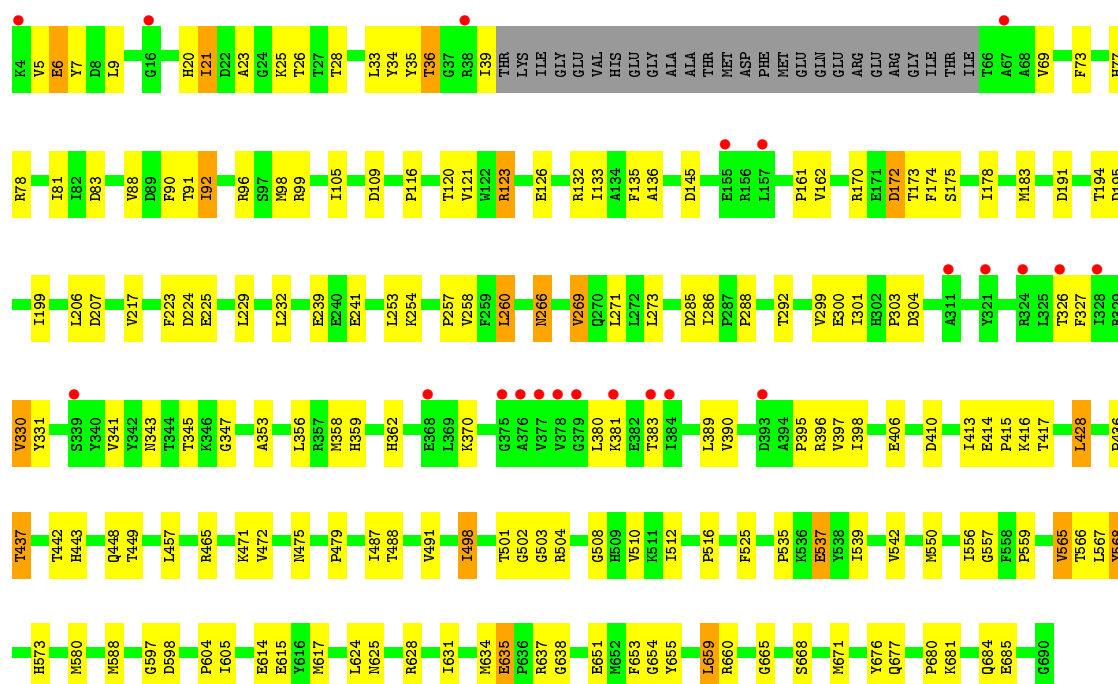
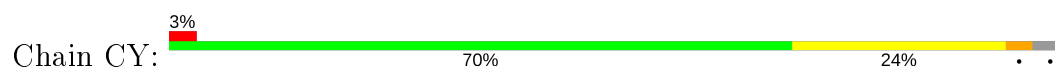


## • Molecule 20: Elongation factor G

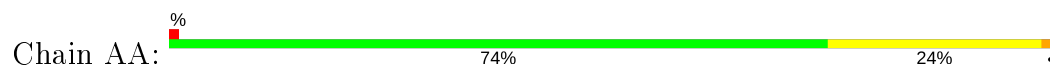


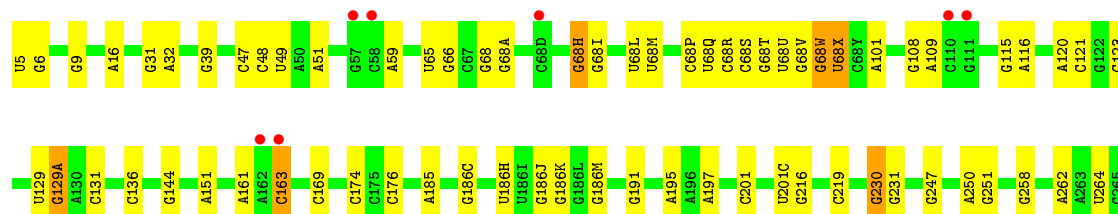
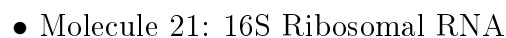


• Molecule 20: Elongation factor G

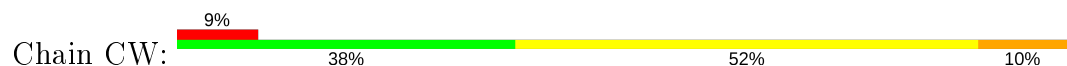


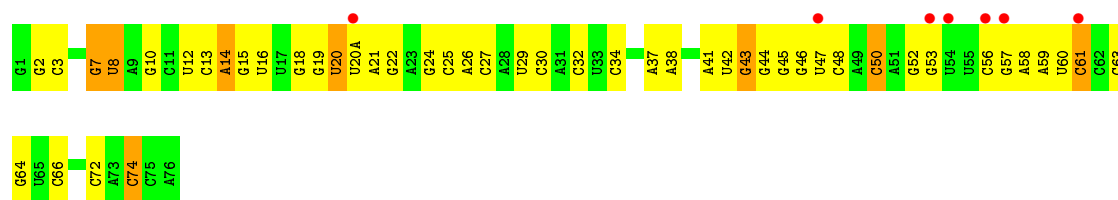
• Molecule 21: 16S Ribosomal RNA







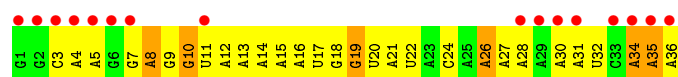




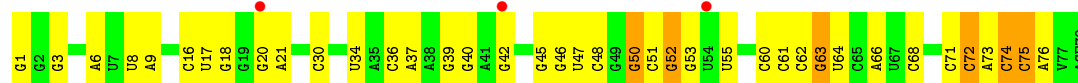
- Molecule 23: mRNA



- Molecule 23: mRNA



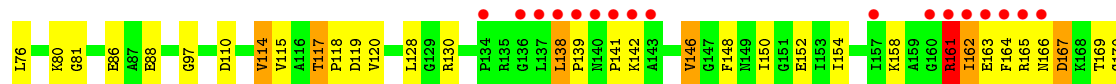
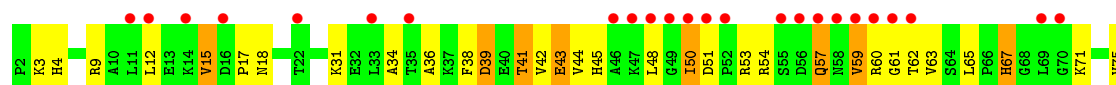
- Molecule 24: tRNA



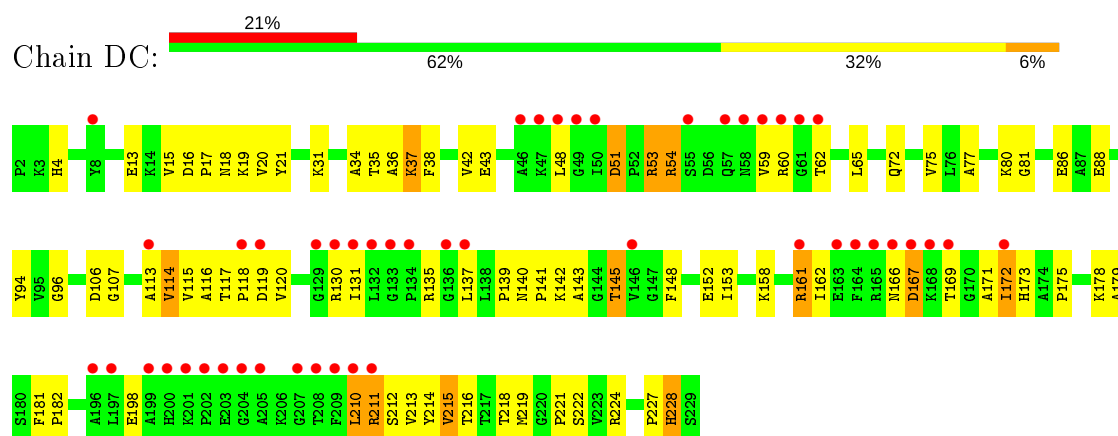
- Molecule 24: tRNA



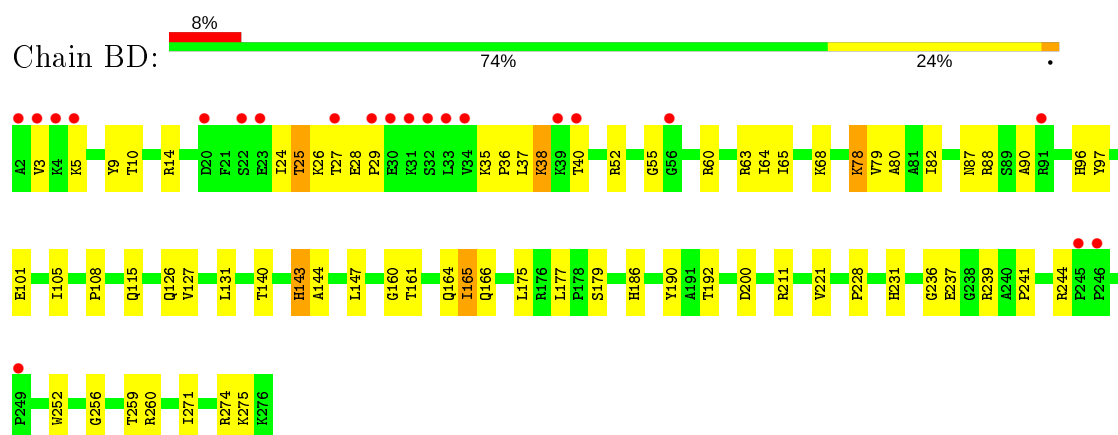
- Molecule 25: 50S ribosomal protein L1



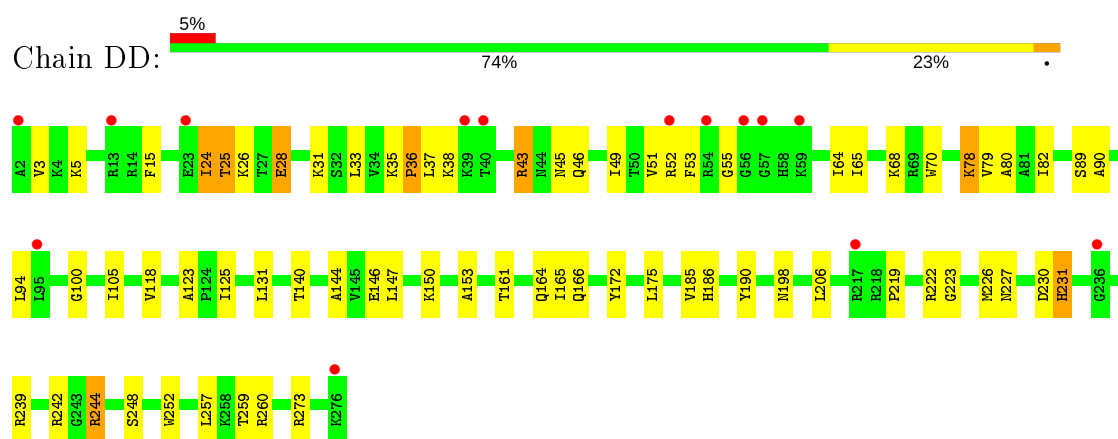
- Molecule 25: 50S ribosomal protein L1



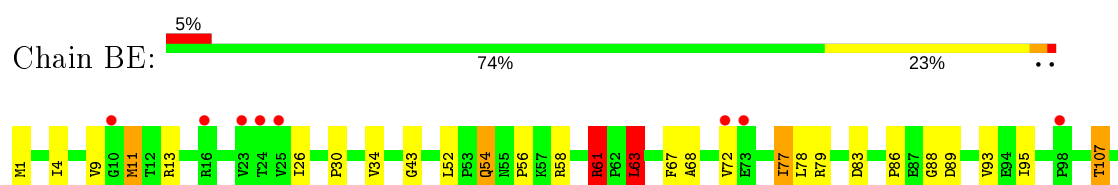
- Molecule 26: 50S ribosomal protein L2

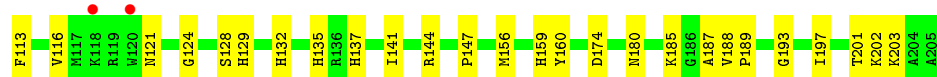


- Molecule 26: 50S ribosomal protein L2

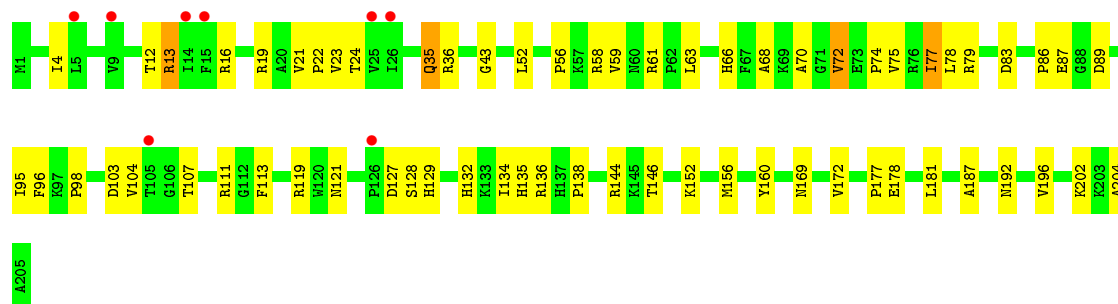


- Molecule 27: 50S ribosomal protein L3

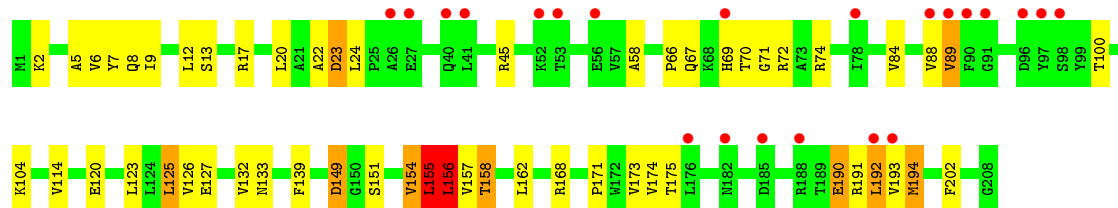
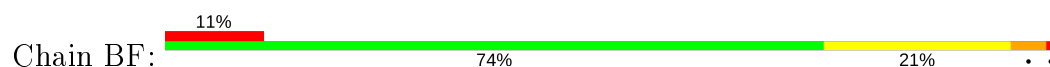




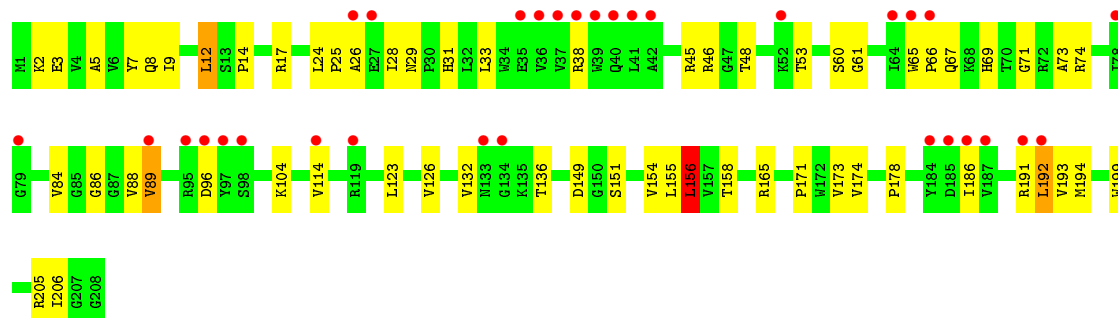
- Molecule 27: 50S ribosomal protein L3



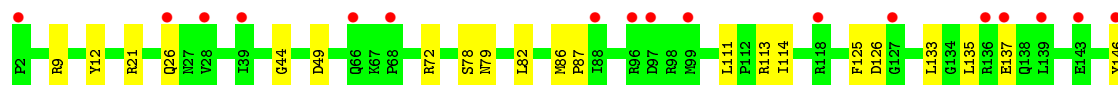
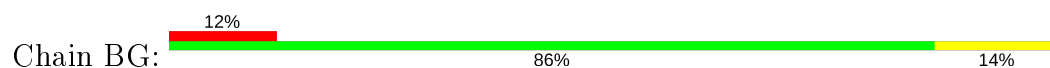
- Molecule 28: 50S ribosomal protein L4



- Molecule 28: 50S ribosomal protein L4

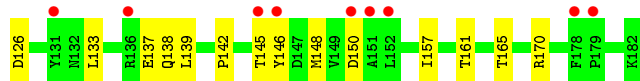
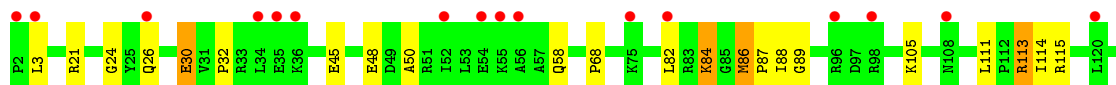
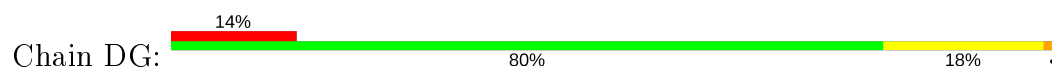


- Molecule 29: 50S ribosomal protein L5

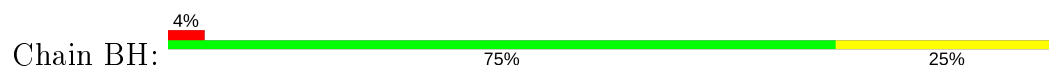




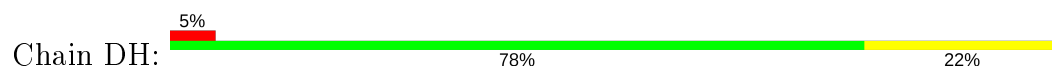
- Molecule 29: 50S ribosomal protein L5



- Molecule 30: 50S ribosomal protein L6



- Molecule 30: 50S ribosomal protein L6



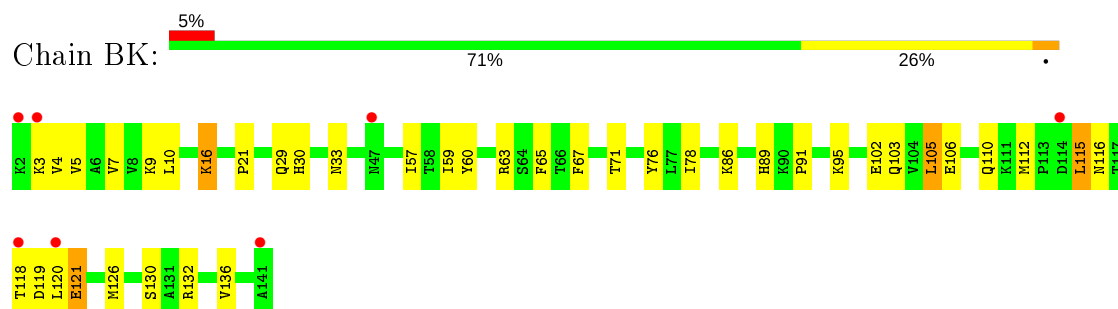
- Molecule 31: 50S ribosomal protein l10



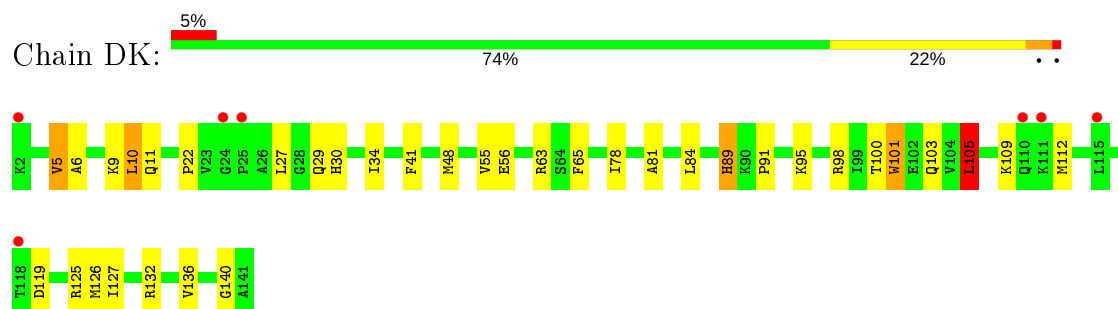
- Molecule 31: 50S ribosomal protein l10



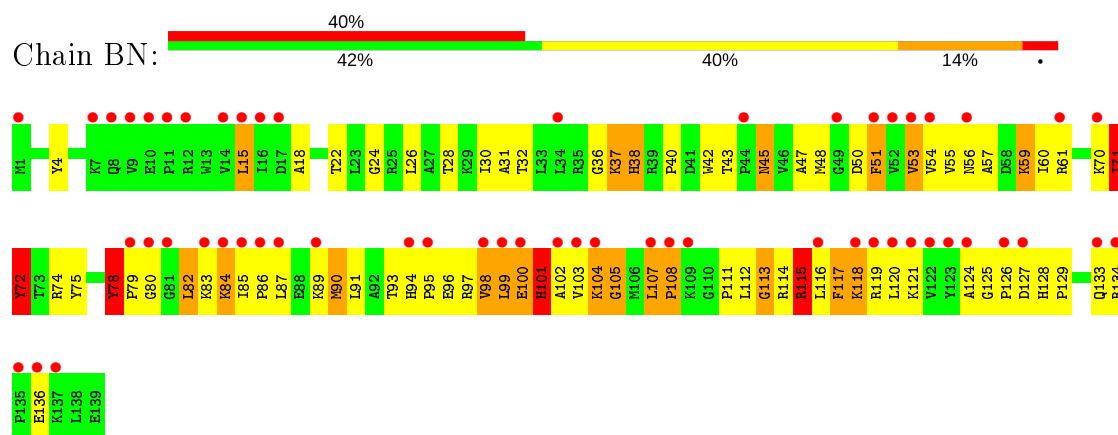
- Molecule 32: 50S ribosomal protein L11



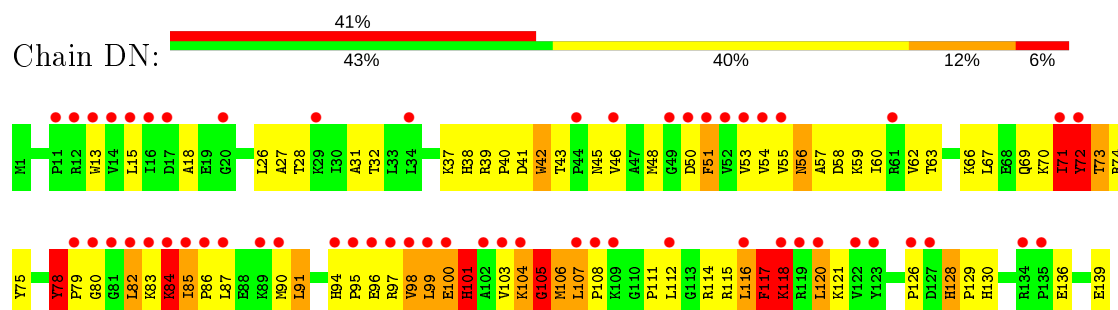
- Molecule 32: 50S ribosomal protein L11



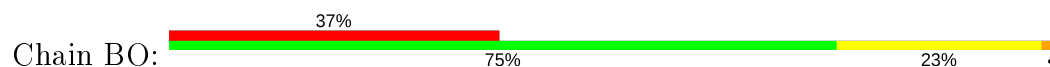
- Molecule 33: 50S ribosomal protein L13

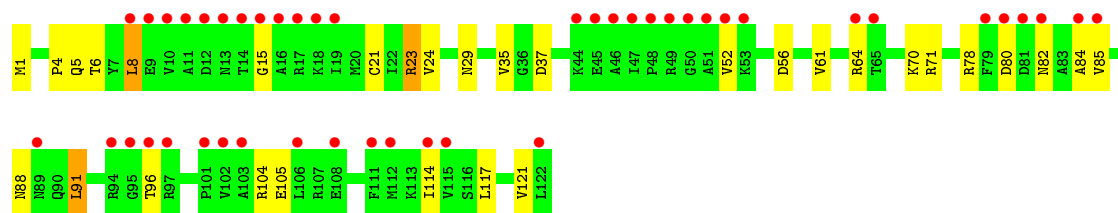


- Molecule 33: 50S ribosomal protein L13

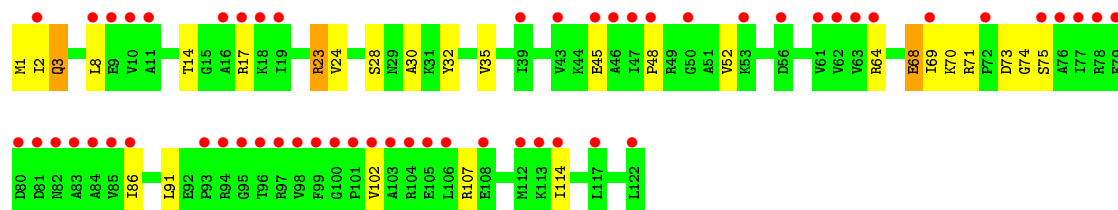
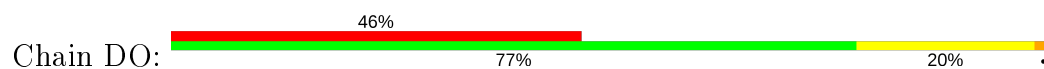


- Molecule 34: 50S ribosomal protein L14

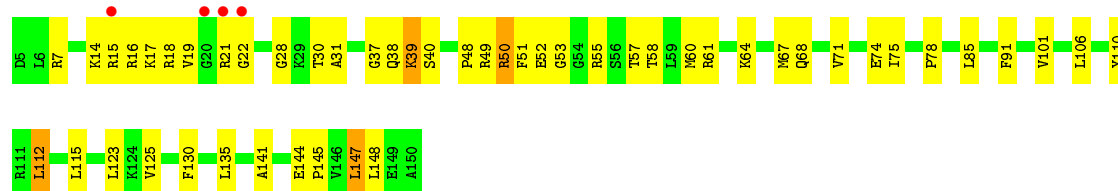




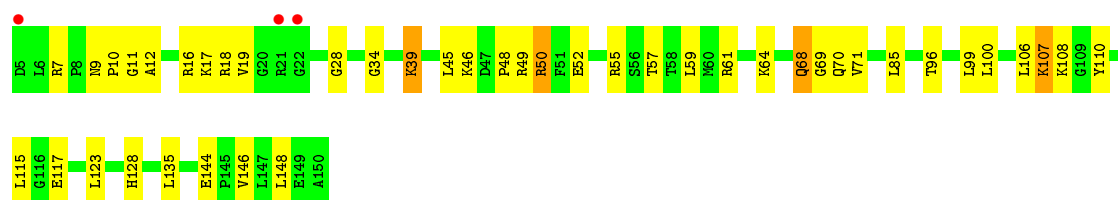
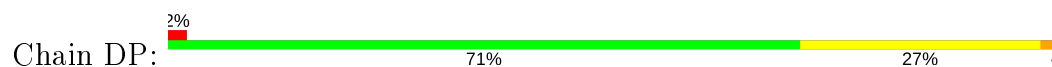
• Molecule 34: 50S ribosomal protein L14



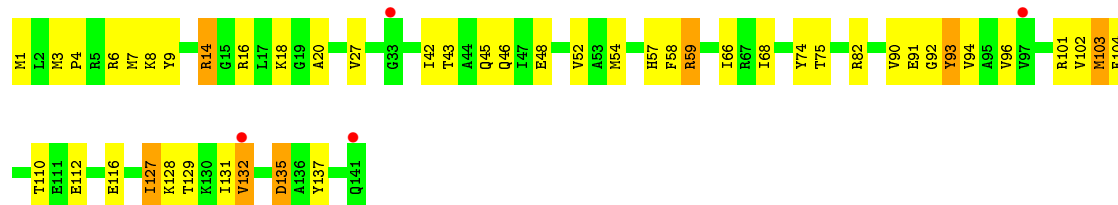
• Molecule 35: 50S ribosomal protein L15



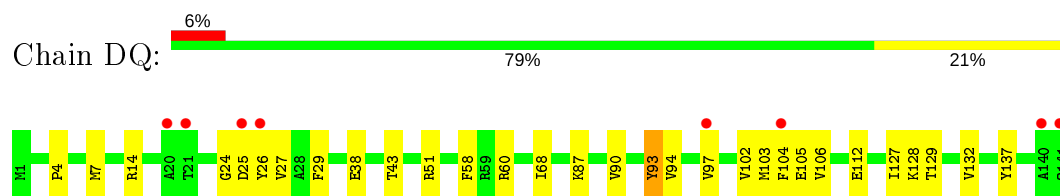
• Molecule 35: 50S ribosomal protein L15



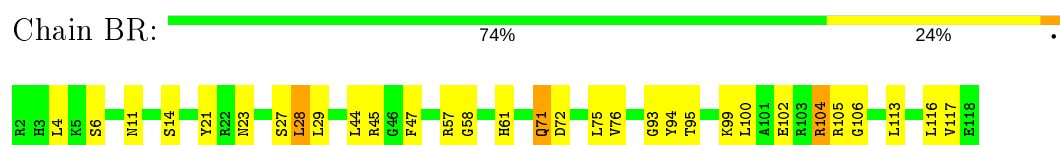
• Molecule 36: 50S ribosomal protein L16



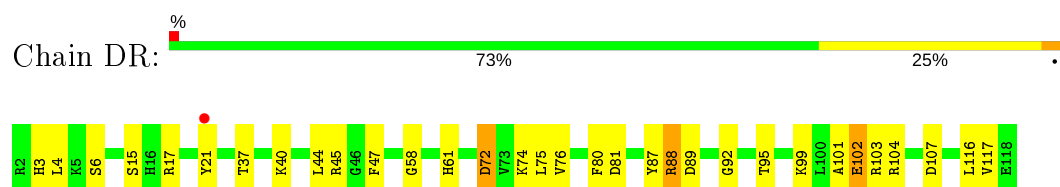
- Molecule 36: 50S ribosomal protein L16



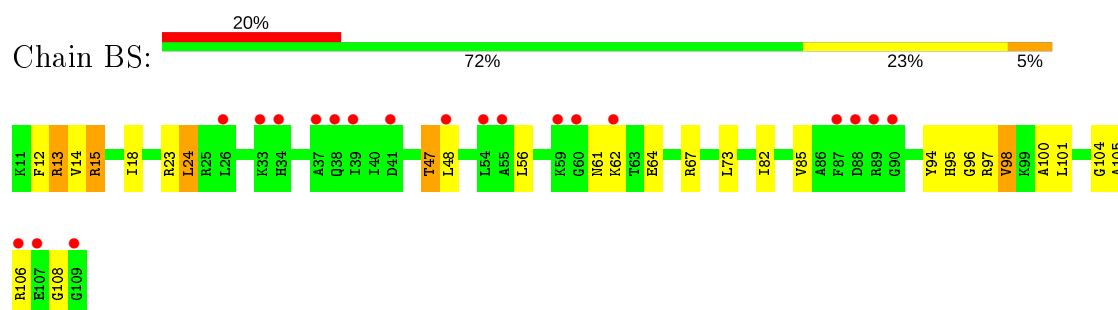
- Molecule 37: 50S ribosomal protein L17



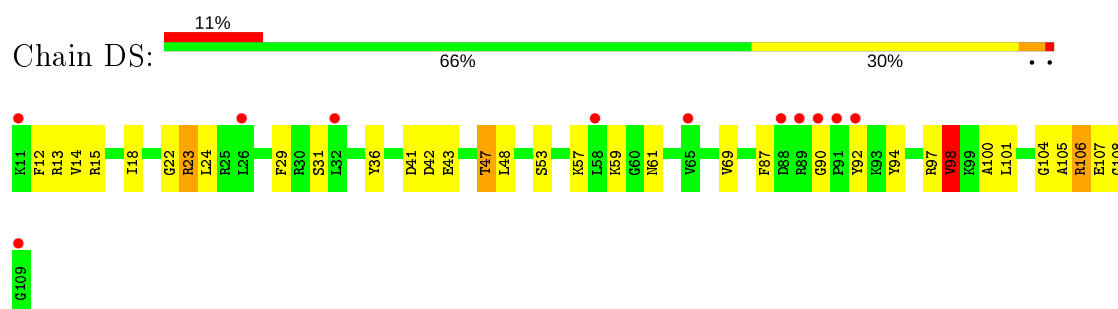
- Molecule 37: 50S ribosomal protein L17



- Molecule 38: 50S ribosomal protein L18



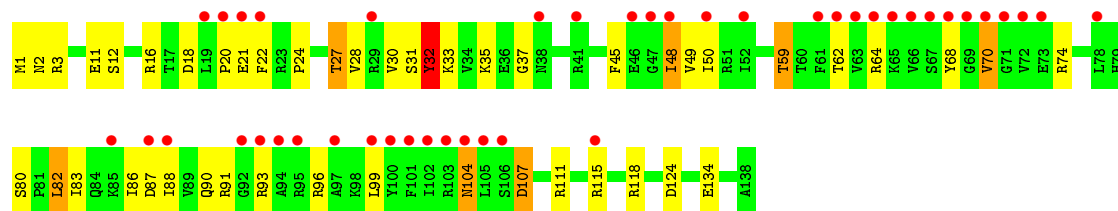
- Molecule 38: 50S ribosomal protein L18



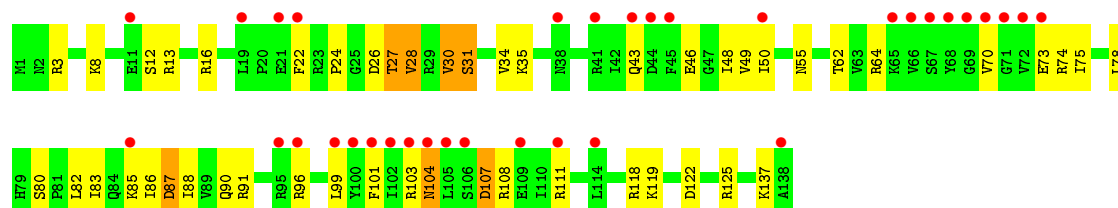
- Molecule 39: 50S ribosomal protein L19



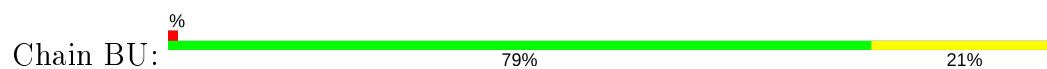




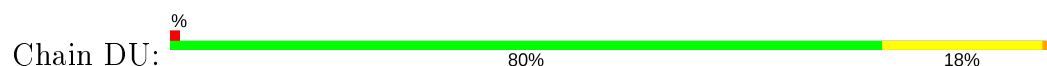
• Molecule 39: 50S ribosomal protein L19



• Molecule 40: 50S ribosomal protein L20



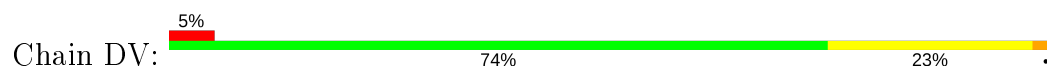
• Molecule 40: 50S ribosomal protein L20



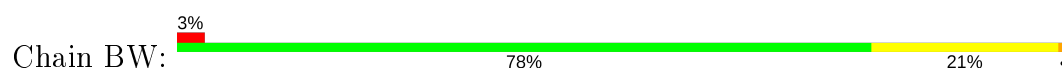
• Molecule 41: 50S ribosomal protein L21



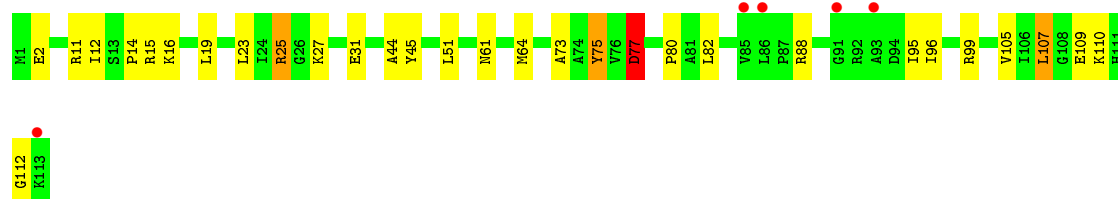
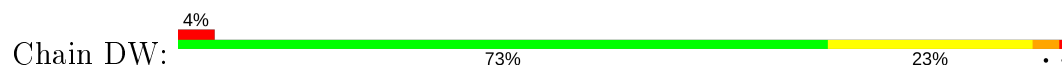
• Molecule 41: 50S ribosomal protein L21



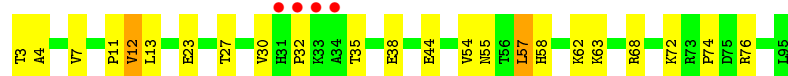
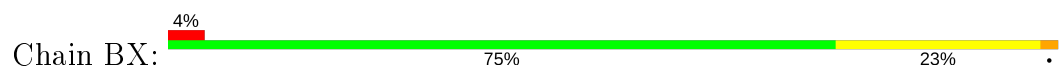
• Molecule 42: 50S ribosomal protein L22



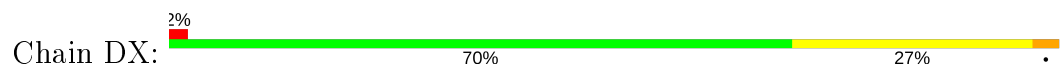
- Molecule 42: 50S ribosomal protein L22



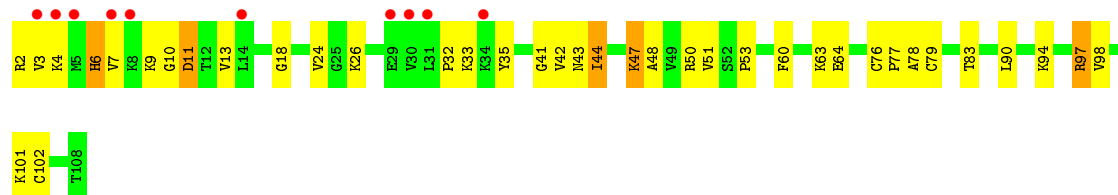
- Molecule 43: 50S ribosomal protein L23



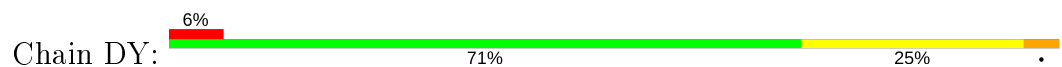
- Molecule 43: 50S ribosomal protein L23



- Molecule 44: 50S ribosomal protein L24

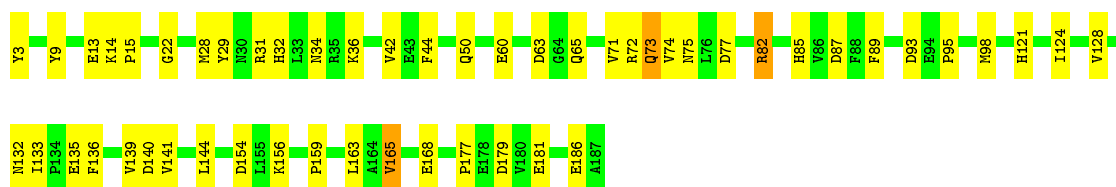


- Molecule 44: 50S ribosomal protein L24




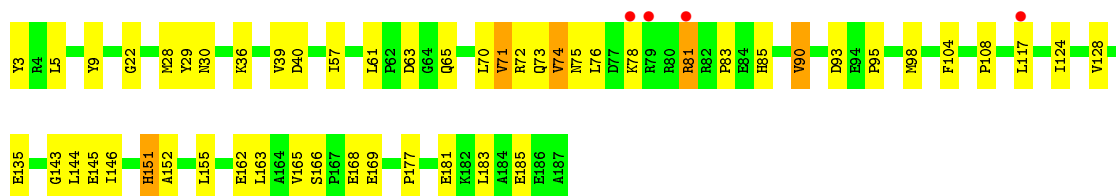
- Molecule 45: 50S ribosomal protein L25

Chain BZ:  72% 26% .




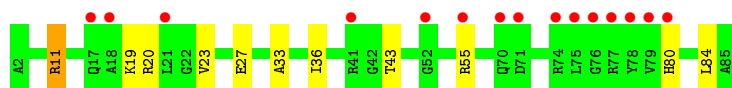
- Molecule 45: 50S ribosomal protein L25

Chain DZ:  72% 25% .




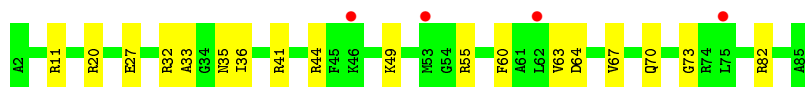
- Molecule 46: 50S ribosomal protein L27

Chain B0:  87% 12% .



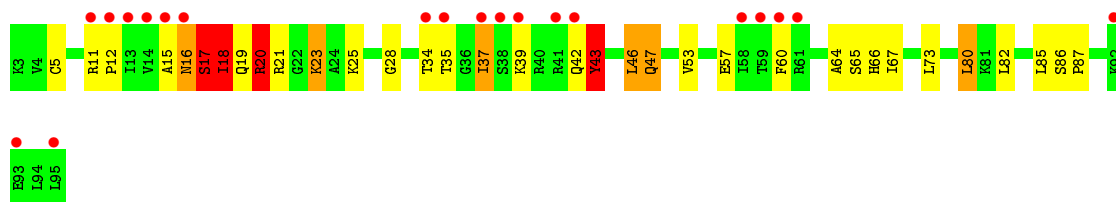
- Molecule 46: 50S ribosomal protein L27

Chain D0:  79% 21% .



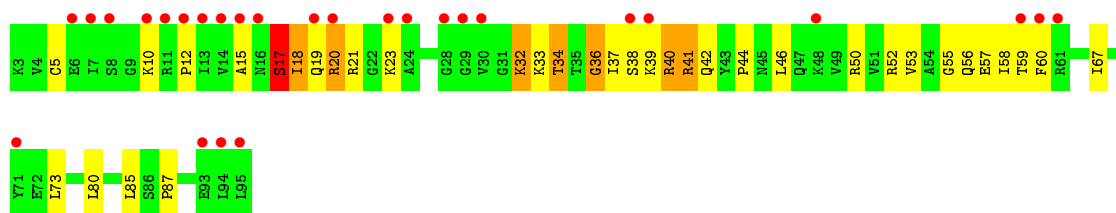
- Molecule 47: 50S ribosomal protein L28

Chain B1:  63% 26% 6% .

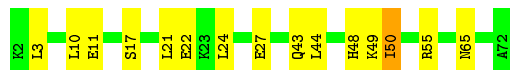
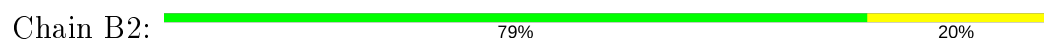


- Molecule 47: 50S ribosomal protein L28

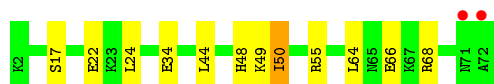
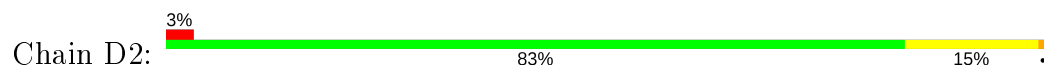
Chain D1:  61% 30% 8% .



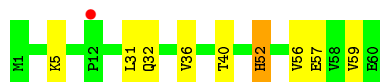
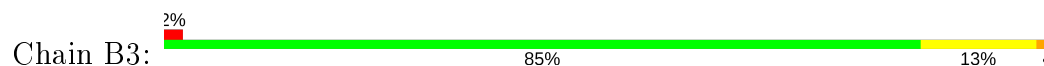
- Molecule 48: 50S ribosomal protein L29



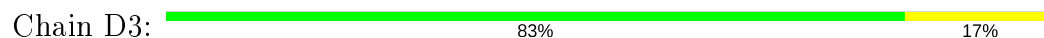
- Molecule 48: 50S ribosomal protein L29



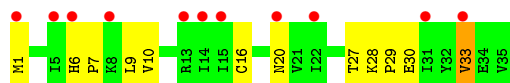
- Molecule 49: 50S ribosomal protein L30



- Molecule 49: 50S ribosomal protein L30



- Molecule 50: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L31



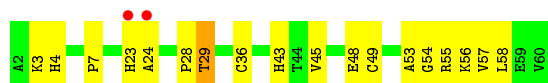
- Molecule 51: 50S ribosomal protein L32

Chain B5:  69% 27%



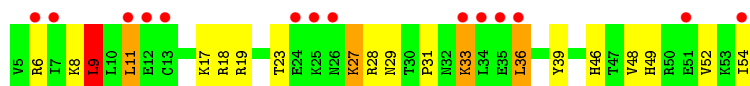
- Molecule 51: 50S ribosomal protein L32

Chain D5:  3% 69% 29%



- Molecule 52: 50S ribosomal protein L33

Chain B6:  28% 60% 30% 8%




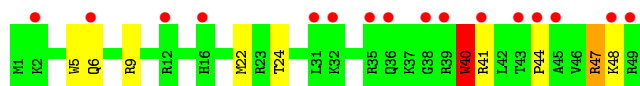
- Molecule 52: 50S ribosomal protein L33

Chain D6:  26% 50% 42% 8%




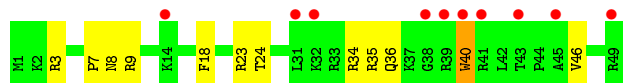
- Molecule 53: 50S ribosomal protein L34

Chain B7:  33% 80% 16%




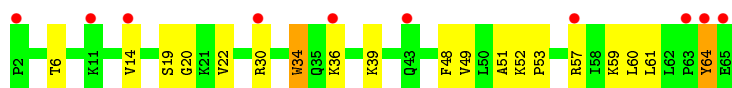
- Molecule 53: 50S ribosomal protein L34

Chain D7:  20% 76% 22%



- Molecule 54: 50S ribosomal protein L35

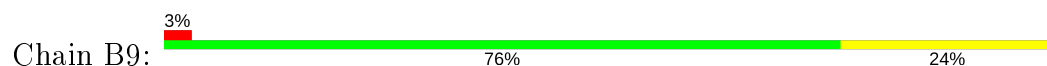
Chain B8:  16% 70% 27%



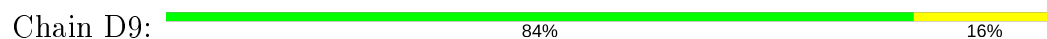
- Molecule 54: 50S ribosomal protein L35



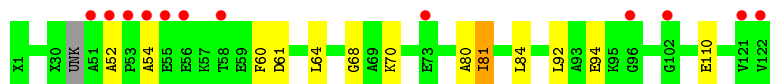
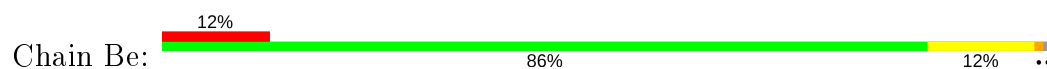
- Molecule 55: 50S ribosomal protein L36



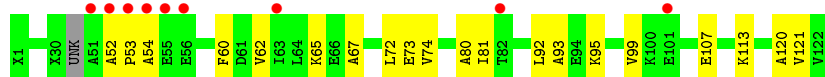
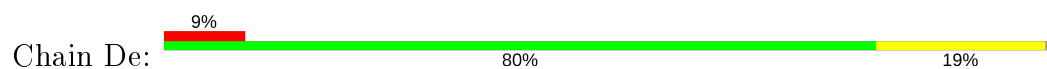
- Molecule 55: 50S ribosomal protein L36



- 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

Chain Df:  100%

There are no outlier residues recorded for this chain.

- Molecule 57: 50S ribosomal protein L7/L12

Chain Dg:  100%

There are no outlier residues recorded for this chain.

- Molecule 58: 50S ribosomal protein L7/L12

Chain Bh:  100%


There are no outlier residues recorded for this chain.

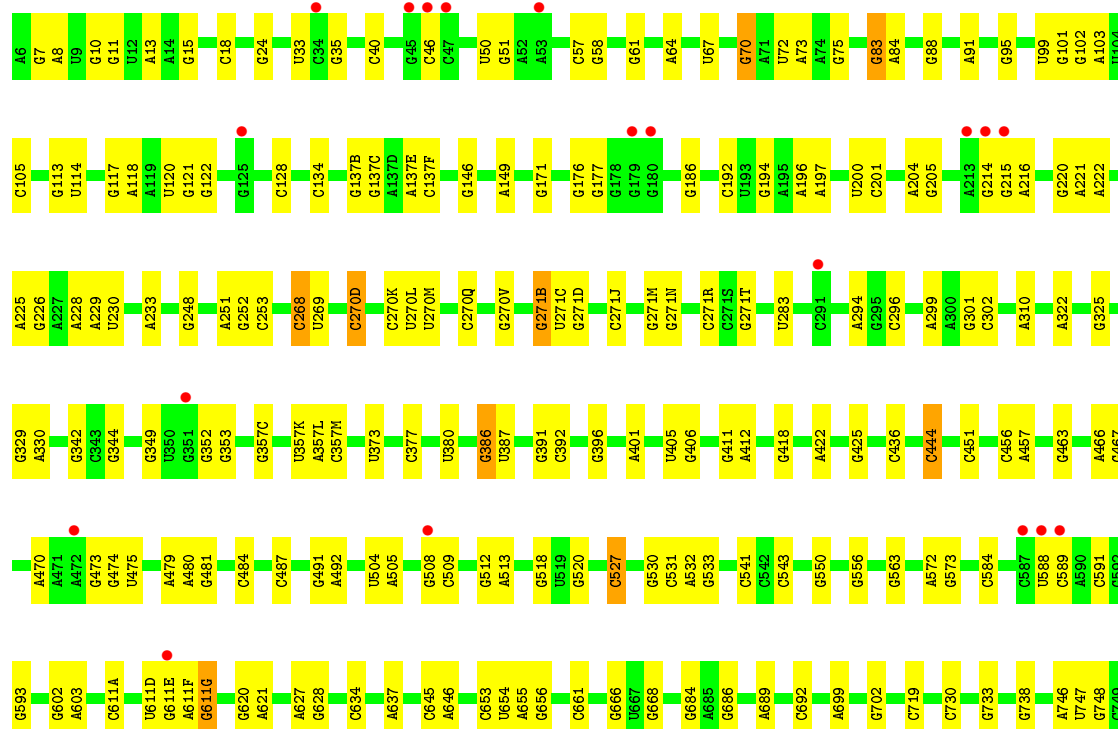
- Molecule 58: 50S ribosomal protein L7/L12

Chain Dh:  100%

There are no outlier residues recorded for this chain.

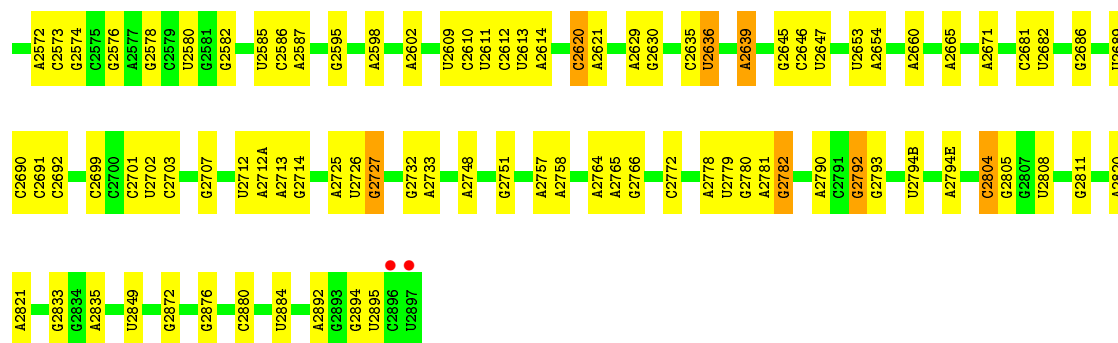
- Molecule 59: 23S Ribosomal RNA

Chain BA:  71% 27%

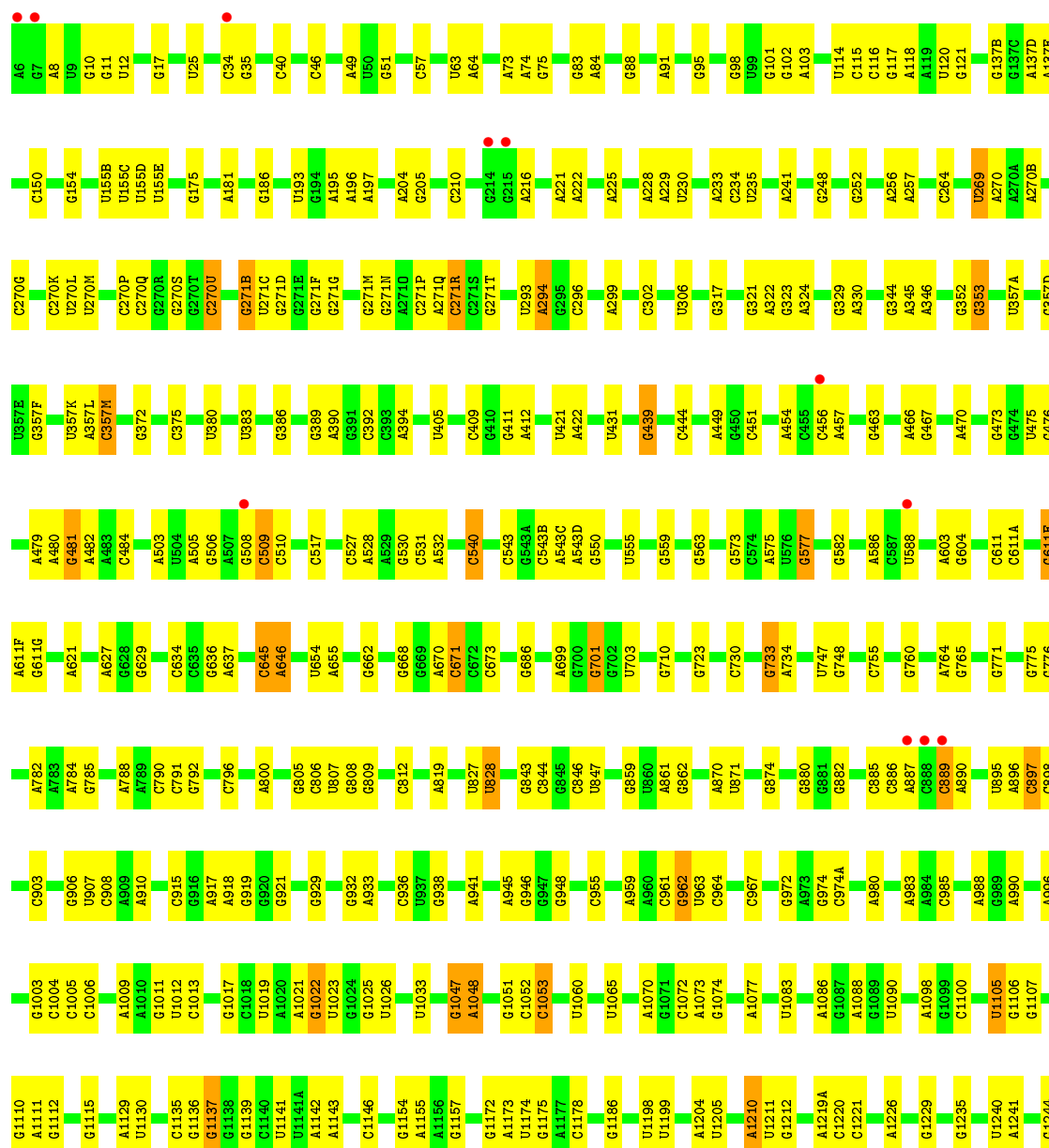
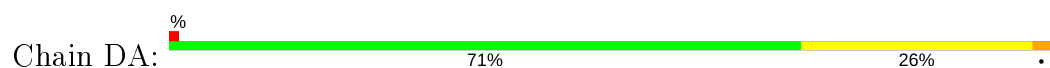


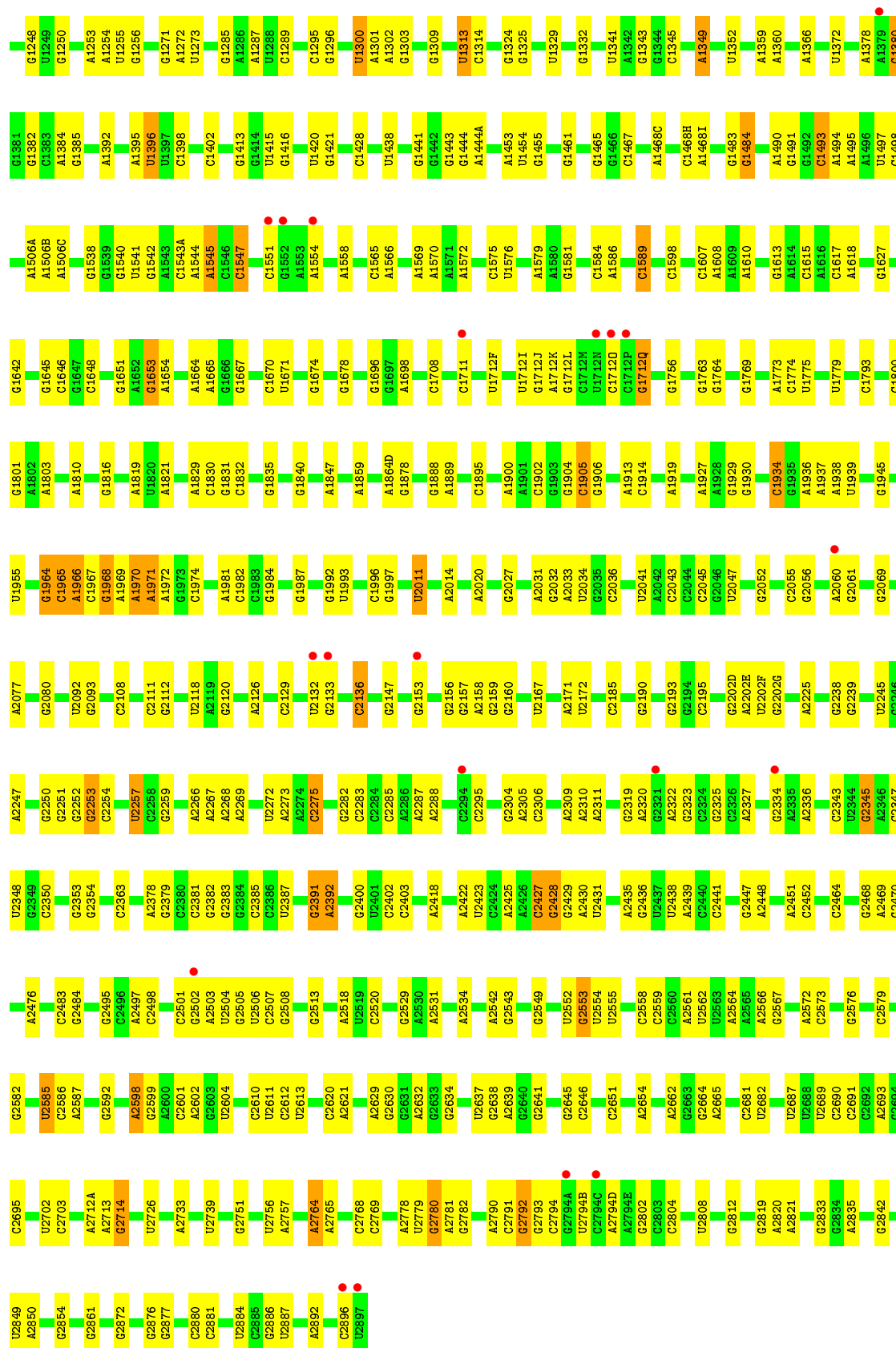
G2446	G2447	A2448	G2449	A2450	G2452	G2456	G2468	A2469	G2470	G2476	G2477	A2478	G2479	G2480	G2484	G2498	G2501	G2502	G2503	G2504	G2505	G2506	G2516	G2520	G2521	G2522	G2529	A2533	G2540	A2541	A2542	G2543	G2544	G2551	G2552	G2553	G2554	G2555	G2556	G2557	G2558	G2559	G2560	A2566	G2567						
A2305	G2306	G2307	G2308	A2309	A2310	G2315	G2319	A2320	G2325	G2334	A2335	A2336	G2337	G2338	G2343	G2344	G2345	A2346	G2347	G2367	G2377	G2378	G2379	G2382	G2383	G2384	G2385	G2402	G2403	G2413	A2422	A2423	A2424	A2425	A2426	G2427	G2428	G2429	A2430	A2435	G2436	A2439	G2440	G2441	G2445	A2446					
U2172	G2181	G2185	G2186	A2198	G2202D	A2202E	U2202F	G2223	G2224	A2235	G2236	G2237	G2238	G2239	U2243	G2244	G2245	G2246	G2247	G2248	G2249	G2250	G2251	G2252	G2253	G2254	G2255	G2256	G2257	G2258	G2259	A2266	A2267	A2268	A2269	G2270	G2275	G2276	G2277	A2278	G2283	G2284	G2285	A2286	A2287	G2304					
G2046	U2047	C2050	A2051	G2055	G2056	A2059	A2060	G2061	U2068	G2069	U2075	G2076	A2077	G2104	G2105	G2106	G2107	G2111	G2112	U2113	A2114	G2115	G2116	G2120	G2131	G2132	G2133	G2136	G2141	U2144	G2145	G2148	G2149	G2154	G2155	G2156	G2157	A2158	G2159	G2160	G2161	A2169	A2170	A2171							
C1934	G1935	A1936	A1937	A1938	U1939	U1940	U1944	G1945	U1951	U1955	C1961	G1962	U1963	G1964	G1965	A1966	C1967	G1968	A1969	A1970	A1971	A1972	A1981	C1982	U1991	G1992	U1993	G1997	G1998	G2009	A2015	A2019	A2020	G2023	G2024	G2025	A2031	G2032	C2033	G2036	U2041	A2042	G2043	A2044	A2045						
G1793	U1794	C1800	G1801	C1806	G1810	C1815	G1816	A1821	A1829	C1830	G1831	G1832	G1835	G1839	G1840	U1841	A1847	A1848	G1860	A1864D	G1878	G1888	G1895	G1899	A1900	A1901	C1902	G1906	A1913	C1914	U1915	A1916	U1917	U1923	G1927	A1928	G1929	G1930	G1933												
G1635	C1640	G1646	G1647	G1648	G1651	A1652	G1653	A1654	C1663	A1664	U1671	G1672	U1673	G1674	A1690	G1695	G1696	G1697	A1698	G1702	G1705	U1706	A1712H	U1712I	G1712J	A1712K	G1712O	G1750	A1755	G1756	G1757	A1758	A1759	G1763	G1764	A1773	G1781	G1782	A1783	A1784	A1787	G1788									
C1498	A1506C	C1506K	G1506O	A1536	C1537	G1538	U1541	G1542	A1543	C1543A	U1544	A1545	C1546	C1547	A1553	A1554	G1555	G1558	G1559	G1560	G1563	C1564	A1565	A1566	A1569	A1570	A1579	A1580	G1581	C1584	A1586	C1598	A1603	C1607	A1610	C1615	A1616	C1617	A1618	G1619	A1631										
G1371	A1378	A1379	G1380	A1384	G1385	C1386	A1395	U1396	G1414	U1415	G1416	C1417	U1420	G1421	G1422	A1427	C1428	G1429	C1430	U1438	A1444A	A1453	U1454	G1455	C1458	G1459	A1460	G1461	G1465	G1466	C1467	A1468C	A1468D	G1483	A1486	A1490	G1491	G1492	C1493	A1494	A1495	U1497									
G1239	U1240	A1241	G1248	U1249	G1250	C1251	A1253	G1256	C1257	A1265	G1266	A1272	U1273	A1274	A1275	A1284	A1287	U1288	C1297	C1298	G1299	U1300	A1301	A1302	G1303	U1313	C1314	A1321	U1326	U1329	C1330	A1331	G1332	U1341	C1345	G1346	G1347	G1348	A1349	U1352	A1359	A1360									
A983	A1095	A988	G989	A990	A996	G1003	C1004	C1005	U1008	U1009	A1010	G1011	U1012	C1013	U1019	G1022	U1023	G1024	U1025	U1026	A1027	U1033	G1034	U1035	G931	G932	A933	A1046	G1047	A1048	C1049	C1052	U1061	G1062	G946	C1063	C955	G956	A1070	G1071	G958	A1073	A1077	U1078	C1079	U1082	G974	C974A	A1083	A1088	A1090
U868	A872	A872	G880	G881	G882	G883	C884	G885	C886	A887	C888	C889	A890	U895	A896	C897	A898	A899	A906	A910	G910	G912	G914	A917	A918	G919	U930	G931	G932	A933	C938	G939	G940	A941	G942	U943	G944	G945	U957	U958	A959	A960	C961	G962	U963	C964	C965	A866	C967		
A750	A751	A752	U757	A761	A761	A764	G765	G766	A777	A782	A783	A784	G785	A910	G910	G912	G914	A917	A918	G919	U930	G931	G932	A933	C938	A919	U827	U828	G831	G832	U833	G836	G839	C844	C846	U847	C857	A861	C865	A866	C867										



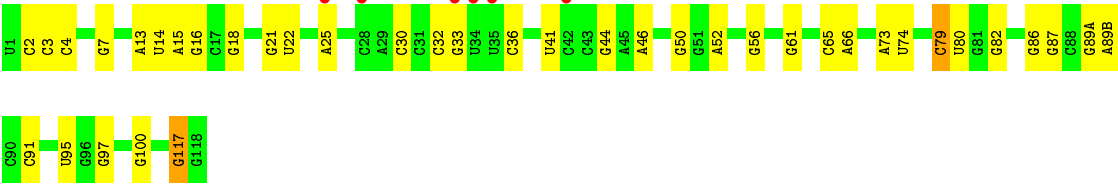


• Molecule 59: 23S Ribosomal RNA

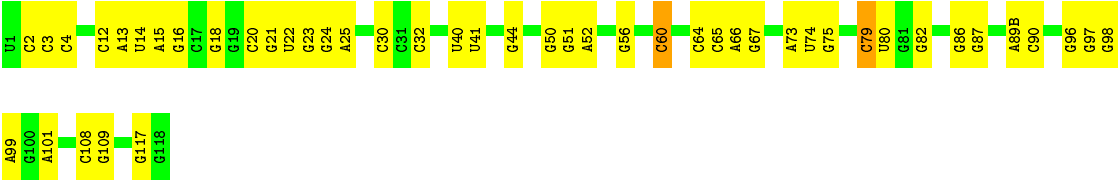




• Molecule 60: 5S Ribosomal RNA



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

<sup>1</sup>Intensities estimated from amplitudes.

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

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

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

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

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

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

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

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

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

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

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

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	163	PHE	Peptide
10	AK	43	SER	Peptide
15	AP	34	GLU	Peptide
20	AY	34	TYR	Peptide
20	AY	630	GLN	Peptide

## 5.2 Too-close contacts [i](#)

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

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AB	233/235 (99%)	168 (72%)	45 (19%)	20 (9%)	1	12
1	CB	233/235 (99%)	171 (73%)	45 (19%)	17 (7%)	1	16

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

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

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

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

5 of 1682 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

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

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

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

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

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

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

Mol	Chain	Res	Type
46	B0	80	HIS
4	CE	112	LEU
43	DX	23	GLU
48	B2	44	LEU
1	CB	121	LEU

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

Mol	Chain	Res	Type
3	CD	125	HIS
12	CM	101	GLN
44	DY	68	HIS
5	CF	7	ASN
10	CK	116	HIS

### 5.3.3 RNA ⓘ

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

5 of 2446 RNA backbone outliers are listed below:

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

5 of 109 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
59	BA	2250	G
21	CA	748	C
59	DA	2438	U
59	BA	2422	A
21	CA	5	U

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 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	DA	2901	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
62	FUA	CY	702	-	36,40,40	1.76	6 (16%)	46,64,64	1.52	6 (13%)
63	NMY	BA	2903	-	45,45,45	0.60	0	63,67,67	0.97	4 (6%)
62	FUA	AY	702	-	36,40,40	1.75	6 (16%)	46,64,64	1.52	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
63	NMY	BA	2902	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
63	NMY	CA	1601	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)
61	GDP	CY	701	-	24,30,30	1.34	4 (16%)	31,47,47	2.01	8 (25%)
61	GDP	AY	701	-	24,30,30	1.37	3 (12%)	31,47,47	2.21	10 (32%)
63	NMY	BA	2904	-	45,45,45	0.59	0	63,67,67	0.97	4 (6%)
63	NMY	AA	1601	-	45,45,45	0.58	0	63,67,67	0.97	4 (6%)

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	DA	2901	-	-	12/18/94/94	0/4/4/4
62	FUA	CY	702	-	-	6/11/92/92	0/4/4/4
63	NMY	BA	2903	-	-	12/18/94/94	0/4/4/4
62	FUA	AY	702	-	-	6/11/92/92	0/4/4/4
63	NMY	BA	2902	-	-	12/18/94/94	0/4/4/4
63	NMY	CA	1601	-	-	12/18/94/94	0/4/4/4
61	GDP	CY	701	-	-	5/12/32/32	0/3/3/3
61	GDP	AY	701	-	-	3/12/32/32	0/3/3/3
63	NMY	BA	2904	-	-	12/18/94/94	0/4/4/4
63	NMY	AA	1601	-	-	12/18/94/94	0/4/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	CY	702	FUA	C23-C22	-6.56	1.39	1.51
62	AY	702	FUA	C23-C22	-6.47	1.40	1.51
62	AY	702	FUA	C23-C24	-4.28	1.39	1.53
62	CY	702	FUA	C23-C24	-4.26	1.39	1.53
61	CY	701	GDP	C6-N1	4.01	1.40	1.33

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	GDP	C2-N3-C4	6.16	122.40	115.36
61	AY	701	GDP	N3-C2-N1	-5.96	119.28	127.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	CY	701	GDP	N3-C2-N1	-5.12	120.39	127.22
61	AY	701	GDP	C2-N3-C4	4.80	120.84	115.36
62	CY	702	FUA	C13-C12-C11	-4.32	105.84	111.90

There are no chirality outliers.

5 of 92 torsion outliers are listed below:

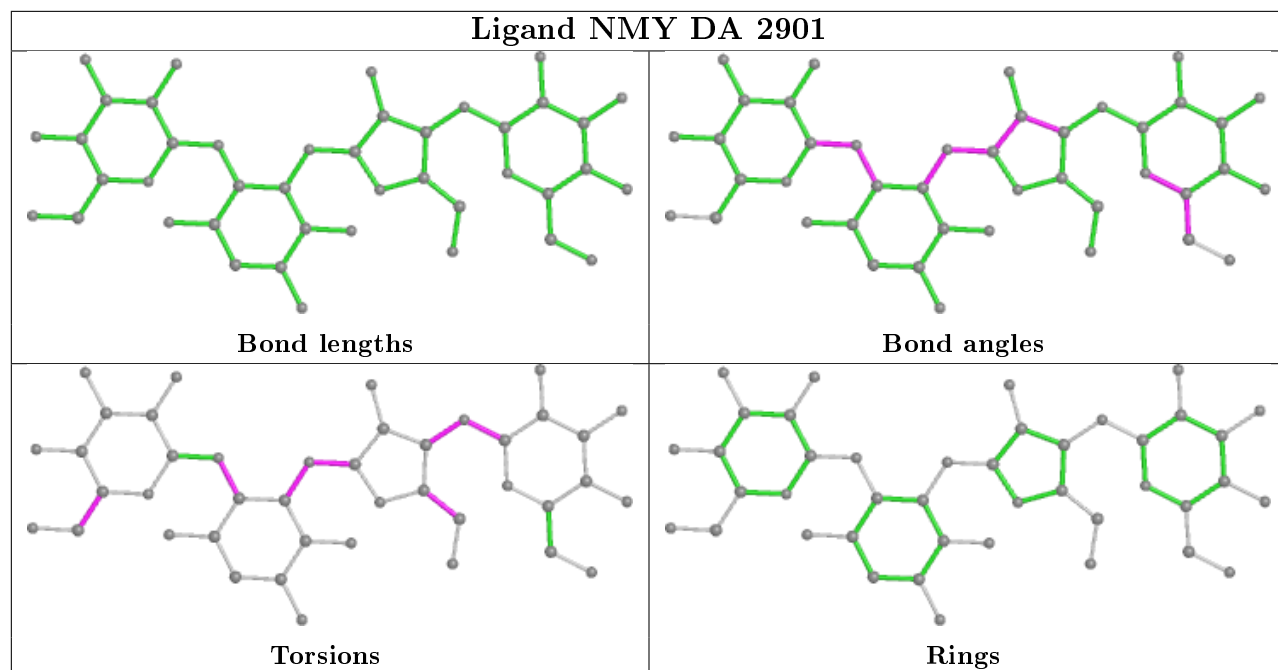
Mol	Chain	Res	Type	Atoms
63	DA	2901	NMY	C4-C5-C6-N6
63	DA	2901	NMY	O5-C5-C6-N6
63	DA	2901	NMY	C14-C13-O11-C11
63	DA	2901	NMY	C16-C15-O18-C18
63	DA	2901	NMY	C19-C18-O18-C15

There are no ring outliers.

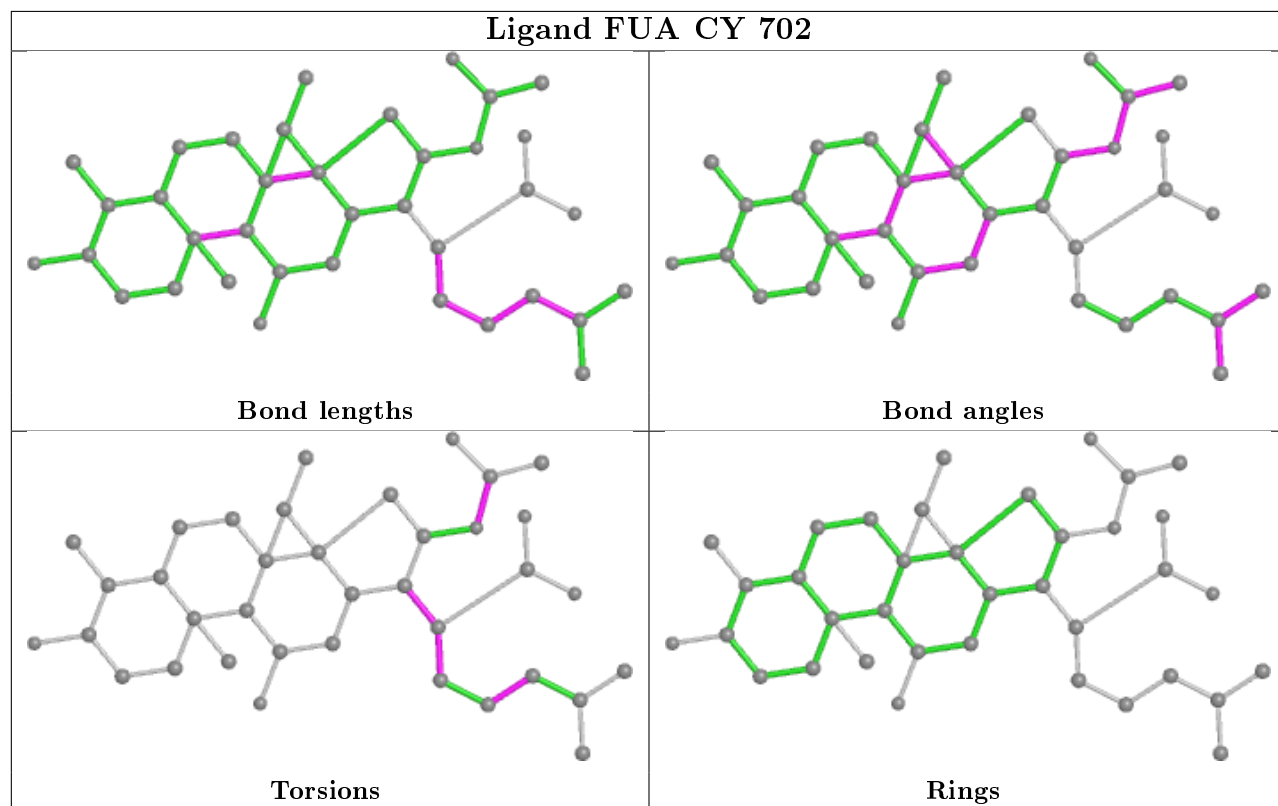
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

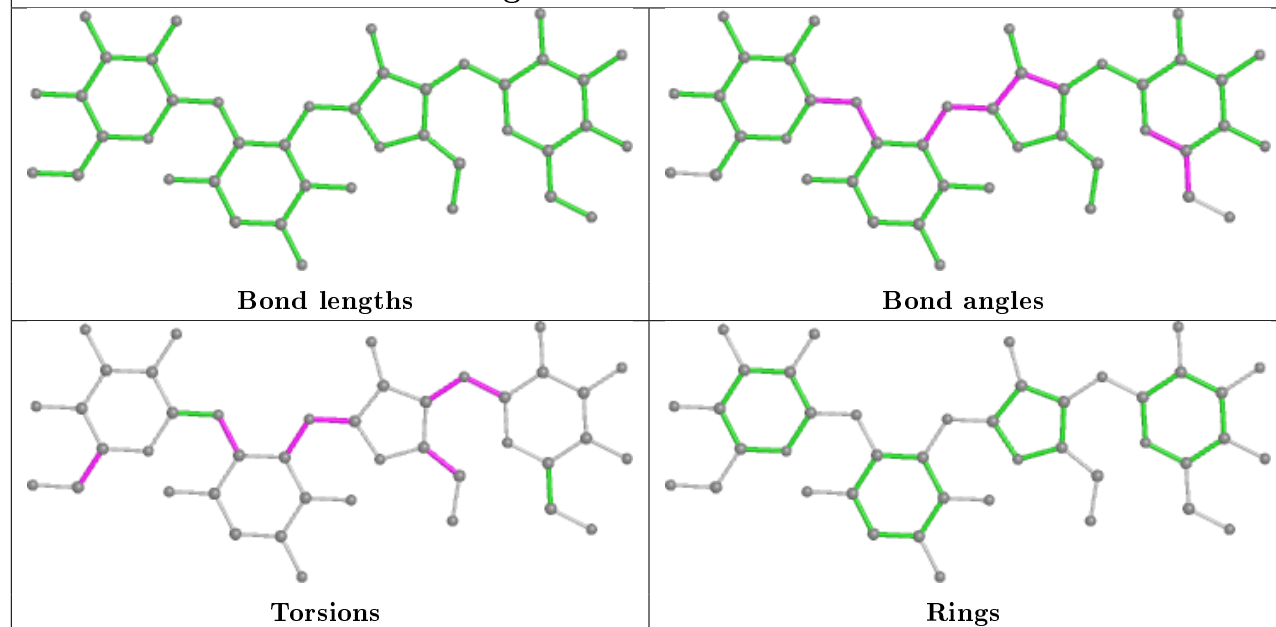
## Ligand NMY DA 2901



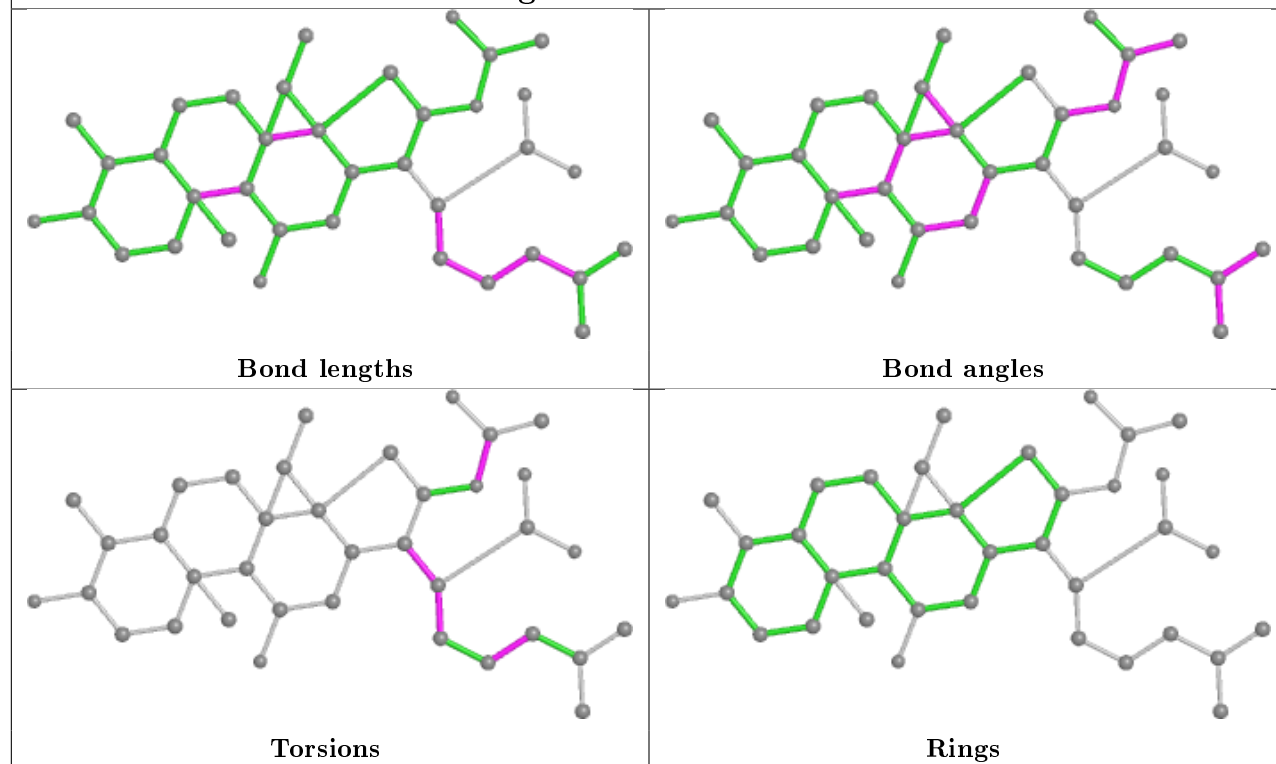
## Ligand FUA CY 702



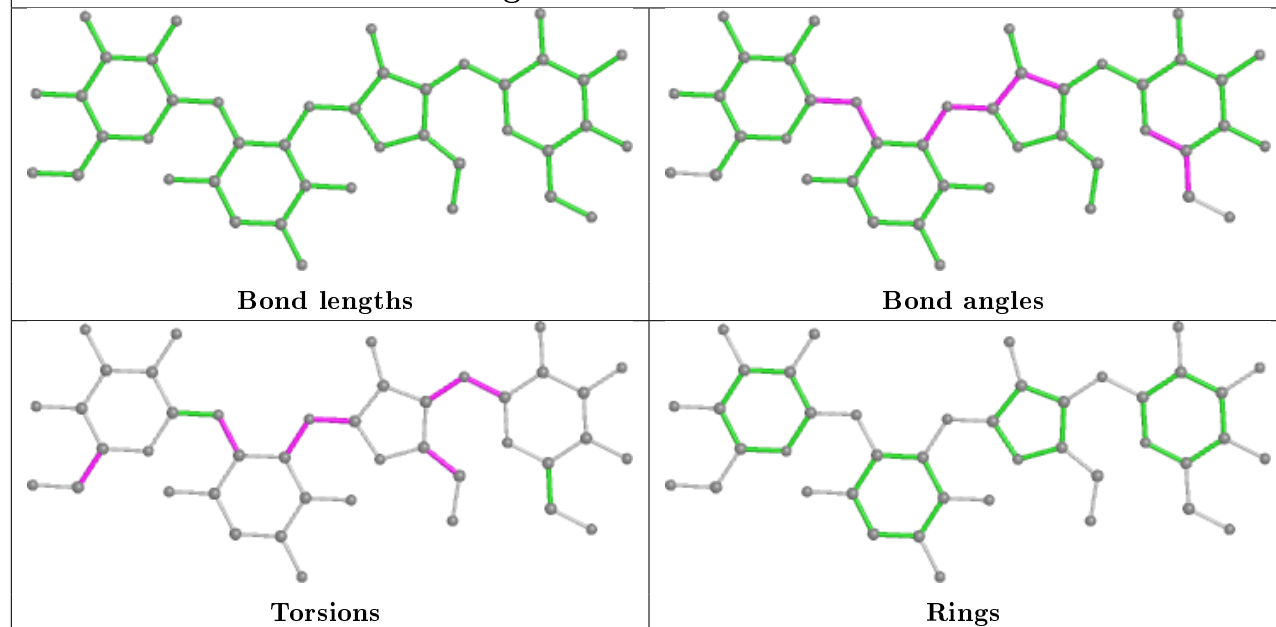
## Ligand NMY BA 2903



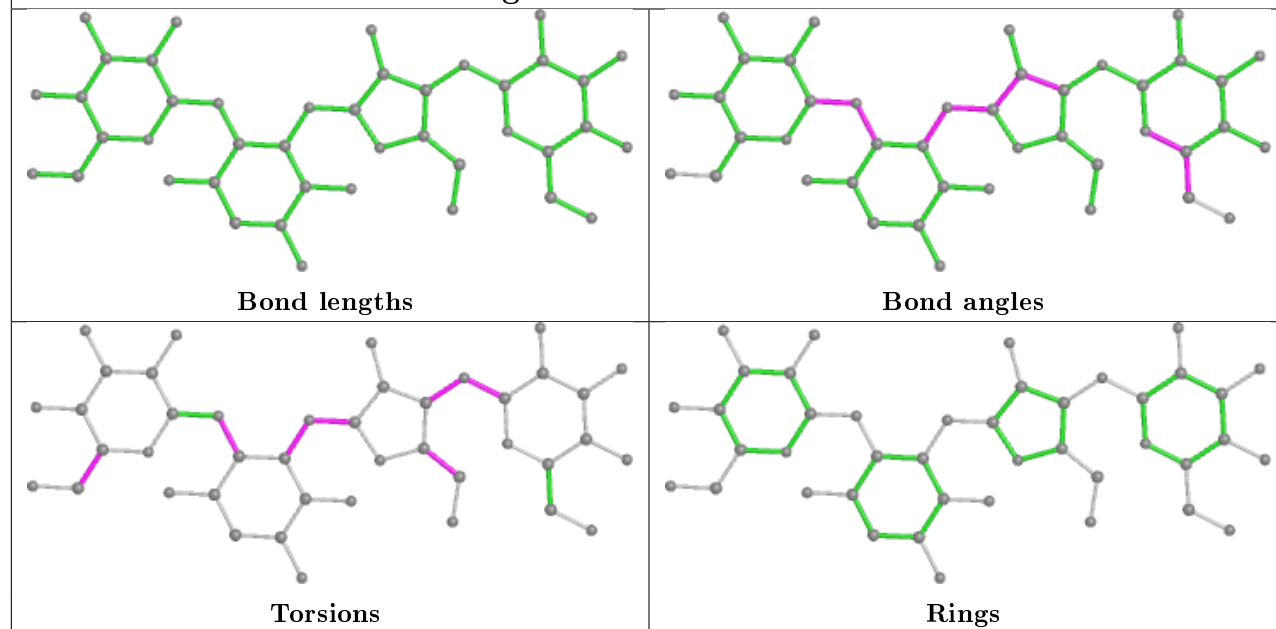
## Ligand FUA AY 702



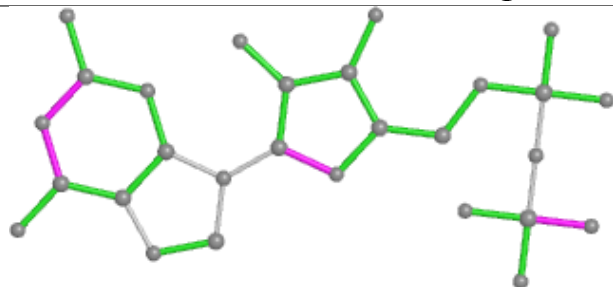
## Ligand NMY BA 2902



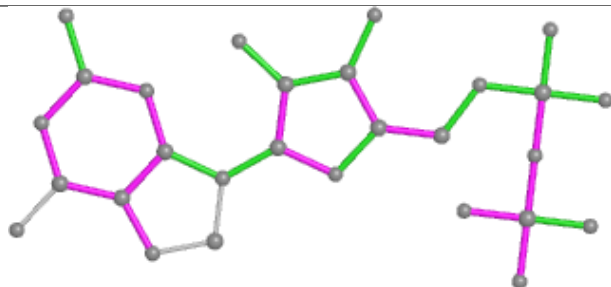
## Ligand NMY CA 1601



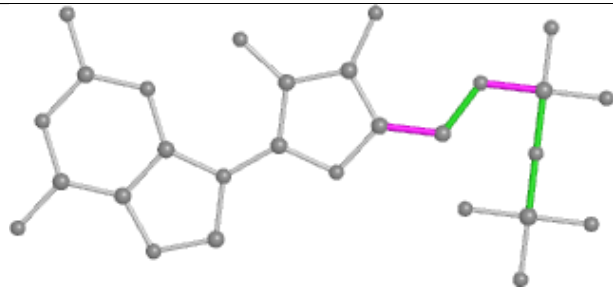
## Ligand GDP CY 701



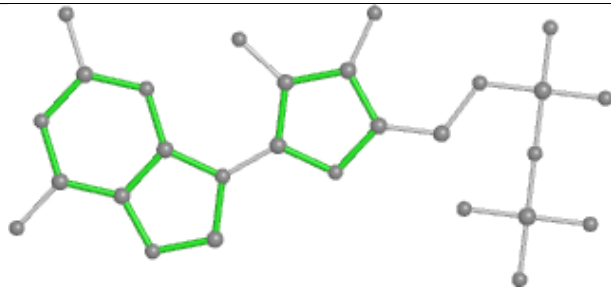
Bond lengths



Bond angles

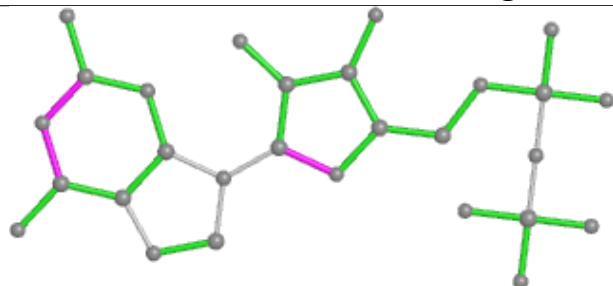


Torsions

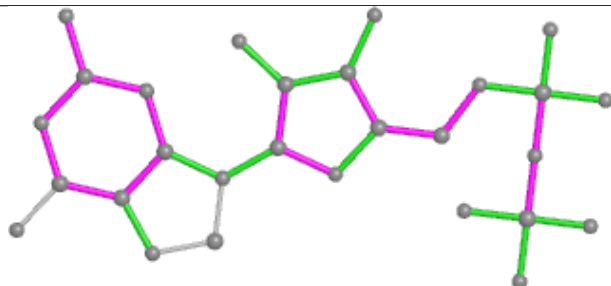


Rings

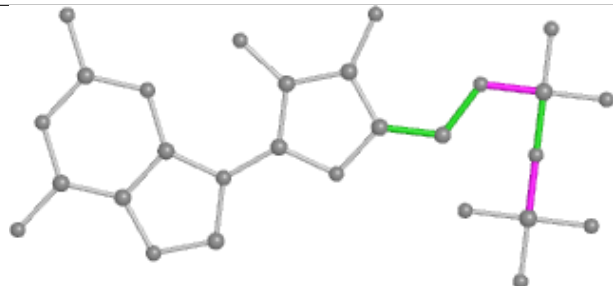
## Ligand GDP AY 701



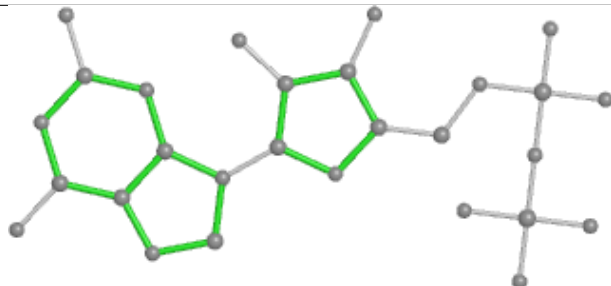
Bond lengths



Bond angles

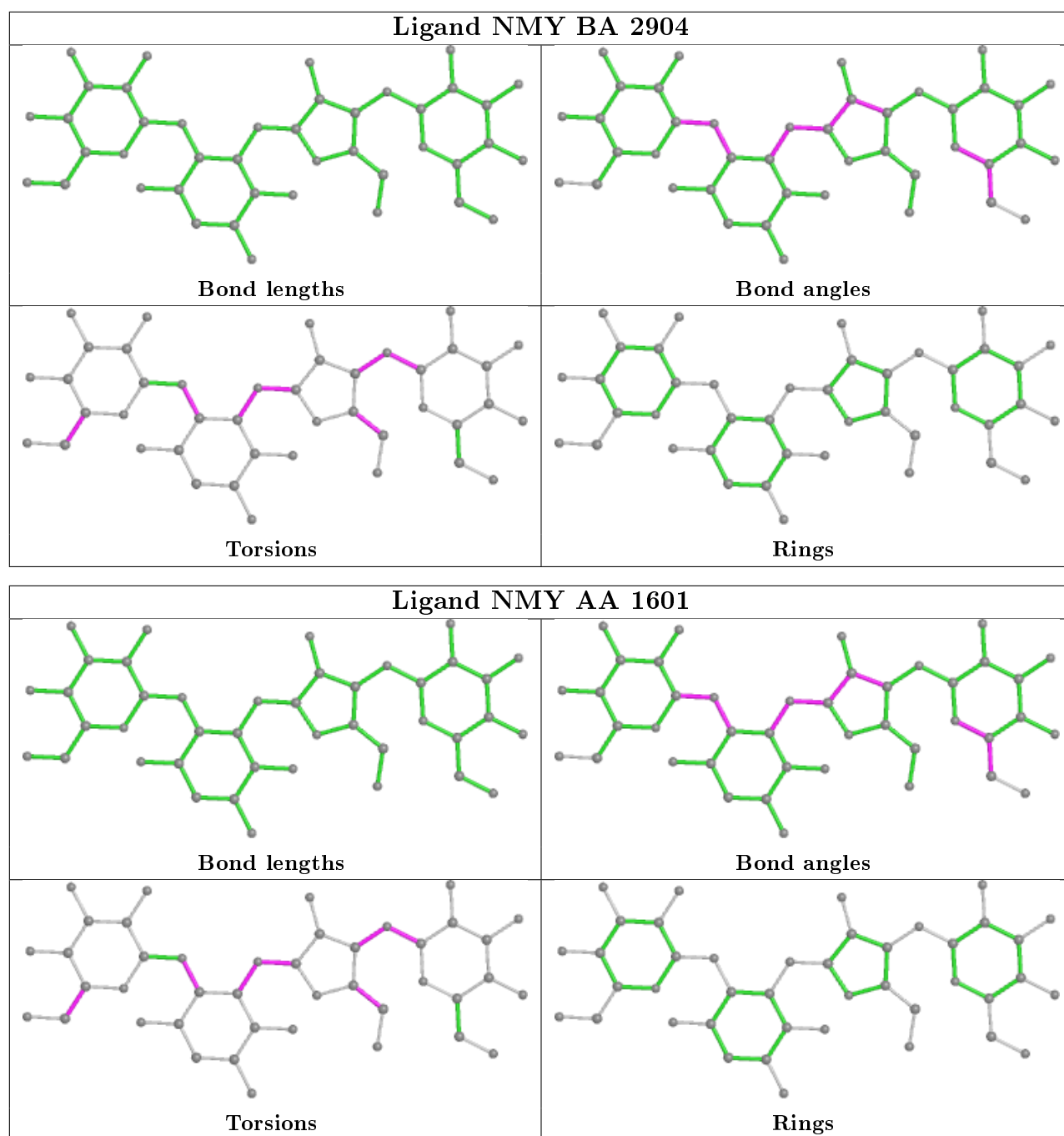


Torsions



Rings





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AB	235/235 (100%)	-0.33	4 (1%) 70 62	17, 55, 103, 129	0
1	CB	235/235 (100%)	-0.09	3 (1%) 77 70	17, 63, 111, 140	0
2	AC	207/207 (100%)	1.77	89 (42%) 0 0	18, 52, 99, 118	0
2	CC	207/207 (100%)	1.85	81 (39%) 0 0	15, 58, 99, 132	0
3	AD	208/208 (100%)	-0.46	2 (0%) 82 76	14, 59, 107, 137	0
3	CD	208/208 (100%)	-0.32	1 (0%) 91 87	20, 52, 102, 136	0
4	AE	151/151 (100%)	0.08	15 (9%) 7 6	26, 62, 96, 129	0
4	CE	151/151 (100%)	-0.05	9 (5%) 21 17	19, 56, 99, 143	0
5	AF	101/101 (100%)	-0.60	0 100 100	22, 57, 111, 128	0
5	CF	101/101 (100%)	-0.65	0 100 100	19, 56, 106, 128	0
6	AG	155/155 (100%)	-0.28	7 (4%) 33 28	26, 78, 122, 150	0
6	CG	155/155 (100%)	-0.32	6 (3%) 39 32	38, 85, 120, 147	0
7	AH	138/138 (100%)	-0.75	0 100 100	16, 43, 87, 109	0
7	CH	138/138 (100%)	-0.63	0 100 100	10, 49, 86, 102	0
8	AI	127/127 (100%)	-0.59	3 (2%) 59 50	30, 64, 101, 127	0
8	CI	127/127 (100%)	-0.59	1 (0%) 86 81	9, 77, 108, 134	0
9	AJ	99/99 (100%)	1.69	37 (37%) 0 0	34, 64, 104, 146	0
9	CJ	99/99 (100%)	1.63	35 (35%) 0 0	22, 57, 107, 115	0
10	AK	119/119 (100%)	0.03	10 (8%) 11 9	13, 74, 139, 160	0
10	CK	119/119 (100%)	-0.03	3 (2%) 57 49	21, 71, 125, 161	0
11	AL	125/125 (100%)	-0.27	4 (3%) 47 38	15, 73, 145, 164	0
11	CL	125/125 (100%)	0.00	6 (4%) 30 26	27, 85, 148, 170	0
12	AM	125/125 (100%)	0.06	6 (4%) 30 26	43, 86, 129, 159	0
12	CM	125/125 (100%)	-0.10	8 (6%) 19 15	27, 63, 103, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	60/60 (100%)	1.04	13 (21%) 0 1	33, 70, 116, 128	0
13	CN	60/60 (100%)	0.81	10 (16%) 1 2	30, 58, 105, 128	0
14	AO	88/88 (100%)	-0.36	1 (1%) 80 74	26, 53, 99, 110	0
14	CO	88/88 (100%)	-0.42	0 100 100	8, 44, 84, 109	0
15	AP	84/84 (100%)	0.40	7 (8%) 11 9	33, 71, 110, 143	0
15	CP	84/84 (100%)	0.45	10 (11%) 4 5	39, 69, 111, 165	0
16	AQ	100/100 (100%)	-0.52	0 100 100	27, 62, 107, 131	0
16	CQ	100/100 (100%)	-0.34	2 (2%) 65 58	22, 66, 120, 135	0
17	AR	70/70 (100%)	-0.30	4 (5%) 23 19	19, 61, 102, 130	0
17	CR	70/70 (100%)	-0.29	3 (4%) 35 30	24, 56, 100, 125	0
18	AS	79/79 (100%)	-0.49	1 (1%) 77 70	17, 69, 111, 124	0
18	CS	79/79 (100%)	-0.13	5 (6%) 20 15	28, 65, 108, 130	0
19	AT	99/99 (100%)	-0.17	5 (5%) 28 24	17, 51, 85, 128	0
19	CT	99/99 (100%)	0.52	16 (16%) 1 2	26, 69, 110, 139	0
20	AY	661/687 (96%)	-0.44	23 (3%) 44 36	19, 64, 113, 178	0
20	CY	661/687 (96%)	-0.36	22 (3%) 46 38	11, 66, 108, 152	0
21	AA	1511/1511 (100%)	-0.46	14 (0%) 84 79	10, 90, 161, 248	0
21	CA	1511/1511 (100%)	-0.47	28 (1%) 66 59	10, 88, 160, 242	0
22	AW	77/77 (100%)	-0.15	9 (11%) 4 5	15, 71, 130, 150	0
22	CW	77/77 (100%)	0.09	7 (9%) 9 7	30, 88, 145, 178	0
23	AV	36/36 (100%)	1.73	8 (22%) 0 0	32, 89, 137, 186	0
23	CV	36/36 (100%)	3.53	16 (44%) 0 0	23, 139, 232, 237	0
24	AX	77/78 (98%)	-0.49	3 (3%) 39 32	3, 65, 233, 320	0
24	CX	77/78 (98%)	-0.36	2 (2%) 56 47	37, 123, 185, 285	0
25	BC	228/228 (100%)	1.24	65 (28%) 0 0	55, 104, 139, 159	0
25	DC	228/228 (100%)	0.75	48 (21%) 1 1	37, 90, 130, 169	0
26	BD	275/275 (100%)	-0.08	21 (7%) 13 11	10, 61, 103, 125	0
26	DD	275/275 (100%)	-0.03	14 (5%) 28 24	16, 57, 100, 127	0
27	BE	205/205 (100%)	0.16	10 (4%) 29 25	21, 60, 107, 131	0
27	DE	205/205 (100%)	0.15	8 (3%) 39 32	22, 57, 97, 142	0
28	BF	208/208 (100%)	0.37	22 (10%) 6 5	20, 67, 108, 149	0

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

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

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

The worst 5 of 1472 RSRZ outliers are listed below:

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

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
64	MG	CY	703	1/1	0.74	0.18	6,6,6,6	0
64	MG	BA	2901	1/1	0.75	0.12	2,2,2,2	0
63	NMY	BA	2904	42/42	0.79	0.26	42,50,59,62	42
61	GDP	AY	701	28/28	0.80	0.24	179,183,185,185	0
62	FUA	AY	702	37/37	0.81	0.69	198,199,200,201	0
63	NMY	DA	2901	42/42	0.81	0.24	31,42,51,53	42
63	NMY	BA	2902	42/42	0.82	0.22	14,24,43,44	42
62	FUA	CY	702	37/37	0.82	0.89	194,196,197,197	0
63	NMY	BA	2903	42/42	0.87	0.28	18,29,38,41	42
63	NMY	AA	1601	42/42	0.87	0.31	16,27,36,38	42

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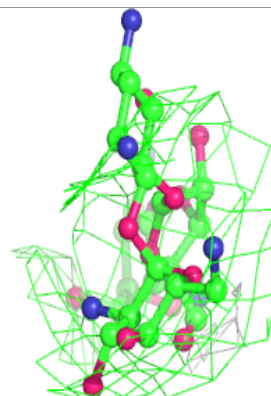
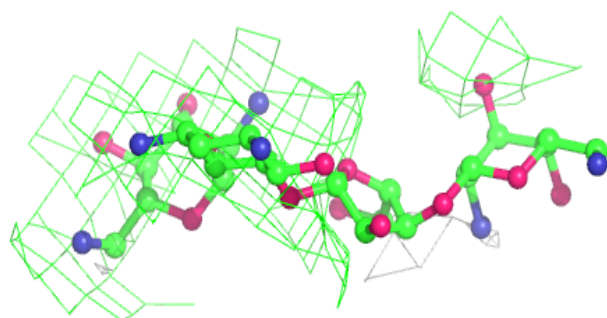
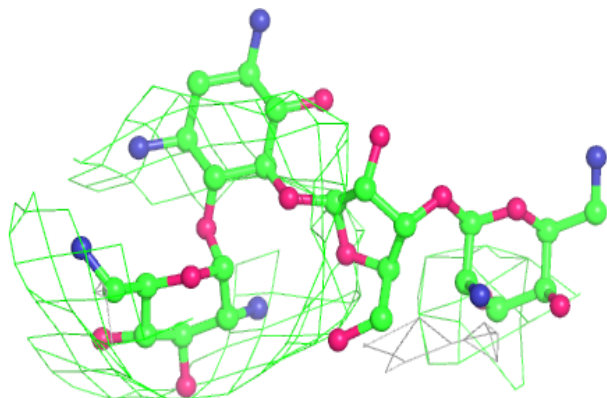
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
61	GDP	CY	701	28/28	0.88	0.14	104,108,109,110	0
63	NMY	CA	1601	42/42	0.90	0.23	14,25,34,37	42

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

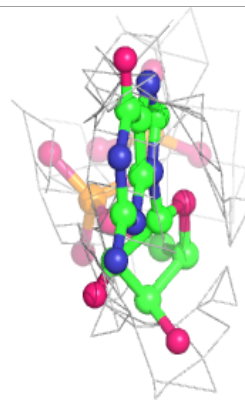
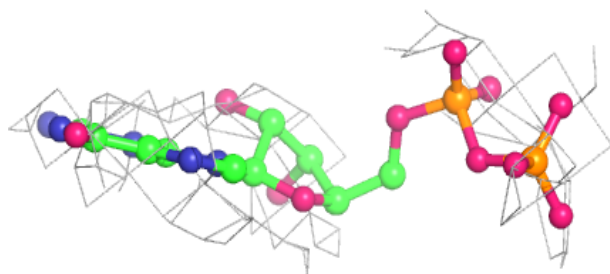
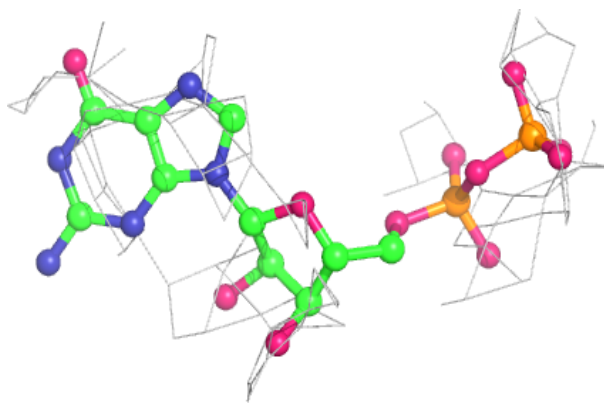
**Electron density around NMY BA 2904:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around GDP AY 701:**

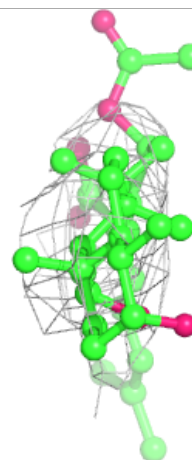
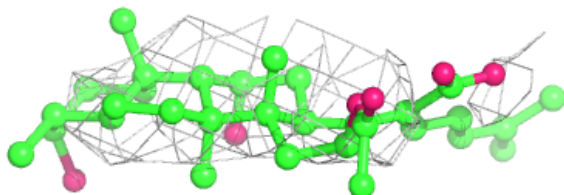
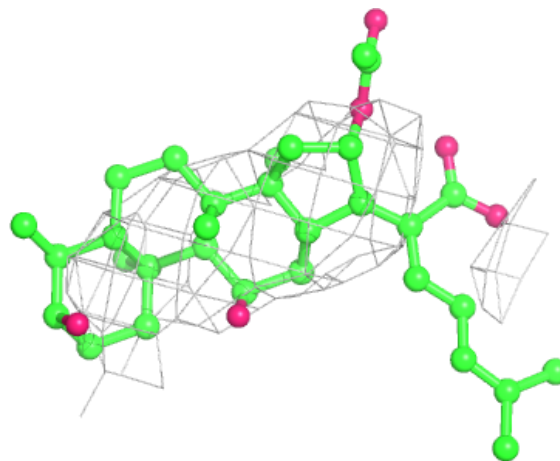
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





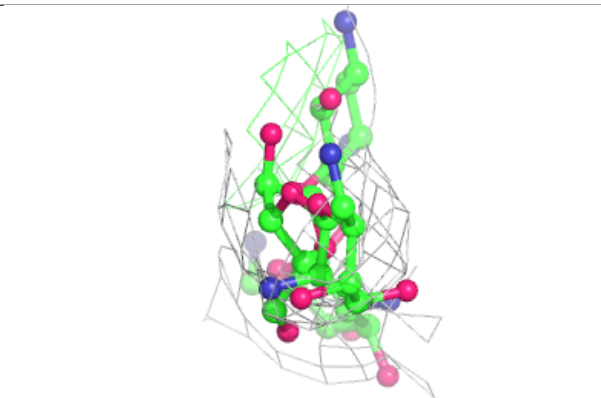
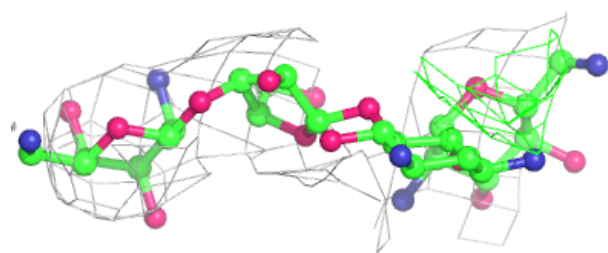
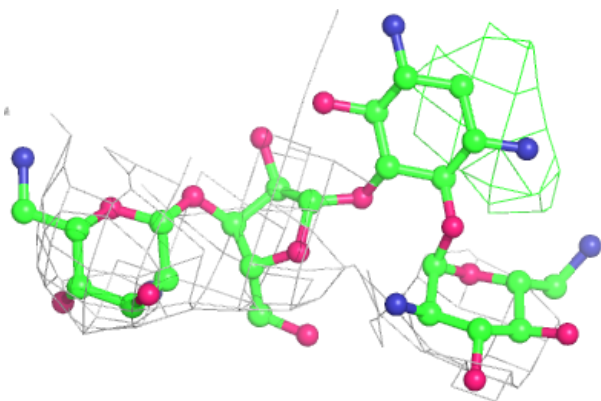
**Electron density around FUA AY 702:**

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

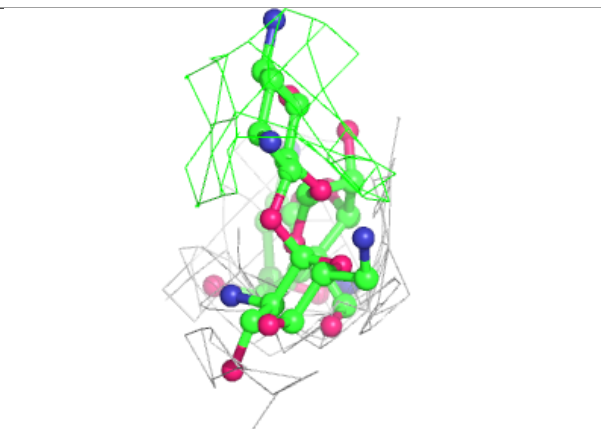
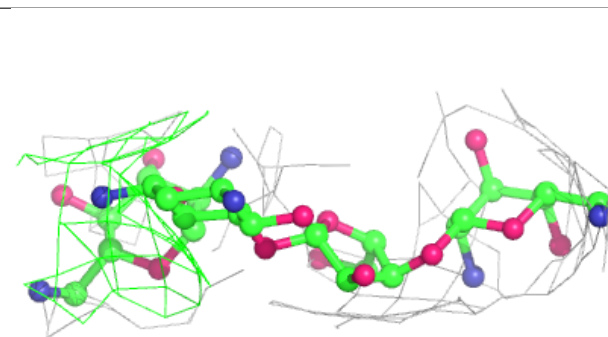
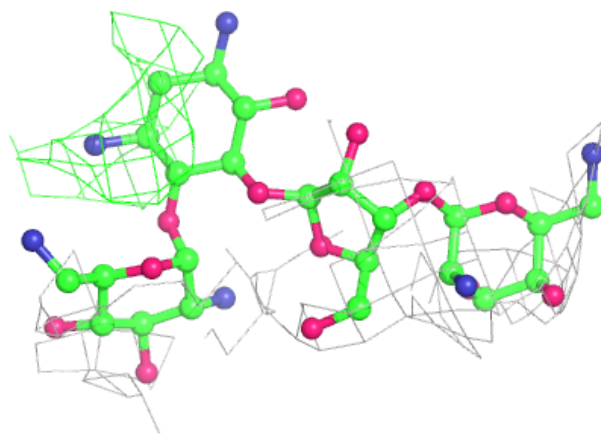


**Electron density around NMY DA 2901:**

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

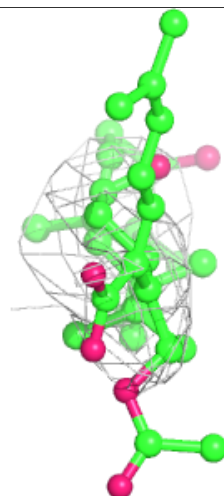
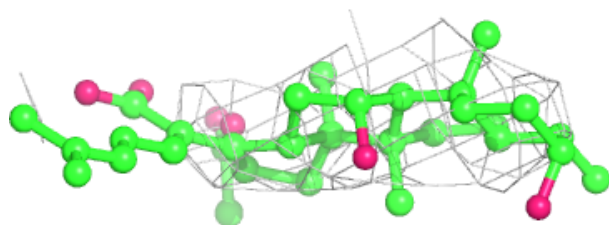
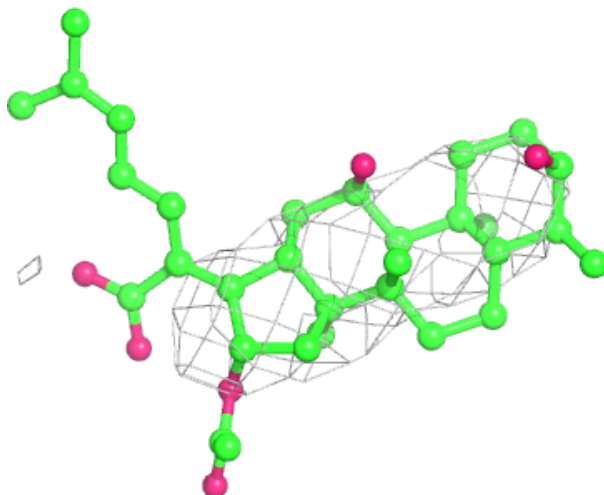
**Electron density around NMY BA 2902:**

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



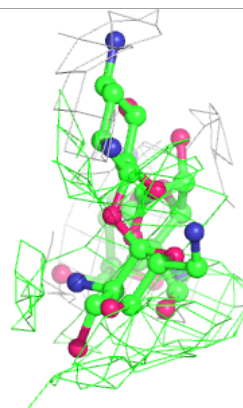
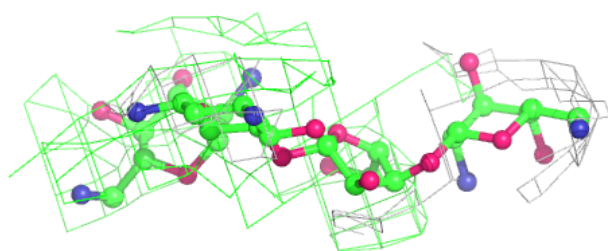
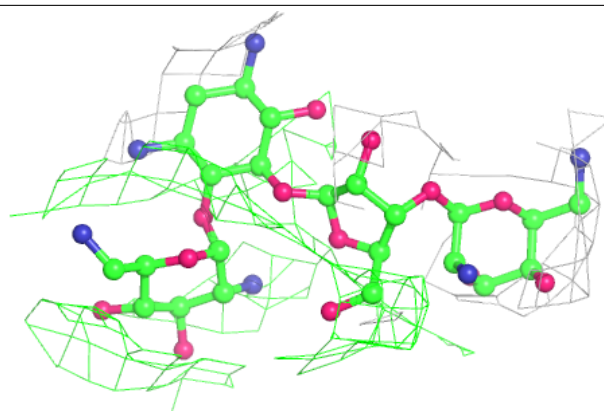
**Electron density around FUA CY 702:**

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



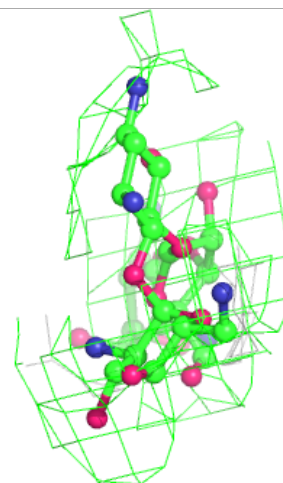
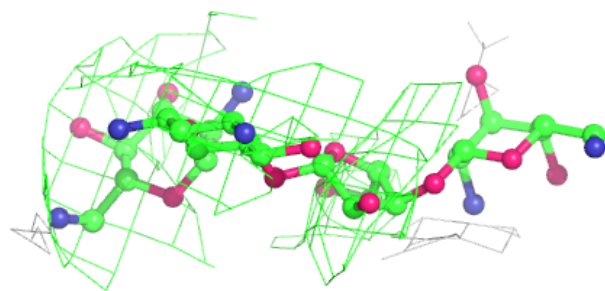
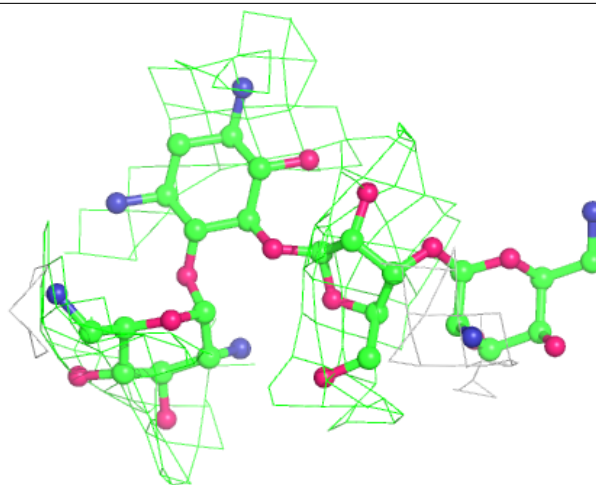
**Electron density around NMY BA 2903:**

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



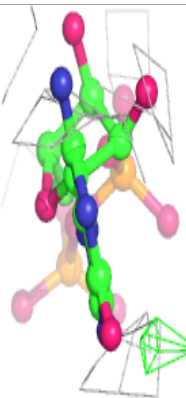
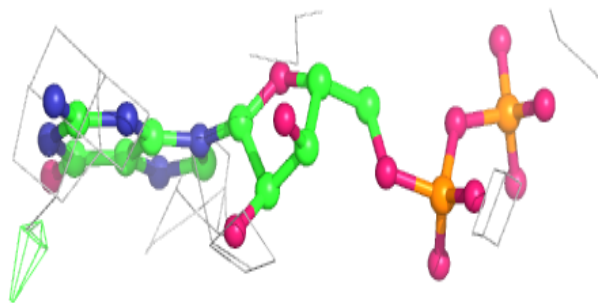
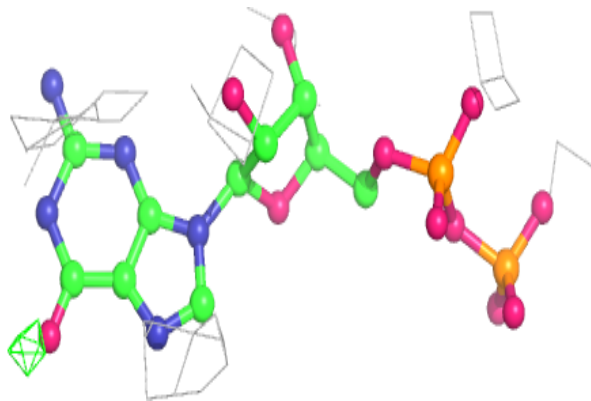
**Electron density around NMY AA 1601:**

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

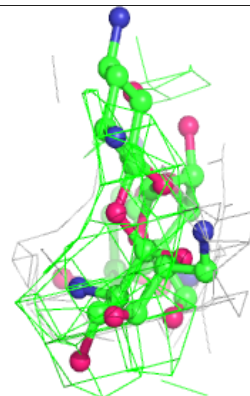
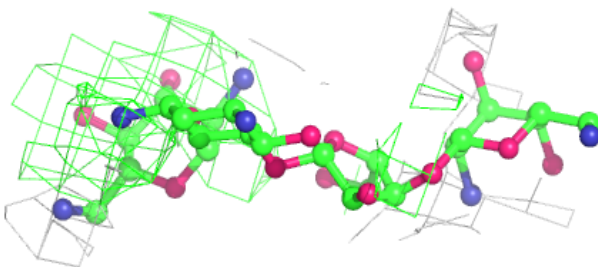
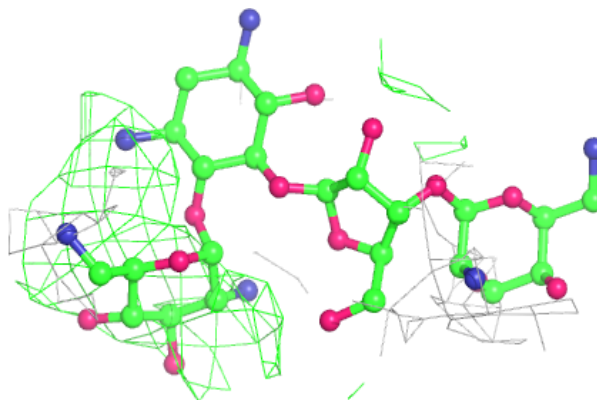


**Electron density around GDP CY 701:**

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

**Electron density around NMY CA 1601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.