



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2026 – 04:51 PM UTC

PDB ID : 4V5G / pdb_00004v5g
Title : The crystal structure of the 70S ribosome bound to EF-Tu and tRNA
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.
Deposited on : 2009-09-01
Resolution : 3.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

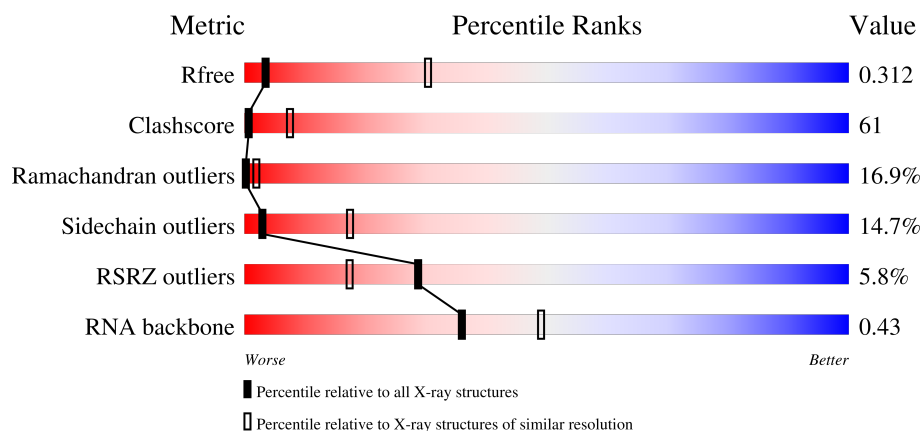
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 Å.

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



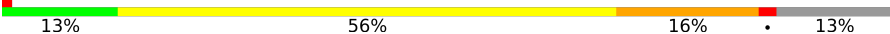
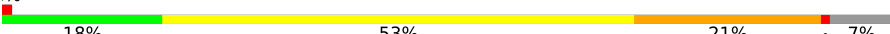
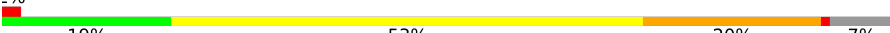
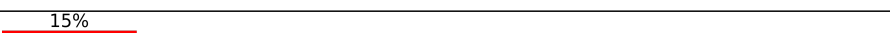
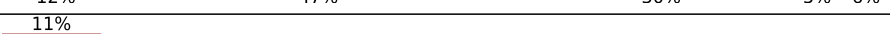
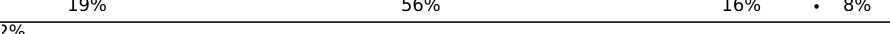
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)
RNA backbone	3983	1014 (4.14-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	4% 11% 66% 18% • •
1	CA	1522	3% 11% 67% 17% • •
2	AB	256	11% 56% 23% • 8%
2	CB	256	% 10% 57% 22% • 8%

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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	406	
25	CZ	406	
26	B0	85	
26	D0	85	

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Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	

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Mol	Chain	Length	Quality of chain
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	

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Mol	Chain	Length	Quality of chain
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	PSU	CY	55	-	-	X	-
60	ZN	D9	101	-	-	X	-
62	GDP	AZ	501	-	-	X	-
62	GDP	CZ	501	-	-	X	-

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 306876 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 RNA chain called 16S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

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

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	13	Total	C	N	O	P	0	0	0
			272	124	50	86	12			
23	CX	13	Total	C	N	O	P	0	0	0
			272	124	50	86	12			

- Molecule 24 is a RNA chain called A-SITE TRNA THR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	0	0	0
			1650	741	292	541	76			
24	CY	77	Total	C	N	O	P	0	0	0
			1650	741	292	541	76			

- Molecule 25 is a protein called ELONGATION FACTOR TU-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	374	Total	C	N	O	S	0	0	0
			2900	1832	508	548	12			
25	CZ	374	Total	C	N	O	S	0	0	0
			2900	1832	508	548	12			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
27	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
29	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			
30	D4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
33	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
34	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
40	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
41	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
43	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	131	Total	C	N	O		0	0	1
			651	390	131	130				
44	DJ	131	Total	C	N	O		0	0	1
			651	390	131	130				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	141	Total	C	N	O		0	0	1
			701	420	141	140				
45	DK	141	Total	C	N	O		0	0	1
			701	420	141	140				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
46	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
51	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
52	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
53	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
55	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

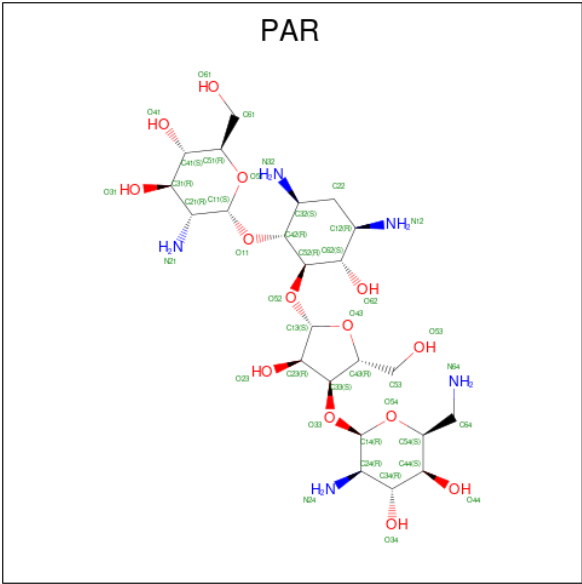
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
57	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			
58	DZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 59 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	N	O	0	0
			42	23	5	14		
59	CA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AD	1	Total	Zn	0	0
			1	1		
60	AN	1	Total	Zn	0	0
			1	1		
60	B4	1	Total	Zn	0	0
			1	1		
60	B9	1	Total	Zn	0	0
			1	1		
60	CD	1	Total	Zn	0	0
			1	1		
60	CN	1	Total	Zn	0	0
			1	1		

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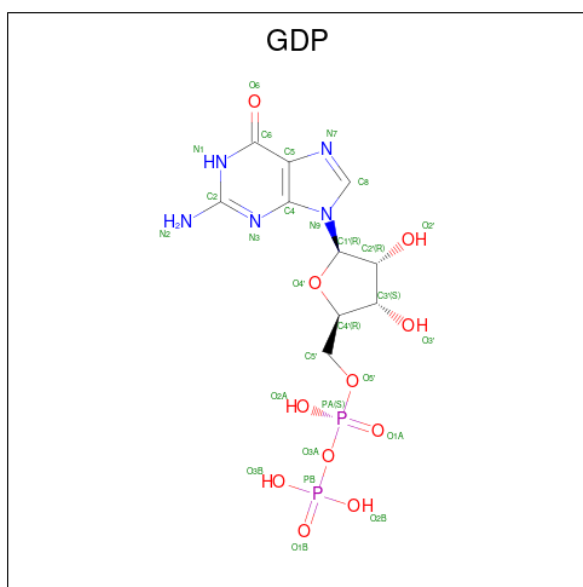
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	D4	1	Total	Zn	0	0
			1	1		
60	D9	1	Total	Zn	0	0
			1	1		

- Molecule 61 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

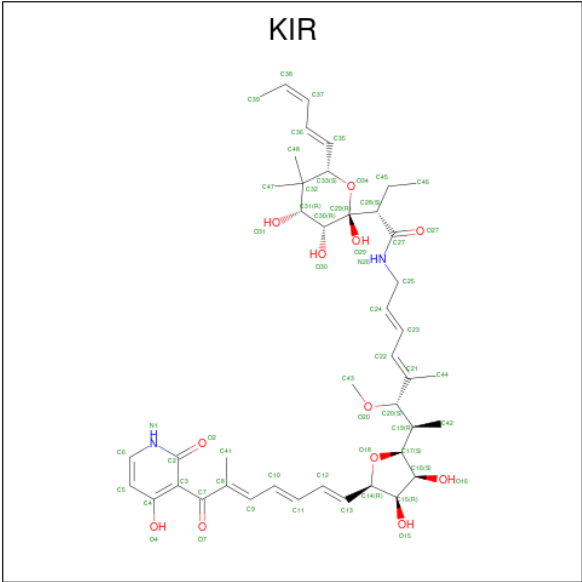
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AY	1	Total	Mg	0	0
			1	1		
61	CY	1	Total	Mg	0	0
			1	1		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AZ	1	Total 28	C 10	N 5	O 11	P 2	0	0
62	CZ	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 63 is KIRROMYCIN (CCD ID: KIR) (formula: C₄₃H₆₀N₂O₁₂).

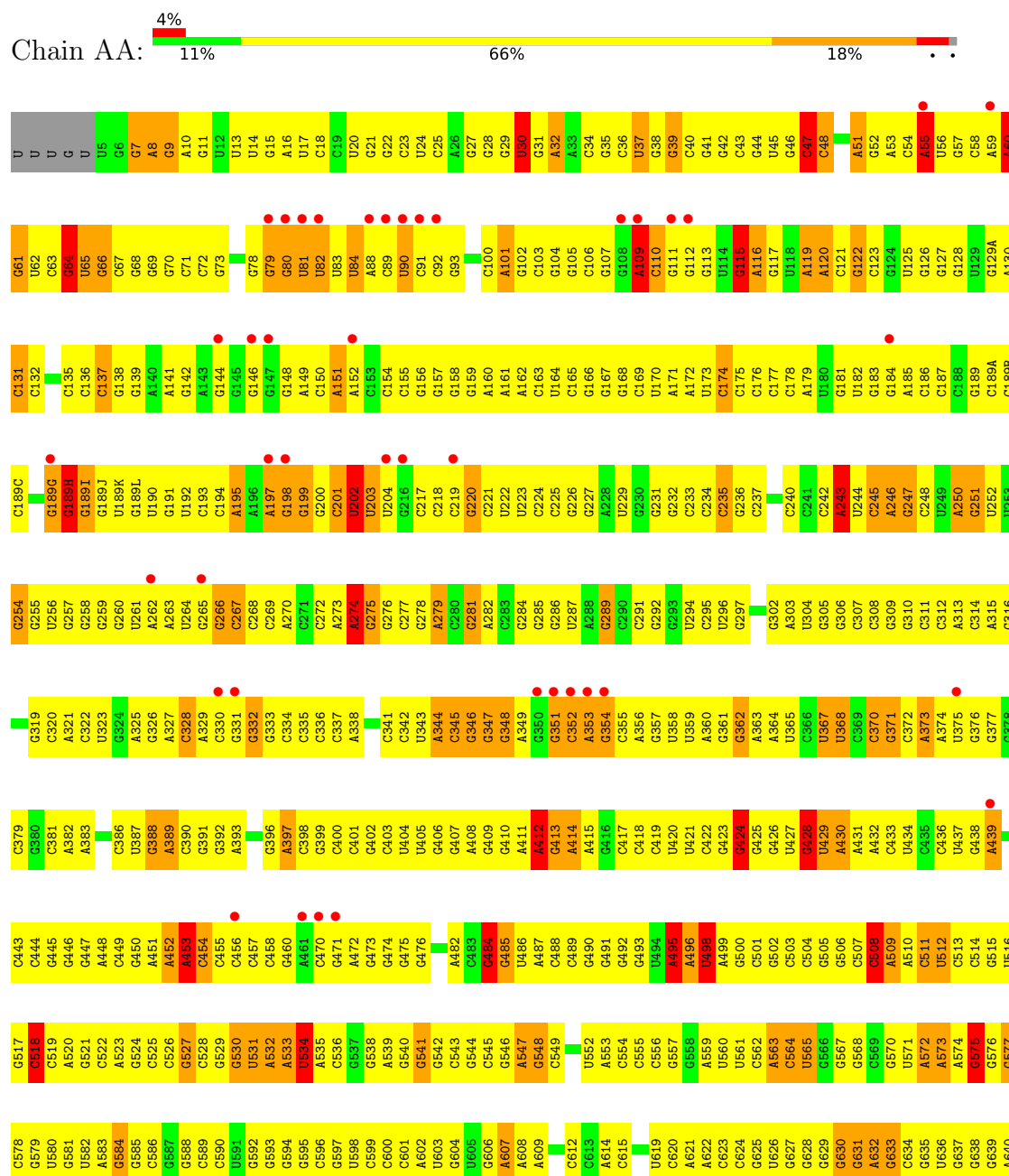


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
63	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
63	CZ	1	Total	C	N	O	0	0
			57	43	2	12		

3 Residue-property plots

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

• Molecule 1: 16S RIBOSOMAL RNA

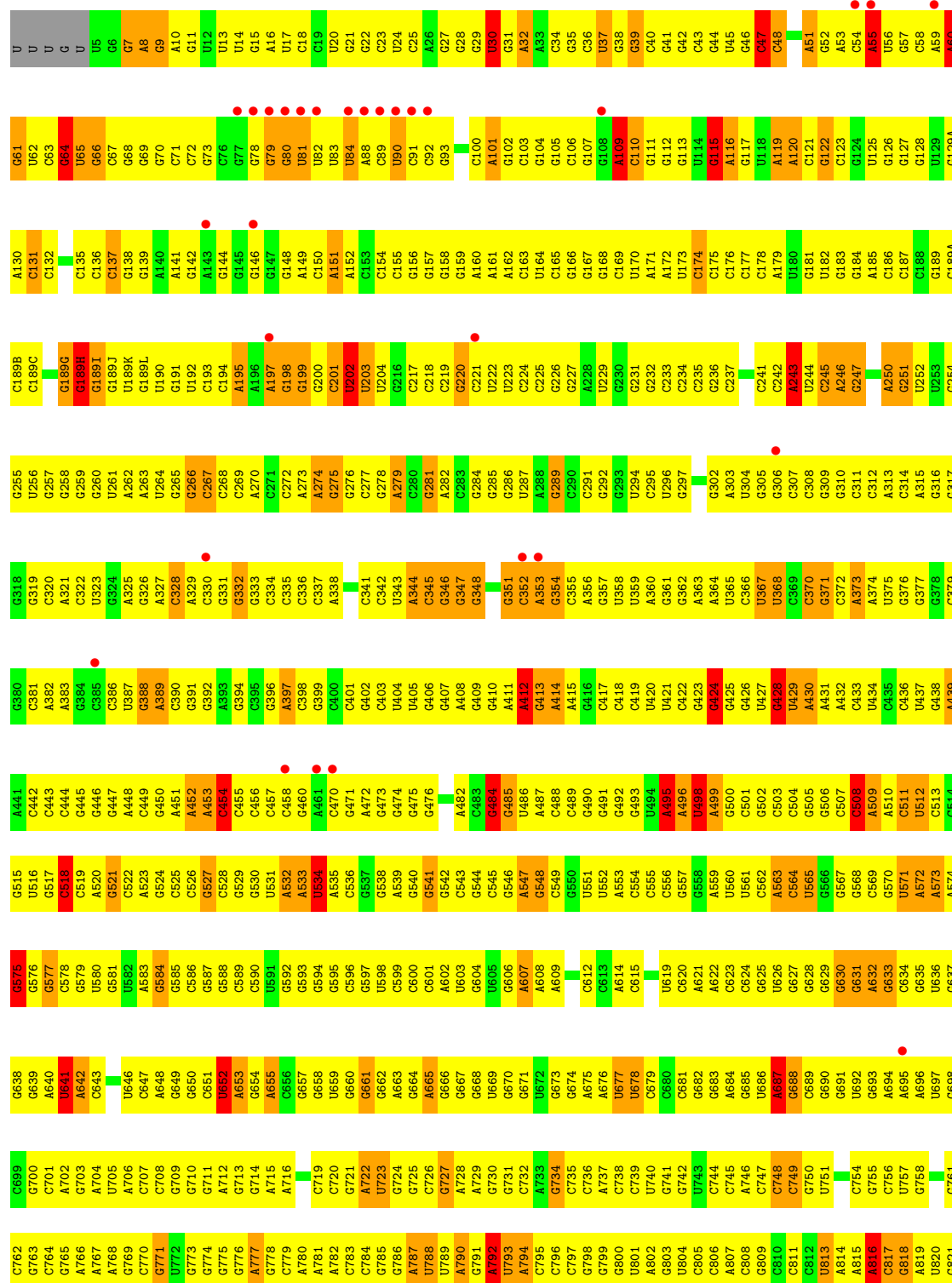


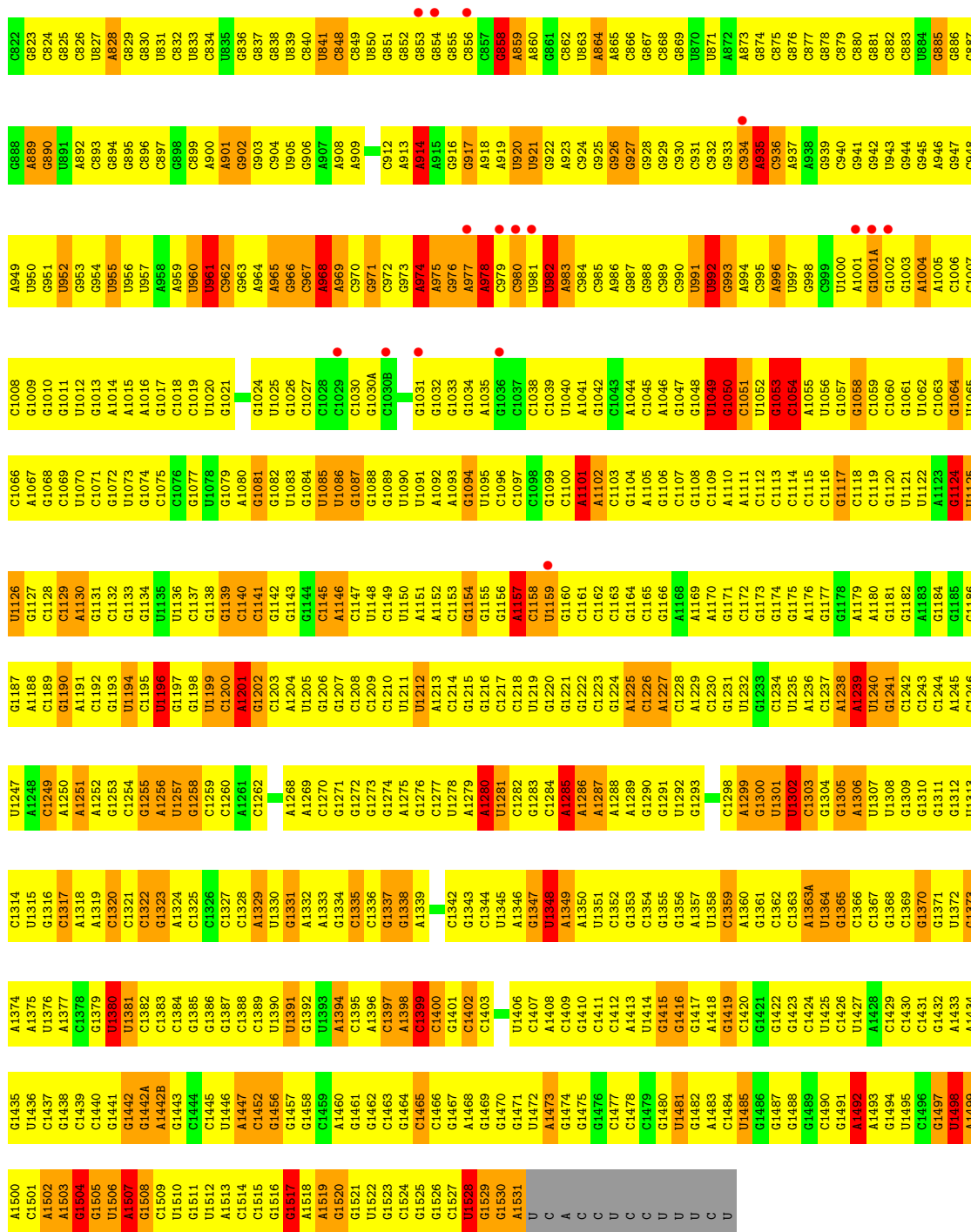
C1440	C1441	C1442	C1443	C1444	C1445	C1446	C1447	C1448	C1449	C1450	C1451	C1452	C1453	C1454	C1455	C1456	C1457	C1458	C1459	C1460	C1461	C1462	C1463	C1464	C1465	C1466	C1467	C1468	C1469	C1470	C1471	C1472	C1473	C1474	C1475	C1476	C1477	C1478	C1479	C1480	C1481	C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505																								
U1380	U1381	C1382	C1383	C1384	C1385	C1386	C1387	C1388	C1389	C1390	U1391	C1392	U1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	U1406	U1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438	C1439	C1504																													
C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	C1329	C1330	C1331	C1332	C1333	C1334	C1335	C1336	C1337	C1338	C1339	C1340	C1341	C1342	C1343	C1344	C1345	C1346	C1347	C1348	C1349	C1350	C1351	C1352	C1353	C1354	C1355	C1356	C1357	C1358	C1359	C1360	C1361	C1362	C1363	C1364	C1365	C1366	C1367	C1368	C1369	C1370	C1371	C1372	C1373	C1374	C1375	C1376	C1377	C1378	C1379																														
A1252	G1253	C1254	G1255	A1256	U1257	G1258	C1259	C1260	A1261	C1262	A1269	C1270	G1271	G1272	G1273	G1274	A1275	G1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	G1291	U1292	G1293	C1298	C1299	C1300	C1301	C1302	C1303	C1304	G1305	C1306	U1307	U1308	U1309	G1310	C1311	C1312	U1313	C1314	U1315	C1316	C1317	A1318	C1319	A1320																															
C1192	G1193	U1194	C1195	U1196	G1197	G1198	U1199	C1200	A1201	C1202	C1203	A1204	U1205	G1206	C1207	C1208	C1209	C1210	U1211	U1212	C1213	C1214	G1215	G1216	C1217	C1218	U1219	C1220	G1221	C1222	C1223	C1224	C1225	A1226	A1227	C1228	A1229	C1230	G1231	U1232	C1233	C1234	U1235	A1236	C1237	A1238	A1239	U1240	G1241	C1242	C1243	C1244	C1245	C1246	U1247	A1248	C1249	A1250																															
G1131	C1132	G1133	C1134	U1135	U1136	C1137	G1138	C1139	C1140	C1141	G1142	U1143	G1144	C1145	G1146	U1147	C1148	C1149	U1150	U1151	A1152	C1153	G1154	G1155	G1156	A1157	U1158	U1159	G1160	C1161	C1162	C1163	G1164	C1165	G1166	A1168	A1169	A1170	G1171	C1172	G1173	C1174	G1175	A1176	G1177	A1178	A1179	A1180	G1181	A1182	A1183	G1184	G1185	G1186	G1187	A1188	C1189	A1190																															
C1071	G1072	U1073	G1074	C1075	U1076	G1077	U1078	C1079	A1080	G1081	G1082	U1083	G1084	U1085	U1086	G1087	G1088	U1089	U1090	U1091	A1092	C1093	U1094	U1095	C1096	C1097	C1098	C1099	C1100	A1101	A1102	C1103	G1104	A1105	G1106	C1107	G1108	C1109	A1110	A1111	C1112	C1113	C1114	C1115	C1116	G1117	C1118	C1119	G1120	U1121	U1122	A1123	G1124	U1125	U1126	G1127	C1128	C1129	A1130																														
G1011	U1012	A1013	G1014	C1015	U1016	C1017	C1018	C1019	U1020	G1021	G1024	U1025	C1026	C1027	C1028	C1029	C1030	G1030A	G1031	G1032	G1033	G1034	A1035	G1036	C1037	C1038	C1039	U1040	U1041	C1042	C1043	A1044	C1045	A1046	G1047	G1048	U1049	G1050	C1051	U1052	G1053	C1054	A1055	U1056	G1057	C1058	C1059	U1060	G1061	U1062	C1063	G1064	U1065	C1066	A1067	C1068	U1069	U1070																															
G951	U952	G953	C954	C955	U956	U957	U960	U961	C962	G963	A964	A965	G966	C967	A968	A969	C970	G971	C972	G973	A974	C975	G976	G977	A978	C979	U980	U981	U982	A983	C984	C985	A986	G987	G988	C989	C990	U991	U992	G993	C994	C995	A996	U997	G998	C999	U1000	A1001	G1001A	G1002	U1003	A1004	C1005	C1006	C1007	C1008	G1009	G1010																															
A889	C890	U891	C892	C893	C894	C895	C896	C897	U898	C899	A900	G901	G902	C903	C904	U905	A908	A909	C912	A913	C914	A915	A916	C917	C918	C919	C920	C921	C922	A923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	A935	C936	A937	C938	C939	C940	C941	C942	U943	C944	C945	C946	C947	C948	U950																																	
G823	C824	C825	C826	U827	A828	C829	C830	U831	C832	U833	C834	U835	C836	C837	C838	U839	C840	U841	C843	C849	U850	C851	C852	C853	C854	C855	C856	C857	C858	A859	U793	A860	C861	C862	U863	A864	A865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	U884	C885	C886	C887	C888																													
A702	G703	U704	U705	G706	C707	C708	C709	G710	G711	U712	G713	G714	A715	G716	C719	C720	G721	A722	U723	G724	G725	C726	G727	A728	C729	A730	G731	C732	A733	G734	C735	C736	A737	C738	C739	U740	G741	G742	U743	C744	C745	A746	C747	C748	C749	G750	U751	G752	A753	C754	G755	C756	U757	A758	G759	C760	C761	C762																															
U641	A642	C643	U646	C647	A648	C649	C650	C651	U652	A653	G654	A655	C656	C657	C658	U659	G660	C661	C662	A663	G664	A665	C666	C667	C668	U669	C670	C671	U672	C763	C764	G765	A766	U767	C768	C769	C770	C771	U772	C773	G774	G775	G776	A777	A716	C719	C720	G721	A722	U723	G724	G725	C726	G727	A728	C729	A730	G731	C732	A733	G734	C735	C736	A737	C738	C739	U740	G741	G742	U743	C744	C745	A746	C747	C748	C749	G750	U751	G752	A753	C754	G755	C756	U757	A758	G759	C760	C761	C762

U1506	U1507	C1508	C1509	U1510	G1511	U1512	A1513	C1514	C1515	C1516	G1517	A1518	A1519	G1520	G1521	U1522	G1523	C1524	G1525	G1526	C1527	U1528	G1529	G1530	G1531	U	C	A	C	U	C	C	U	U	U	C	U
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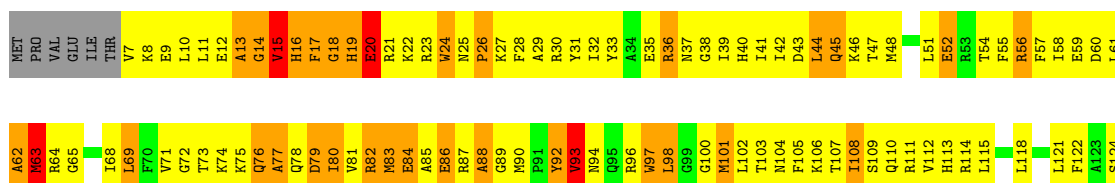
● Molecule 1: 16S RIBOSOMAL RNA

Chain CA: 3% 11% 67% 17%

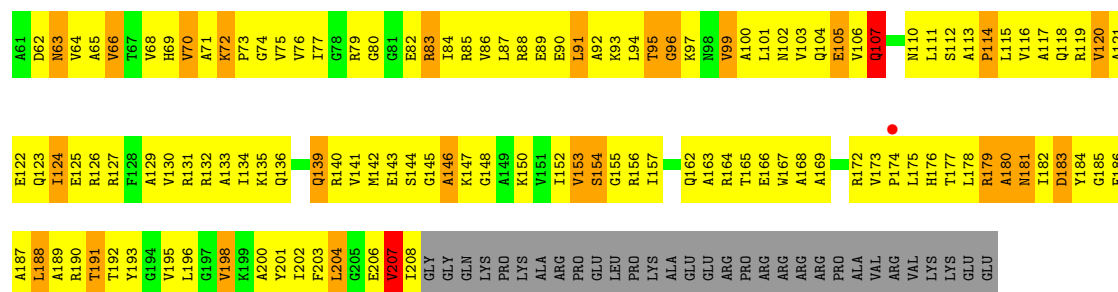




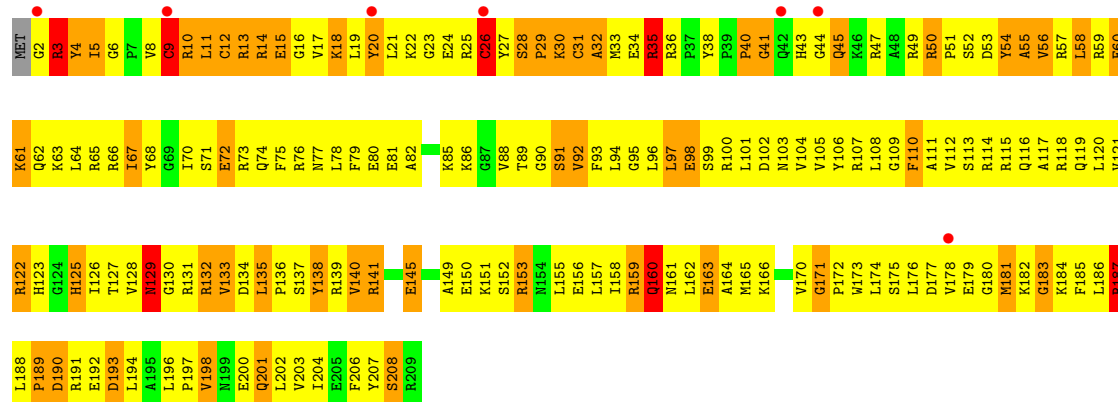
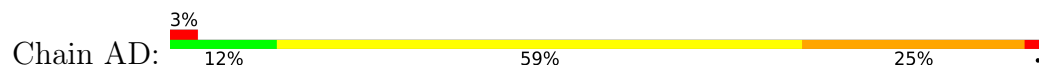
Chain AB: 11% 56% 23% 8%



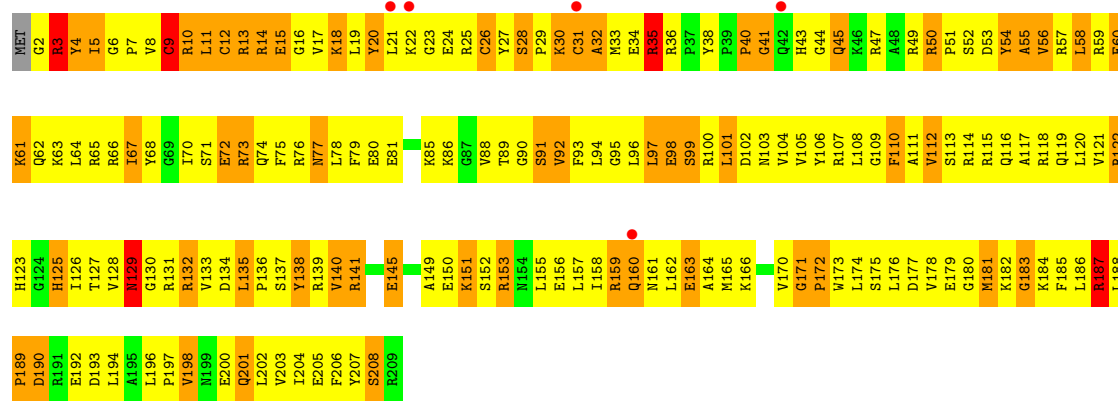
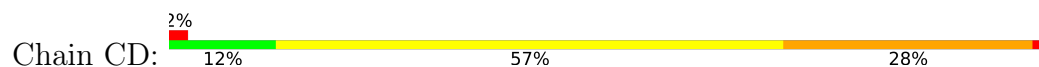




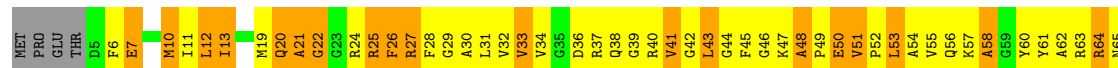
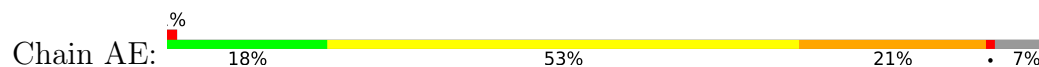
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

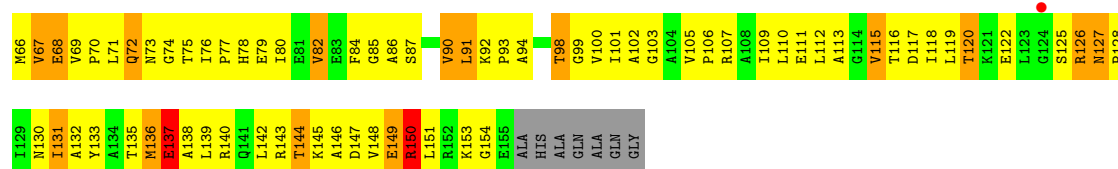


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

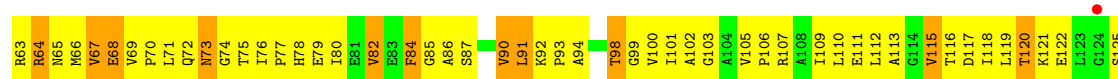
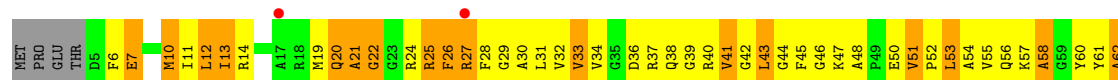
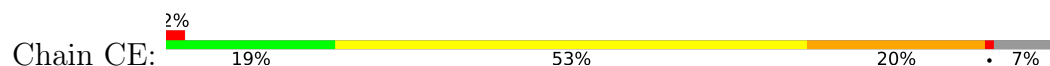


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

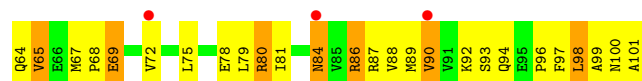
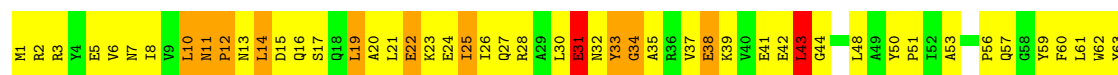




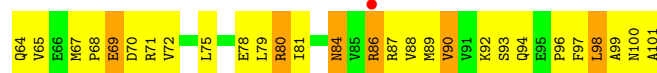
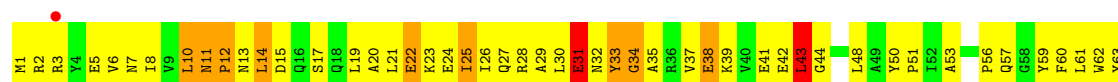
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



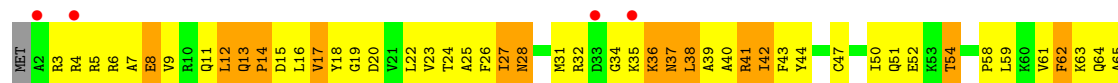
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

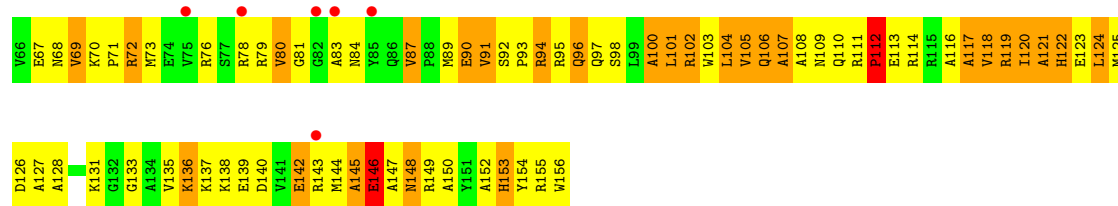


• Molecule 6: 30S RIBOSOMAL PROTEIN S6

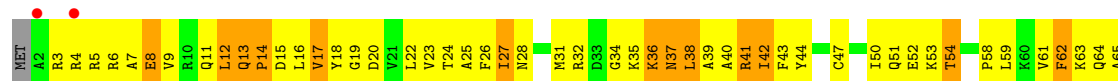


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

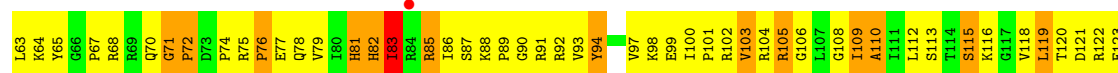
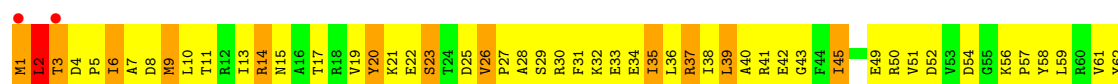




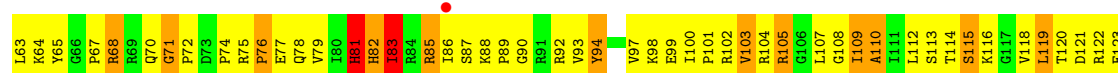
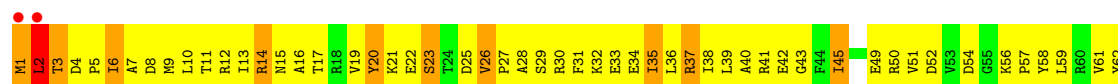
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



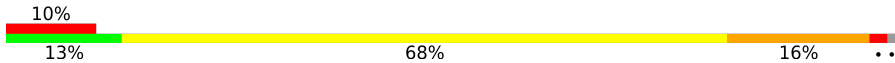
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

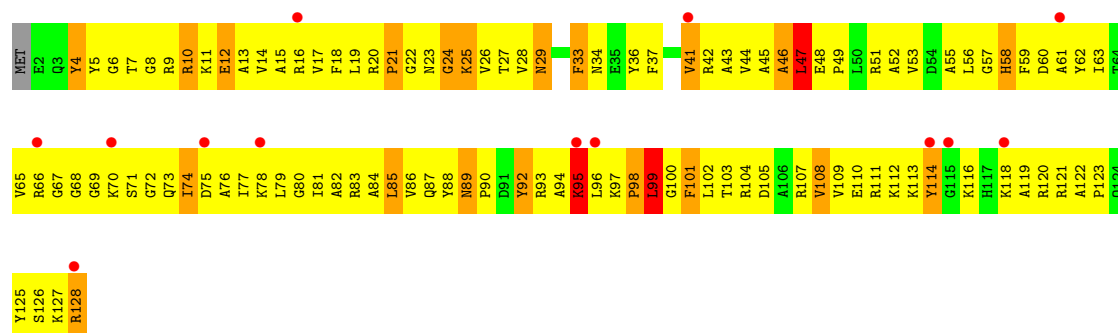


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

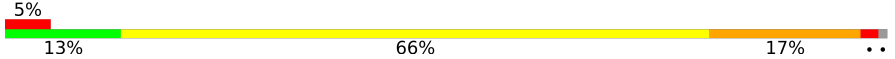


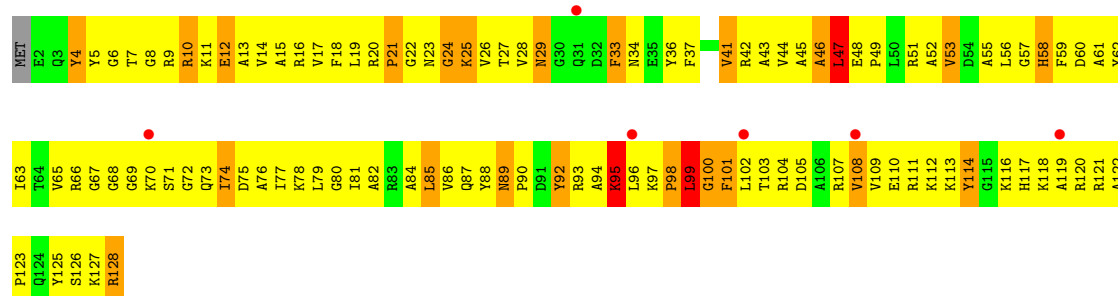
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI: 

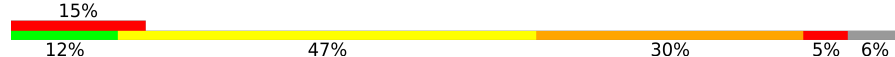


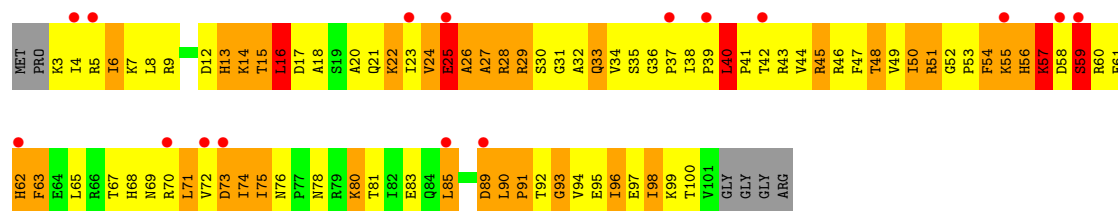
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI: 



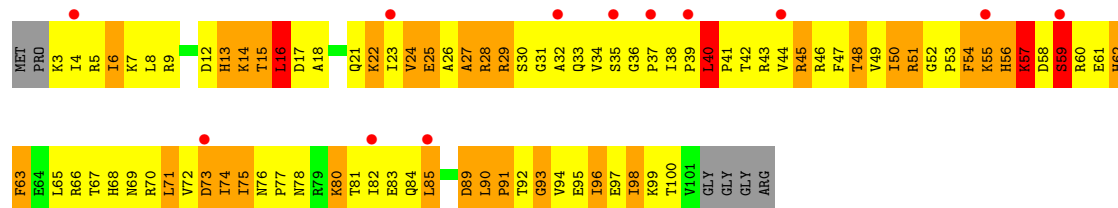
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ: 

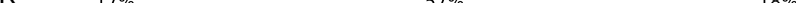


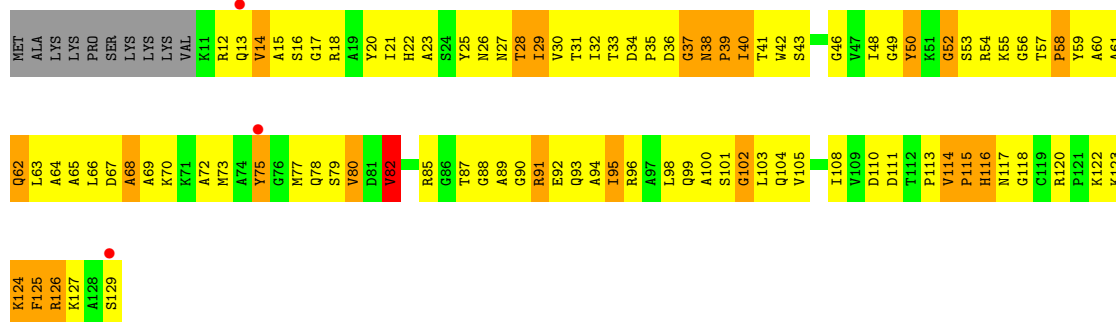
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ: 

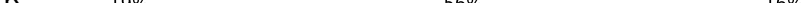


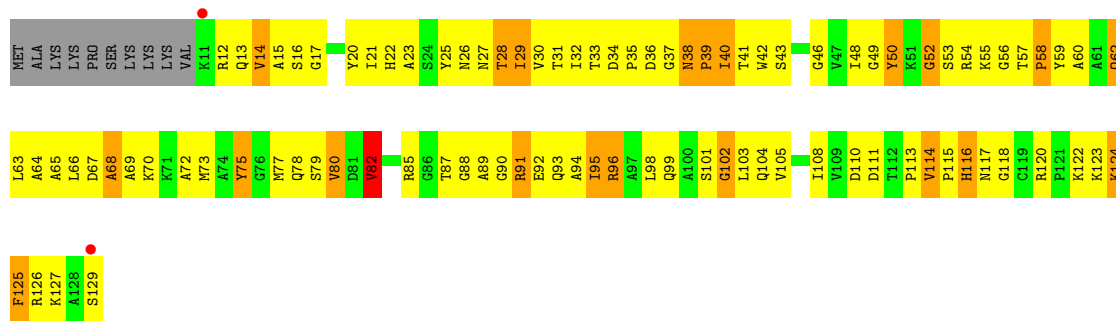
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK: 



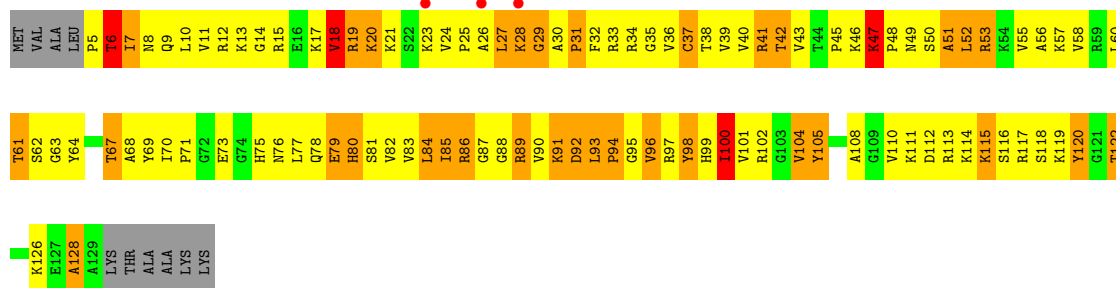
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK: 



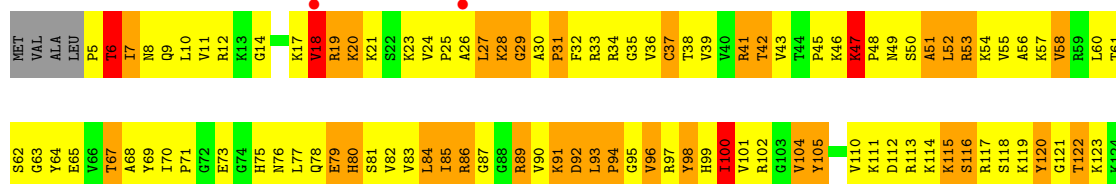
● Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



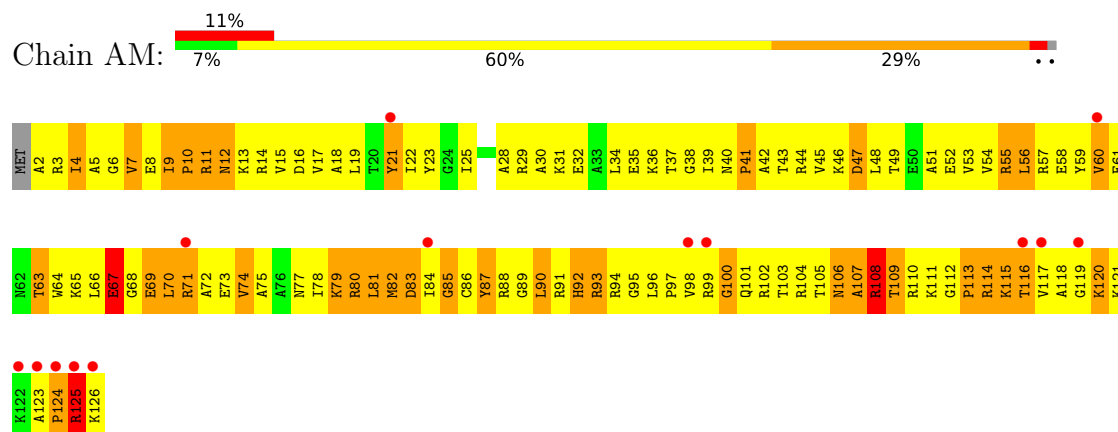
● Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL: 

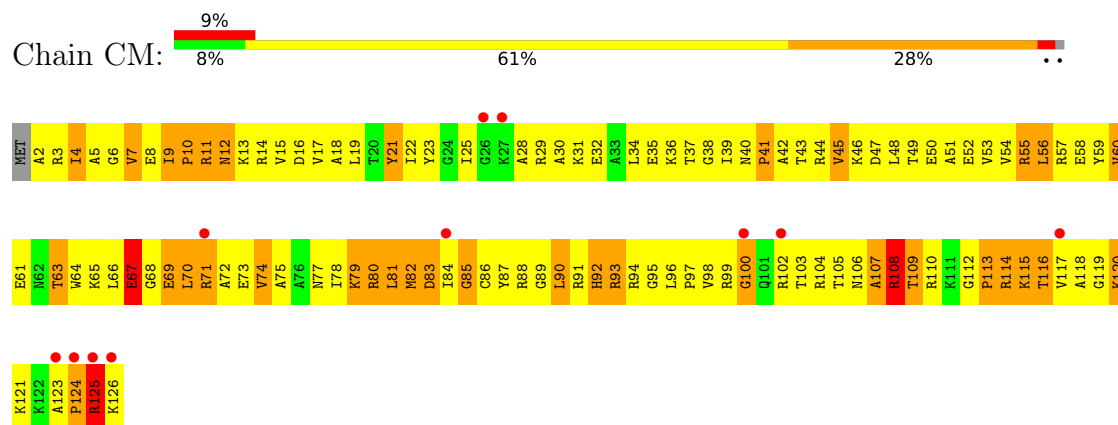




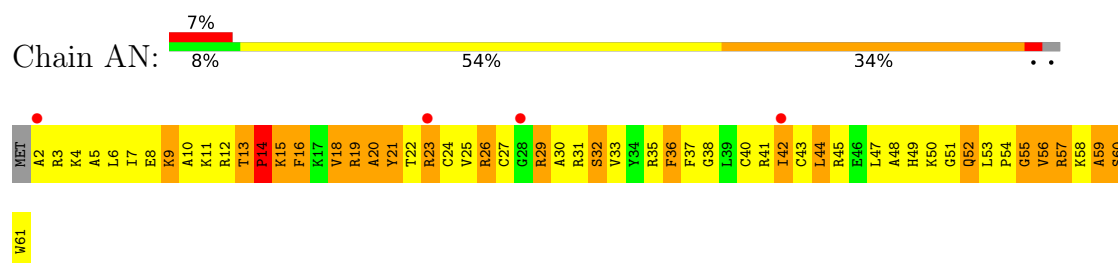
● Molecule 13: 30S RIBOSOMAL PROTEIN S13



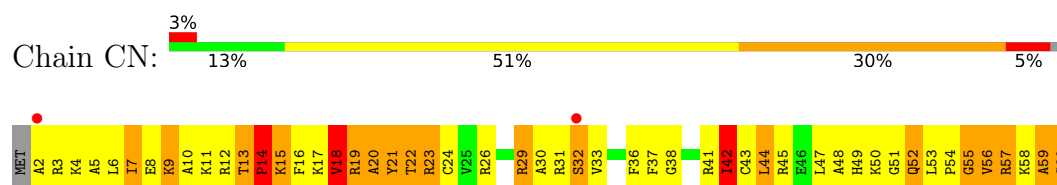
● Molecule 13: 30S RIBOSOMAL PROTEIN S13



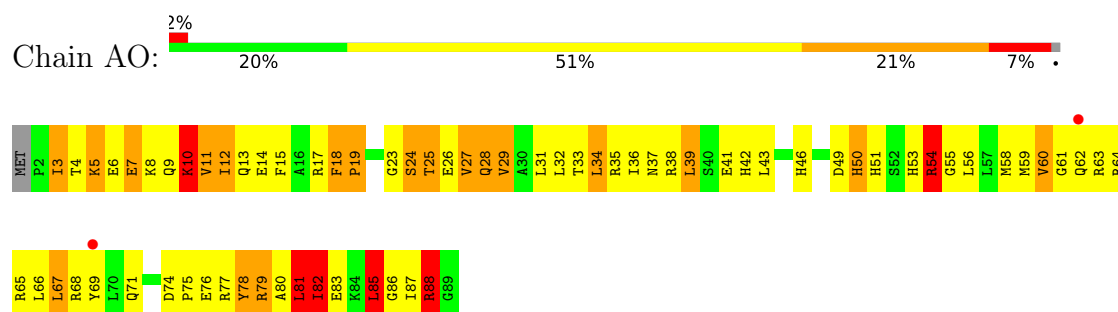
● Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



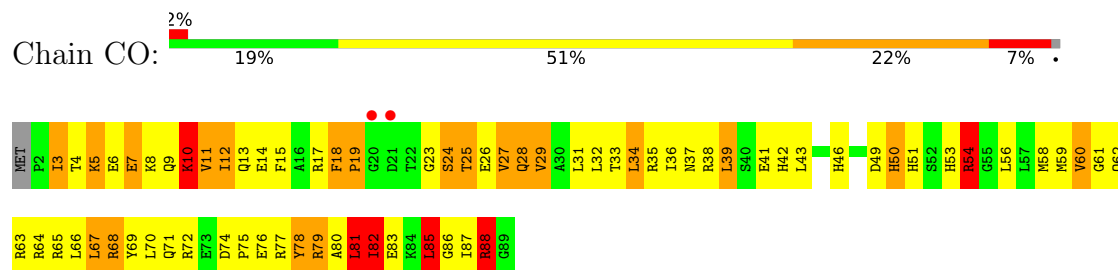
● Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



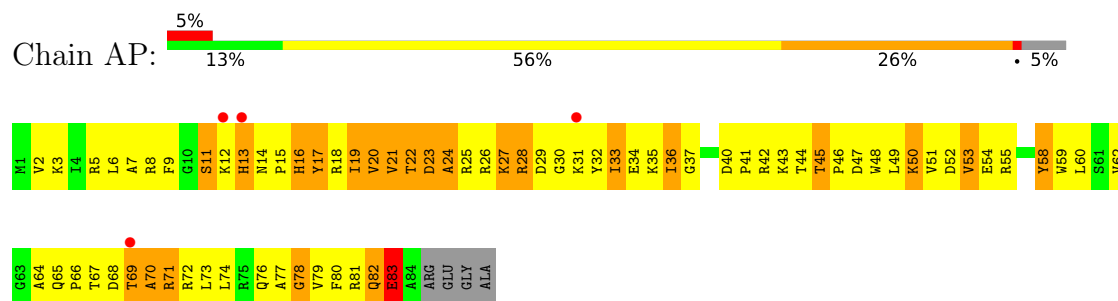
● Molecule 15: 30S RIBOSOMAL PROTEIN S15



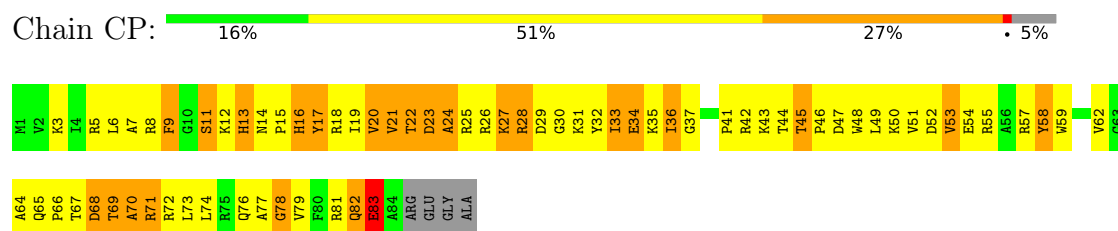
• Molecule 15: 30S RIBOSOMAL PROTEIN S15



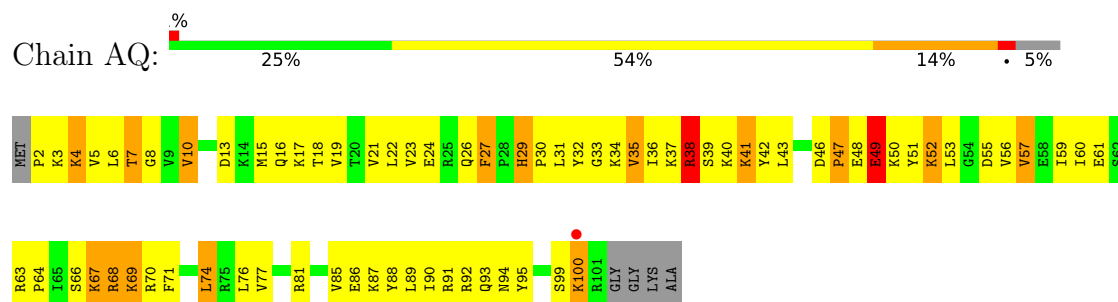
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



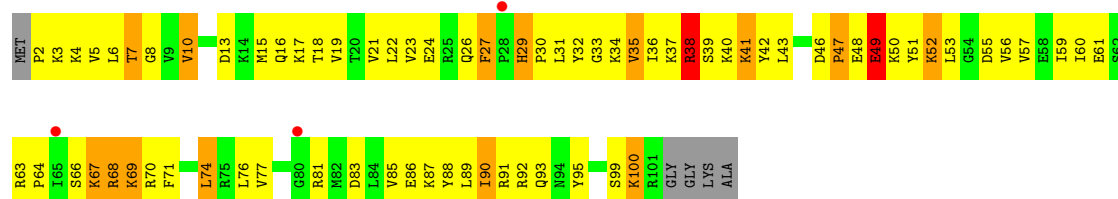
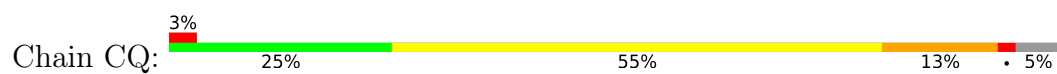
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



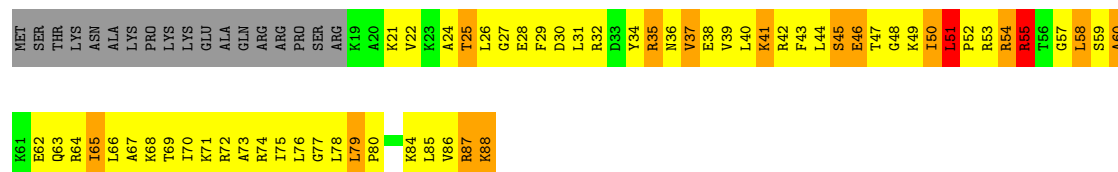
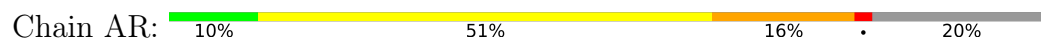
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



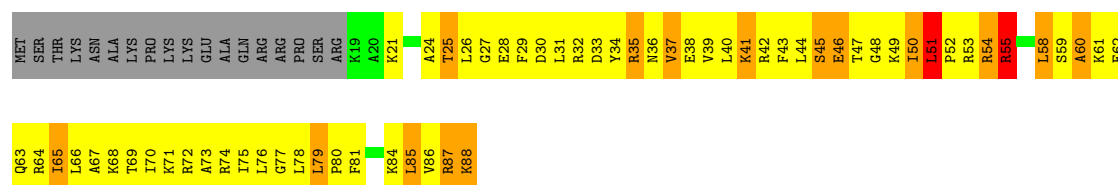
• Molecule 17: 30S RIBOSOMAL PROTEIN S17



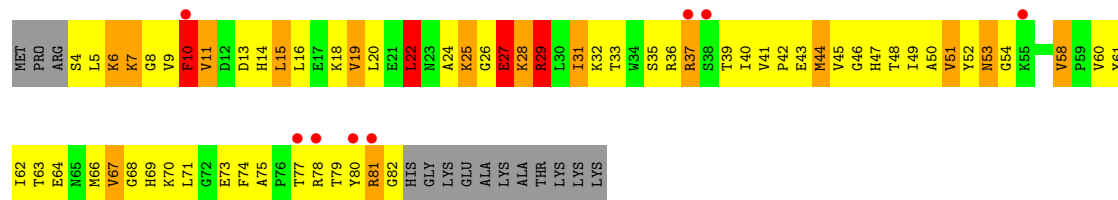
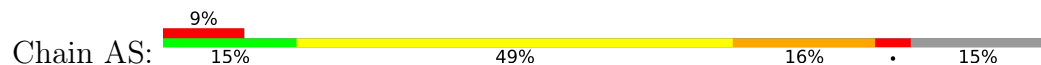
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



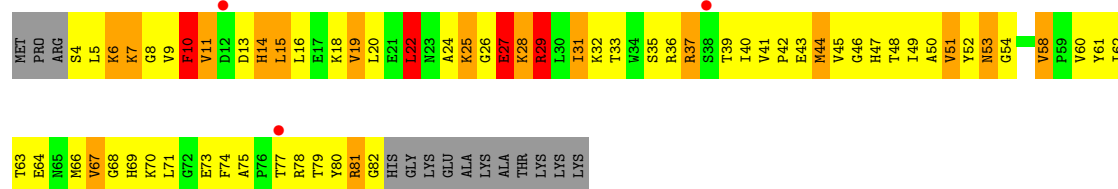
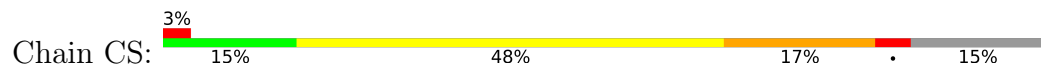
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



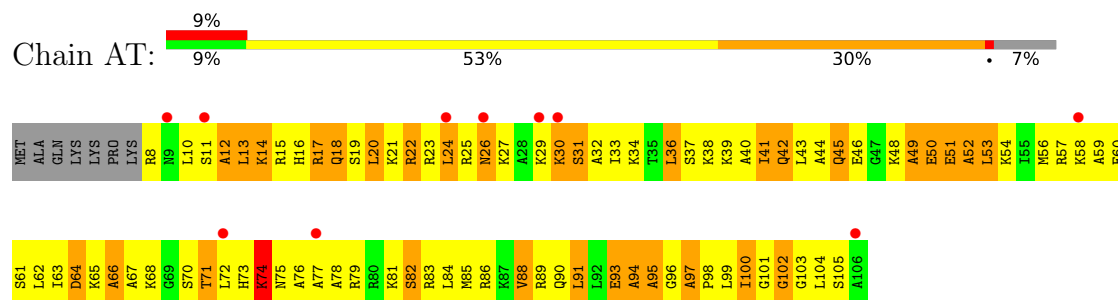
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



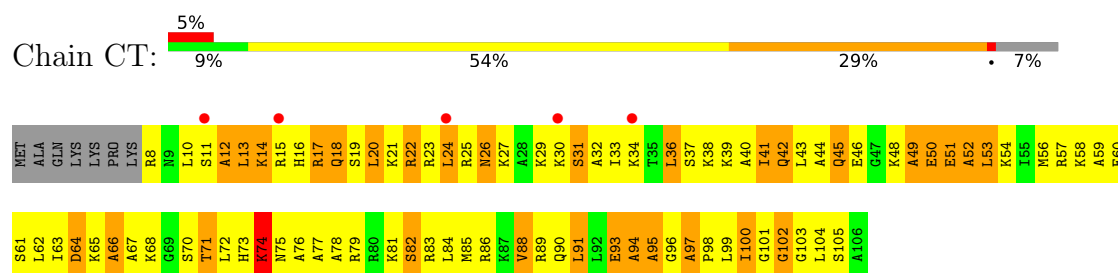
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



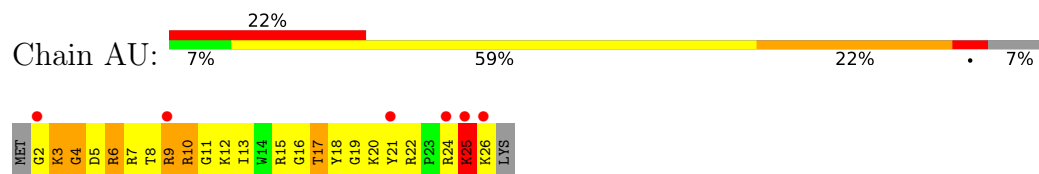
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



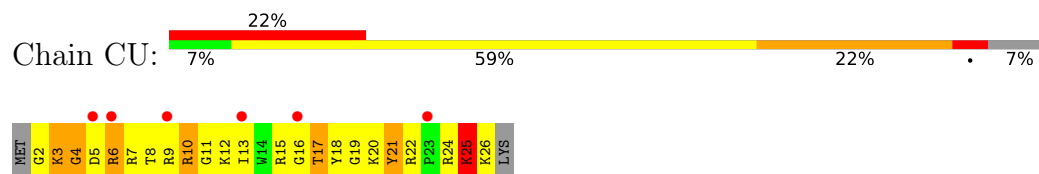
- Molecule 20: 30S RIBOSOMAL PROTEIN S20



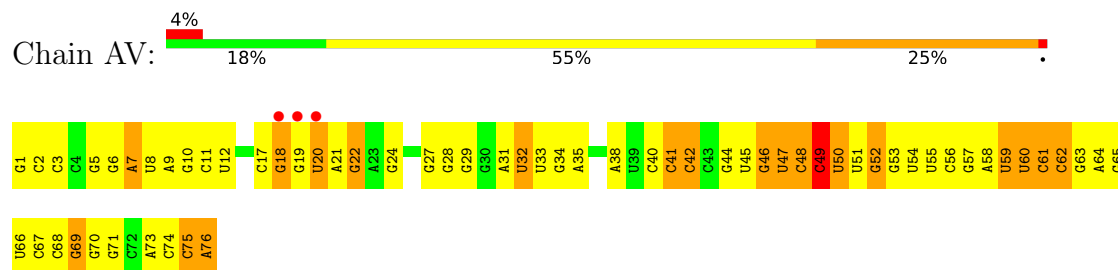
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



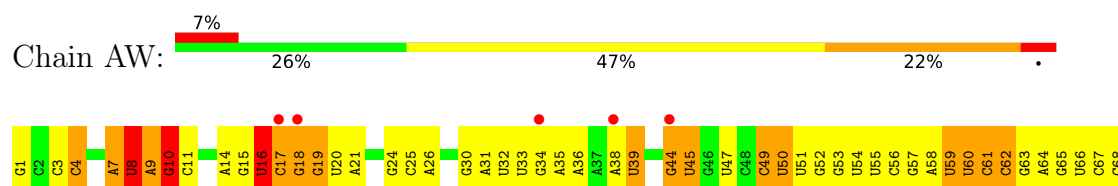
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

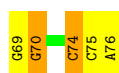


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

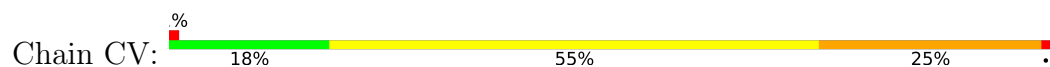


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

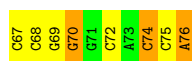




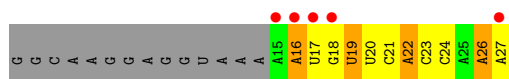
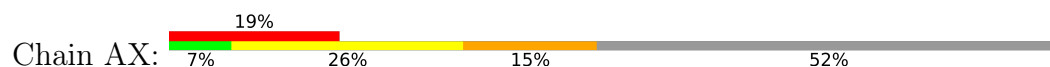
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



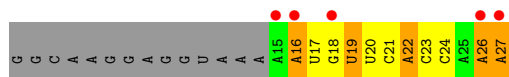
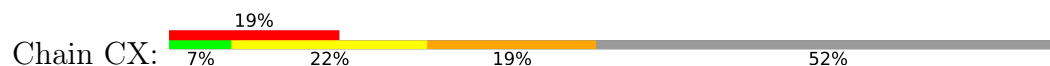
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



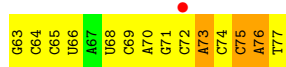
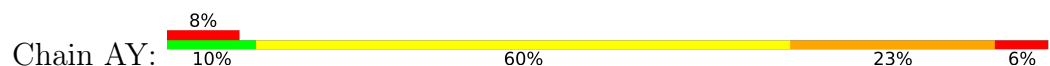
- Molecule 23: MRNA



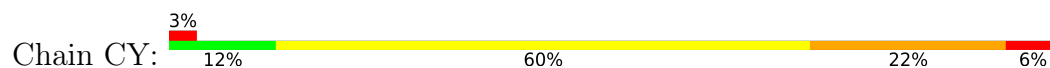
- Molecule 23: MRNA

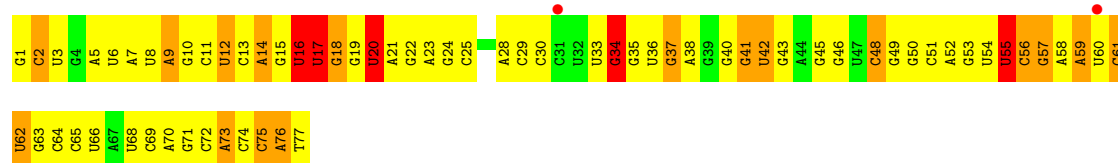


- Molecule 24: A-SITE TRNA THR

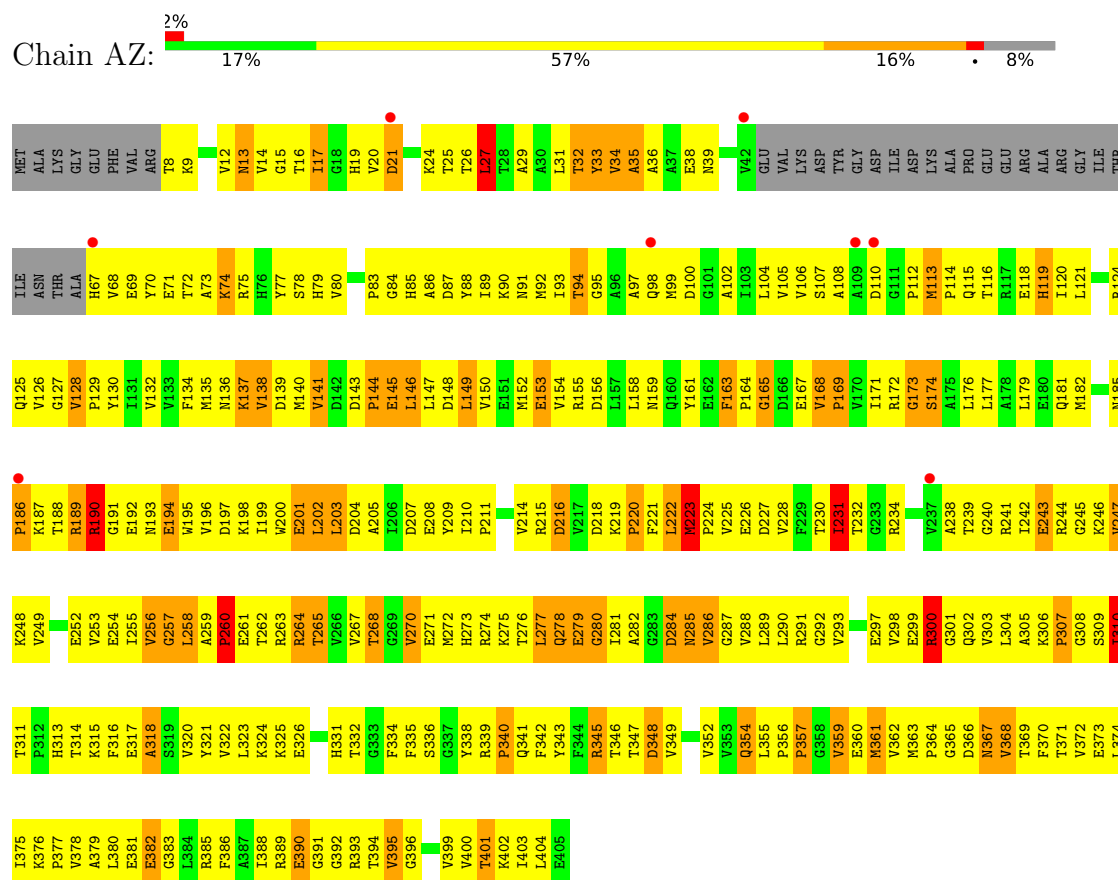


- Molecule 24: A-SITE TRNA THR

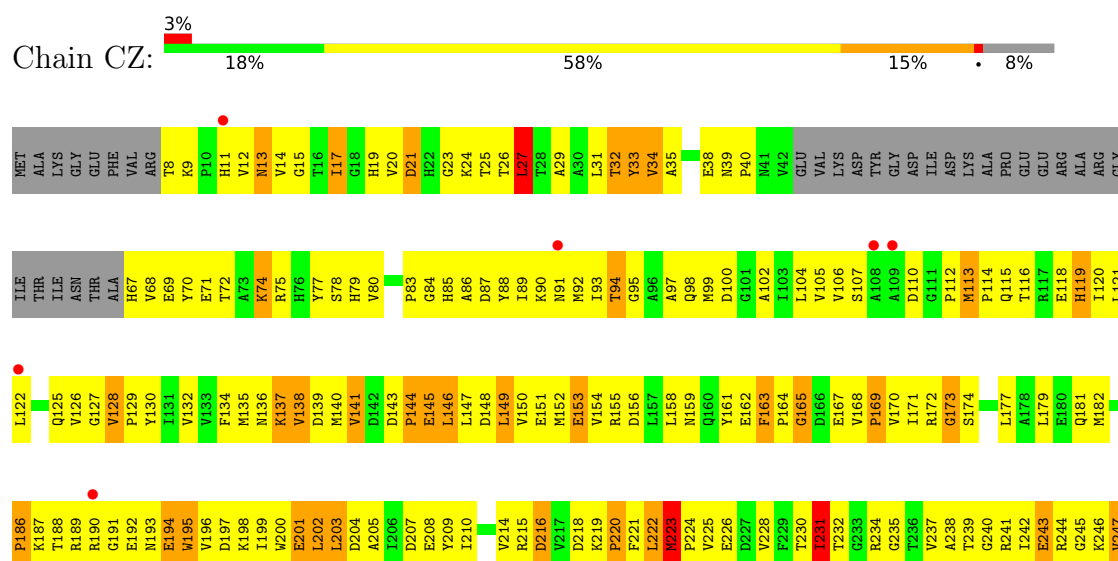


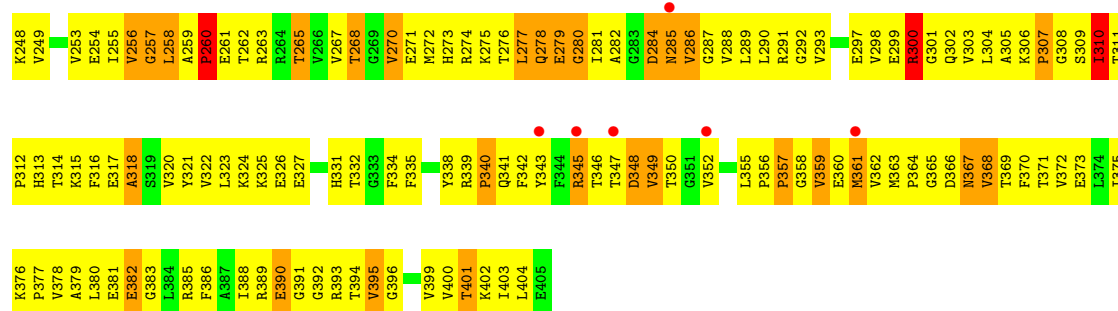


• Molecule 25: ELONGATION FACTOR TU-A

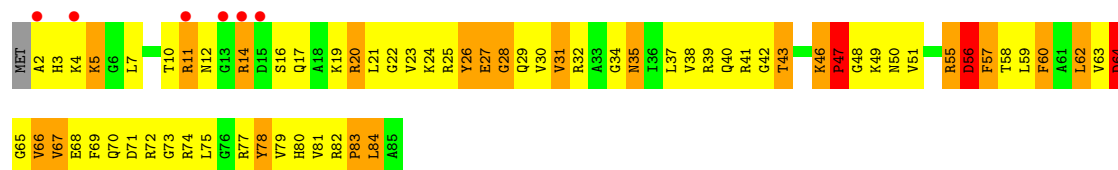
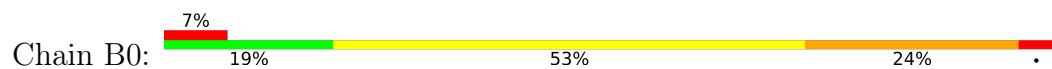


• Molecule 25: ELONGATION FACTOR TU-A

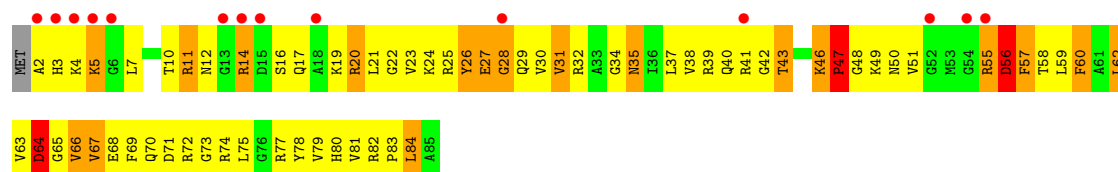
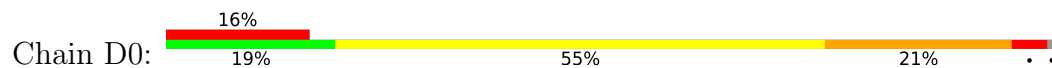




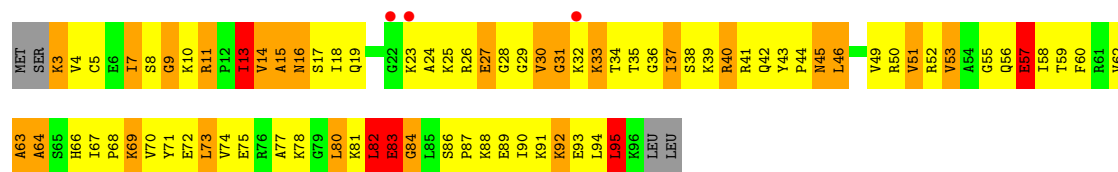
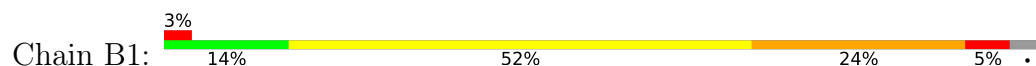
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



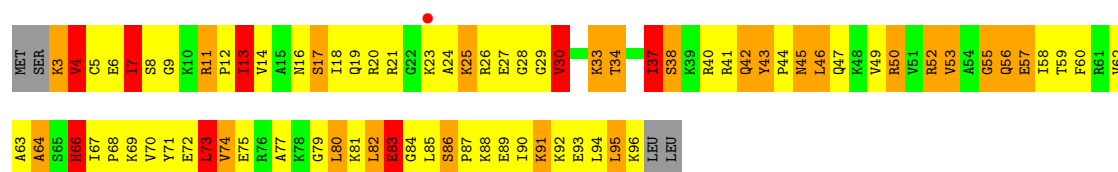
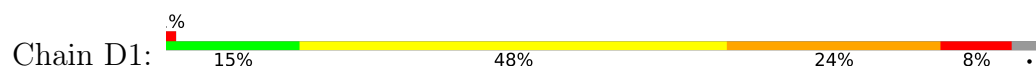
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



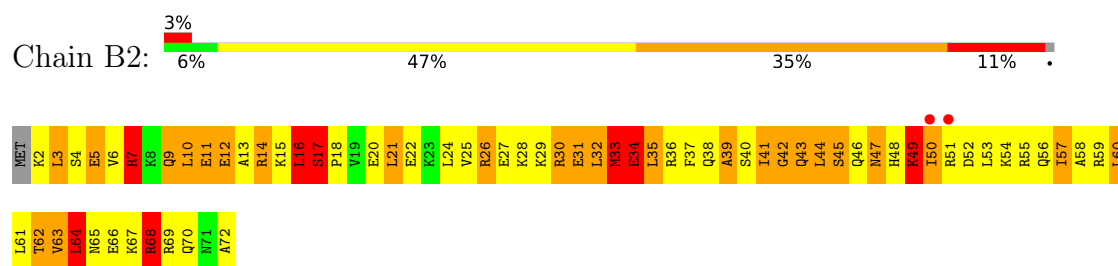
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



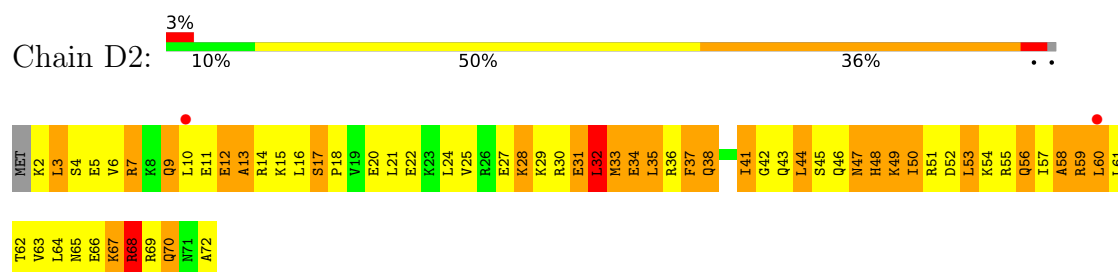
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



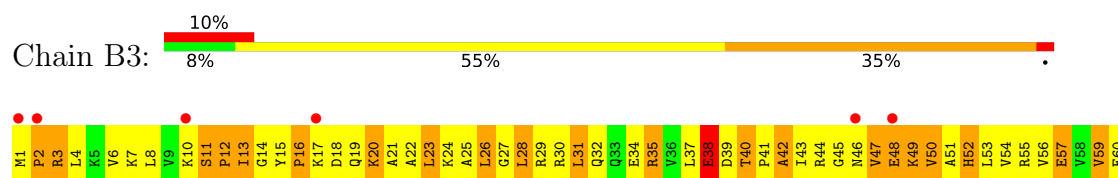
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



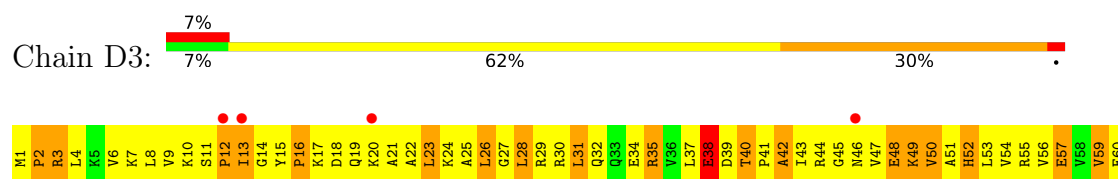
• Molecule 28: 50S RIBOSOMAL PROTEIN L29



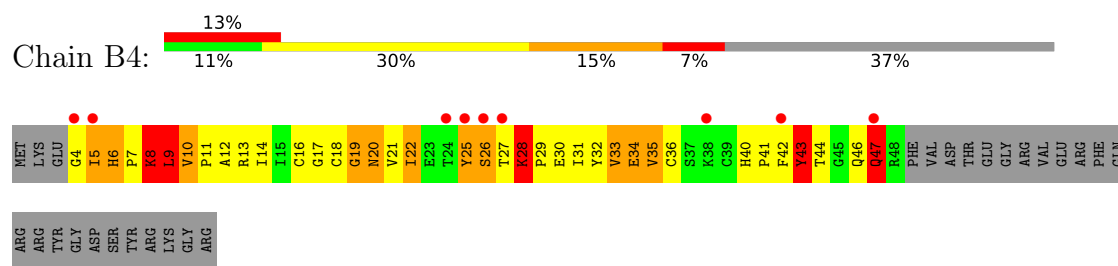
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



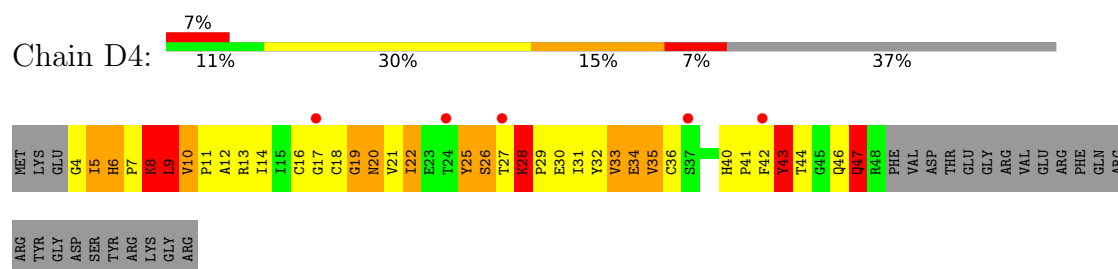
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



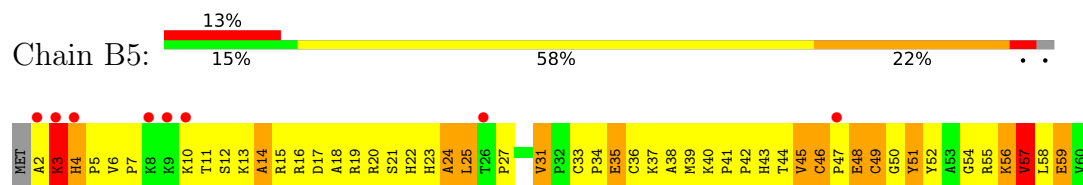
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



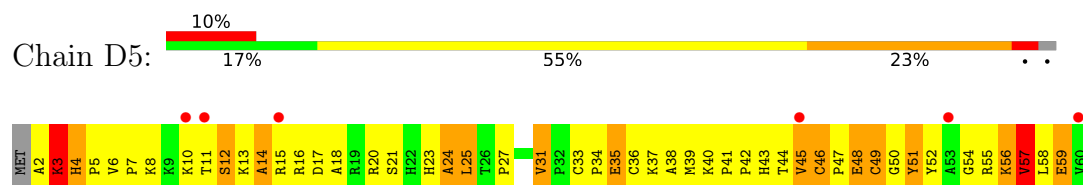
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



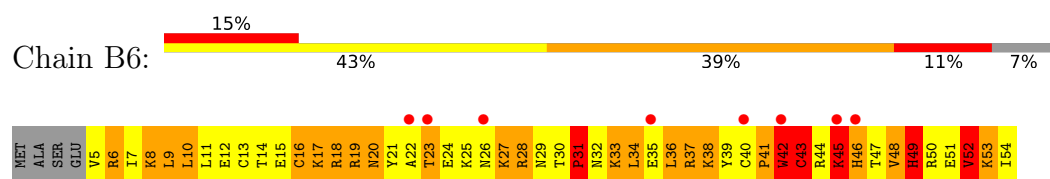
● Molecule 31: 50S RIBOSOMAL PROTEIN L32



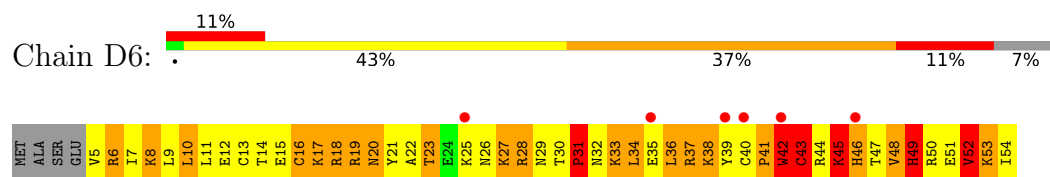
● Molecule 31: 50S RIBOSOMAL PROTEIN L32



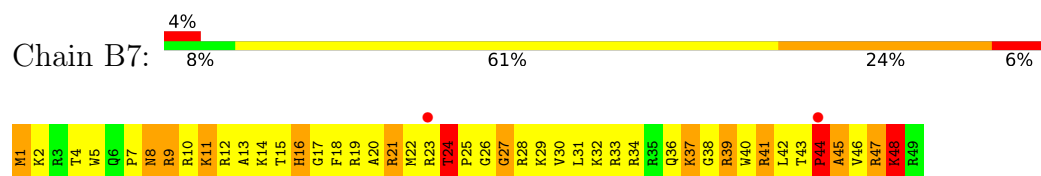
● Molecule 32: 50S RIBOSOMAL PROTEIN L33



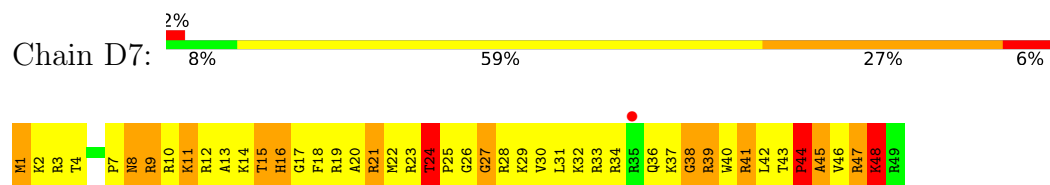
● Molecule 32: 50S RIBOSOMAL PROTEIN L33



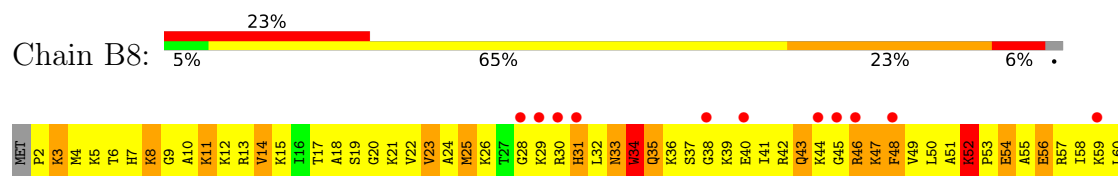
● Molecule 33: 50S RIBOSOMAL PROTEIN L34



● Molecule 33: 50S RIBOSOMAL PROTEIN L34

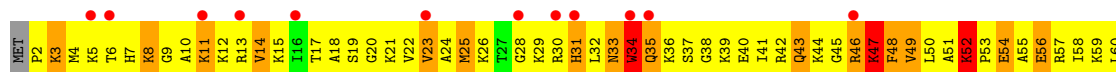
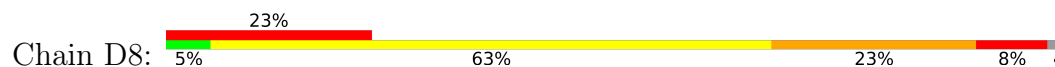


● Molecule 34: 50S RIBOSOMAL PROTEIN L35

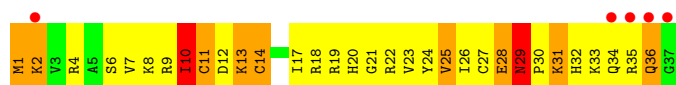
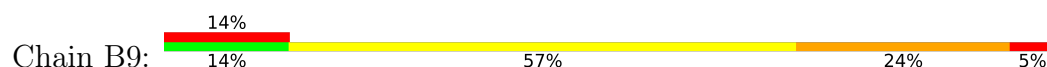




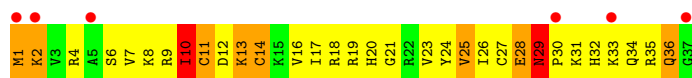
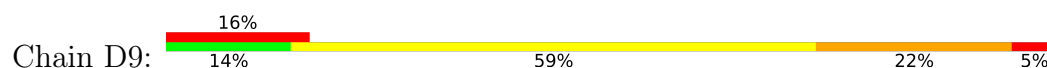
• Molecule 34: 50S RIBOSOMAL PROTEIN L35



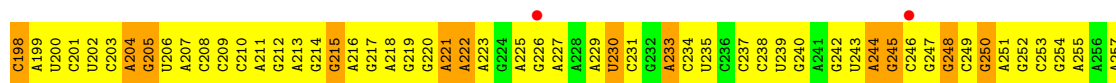
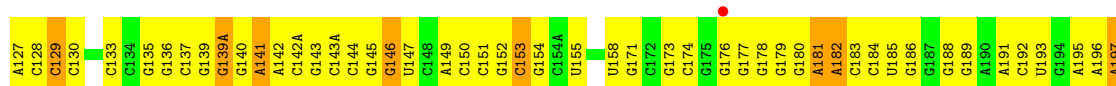
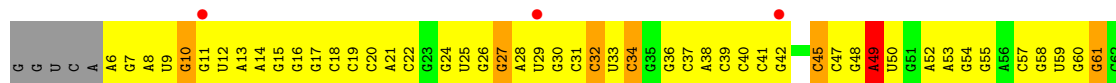
• Molecule 35: 50S RIBOSOMAL PROTEIN L36



• Molecule 35: 50S RIBOSOMAL PROTEIN L36



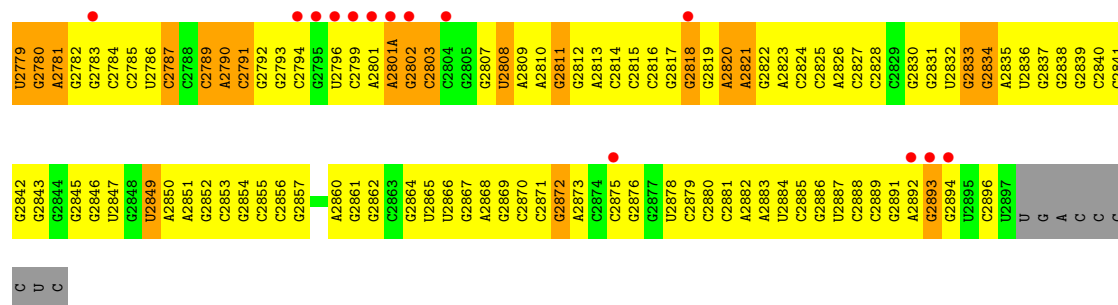
• Molecule 36: 23S RIBOSOMAL RNA



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U1067	C1005	C1006	U943	G877	C815	C755	C693	G654A	U597	G533	A472	G411	G352	C287
A1068	A1067	C1006	U943	A878	C816	C756	C694	G654B	G598	U534	G473	A412	G353	C288
G1069	G1068	C1007	A945	G879	C817	U757	C696	G654C	G600	C535	G474	C413	G353	C289
A1069	A1068	C1008	G946	G880	G818	C758	C697	G654D	G601	A536	U475	C414	G354	C290
U1070	U1069	A1009	G947	G881	A819	C759	C698	G654E	G602	C537	G476	C415	G355	C291
G1071	G1070	A1010	G948	G882	A820	C760	C699	G654F	G603	G538	A477	C416	G356	C292
C1072	C1071	C949	G949	G883	A821	A761	C700	G654G	A604	C540	A479	C417	U357	C293
A1073	A1072	C950	G950	C884	U822	U762	G701	G654H	G605	C541	A480	C418	A357	C294
G1074	G1073	C951	C885	C885	G823	C763	G702	G654I	U606	C542	C481	C419	A359	C295
		G952	C886	C886	U826	A764	U703	A654J	U607	C543	G482	U421	G360	C296
U1077	U1076	A953	A887	C887	U826	C765	G704	G654K	C607	C543	A482	U421	G361	C297
C1079	C1078	G954	G954	C888	U827	C766	A705	G654L	A608	A547	C484	A422	U362	C298
G1080	G1079	C955	C889	C889	U828	U767	A706	G654M	G610	A548	C485	A423	G363	C299
A1086	A1085	G956	U919	A890	A829	C768	G707	G654N	C611	C486	C486	G425	A363A	
U1087	U1086	A1020	A957	G892	G830	C769	C708	C654P	C612	C551	C487	C426	A363F	
G1087	G1086	A1021	U958	C893	G831	C770	U709	C654Q	G613	G552	G488	U427	A364	
A1088	A1087	G1022	A959	C894	G832	C771	G710	C654R	U614	G553	C489	A428	C365	
G1089	G1088	U1023	C960	U895	U833	C772	G711	G654S	U614A	C491	A429	A429	C366	
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U1092	U1091	U1026	U963	C898	G836	C775	U714	A654V	G615	U557	G494	A432	G372	
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G1099	G1098	C970	U1033	U907	G843	C782	G721	C661	G623	C564	A501	C440	C379	
U1099	U1098	G1034	C971	C908	C844	A783	A722	G662	C624	C565	A502	U441	U380	
C1100	C1100	U1035	A972	A909	G845	C784	G723	G663	G625	U566	A503	C442	G382	
U1101	U1101	G1036	G973	G916	C846	C785	U724	C664	U626	A667	U504	C443	C381	
C1102	C1102	G1037	G974	A911	U847	C786	G725	C665	A627	U568	A505	C444	U363	
A1103	A1103	C1038	C975	C912	G848	U787	G726	C666	G628	U569	G506	C445	U384	
C1104	C1104	G1039	G975	U913	A849	A788	A727	U657	G629	C570	A507	C446	C385	
U1105	U1105	A1045	G981	C913	C850	C789	G728	G668	G630	A571	C508	A447	C385	
G1106	G1106	C1041	G977	C915	U851	C790	G729	G669	A631	A572	C509	U448	U387	
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U1108	U1108	C1043	G979	A917	G853	C792	C731	A671	A633	C574	U511	C450	G327	
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G1112	G1112	G1047	A983	G921	C857	C796	C736	A675	A637	C579	A514	C453	C392	
U1113	U1113	A1048	U922	U922	U858	C797	C737	A676	G638	C580	A515	C454	C393	
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C1117	C1117	C1052	A987	A926	G862	C801	G741	C680	C642	G583	U519	C458	G397	
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U1119	U1119	A1054	A990	C928	G864	U803	G743	G682	A644	A586	C521	C461	G399	
C1120	C1120	G1055	C991	G832	C865	A804	G744	G683	C645	C587	C523	C462	C400	
C1121	C1121	G1056	C992	A833	A866	C805	G745	G684	A646	U588	U524	C463	A401	
G1122	G1122	A1057	G993	C934	U874	C806	G746	A685	C647	C589	U525	C464	A402	
C1123	C1123	C994	C994	C935	G869	U807	U747	G686	G648	C590	A526	U464	U403	
U1124	U1124	G1059	C995	A870	C808	G808	G748	C687	C591	A466	C527	C465	C343	
G1125	G1125	U1060	A996	U937	U871	C809	C749	U688	C550	G592	A528	C467	U405	
U1126	U1126	C1061	G997	C936	A872	U810	A750	A689	G551	G593	A529	C468	A346	
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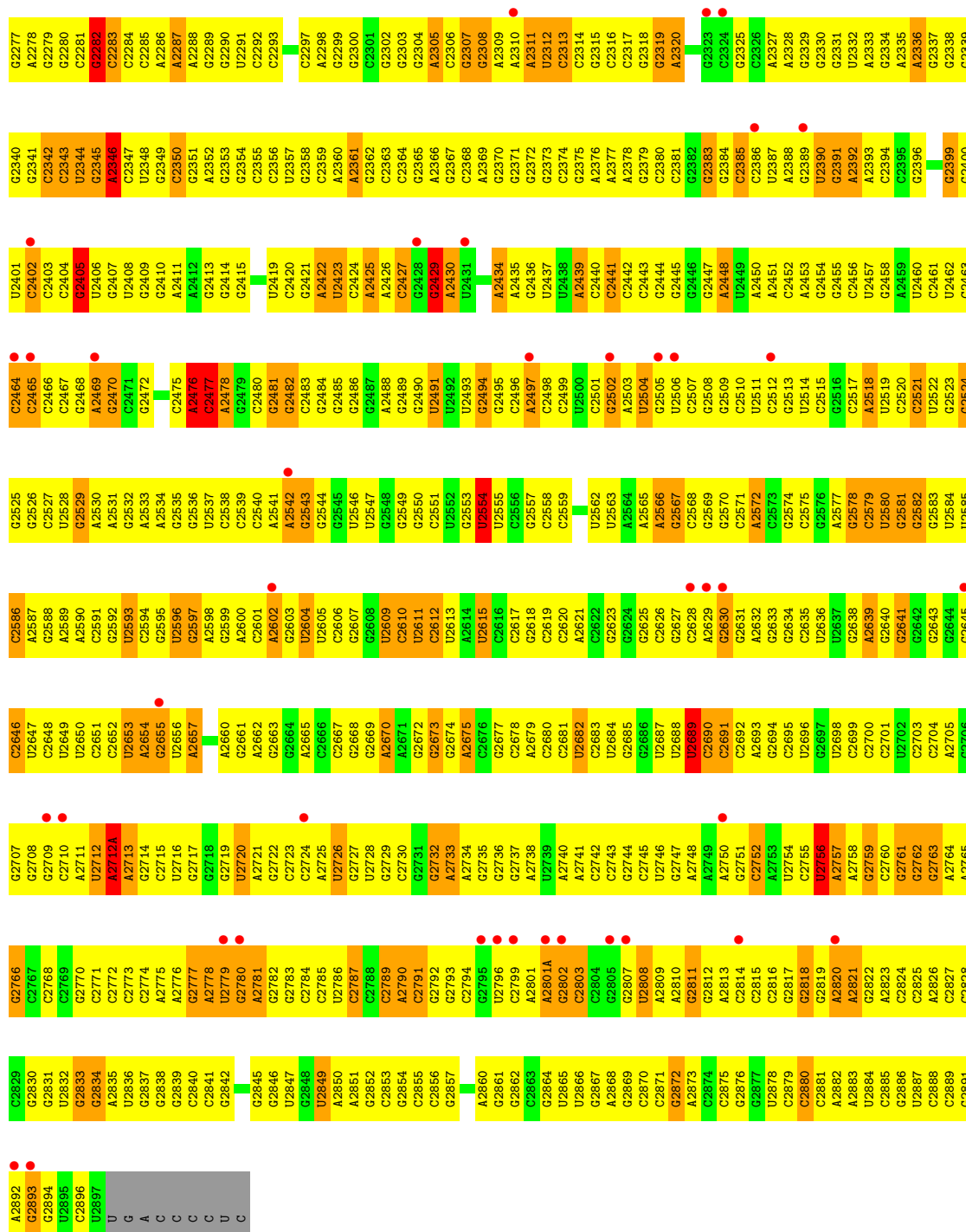


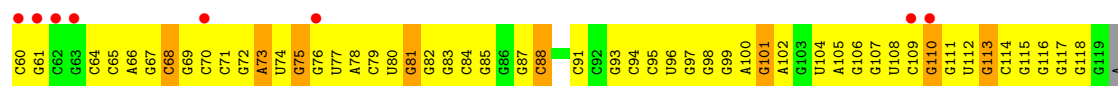
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G1966	G2032	C2095	G2156	C2226	G2288	G2352	G2415	A2478	G2538	A2600	G2672	G2722
C1967	U2033	U2096	G2157	G2227	G2289	G2353	G2416	G2479	C2539	G2601	G2673	G2723
G1968	U2034	C2097	A2158	G2228	G2290	G2354	U2419	C2480	C2540	A2602	G2674	G2724
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A1970	G2036	U2099	G2160	G2230	U2292	C2356	G2421	G2482	A2542	G2604	G2676	U2726
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A1972	G2038	G2101	G2162	U2232	U2294	G2358	A2423	G2484	G2544	G2606	G2678	U2728
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	U2041	G2104	G2165	G2235	U2297	A2361	A2425	G2487	U2547	U2609	G2672	G2731
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G2009	A2071	U2130	G2193	U2262	A2327	U2387	C2452	G2513	G2575	G2636	G2699	A2758
G2010	G2072	G2132	G2194	C2263	G2328	A2388	A2453	U2514	G2576	U2637	C2700	G2759
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G2012	U2074	A2135	C2136	A2195	U2331	U2390	G2455	G2516	G2578	A2639	U2702	G2761
A2015	U2075	G2137	C2138	C2196	U2332	G2391	C2456	A2517	U2580	G2640	G2703	G2762
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U2017	C2078	G2140	C2141	A2198	G2334	G2393	G2458	U2519	U2582	G2642	G2705	A2764
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A2019	A2082	U2144	U2145	C2201	G2273	G2400	U2460	U2521	U2584	G2644	G2707	G2766
A2020	G2083	C2146	C2147	C2202	A2268	G2401	C2461	U2522	U2585	G2645	G2708	C2767
C2021	C2084	G2148	G2149	U2203	A2269	U2402	C2462	G2523	G2586	G2646	G2709	G2768
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					G2283	A2546	G2470	A2531	U2594	A2654	U2716	A2776
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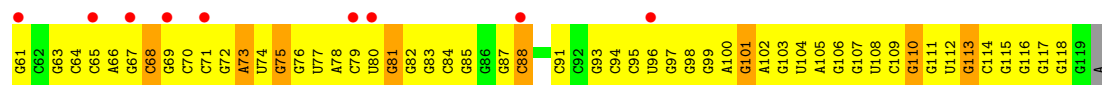
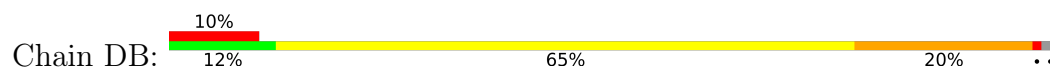
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A933	G934	C935	C936	U937	G938	C939	G940	A941	C942	U943	G944	A945	G946	G947	C948	C949	G950	C951	G952	A953	C954	C955	G956	A957	U958	A959	A960	C961	G962	U963	C964	C965	C966	C967	U968	G969	C970	C971	G972	A973	G974	C975	G976	C977	C978	G979	A980	A981	C982	A983	A984	C985	C986	G987	A988	G989	A990	C991	
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C647	C648	C649	C650	C651	C652	A653	A654	C654A	C654B	C654C	C654D	C654E	C654F	C654G	C654H	C654I	A654J	C654K	C654L	C654M	C654N	C654O	C654P	C654Q	C654R	C654S	C654T	A654U	A654V	A655	C656	U657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	A670	C671	C672	C673	C674	A675	A676	C677	C678	C679	C680	C681	C682	C683	C684
C589	A590	C591	G592	G593	U594	C595	C596	U597	G598	G599	G600	C601	G602	A603	G604	C605	U606	U607	A608	A609	G610	C611	C612	G613	U614	U614A	G614B	A614C	G615	G616	C618	G619	G620	A621	G622	G623	C624	G625	U626	A627	G628	G629	G630	A631	A632	C633	C634	C635	G636	A637	G638	U639	C640	C641	C642	A643	A644	C645	A646

G2207	C2145	G1959	G1824	A1762	G1684	G1624	G1560	A1495	C1432
A2208	C2146	A1960	A1825	G1763	C1685	C1625	G1561	A1496	U1433
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G2259	U2189	G2002	G1878	G1807	C1745	G1667	C1607	C1476	
G2260	G2190	G2003	C1879	U1808	A1668	A1608	A1608	A1477	
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	C2195	G2011	A1884	G1813	U1673	G1613	C1549		
	C2196	U2011	A1885	G1814	G1674	A1614	C1550		
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G2272	C2201	U2016	G1891	A1819	U1757	G1620	C1556		
U2273	C2202	U2017	G1892	U1820	U1680	U1621	C1557		
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G2275	C2205	A2019	C1957	G1822	G1682	C1558	C1492		
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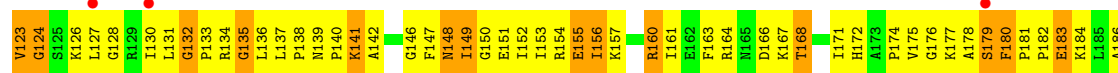
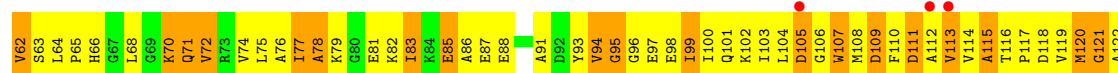
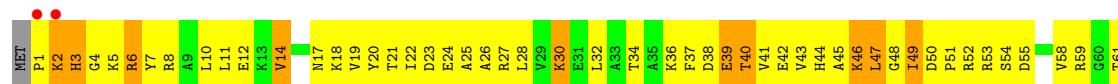




• Molecule 37: 5S RIBOSOMAL RNA



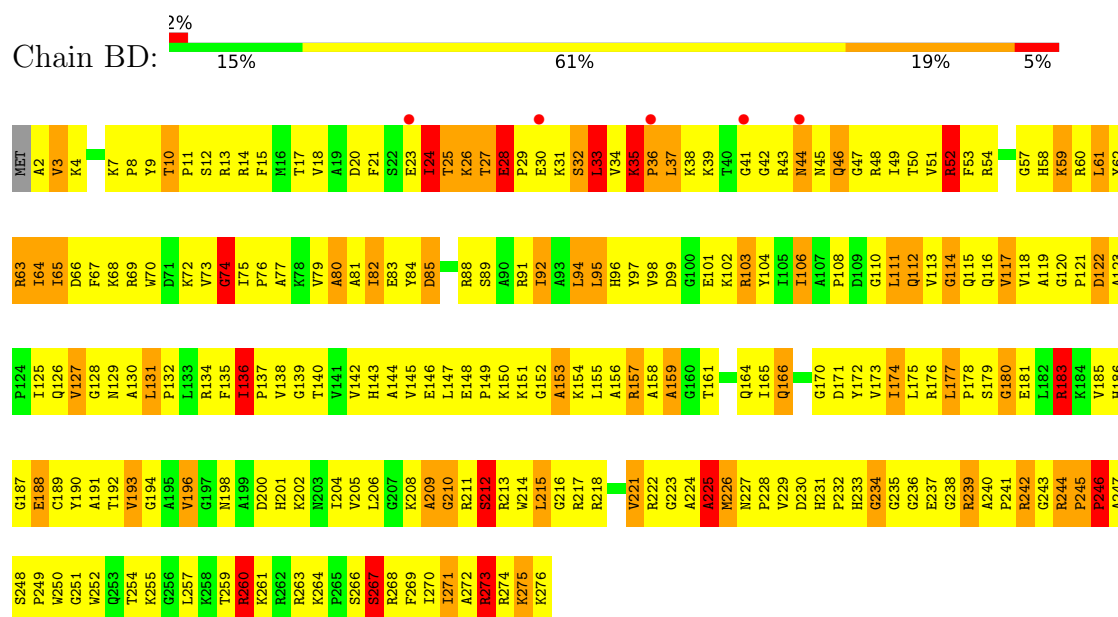
• Molecule 38: 50S RIBOSOMAL PROTEIN L1



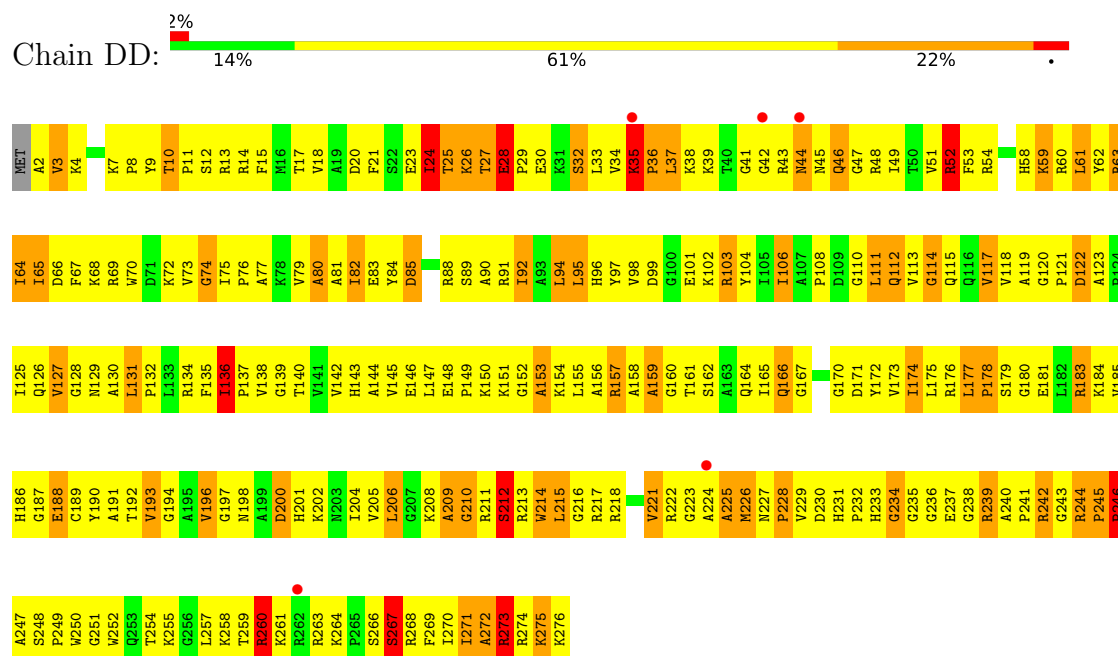
• Molecule 38: 50S RIBOSOMAL PROTEIN L1



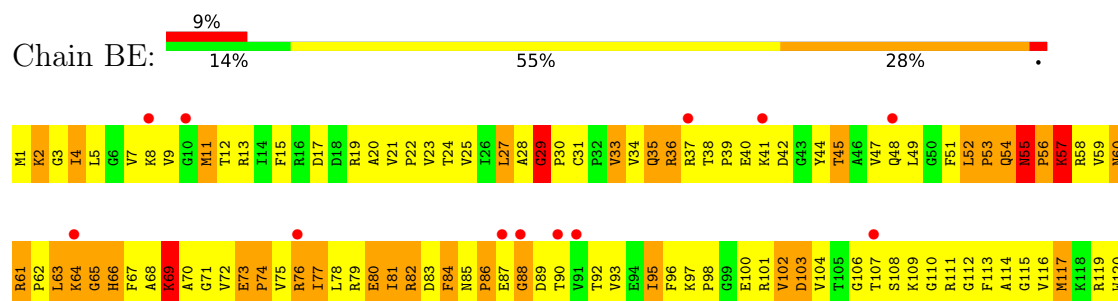
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

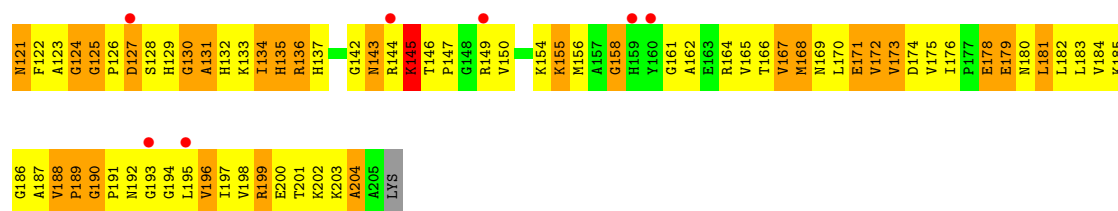


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

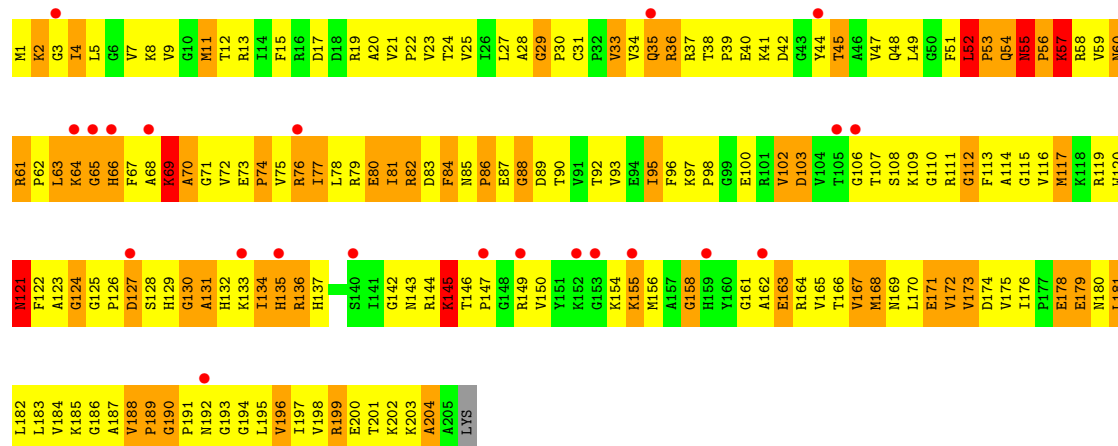
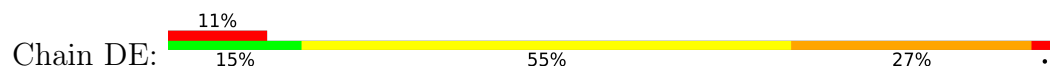


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

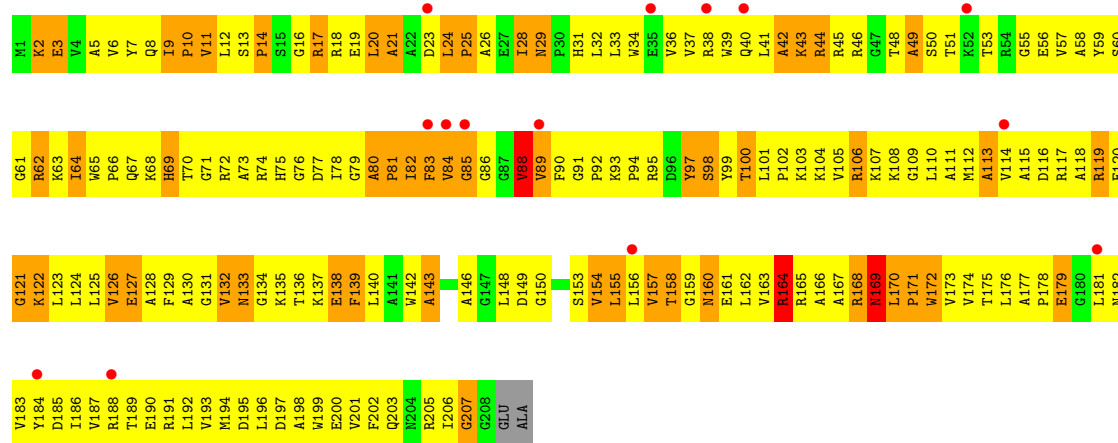
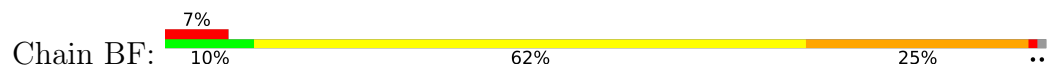




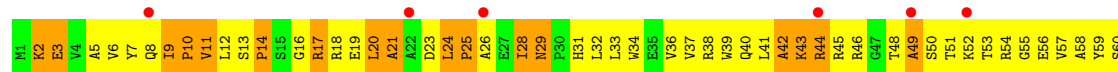
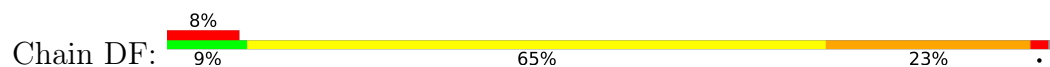
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

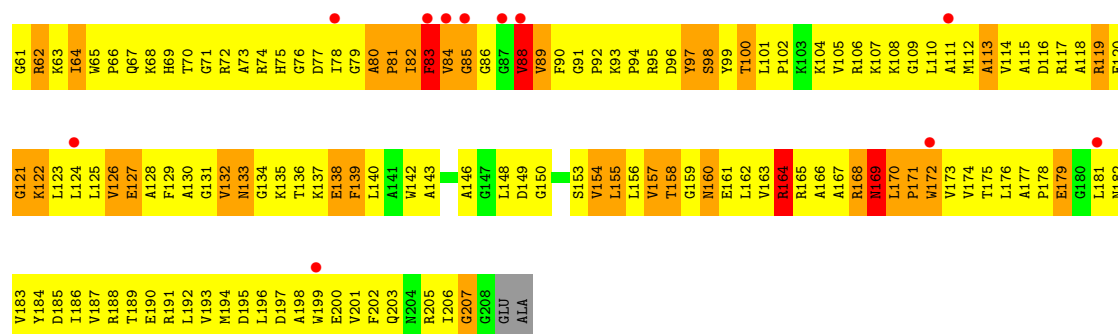


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

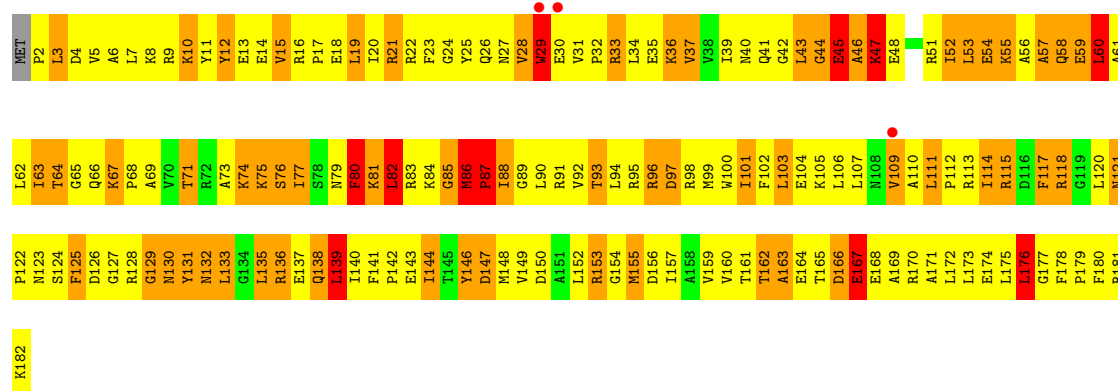


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

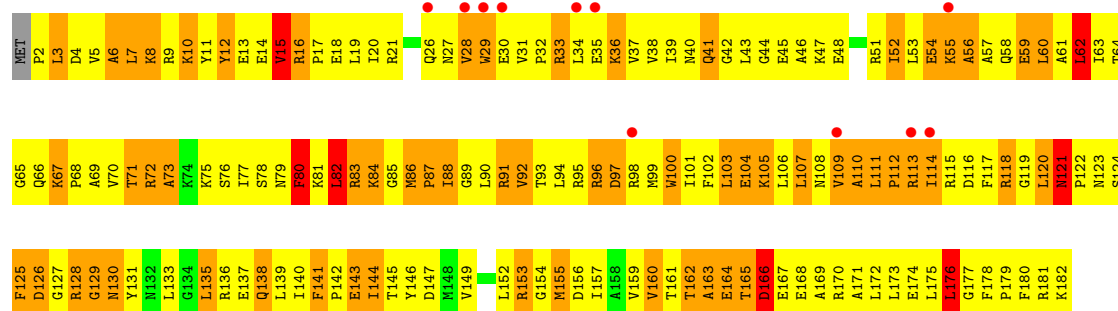




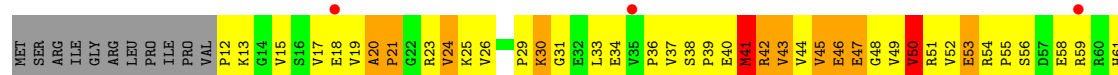
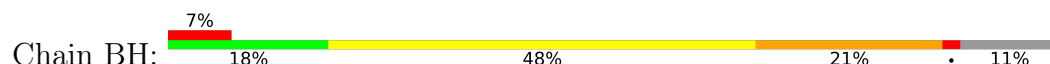
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

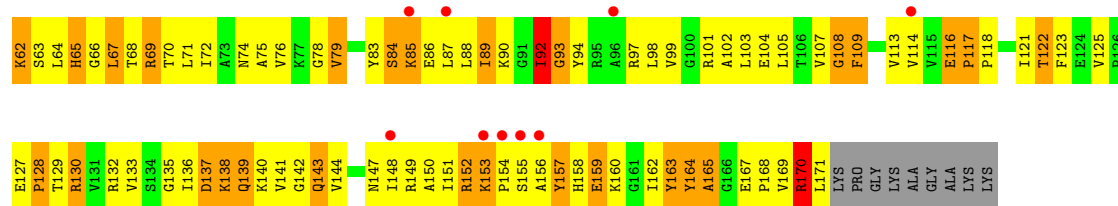


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

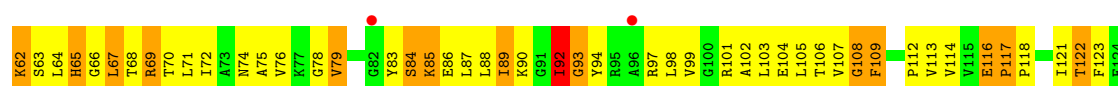
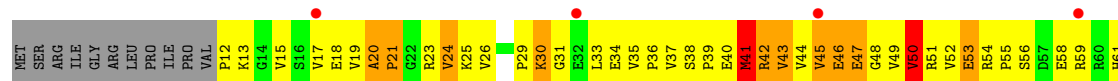
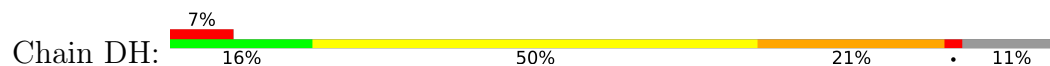


• Molecule 43: 50S RIBOSOMAL PROTEIN L6

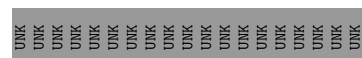
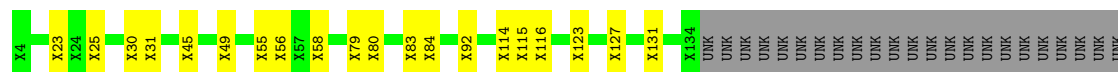




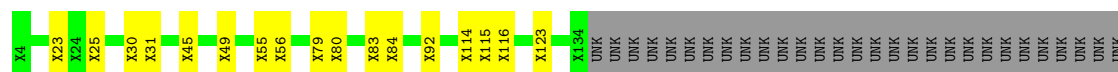
- Molecule 43: 50S RIBOSOMAL PROTEIN L6



- Molecule 44: 50S RIBOSOMAL PROTEIN L10



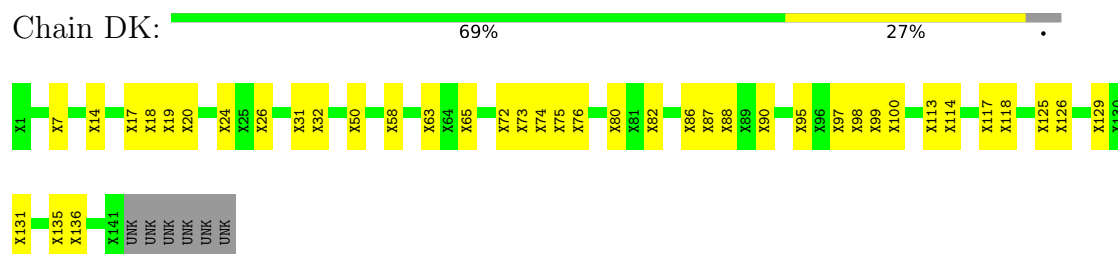
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



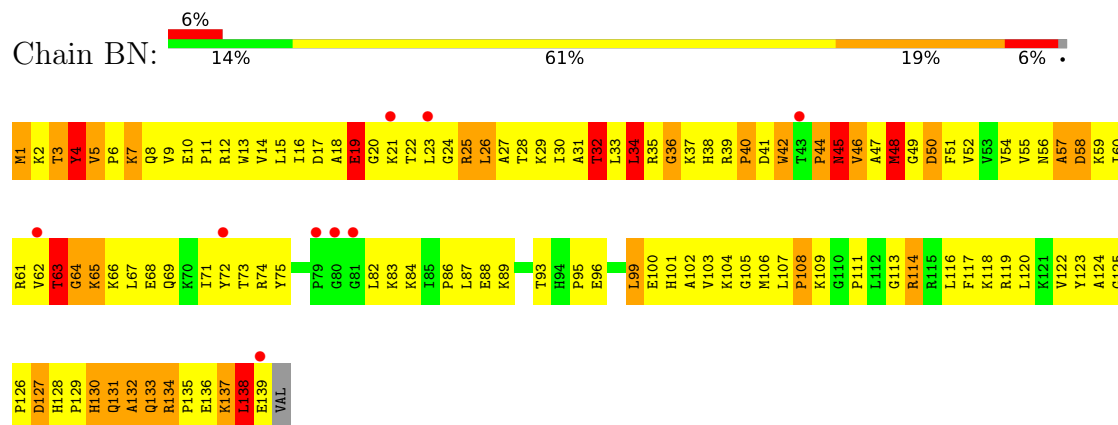
- Molecule 45: 50S RIBOSOMAL PROTEIN L11



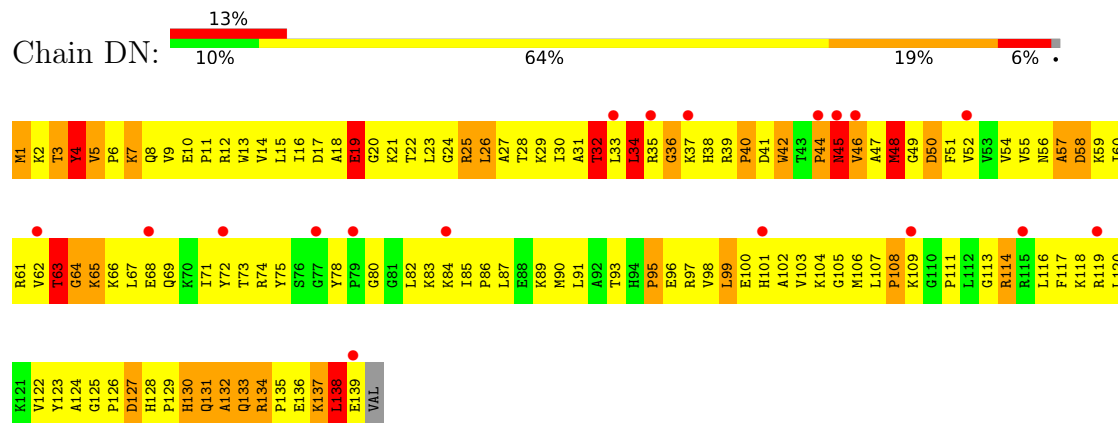
• Molecule 45: 50S RIBOSOMAL PROTEIN L11



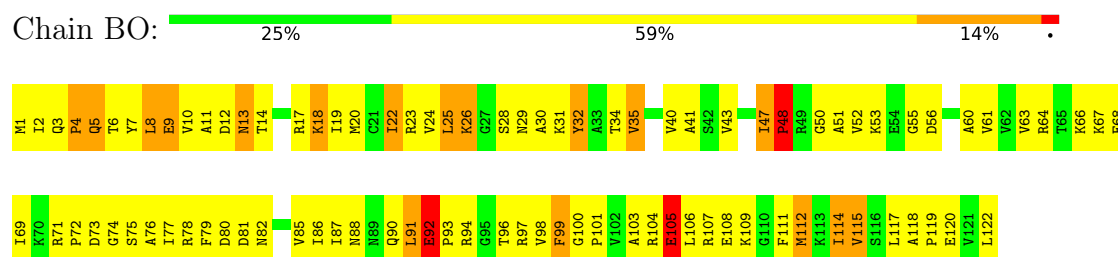
• Molecule 46: 50S RIBOSOMAL PROTEIN L13



• Molecule 46: 50S RIBOSOMAL PROTEIN L13



• Molecule 47: 50S RIBOSOMAL PROTEIN L14



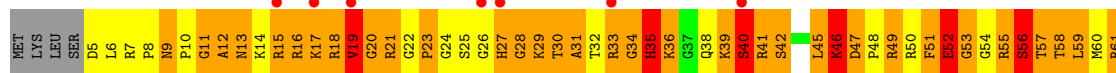
• Molecule 47: 50S RIBOSOMAL PROTEIN L14



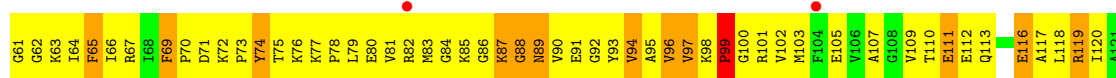
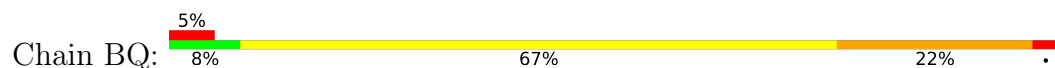
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



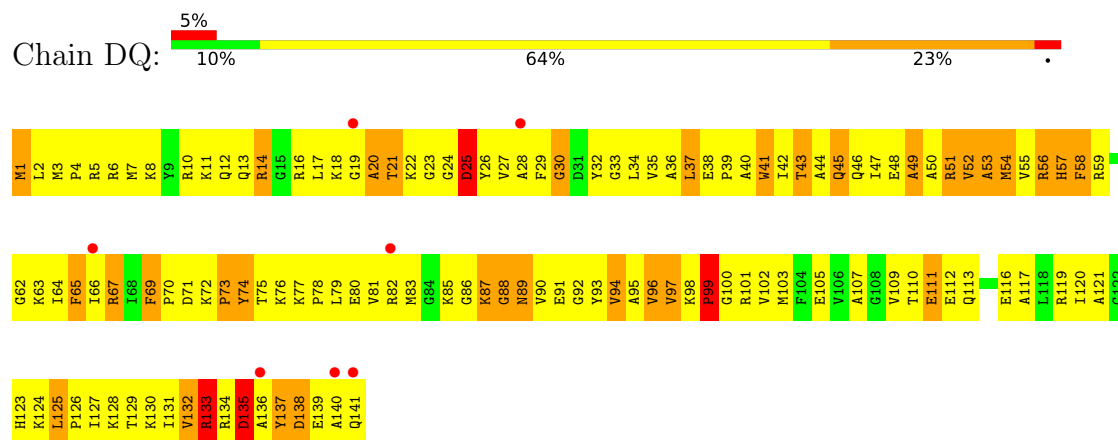
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



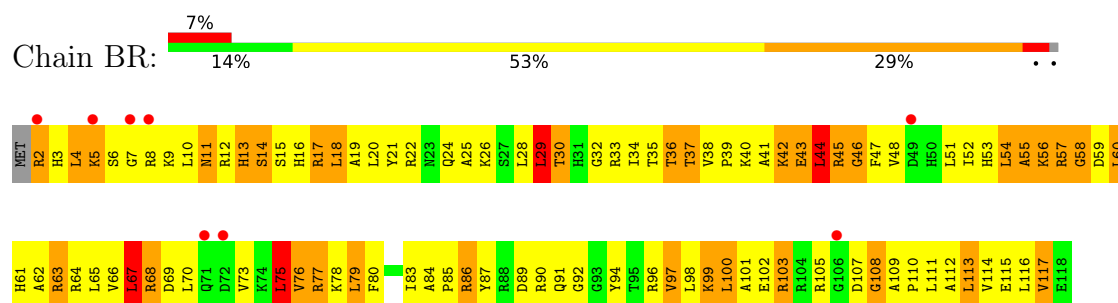
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



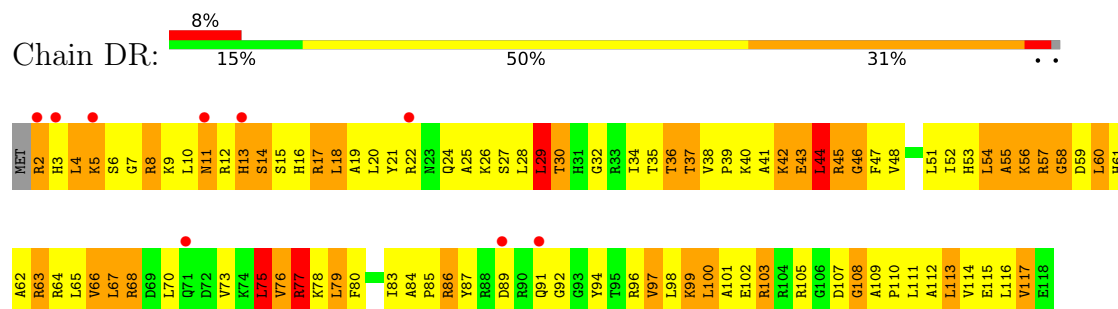
- Molecule 49: 50S RIBOSOMAL PROTEIN L16



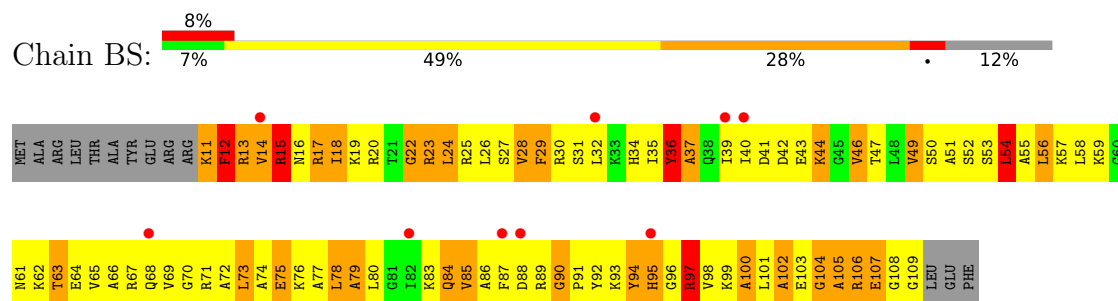
- Molecule 50: 50S RIBOSOMAL PROTEIN L17



- Molecule 50: 50S RIBOSOMAL PROTEIN L17

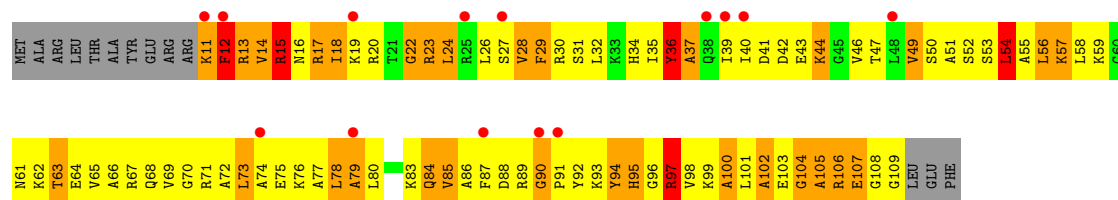


- Molecule 51: 50S RIBOSOMAL PROTEIN L18

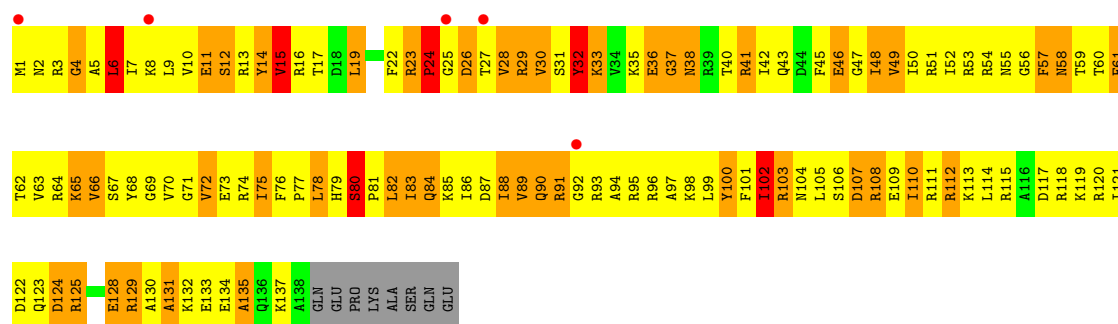


- Molecule 51: 50S RIBOSOMAL PROTEIN L18

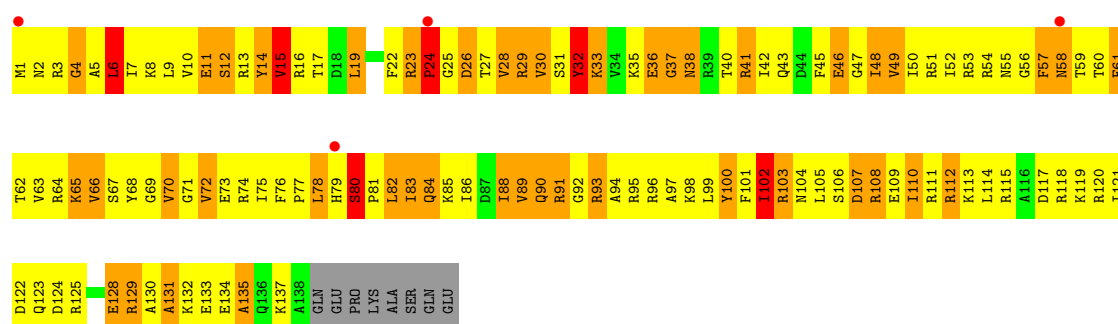




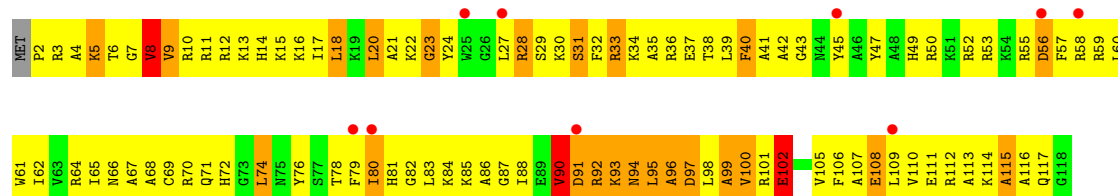
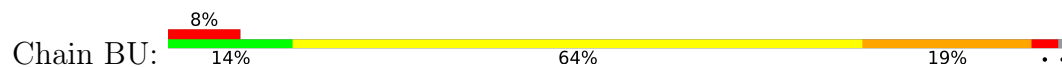
• Molecule 52: 50S RIBOSOMAL PROTEIN L19



• Molecule 52: 50S RIBOSOMAL PROTEIN L19

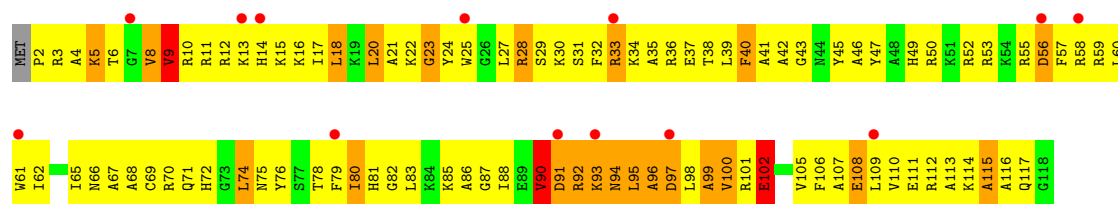


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

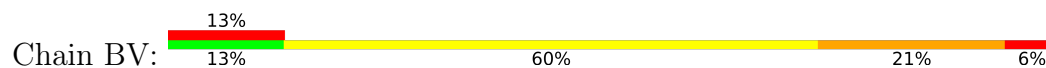


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

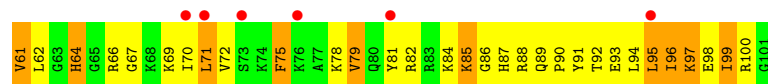
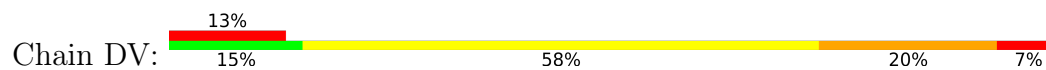




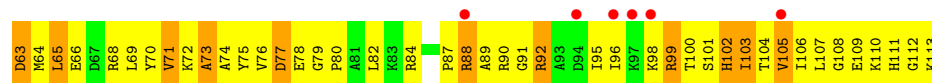
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



• Molecule 54: 50S RIBOSOMAL PROTEIN L21



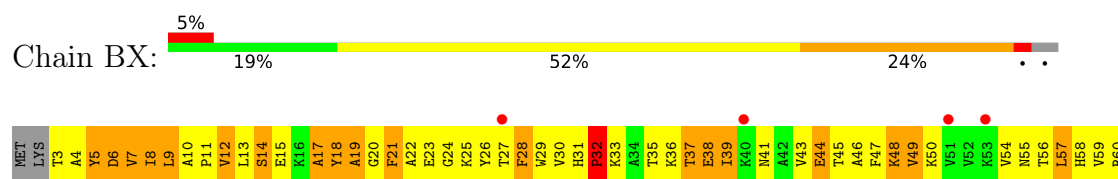
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



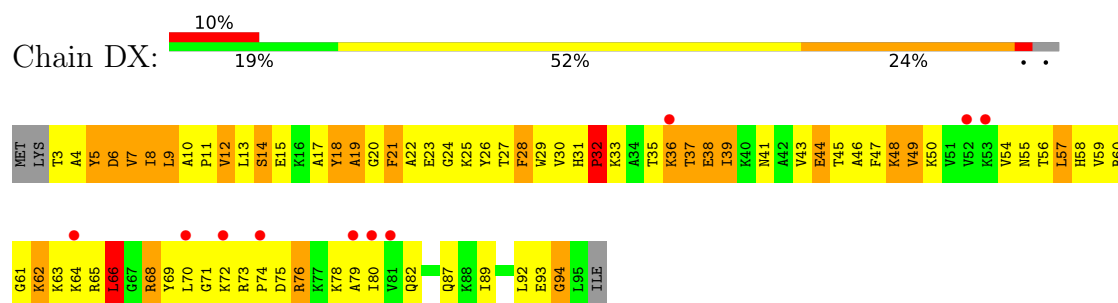
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



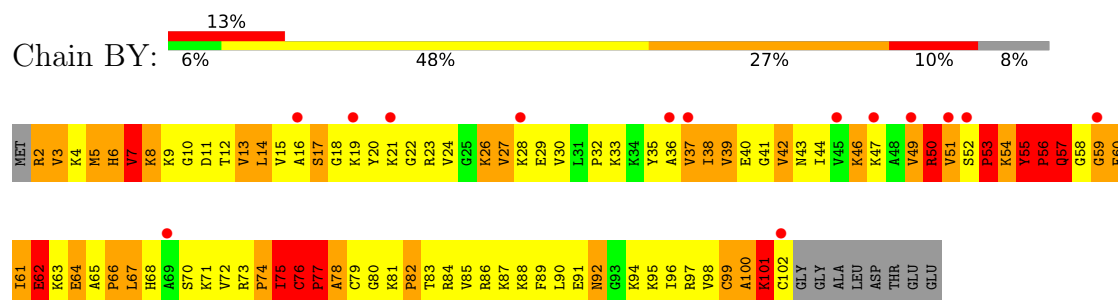
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



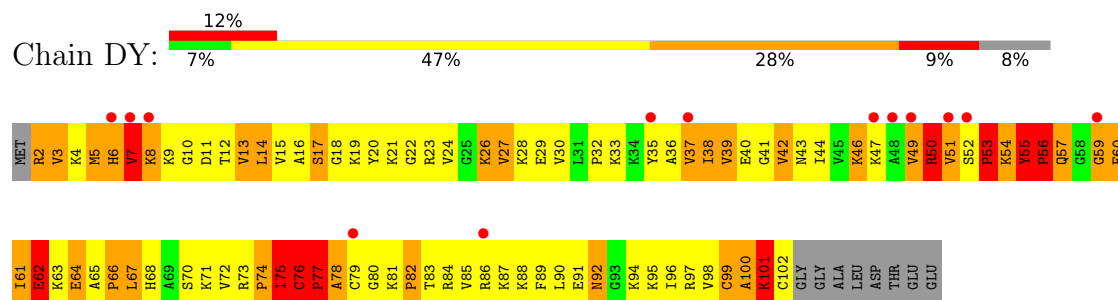
- Molecule 56: 50S RIBOSOMAL PROTEIN L23



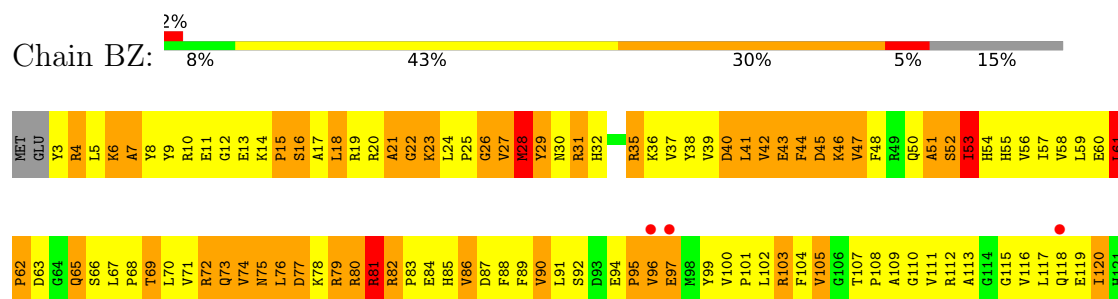
- Molecule 57: 50S RIBOSOMAL PROTEIN L24

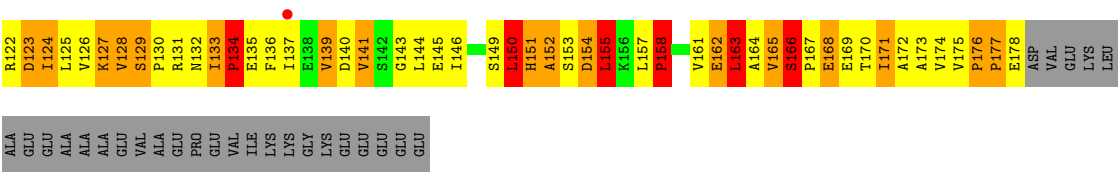


- Molecule 57: 50S RIBOSOMAL PROTEIN L24

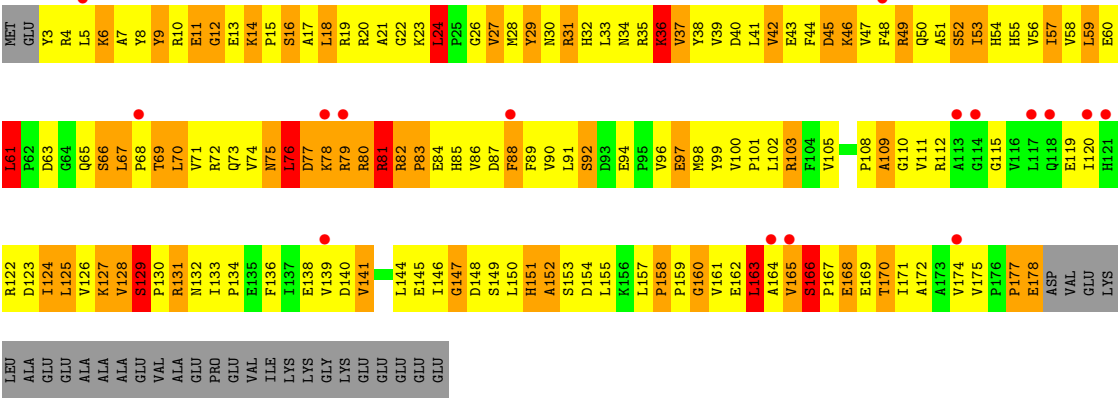


- Molecule 58: 50S RIBOSOMAL PROTEIN L25





● Molecule 58: 50S RIBOSOMAL PROTEIN L25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	289.57Å 268.36Å 403.88Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 50.00 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-3.60) 93.5 (50.00-3.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.281 , 0.315 0.278 , 0.312	Depositor DCC
R_{free} test set	35772 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	102.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 92.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	306876	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: YG, MG, 7MG, GDP, KIR, H2U, ZN, 5MU, PAR, PSU

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	AA	0.53	0/36190	0.76	56/56486 (0.1%)
1	CA	0.53	0/36190	0.76	51/56486 (0.1%)
2	AB	0.58	1/1936 (0.1%)	1.05	10/2611 (0.4%)
2	CB	0.54	1/1936 (0.1%)	1.04	11/2611 (0.4%)
3	AC	0.61	1/1637 (0.1%)	1.07	15/2207 (0.7%)
3	CC	0.59	1/1637 (0.1%)	1.08	13/2207 (0.6%)
4	AD	0.58	0/1733	1.13	16/2318 (0.7%)
4	CD	0.54	0/1733	1.11	13/2318 (0.6%)
5	AE	0.72	1/1163 (0.1%)	1.15	8/1566 (0.5%)
5	CE	0.70	1/1163 (0.1%)	1.15	10/1566 (0.6%)
6	AF	0.50	0/856	0.98	3/1154 (0.3%)
6	CF	0.51	0/856	0.96	2/1154 (0.2%)
7	AG	0.52	0/1276	0.98	6/1709 (0.4%)
7	CG	0.49	0/1276	0.97	6/1709 (0.4%)
8	AH	0.64	0/1136	1.08	5/1527 (0.3%)
8	CH	0.60	0/1136	1.07	5/1527 (0.3%)
9	AI	0.47	0/1029	0.98	3/1379 (0.2%)
9	CI	0.45	0/1029	0.99	3/1379 (0.2%)
10	AJ	0.63	1/808 (0.1%)	1.11	10/1087 (0.9%)
10	CJ	0.64	1/808 (0.1%)	1.11	9/1087 (0.8%)
11	AK	0.62	0/900	1.13	11/1213 (0.9%)
11	CK	0.61	0/900	1.13	8/1213 (0.7%)
12	AL	0.66	1/987 (0.1%)	1.15	7/1322 (0.5%)
12	CL	0.66	1/987 (0.1%)	1.13	8/1322 (0.6%)
13	AM	0.57	1/999 (0.1%)	1.17	8/1338 (0.6%)
13	CM	0.56	1/999 (0.1%)	1.16	7/1338 (0.5%)
14	AN	0.61	0/501	1.06	3/664 (0.5%)
14	CN	0.61	0/501	1.06	3/664 (0.5%)
15	AO	0.59	0/745	1.13	7/992 (0.7%)
15	CO	0.56	0/745	1.12	7/992 (0.7%)
16	AP	0.61	1/717 (0.1%)	1.09	5/965 (0.5%)
16	CP	0.60	1/717 (0.1%)	1.10	8/965 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.56	1/837 (0.1%)	1.07	6/1119 (0.5%)
17	CQ	0.57	1/837 (0.1%)	1.07	5/1119 (0.4%)
18	AR	0.62	0/579	1.06	4/768 (0.5%)
18	CR	0.61	0/579	1.07	5/768 (0.7%)
19	AS	0.59	1/643 (0.2%)	0.94	2/867 (0.2%)
19	CS	0.57	1/643 (0.2%)	0.94	2/867 (0.2%)
20	AT	0.48	0/765	1.20	9/1007 (0.9%)
20	CT	0.47	0/765	1.20	9/1007 (0.9%)
21	AU	0.66	1/213 (0.5%)	0.95	0/279
21	CU	0.70	1/213 (0.5%)	0.97	1/279 (0.4%)
22	AV	0.44	0/1809	0.73	1/2819 (0.0%)
22	AW	0.43	0/1809	0.66	0/2819
22	CV	0.43	0/1809	0.73	1/2819 (0.0%)
22	CW	0.43	0/1809	0.66	1/2819 (0.0%)
23	AX	0.60	0/304	0.91	0/471
23	CX	0.62	0/304	0.89	0/471
24	AY	0.45	0/1660	0.65	1/2583 (0.0%)
24	CY	0.47	0/1660	0.66	1/2583 (0.0%)
25	AZ	0.49	0/2957	1.03	15/4015 (0.4%)
25	CZ	0.48	0/2957	1.03	12/4015 (0.3%)
26	B0	0.49	0/671	1.00	5/892 (0.6%)
26	D0	0.48	0/671	0.99	5/892 (0.6%)
27	B1	0.79	1/739 (0.1%)	1.26	6/983 (0.6%)
27	D1	0.73	0/739	1.36	14/983 (1.4%)
28	B2	0.53	0/600	1.38	11/793 (1.4%)
28	D2	0.54	0/600	1.27	5/793 (0.6%)
29	B3	0.58	1/473 (0.2%)	1.21	7/636 (1.1%)
29	D3	0.58	1/473 (0.2%)	1.21	7/636 (1.1%)
30	B4	0.88	1/350 (0.3%)	1.10	0/476
30	D4	0.97	1/350 (0.3%)	1.09	0/476
31	B5	0.55	0/473	1.16	5/639 (0.8%)
31	D5	0.56	0/473	1.14	5/639 (0.8%)
32	B6	0.66	0/440	1.35	10/586 (1.7%)
32	D6	0.70	0/440	1.37	10/586 (1.7%)
33	B7	0.62	1/427 (0.2%)	1.10	6/563 (1.1%)
33	D7	0.62	1/427 (0.2%)	1.08	5/563 (0.9%)
34	B8	0.63	1/516 (0.2%)	1.14	7/681 (1.0%)
34	D8	0.63	1/516 (0.2%)	1.15	8/681 (1.2%)
35	B9	0.53	0/310	1.00	2/407 (0.5%)
35	D9	0.56	0/310	1.03	2/407 (0.5%)
36	BA	0.52	0/69972	0.74	58/109237 (0.1%)
36	DA	0.52	0/69972	0.74	63/109237 (0.1%)
37	BB	0.46	0/2853	0.66	1/4451 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.45	0/2853	0.66	1/4451 (0.0%)
38	BC	0.58	4/1774 (0.2%)	1.10	10/2391 (0.4%)
38	DC	0.56	4/1774 (0.2%)	1.08	11/2391 (0.5%)
39	BD	0.72	0/2195	1.28	23/2955 (0.8%)
39	DD	0.68	0/2195	1.25	23/2955 (0.8%)
40	BE	0.61	1/1597 (0.1%)	1.15	17/2155 (0.8%)
40	DE	0.59	1/1597 (0.1%)	1.15	16/2155 (0.7%)
41	BF	0.56	1/1659 (0.1%)	1.14	16/2246 (0.7%)
41	DF	0.53	1/1659 (0.1%)	1.13	15/2246 (0.7%)
42	BG	0.58	0/1499	1.30	19/2016 (0.9%)
42	DG	0.57	0/1499	1.17	19/2016 (0.9%)
43	BH	0.49	1/1246 (0.1%)	1.20	12/1684 (0.7%)
43	DH	0.50	1/1246 (0.1%)	1.20	12/1684 (0.7%)
46	BN	0.53	1/1132 (0.1%)	1.16	10/1527 (0.7%)
46	DN	0.52	1/1132 (0.1%)	1.14	10/1527 (0.7%)
47	BO	0.64	0/943	1.15	11/1269 (0.9%)
47	DO	0.63	0/943	1.16	11/1269 (0.9%)
48	BP	0.61	0/1131	1.48	27/1504 (1.8%)
48	DP	0.59	0/1131	1.47	28/1504 (1.9%)
49	BQ	0.56	0/1143	1.16	14/1527 (0.9%)
49	DQ	0.56	0/1143	1.16	13/1527 (0.9%)
50	BR	0.51	0/974	1.12	6/1302 (0.5%)
50	DR	0.51	0/974	1.15	8/1302 (0.6%)
51	BS	0.51	1/779 (0.1%)	1.02	7/1038 (0.7%)
51	DS	0.52	1/779 (0.1%)	1.04	8/1038 (0.8%)
52	BT	0.57	1/1156 (0.1%)	1.14	11/1544 (0.7%)
52	DT	0.54	1/1156 (0.1%)	1.13	11/1544 (0.7%)
53	BU	0.51	0/975	1.19	11/1297 (0.8%)
53	DU	0.52	0/975	1.17	10/1297 (0.8%)
54	BV	0.50	0/790	1.02	3/1057 (0.3%)
54	DV	0.49	0/790	1.02	3/1057 (0.3%)
55	BW	0.55	0/907	1.04	6/1216 (0.5%)
55	DW	0.54	0/907	1.06	6/1216 (0.5%)
56	BX	0.54	1/740 (0.1%)	1.11	6/995 (0.6%)
56	DX	0.54	1/740 (0.1%)	1.10	7/995 (0.7%)
57	BY	0.56	1/789 (0.1%)	1.25	10/1053 (0.9%)
57	DY	0.57	1/789 (0.1%)	1.25	9/1053 (0.9%)
58	BZ	0.57	0/1435	1.21	19/1949 (1.0%)
58	DZ	0.58	0/1435	1.19	19/1949 (1.0%)
All	All	0.54	53/329754 (0.0%)	0.87	1132/492708 (0.2%)

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	AA	1	68
1	CA	0	63
22	AV	0	2
22	AW	0	3
22	CV	0	2
22	CW	0	3
23	AX	0	1
23	CX	0	1
30	B4	0	1
30	D4	0	1
36	BA	2	84
36	DA	1	84
46	BN	0	1
46	DN	0	1
All	All	4	315

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	D4	47	GLN	C-N	-10.02	1.19	1.33
30	B4	47	GLN	C-N	-7.06	1.23	1.33
38	BC	218	MET	SD-CE	6.92	1.96	1.79
38	BC	218	MET	CG-SD	6.62	1.97	1.80
38	BC	120	MET	CG-SD	6.37	1.96	1.80

The worst 5 of 1132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1498	U	C2'-C3'-O3'	16.34	134.01	109.50
28	D2	32	LEU	N-CA-C	-15.06	94.86	111.28
4	AD	12	CYS	N-CA-C	-14.86	95.09	111.28
4	CD	12	CYS	N-CA-C	-14.46	95.52	111.28
42	BG	88	ILE	N-CA-C	13.25	127.56	108.48

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1498	U	C3'
36	BA	1799	G	C3'
36	BA	1819	A	C3'

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Mol	Chain	Res	Type	Atom
36	DA	1819	A	C3'

5 of 315 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	109	A	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	24	U	Sidechain
1	AA	37	U	Sidechain
1	AA	7	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	2220	0
1	CA	32329	0	16318	2219	0
2	AB	1901	0	1951	401	1
2	CB	1901	0	1951	411	1
3	AC	1613	0	1677	283	0
3	CC	1613	0	1677	275	0
4	AD	1703	0	1764	310	0
4	CD	1703	0	1765	323	0
5	AE	1147	0	1207	208	0
5	CE	1147	0	1207	208	0
6	AF	843	0	857	96	0
6	CF	843	0	857	108	0
7	AG	1257	0	1296	198	0
7	CG	1257	0	1296	199	0
8	AH	1116	0	1177	196	0
8	CH	1116	0	1177	207	0
9	AI	1010	0	1037	173	0
9	CI	1010	0	1037	181	0
10	AJ	795	0	840	208	0
10	CJ	795	0	840	216	0
11	AK	885	0	904	142	0
11	CK	885	0	904	131	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	971	0	1057	162	0
12	CL	971	0	1057	160	0
13	AM	988	0	1059	230	0
13	CM	988	0	1059	221	0
14	AN	492	0	529	136	0
14	CN	492	0	529	135	0
15	AO	734	0	771	102	0
15	CO	734	0	771	106	0
16	AP	701	0	720	125	0
16	CP	701	0	720	124	0
17	AQ	824	0	891	92	0
17	CQ	824	0	891	93	0
18	AR	574	0	644	100	0
18	CR	574	0	644	99	0
19	AS	630	0	652	135	0
19	CS	630	0	652	135	0
20	AT	763	0	861	156	0
20	CT	763	0	861	147	0
21	AU	209	0	221	31	0
21	CU	209	0	221	33	0
22	AV	1619	0	822	99	0
22	AW	1619	0	822	83	0
22	CV	1619	0	822	88	0
22	CW	1619	0	822	88	0
23	AX	272	0	142	23	0
23	CX	272	0	142	21	0
24	AY	1650	0	851	116	0
24	CY	1650	0	851	114	0
25	AZ	2900	0	2907	521	0
25	CZ	2900	0	2907	503	0
26	B0	662	0	688	114	0
26	D0	662	0	688	117	0
27	B1	732	0	808	157	0
27	D1	732	0	808	161	0
28	B2	598	0	653	175	0
28	D2	598	0	653	159	0
29	B3	468	0	523	78	0
29	D3	468	0	523	81	0
30	B4	341	0	337	71	0
30	D4	341	0	337	63	0
31	B5	459	0	480	105	0
31	D5	459	0	480	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B6	433	0	461	159	0
32	D6	433	0	461	164	0
33	B7	419	0	467	78	0
33	D7	419	0	467	81	0
34	B8	508	0	576	148	0
34	D8	508	0	576	153	0
35	B9	307	0	335	77	0
35	D9	307	0	337	80	0
36	BA	62474	0	31497	4310	0
36	DA	62474	0	31497	4324	0
37	BB	2551	0	1295	152	0
37	DB	2551	0	1295	163	0
38	BC	1742	0	1800	282	1
38	DC	1742	0	1800	283	1
39	BD	2145	0	2234	459	0
39	DD	2145	0	2234	455	0
40	BE	1564	0	1629	344	0
40	DE	1564	0	1629	335	0
41	BF	1624	0	1677	374	0
41	DF	1624	0	1677	370	0
42	BG	1474	0	1535	420	0
42	DG	1474	0	1535	380	0
43	BH	1223	0	1282	223	0
43	DH	1223	0	1282	226	0
44	BJ	651	0	136	11	0
44	DJ	651	0	136	9	0
45	BK	701	0	157	35	0
45	DK	701	0	157	34	0
46	BN	1105	0	1180	246	0
46	DN	1105	0	1180	248	0
47	BO	933	0	996	126	0
47	DO	933	0	996	128	0
48	BP	1114	0	1187	323	0
48	DP	1114	0	1187	321	0
49	BQ	1122	0	1179	252	0
49	DQ	1122	0	1179	240	0
50	BR	960	0	1021	205	0
50	DR	960	0	1021	202	0
51	BS	771	0	832	202	0
51	DS	771	0	832	197	0
52	BT	1142	0	1202	283	0
52	DT	1142	0	1202	285	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	BU	958	0	1015	235	0
53	DU	958	0	1015	237	0
54	BV	779	0	852	168	0
54	DV	779	0	852	172	0
55	BW	896	0	953	161	0
55	DW	896	0	953	167	0
56	BX	726	0	778	129	0
56	DX	726	0	778	123	0
57	BY	776	0	870	210	0
57	DY	776	0	870	205	0
58	BZ	1403	0	1432	327	0
58	DZ	1403	0	1432	306	0
59	AA	42	0	45	4	0
59	CA	42	0	45	3	0
60	AD	1	0	0	1	0
60	AN	1	0	0	0	0
60	B4	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D4	1	0	0	0	0
60	D9	1	0	0	2	0
61	AY	1	0	0	0	0
61	CY	1	0	0	0	0
62	AZ	28	0	12	15	0
62	CZ	28	0	12	15	0
63	AZ	57	0	58	4	0
63	CZ	57	0	59	8	0
All	All	306876	0	208322	31193	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 61.

The worst 5 of 31193 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:AZ:356:PRO:O	25:AZ:359:VAL:CG2	1.74	1.32
27:B1:41:ARG:NH2	36:BA:1365:A:H5''	1.53	1.24
25:CZ:356:PRO:O	25:CZ:359:VAL:HG22	1.38	1.20
24:CY:41:G:H2'	24:CY:42:U:H5''	1.24	1.19
32:B6:45:LYS:H	32:B6:45:LYS:CD	1.48	1.19

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_445]	1.63	0.57
2:CB:65:GLY:O	38:DC:27:ARG:NH2[2_646]	1.66	0.54

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	
2	AB	233/256 (91%)	116 (50%)	72 (31%)	45 (19%)	0	1
2	CB	233/256 (91%)	115 (49%)	74 (32%)	44 (19%)	0	1
3	AC	205/239 (86%)	117 (57%)	52 (25%)	36 (18%)	0	1
3	CC	205/239 (86%)	113 (55%)	57 (28%)	35 (17%)	0	2
4	AD	206/209 (99%)	123 (60%)	49 (24%)	34 (16%)	0	2
4	CD	206/209 (99%)	122 (59%)	48 (23%)	36 (18%)	0	1
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0	5
5	CE	149/162 (92%)	98 (66%)	37 (25%)	14 (9%)	0	6
6	AF	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	0	6
6	CF	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	0	6
7	AG	153/156 (98%)	86 (56%)	35 (23%)	32 (21%)	0	1
7	CG	153/156 (98%)	86 (56%)	37 (24%)	30 (20%)	0	1
8	AH	136/138 (99%)	88 (65%)	34 (25%)	14 (10%)	0	5
8	CH	136/138 (99%)	89 (65%)	35 (26%)	12 (9%)	0	7
9	AI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	3
9	CI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	3
10	AJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	3
10	CJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	80 (68%)	29 (25%)	8 (7%)	1	11
11	CK	117/129 (91%)	77 (66%)	32 (27%)	8 (7%)	1	11
12	AL	123/135 (91%)	71 (58%)	32 (26%)	20 (16%)	0	2
12	CL	123/135 (91%)	73 (59%)	31 (25%)	19 (15%)	0	2
13	AM	123/126 (98%)	58 (47%)	39 (32%)	26 (21%)	0	1
13	CM	123/126 (98%)	58 (47%)	39 (32%)	26 (21%)	0	1
14	AN	58/61 (95%)	28 (48%)	17 (29%)	13 (22%)	0	0
14	CN	58/61 (95%)	29 (50%)	14 (24%)	15 (26%)	0	0
15	AO	86/89 (97%)	54 (63%)	16 (19%)	16 (19%)	0	1
15	CO	86/89 (97%)	55 (64%)	15 (17%)	16 (19%)	0	1
16	AP	82/88 (93%)	50 (61%)	18 (22%)	14 (17%)	0	2
16	CP	82/88 (93%)	50 (61%)	18 (22%)	14 (17%)	0	2
17	AQ	98/105 (93%)	70 (71%)	21 (21%)	7 (7%)	1	10
17	CQ	98/105 (93%)	69 (70%)	21 (21%)	8 (8%)	0	8
18	AR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	1
18	CR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	1
19	AS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	3
19	CS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	3
20	AT	97/106 (92%)	49 (50%)	30 (31%)	18 (19%)	0	1
20	CT	97/106 (92%)	50 (52%)	29 (30%)	18 (19%)	0	1
21	AU	23/27 (85%)	10 (44%)	7 (30%)	6 (26%)	0	0
21	CU	23/27 (85%)	10 (44%)	8 (35%)	5 (22%)	0	0
25	AZ	370/406 (91%)	254 (69%)	77 (21%)	39 (10%)	0	5
25	CZ	370/406 (91%)	252 (68%)	81 (22%)	37 (10%)	0	5
26	B0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	0	6
26	D0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	0	6
27	B1	92/98 (94%)	55 (60%)	22 (24%)	15 (16%)	0	2
27	D1	92/98 (94%)	54 (59%)	25 (27%)	13 (14%)	0	3
28	B2	69/72 (96%)	43 (62%)	10 (14%)	16 (23%)	0	0
28	D2	69/72 (96%)	44 (64%)	14 (20%)	11 (16%)	0	2
29	B3	58/60 (97%)	28 (48%)	15 (26%)	15 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	D3	58/60 (97%)	28 (48%)	16 (28%)	14 (24%)	0	0
30	B4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	1
30	D4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	1
31	B5	57/60 (95%)	33 (58%)	13 (23%)	11 (19%)	0	1
31	D5	57/60 (95%)	32 (56%)	14 (25%)	11 (19%)	0	1
32	B6	48/54 (89%)	17 (35%)	14 (29%)	17 (35%)	0	0
32	D6	48/54 (89%)	18 (38%)	14 (29%)	16 (33%)	0	0
33	B7	47/49 (96%)	27 (57%)	12 (26%)	8 (17%)	0	2
33	D7	47/49 (96%)	27 (57%)	12 (26%)	8 (17%)	0	2
34	B8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	1
34	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	1
35	B9	35/37 (95%)	18 (51%)	9 (26%)	8 (23%)	0	0
35	D9	35/37 (95%)	18 (51%)	10 (29%)	7 (20%)	0	1
38	BC	226/229 (99%)	143 (63%)	53 (24%)	30 (13%)	0	3
38	DC	226/229 (99%)	141 (62%)	55 (24%)	30 (13%)	0	3
39	BD	273/276 (99%)	176 (64%)	63 (23%)	34 (12%)	0	4
39	DD	273/276 (99%)	172 (63%)	66 (24%)	35 (13%)	0	3
40	BE	203/206 (98%)	109 (54%)	45 (22%)	49 (24%)	0	0
40	DE	203/206 (98%)	108 (53%)	46 (23%)	49 (24%)	0	0
41	BF	206/210 (98%)	120 (58%)	47 (23%)	39 (19%)	0	1
41	DF	206/210 (98%)	121 (59%)	46 (22%)	39 (19%)	0	1
42	BG	179/182 (98%)	86 (48%)	52 (29%)	41 (23%)	0	0
42	DG	179/182 (98%)	96 (54%)	45 (25%)	38 (21%)	0	1
43	BH	158/180 (88%)	98 (62%)	36 (23%)	24 (15%)	0	2
43	DH	158/180 (88%)	99 (63%)	35 (22%)	24 (15%)	0	2
46	BN	137/140 (98%)	75 (55%)	39 (28%)	23 (17%)	0	2
46	DN	137/140 (98%)	74 (54%)	40 (29%)	23 (17%)	0	2
47	BO	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	0	5
47	DO	120/122 (98%)	93 (78%)	15 (12%)	12 (10%)	0	5
48	BP	144/150 (96%)	72 (50%)	35 (24%)	37 (26%)	0	0
48	DP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	BQ	139/141 (99%)	77 (55%)	46 (33%)	16 (12%)	0	4
49	DQ	139/141 (99%)	81 (58%)	39 (28%)	19 (14%)	0	3
50	BR	115/118 (98%)	68 (59%)	25 (22%)	22 (19%)	0	1
50	DR	115/118 (98%)	70 (61%)	23 (20%)	22 (19%)	0	1
51	BS	97/112 (87%)	37 (38%)	35 (36%)	25 (26%)	0	0
51	DS	97/112 (87%)	36 (37%)	37 (38%)	24 (25%)	0	0
52	BT	136/146 (93%)	63 (46%)	40 (29%)	33 (24%)	0	0
52	DT	136/146 (93%)	63 (46%)	40 (29%)	33 (24%)	0	0
53	BU	115/118 (98%)	69 (60%)	34 (30%)	12 (10%)	0	5
53	DU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	0	5
54	BV	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	1
54	DV	99/101 (98%)	61 (62%)	18 (18%)	20 (20%)	0	1
55	BW	111/113 (98%)	73 (66%)	24 (22%)	14 (13%)	0	4
55	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	4
56	BX	91/96 (95%)	55 (60%)	20 (22%)	16 (18%)	0	1
56	DX	91/96 (95%)	54 (59%)	22 (24%)	15 (16%)	0	2
57	BY	99/110 (90%)	37 (37%)	29 (29%)	33 (33%)	0	0
57	DY	99/110 (90%)	38 (38%)	28 (28%)	33 (33%)	0	0
58	BZ	174/206 (84%)	87 (50%)	47 (27%)	40 (23%)	0	0
58	DZ	174/206 (84%)	96 (55%)	41 (24%)	37 (21%)	0	1
All	All	12280/13108 (94%)	7151 (58%)	3059 (25%)	2070 (17%)	0	2

5 of 2070 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	19	HIS
2	AB	76	GLN
2	AB	77	ALA
2	AB	93	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	
2	AB	202/220 (92%)	178 (88%)	24 (12%)	5	24
2	CB	202/220 (92%)	178 (88%)	24 (12%)	5	24
3	AC	160/188 (85%)	148 (92%)	12 (8%)	12	39
3	CC	160/188 (85%)	148 (92%)	12 (8%)	12	39
4	AD	180/181 (99%)	153 (85%)	27 (15%)	3	17
4	CD	180/181 (99%)	151 (84%)	29 (16%)	2	15
5	AE	115/123 (94%)	92 (80%)	23 (20%)	1	8
5	CE	115/123 (94%)	93 (81%)	22 (19%)	1	9
6	AF	90/90 (100%)	78 (87%)	12 (13%)	4	21
6	CF	90/90 (100%)	79 (88%)	11 (12%)	5	23
7	AG	126/127 (99%)	113 (90%)	13 (10%)	7	30
7	CG	126/127 (99%)	113 (90%)	13 (10%)	7	30
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	17
8	CH	119/119 (100%)	102 (86%)	17 (14%)	3	19
9	AI	98/99 (99%)	88 (90%)	10 (10%)	7	30
9	CI	98/99 (99%)	88 (90%)	10 (10%)	7	30
10	AJ	88/92 (96%)	69 (78%)	19 (22%)	1	7
10	CJ	88/92 (96%)	69 (78%)	19 (22%)	1	7
11	AK	90/99 (91%)	79 (88%)	11 (12%)	5	23
11	CK	90/99 (91%)	80 (89%)	10 (11%)	6	27
12	AL	104/111 (94%)	80 (77%)	24 (23%)	1	6
12	CL	104/111 (94%)	80 (77%)	24 (23%)	1	6
13	AM	99/101 (98%)	87 (88%)	12 (12%)	5	23
13	CM	99/101 (98%)	87 (88%)	12 (12%)	5	23
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	15
14	CN	49/50 (98%)	40 (82%)	9 (18%)	1	10
15	AO	79/80 (99%)	68 (86%)	11 (14%)	3	19
15	CO	79/80 (99%)	68 (86%)	11 (14%)	3	19
16	AP	72/74 (97%)	62 (86%)	10 (14%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	63 (88%)	9 (12%)	4	22
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	35
17	CQ	94/97 (97%)	86 (92%)	8 (8%)	10	35
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5	25
18	CR	61/77 (79%)	53 (87%)	8 (13%)	4	21
19	AS	69/80 (86%)	58 (84%)	11 (16%)	2	15
19	CS	69/80 (86%)	58 (84%)	11 (16%)	2	15
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	18
20	CT	76/82 (93%)	65 (86%)	11 (14%)	3	18
21	AU	19/22 (86%)	18 (95%)	1 (5%)	20	48
21	CU	19/22 (86%)	18 (95%)	1 (5%)	20	48
25	AZ	314/339 (93%)	274 (87%)	40 (13%)	4	22
25	CZ	314/339 (93%)	275 (88%)	39 (12%)	4	23
26	B0	66/67 (98%)	50 (76%)	16 (24%)	1	5
26	D0	66/67 (98%)	51 (77%)	15 (23%)	1	6
27	B1	78/83 (94%)	58 (74%)	20 (26%)	0	4
27	D1	78/83 (94%)	59 (76%)	19 (24%)	1	4
28	B2	66/67 (98%)	47 (71%)	19 (29%)	0	2
28	D2	66/67 (98%)	50 (76%)	16 (24%)	1	5
29	B3	51/52 (98%)	44 (86%)	7 (14%)	3	20
29	D3	51/52 (98%)	44 (86%)	7 (14%)	3	20
30	B4	39/63 (62%)	25 (64%)	14 (36%)	0	1
30	D4	39/63 (62%)	25 (64%)	14 (36%)	0	1
31	B5	51/52 (98%)	47 (92%)	4 (8%)	11	38
31	D5	51/52 (98%)	47 (92%)	4 (8%)	11	38
32	B6	49/52 (94%)	39 (80%)	10 (20%)	1	8
32	D6	49/52 (94%)	39 (80%)	10 (20%)	1	8
33	B7	41/42 (98%)	32 (78%)	9 (22%)	1	6
33	D7	41/42 (98%)	31 (76%)	10 (24%)	1	4
34	B8	53/55 (96%)	46 (87%)	7 (13%)	4	21
34	D8	53/55 (96%)	45 (85%)	8 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	B9	34/34 (100%)	27 (79%)	7 (21%)	1	8
35	D9	34/34 (100%)	27 (79%)	7 (21%)	1	8
38	BC	180/181 (99%)	156 (87%)	24 (13%)	4	21
38	DC	180/181 (99%)	154 (86%)	26 (14%)	3	18
39	BD	217/218 (100%)	178 (82%)	39 (18%)	2	11
39	DD	217/218 (100%)	178 (82%)	39 (18%)	2	11
40	BE	165/166 (99%)	150 (91%)	15 (9%)	9	33
40	DE	165/166 (99%)	151 (92%)	14 (8%)	10	35
41	BF	165/166 (99%)	152 (92%)	13 (8%)	11	37
41	DF	165/166 (99%)	152 (92%)	13 (8%)	11	37
42	BG	155/156 (99%)	128 (83%)	27 (17%)	2	12
42	DG	155/156 (99%)	129 (83%)	26 (17%)	2	13
43	BH	132/148 (89%)	116 (88%)	16 (12%)	5	23
43	DH	132/148 (89%)	116 (88%)	16 (12%)	5	23
46	BN	117/119 (98%)	106 (91%)	11 (9%)	8	32
46	DN	117/119 (98%)	106 (91%)	11 (9%)	8	32
47	BO	100/100 (100%)	89 (89%)	11 (11%)	6	27
47	DO	100/100 (100%)	88 (88%)	12 (12%)	5	24
48	BP	112/116 (97%)	85 (76%)	27 (24%)	1	5
48	DP	112/116 (97%)	85 (76%)	27 (24%)	1	5
49	BQ	111/111 (100%)	93 (84%)	18 (16%)	2	15
49	DQ	111/111 (100%)	93 (84%)	18 (16%)	2	15
50	BR	100/101 (99%)	85 (85%)	15 (15%)	3	17
50	DR	100/101 (99%)	85 (85%)	15 (15%)	3	17
51	BS	77/88 (88%)	66 (86%)	11 (14%)	3	19
51	DS	77/88 (88%)	67 (87%)	10 (13%)	4	21
52	BT	120/127 (94%)	100 (83%)	20 (17%)	2	14
52	DT	120/127 (94%)	101 (84%)	19 (16%)	2	15
53	BU	92/94 (98%)	84 (91%)	8 (9%)	9	34
53	DU	92/94 (98%)	84 (91%)	8 (9%)	9	34
54	BV	82/82 (100%)	67 (82%)	15 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	DV	82/82 (100%)	67 (82%)	15 (18%)	2	11
55	BW	91/92 (99%)	77 (85%)	14 (15%)	2	16
55	DW	91/92 (99%)	77 (85%)	14 (15%)	2	16
56	BX	74/78 (95%)	65 (88%)	9 (12%)	5	23
56	DX	74/78 (95%)	65 (88%)	9 (12%)	5	23
57	BY	84/91 (92%)	68 (81%)	16 (19%)	1	9
57	DY	84/91 (92%)	69 (82%)	15 (18%)	2	11
58	BZ	155/179 (87%)	126 (81%)	29 (19%)	1	10
58	DZ	155/179 (87%)	127 (82%)	28 (18%)	2	11
All	All	10322/10862 (95%)	8804 (85%)	1518 (15%)	3	17

5 of 1518 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	CK	91	ARG
31	D5	56	LYS
12	CL	105	TYR
11	CK	82	VAL
25	CZ	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 372 such sidechains are listed below:

Mol	Chain	Res	Type
10	CJ	78	ASN
32	D6	32	ASN
13	CM	77	ASN
25	CZ	119	HIS
39	DD	126	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	288 (19%)	59 (3%)
1	CA	1503/1522 (98%)	284 (18%)	59 (3%)
22	AV	75/76 (98%)	20 (26%)	0
22	AW	75/76 (98%)	21 (28%)	2 (2%)
22	CV	75/76 (98%)	20 (26%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	CW	75/76 (98%)	21 (28%)	2 (2%)
23	AX	12/27 (44%)	4 (33%)	0
23	CX	12/27 (44%)	4 (33%)	0
24	AY	73/77 (94%)	29 (39%)	0
24	CY	73/77 (94%)	28 (38%)	0
36	BA	2900/2915 (99%)	648 (22%)	55 (1%)
36	DA	2900/2915 (99%)	654 (22%)	55 (1%)
37	BB	118/122 (96%)	29 (24%)	1 (0%)
37	DB	118/122 (96%)	29 (24%)	1 (0%)
All	All	9512/9630 (98%)	2079 (21%)	234 (2%)

5 of 2079 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 234 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2762	G
36	DA	2110	G
1	CA	575	G
36	DA	1992	G
36	DA	790	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	YG	AY	37	24	38,42,43	1.32	3 (7%)	45,62,65	2.09	15 (33%)
24	H2U	CY	17	24	18,21,22	0.88	0	19,30,33	1.62	3 (15%)
24	5MU	CY	54	24	19,22,23	0.25	0	27,32,35	0.38	0
24	7MG	CY	46	24	23,26,27	2.60	3 (13%)	27,39,42	1.69	3 (11%)
24	H2U	CY	20	24	18,21,22	0.85	0	19,30,33	1.60	3 (15%)
24	H2U	AY	17	24	18,21,22	0.87	0	19,30,33	1.63	3 (15%)
24	YG	CY	37	24	38,42,43	1.30	3 (7%)	45,62,65	2.09	15 (33%)
24	7MG	AY	46	24	23,26,27	2.54	3 (13%)	27,39,42	1.70	3 (11%)
24	PSU	CY	55	24	18,21,22	1.07	2 (11%)	21,30,33	2.10	6 (28%)
24	H2U	AY	20	24	18,21,22	0.86	0	19,30,33	1.58	3 (15%)
24	H2U	CY	16	24	18,21,22	0.90	1 (5%)	19,30,33	1.49	3 (15%)
24	PSU	AY	55	24	18,21,22	1.07	2 (11%)	21,30,33	2.06	6 (28%)
24	5MU	AY	54	24	19,22,23	0.25	0	27,32,35	0.39	0
24	H2U	AY	16	24	18,21,22	0.96	1 (5%)	19,30,33	1.48	3 (15%)

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
24	YG	AY	37	24	-	2/24/42/43	0/4/4/4
24	H2U	CY	17	24	-	5/7/38/39	0/2/2/2
24	5MU	CY	54	24	-	0/7/25/26	0/2/2/2
24	7MG	CY	46	24	-	0/7/37/38	0/3/3/3
24	H2U	CY	20	24	-	3/7/38/39	0/2/2/2
24	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	YG	CY	37	24	-	2/24/42/43	0/4/4/4
24	7MG	AY	46	24	-	0/7/37/38	0/3/3/3
24	PSU	CY	55	24	-	0/7/25/26	0/2/2/2
24	H2U	AY	20	24	-	3/7/38/39	0/2/2/2
24	H2U	CY	16	24	-	2/7/38/39	0/2/2/2
24	PSU	AY	55	24	-	0/7/25/26	0/2/2/2
24	5MU	AY	54	24	-	0/7/25/26	0/2/2/2
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-11.77	1.38	1.45
24	AY	46	7MG	C8-N9	-11.49	1.38	1.45
24	AY	37	YG	C13-C12	5.15	1.56	1.50
24	CY	37	YG	C13-C12	4.61	1.56	1.50
24	CY	46	7MG	C5-N7	3.09	1.39	1.35

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	46	7MG	N9-C8-N7	6.88	113.11	103.37
24	CY	46	7MG	N9-C8-N7	6.83	113.05	103.37
24	CY	37	YG	C24-O23-C21	5.54	122.04	115.63
24	AY	37	YG	C24-O23-C21	5.28	121.74	115.63
24	AY	37	YG	C5-C4-N3	-5.10	119.86	123.99

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	17	H2U	O4'-C1'-N1-C2
24	AY	17	H2U	O4'-C1'-N1-C6
24	AY	20	H2U	O4'-C4'-C5'-O5'
24	AY	20	H2U	C3'-C4'-C5'-O5'
24	CY	17	H2U	O4'-C1'-N1-C2

There are no ring outliers.

12 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	37	YG	7	0
24	CY	17	H2U	1	0
24	CY	54	5MU	5	0
24	CY	20	H2U	2	0
24	AY	17	H2U	1	0
24	CY	37	YG	4	0
24	CY	55	PSU	7	0
24	AY	20	H2U	2	0
24	CY	16	H2U	3	0
24	AY	55	PSU	6	0
24	AY	54	5MU	4	0
24	AY	16	H2U	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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	KIR	CZ	502	-	56,59,59	3.69	21 (37%)	60,84,84	1.67	11 (18%)
62	GDP	AZ	501	-	29,30,30	1.08	3 (10%)	45,47,47	1.69	8 (17%)
59	PAR	AA	1601	-	44,45,45	1.38	4 (9%)	63,67,67	1.38	7 (11%)
62	GDP	CZ	501	-	29,30,30	1.08	2 (6%)	45,47,47	1.80	10 (22%)
63	KIR	AZ	502	-	56,59,59	3.64	21 (37%)	60,84,84	1.65	10 (16%)
59	PAR	CA	1601	-	44,45,45	1.36	5 (11%)	63,67,67	1.34	8 (12%)

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	KIR	CZ	502	-	-	7/54/98/98	0/3/3/3
62	GDP	AZ	501	-	-	2/16/32/32	0/3/3/3
59	PAR	AA	1601	-	-	8/18/94/94	0/4/4/4
62	GDP	CZ	501	-	-	3/16/32/32	0/3/3/3
63	KIR	AZ	502	-	-	7/54/98/98	0/3/3/3
59	PAR	CA	1601	-	-	5/18/94/94	0/4/4/4

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	AZ	502	KIR	O18-C17	-14.90	1.22	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	CZ	502	KIR	O18-C17	-14.79	1.22	1.44
63	CZ	502	KIR	O30-C30	-12.48	1.18	1.42
63	AZ	502	KIR	O30-C30	-12.39	1.18	1.42
63	AZ	502	KIR	O34-C33	-9.42	1.29	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	AZ	501	GDP	C2-N3-C4	5.23	121.30	112.30
62	CZ	501	GDP	C2-N3-C4	5.16	121.19	112.30
62	CZ	501	GDP	C5-C4-N3	-5.01	120.42	128.39
59	AA	1601	PAR	O33-C14-C24	4.74	115.83	108.08
62	AZ	501	GDP	C5-C4-N3	-4.62	121.04	128.39

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AA	1601	PAR	C44-C54-C64-N64
59	AA	1601	PAR	O54-C54-C64-N64
62	AZ	501	GDP	PA-O3A-PB-O2B
62	AZ	501	GDP	PA-O3A-PB-O3B
62	CZ	501	GDP	PA-O3A-PB-O2B

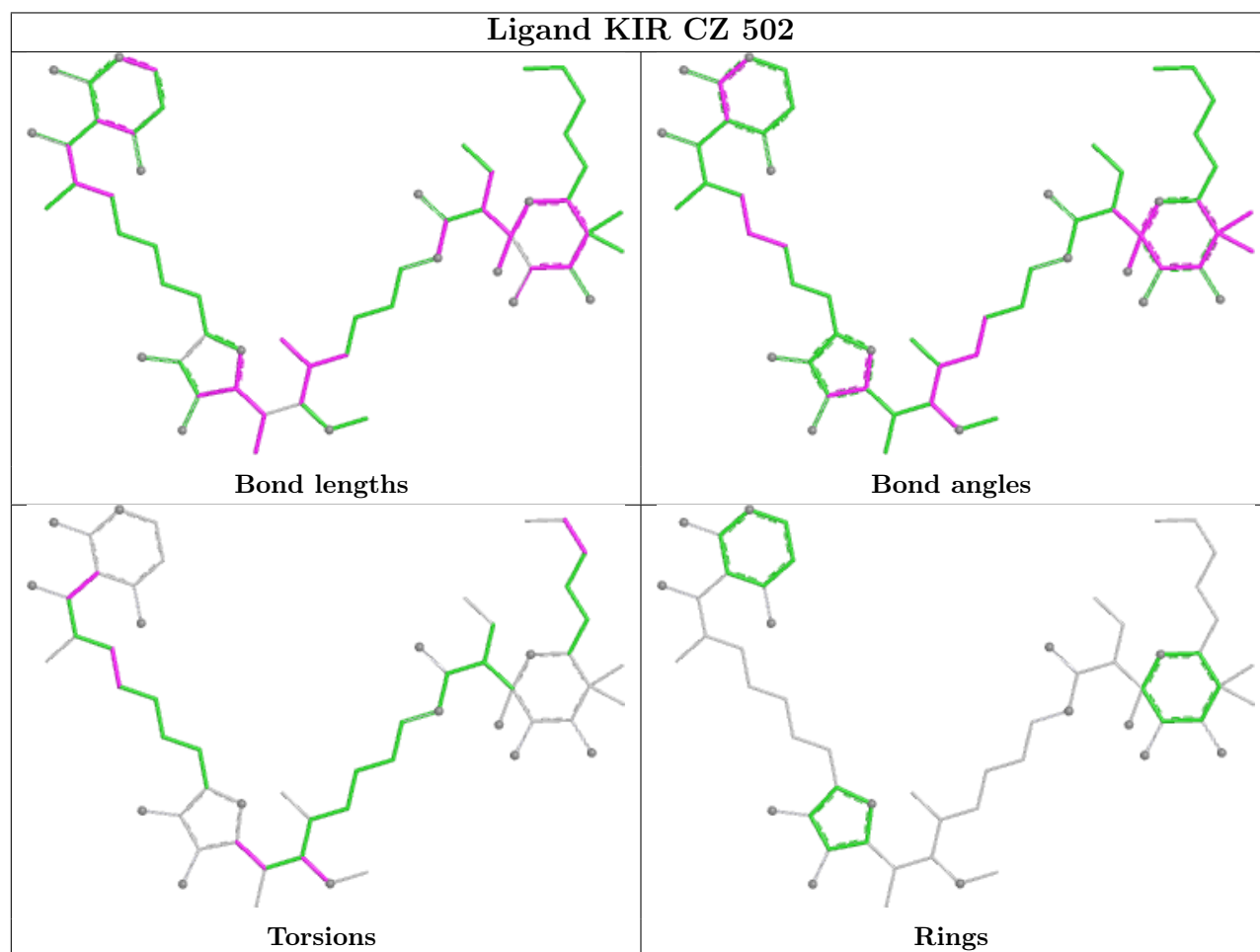
There are no ring outliers.

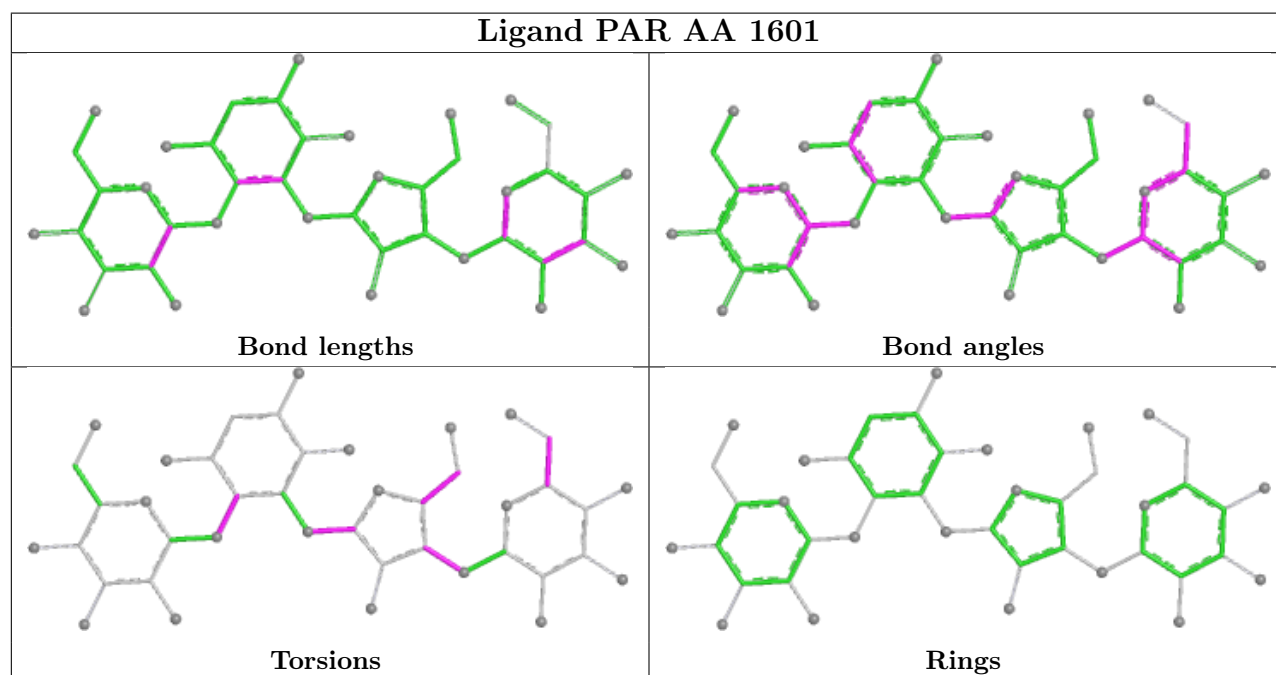
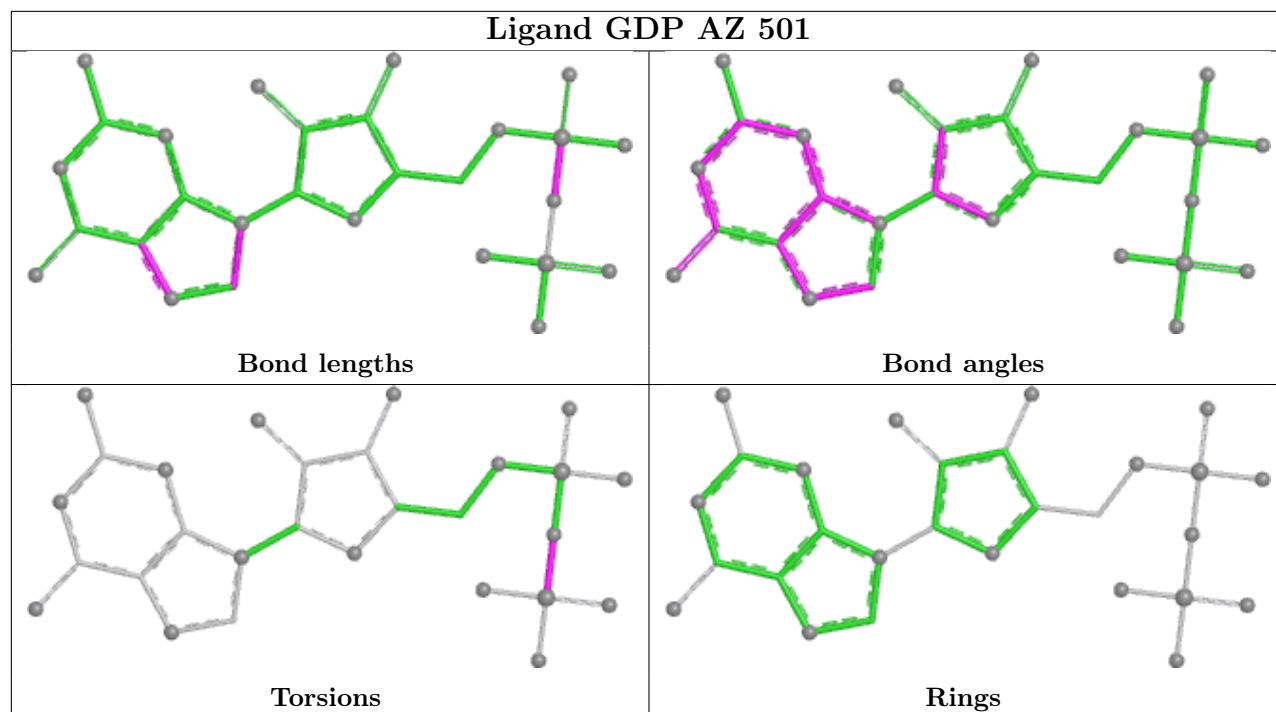
6 monomers are involved in 49 short contacts:

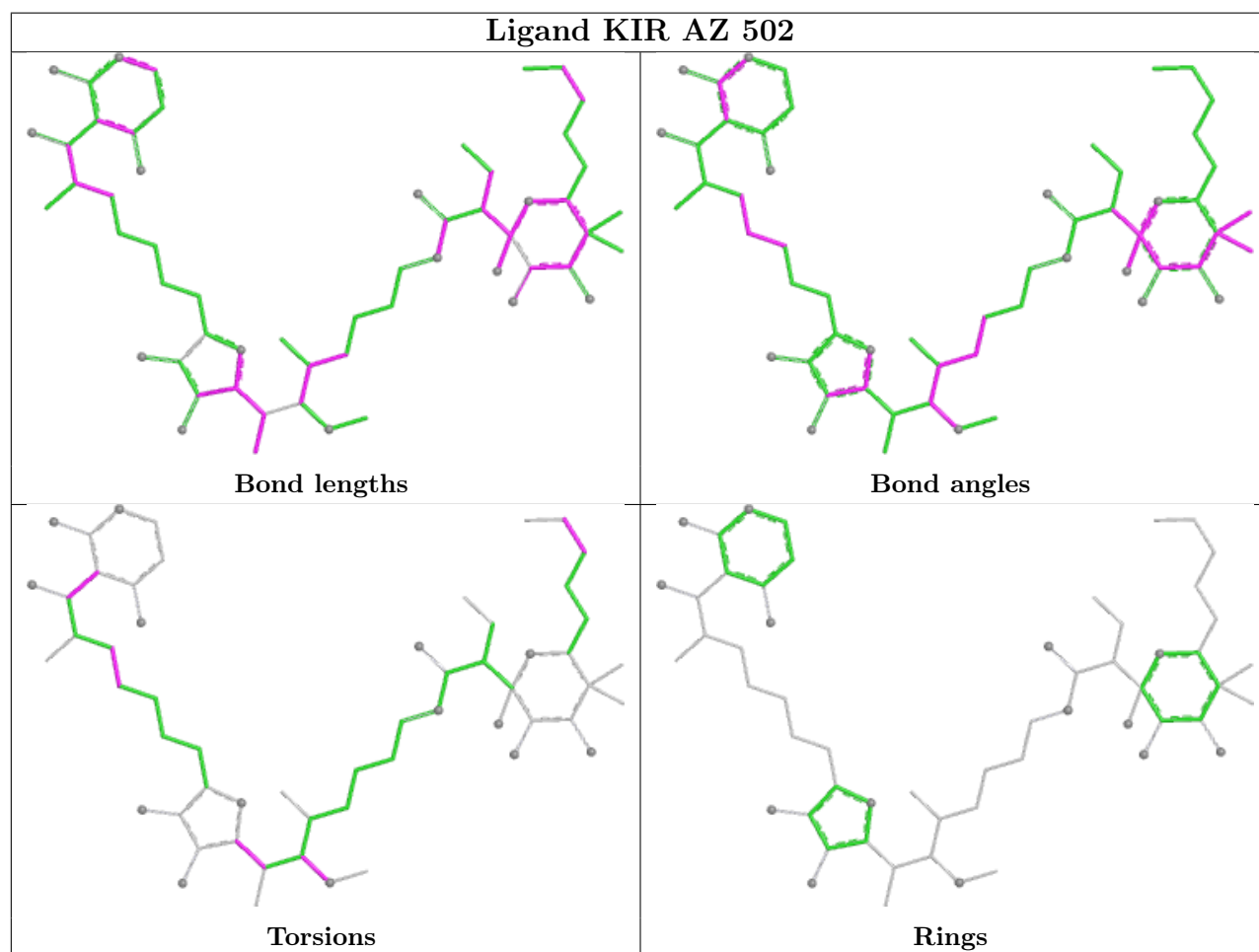
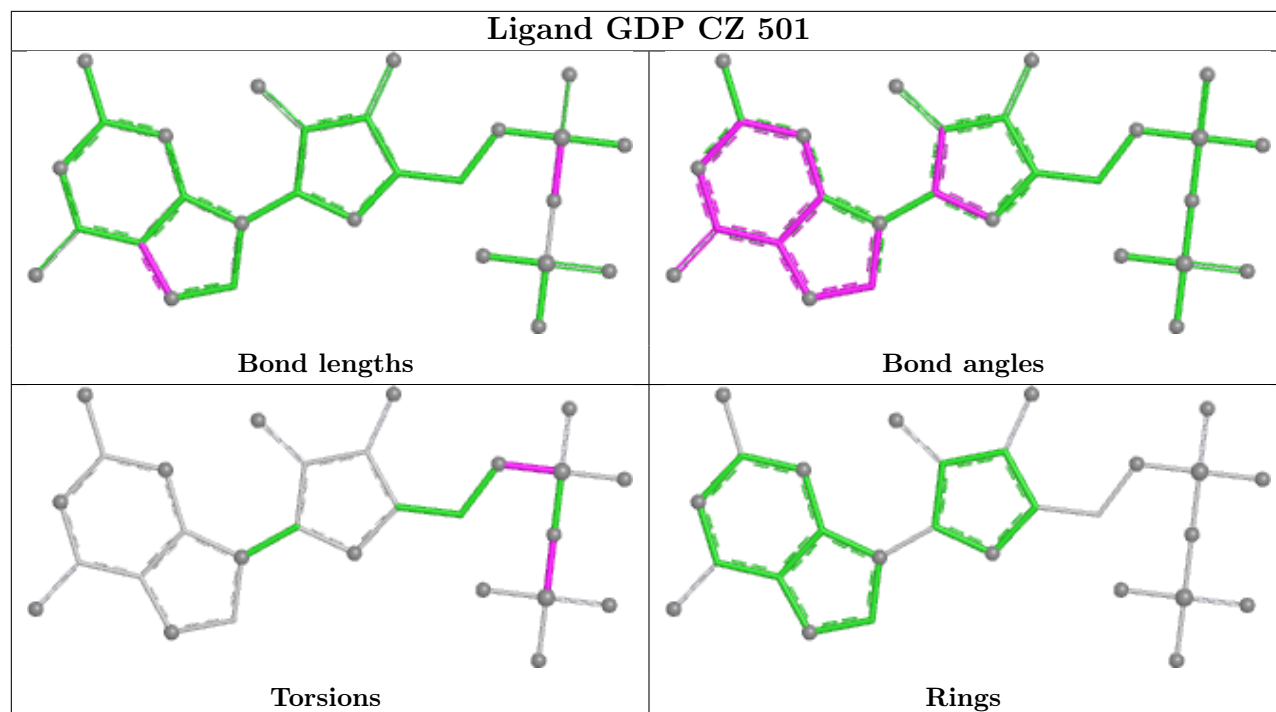
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	CZ	502	KIR	8	0
62	AZ	501	GDP	15	0
59	AA	1601	PAR	4	0
62	CZ	501	GDP	15	0
63	AZ	502	KIR	4	0
59	CA	1601	PAR	3	0

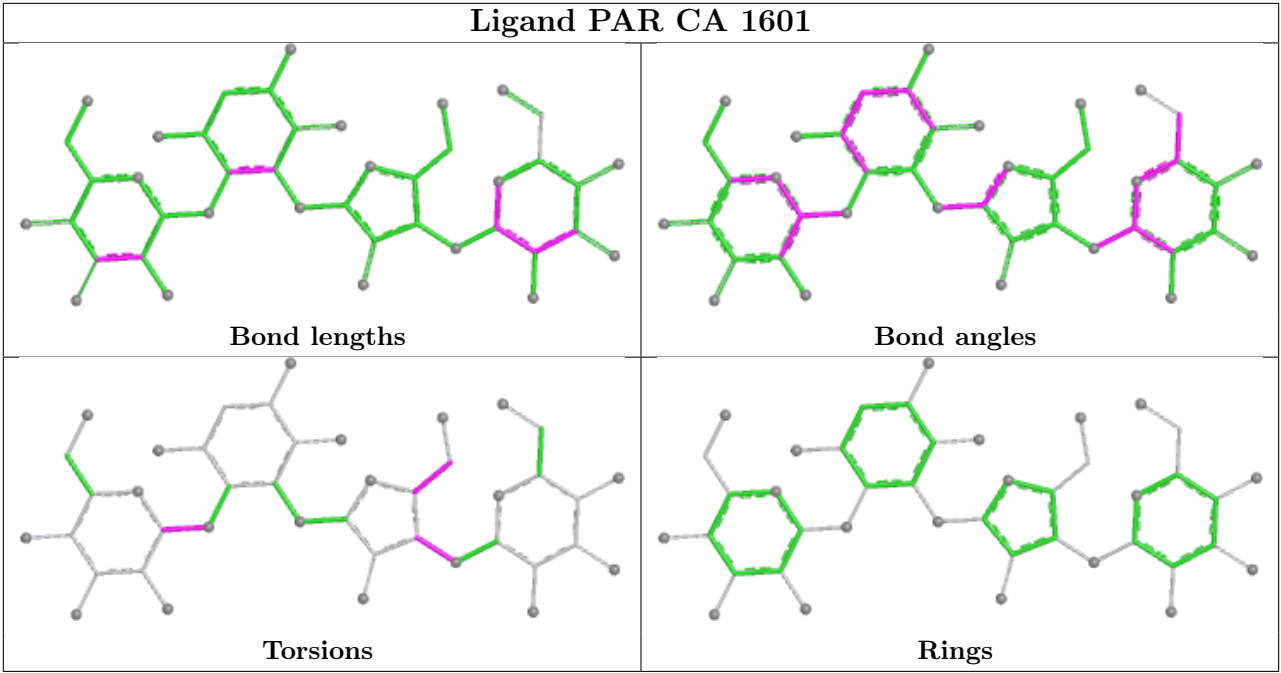
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	D4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D4	47:GLN	C	48:ARG	N	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.47	67 (4%) 38 21	29, 82, 163, 200	0
1	CA	1504/1522 (98%)	0.44	45 (2%) 52 30	28, 83, 163, 200	0
2	AB	235/256 (91%)	0.29	0 100 100	63, 102, 151, 161	0
2	CB	235/256 (91%)	0.24	3 (1%) 75 48	63, 102, 151, 162	0
3	AC	207/239 (86%)	0.17	1 (0%) 87 66	54, 91, 111, 117	0
3	CC	207/239 (86%)	0.11	2 (0%) 79 54	59, 91, 111, 117	0
4	AD	208/209 (99%)	0.29	7 (3%) 48 27	60, 91, 116, 122	0
4	CD	208/209 (99%)	0.21	5 (2%) 59 34	61, 92, 117, 123	0
5	AE	151/162 (93%)	0.00	1 (0%) 84 61	44, 72, 90, 108	0
5	CE	151/162 (93%)	0.08	3 (1%) 65 38	43, 73, 91, 109	0
6	AF	101/101 (100%)	0.36	3 (2%) 52 30	91, 102, 110, 118	0
6	CF	101/101 (100%)	0.27	2 (1%) 65 38	92, 103, 111, 118	0
7	AG	155/156 (99%)	0.33	10 (6%) 25 16	79, 104, 134, 141	0
7	CG	155/156 (99%)	0.17	3 (1%) 66 39	81, 104, 134, 141	0
8	AH	138/138 (100%)	0.29	3 (2%) 62 36	62, 80, 97, 116	0
8	CH	138/138 (100%)	0.21	3 (2%) 62 36	61, 82, 97, 115	0
9	AI	127/128 (99%)	0.96	13 (10%) 12 10	73, 126, 153, 158	0
9	CI	127/128 (99%)	0.57	6 (4%) 36 20	74, 126, 154, 159	0
10	AJ	99/105 (94%)	0.93	16 (16%) 4 5	79, 121, 149, 154	0
10	CJ	99/105 (94%)	0.92	12 (12%) 8 7	80, 121, 148, 153	0
11	AK	119/129 (92%)	0.40	3 (2%) 58 34	63, 84, 125, 150	0
11	CK	119/129 (92%)	0.30	2 (1%) 69 41	65, 85, 126, 151	0
12	AL	125/135 (92%)	0.25	3 (2%) 59 34	47, 70, 100, 125	0
12	CL	125/135 (92%)	0.36	2 (1%) 70 43	52, 71, 101, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	125/126 (99%)	0.76	14 (11%) 10 8	79, 119, 143, 159	0
13	CM	125/126 (99%)	0.51	11 (8%) 15 11	80, 118, 143, 159	0
14	AN	60/61 (98%)	0.36	4 (6%) 24 15	60, 77, 96, 101	0
14	CN	60/61 (98%)	0.32	2 (3%) 49 28	61, 77, 95, 103	0
15	AO	88/89 (98%)	0.43	2 (2%) 61 35	69, 92, 109, 112	0
15	CO	88/89 (98%)	0.26	2 (2%) 61 35	72, 91, 109, 112	0
16	AP	84/88 (95%)	0.50	4 (4%) 35 20	76, 89, 119, 137	0
16	CP	84/88 (95%)	0.27	0 100 100	74, 89, 118, 137	0
17	AQ	100/105 (95%)	0.28	1 (1%) 79 54	65, 92, 115, 121	0
17	CQ	100/105 (95%)	0.38	3 (3%) 52 30	67, 92, 115, 121	0
18	AR	70/88 (79%)	0.04	0 100 100	55, 86, 114, 121	0
18	CR	70/88 (79%)	-0.02	0 100 100	57, 87, 115, 121	0
19	AS	79/93 (84%)	0.70	8 (10%) 12 10	82, 120, 143, 146	0
19	CS	79/93 (84%)	0.53	3 (3%) 44 25	83, 120, 144, 146	0
20	AT	99/106 (93%)	0.59	10 (10%) 12 10	94, 109, 129, 132	0
20	CT	99/106 (93%)	0.40	5 (5%) 33 19	93, 109, 129, 132	0
21	AU	25/27 (92%)	1.48	6 (24%) 2 2	104, 116, 137, 139	0
21	CU	25/27 (92%)	1.52	6 (24%) 2 2	104, 116, 136, 138	0
22	AV	76/76 (100%)	0.67	3 (3%) 43 24	54, 120, 170, 179	0
22	AW	76/76 (100%)	0.89	5 (6%) 24 15	82, 147, 186, 199	0
22	CV	76/76 (100%)	0.61	1 (1%) 75 48	54, 121, 170, 179	0
22	CW	76/76 (100%)	1.11	10 (13%) 7 6	84, 148, 185, 199	0
23	AX	13/27 (48%)	1.18	5 (38%) 1 1	45, 63, 136, 154	0
23	CX	13/27 (48%)	1.26	5 (38%) 1 1	47, 62, 136, 154	0
24	AY	70/77 (90%)	0.88	6 (8%) 16 12	74, 155, 194, 200	0
24	CY	70/77 (90%)	0.74	2 (2%) 53 30	76, 156, 194, 200	0
25	AZ	374/406 (92%)	0.35	8 (2%) 63 37	97, 139, 158, 177	0
25	CZ	374/406 (92%)	0.44	12 (3%) 50 29	98, 139, 158, 176	0
26	B0	84/85 (98%)	0.79	6 (7%) 22 14	104, 116, 128, 137	0
26	D0	84/85 (98%)	0.99	14 (16%) 4 5	104, 116, 129, 137	0
27	B1	94/98 (95%)	0.18	3 (3%) 50 29	41, 71, 107, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D1	94/98 (95%)	0.32	1 (1%) 78 52	63, 85, 115, 122	0
28	B2	71/72 (98%)	0.17	2 (2%) 55 31	84, 115, 128, 130	0
28	D2	71/72 (98%)	0.29	2 (2%) 55 31	104, 125, 144, 163	0
29	B3	60/60 (100%)	0.98	6 (10%) 12 10	106, 122, 132, 148	0
29	D3	60/60 (100%)	0.73	4 (6%) 24 15	107, 122, 132, 148	0
30	B4	45/71 (63%)	0.99	9 (20%) 3 3	107, 169, 196, 198	0
30	D4	45/71 (63%)	0.78	5 (11%) 10 8	107, 170, 195, 197	0
31	B5	59/60 (98%)	0.99	8 (13%) 7 6	89, 116, 175, 187	0
31	D5	59/60 (98%)	0.93	6 (10%) 12 10	90, 115, 175, 186	0
32	B6	50/54 (92%)	0.96	8 (16%) 5 5	78, 119, 146, 152	0
32	D6	50/54 (92%)	0.76	6 (12%) 9 7	79, 119, 147, 152	0
33	B7	49/49 (100%)	0.46	2 (4%) 41 23	59, 77, 144, 152	0
33	D7	49/49 (100%)	0.49	1 (2%) 65 38	60, 78, 145, 152	0
34	B8	64/65 (98%)	1.37	15 (23%) 2 2	80, 104, 124, 138	0
34	D8	64/65 (98%)	1.68	15 (23%) 2 2	83, 104, 125, 138	0
35	B9	37/37 (100%)	0.85	5 (13%) 7 6	104, 117, 124, 128	0
35	D9	37/37 (100%)	1.19	6 (16%) 4 5	103, 118, 125, 126	0
36	BA	2901/2915 (99%)	0.76	191 (6%) 24 15	31, 100, 192, 200	0
36	DA	2901/2915 (99%)	0.74	181 (6%) 26 16	31, 101, 192, 200	0
37	BB	119/122 (97%)	1.13	20 (16%) 4 5	103, 142, 169, 175	0
37	DB	119/122 (97%)	1.00	12 (10%) 12 10	102, 142, 168, 174	0
38	BC	228/229 (99%)	0.43	9 (3%) 43 24	92, 122, 168, 178	0
38	DC	228/229 (99%)	0.41	8 (3%) 47 27	92, 122, 167, 179	0
39	BD	275/276 (99%)	0.24	5 (1%) 67 40	30, 67, 96, 110	0
39	DD	275/276 (99%)	0.29	5 (1%) 67 40	38, 68, 96, 109	0
40	BE	205/206 (99%)	0.82	19 (9%) 14 10	67, 106, 143, 154	0
40	DE	205/206 (99%)	0.78	22 (10%) 11 9	67, 106, 143, 153	0
41	BF	208/210 (99%)	0.64	14 (6%) 24 15	61, 123, 160, 167	0
41	DF	208/210 (99%)	0.65	17 (8%) 17 12	62, 123, 160, 166	0
42	BG	181/182 (99%)	0.29	3 (1%) 69 41	103, 128, 146, 163	0
42	DG	181/182 (99%)	0.49	11 (6%) 27 16	111, 133, 151, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
43	BH	160/180 (88%)	0.73	12 (7%)	20	14	131, 155, 174, 176	0
43	DH	160/180 (88%)	0.80	12 (7%)	20	14	131, 155, 174, 176	0
44	BJ	0/173	-	-	-	-	-	-
44	DJ	0/173	-	-	-	-	-	-
45	BK	0/147	-	-	-	-	-	-
45	DK	0/147	-	-	-	-	-	-
46	BN	139/140 (99%)	0.72	9 (6%)	25	16	103, 123, 148, 155	0
46	DN	139/140 (99%)	0.88	18 (12%)	7	7	103, 123, 148, 155	0
47	BO	122/122 (100%)	0.16	0	100	100	60, 80, 96, 104	0
47	DO	122/122 (100%)	0.23	1 (0%)	82	58	61, 80, 96, 106	0
48	BP	146/150 (97%)	0.98	21 (14%)	6	6	71, 113, 133, 140	0
48	DP	146/150 (97%)	0.79	15 (10%)	12	10	70, 114, 133, 139	0
49	BQ	141/141 (100%)	0.59	7 (4%)	34	19	73, 106, 130, 159	0
49	DQ	141/141 (100%)	0.60	7 (4%)	34	19	73, 105, 129, 159	0
50	BR	117/118 (99%)	0.65	8 (6%)	23	15	81, 105, 123, 143	0
50	DR	117/118 (99%)	0.63	9 (7%)	19	13	82, 105, 124, 143	0
51	BS	99/112 (88%)	0.84	9 (9%)	15	11	96, 133, 155, 162	0
51	DS	99/112 (88%)	0.90	14 (14%)	6	6	97, 133, 156, 162	0
52	BT	138/146 (94%)	0.50	5 (3%)	46	26	72, 112, 166, 181	0
52	DT	138/146 (94%)	0.49	4 (2%)	53	30	73, 111, 166, 181	0
53	BU	117/118 (99%)	0.80	9 (7%)	19	13	87, 120, 141, 147	0
53	DU	117/118 (99%)	0.85	13 (11%)	10	8	88, 119, 141, 148	0
54	BV	101/101 (100%)	0.99	13 (12%)	7	7	105, 144, 159, 164	0
54	DV	101/101 (100%)	0.91	13 (12%)	7	7	106, 145, 159, 165	0
55	BW	113/113 (100%)	0.58	8 (7%)	22	14	81, 109, 132, 136	0
55	DW	113/113 (100%)	0.49	5 (4%)	39	22	81, 109, 131, 136	0
56	BX	93/96 (96%)	0.77	5 (5%)	31	18	96, 108, 124, 128	0
56	DX	93/96 (96%)	0.87	10 (10%)	11	9	97, 109, 125, 130	0
57	BY	101/110 (91%)	1.13	14 (13%)	6	6	124, 145, 165, 170	0
57	DY	101/110 (91%)	1.03	13 (12%)	7	7	123, 145, 163, 170	0
58	BZ	176/206 (85%)	0.50	4 (2%)	61	35	107, 133, 161, 164	0
58	DZ	176/206 (85%)	0.84	16 (9%)	15	11	109, 139, 168, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22002/23378 (94%)	0.59	1268 (5%) 29 17	28, 105, 164, 200	0

The worst 5 of 1268 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	D8	65	GLU	20.0
34	B8	65	GLU	11.4
48	BP	65	ARG	6.9
27	B1	22	GLY	6.4
9	AI	66	ARG	6.4

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
24	H2U	CY	20	20/21	0.20	0.12	195,198,200,200	0
24	H2U	AY	16	20/21	0.26	0.21	198,199,200,200	0
24	H2U	CY	16	20/21	0.41	0.15	199,199,200,200	0
24	H2U	CY	17	20/21	0.45	0.16	196,199,200,200	0
24	H2U	AY	20	20/21	0.47	0.13	196,198,200,200	0
24	H2U	AY	17	20/21	0.47	0.18	195,199,199,200	0
24	PSU	CY	55	20/21	0.74	0.12	172,180,180,180	0
24	7MG	AY	46	24/25	0.75	0.15	186,189,190,190	0
24	PSU	AY	55	20/21	0.80	0.10	171,180,181,182	0
24	5MU	CY	54	21/22	0.82	0.11	165,167,168,171	0
24	7MG	CY	46	24/25	0.82	0.15	186,189,190,190	0
24	5MU	AY	54	21/22	0.84	0.12	164,166,168,171	0
24	YG	CY	37	39/40	0.89	0.15	77,108,122,122	0
24	YG	AY	37	39/40	0.92	0.19	77,108,121,122	0

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

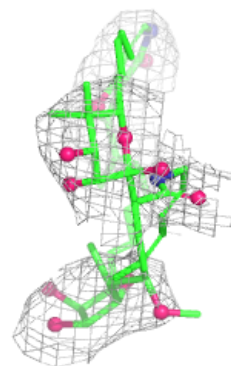
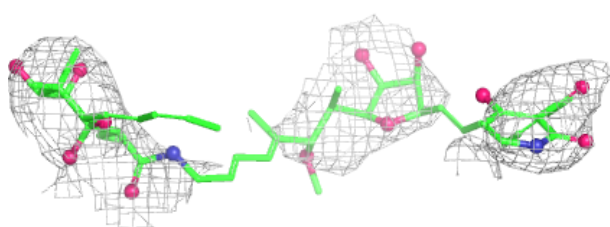
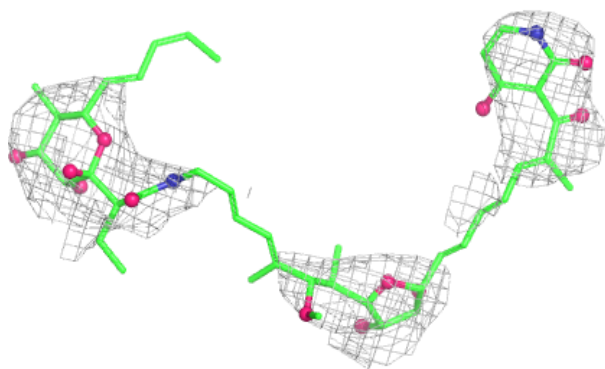
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
61	MG	CY	101	1/1	0.24	0.23	181,181,181,181	0
61	MG	AY	101	1/1	0.70	0.18	109,109,109,109	0
63	KIR	AZ	502	57/57	0.86	0.14	98,106,116,117	0
62	GDP	CZ	501	28/28	0.88	0.08	117,126,128,128	0
63	KIR	CZ	502	57/57	0.88	0.15	99,106,116,117	0
62	GDP	AZ	501	28/28	0.89	0.09	117,124,126,126	0
59	PAR	CA	1601	42/42	0.93	0.11	41,46,64,65	0
59	PAR	AA	1601	42/42	0.94	0.10	40,44,48,49	0
60	ZN	D4	101	1/1	0.98	0.03	133,133,133,133	0
60	ZN	B4	101	1/1	0.99	0.07	97,97,97,97	0
60	ZN	D9	101	1/1	0.99	0.03	126,126,126,126	0
60	ZN	CD	301	1/1	1.00	0.11	56,56,56,56	0
60	ZN	CN	101	1/1	1.00	0.01	100,100,100,100	0
60	ZN	AN	101	1/1	1.00	0.03	45,45,45,45	0
60	ZN	AD	301	1/1	1.00	0.10	52,52,52,52	0
60	ZN	B9	101	1/1	1.00	0.02	113,113,113,113	0

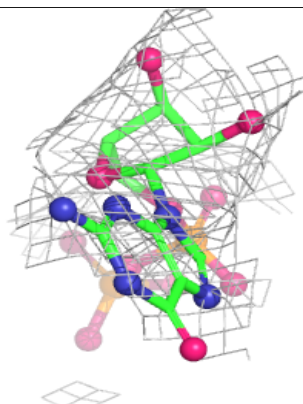
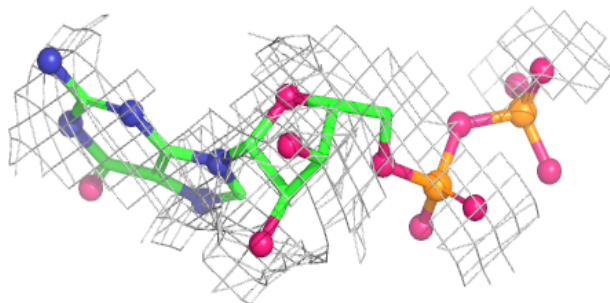
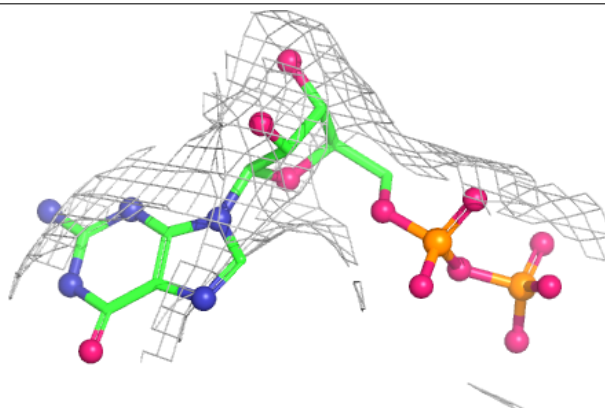
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around KIR AZ 502:

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

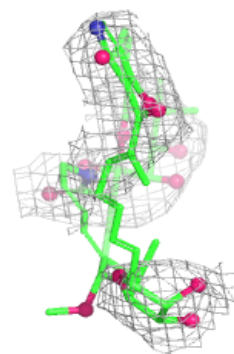
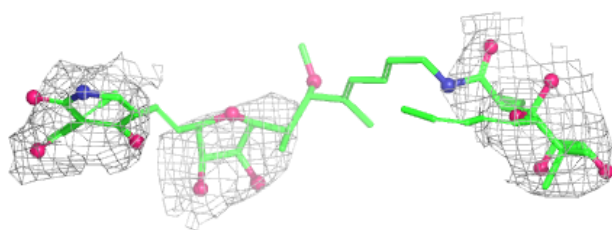
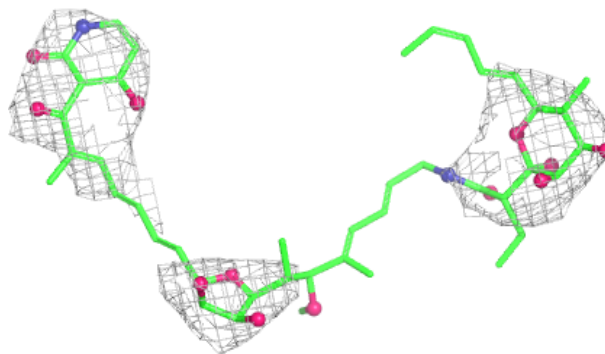
**Electron density around GDP CZ 501:**

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

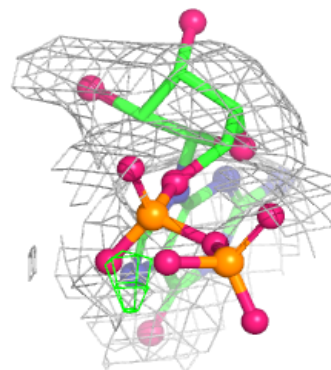
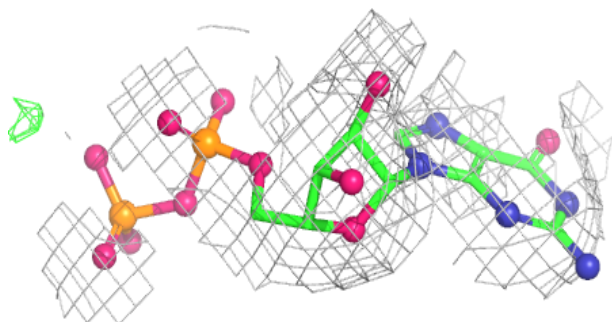
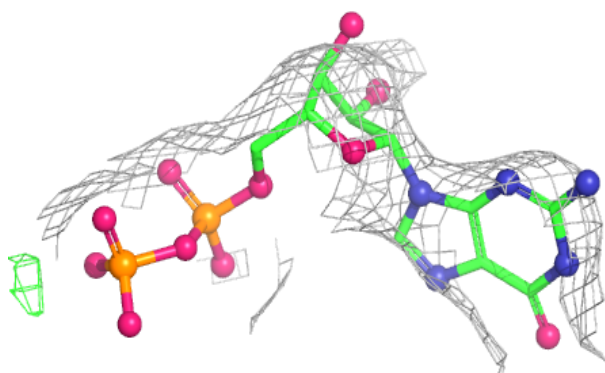


Electron density around KIR CZ 502:

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

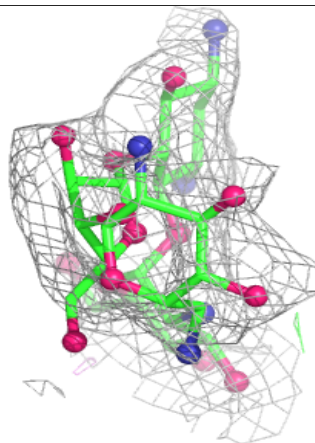
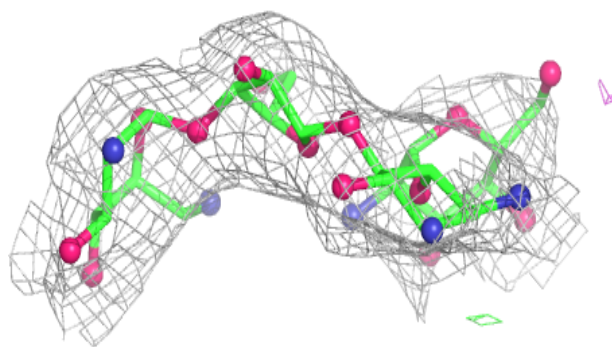
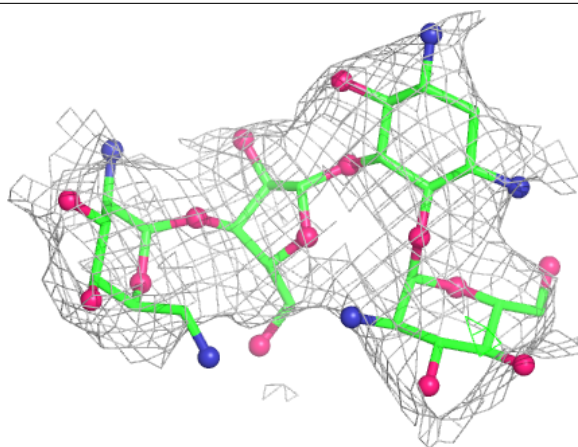
**Electron density around GDP AZ 501:**

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



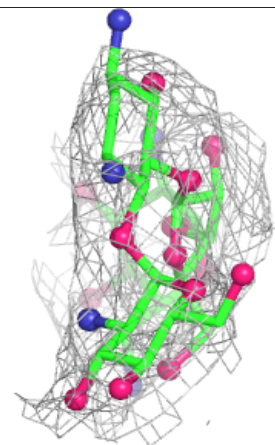
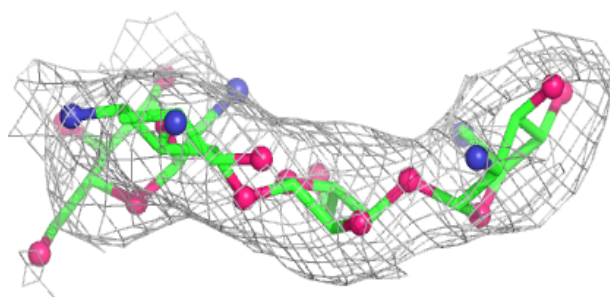
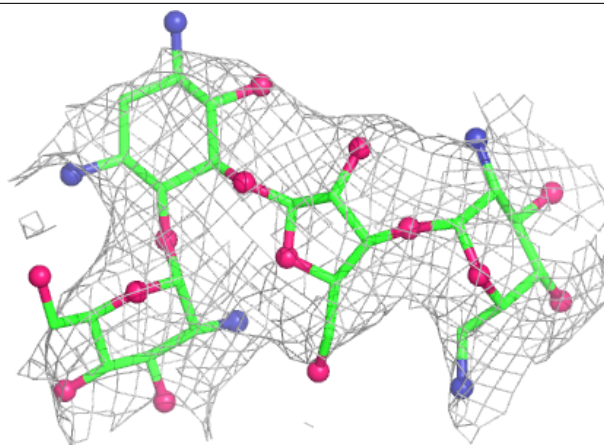
Electron density around PAR CA 1601:

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



Electron density around PAR AA 1601:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.