



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 3, 2020 – 11:04 am BST

PDB ID : 4V5G
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

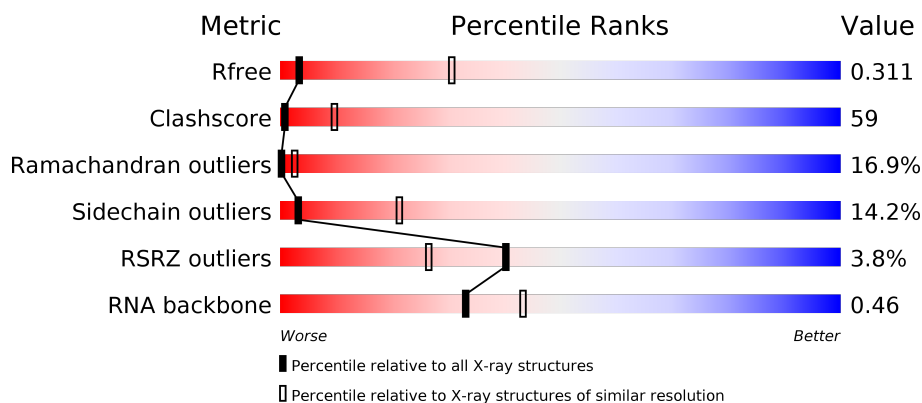
1 Overall quality at a glance

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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)
RNA backbone	3102	1017 (4.20-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>11%</div> <div>66%</div> <div>19%</div> <div>..</div> </div>
1	CA	1522	<div> <div>11%</div> <div>67%</div> <div>18%</div> <div>..</div> </div>
2	AB	256	<div> <div>13%</div> <div>57%</div> <div>20%</div> <div>• 8%</div> </div>
2	CB	256	<div> <div>13%</div> <div>58%</div> <div>18%</div> <div>• 8%</div> </div>

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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	H2U	AY	16	-	-	-	X
24	H2U	CY	16	-	-	-	X
24	H2U	CY	17	-	-	-	X
24	PSU	CY	55	-	-	X	-
60	ZN	D9	101	-	-	X	-
61	MG	CY	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			

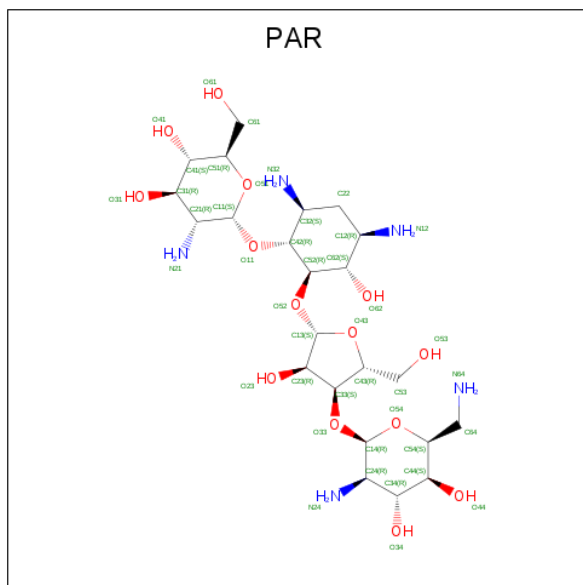
- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

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 1403	C 897	N 252	O 252	S 2	0	0	0
58	DZ	176	Total 1403	C 897	N 252	O 252	S 2	0	0	0

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
60	B4	1	Total Zn 1 1	0	0
60	CN	1	Total Zn 1 1	0	0
60	AN	1	Total Zn 1 1	0	0
60	B9	1	Total Zn 1 1	0	0
60	D9	1	Total Zn 1 1	0	0
60	D4	1	Total Zn 1 1	0	0

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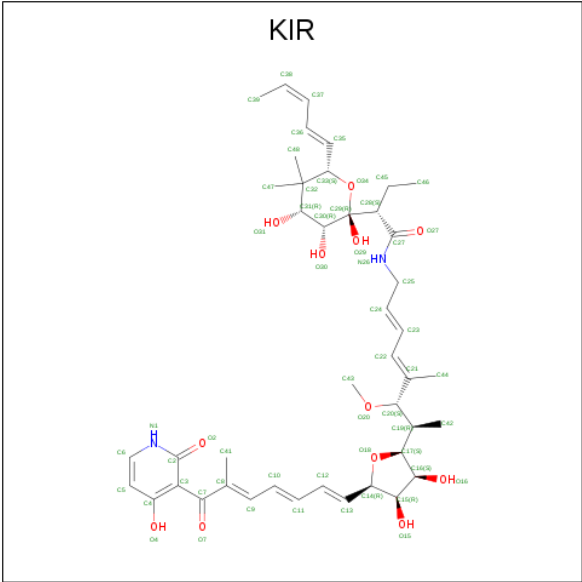
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CD	1	Total 1	Zn 1	0	0
60	AD	1	Total 1	Zn 1	0	0

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

-
- ORTEP diagram of the GDP molecule. The structure shows the guanine base (C1-C6, N1-N7, O6), the ribose sugar (C1', C2', C3', C4', C5'), and the diphosphate group (P1, P2, O1A-O5A, O1B-O5B). The displacement ellipsoids are drawn at the 50% probability level.

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

- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



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		

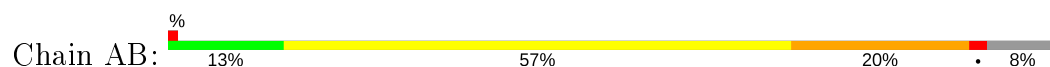
A1507	G1441	U1381	C1321	G1253	G1193	G1132	G1072	G1011	G951	A889	G823	G763	A702	U641
G1508	G1442	C1382	C1322	C1254	U1194	G1133	U1073	U1012	U952	G890	C824	C764	G703	A642
U1509	G1442A	C1383	G1255	G1256	C1195	U1135	G1074	G1013	G953	U891	G825	C765	A704	C643
U1510	A1442B	C1384	A1324	A1256	U1196	U1136	C1075	A1014	G954	A892	C826	A766	U705	
G1511	G1443	G1385	C1325	U1257	G1197	U1137	G1076	A1015	U955	G894	A828	A767	A706	U646
U1512	C1444	G1386	G1326	G1258	G1198	C1137	U1078	A1016	U956	G894	G829	A768	C707	C647
A1513	C1445	G1387	C1327	C1259	U1199	G1138	U1079	C1017	U957	G895	G830	C770	C708	A648
C1514	U1446	C1388	C1328	C1260	C1200	G1139	A1080	C1018	U960	C896	U831	G771	G710	G649
C1515	A1447	C1389	A1261	A1261	A1201	C1140	A1081	U1019	U961	G898	C832	U772	G711	G650
G1516	C1452	U1390	U1330	C1262	G1202	C1141	G1081	U1020	G962	C899	U833	G773	A712	C851
G1517	G1456	U1391	G1331		C1203	G1142	G1082	G1021	G963	C899	U834	G774	G713	A653
A1518	G1457	G1392	A1332		A1204	G1143	U1083		G964	A900	U835	G775	G714	G654
A1519	U1393	U1393	A1333	C1270	U1205	G1144	G1084	G1024	A901	G902	U836	G776	A715	A655
G1520	A1460	A1394	G1334	C1271	G1206	C1145	U1085	U1025	A905	G902	G837	A777	A716	
G1521	G1461	C1395	C1335	G1272	G1207	A1146	U1086	C1026	G906	G903	G838	A778		
U1522	G1462	A1396	C1336	G1273	C1208	C1147	U1087	C1027	G907	C904	G839	G779	G719	G657
G1523	C1463	C1397	G1337	G1274	C1209	U1148	G1088		A908	U905	U839	C779	A780	U659
C1524	G1464	A1398	G1338	A1275	C1210	C1149	G1089		A909		C840	A781	C720	U660
G1525	C1465	C1399	A1339	G1276	U1211	U1150	U1090	G1030	C970	A908	U841	A782	G721	G661
G1526	C1466	C1400		C1277	U1212	A1151	U1091	G1030A	C971	A909	C848	A783	A722	G662
C1527	G1467	G1401	C1342	U1278	A1213	A1152	A1092		C972		C849	C783	G723	G663
U1528	A1468	C1402	G1343	A1279	G1214	C1153	A1093	G1031	C973	C912	U850	C784	G724	A663
G1529	G1469	C1403	C1344	A1280	G1215	G1154	G1094	G1032	G974	A913	G851	G785	G725	G664
G1530	G1470	C1404	U1345	U1281	G1216	G1155	U1095	G1033	A975	A915	G852	G786	G726	A665
A1531	G1471	G1405	U1346	C1282	C1217	G1156	C1096	G1034	G976	A916	G853	A787	G727	A666
U	U1472	U1406	G1347	G1283	C1218	A1157	C1097	A1035	A977	C916	C854	U788	A728	G667
C	A1473	C1407	U1348	C1284	U1219	C1158	C1098		A978	C917	G855	U789	A729	G668
A	G1474	A1408	A1349	U1285	G1220	U1159	G1099	C1039	C979	A918	C856	A790	G730	U669
C	G1475	C1409	A1350	A1286	G1221	G1160	U1100	U1040	C980	A919	G857	G791	G731	G670
C	G1476	G1410	U1351	A1287	C1222	C1161	A1101	A1041	U981	U920	G858	A792	C732	G671
U	C1477	C1411	C1352	A1288	G1223	C1162	A1102	G1042	U982	U921	A859	U793	A733	U672
U	C1478	C1412	G1353	A1289	G1224	C1163	C1103	G1043	A983	C922	A860	A794	G734	G673
C	C1479	A1413	C1354	G1290	A1225	G1164	A1104	A1044	C984	A923	G861	C795	C735	G674
U	G1480	G1414	G1355	G1291	C1226	C1165	A1105	C1045	C985	C925	U863	C796	C736	A675
U	U1481	G1415	G1356	U1292	A1227	G1166	A1106	A1046	A986	G926	U864	C797	A737	A676
U	G1482	G1416	A1357	G1293	C1228	A1168	C1107	G1047	G987	G927	A865	G798	C738	U677
C	A1483	G1417	U1358		A1229	A1169	G1108	G1048	G988		C866	G799	C739	U678
U	C1484	A1418	C1359	C1298	C1230	A1170	C1109	U1049	C989	C928	C867	G800	U740	C679
U	U1485	G1419	A1360	A1299	G1231	G1171	A1110	G1050	C990	G929	G867	U801	U741	C680
U	G1486	C1420	G1361	G1300	U1232	C1172	A1111	C1051	U991	C930	C868	A802	G742	C681
U	G1487	G1421	C1362	U1301	G1233	G1173	A1112	U1052	U992	C931	G869	G803	U743	G682
U	G1488	G1422	C1363	G1302	C1234	G1174	C1113	G1053	G993	C932	U870	U804	C744	G683
U	G1489	C1423	A1363A	C1303	U1235	G1175	C1114	G1054	A994	G933	U871	C805	C745	A684
C1490	U1364	C1424	G1364	G1304	A1236	A1176	C1115	A1055	C995	C934	A872	C806	C746	G685
G1491	G1365	U1425	G1365	G1305	C1237	G1177	C1116	U1056	A996	A935	A873	A807	C747	U686
A1492	C1366	C1426	C1366	A1306	A1238	G1178	G1117	G1057	C997	C936	G874	C808	C748	A687
A1493	C1367	U1427	C1367	U1307	A1239	A1179	C1118	G1058	G998	A937	C875	G809	C749	G688
U1494	U1308	A1428	G1368	U1308	U1240	A1180	C1119	C1059	C999	A938	G876	C810	G750	C689
U1495	C1369	C1429	G1369	G1309	G1241	G1181	G1120	C1060	U1000	G939	C877	C811	U751	G690
C1496	G1370	C1430	G1370	G1310	C1242	G1182	U1121	G1061	A1001	C940	G878	C812	G752	G691
G1497	G1371	C1431	G1371	G1311	C1243	A1183	U1122	U1062	G1001A	G941	C879	U813	A753	U692
U1498	G1432	G1432	U1372	G1312	C1244	G1184	A1123	C1063	G1002	G942	C880	A814	C754	G693
A1499	A1433	C1433	G1373	U1313	A1245	G1185	G1124	G1064	U943	G944	C881	A815	C755	A694
A1500	A1374	A1434	A1374	C1314	C1246	G1186	U1125	U1065	A1004	G944	C882	A816	C756	A695
C1501	G1435	U1375	A1375	U1315	U1247	G1187	U1126	C1066	A1005	G945	C883	C817	C757	A696
A1502	U1436	G1316	A1316	G1316	A1248	G1188	G1127	A1067	A946	G947	U884	G818	C758	U697
A1503	C1437	C1377	A1377	C1317	C1249	C1189	C1128	G1068	C1007	G947	C885	A819	A759	G698
G1504	G1438	C1378	C1378	A1318	A1250	G1190	C1129	C1069	C1008	C948	G886	U820	G760	C699
G1505	C1439	G1379	G1379	A1319	A1251	A1191	A1130	U1070	G1009	A949	G887	G821	G761	C699
U1506	C1440	C1440	U1380	C1320	A1252	C1192	G1131	C1071	G1010	U950	G888	C822	C762	C701

● Molecule 1: 16S RIBOSOMAL RNA



G951	G1010	G1069	G1129	G1190	A1250	A1318	C1378	C1439	G1504
G952	G1011	U1070	A1130	A1191	A1251	A1319	G1379	C1440	G1505
G953	G1012	C1071	G1131	G1192	A1252	C1320	G1380	G1441	U1506
G954	G1013	G1072	C1132	G1193	G1253	G1321	U1381	G1442	A1507
U955	A1014	U1073	G1133	U1194	C1254	C1322	C1382	A1442A	G1508
U956	A1015	G1074	G1134	G1195	G1255	G1323	C1383	G1443	C1509
U957	A1016	C1075	U1135	U1196	A1256	A1324	C1384	G1444	U1510
A958	G1017	C1076	U1136	G1197	U1257	G1325	G1385	C1445	G1511
A959	C1018	U1077	G1137	G1198	U1258	G1326	G1386	U1446	U1512
U960	C1019	U1078	G1138	U1199	C1259	C1327	G1387	A1447	A1513
U961	U1020	U1079	G1139	C1200	C1260	C1328	C1388	A1448	C1514
G962	G1021	A1080	C1140	A1201	U1261	A1329	C1389	C1452	C1515
G963		U1081	C1141	G1202	C1262	U1330	U1390	G1456	A1516
A964	G1024	G1082	G1142	C1203		G1331	U1391	G1457	U1517
A965	U1025	U1083	G1143	A1204	A1269	A1332	G1392	G1458	A1518
G966	G1026	G1084	U1144	U1205	C1270	A1333	U1393	C1459	A1519
C967	C1027	U1085	C1145	G1206	G1271	G1334	A1394	G1460	G1520
A968	G1028	U1086	C1146	G1207	G1272	G1335	C1395	G1461	G1521
A969	C1029	G1087	C1147	C1208	G1273	G1336	A1396	G1462	U1522
C970	C1030	G1088	U1148	C1209	G1274	G1337	C1397	G1463	G1523
G971	G1030A	U1089	C1149	C1210	A1275	A1338	C1398	C1465	G1524
C972	G1030B	U1090	U1150	U1211	G1276	A1339	C1399	C1466	G1525
G973		U1091	A1151	U1212	C1277		C1400	C1467	C1526
A974	G1031	A1092	C1152	A1213	U1278	G1342	G1401	A1468	U1528
A975	G1032	A1093	C1153	C1214	A1279	G1343	C1402	G1469	G1529
G976	G1033	G1094	U1154	G1215	A1280	C1344	C1403	G1470	A1531
A977	G1034	U1095	G1155	C1217	U1281	U1345		G1471	
A978	A1035	C1096	C1156	G1218	C1282	A1346	U1406	U1472	U
C979		G1097	A1157	C1219	G1283	G1347	C1407	A1473	C
C980	G1038	G1098	C1158	U1219	C1284	U1348	A1408	A1474	A
U981	C1039	G1099	U1159	G1220	A1285	A1349	C1409	G1475	C
U982	U1040	C1100	G1160	G1221	A1286	A1350	G1410	C1476	C
A983	A1041	A1101	C1161	G1222	A1287	U1351	C1411	C1477	U
C984	G1042	C1102	C1162	C1223	A1288	G1352	A1412	C1478	C
C985	C1043	C1103	C1163	G1224	A1289	G1353	A1413	C1479	C
A986	A1044	G1104	G1164	A1225	G1290	C1354	U1414	G1480	U
G987	C1045	A1105	C1165	C1226	G1291	G1355	G1415	U1481	U
G988	A1046	G1106	G1166	A1227	U1292	G1356	G1416	G1482	U
C989	G1047	C1107	U1168	C1228	G1293	A1357	G1417	A1483	C
C990	U1048	G1108	A1169	A1229	C1298	U1358	A1418	C1484	U
U991	U1049	C1109	C1170	C1230	A1299	C1359	G1419	U1485	
U992	G1050	A1110	G1171	G1231	G1300	A1360	C1420	G1486	
G993	C1051	C1111	C1172	U1232	U1301	G1361	G1421	G1487	
A994	U1052	C1112	G1173	G1233	U1302	C1362	G1422	G1488	
C995	G1053	C1113	G1174	C1234	C1303	A1363A	G1423	C1489	
A996	A1054	C1114	G1175	U1235	G1304	U1364	C1424	G1490	
U997	U1056	C1115	A1176	A1236	C1305	G1365	U1425	G1491	
G998	U1057	C1116	G1177	C1237	G1306	C1366	C1426	A1492	
C999	G1057	G1117	U1178	A1238	A1307	C1367	U1427	A1493	
U1000	U1058	C1118	A1179	A1239	U1308	G1368	A1428	A1494	
A1001	C1059	C1119	A1180	U1240	U1309	C1369	C1429	U1495	
G1001A	G1060	G1120	G1181	G1241	G1310	C1370	C1430	C1496	
G1002	G1061	U1121	G1182	C1242	G1311	G1371	G1431	G1497	
G1003	U1062	U1122	A1183	C1243	G1312	U1372	G1432	U1498	
A1004	C1063	G1123	G1184	C1244	G1313	A1373	A1433	A1499	
A1005	G1064	G1124	U1185	A1245	C1314	G1374	A1434	A1500	
C1006	U1065	U1125	G1186	C1246	C1315	A1375	G1435	A1501	
C1007	U1066	U1126	U1187	U1247	U1316	U1376	U1436	A1502	
C1008	A1067	G1127	A1188	A1248	C1317	A1377	G1438	A1503	
G1009	G1068	C1128	C1189	C1249					

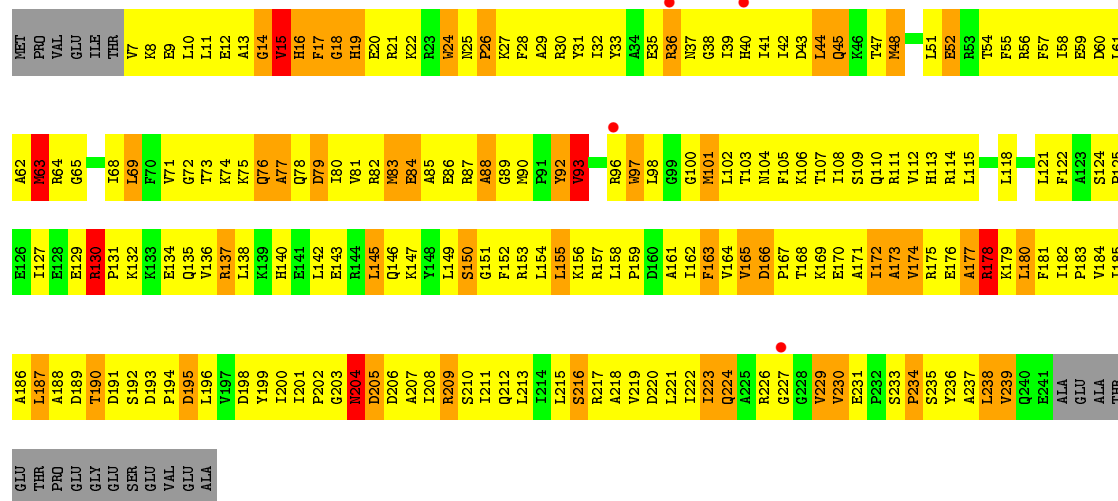
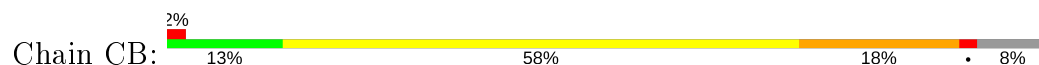
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



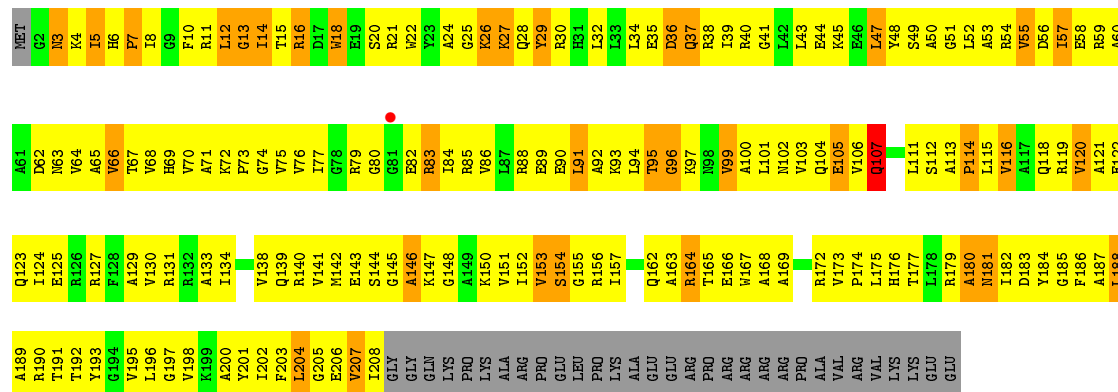
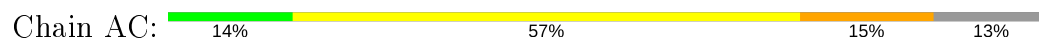
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PRO	A63	E126	A186
VAL	R64	I127	L187
GLU	G65	E128	A188
ILE		E129	D189
THR		A130	T190
V7	I68	P131	D191
K8	L69	K132	S192
E9	F70	K133	D193
L10	V71	E134	P194
L11	G72	Q135	D195
L12	T73	V136	L196
A13	K74	R137	V197
E14	K75	L138	D198
G14	Q76	L139	I199
Y15	A77	H140	I200
H16	Q78	E141	T201
F17	D79	L142	P202
G18	I80	E143	G203
H19	V81	E144	N204
E20	R82	L145	D205
R21	M83	Q146	D206
K22	E84	K147	A207
R23	A85	Y148	I208
W24	E86	L149	R209
N25	R87	S150	S210
P26	A88	G151	I211
R27	G89	F152	Q212
F28	N90	R153	L213
A29	P91	L154	L214
R30	Y92	L155	L215
Y31	Y93	K156	S216
I32	N94	R157	R217
I33	Q95	L158	A218
A34	R96	P159	V219
E35	W97	D160	D220
R36	L98	A161	L221
N37	G99	I162	I222
G38	G100	F163	I223
I39	M101	V164	Q224
H40	T102	V165	A225
I41	N103	D166	R226
I42	N104	P167	G227
D43	F105	T168	G228
L44	K106	K169	V229
Q45	T107	E170	V230
R46	I108	A171	E231
F47	Q110	I172	P232
M48	R111	A173	S233
	R112	V174	P234
L51	H113	R175	S235
E52	R114	E176	Y236
R53	L115	A177	A237
T54	F55	R178	L238
F56	R56	K179	V239
F57	L118	L180	Q240
I58	L121	F181	E241
E59	F122	I182	ALA
D60	A123	G183	GLU
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THR
GLU
THR
PRO
GLU
GLY
GLU
SER
VAL
GLU
ALA

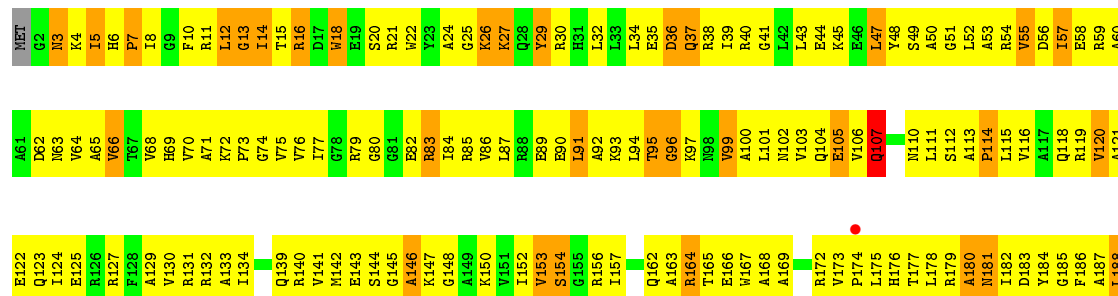
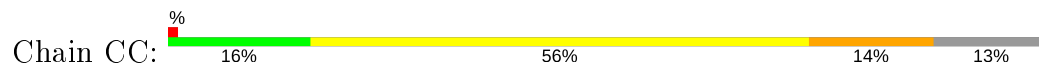
• Molecule 2: 30S RIBOSOMAL PROTEIN S2



• Molecule 3: 30S RIBOSOMAL PROTEIN S3

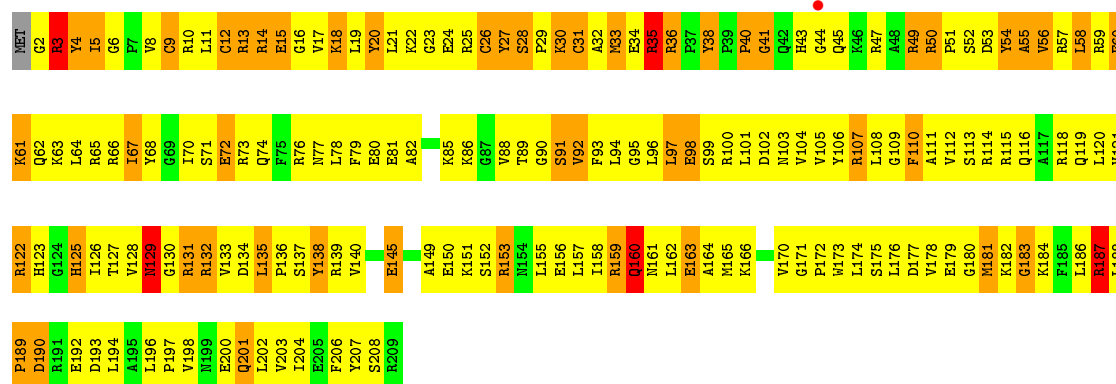


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

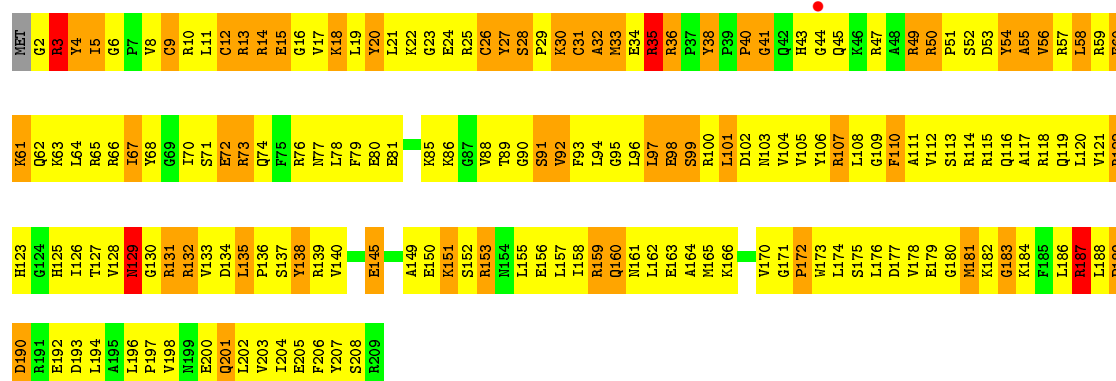
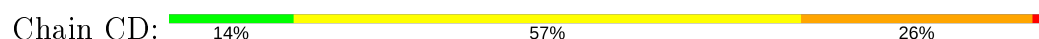




• Molecule 4: 30S RIBOSOMAL PROTEIN S4



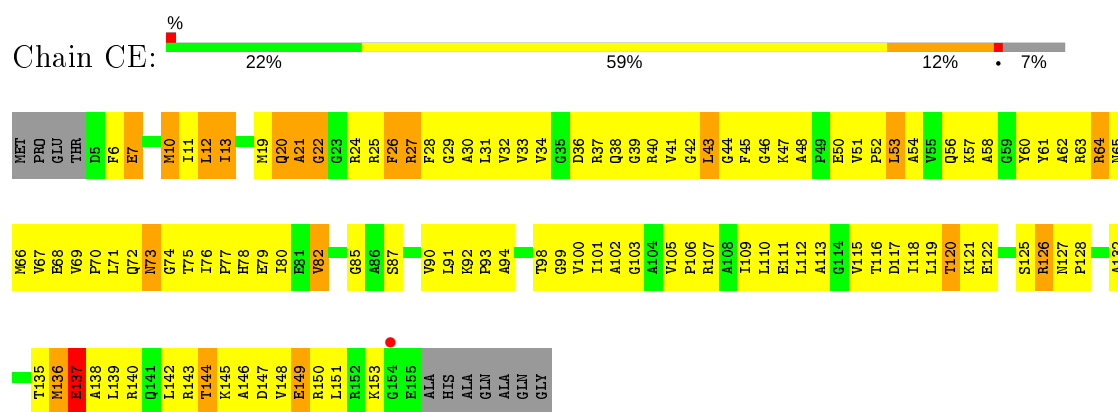
• Molecule 4: 30S RIBOSOMAL PROTEIN S4



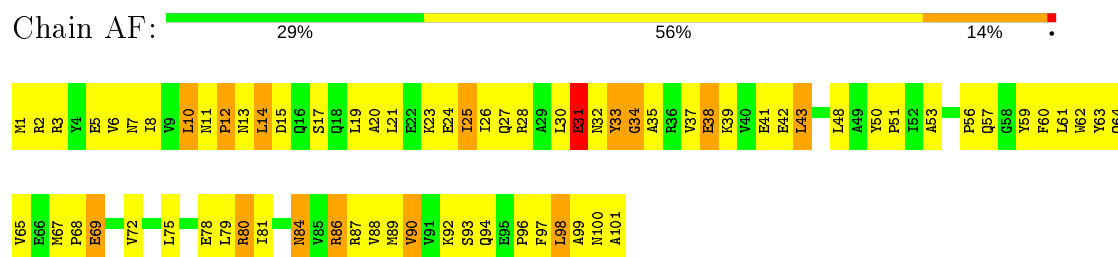
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



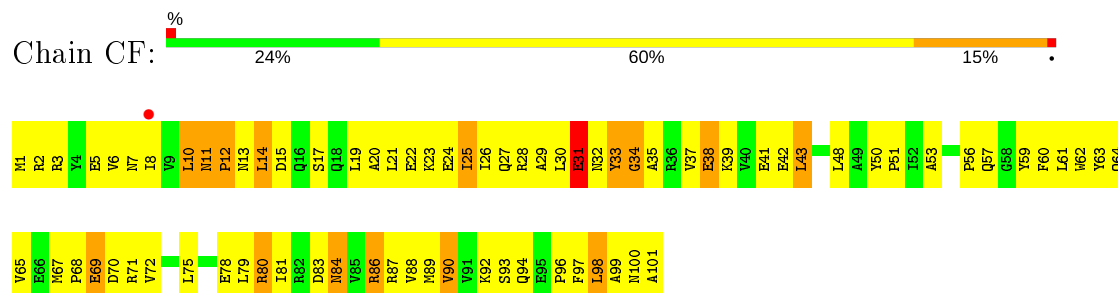
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



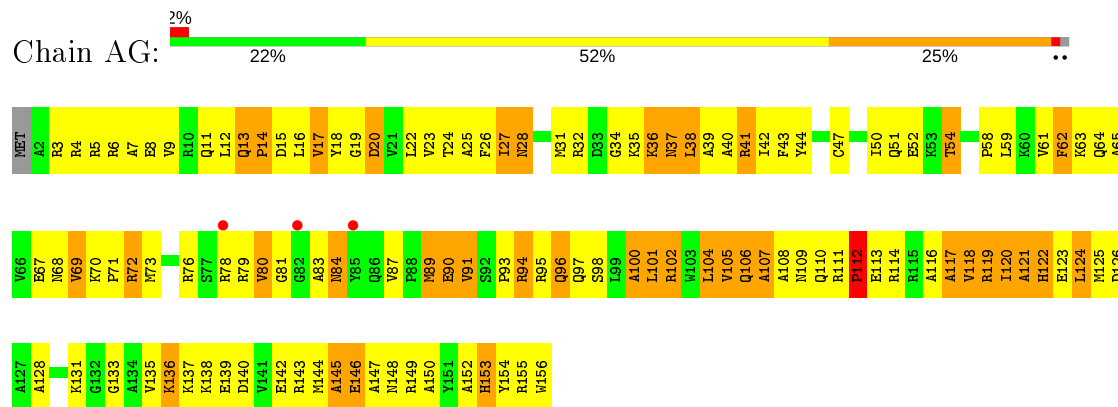
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

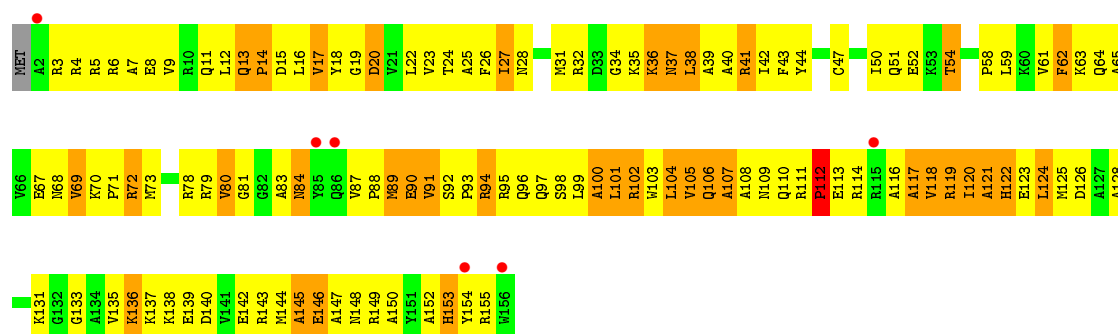


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

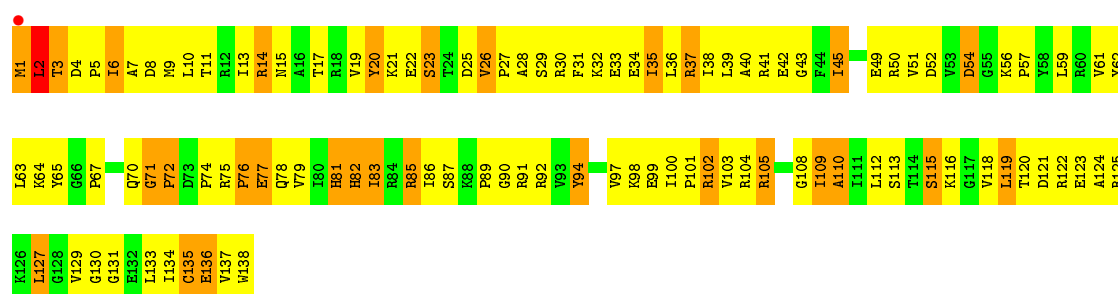


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

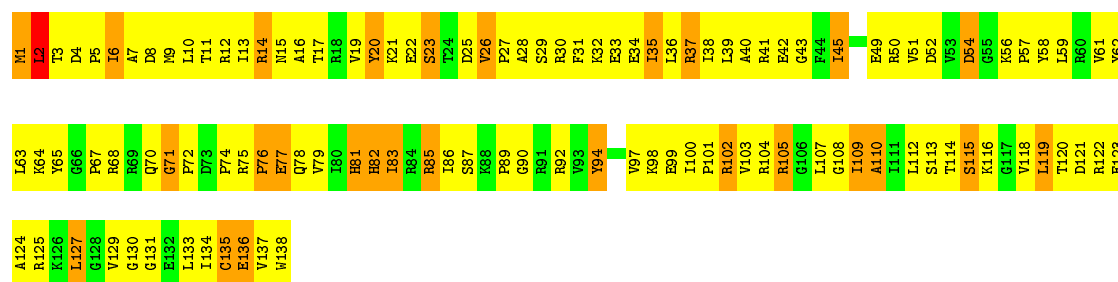




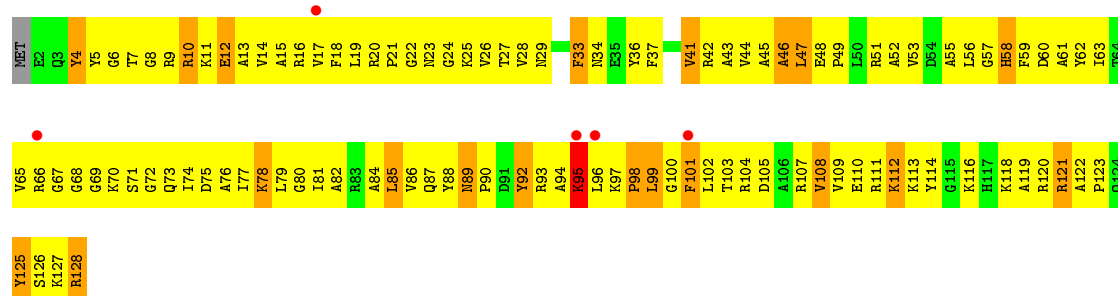
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



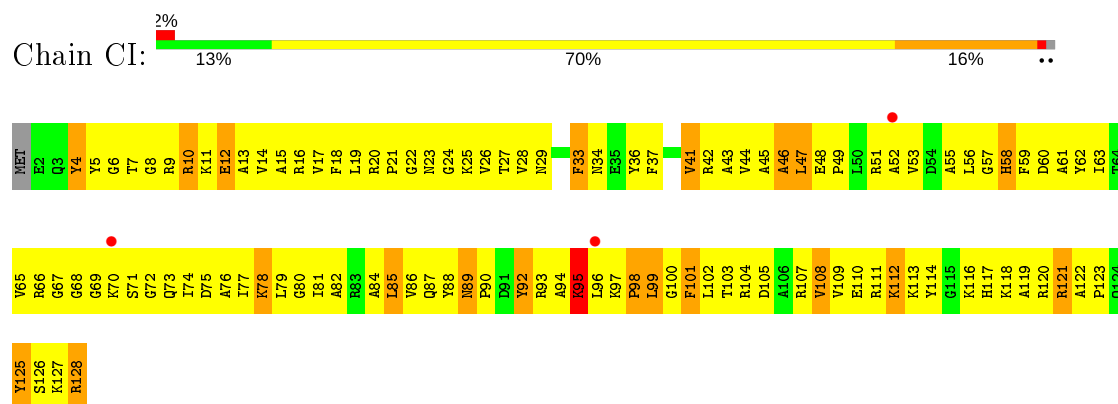
• Molecule 8: 30S RIBOSOMAL PROTEIN S8



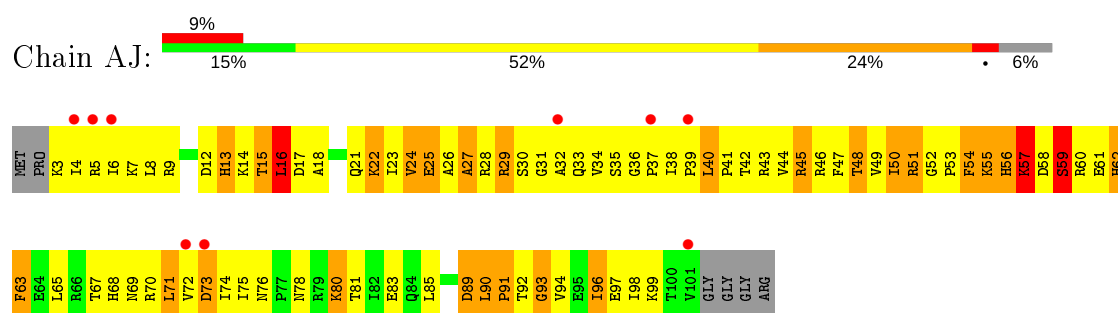
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



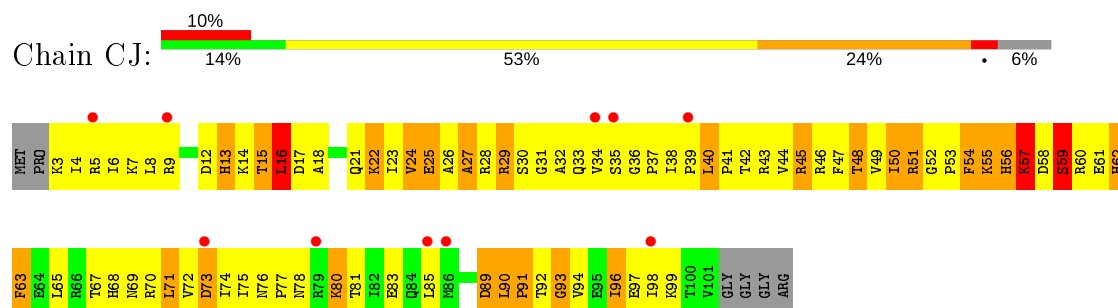
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



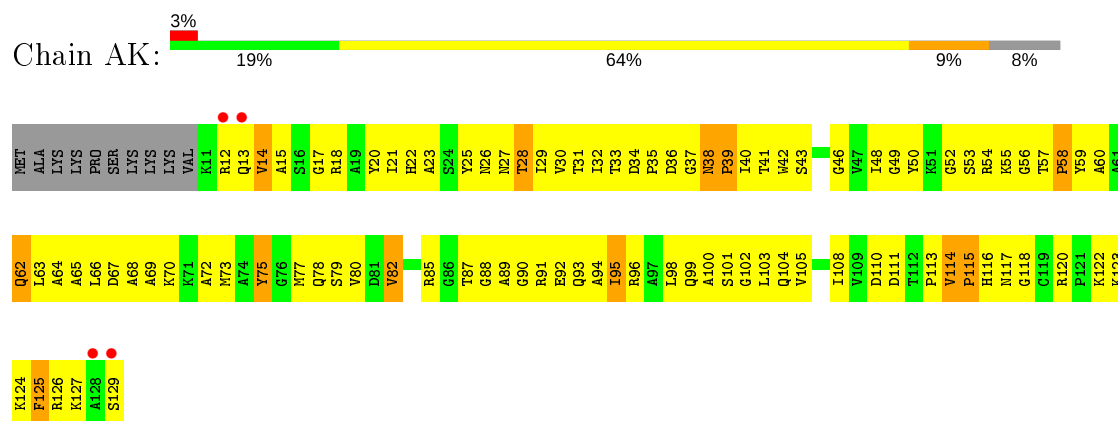
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



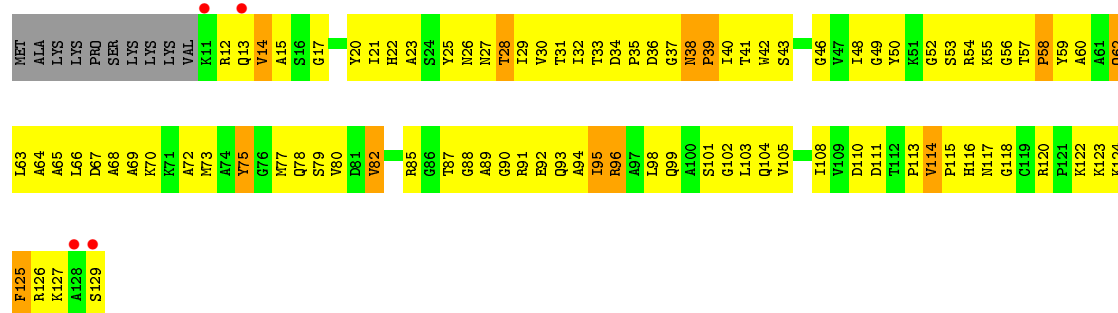
- Molecule 10: 30S RIBOSOMAL PROTEIN S10



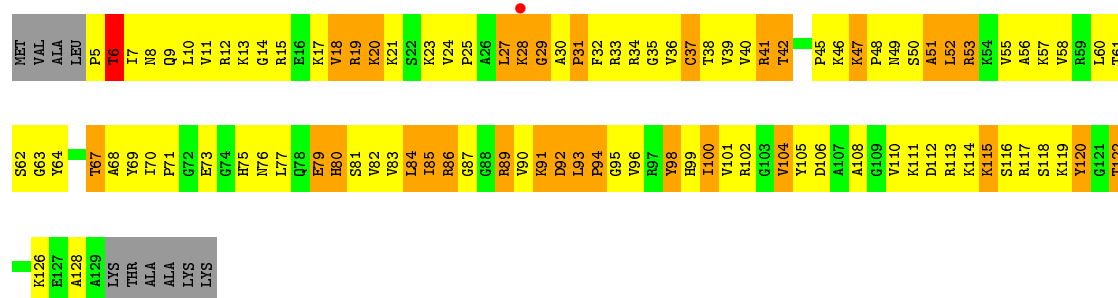
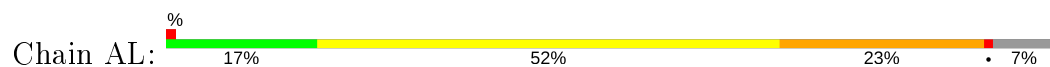
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



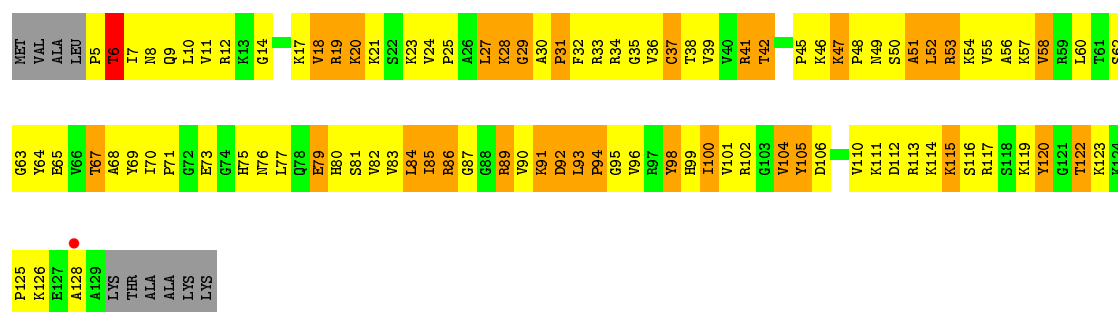
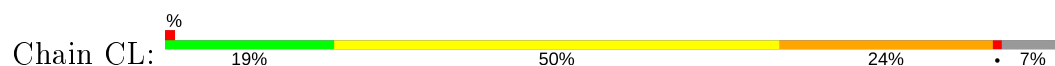
- Molecule 11: 30S RIBOSOMAL PROTEIN S11



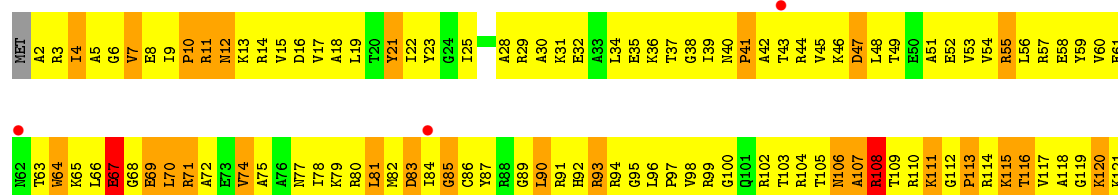
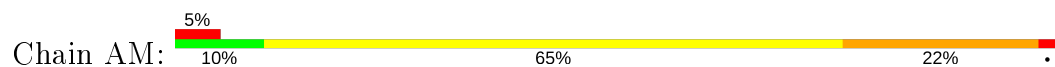
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

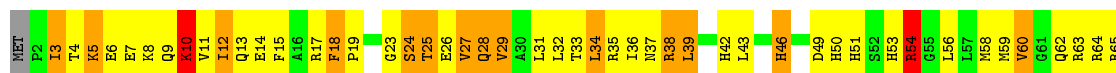


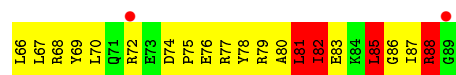
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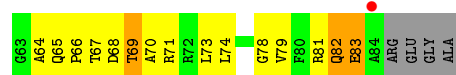
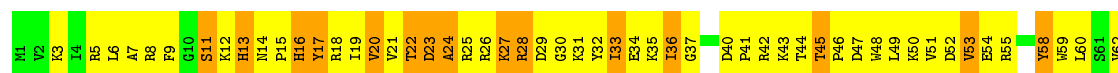
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



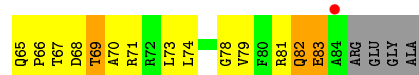
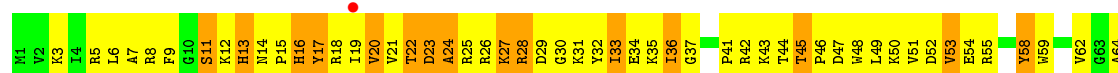




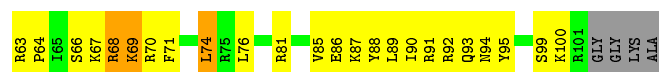
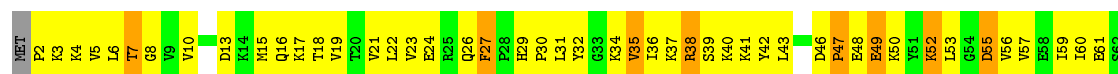
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



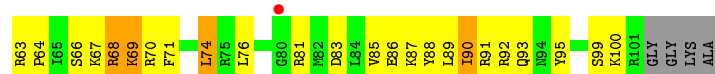
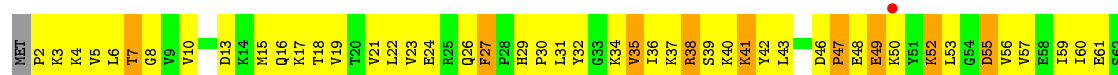
• Molecule 16: 30S RIBOSOMAL PROTEIN S16



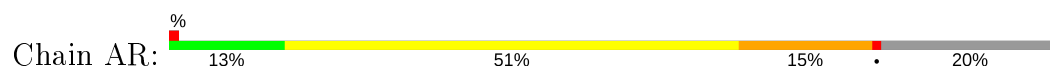
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

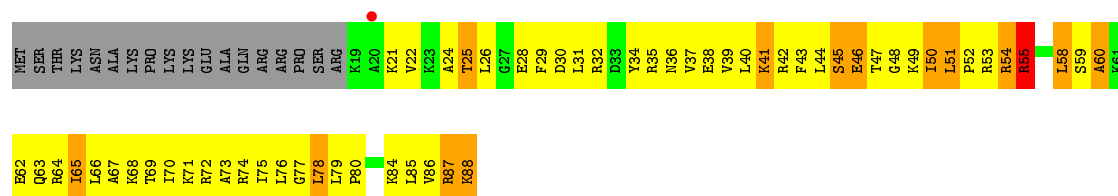


• Molecule 17: 30S RIBOSOMAL PROTEIN S17

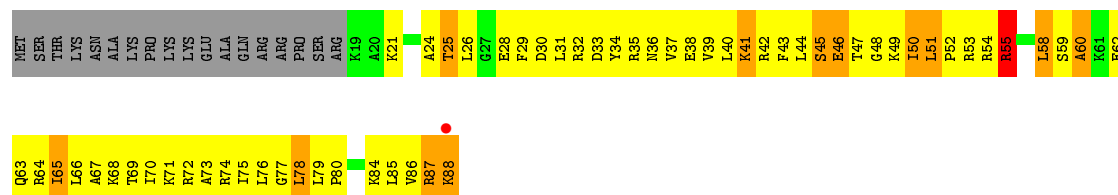
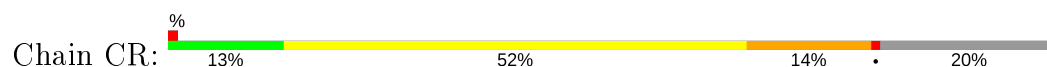


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

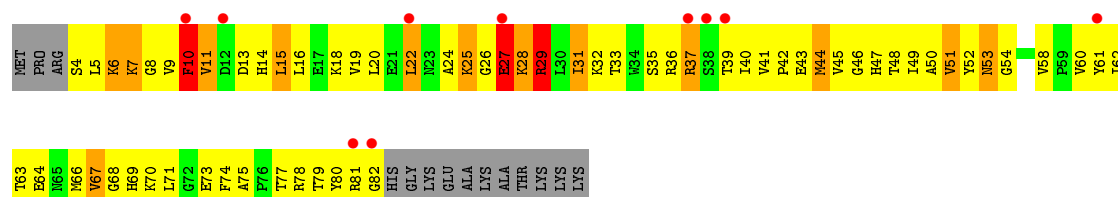
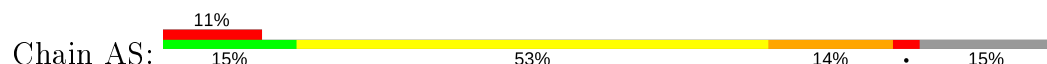




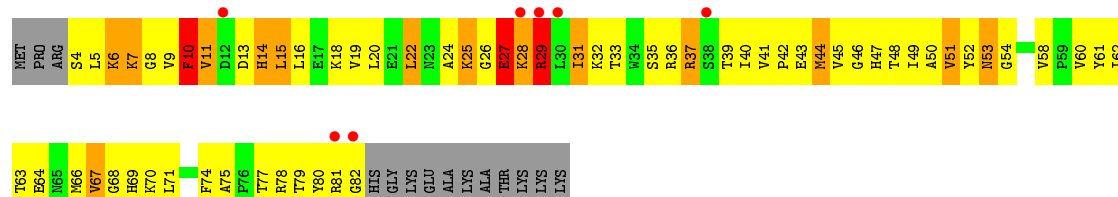
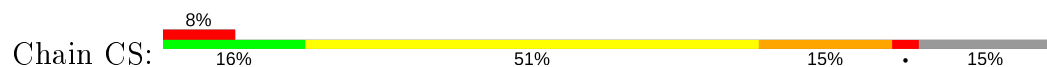
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



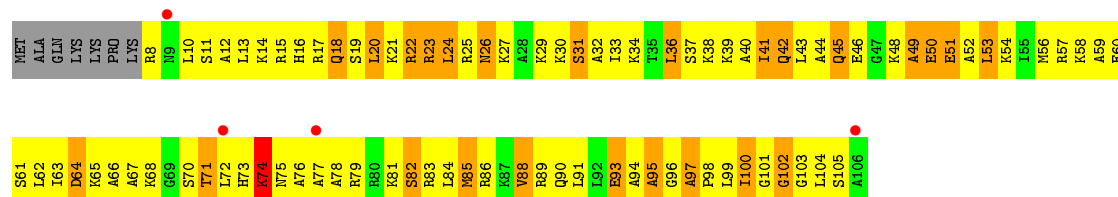
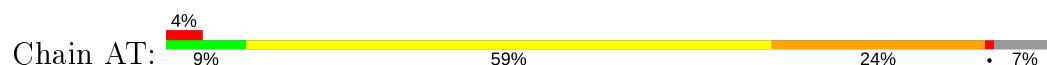
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



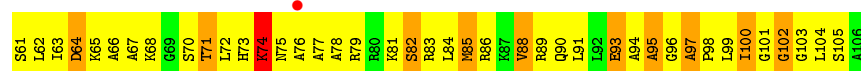
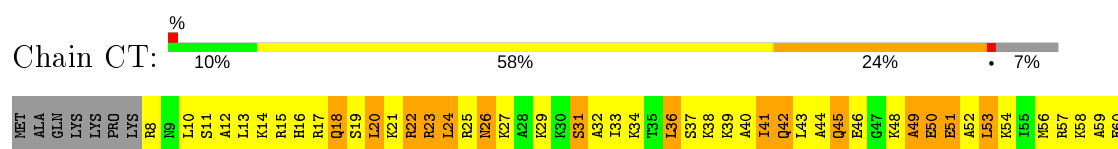
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



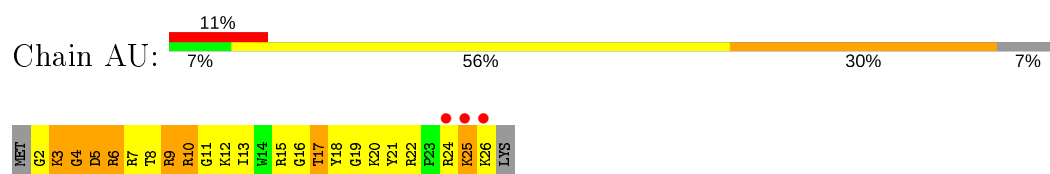
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



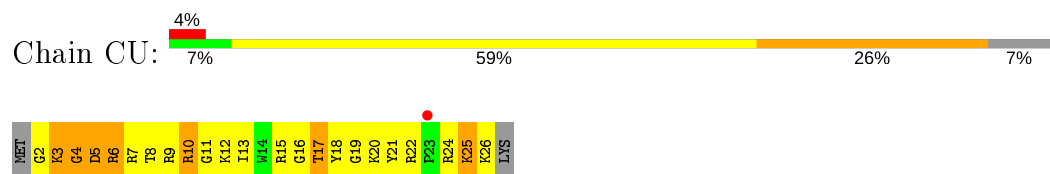
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



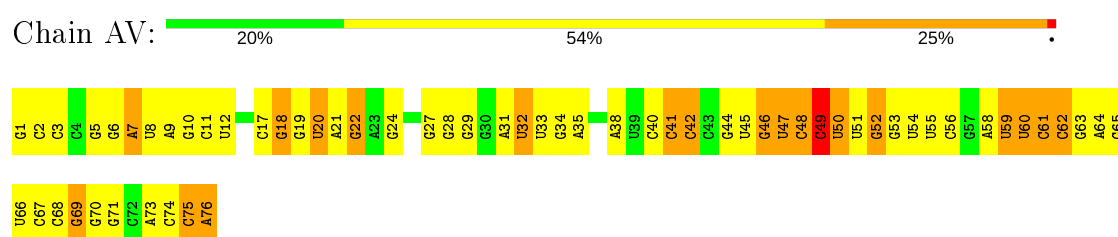
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



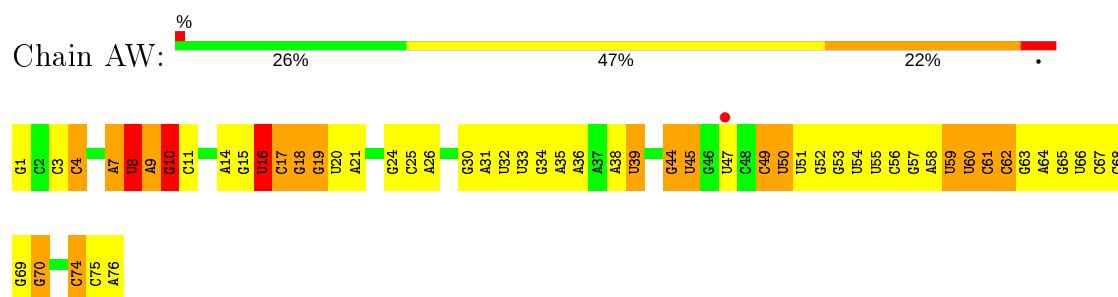
• Molecule 21: 30S RIBOSOMAL PROTEIN THX



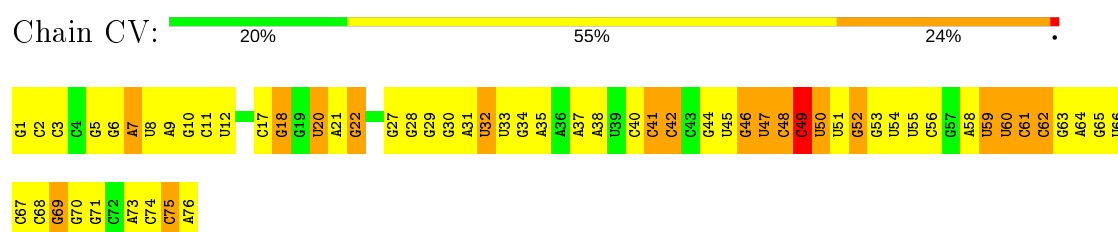
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



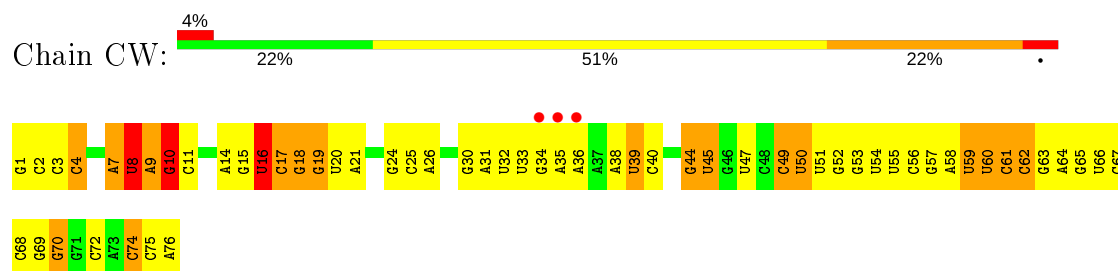
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



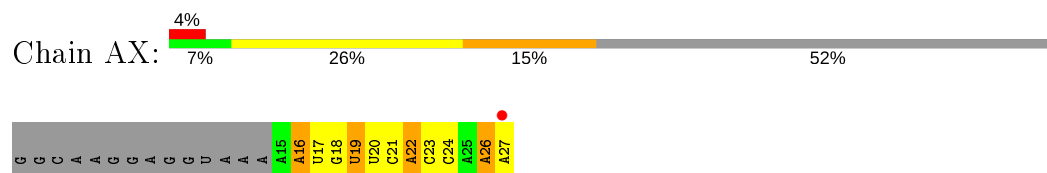
• Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



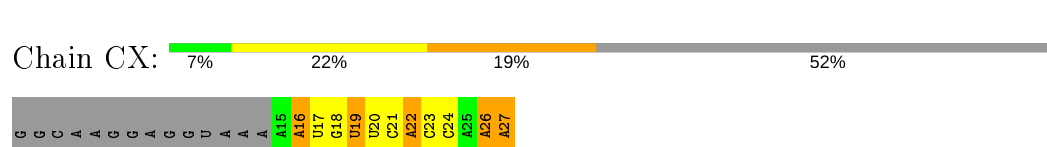
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE



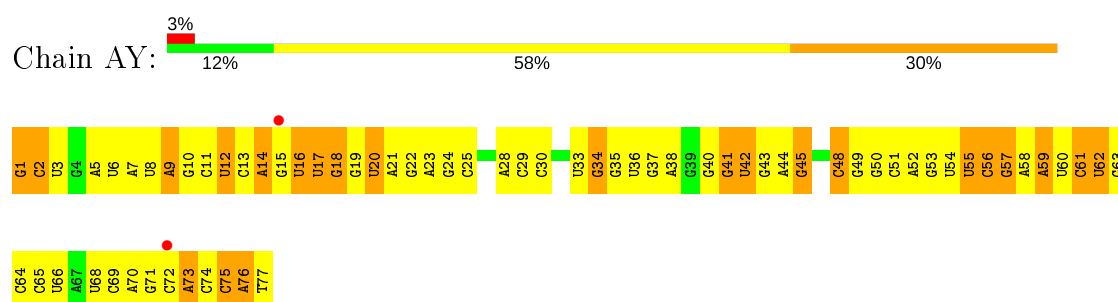
- Molecule 23: MRNA



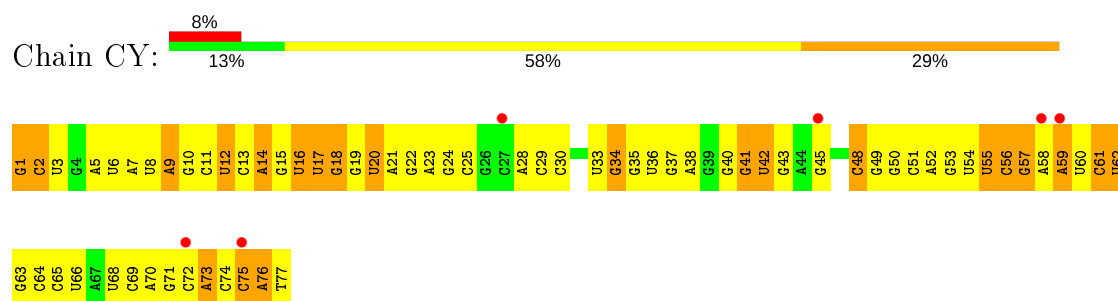
- Molecule 23: MRNA



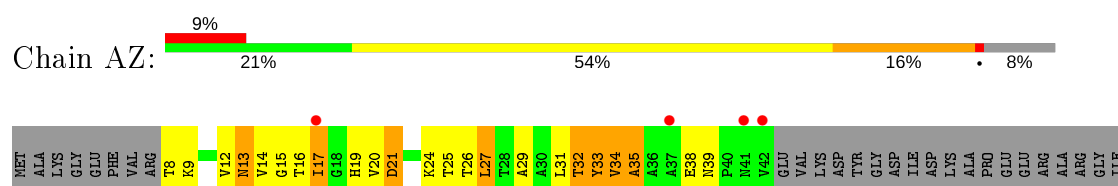
- Molecule 24: A-SITE TRNA THR

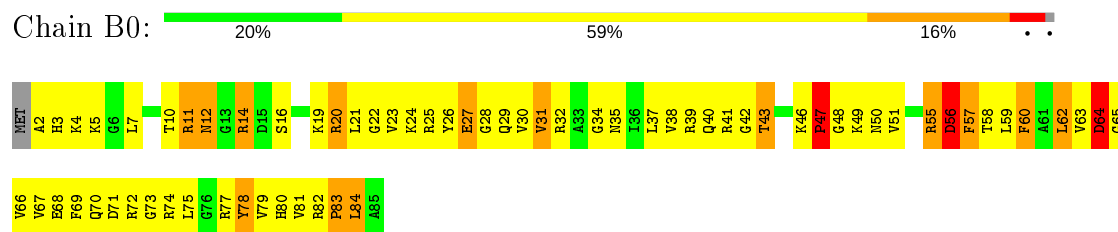


- Molecule 24: A-SITE TRNA THR

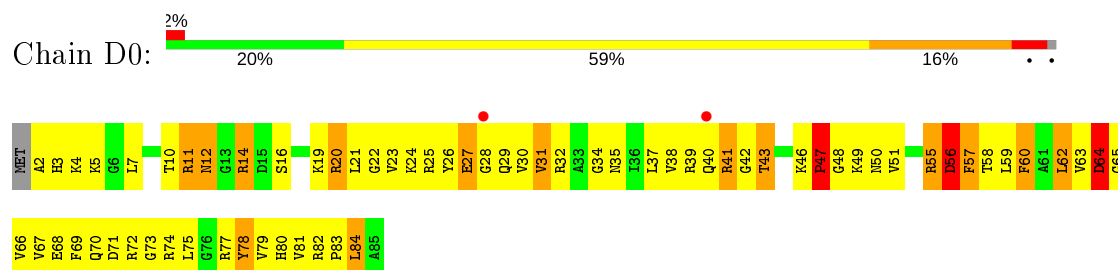


- Molecule 25: ELONGATION FACTOR TU-A

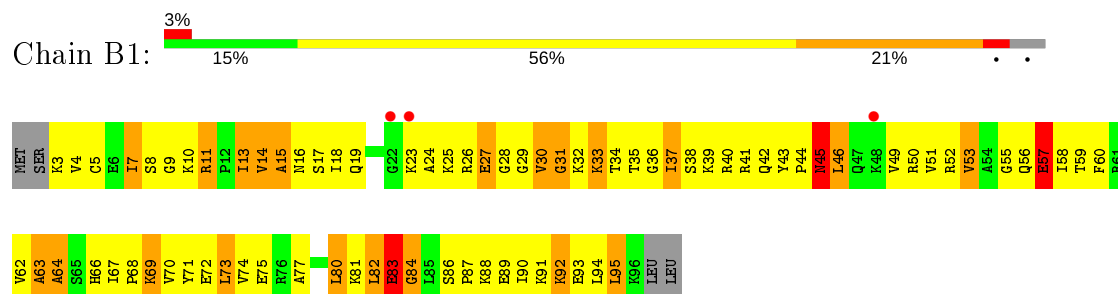




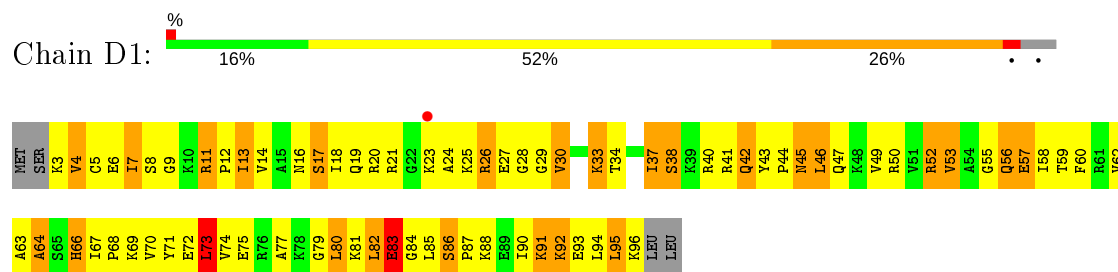
• Molecule 26: 50S RIBOSOMAL PROTEIN L27



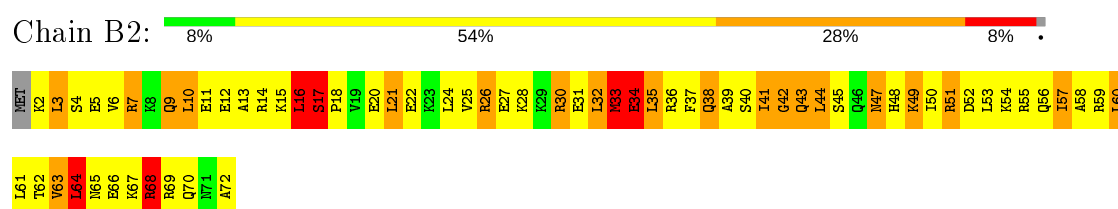
• Molecule 27: 50S RIBOSOMAL PROTEIN L28



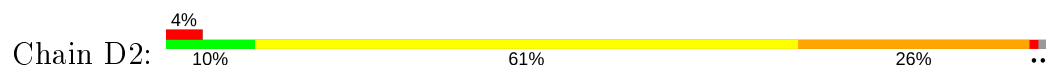
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

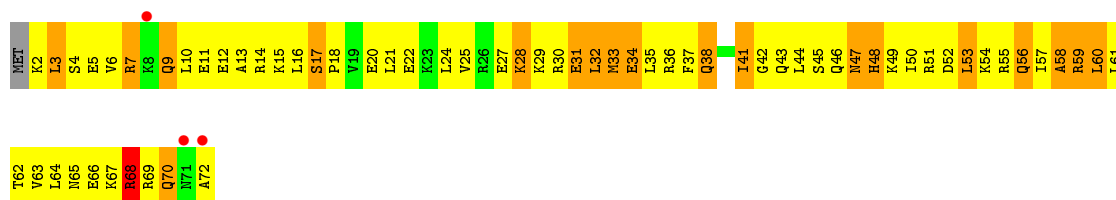


• Molecule 28: 50S RIBOSOMAL PROTEIN L29

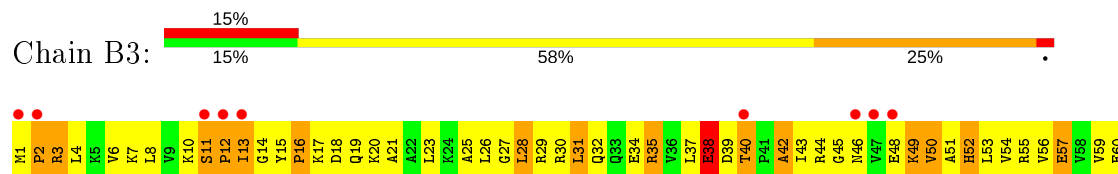


• Molecule 28: 50S RIBOSOMAL PROTEIN L29

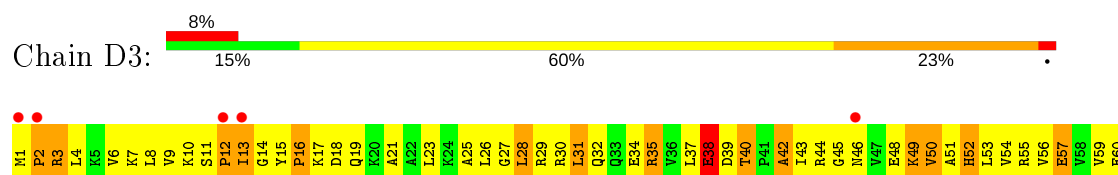




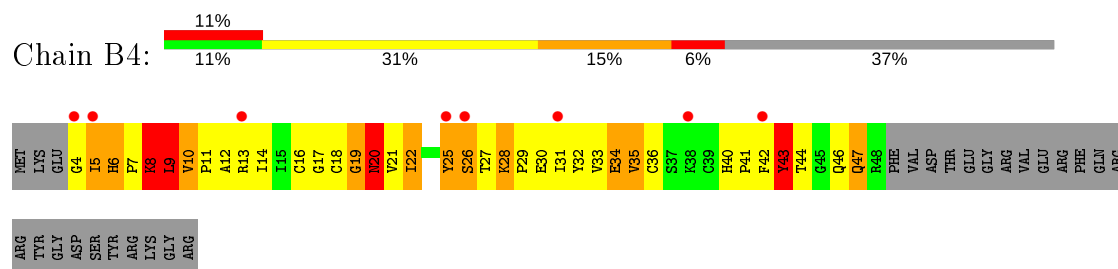
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



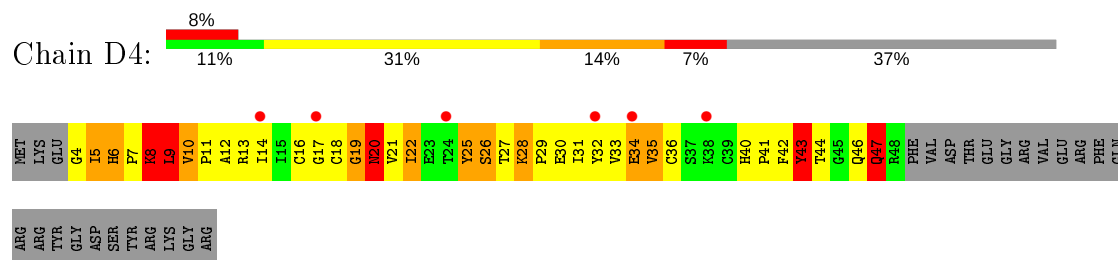
• Molecule 29: 50S RIBOSOMAL PROTEIN L30



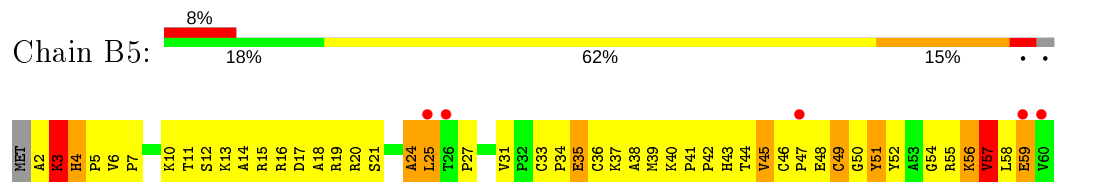
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



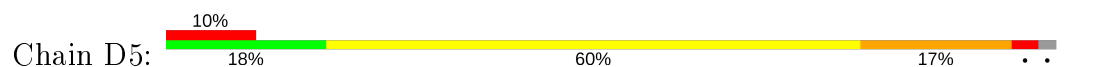
• Molecule 30: 50S RIBOSOMAL PROTEIN L31



• Molecule 31: 50S RIBOSOMAL PROTEIN L32



• Molecule 31: 50S RIBOSOMAL PROTEIN L32





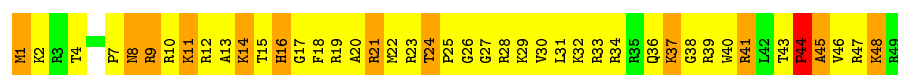
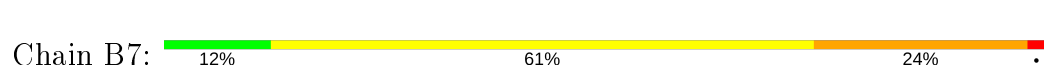
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



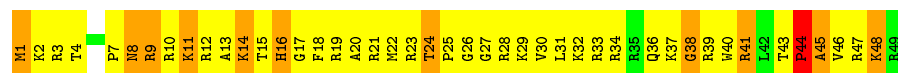
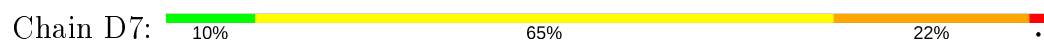
• Molecule 32: 50S RIBOSOMAL PROTEIN L33



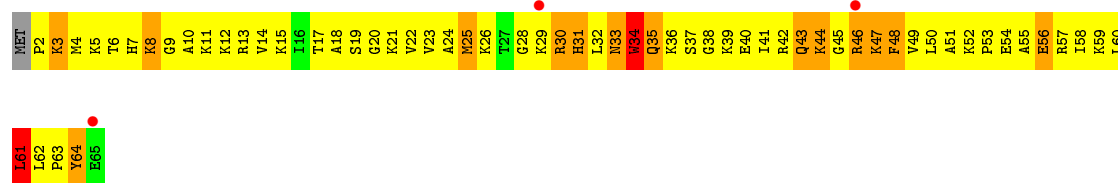
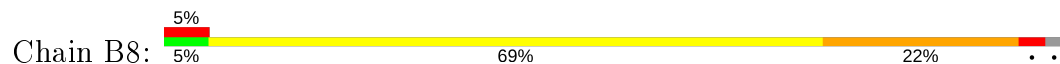
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



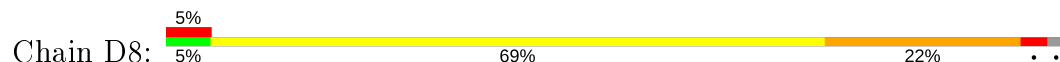
• Molecule 33: 50S RIBOSOMAL PROTEIN L34



• Molecule 34: 50S RIBOSOMAL PROTEIN L35

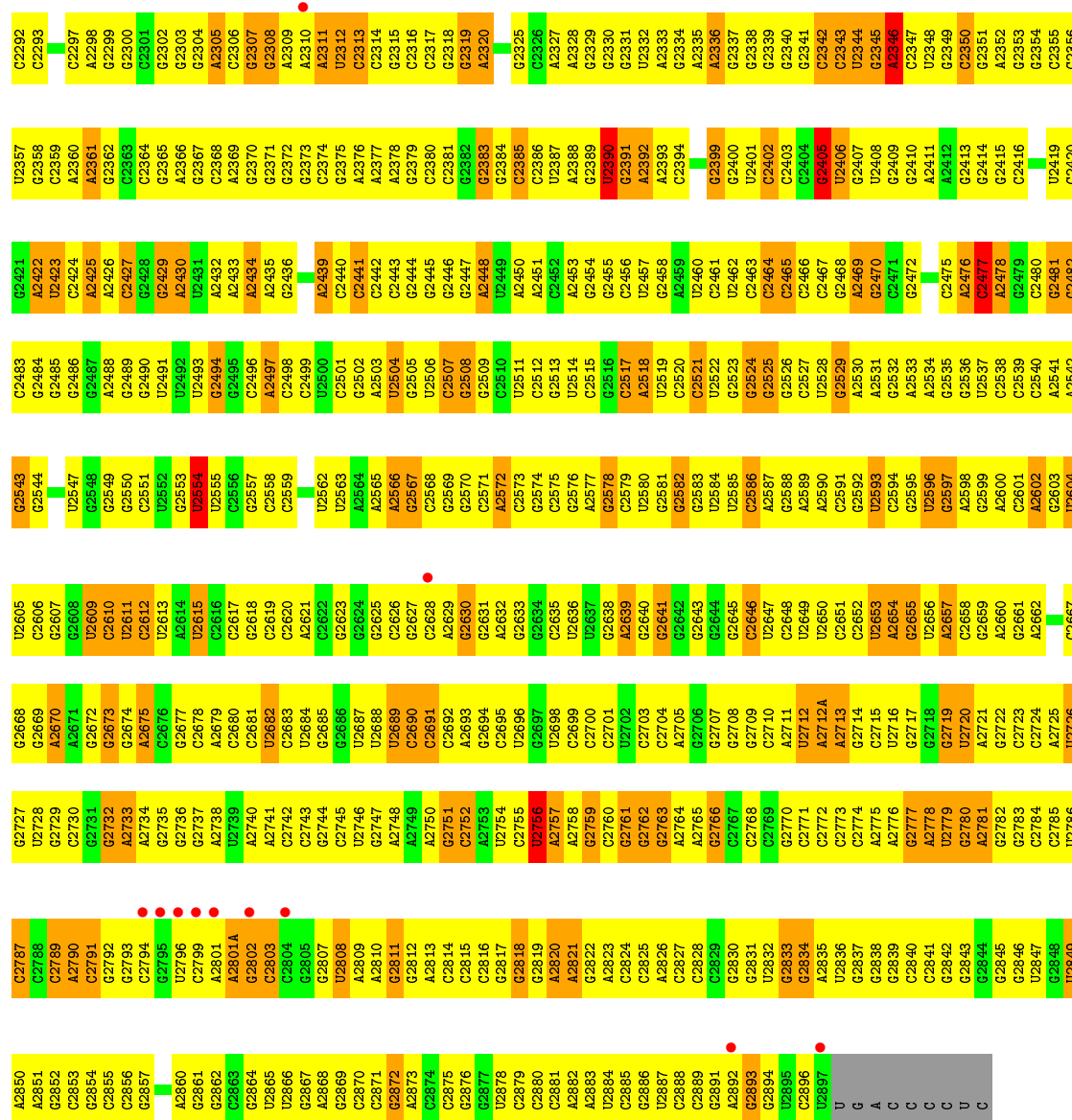


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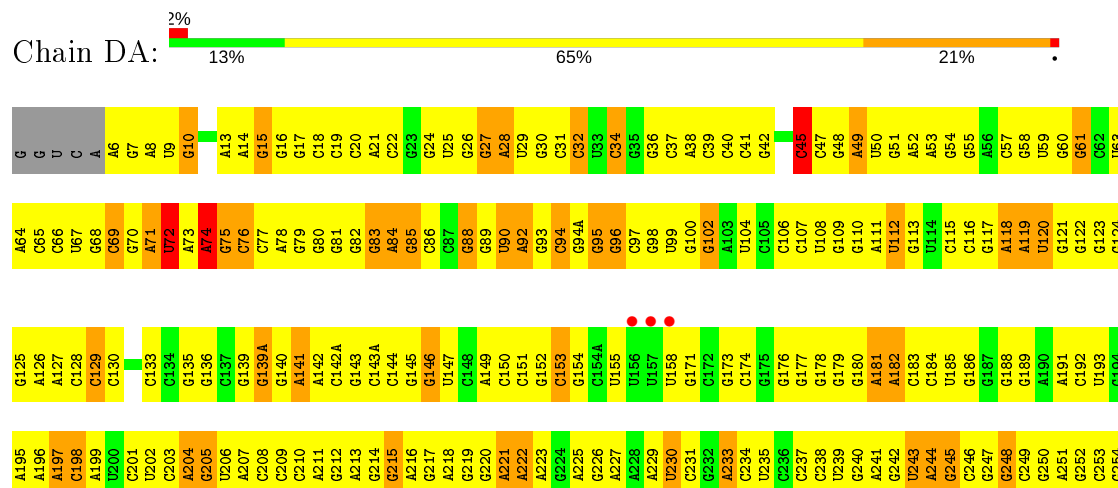


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C1375	G1315	G1250	G1188	G1125	A1057	C991	G932	C865	A804	G744	C645	C587
U1316	U1316	C1251	U1189	A1126	G1058	C992	A933	A866	G805	G745	A646	U588
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C2205	C2205	G2083	A2019	A1953	G1888	A1819	U1757	C1680	U1621	C1555	C1493	C1430
G2206	G2206	C2084	A2020	G1954	A1889	U1820	G1758	G1681	G1622	C1556	C1494	U1431
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A2208	G2208	U2086	U2022	U1956	G1891	G1822	A1760	C1683	G1624	A1558	A1496	U1433
G2279	G2279	G2147	G2023	C1957	C1892	G1823	C1761	C1684	C1625	G1559	U1497	G1434
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• Molecule 36: 23S RIBOSOMAL RNA

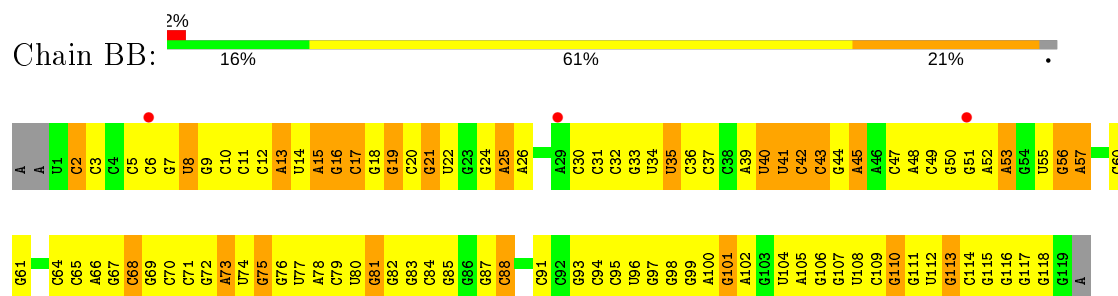


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A1070	A1009	G946	G880	C917	C757	G697	G654E	G801	A536	G355	U294	A265
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C1072	G1011	G948	G882	A819	C759	A699	G654G	G803	G538	A357	G295	G267
A1073	U1012	C949	G883	A820	G760	G700	G654H	G804	U539	U358	C296	C268
G1074	C1013	G950	C884	A821	A761	G701	G654I	U806	C540	A359	C297	U269
	U1014	G952	C885	U822	U762	G702	G654J	U807	C541	A360	G298	A270
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G1089	U1024	A959	C894	G831	G770	G710	C654R	U614	G553	G364	U306	C271G
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G1091	U1026	C961	A896	U833	C772	G712	G654T	G814B	U555	C366	G308	G271I
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U1097	A1032	G968	U905	A841	G778	A718	C658	G820	G561	C375	A314	C271O
A1098	U1033	U969	G906	G842	U779	C719	C659	A621	U562	G376	G315	C271P
G1099	G1034	C970	U907	G843	G780	C720	G660	G822	G498	C377	C316	G271Q
C1100	U1035	C971	C908	C844	A781	G721	G661	G823	U499	C378	G317	G271R
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A1103	U1038	G974	A911	U847	A784	U724	C664	U826	A567	G381	A320	G271U
G1039	C1039	C975	C912	G848	G785	G725	C665	G827	U568	G382	G321	G271V
U1105	C1040	G976	U913	A849	G786	G726	G666	G828	U569	U383	A322	G271W
G1106	C1041	G977	C914	C850	U787	A727	U667	G829	G570	U384	G323	G271X
U1107	G1042	G978	C915	U851	A788	G728	G668	G630	A571	C385	A324	U271Y
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G1104	A1045	G979	A917	G853	C790	G730	A670	A632	G573	U387	G326	G272
A1046	A1046	A980	A918	G854	C791	C731	C671	A633	G574	G388	G327	U272A
G1047	C1047	A981	G919	G855	G792	G732	C672	C834	U576	G389	U328	G272B
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C1049	C1049	A983	G921	C857	G794	A734	A674	G636	C451	G391	A330	G272D
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C1122	G1058	G993	G934	A867	A804	G744	G684	A646	U588	A401	A340	
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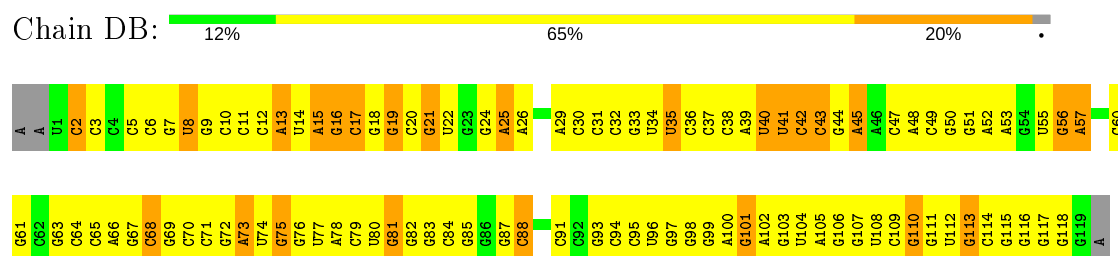


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C	G2839	A2776	A2656	G2596	G2535	C2476	G2410	G2349	C2284	G2223	G2152	G2091	U2028
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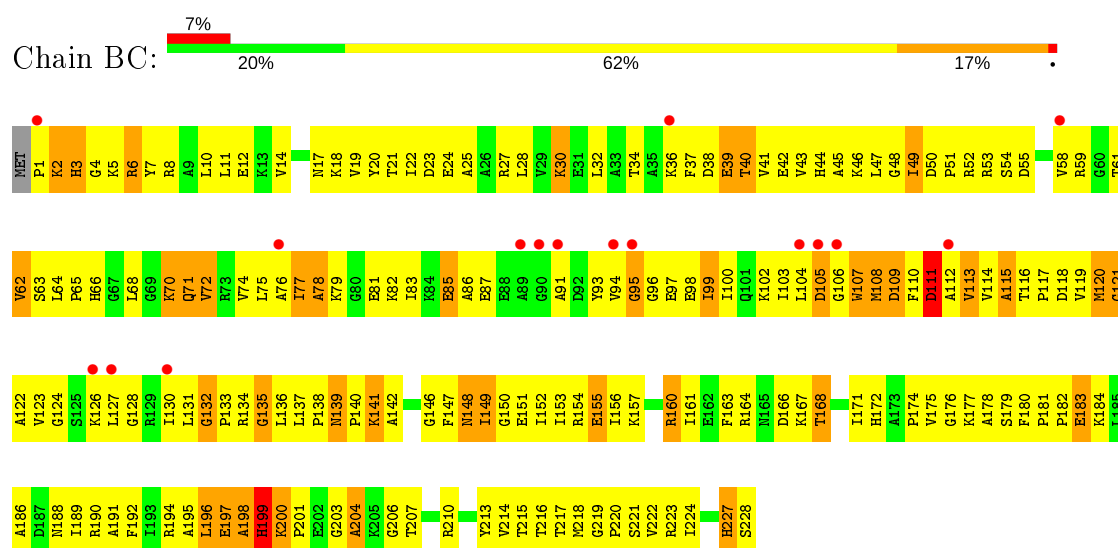
- Molecule 37: 5S RIBOSOMAL RNA



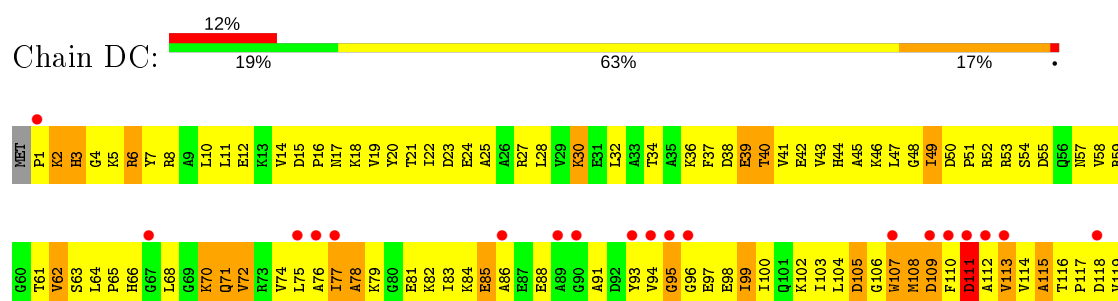
- Molecule 37: 5S RIBOSOMAL RNA

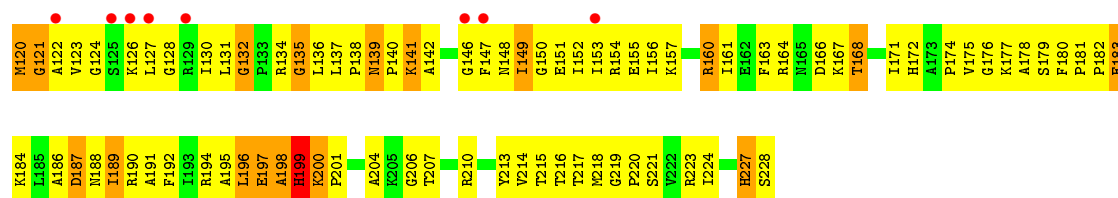


- Molecule 38: 50S RIBOSOMAL PROTEIN L1

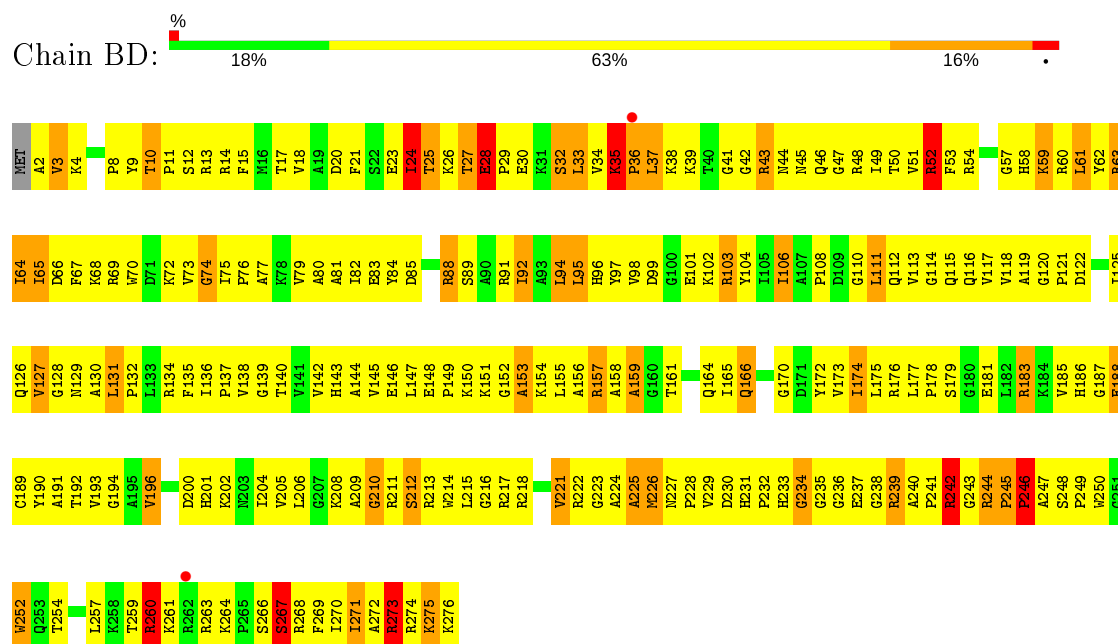


- Molecule 38: 50S RIBOSOMAL PROTEIN L1

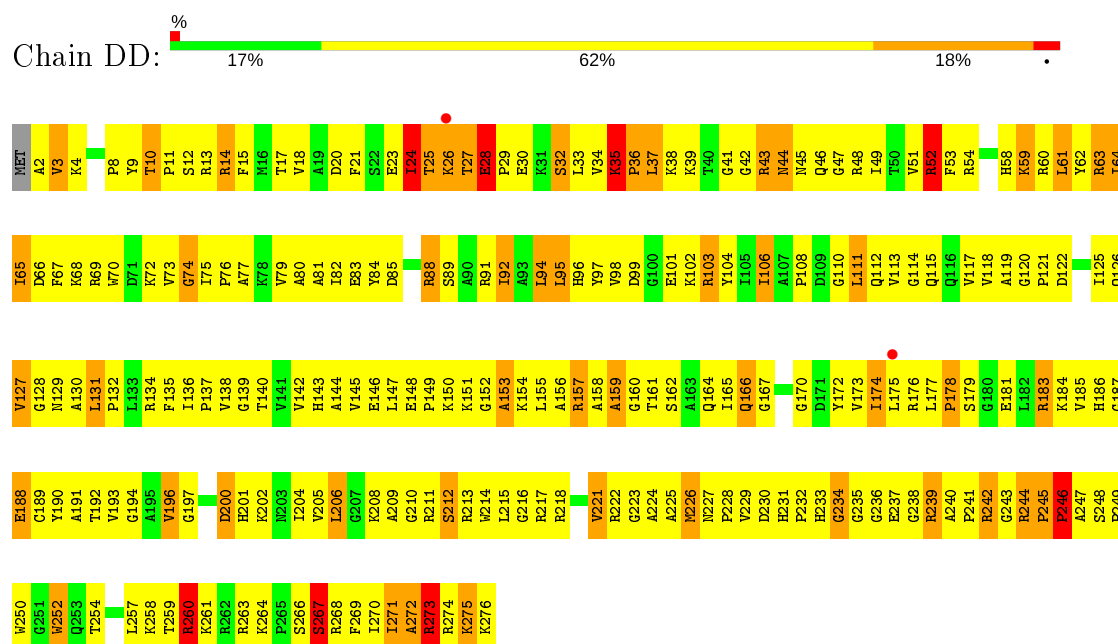




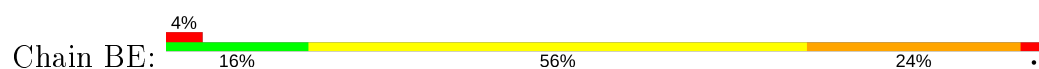
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

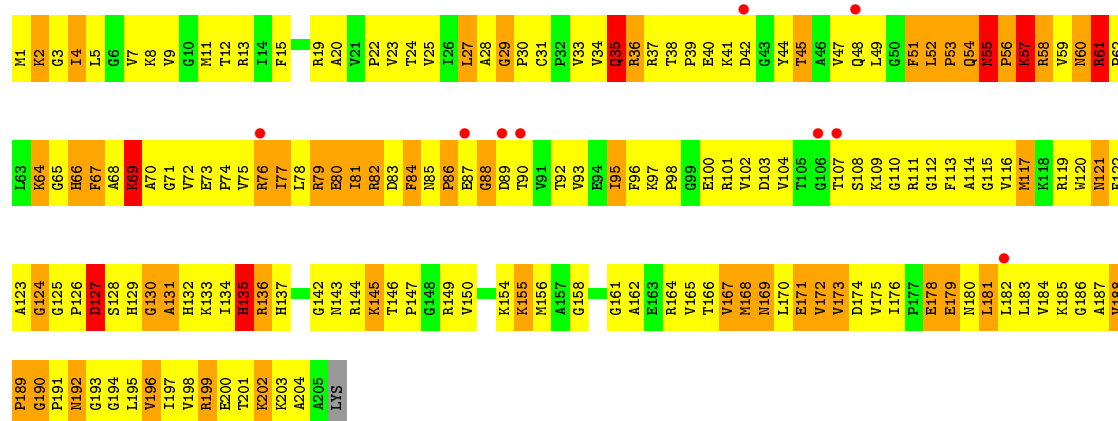


• Molecule 39: 50S RIBOSOMAL PROTEIN L2

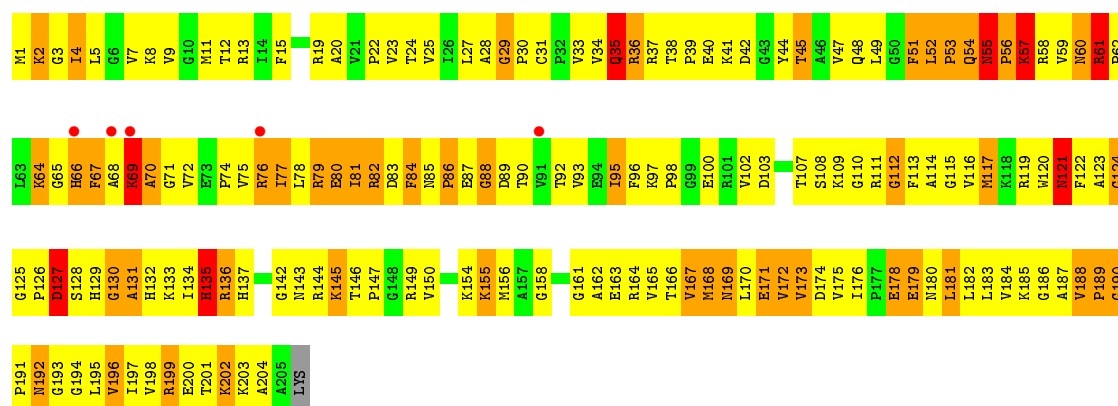
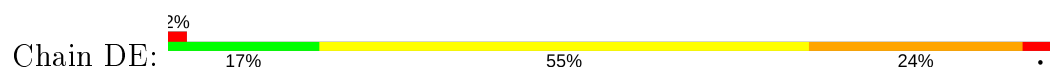


• Molecule 40: 50S RIBOSOMAL PROTEIN L3

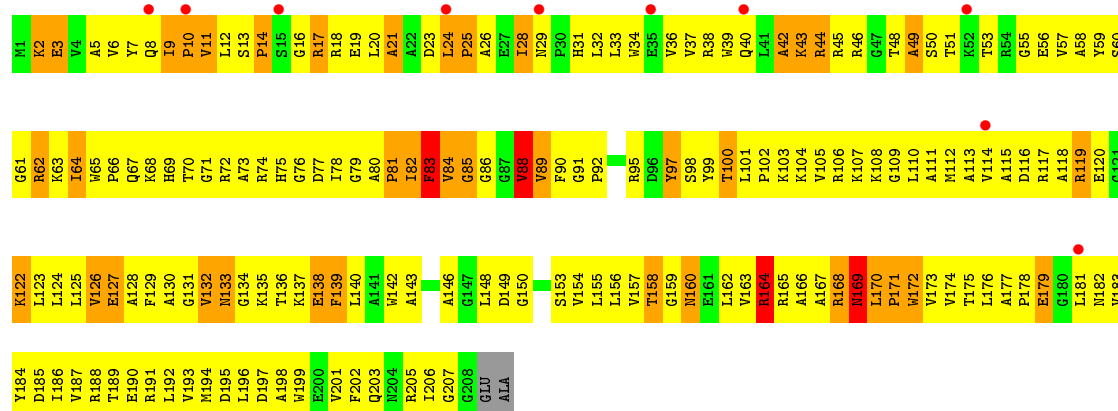
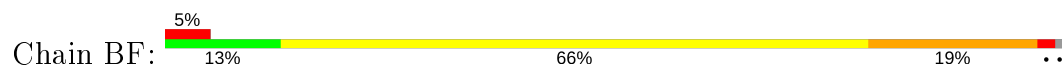




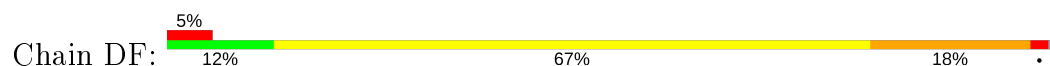
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

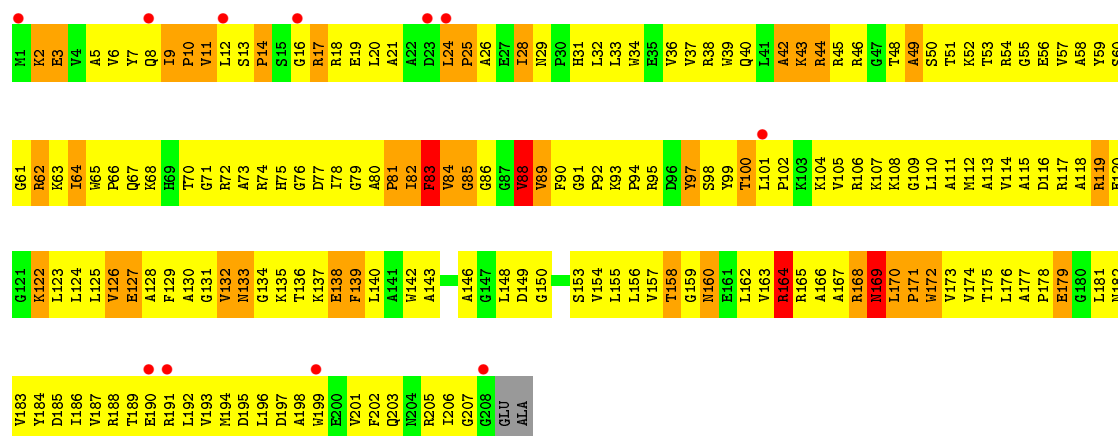


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

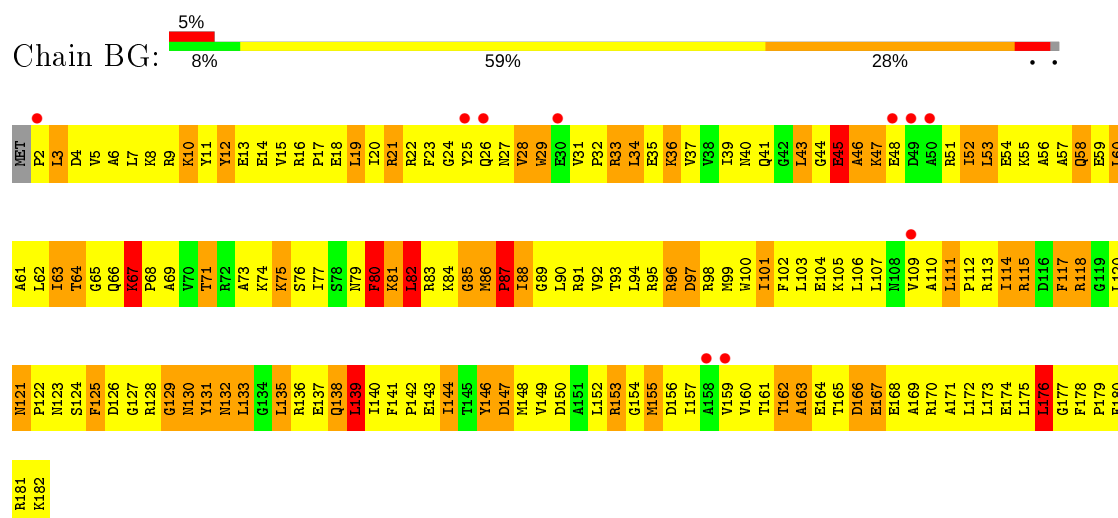


• Molecule 41: 50S RIBOSOMAL PROTEIN L4

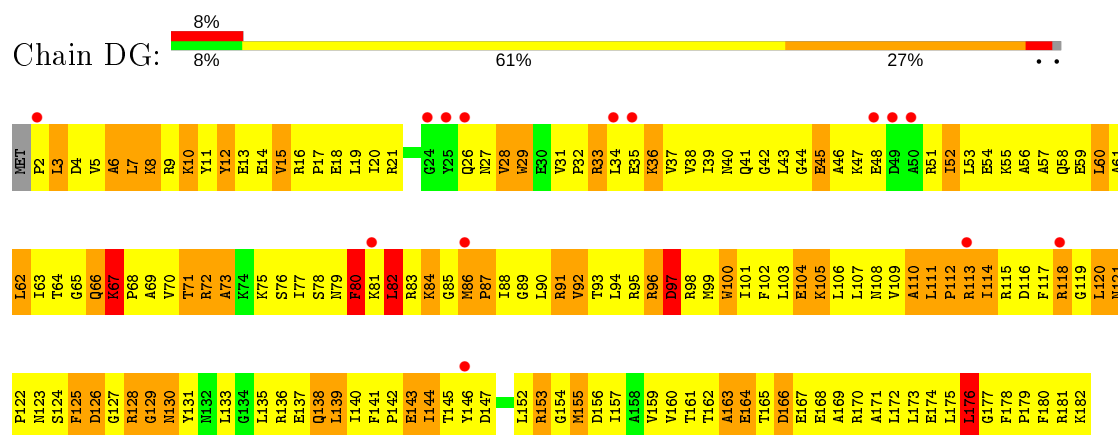




• Molecule 42: 50S RIBOSOMAL PROTEIN L5

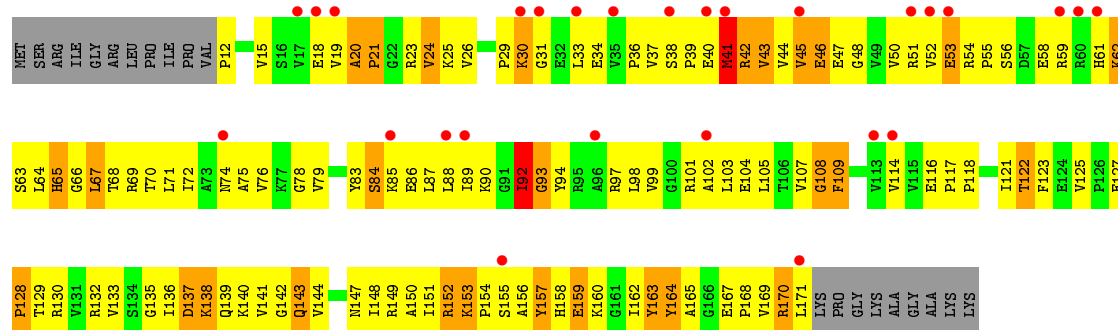


• Molecule 42: 50S RIBOSOMAL PROTEIN L5

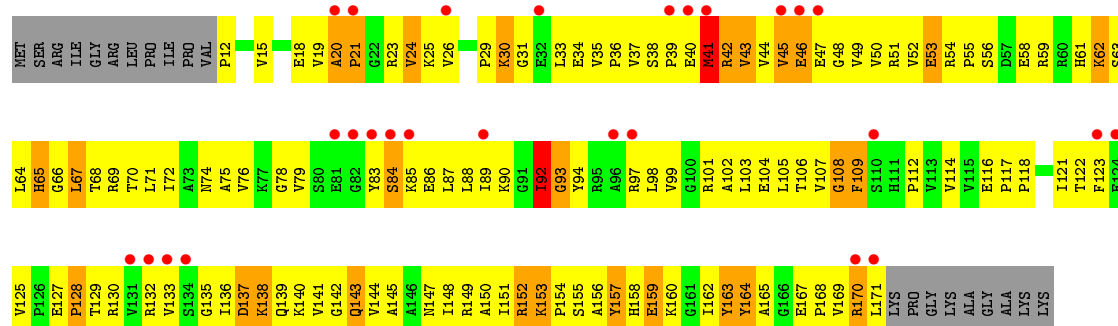


• Molecule 43: 50S RIBOSOMAL PROTEIN L6





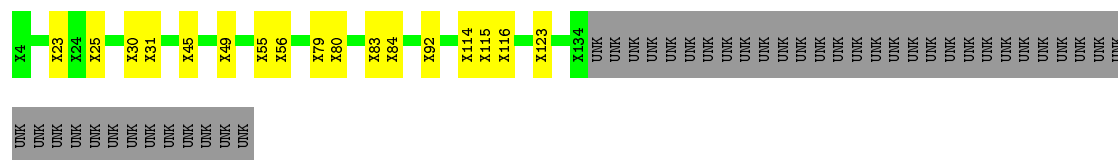
• Molecule 43: 50S RIBOSOMAL PROTEIN L6



• Molecule 44: 50S RIBOSOMAL PROTEIN L10



• Molecule 44: 50S RIBOSOMAL PROTEIN L10



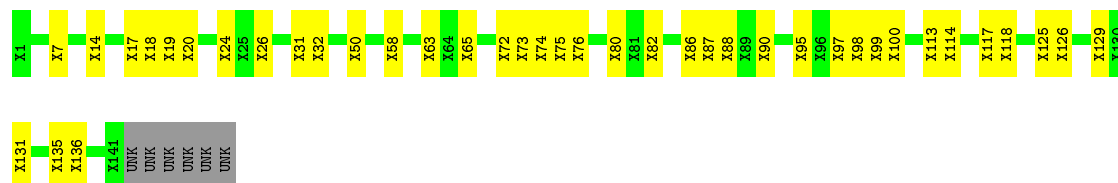
• Molecule 45: 50S RIBOSOMAL PROTEIN L11





• Molecule 45: 50S RIBOSOMAL PROTEIN L11

Chain DK: 69% 27%



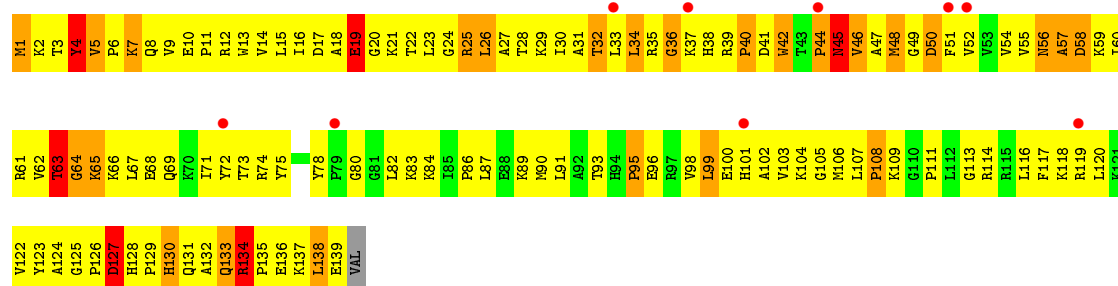
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN: 4% 15% 63% 18%



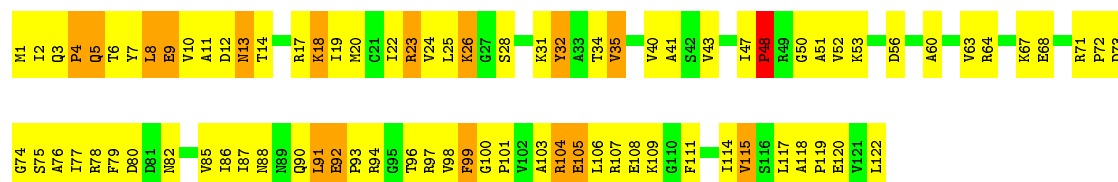
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN: 6% 11% 66% 18%

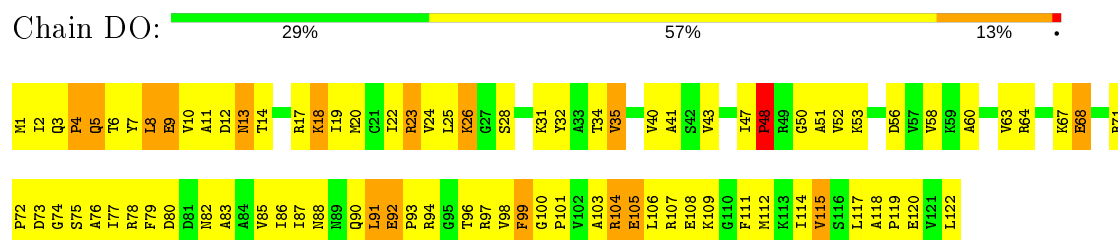


• Molecule 47: 50S RIBOSOMAL PROTEIN L14

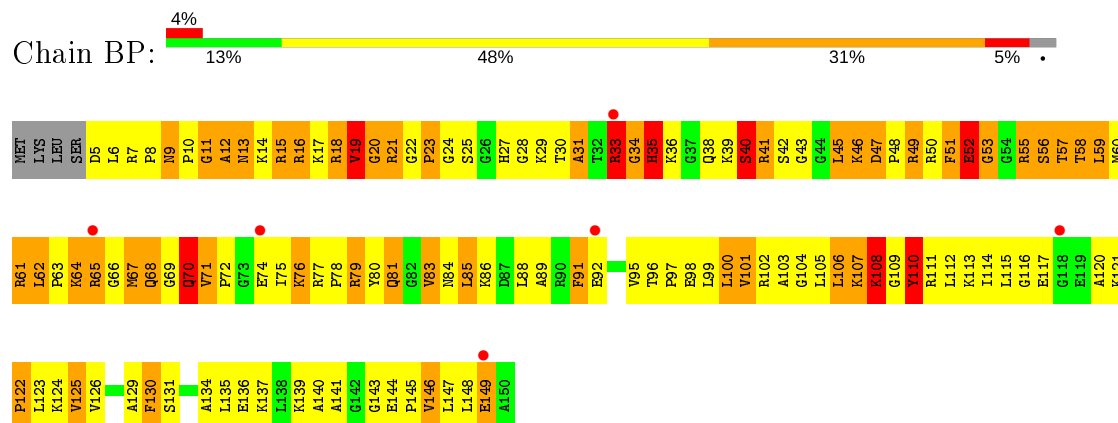
Chain BO: 31% 55% 13%



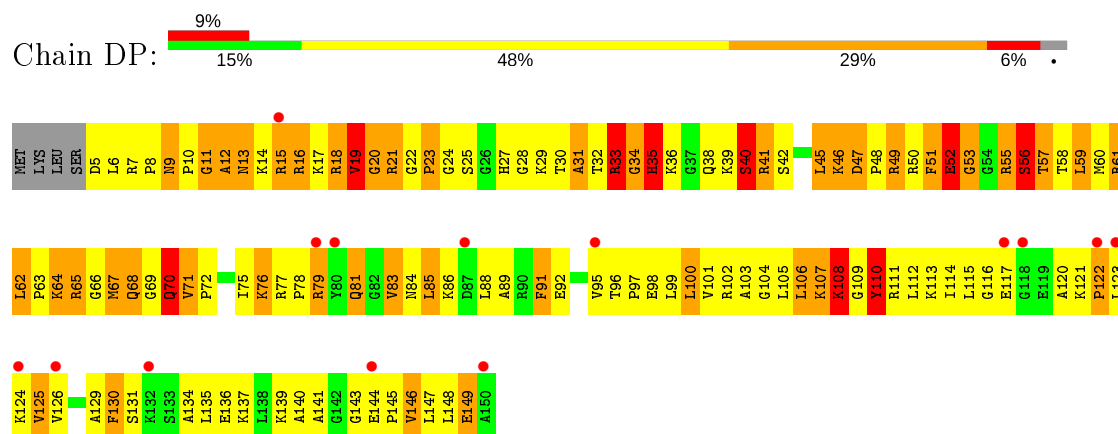
• Molecule 47: 50S RIBOSOMAL PROTEIN L14



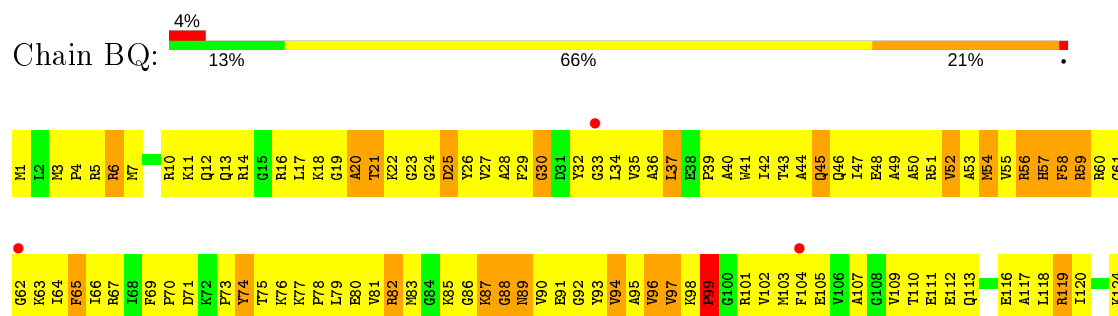
• Molecule 48: 50S RIBOSOMAL PROTEIN L15



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

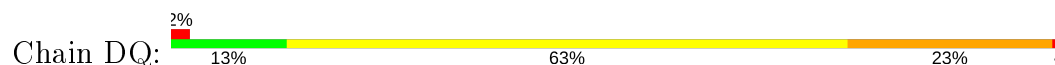


• Molecule 49: 50S RIBOSOMAL PROTEIN L16

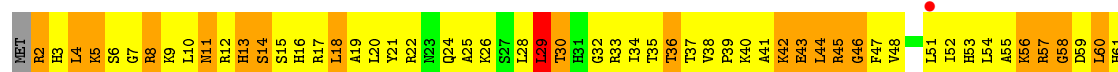
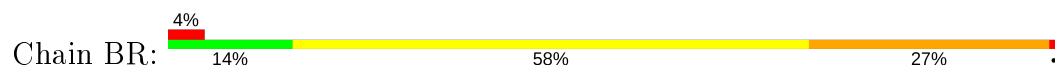




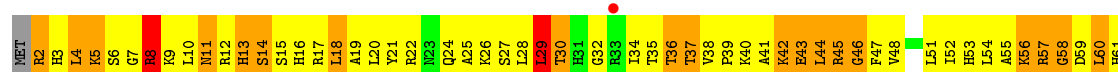
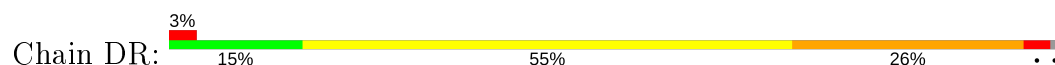
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



• Molecule 50: 50S RIBOSOMAL PROTEIN L17




• Molecule 50: 50S RIBOSOMAL PROTEIN L17

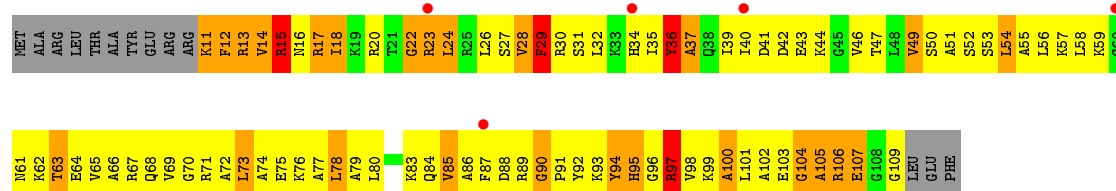


• Molecule 51: 50S RIBOSOMAL PROTEIN L18




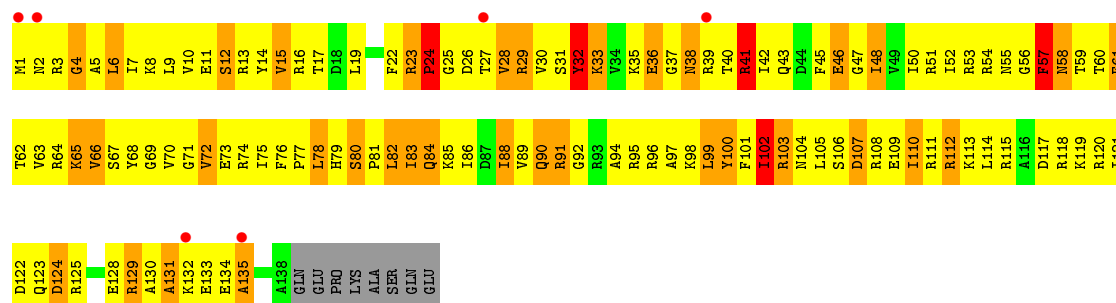
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS: 




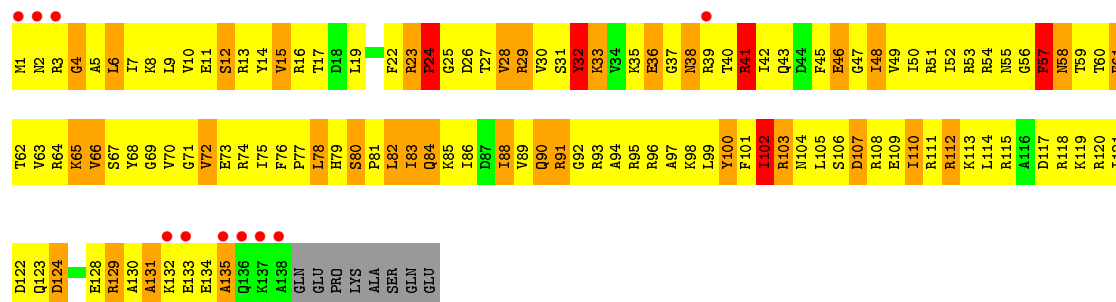
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT: 



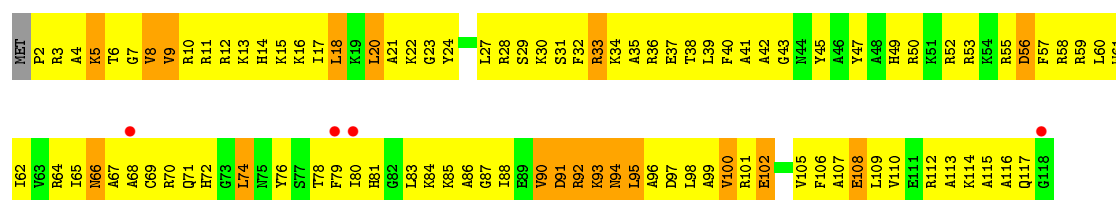
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT: 



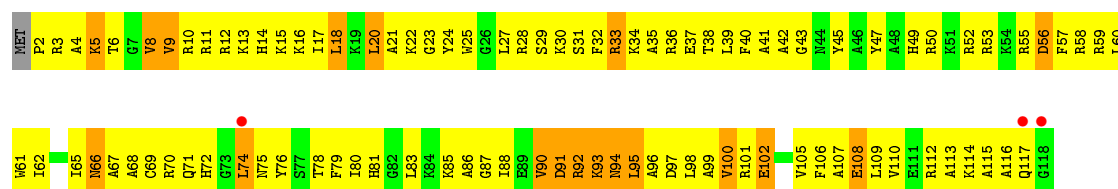
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU: 

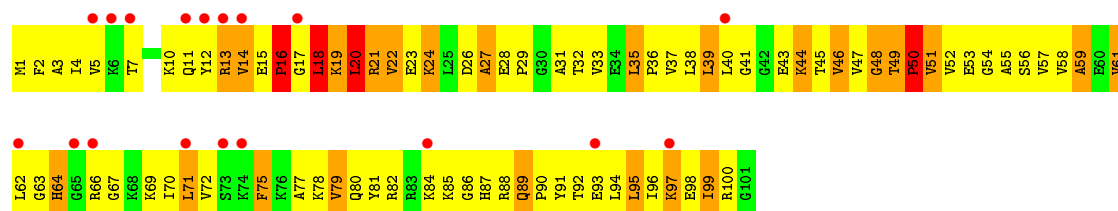
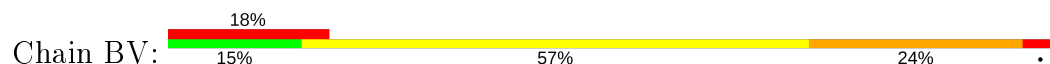


• Molecule 53: 50S RIBOSOMAL PROTEIN L20

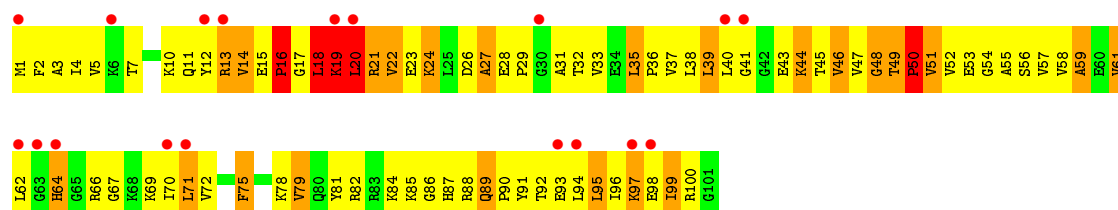
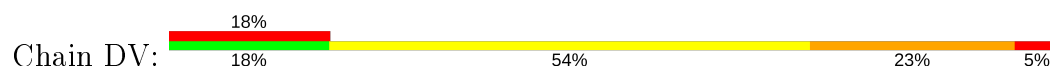
Chain DU: 



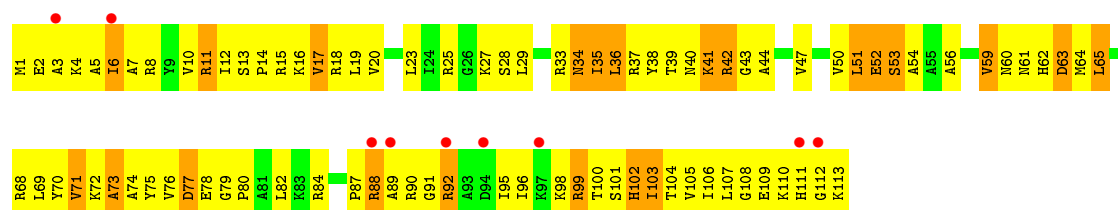
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



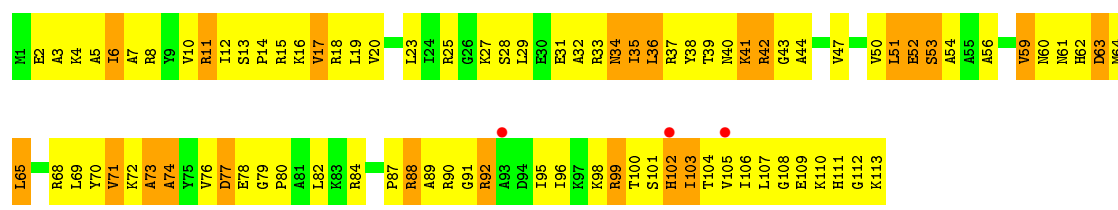
• Molecule 54: 50S RIBOSOMAL PROTEIN L21



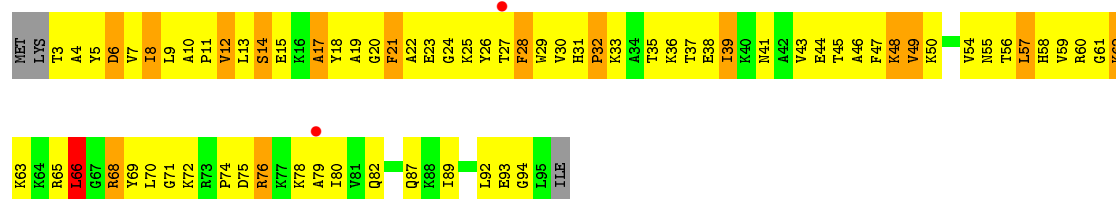
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



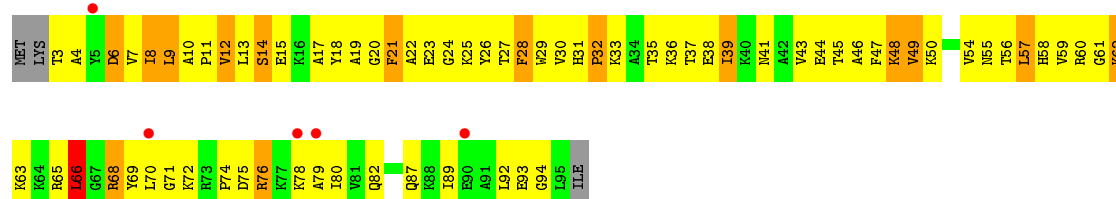
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



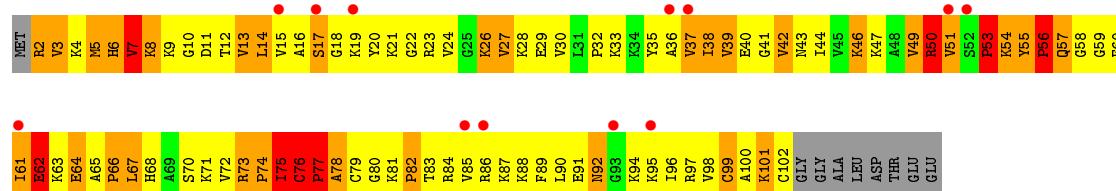
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



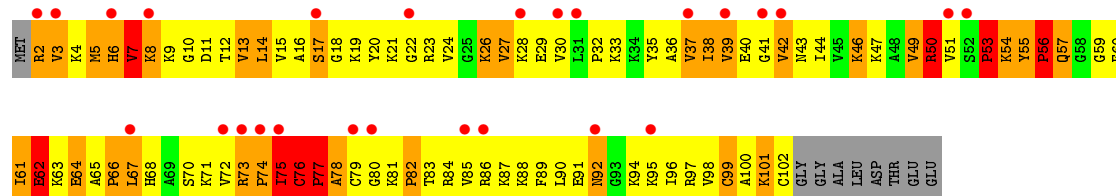
• Molecule 56: 50S RIBOSOMAL PROTEIN L23



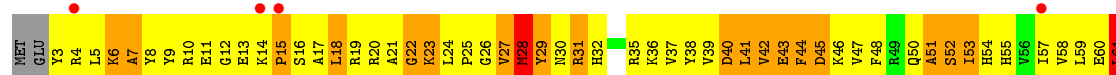
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

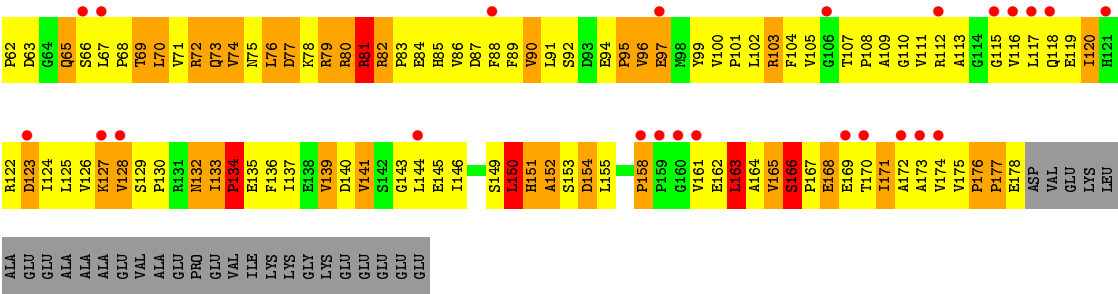


• Molecule 57: 50S RIBOSOMAL PROTEIN L24

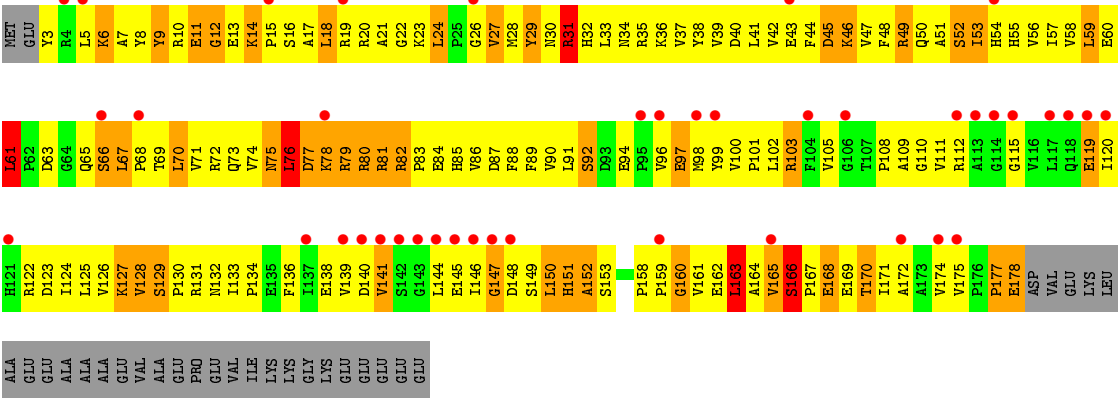
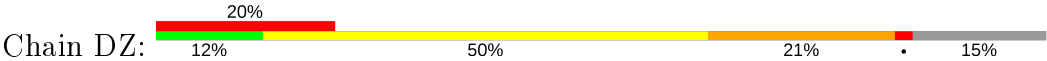


• Molecule 58: 50S RIBOSOMAL PROTEIN L25





● 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 49.91 – 3.48	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-3.60) 87.3 (49.91-3.48)	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 0.277 , 0.311	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 , 68.0	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	0.89	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: 5MU, GDP, PAR, H2U, MG, ZN, YG, KIR, 7MG, 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	0.64	1/36190 (0.0%)	0.78	23/56486 (0.0%)
1	CA	0.64	0/36190	0.77	20/56486 (0.0%)
2	AB	0.44	0/1936	0.71	0/2611
2	CB	0.44	0/1936	0.72	0/2611
3	AC	0.46	0/1637	0.73	1/2207 (0.0%)
3	CC	0.47	0/1637	0.73	0/2207
4	AD	0.46	0/1733	0.75	1/2318 (0.0%)
4	CD	0.44	0/1733	0.73	2/2318 (0.1%)
5	AE	0.57	0/1163	0.79	1/1566 (0.1%)
5	CE	0.56	0/1163	0.78	0/1566
6	AF	0.42	0/856	0.67	0/1154
6	CF	0.42	0/856	0.67	0/1154
7	AG	0.41	0/1276	0.66	0/1709
7	CG	0.42	0/1276	0.66	0/1709
8	AH	0.51	0/1136	0.72	0/1527
8	CH	0.49	0/1136	0.74	0/1527
9	AI	0.39	0/1029	0.65	0/1379
9	CI	0.39	0/1029	0.65	0/1379
10	AJ	0.46	0/808	0.71	1/1087 (0.1%)
10	CJ	0.48	0/808	0.71	1/1087 (0.1%)
11	AK	0.48	0/900	0.73	0/1213
11	CK	0.48	0/900	0.73	0/1213
12	AL	0.52	0/987	0.81	0/1322
12	CL	0.54	0/987	0.81	0/1322
13	AM	0.43	0/999	0.75	0/1338
13	CM	0.43	0/999	0.74	0/1338
14	AN	0.52	0/501	0.73	0/664
14	CN	0.51	0/501	0.74	0/664
15	AO	0.45	0/745	0.73	0/992
15	CO	0.44	0/745	0.73	0/992
16	AP	0.48	0/717	0.72	0/965
16	CP	0.46	0/717	0.72	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.46	0/837	0.74	0/1119
17	CQ	0.48	0/837	0.74	0/1119
18	AR	0.50	0/579	0.75	1/768 (0.1%)
18	CR	0.49	0/579	0.75	1/768 (0.1%)
19	AS	0.47	0/643	0.67	0/867
19	CS	0.45	0/643	0.67	0/867
20	AT	0.38	0/765	0.70	0/1007
20	CT	0.36	0/765	0.70	0/1007
21	AU	0.55	0/213	0.63	0/279
21	CU	0.56	0/213	0.64	0/279
22	AV	0.53	0/1809	0.76	0/2819
22	AW	0.45	0/1809	0.73	0/2819
22	CV	0.49	0/1809	0.76	0/2819
22	CW	0.45	0/1809	0.72	0/2819
23	AX	0.71	0/304	0.83	0/471
23	CX	0.72	0/304	0.81	0/471
24	AY	0.50	1/1660 (0.1%)	0.72	1/2583 (0.0%)
24	CY	0.51	1/1660 (0.1%)	0.72	1/2583 (0.0%)
25	AZ	0.38	0/2957	0.65	0/4015
25	CZ	0.38	0/2957	0.65	0/4015
26	B0	0.40	0/671	0.67	0/892
26	D0	0.40	0/671	0.66	0/892
27	B1	0.57	0/739	0.91	0/983
27	D1	0.60	0/739	0.92	1/983 (0.1%)
28	B2	0.44	0/600	0.87	2/793 (0.3%)
28	D2	0.43	0/600	0.80	1/793 (0.1%)
29	B3	0.44	0/473	0.74	0/636
29	D3	0.42	0/473	0.75	0/636
30	B4	0.71	0/350	0.79	0/476
30	D4	0.73	1/350 (0.3%)	0.75	0/476
31	B5	0.44	0/473	0.72	0/639
31	D5	0.43	0/473	0.71	0/639
32	B6	0.53	0/440	0.91	0/586
32	D6	0.56	0/440	0.93	0/586
33	B7	0.50	0/427	0.75	0/563
33	D7	0.50	0/427	0.74	0/563
34	B8	0.51	0/516	0.78	0/681
34	D8	0.51	0/516	0.77	0/681
35	B9	0.42	0/310	0.66	0/407
35	D9	0.44	0/310	0.67	0/407
36	BA	0.61	2/69972 (0.0%)	0.76	36/109237 (0.0%)
36	DA	0.61	2/69972 (0.0%)	0.77	37/109237 (0.0%)
37	BB	0.46	0/2853	0.72	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DB	0.45	0/2853	0.72	0/4451
38	BC	0.45	2/1774 (0.1%)	0.69	0/2391
38	DC	0.44	2/1774 (0.1%)	0.69	0/2391
39	BD	0.59	0/2195	0.86	1/2955 (0.0%)
39	DD	0.57	0/2195	0.86	0/2955
40	BE	0.48	0/1597	0.75	0/2155
40	DE	0.47	0/1597	0.75	0/2155
41	BF	0.45	0/1659	0.73	0/2246
41	DF	0.43	0/1659	0.72	0/2246
42	BG	0.46	0/1499	0.81	3/2016 (0.1%)
42	DG	0.50	1/1499 (0.1%)	0.77	0/2016
43	BH	0.37	0/1246	0.70	0/1684
43	DH	0.36	0/1246	0.70	0/1684
46	BN	0.42	0/1132	0.75	1/1527 (0.1%)
46	DN	0.43	0/1132	0.75	1/1527 (0.1%)
47	BO	0.49	0/943	0.79	0/1269
47	DO	0.52	0/943	0.78	0/1269
48	BP	0.49	0/1131	1.00	7/1504 (0.5%)
48	DP	0.48	0/1131	0.99	6/1504 (0.4%)
49	BQ	0.44	0/1143	0.71	0/1527
49	DQ	0.43	0/1143	0.72	0/1527
50	BR	0.41	0/974	0.74	0/1302
50	DR	0.39	0/974	0.74	0/1302
51	BS	0.41	0/779	0.72	0/1038
51	DS	0.41	0/779	0.72	0/1038
52	BT	0.47	0/1156	0.75	0/1544
52	DT	0.44	0/1156	0.75	0/1544
53	BU	0.43	0/975	0.74	0/1297
53	DU	0.45	0/975	0.75	0/1297
54	BV	0.39	0/790	0.73	0/1057
54	DV	0.40	0/790	0.73	0/1057
55	BW	0.44	0/907	0.71	0/1216
55	DW	0.42	0/907	0.72	0/1216
56	BX	0.47	0/740	0.71	0/995
56	DX	0.45	0/740	0.71	0/995
57	BY	0.44	0/789	0.81	1/1053 (0.1%)
57	DY	0.43	0/789	0.81	1/1053 (0.1%)
58	BZ	0.43	0/1435	0.77	0/1949
58	DZ	0.45	0/1435	0.78	0/1949
All	All	0.57	13/329754 (0.0%)	0.76	152/492708 (0.0%)

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 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	1	G	OP3-P	-7.09	1.52	1.61
24	AY	1	G	OP3-P	-7.06	1.52	1.61
30	D4	47	GLN	C-N	-6.41	1.19	1.34
38	BC	218	MET	CG-SD	6.21	1.97	1.81
36	DA	2551	C	N1-C2	6.07	1.46	1.40

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1498	U	C2'-C3'-O3'	11.14	134.01	109.50
1	AA	1050	G	N9-C1'-C2'	-9.97	101.03	112.00
1	CA	1050	G	N9-C1'-C2'	-9.73	101.29	112.00
1	AA	961	U	N1-C1'-C2'	-9.15	101.93	112.00
1	CA	961	U	N1-C1'-C2'	-9.06	102.03	112.00

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

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	2215	0
1	CA	32329	0	16318	2218	0
2	AB	1901	0	1951	376	1
2	CB	1901	0	1951	383	1
3	AC	1613	0	1677	265	0
3	CC	1613	0	1677	260	0
4	AD	1703	0	1764	296	0
4	CD	1703	0	1765	305	0
5	AE	1147	0	1207	196	0
5	CE	1147	0	1207	198	0
6	AF	843	0	857	86	0
6	CF	843	0	857	101	0
7	AG	1257	0	1296	187	0
7	CG	1257	0	1296	187	0
8	AH	1116	0	1177	192	0
8	CH	1116	0	1177	204	0
9	AI	1010	0	1037	165	0
9	CI	1010	0	1037	168	0
10	AJ	795	0	840	197	0
10	CJ	795	0	840	209	0
11	AK	885	0	904	130	0
11	CK	885	0	904	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	AL	971	0	1057	156	0
12	CL	971	0	1057	149	0
13	AM	988	0	1059	215	0
13	CM	988	0	1059	208	0
14	AN	492	0	529	130	0
14	CN	492	0	529	129	0
15	AO	734	0	771	94	0
15	CO	734	0	771	97	0
16	AP	701	0	720	116	0
16	CP	701	0	720	114	0
17	AQ	824	0	891	88	0
17	CQ	824	0	891	89	0
18	AR	574	0	644	97	0
18	CR	574	0	644	95	0
19	AS	630	0	652	129	0
19	CS	630	0	652	129	0
20	AT	763	0	861	148	0
20	CT	763	0	861	141	0
21	AU	209	0	221	30	0
21	CU	209	0	221	33	0
22	AV	1619	0	822	99	0
22	AW	1619	0	822	82	0
22	CV	1619	0	822	87	0
22	CW	1619	0	822	90	0
23	AX	272	0	142	23	0
23	CX	272	0	142	21	0
24	AY	1650	0	851	118	0
24	CY	1650	0	851	115	0
25	AZ	2900	0	2907	491	0
25	CZ	2900	0	2907	478	0
26	B0	662	0	688	112	0
26	D0	662	0	688	112	0
27	B1	732	0	808	156	0
27	D1	732	0	808	158	0
28	B2	598	0	653	166	0
28	D2	598	0	653	153	0
29	B3	468	0	523	74	0
29	D3	468	0	523	76	0
30	B4	341	0	337	72	0
30	D4	341	0	337	63	0
31	B5	459	0	480	98	0
31	D5	459	0	480	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	B6	433	0	461	157	0
32	D6	433	0	461	162	0
33	B7	419	0	467	71	0
33	D7	419	0	467	76	0
34	B8	508	0	576	141	0
34	D8	508	0	576	147	0
35	B9	307	0	335	74	0
35	D9	307	0	337	78	0
36	BA	62474	0	31497	4307	0
36	DA	62474	0	31497	4322	0
37	BB	2551	0	1295	152	0
37	DB	2551	0	1295	162	0
38	BC	1742	0	1800	269	1
38	DC	1742	0	1800	272	1
39	BD	2145	0	2234	441	0
39	DD	2145	0	2234	438	0
40	BE	1564	0	1629	331	0
40	DE	1564	0	1629	327	0
41	BF	1624	0	1677	362	0
41	DF	1624	0	1677	351	0
42	BG	1474	0	1535	396	0
42	DG	1474	0	1535	365	0
43	BH	1223	0	1282	214	0
43	DH	1223	0	1282	215	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	233	0
46	DN	1105	0	1180	232	0
47	BO	933	0	996	121	0
47	DO	933	0	996	120	0
48	BP	1114	0	1187	309	0
48	DP	1114	0	1187	308	0
49	BQ	1122	0	1179	240	0
49	DQ	1122	0	1179	226	0
50	BR	960	0	1021	198	0
50	DR	960	0	1021	197	0
51	BS	771	0	832	195	0
51	DS	771	0	832	189	0
52	BT	1142	0	1202	274	0
52	DT	1142	0	1202	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	BU	958	0	1015	223	0
53	DU	958	0	1015	223	0
54	BV	779	0	852	167	0
54	DV	779	0	852	169	0
55	BW	896	0	953	153	0
55	DW	896	0	953	160	0
56	BX	726	0	778	118	0
56	DX	726	0	778	115	0
57	BY	776	0	870	208	0
57	DY	776	0	870	203	0
58	BZ	1403	0	1432	320	0
58	DZ	1403	0	1432	293	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	30310	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 59.

The worst 5 of 30310 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	2
2	CB	233/256 (91%)	115 (49%)	74 (32%)	44 (19%)	0	2
3	AC	205/239 (86%)	117 (57%)	52 (25%)	36 (18%)	0	2
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	3
4	CD	206/209 (99%)	122 (59%)	48 (23%)	36 (18%)	0	2
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	0	7
5	CE	149/162 (92%)	98 (66%)	37 (25%)	14 (9%)	0	8
6	AF	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	9
6	CF	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	9
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	2
8	AH	136/138 (99%)	88 (65%)	34 (25%)	14 (10%)	0	7
8	CH	136/138 (99%)	89 (65%)	35 (26%)	12 (9%)	1	9
9	AI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	4
9	CI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	4
10	AJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	4
10	CJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	80 (68%)	29 (25%)	8 (7%)	1	15
11	CK	117/129 (91%)	77 (66%)	32 (27%)	8 (7%)	1	15
12	AL	123/135 (91%)	71 (58%)	32 (26%)	20 (16%)	0	3
12	CL	123/135 (91%)	73 (59%)	31 (25%)	19 (15%)	0	3
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	1
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	2
15	CO	86/89 (97%)	55 (64%)	15 (17%)	16 (19%)	0	2
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	14
17	CQ	98/105 (93%)	69 (70%)	21 (21%)	8 (8%)	1	10
18	AR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	2
18	CR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	2
19	AS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	4
19	CS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	4
20	AT	97/106 (92%)	49 (50%)	30 (31%)	18 (19%)	0	2
20	CT	97/106 (92%)	50 (52%)	29 (30%)	18 (19%)	0	2
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	1
25	AZ	370/406 (91%)	254 (69%)	77 (21%)	39 (10%)	0	7
25	CZ	370/406 (91%)	252 (68%)	81 (22%)	37 (10%)	0	8
26	B0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	0	8
26	D0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	0	8
27	B1	92/98 (94%)	55 (60%)	22 (24%)	15 (16%)	0	3
27	D1	92/98 (94%)	54 (59%)	25 (27%)	13 (14%)	0	4
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	3
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	2
30	D4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	2
31	B5	57/60 (95%)	33 (58%)	13 (23%)	11 (19%)	0	2
31	D5	57/60 (95%)	32 (56%)	14 (25%)	11 (19%)	0	2
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	2
34	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	2
35	B9	35/37 (95%)	18 (51%)	9 (26%)	8 (23%)	0	1
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	4
38	DC	226/229 (99%)	141 (62%)	55 (24%)	30 (13%)	0	4
39	BD	273/276 (99%)	176 (64%)	63 (23%)	34 (12%)	0	5
39	DD	273/276 (99%)	172 (63%)	66 (24%)	35 (13%)	0	5
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	2
41	DF	206/210 (98%)	121 (59%)	46 (22%)	39 (19%)	0	2
42	BG	179/182 (98%)	86 (48%)	52 (29%)	41 (23%)	0	1
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	3
43	DH	158/180 (88%)	99 (63%)	35 (22%)	24 (15%)	0	3
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	8
47	DO	120/122 (98%)	93 (78%)	15 (12%)	12 (10%)	0	8
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	6
49	DQ	139/141 (99%)	81 (58%)	39 (28%)	19 (14%)	0	4
50	BR	115/118 (98%)	68 (59%)	25 (22%)	22 (19%)	0	2
50	DR	115/118 (98%)	70 (61%)	23 (20%)	22 (19%)	0	2
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	7
53	DU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	0	7
54	BV	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	2
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	5
55	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	5
56	BX	91/96 (95%)	55 (60%)	20 (22%)	16 (18%)	0	2
56	DX	91/96 (95%)	54 (59%)	22 (24%)	15 (16%)	0	3
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	27
2	CB	202/220 (92%)	179 (89%)	23 (11%)	5	29
3	AC	160/188 (85%)	148 (92%)	12 (8%)	13	45
3	CC	160/188 (85%)	148 (92%)	12 (8%)	13	45
4	AD	180/181 (99%)	147 (82%)	33 (18%)	1	10
4	CD	180/181 (99%)	146 (81%)	34 (19%)	1	9
5	AE	115/123 (94%)	103 (90%)	12 (10%)	7	33
5	CE	115/123 (94%)	103 (90%)	12 (10%)	7	33
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	26
6	CF	90/90 (100%)	78 (87%)	12 (13%)	4	23
7	AG	126/127 (99%)	113 (90%)	13 (10%)	7	34
7	CG	126/127 (99%)	113 (90%)	13 (10%)	7	34
8	AH	119/119 (100%)	100 (84%)	19 (16%)	2	16
8	CH	119/119 (100%)	101 (85%)	18 (15%)	3	19
9	AI	98/99 (99%)	86 (88%)	12 (12%)	5	26
9	CI	98/99 (99%)	86 (88%)	12 (12%)	5	26
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	1	9
10	CJ	88/92 (96%)	71 (81%)	17 (19%)	1	9
11	AK	90/99 (91%)	81 (90%)	9 (10%)	7	35
11	CK	90/99 (91%)	82 (91%)	8 (9%)	9	40
12	AL	104/111 (94%)	82 (79%)	22 (21%)	1	7
12	CL	104/111 (94%)	82 (79%)	22 (21%)	1	7
13	AM	99/101 (98%)	88 (89%)	11 (11%)	6	31
13	CM	99/101 (98%)	88 (89%)	11 (11%)	6	31
14	AN	49/50 (98%)	40 (82%)	9 (18%)	1	10
14	CN	49/50 (98%)	40 (82%)	9 (18%)	1	10
15	AO	79/80 (99%)	69 (87%)	10 (13%)	4	24
15	CO	79/80 (99%)	68 (86%)	11 (14%)	3	22
16	AP	72/74 (97%)	65 (90%)	7 (10%)	8	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	65 (90%)	7 (10%)	8	36
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	17	52
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	13	46
18	AR	61/77 (79%)	56 (92%)	5 (8%)	11	42
18	CR	61/77 (79%)	56 (92%)	5 (8%)	11	42
19	AS	69/80 (86%)	59 (86%)	10 (14%)	3	20
19	CS	69/80 (86%)	59 (86%)	10 (14%)	3	20
20	AT	76/82 (93%)	63 (83%)	13 (17%)	2	13
20	CT	76/82 (93%)	63 (83%)	13 (17%)	2	13
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	33
21	CU	19/22 (86%)	17 (90%)	2 (10%)	7	33
25	AZ	314/339 (93%)	272 (87%)	42 (13%)	4	23
25	CZ	314/339 (93%)	273 (87%)	41 (13%)	4	23
26	B0	66/67 (98%)	52 (79%)	14 (21%)	1	7
26	D0	66/67 (98%)	51 (77%)	15 (23%)	1	5
27	B1	78/83 (94%)	59 (76%)	19 (24%)	0	4
27	D1	78/83 (94%)	59 (76%)	19 (24%)	0	4
28	B2	66/67 (98%)	49 (74%)	17 (26%)	0	4
28	D2	66/67 (98%)	56 (85%)	10 (15%)	3	19
29	B3	51/52 (98%)	44 (86%)	7 (14%)	3	22
29	D3	51/52 (98%)	44 (86%)	7 (14%)	3	22
30	B4	39/63 (62%)	26 (67%)	13 (33%)	0	2
30	D4	39/63 (62%)	26 (67%)	13 (33%)	0	2
31	B5	51/52 (98%)	47 (92%)	4 (8%)	12	44
31	D5	51/52 (98%)	47 (92%)	4 (8%)	12	44
32	B6	49/52 (94%)	41 (84%)	8 (16%)	2	15
32	D6	49/52 (94%)	40 (82%)	9 (18%)	1	10
33	B7	41/42 (98%)	32 (78%)	9 (22%)	1	6
33	D7	41/42 (98%)	33 (80%)	8 (20%)	1	9
34	B8	53/55 (96%)	45 (85%)	8 (15%)	3	19
34	D8	53/55 (96%)	45 (85%)	8 (15%)	3	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	B9	34/34 (100%)	30 (88%)	4 (12%)	5	28
35	D9	34/34 (100%)	30 (88%)	4 (12%)	5	28
38	BC	180/181 (99%)	157 (87%)	23 (13%)	4	24
38	DC	180/181 (99%)	157 (87%)	23 (13%)	4	24
39	BD	217/218 (100%)	180 (83%)	37 (17%)	2	13
39	DD	217/218 (100%)	178 (82%)	39 (18%)	1	11
40	BE	165/166 (99%)	142 (86%)	23 (14%)	3	22
40	DE	165/166 (99%)	143 (87%)	22 (13%)	4	23
41	BF	165/166 (99%)	152 (92%)	13 (8%)	12	44
41	DF	165/166 (99%)	152 (92%)	13 (8%)	12	44
42	BG	155/156 (99%)	130 (84%)	25 (16%)	2	16
42	DG	155/156 (99%)	129 (83%)	26 (17%)	2	14
43	BH	132/148 (89%)	118 (89%)	14 (11%)	6	32
43	DH	132/148 (89%)	119 (90%)	13 (10%)	8	36
46	BN	117/119 (98%)	103 (88%)	14 (12%)	5	27
46	DN	117/119 (98%)	102 (87%)	15 (13%)	4	24
47	BO	100/100 (100%)	90 (90%)	10 (10%)	7	35
47	DO	100/100 (100%)	90 (90%)	10 (10%)	7	35
48	BP	112/116 (97%)	88 (79%)	24 (21%)	1	7
48	DP	112/116 (97%)	89 (80%)	23 (20%)	1	7
49	BQ	111/111 (100%)	91 (82%)	20 (18%)	1	11
49	DQ	111/111 (100%)	91 (82%)	20 (18%)	1	11
50	BR	100/101 (99%)	86 (86%)	14 (14%)	3	21
50	DR	100/101 (99%)	82 (82%)	18 (18%)	1	11
51	BS	77/88 (88%)	66 (86%)	11 (14%)	3	21
51	DS	77/88 (88%)	66 (86%)	11 (14%)	3	21
52	BT	120/127 (94%)	99 (82%)	21 (18%)	2	12
52	DT	120/127 (94%)	100 (83%)	20 (17%)	2	14
53	BU	92/94 (98%)	84 (91%)	8 (9%)	10	41
53	DU	92/94 (98%)	84 (91%)	8 (9%)	10	41
54	BV	82/82 (100%)	66 (80%)	16 (20%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	DV	82/82 (100%)	66 (80%)	16 (20%)	1	9
55	BW	91/92 (99%)	79 (87%)	12 (13%)	4	23
55	DW	91/92 (99%)	79 (87%)	12 (13%)	4	23
56	BX	74/78 (95%)	67 (90%)	7 (10%)	8	37
56	DX	74/78 (95%)	67 (90%)	7 (10%)	8	37
57	BY	84/91 (92%)	68 (81%)	16 (19%)	1	9
57	DY	84/91 (92%)	68 (81%)	16 (19%)	1	9
58	BZ	155/179 (87%)	127 (82%)	28 (18%)	1	11
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	2	18
All	All	10322/10862 (95%)	8852 (86%)	1470 (14%)	3	21

5 of 1470 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	20	LEU
6	CF	31	GLU
51	DS	15	ARG
55	BW	92	ARG
2	CB	63	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
54	BV	11	GLN
5	CE	73	ASN
50	DR	23	ASN
56	BX	41	ASN
2	CB	146	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	75/77 (97%)	29 (38%)	0
24	CY	75/77 (97%)	28 (37%)	0
36	BA	2900/2915 (99%)	647 (22%)	55 (1%)
36	DA	2900/2915 (99%)	653 (22%)	55 (1%)
37	BB	118/122 (96%)	29 (24%)	1 (0%)
37	DB	118/122 (96%)	29 (24%)	1 (0%)
All	All	9516/9630 (98%)	2077 (21%)	234 (2%)

5 of 2077 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	2126	A
1	CA	266	G
36	DA	1819	A
36	BA	2282	G
1	CA	30	U

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	PSU	AY	55	24	17,21,22	1.72	4 (23%)	20,30,33	3.41	7 (35%)
24	H2U	AY	17	24	18,21,22	0.84	0	21,30,33	1.89	4 (19%)
24	7MG	AY	46	24	22,26,27	1.22	2 (9%)	28,39,42	2.26	5 (17%)
24	H2U	AY	20	24	18,21,22	0.83	0	21,30,33	1.75	4 (19%)
24	H2U	AY	16	24	18,21,22	0.95	1 (5%)	21,30,33	1.79	4 (19%)
24	7MG	CY	46	24	22,26,27	1.20	2 (9%)	28,39,42	2.26	5 (17%)
24	YG	CY	37	24	29,42,43	1.20	2 (6%)	29,62,65	1.96	7 (24%)
24	H2U	CY	16	24	18,21,22	0.88	1 (5%)	21,30,33	1.80	4 (19%)
24	5MU	AY	54	24	15,22,23	1.16	2 (13%)	16,32,35	3.70	1 (6%)
24	PSU	CY	55	24	17,21,22	1.70	4 (23%)	20,30,33	3.38	8 (40%)
24	H2U	CY	20	24	18,21,22	0.82	0	21,30,33	1.77	4 (19%)
24	YG	AY	37	24	29,42,43	1.29	4 (13%)	29,62,65	1.96	8 (27%)
24	H2U	CY	17	24	18,21,22	0.85	0	21,30,33	1.90	4 (19%)
24	5MU	CY	54	24	15,22,23	1.18	2 (13%)	16,32,35	3.72	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PSU	AY	55	24	-	4/7/25/26	0/2/2/2
24	H2U	AY	17	24	-	5/7/38/39	0/2/2/2
24	7MG	AY	46	24	-	0/7/37/38	0/3/3/3
24	H2U	AY	20	24	-	3/7/38/39	0/2/2/2
24	H2U	AY	16	24	-	2/7/38/39	0/2/2/2
24	7MG	CY	46	24	-	0/7/37/38	0/3/3/3
24	YG	CY	37	24	-	2/20/42/43	0/4/4/4
24	H2U	CY	16	24	-	2/7/38/39	0/2/2/2
24	5MU	AY	54	24	-	0/5/25/26	0/2/2/2
24	PSU	CY	55	24	-	4/7/25/26	0/2/2/2
24	H2U	CY	20	24	-	3/7/38/39	0/2/2/2
24	YG	AY	37	24	-	2/20/42/43	0/4/4/4
24	H2U	CY	17	24	-	5/7/38/39	0/2/2/2
24	5MU	CY	54	24	-	0/5/25/26	0/2/2/2

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	55	PSU	C5-C1'	4.64	1.56	1.52
24	CY	55	PSU	C5-C1'	4.56	1.56	1.52
24	AY	37	YG	C2-N2	-3.99	1.29	1.35
24	AY	46	7MG	C6-N1	3.86	1.39	1.33
24	CY	37	YG	C2-N2	-3.81	1.30	1.35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	54	5MU	C4-N3-C2	14.57	127.44	115.14
24	AY	54	5MU	C4-N3-C2	14.49	127.37	115.14
24	AY	55	PSU	N1-C2-N3	-10.24	120.29	128.43
24	CY	55	PSU	N1-C2-N3	-10.19	120.33	128.43
24	AY	55	PSU	C4-N3-C2	6.81	120.89	115.14

There are no chirality outliers.

5 of 32 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	20	H2U	O4'-C4'-C5'-O5'

There are no ring outliers.

12 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	AY	55	PSU	5	0
24	AY	17	H2U	1	0
24	AY	20	H2U	2	0
24	AY	16	H2U	3	0
24	CY	37	YG	5	0
24	CY	16	H2U	3	0
24	AY	54	5MU	4	0
24	CY	55	PSU	7	0
24	CY	20	H2U	2	0
24	AY	37	YG	8	0
24	CY	17	H2U	1	0
24	CY	54	5MU	6	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	3.43	24 (42%)	62,84,84	1.66	14 (22%)
59	PAR	CA	1601	-	45,45,45	1.43	5 (11%)	64,67,67	1.36	9 (14%)
63	KIR	AZ	502	-	56,59,59	3.40	23 (41%)	62,84,84	1.65	10 (16%)
62	GDP	CZ	501	-	24,30,30	1.40	3 (12%)	31,47,47	2.02	6 (19%)
62	GDP	AZ	501	-	24,30,30	1.37	3 (12%)	31,47,47	2.15	8 (25%)
59	PAR	AA	1601	-	45,45,45	1.49	5 (11%)	64,67,67	1.42	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	-	-	6/54/98/98	0/3/3/3
59	PAR	CA	1601	-	-	5/18/94/94	0/4/4/4
63	KIR	AZ	502	-	-	7/54/98/98	0/3/3/3
62	GDP	CZ	501	-	-	3/12/32/32	0/3/3/3
62	GDP	AZ	501	-	-	2/12/32/32	0/3/3/3
59	PAR	AA	1601	-	-	7/18/94/94	0/4/4/4

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	AZ	502	KIR	O18-C17	-14.60	1.22	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	CZ	502	KIR	O18-C17	-14.49	1.22	1.44
63	CZ	502	KIR	O30-C30	-12.32	1.18	1.42
63	AZ	502	KIR	O30-C30	-12.23	1.18	1.42
63	CZ	502	KIR	C22-C21	6.04	1.39	1.33

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	AZ	501	GDP	N3-C2-N1	-5.58	119.78	127.22
62	AZ	501	GDP	C2-N3-C4	5.20	121.30	115.36
62	CZ	501	GDP	C2-N3-C4	5.11	121.19	115.36
62	CZ	501	GDP	N3-C2-N1	-4.81	120.81	127.22
63	CZ	502	KIR	O29-C29-O34	-4.52	102.64	110.21

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	AZ	502	KIR	O18-C17-C19-C42
62	CZ	501	GDP	PA-O3A-PB-O2B
62	CZ	501	GDP	PA-O3A-PB-O3B
62	AZ	501	GDP	PA-O3A-PB-O2B
62	AZ	501	GDP	PA-O3A-PB-O3B

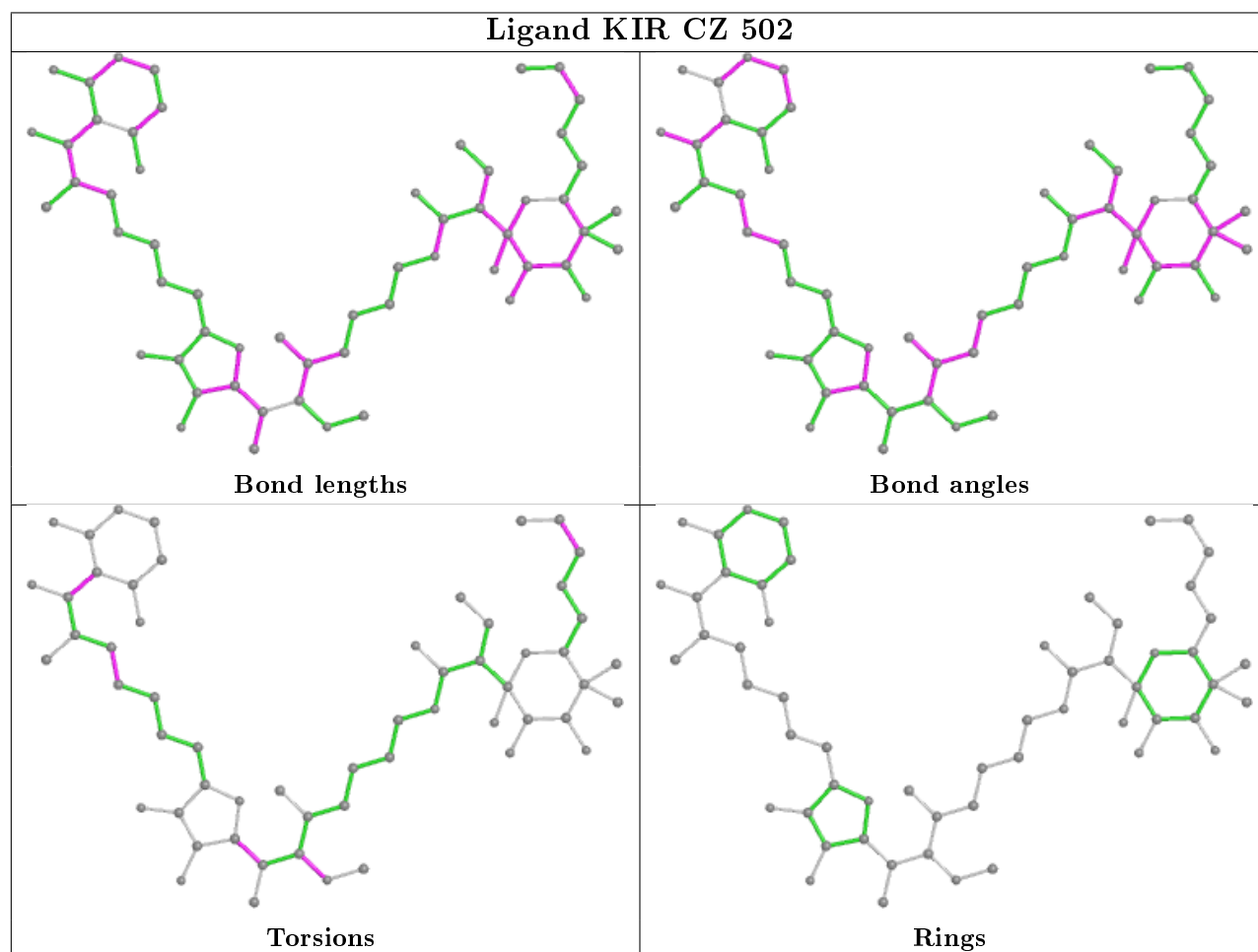
There are no ring outliers.

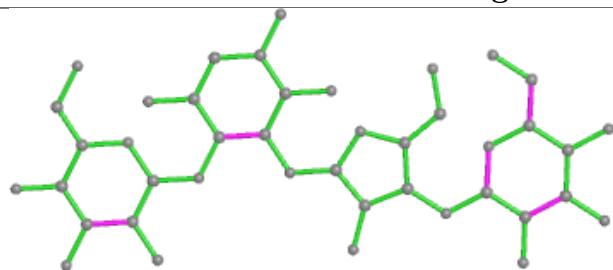
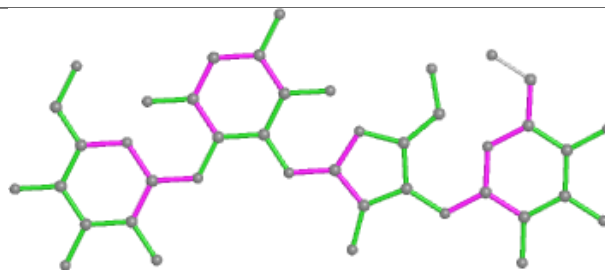
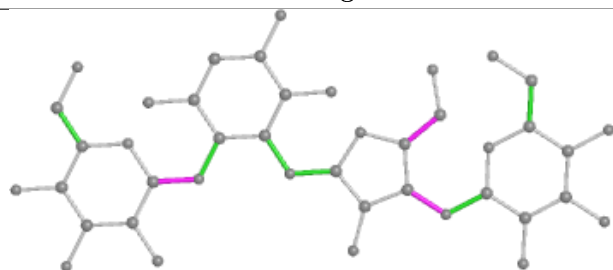
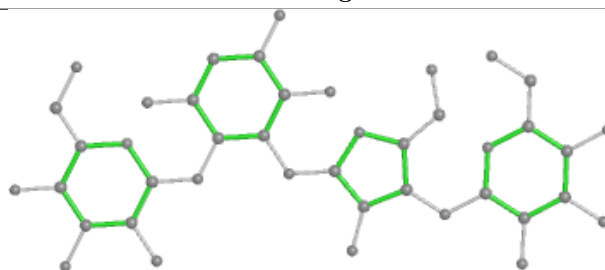
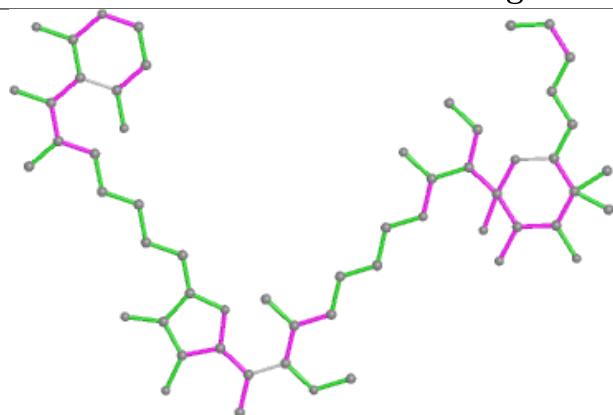
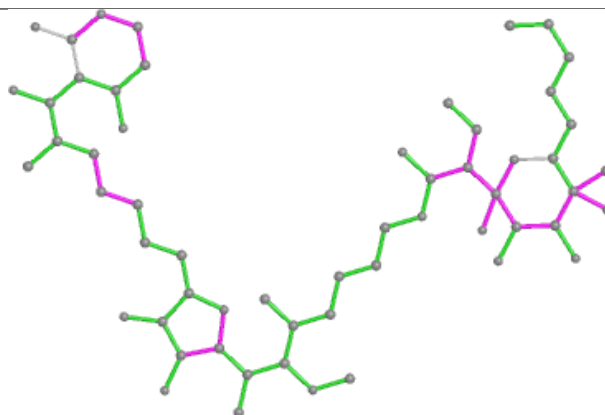
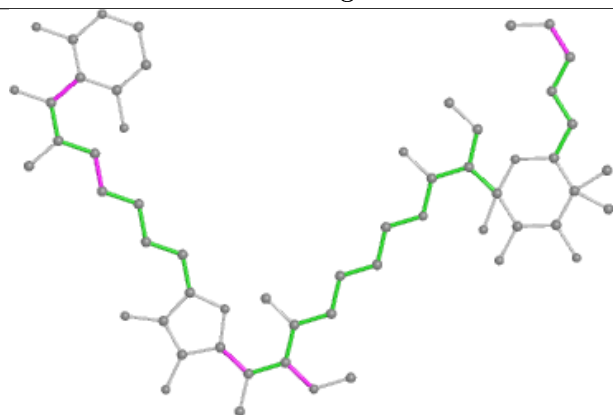
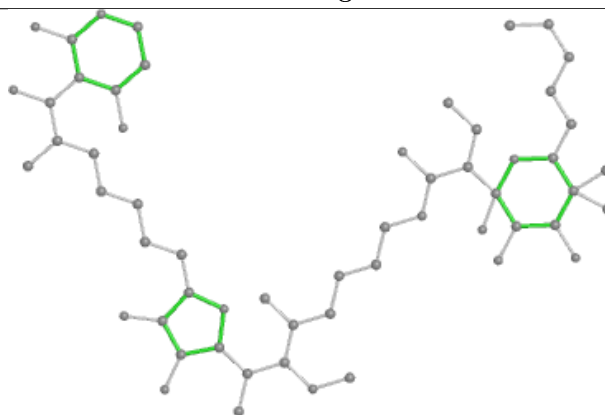
6 monomers are involved in 49 short contacts:

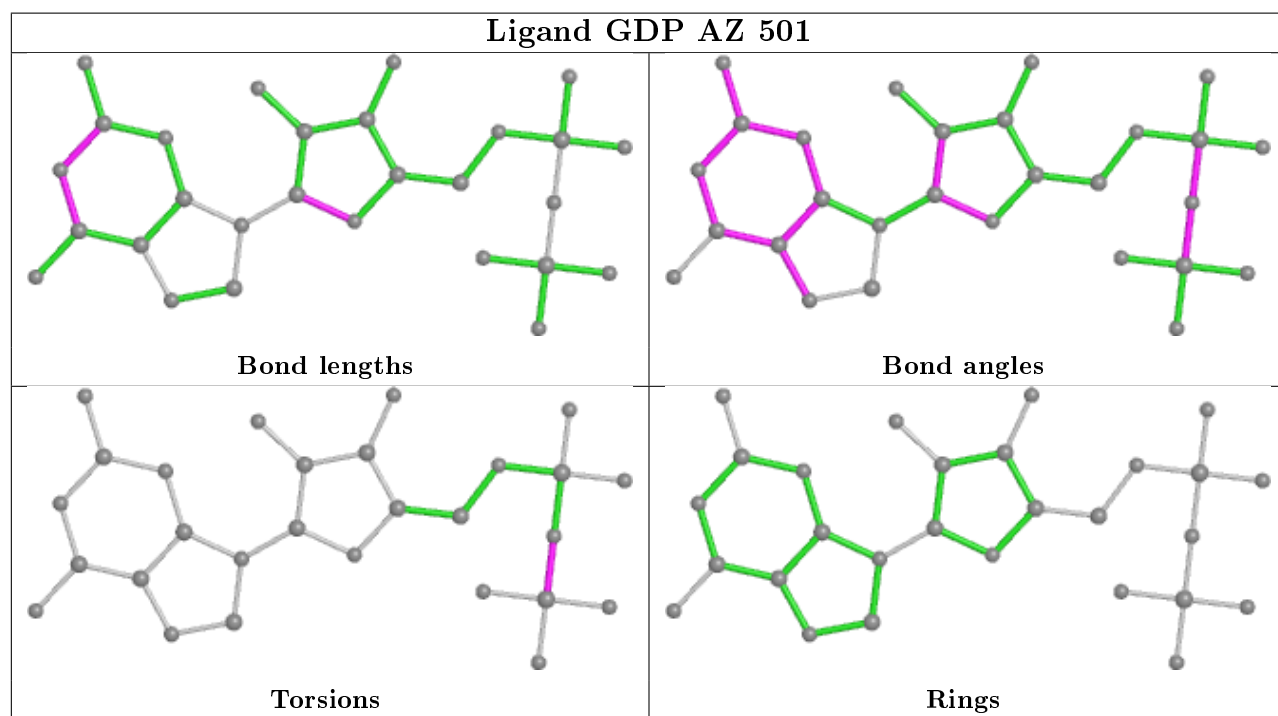
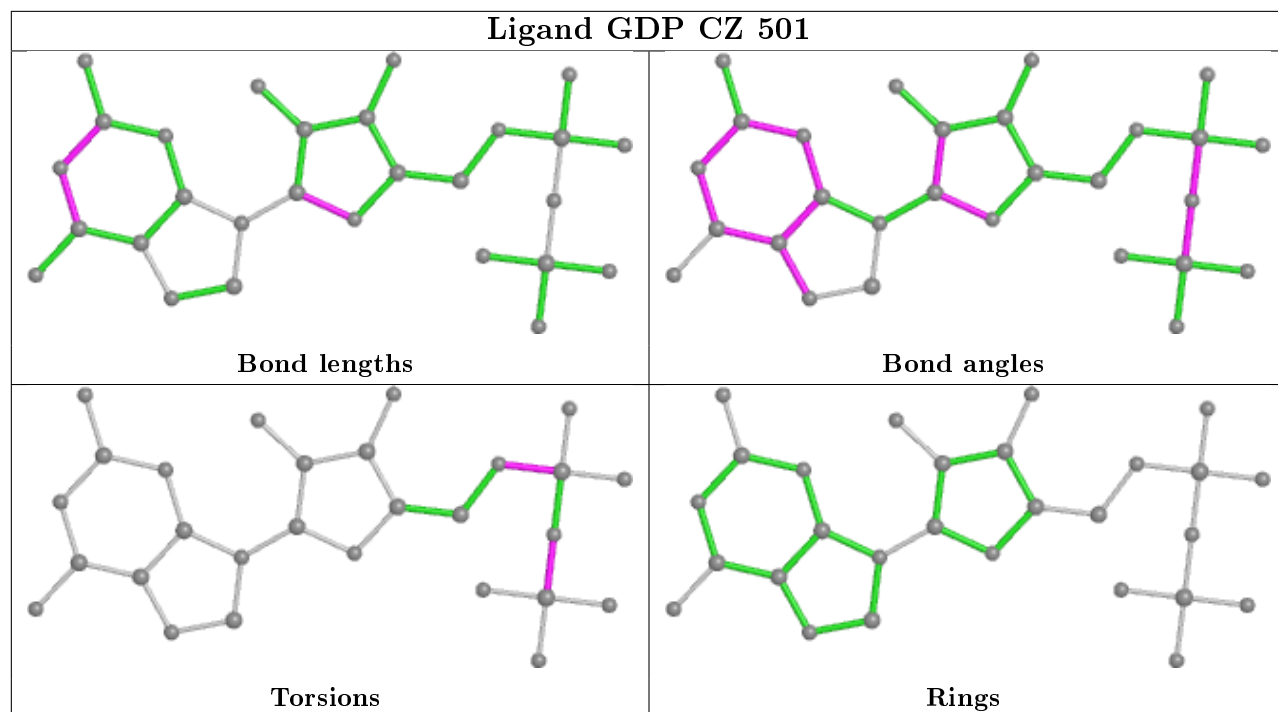
Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	CZ	502	KIR	8	0
59	CA	1601	PAR	3	0
63	AZ	502	KIR	4	0
62	CZ	501	GDP	15	0
62	AZ	501	GDP	15	0
59	AA	1601	PAR	4	0

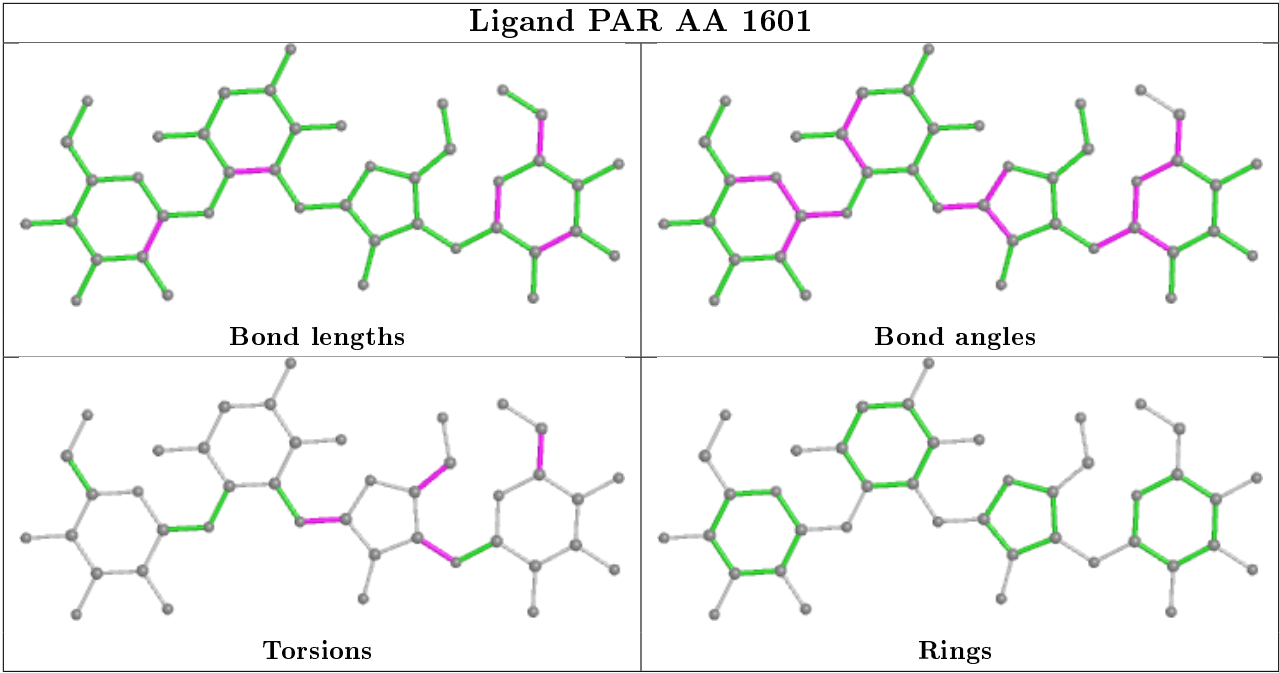
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

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



Ligand PAR CA 1601**Bond lengths****Bond angles****Torsions****Rings****Ligand KIR AZ 502****Bond lengths****Bond angles****Torsions****Rings**





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%)	-0.07	10 (0%) 87 78	29, 82, 163, 200	0
1	CA	1504/1522 (98%)	-0.17	13 (0%) 84 73	28, 83, 163, 200	0
2	AB	235/256 (91%)	-0.06	3 (1%) 77 63	63, 102, 151, 161	0
2	CB	235/256 (91%)	-0.15	4 (1%) 70 55	63, 102, 151, 162	0
3	AC	207/239 (86%)	-0.19	1 (0%) 91 83	54, 91, 111, 117	0
3	CC	207/239 (86%)	-0.20	2 (0%) 82 70	59, 91, 111, 117	0
4	AD	208/209 (99%)	-0.23	1 (0%) 91 83	60, 91, 116, 122	0
4	CD	208/209 (99%)	-0.15	1 (0%) 91 83	61, 92, 117, 123	0
5	AE	151/162 (93%)	-0.30	0 100 100	44, 72, 90, 108	0
5	CE	151/162 (93%)	-0.25	1 (0%) 87 78	43, 73, 91, 109	0
6	AF	101/101 (100%)	-0.20	0 100 100	91, 102, 110, 118	0
6	CF	101/101 (100%)	-0.03	1 (0%) 82 70	92, 103, 111, 118	0
7	AG	155/156 (99%)	-0.10	3 (1%) 66 51	79, 104, 134, 141	0
7	CG	155/156 (99%)	-0.13	6 (3%) 39 25	81, 104, 134, 141	0
8	AH	138/138 (100%)	-0.04	1 (0%) 87 78	62, 80, 97, 116	0
8	CH	138/138 (100%)	-0.14	0 100 100	61, 82, 97, 115	0
9	AI	127/128 (99%)	0.08	5 (3%) 39 25	73, 126, 153, 158	0
9	CI	127/128 (99%)	0.11	3 (2%) 59 42	74, 126, 154, 159	0
10	AJ	99/105 (94%)	0.41	9 (9%) 9 5	79, 121, 149, 154	0
10	CJ	99/105 (94%)	0.42	10 (10%) 7 4	80, 121, 148, 153	0
11	AK	119/129 (92%)	-0.10	4 (3%) 45 30	63, 84, 125, 150	0
11	CK	119/129 (92%)	-0.01	4 (3%) 45 30	65, 85, 126, 151	0
12	AL	125/135 (92%)	-0.24	1 (0%) 86 75	47, 70, 100, 125	0
12	CL	125/135 (92%)	-0.09	1 (0%) 86 75	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%)	0.12	6 (4%) 30 19	79, 119, 143, 159	0
13	CM	125/126 (99%)	0.12	5 (4%) 38 25	81, 118, 143, 159	0
14	AN	60/61 (98%)	-0.22	1 (1%) 70 55	60, 77, 96, 101	0
14	CN	60/61 (98%)	-0.12	1 (1%) 70 55	61, 77, 95, 103	0
15	AO	88/89 (98%)	-0.05	1 (1%) 80 68	69, 92, 109, 112	0
15	CO	88/89 (98%)	0.00	2 (2%) 60 44	72, 91, 109, 112	0
16	AP	84/88 (95%)	-0.05	1 (1%) 79 66	76, 89, 119, 137	0
16	CP	84/88 (95%)	0.01	2 (2%) 59 42	74, 89, 118, 137	0
17	AQ	100/105 (95%)	-0.05	0 100 100	65, 92, 115, 121	0
17	CQ	100/105 (95%)	0.03	2 (2%) 65 49	67, 93, 115, 121	0
18	AR	70/88 (79%)	-0.20	1 (1%) 75 61	55, 86, 114, 121	0
18	CR	70/88 (79%)	-0.22	1 (1%) 75 61	57, 87, 115, 121	0
19	AS	79/93 (84%)	0.42	10 (12%) 3 2	82, 120, 143, 146	0
19	CS	79/93 (84%)	0.27	7 (8%) 9 5	83, 120, 144, 146	0
20	AT	99/106 (93%)	-0.14	4 (4%) 38 25	94, 109, 129, 132	0
20	CT	99/106 (93%)	-0.15	1 (1%) 82 70	93, 109, 129, 132	0
21	AU	25/27 (92%)	0.64	3 (12%) 4 3	104, 116, 137, 139	0
21	CU	25/27 (92%)	0.38	1 (4%) 38 25	104, 116, 136, 138	0
22	AV	76/76 (100%)	-0.15	0 100 100	54, 120, 170, 179	0
22	AW	76/76 (100%)	-0.06	1 (1%) 77 63	82, 147, 186, 199	0
22	CV	76/76 (100%)	-0.21	0 100 100	54, 121, 170, 179	0
22	CW	76/76 (100%)	0.06	3 (3%) 39 25	84, 148, 185, 199	0
23	AX	13/27 (48%)	0.32	1 (7%) 13 8	45, 63, 136, 154	0
23	CX	13/27 (48%)	0.16	0 100 100	47, 63, 136, 154	0
24	AY	70/77 (90%)	0.23	2 (2%) 51 35	74, 155, 194, 200	0
24	CY	70/77 (90%)	0.47	6 (8%) 10 6	76, 156, 195, 200	0
25	AZ	374/406 (92%)	0.49	36 (9%) 8 4	97, 139, 158, 177	0
25	CZ	374/406 (92%)	0.78	67 (17%) 1 0	98, 139, 158, 176	0
26	B0	84/85 (98%)	0.16	0 100 100	104, 116, 128, 137	0
26	D0	84/85 (98%)	0.27	2 (2%) 59 42	104, 116, 129, 137	0
27	B1	94/98 (95%)	-0.21	3 (3%) 47 32	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%)	-0.19	1 (1%) 80 68	63, 85, 115, 122	0
28	B2	71/72 (98%)	-0.24	0 100 100	84, 115, 128, 130	0
28	D2	71/72 (98%)	0.14	3 (4%) 36 23	104, 125, 144, 163	0
29	B3	60/60 (100%)	0.85	9 (15%) 2 1	106, 122, 132, 148	0
29	D3	60/60 (100%)	0.48	5 (8%) 11 7	107, 122, 132, 148	0
30	B4	45/71 (63%)	0.75	8 (17%) 1 1	107, 169, 196, 198	0
30	D4	45/71 (63%)	0.61	6 (13%) 3 2	107, 170, 195, 197	0
31	B5	59/60 (98%)	0.63	5 (8%) 10 6	89, 116, 175, 187	0
31	D5	59/60 (98%)	0.42	6 (10%) 6 4	90, 115, 175, 186	0
32	B6	50/54 (92%)	0.47	7 (14%) 2 2	78, 119, 146, 152	0
32	D6	50/54 (92%)	0.48	6 (12%) 4 3	79, 119, 147, 152	0
33	B7	49/49 (100%)	-0.18	0 100 100	59, 77, 144, 152	0
33	D7	49/49 (100%)	-0.41	0 100 100	60, 78, 145, 152	0
34	B8	64/65 (98%)	0.12	3 (4%) 31 19	80, 104, 124, 138	0
34	D8	64/65 (98%)	0.24	3 (4%) 31 19	83, 104, 125, 138	0
35	B9	37/37 (100%)	0.21	2 (5%) 25 16	104, 117, 124, 128	0
35	D9	37/37 (100%)	0.71	4 (10%) 5 3	103, 118, 125, 126	0
36	BA	2901/2915 (99%)	-0.04	49 (1%) 70 55	31, 100, 192, 200	0
36	DA	2901/2915 (99%)	-0.05	59 (2%) 65 49	31, 101, 192, 200	0
37	BB	119/122 (97%)	0.04	3 (2%) 57 41	103, 142, 169, 175	0
37	DB	119/122 (97%)	-0.15	0 100 100	102, 142, 168, 174	0
38	BC	228/229 (99%)	0.37	16 (7%) 16 9	92, 122, 168, 178	0
38	DC	228/229 (99%)	0.54	27 (11%) 4 3	92, 122, 167, 179	0
39	BD	275/276 (99%)	-0.13	2 (0%) 87 78	30, 67, 96, 110	0
39	DD	275/276 (99%)	-0.17	2 (0%) 87 78	38, 68, 96, 109	0
40	BE	205/206 (99%)	0.18	9 (4%) 34 21	67, 106, 143, 154	0
40	DE	205/206 (99%)	0.12	5 (2%) 59 42	67, 106, 143, 153	0
41	BF	208/210 (99%)	0.14	10 (4%) 30 19	61, 123, 160, 167	0
41	DF	208/210 (99%)	0.28	11 (5%) 26 16	62, 123, 160, 166	0
42	BG	181/182 (99%)	0.08	10 (5%) 25 15	103, 128, 146, 163	0
42	DG	181/182 (99%)	0.34	14 (7%) 13 8	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%)	0.67	27 (16%) 1 1	131, 155, 174, 176	0
43	DH	160/180 (88%)	0.92	27 (16%) 1 1	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%)	0.20	6 (4%) 35 22	103, 123, 148, 155	0
46	DN	139/140 (99%)	0.22	9 (6%) 18 11	103, 123, 148, 155	0
47	BO	122/122 (100%)	-0.14	0 100 100	60, 80, 96, 105	0
47	DO	122/122 (100%)	-0.05	0 100 100	61, 80, 96, 106	0
48	BP	146/150 (97%)	0.02	6 (4%) 37 24	71, 113, 133, 140	0
48	DP	146/150 (97%)	0.35	14 (9%) 8 4	70, 114, 133, 139	0
49	BQ	141/141 (100%)	0.10	5 (3%) 44 29	73, 106, 130, 159	0
49	DQ	141/141 (100%)	0.14	3 (2%) 63 48	73, 105, 129, 159	0
50	BR	117/118 (99%)	0.11	5 (4%) 35 22	81, 105, 123, 143	0
50	DR	117/118 (99%)	0.18	4 (3%) 45 30	82, 105, 124, 143	0
51	BS	99/112 (88%)	0.22	3 (3%) 50 34	96, 133, 155, 162	0
51	DS	99/112 (88%)	0.35	5 (5%) 28 17	97, 133, 156, 162	0
52	BT	138/146 (94%)	0.09	6 (4%) 35 22	72, 112, 166, 181	0
52	DT	138/146 (94%)	0.21	10 (7%) 15 9	73, 111, 166, 181	0
53	BU	117/118 (99%)	0.17	4 (3%) 45 30	87, 120, 141, 147	0
53	DU	117/118 (99%)	-0.07	3 (2%) 56 40	88, 119, 141, 148	0
54	BV	101/101 (100%)	0.77	18 (17%) 1 1	105, 144, 159, 164	0
54	DV	101/101 (100%)	0.73	18 (17%) 1 1	106, 145, 159, 165	0
55	BW	113/113 (100%)	0.14	9 (7%) 12 7	81, 109, 132, 136	0
55	DW	113/113 (100%)	0.17	3 (2%) 54 38	81, 109, 131, 136	0
56	BX	93/96 (96%)	0.04	2 (2%) 62 45	96, 108, 124, 128	0
56	DX	93/96 (96%)	0.14	5 (5%) 25 16	97, 109, 125, 130	0
57	BY	101/110 (91%)	0.66	12 (11%) 4 3	124, 145, 165, 170	0
57	DY	101/110 (91%)	1.18	26 (25%) 0 0	123, 145, 163, 170	0
58	BZ	176/206 (85%)	0.71	28 (15%) 1 1	107, 133, 161, 164	0
58	DZ	176/206 (85%)	1.00	41 (23%) 0 0	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%)	0.06	838 (3%) 40 26	28, 105, 164, 200	0

The worst 5 of 838 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	DQ	140	ALA	16.1
31	B5	60	VAL	14.7
57	DY	52	SER	12.2
1	AA	89	C	11.2
36	DA	654(I)	C	11.0

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	16	20/21	0.53	0.47	199,199,200,200	0
24	H2U	AY	17	20/21	0.58	0.40	195,199,199,200	0
24	H2U	AY	16	20/21	0.62	0.66	198,199,200,200	0
24	PSU	CY	55	20/21	0.66	0.31	172,180,180,180	0
24	H2U	CY	17	20/21	0.67	0.48	196,199,200,200	0
24	H2U	CY	20	20/21	0.72	0.18	195,198,200,200	0
24	PSU	AY	55	20/21	0.76	0.19	171,180,181,182	0
24	7MG	AY	46	24/25	0.78	0.22	186,189,190,190	0
24	7MG	CY	46	24/25	0.78	0.24	186,189,190,190	0
24	H2U	AY	20	20/21	0.83	0.21	196,198,200,200	0
24	5MU	AY	54	21/22	0.85	0.23	164,166,168,171	0
24	5MU	CY	54	21/22	0.87	0.35	165,167,168,171	0
24	YG	CY	37	39/40	0.90	0.26	77,108,122,122	0
24	YG	AY	37	39/40	0.90	0.30	77,108,121,122	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

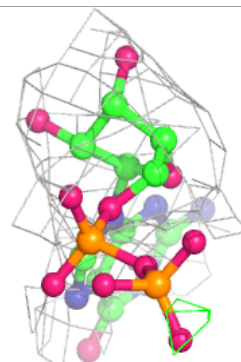
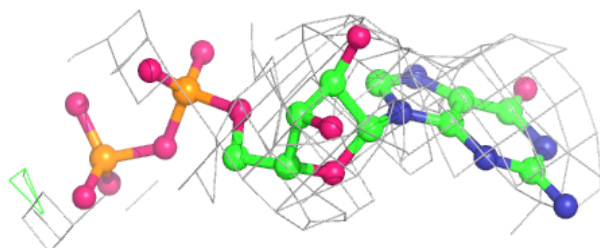
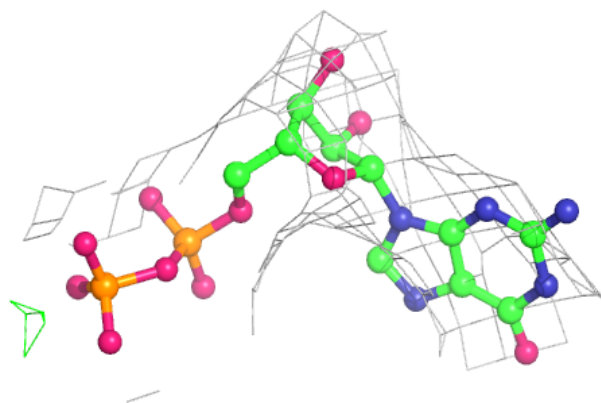
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	-0.22	2.02	181,181,181,181	0
61	MG	AY	101	1/1	0.32	0.24	109,109,109,109	0
62	GDP	CZ	501	28/28	0.84	0.19	117,126,128,128	0
63	KIR	AZ	502	57/57	0.85	0.46	98,106,116,117	0
63	KIR	CZ	502	57/57	0.89	0.44	99,106,116,117	0
62	GDP	AZ	501	28/28	0.89	0.20	117,124,126,126	0
59	PAR	CA	1601	42/42	0.94	0.21	41,46,64,65	0
60	ZN	D4	101	1/1	0.94	0.12	133,133,133,133	0
59	PAR	AA	1601	42/42	0.94	0.20	40,44,48,49	0
60	ZN	D9	101	1/1	0.96	0.09	126,126,126,126	0
60	ZN	B4	101	1/1	0.97	0.15	97,97,97,97	0
60	ZN	CN	101	1/1	0.98	0.19	100,100,100,100	0
60	ZN	AD	301	1/1	0.99	0.28	52,52,52,52	0
60	ZN	B9	101	1/1	0.99	0.18	113,113,113,113	0
60	ZN	CD	301	1/1	0.99	0.29	56,56,56,56	0
60	ZN	AN	101	1/1	1.00	0.16	45,45,45,45	0

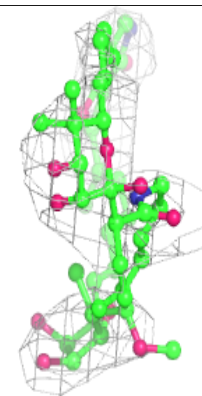
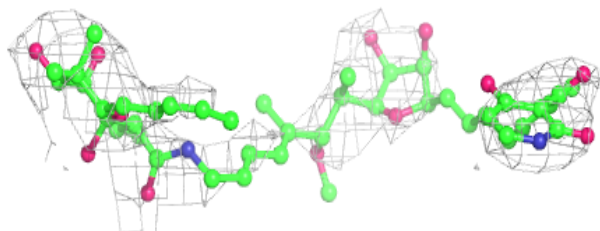
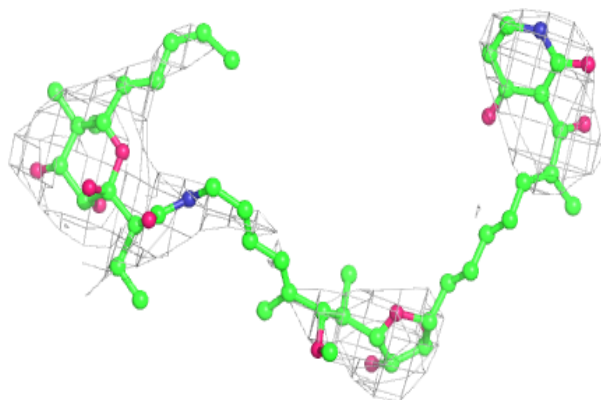
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

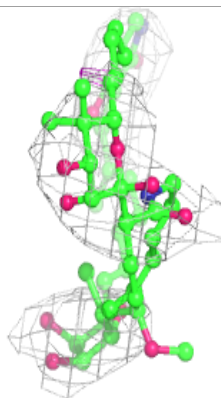
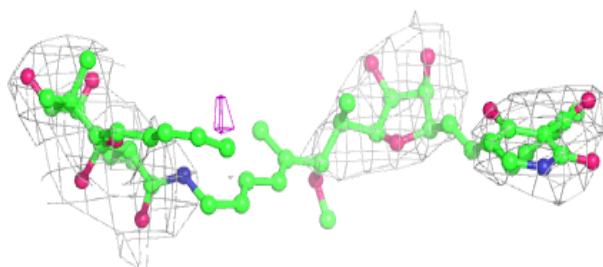
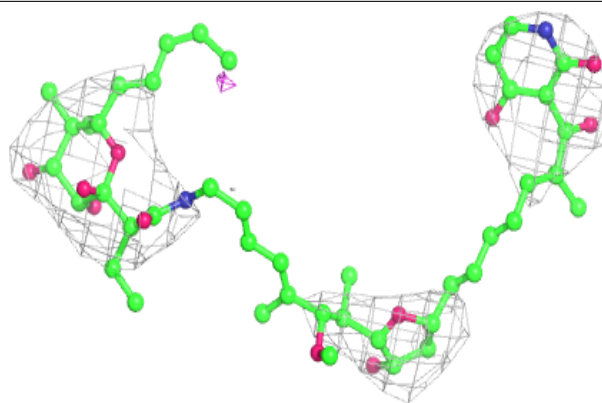
**Electron density around KIR AZ 502:**

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

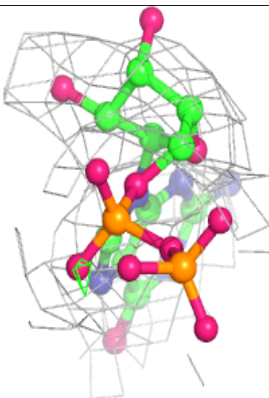
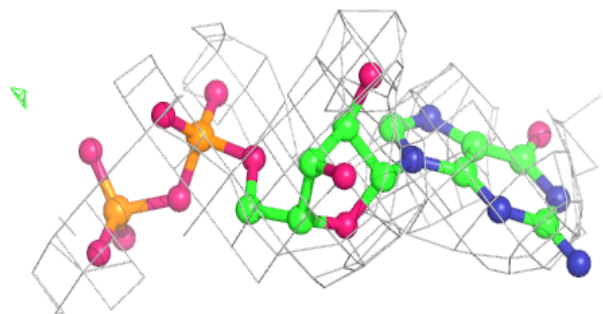
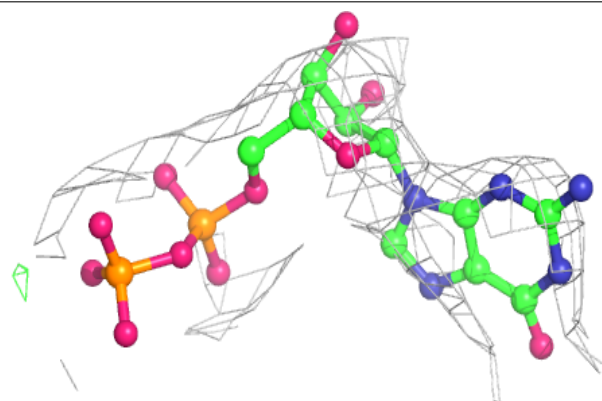


Electron density around KIR CZ 502:

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

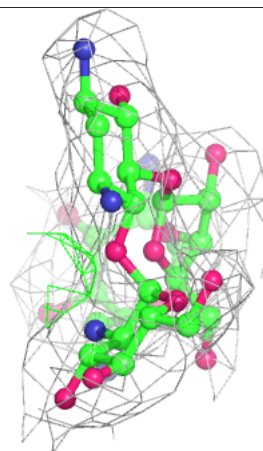
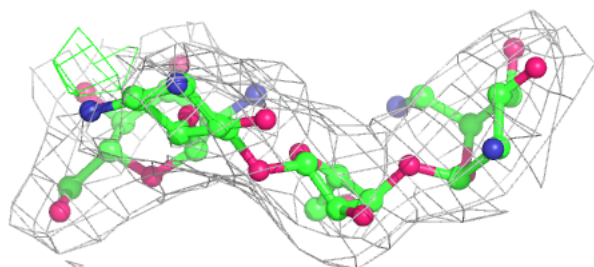
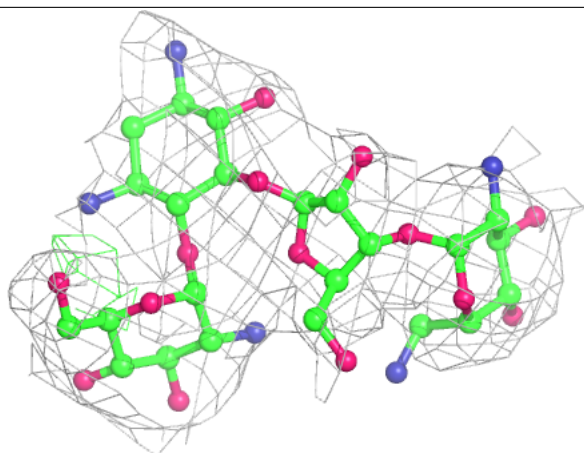
**Electron density around GDP AZ 501:**

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

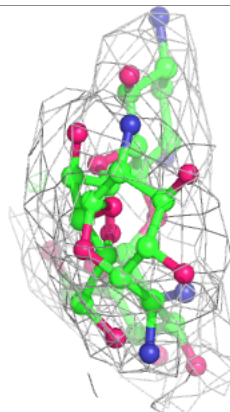
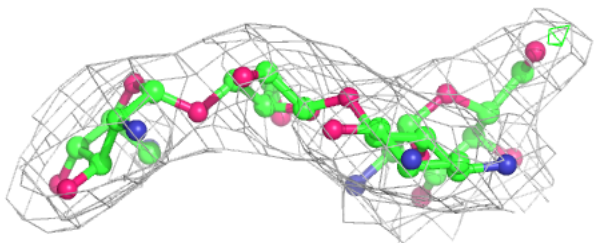
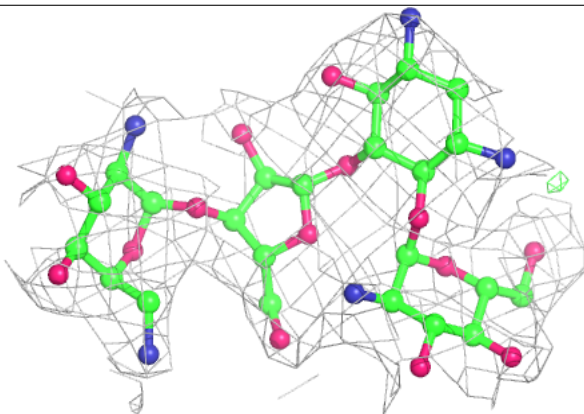


Electron density around PAR CA 1601:

$2mF_o-DF_c$ (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.