



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 2, 2024 – 04:12 pm GMT

PDB ID : 4V8O
Title : Crystal structure of the hybrid state of ribosome in complex with the guanosine triphosphatase release factor 3
Authors : Jin, H.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2011-07-26
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

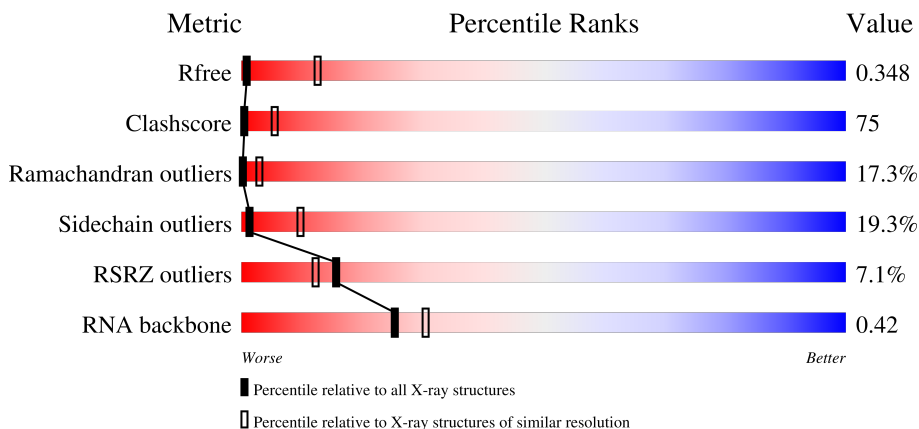
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)
RNA backbone	3102	1036 (4.60-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	AB	256	
3	AC	239	
4	AD	209	

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Mol	Chain	Length	Quality of chain
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	77	
23	AX	9	
24	AY	529	
25	B0	85	
26	B1	98	
27	B2	72	
28	B3	60	
29	B4	71	

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Mol	Chain	Length	Quality of chain
30	B5	60	
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BJ	173	
44	BK	147	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	
52	BU	118	
53	BV	101	
54	BW	113	

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Mol	Chain	Length	Quality of chain
55	BX	96	
56	BY	110	
57	BZ	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
58	GCP	AY	1000	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 151017 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 RRNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
9	AI	127	1011	639	198	174	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	conflict	UNP P80374

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

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

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

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

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

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	expression tag	UNP P17293
AL	2	VAL	-	expression tag	UNP P17293
AL	3	ALA	-	expression tag	UNP P17293
AL	4	LEU	-	expression tag	UNP P17293

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

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

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

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

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

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

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

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

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

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

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

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

- 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			

- 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			

- 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			

- Molecule 22 is a RNA chain called PE HYBRID STATE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			192	88	39	57	8			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	496	Total	C	N	O	S	0	0	0
			3934	2492	677	744	21			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	BA	2901	62477	27807	11683	20087	2900	0	0	0

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	BC	228	1742	1101	318	319	4	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	19	ILE	VAL	conflict	UNP Q5SLP7
BC	27	HIS	ARG	conflict	UNP Q5SLP7
BC	127	MET	LEU	conflict	UNP Q5SLP7

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	BH	156	1189	752	222	214	1	0	0	1

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
43	BJ	131	654	393	131	130	0	0	1

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

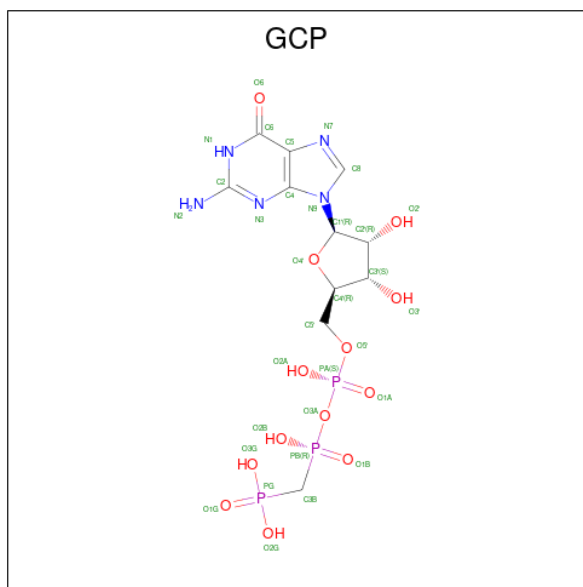
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L25.

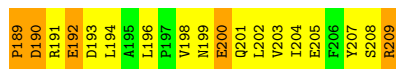
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
57	BZ	176	1403	897	252	252	2	0	0	0

- Molecule 58 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).

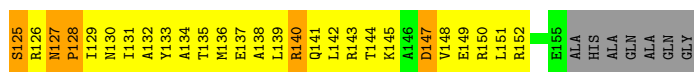
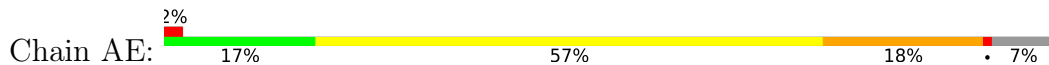


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
58	AY	1	32	11	5	13	3	0	0

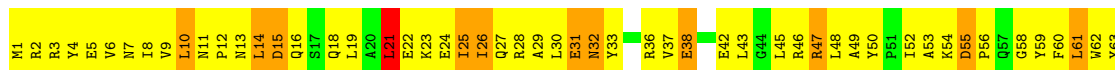
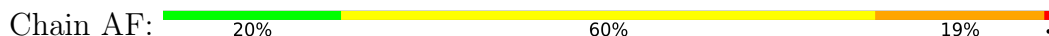
A1503	G1438	A1375	G1316	A1256	A1194	C1132	G1072	U1012	U952	A892	G836	A766	U705	G643
G1504	C1439	U1376	C1317	U1257	C1195	G1133	U1073	G1013	G953	C893	U827	A767	A706	G644
U1505	G1440	C1378	A1318	G1258	U1196	G1134	G1074	A1014	G954	G894	A814	A768	C707	C645
U1506	G1441	C1377	A1319	C1259	G1197	U1135	G1075	A1015	U955	G895	G829	A769	C708	U646
A1507	G1442	G1379	C1320	A1260	U1198	U1136	G1076	A1016	U956	C896	U830	C770	C709	C647
U1508	G1443	U1380	C1321	A1261	U1199	U1137	G1077	G1017	U957	C897	U831	G771	G710	A648
C1509	A1442B	U1381	G1322	C1262	C1200	G1138	U1078	C1018	A958	C898	C832	U772	G711	G649
U1510	G1443	C1382	G1323	C1263	A1201	U1139	A1079	C1019	A959	C899	U833	G773	A712	G650
C1511	C1444	A1383	A1324	G1264	G1202	C1140	G1080	U1020	U960	A900	C834	G774	G713	G651
U1512	G1445	C1384	C1325	G1265	C1203	C1141	G1081	G1021	U961	A901	U835	G775	G714	A652
A1513	U1446	G1385	C1326	A1266	A1204	G1142	G1082	G1022	C962	G902	G836	G776	A715	A653
C1514	A1447	G1386	C1327	C1267	U1205	G1143	U1083	U1023	G963	C903	G837	A777	A716	G657
U1515	G1452	G1387	C1328	A1268	G1206	G1144	G1084	U1024	A964	C904	G838	G778	C717	G658
G1516	G1456	C1388	A1329	A1269	G1207	C1145	U1085	C1027	A965	U965	U839	C779	G718	U659
G1517	A1457	C1389	U1330	C1270	C1208	A1146	U1086	C1028	G966	G906	C840	C780	G719	G660
A1518	G1458	G1391	G1331	G1271	C1209	C1147	G1087	C1029	C967	A907	U841	A781	C720	G661
U1519	A1459	C1392	A1332	G1272	C1210	U1148	G1088	C1030	A968	C848	A782	G782	G721	G662
G1520	A1460	G1393	G1333	G1273	U1211	C1149	G1089	G1030A	A969	C849	C783	A783	A722	G663
U1521	G1461	U1393	G1334	G1274	U1212	U1150	U1090	C1030B	C970	U850	G784	C784	U723	A663
G1522	A1462	C1394	C1335	A1275	A1213	A1151	U1091	G1030C	G971	U911	G851	G785	G724	G664
U1523	G1463	C1395	C1336	G1276	C1214	A1152	U1092	A1030D	C972	C912	G852	G786	G725	A665
G1526	G1464	A1396	G1337	U1277	G1215	C1153	A1093	G1031	G973	A913	G853	A787	C726	G666
C1527	G1465	C1397	G1338	U1278	G1216	G1154	U1094	G1032	A974	A914	G854	U788	G727	G667
U1528	G1466	A1398	A1339	A1279	C1217	G1155	U1095	G1033	A975	A915	G855	U789	A728	G668
G1529	G1467	C1399	A1340	A1280	C1218	G1156	C1096	G1034	G976	G916	C856	A790	A729	U669
U1530	A1468	C1400	U1341	U1281	U1219	A1157	C1097	A1035	A977	G917	C857	G791	G730	G670
A1531	G1469	G1401	C1342	C1282	G1220	U1158	U1098	G1036	A978	A918	G858	A792	G731	G671
U	G1470	C1402	G1343	G1283	G1221	U1159	C1099	C1037	C979	A919	A859	U793	G732	U672
C	G1471	C1403	C1344	C1284	G1222	G1160	C1100	C1038	C980	U920	A860	A794	G734	G673
U	A1472	C1404	U1345	A1285	C1223	C1161	A1101	C1039	U981	U921	C861	C795	G735	G674
C	G1473	G1405	G1346	A1286	C1224	C1162	A1102	U1040	U982	G922	C862	C796	G736	A675
C	G1474	U1406	G1347	A1287	A1225	C1163	A1103	A1041	A983	A923	U863	C797	A737	A676
U	G1475	C1407	U1348	A1288	C1226	C1165	G1104	G1042	C984	C924	A864	G798	C738	U677
U	A1476	A1408	A1349	A1289	A1227	G1166	G1105	A1046	A985	G925	A865	G799	C739	U678
C	C1477	C1409	A1350	G1290	C1228	U1168	G1106	G1047	A986	G926	C866	G800	U740	C679
U	G1478	G1410	U1351	G1291	A1229	A1169	C1107	G1048	G987	U927	C867	U801	G741	U679
C	C1479	C1411	C1352	U1292	C1230	A1170	G1108	G1049	G988	G928	C868	A802	G742	C680
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C	A1483	G1415	C1356	C1296	C1234	G1174	C1112	U1052	U992	C932	A872	C806	A746	G685
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U	G1487	G1419	A1360	G1300	A1238	G1178	C1116	U1056	A996	G936	C876	C810	G750	C689
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U	C1424	C1363	G1363	G1303	G1241	G1181	C1119	C1059	C999	G939	C879	U813	A753	U692
U	U1490	A1363A	G1364	G1304	C1242	G1182	G1120	U1060	U1000	C940	C880	A814	C754	G693
U	A1492	U1364	G1364	G1305	C1243	A1183	U1121	G1061	A1001	G941	C881	A815	G755	A694
U	A1493	G1365	G1365	A1306	C1244	G1184	U1122	U1062	G942	G942	C882	A816	C756	A695
U	U1494	C1366	U1307	U1307	G1248	G1185	A1123	G1063	U943	U943	C883	C817	U757	A696
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U	C1431	C1368	G1309	G1309	C1249	G1187	U1125	U1065	G945	A885	U884	A819	A759	G698
U	G1432	C1369	G1310	G1310	A1250	A1188	U1126	C1066	U946	G886	U820	G820	G760	C699
U	G1433	G1370	G1311	G1311	A1251	C1189	G1127	A1067	G947	G887	U821	U821	G761	G700
U	A1434	G1371	G1312	G1312	A1252	G1190	C1128	G1068	C948	G888	C822	C822	C762	C701
U	U1500	U1372	U1313	U1313	G1253	A1191	A1129	C1069	A949	A899	G823	G823	G763	A702
U	U1501	G1373	C1264	C1264	C1254	A1192	A1130	U1070	U950	G890	C824	C824	C764	G703
U	A1502	A1374	G1315	U1315	G1255	G1193	G1131	C1071	G1011	U951	U891	G825	G765	A704



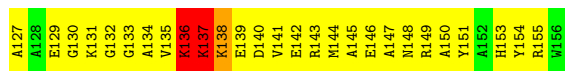
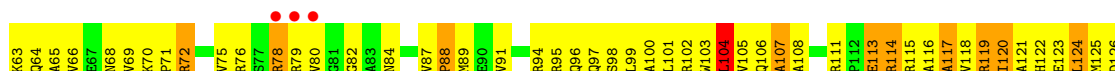
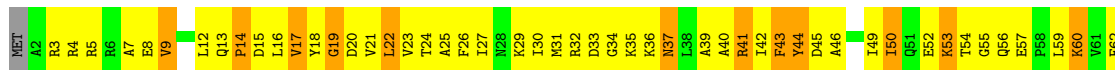
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



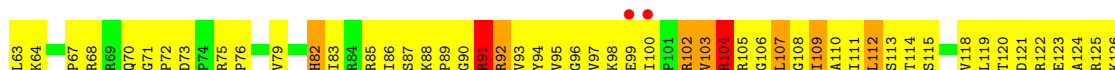
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

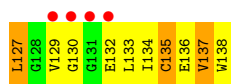


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

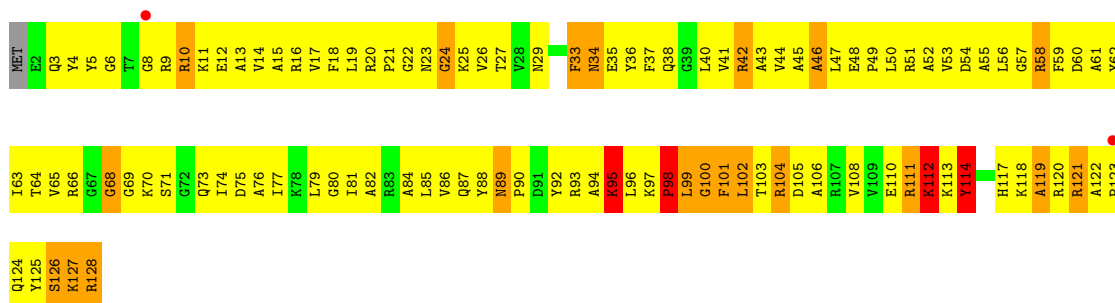
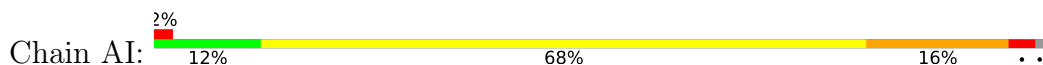


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

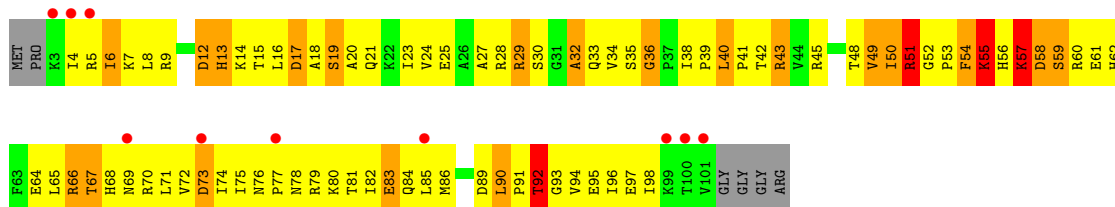
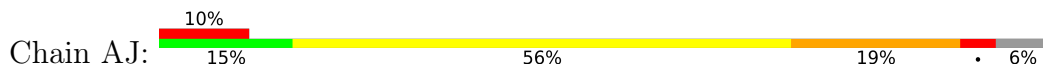




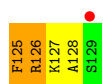
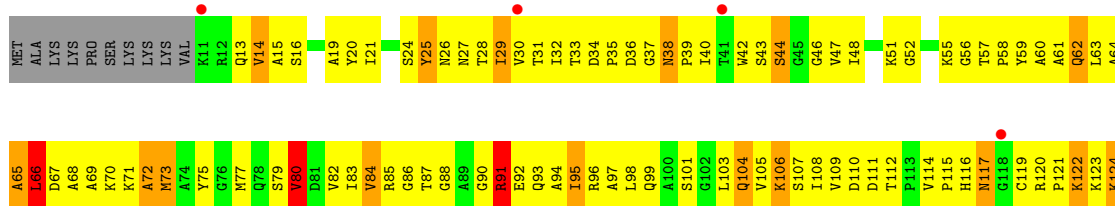
- Molecule 9: 30S RIBOSOMAL PROTEIN S9



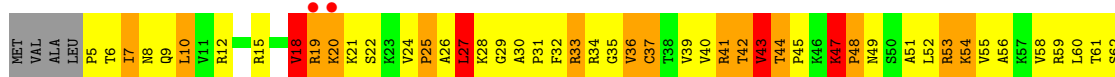
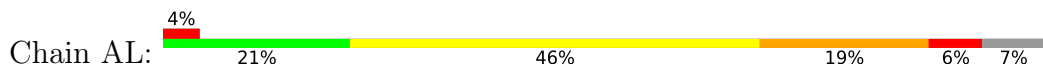
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

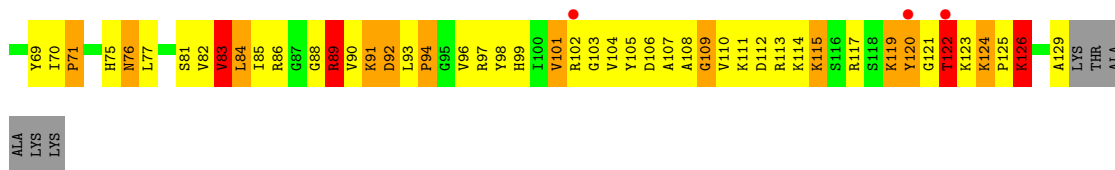


- Molecule 11: 30S RIBOSOMAL PROTEIN S11

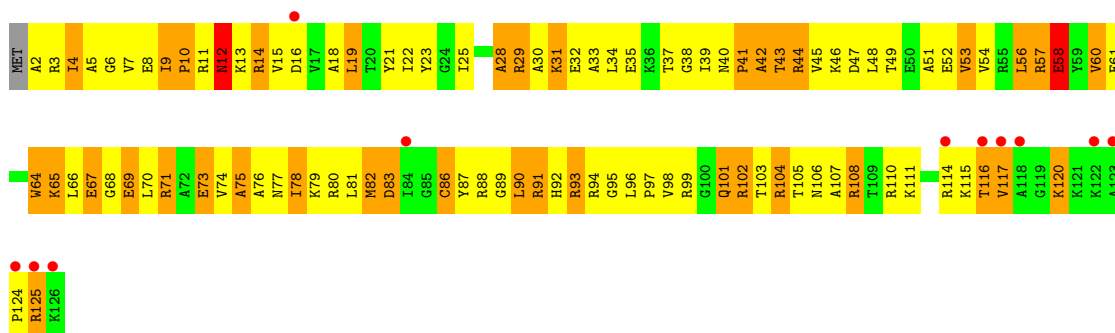
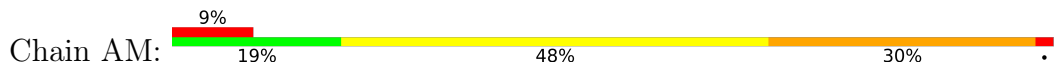


- Molecule 12: 30S RIBOSOMAL PROTEIN S12

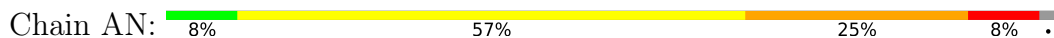




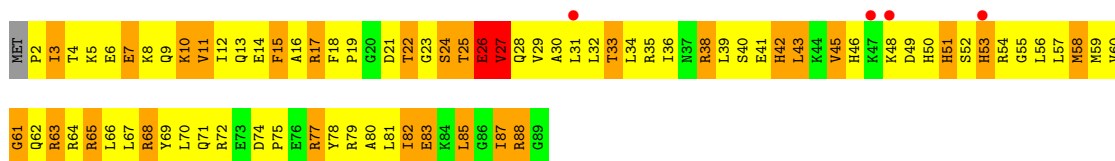
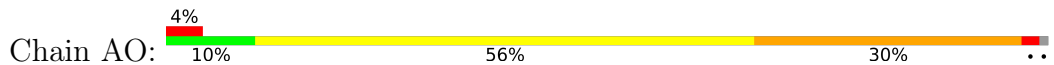
- Molecule 13: 30S RIBOSOMAL PROTEIN S13



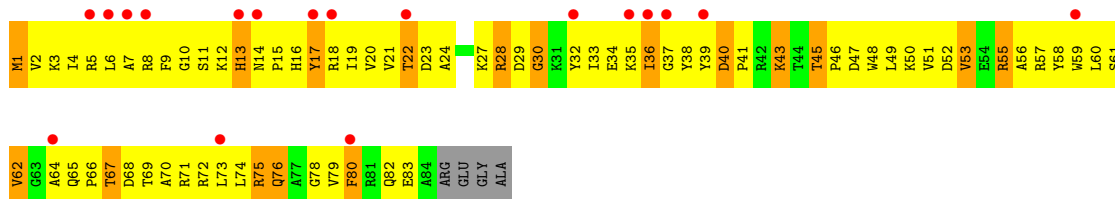
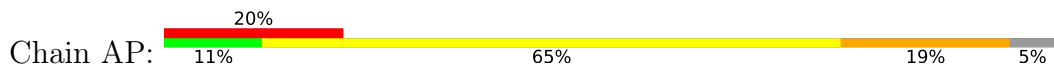
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



- Molecule 15: 30S RIBOSOMAL PROTEIN S15

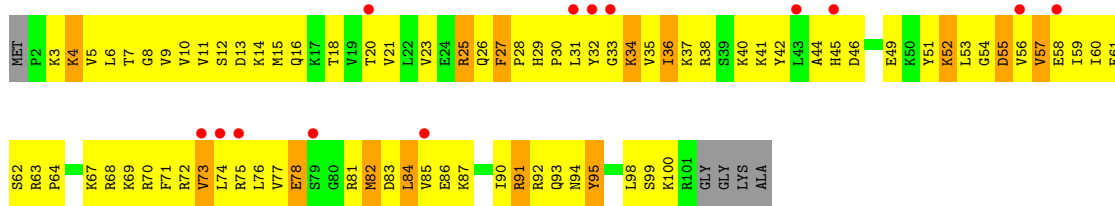


- Molecule 16: 30S RIBOSOMAL PROTEIN S16

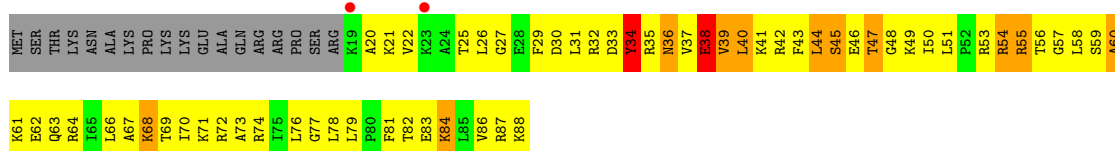
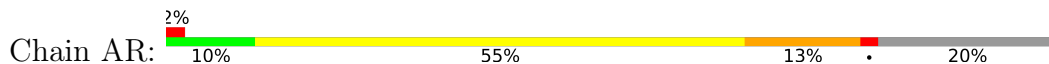


- Molecule 17: 30S RIBOSOMAL PROTEIN S17

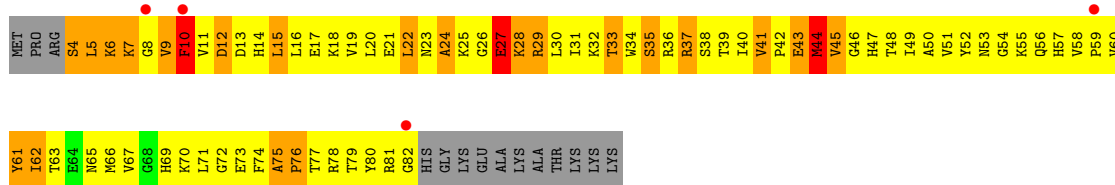




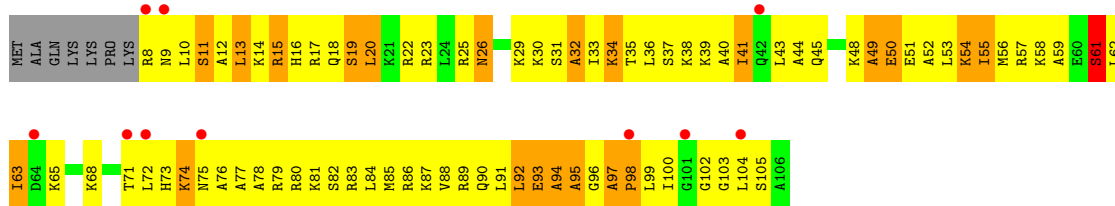
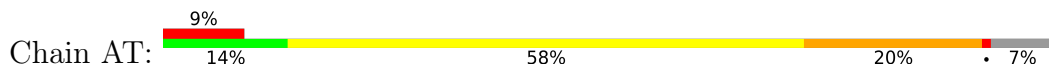
• Molecule 18: 30S RIBOSOMAL PROTEIN S18



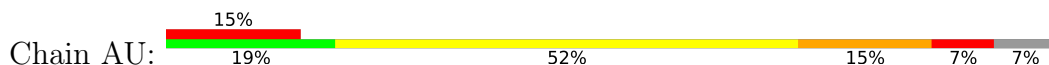
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

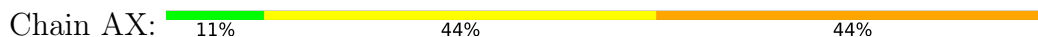


• Molecule 22: PE HYBRID STATE TRNA FMET

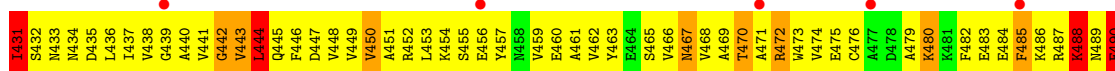
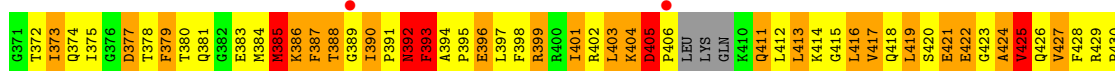
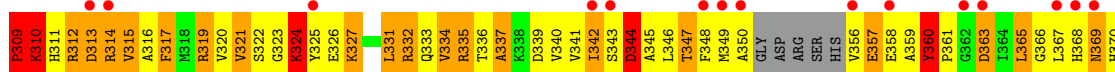
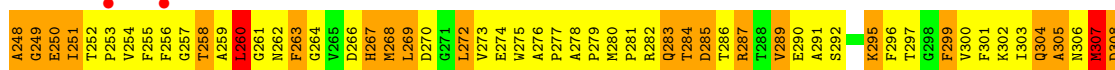
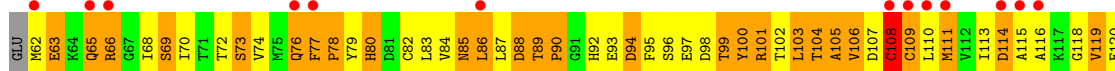
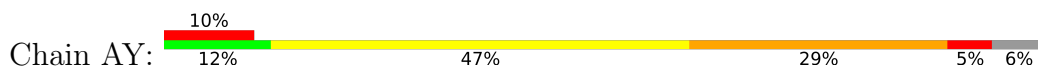




• Molecule 23: MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

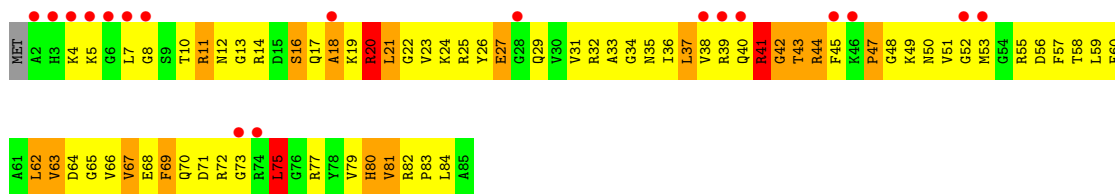


• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3

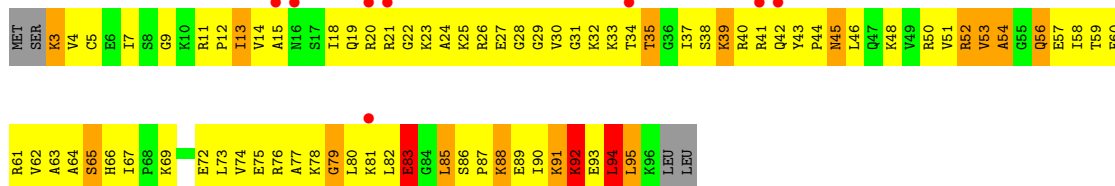


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

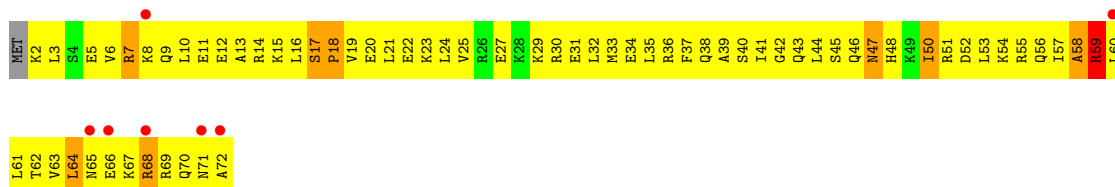




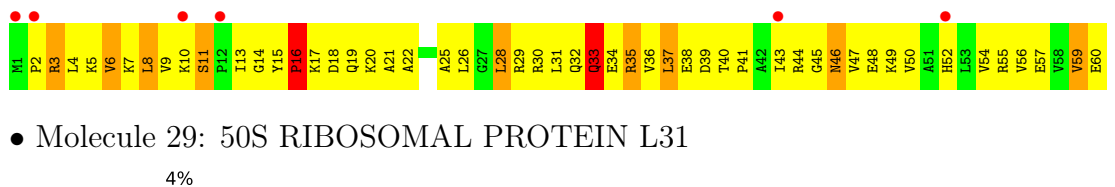
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



• Molecule 27: 50S RIBOSOMAL PROTEIN L29



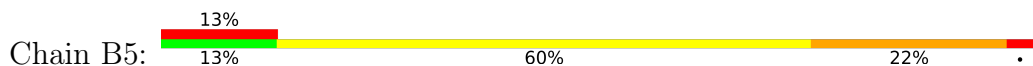
• Molecule 28: 50S RIBOSOMAL PROTEIN L30

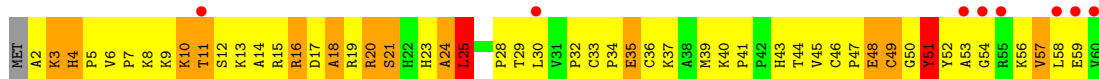


• Molecule 29: 50S RIBOSOMAL PROTEIN L31

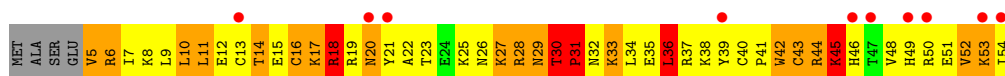


• Molecule 30: 50S RIBOSOMAL PROTEIN L32





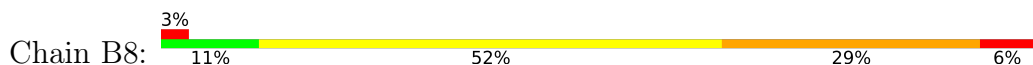
- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 32: 50S RIBOSOMAL PROTEIN L34



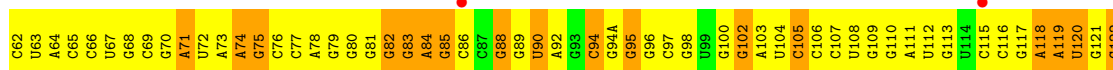
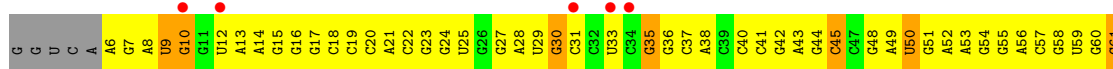
- Molecule 33: 50S RIBOSOMAL PROTEIN L35



- Molecule 34: 50S RIBOSOMAL PROTEIN L36

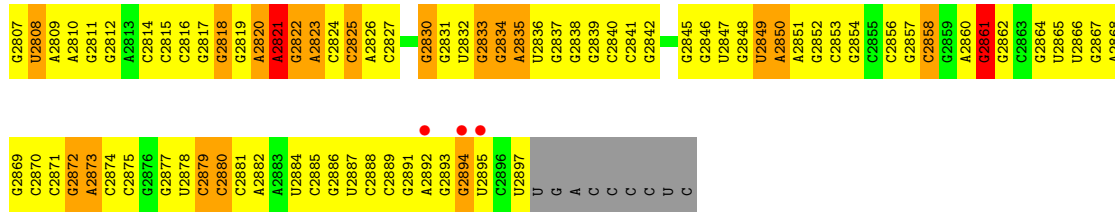


- Molecule 35: 23S RIBOSOMAL RNA

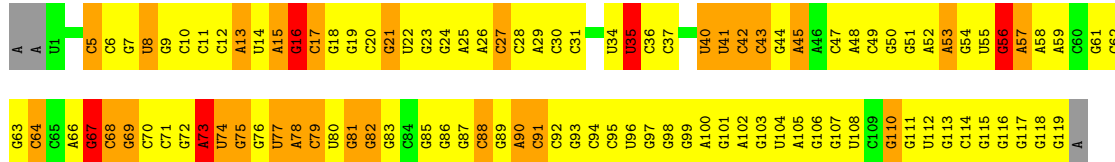
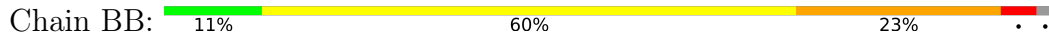


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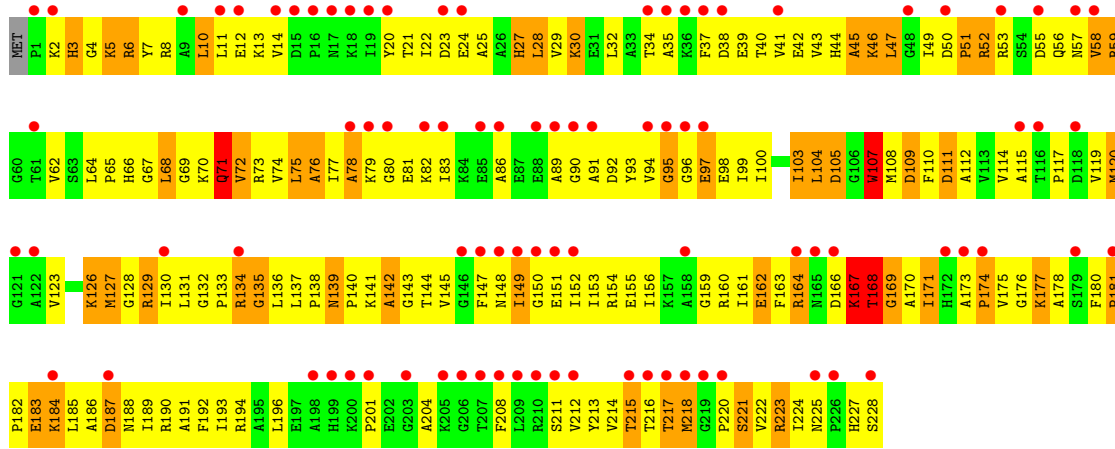
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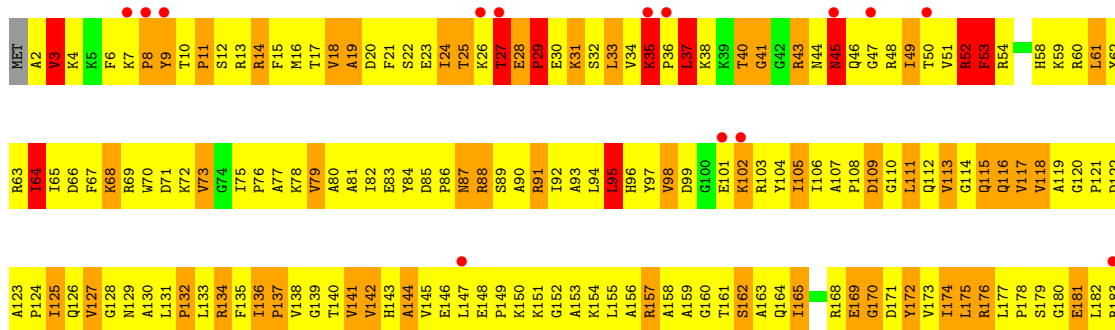
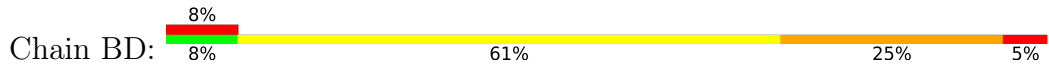
● Molecule 36: 5S RIBOSOMAL RNA

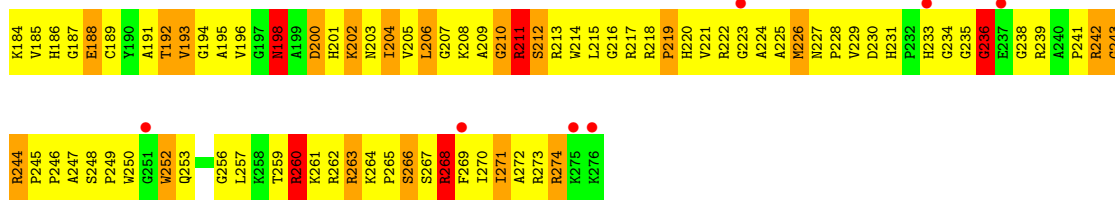


● Molecule 37: 50S RIBOSOMAL PROTEIN L1

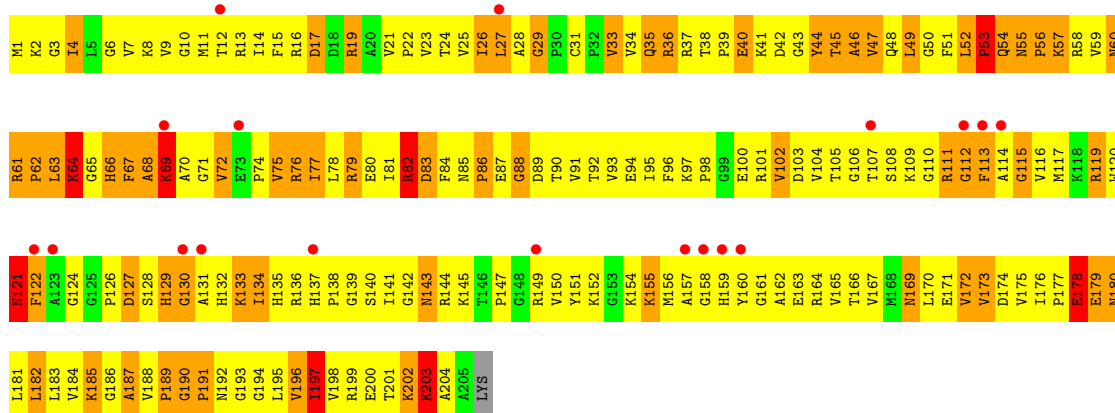
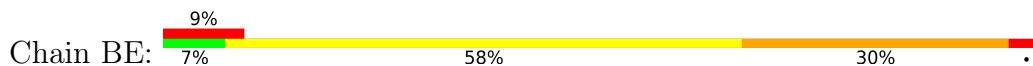


● Molecule 38: 50S RIBOSOMAL PROTEIN L2

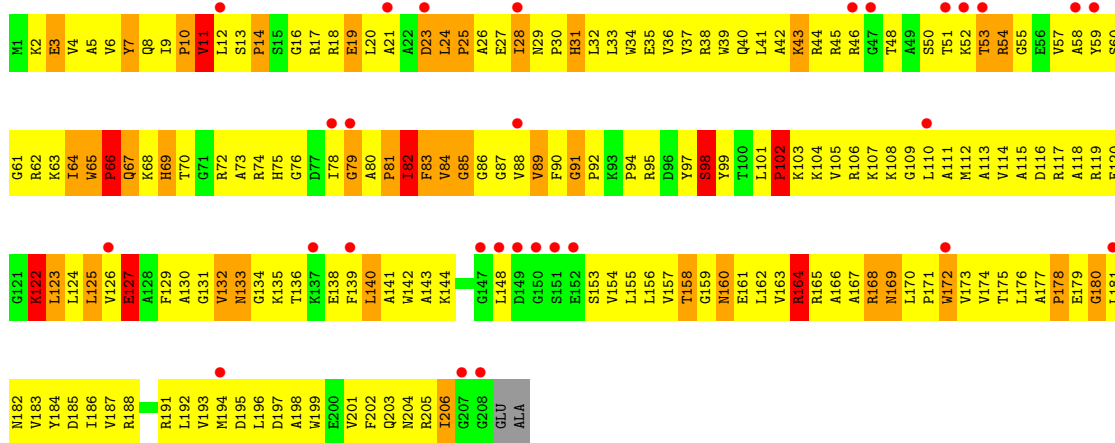
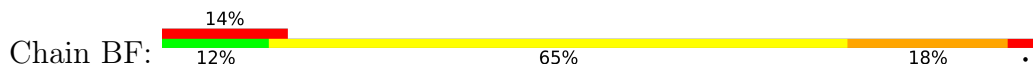




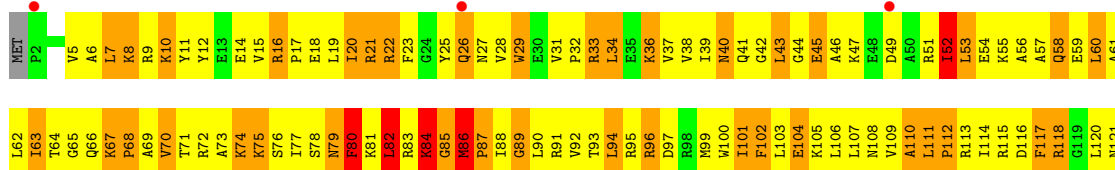
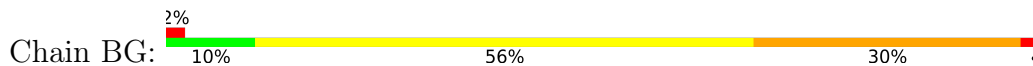
● Molecule 39: 50S RIBOSOMAL PROTEIN L3



● Molecule 40: 50S RIBOSOMAL PROTEIN L4

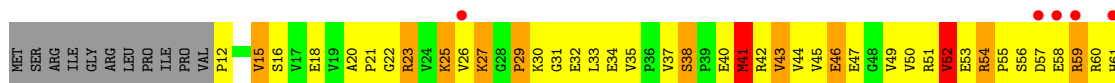
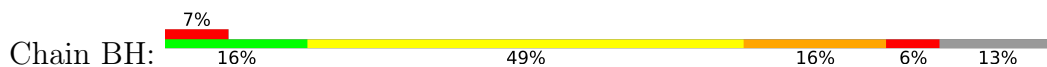


● Molecule 41: 50S RIBOSOMAL PROTEIN L5

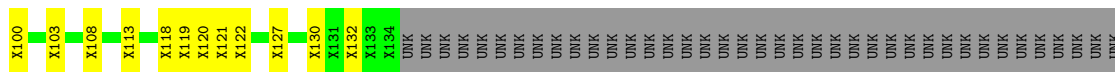
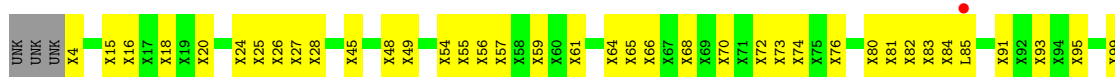




• Molecule 42: 50S RIBOSOMAL PROTEIN L6



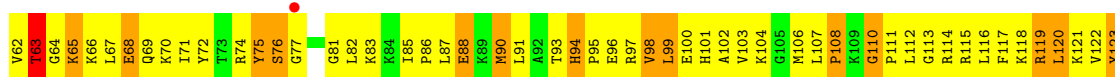
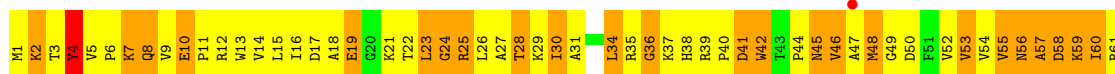
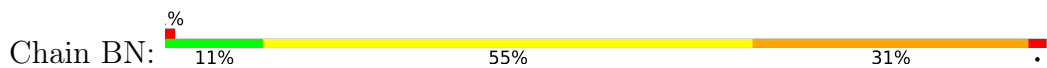
• Molecule 43: 50S RIBOSOMAL PROTEIN L10



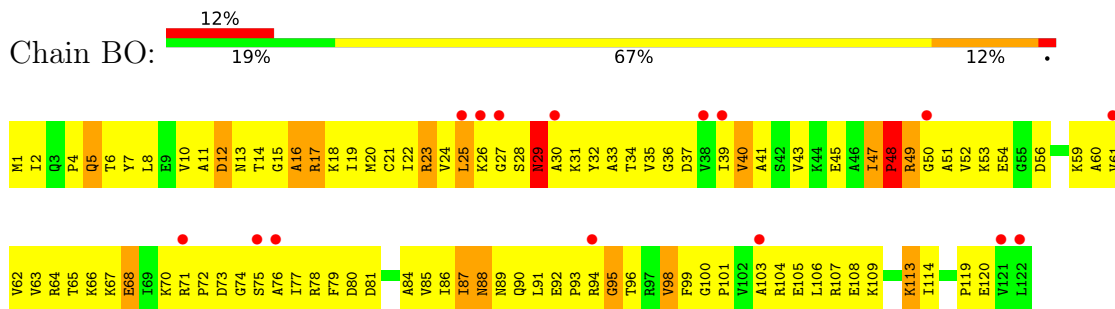
• Molecule 44: 50S RIBOSOMAL PROTEIN L11



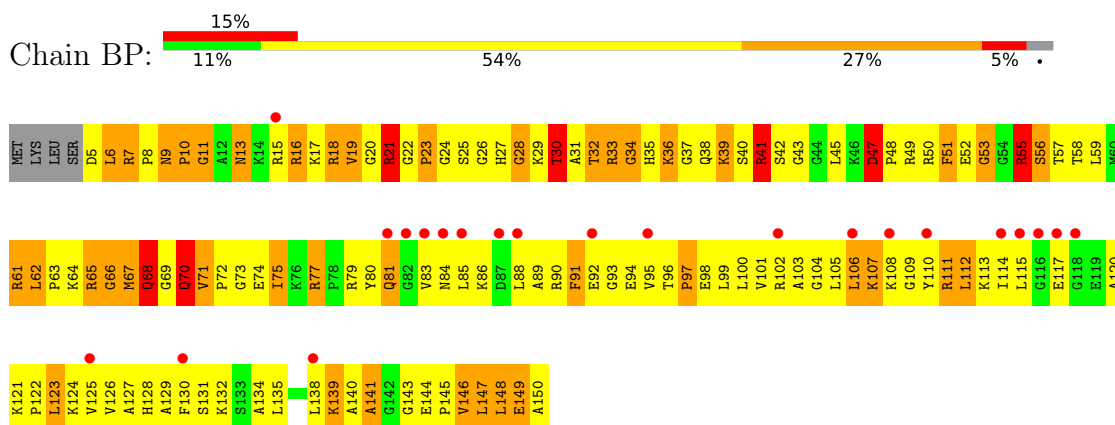
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



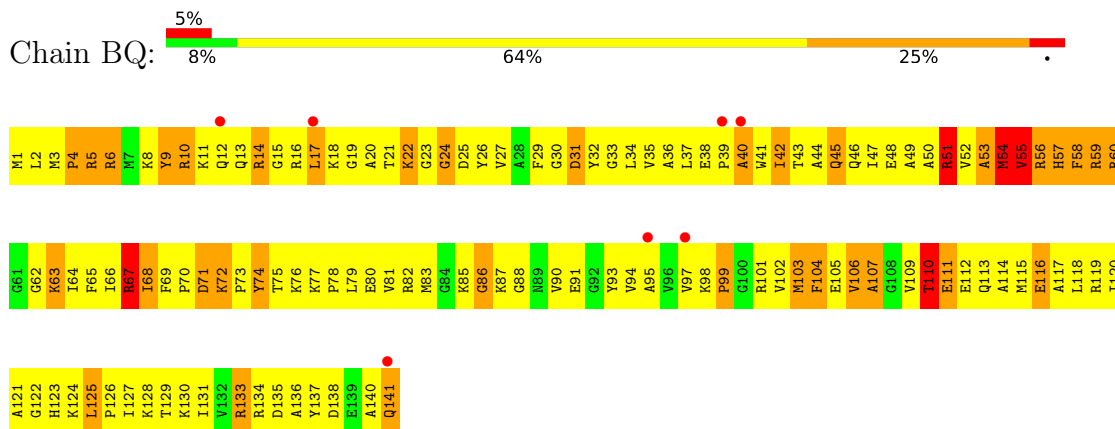
- Molecule 46: 50S RIBOSOMAL PROTEIN L14



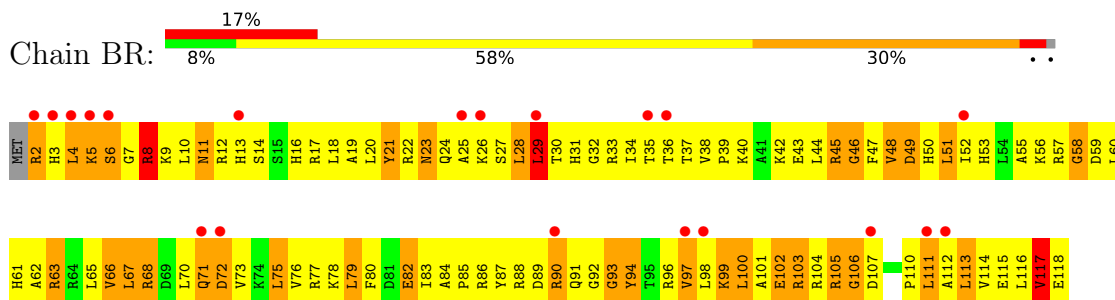
- Molecule 47: 50S RIBOSOMAL PROTEIN L15



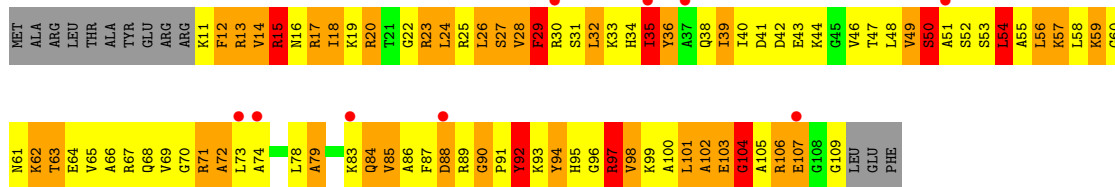
- Molecule 48: 50S RIBOSOMAL PROTEIN L16



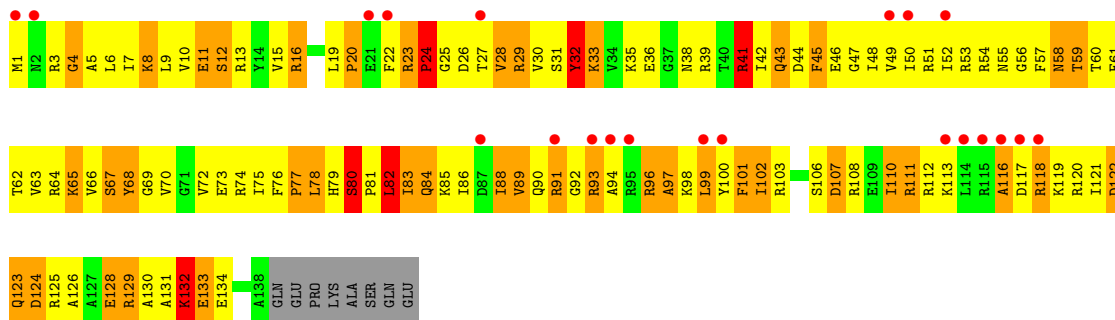
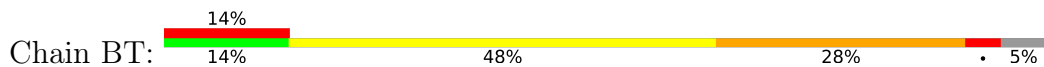
- Molecule 49: 50S RIBOSOMAL PROTEIN L17



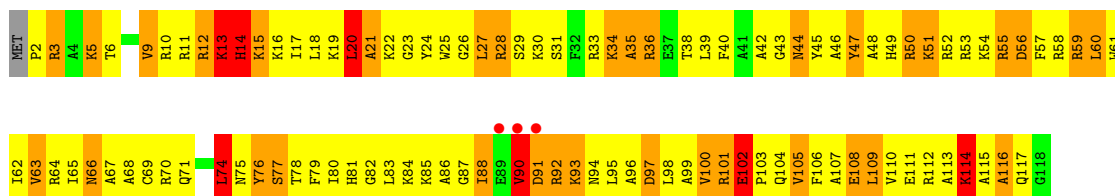
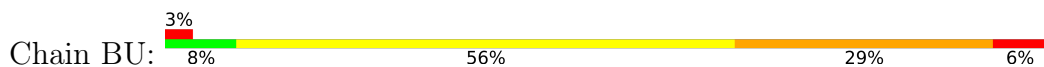
- Molecule 50: 50S RIBOSOMAL PROTEIN L18



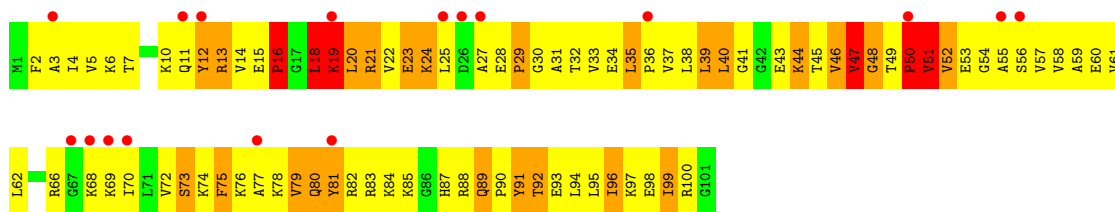
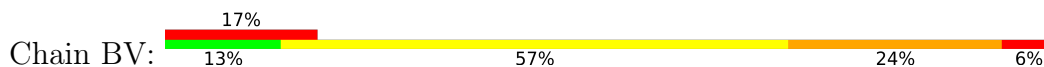
• Molecule 51: 50S RIBOSOMAL PROTEIN L19



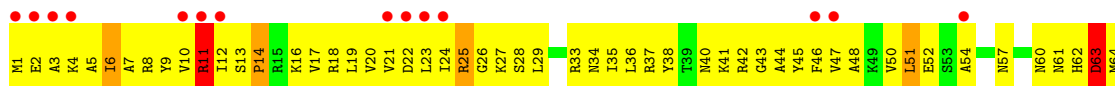
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

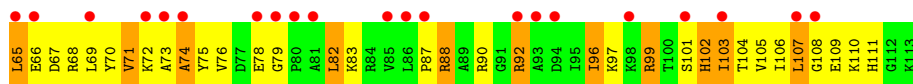


• Molecule 53: 50S RIBOSOMAL PROTEIN L21

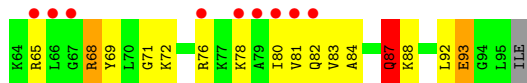
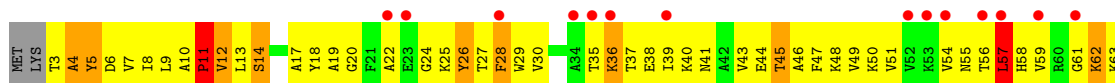


• Molecule 54: 50S RIBOSOMAL PROTEIN L22

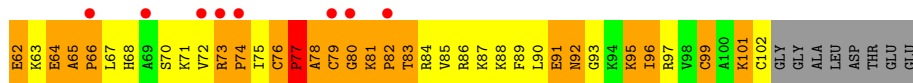
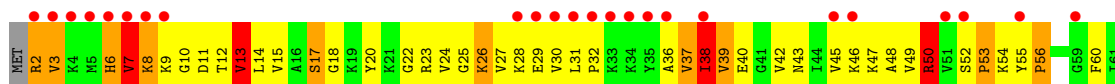
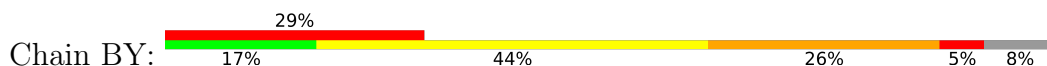




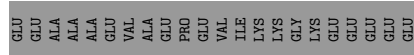
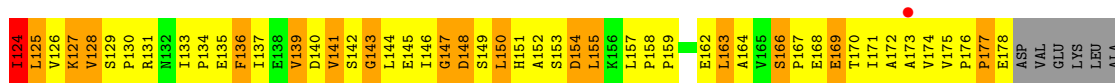
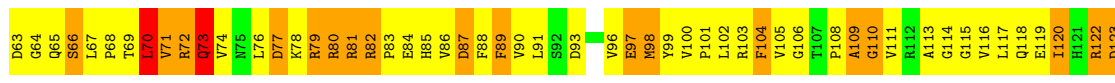
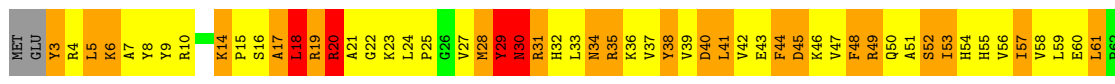
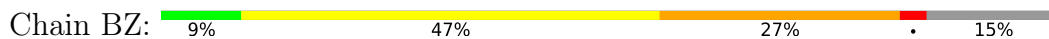
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 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	204.70Å 229.30Å 307.00Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	44.90 – 3.80 44.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.90-3.80) 96.6 (44.91-3.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.57Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.351 0.298 , 0.348	Depositor DCC
R_{free} test set	53888 reflections (2.37%)	wwPDB-VP
Wilson B-factor (Å ²)	110.2	Xtrriage
Anisotropy	0.390	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtrriage
Estimated twinning fraction	0.166 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	151017	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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 i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

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	0.79	12/36190 (0.0%)	0.89	56/56486 (0.1%)
2	AB	0.62	0/1936	0.96	1/2611 (0.0%)
3	AC	0.60	0/1637	0.93	3/2207 (0.1%)
4	AD	0.50	0/1733	0.86	2/2318 (0.1%)
5	AE	0.63	0/1163	0.94	1/1566 (0.1%)
6	AF	0.56	0/856	0.88	0/1154
7	AG	0.59	0/1276	0.85	0/1709
8	AH	0.56	0/1136	0.91	1/1527 (0.1%)
9	AI	0.56	0/1029	0.83	0/1378
10	AJ	0.59	0/808	0.88	0/1087
11	AK	0.57	0/900	0.89	0/1213
12	AL	0.59	0/987	1.01	2/1322 (0.2%)
13	AM	0.59	0/999	0.95	0/1338
14	AN	0.71	0/501	1.03	1/664 (0.2%)
15	AO	0.65	0/745	0.86	0/992
16	AP	0.53	0/717	0.88	0/965
17	AQ	0.61	0/837	0.92	1/1119 (0.1%)
18	AR	0.60	0/579	0.89	1/768 (0.1%)
19	AS	0.68	0/643	0.91	1/867 (0.1%)
20	AT	0.54	0/765	0.80	0/1007
21	AU	0.70	0/213	0.95	1/279 (0.4%)
22	AV	0.65	0/1832	0.82	0/2855
23	AX	0.66	0/216	0.77	0/335
24	AY	1.05	19/4005 (0.5%)	1.16	32/5407 (0.6%)
25	B0	0.61	0/671	0.98	2/892 (0.2%)
26	B1	0.49	0/739	0.85	0/983
27	B2	0.51	0/600	0.82	0/793
28	B3	0.57	0/473	0.93	0/636
29	B4	0.69	0/350	0.80	0/476
30	B5	0.64	0/473	0.89	0/639
31	B6	0.79	0/440	1.09	2/586 (0.3%)
32	B7	0.53	0/427	0.79	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.68	0/516	0.92	0/681
34	B9	0.53	0/310	0.85	0/407
35	BA	0.76	16/69976 (0.0%)	0.86	82/109244 (0.1%)
36	BB	0.76	1/2853 (0.0%)	0.89	5/4451 (0.1%)
37	BC	0.81	4/1775 (0.2%)	0.94	4/2392 (0.2%)
38	BD	0.69	0/2195	1.07	9/2955 (0.3%)
39	BE	0.59	0/1597	0.95	1/2155 (0.0%)
40	BF	0.61	0/1659	0.88	0/2246
41	BG	0.58	0/1499	0.92	3/2016 (0.1%)
42	BH	0.66	0/1211	0.88	0/1636
43	BJ	0.53	0/7	0.70	0/8
45	BN	0.57	0/1132	0.91	1/1527 (0.1%)
46	BO	0.60	0/943	0.90	0/1269
47	BP	0.57	0/1131	1.08	6/1504 (0.4%)
48	BQ	0.63	0/1143	1.00	3/1527 (0.2%)
49	BR	0.49	0/974	0.92	1/1302 (0.1%)
50	BS	0.66	0/779	1.12	6/1038 (0.6%)
51	BT	0.60	0/1156	0.92	3/1544 (0.2%)
52	BU	0.63	0/975	0.91	1/1297 (0.1%)
53	BV	0.54	0/790	0.97	2/1057 (0.2%)
54	BW	0.59	0/907	0.82	0/1216
55	BX	0.63	0/740	0.83	1/995 (0.1%)
56	BY	0.61	0/789	0.90	0/1053
57	BZ	0.62	0/1435	0.95	0/1949
All	All	0.73	52/162368 (0.0%)	0.89	235/242211 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	3	125
9	AI	0	1
11	AK	0	1
17	AQ	0	1
21	AU	0	1
22	AV	0	5
24	AY	0	5
30	B5	0	1
35	BA	3	160
36	BB	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	BH	0	1
45	BN	0	1
48	BQ	0	1
53	BV	0	1
All	All	6	316

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	191	TYR	CE2-CZ	11.85	1.53	1.38
24	AY	189	GLU	CG-CD	-10.57	1.36	1.51
24	AY	191	TYR	CD1-CE1	10.46	1.55	1.39
24	AY	504	ILE	C-N	-9.62	1.11	1.34
24	AY	444	LEU	C-N	-9.54	1.12	1.34

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	191	TYR	CB-CG-CD1	-18.01	110.19	121.00
24	AY	307	MET	CG-SD-CE	13.35	121.55	100.20
24	AY	319	ARG	NE-CZ-NH1	12.45	126.52	120.30
24	AY	504	ILE	C-N-CA	-12.18	91.26	121.70
1	AA	1498	U	C2'-C3'-O3'	11.78	135.42	109.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1049	U	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'

5 of 316 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	19	C	Sidechain
1	AA	28	G	Sidechain
1	AA	96	U	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	2580	0
2	AB	1901	0	1951	513	1
3	AC	1613	0	1677	306	0
4	AD	1703	0	1767	335	0
5	AE	1147	0	1207	231	0
6	AF	843	0	857	144	0
7	AG	1257	0	1296	177	0
8	AH	1116	0	1177	205	0
9	AI	1011	0	1043	205	0
10	AJ	795	0	840	196	0
11	AK	885	0	904	152	0
12	AL	971	0	1057	217	0
13	AM	988	0	1059	192	0
14	AN	492	0	533	153	0
15	AO	734	0	771	229	0
16	AP	701	0	720	131	0
17	AQ	824	0	891	158	0
18	AR	574	0	644	122	0
19	AS	630	0	652	209	0
20	AT	763	0	861	150	0
21	AU	209	0	221	48	0
22	AV	1640	0	837	195	0
23	AX	192	0	99	22	0
24	AY	3934	0	3922	1256	0
25	B0	662	0	688	138	0
26	B1	732	0	808	131	0
27	B2	598	0	653	126	0
28	B3	468	0	523	108	0
29	B4	341	0	339	89	0
30	B5	459	0	480	131	0
31	B6	433	0	461	109	0
32	B7	419	0	467	110	0
33	B8	508	0	576	154	0
34	B9	307	0	338	70	0
35	BA	62477	0	31497	5283	0
36	BB	2551	0	1295	229	0
37	BC	1742	0	1794	377	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BD	2145	0	2234	780	0
39	BE	1564	0	1629	448	0
40	BF	1624	0	1677	415	0
41	BG	1474	0	1535	340	0
42	BH	1189	0	1247	282	0
43	BJ	654	0	157	36	0
44	BK	701	0	168	41	0
45	BN	1105	0	1180	270	0
46	BO	933	0	996	182	0
47	BP	1114	0	1187	361	0
48	BQ	1122	0	1179	291	0
49	BR	960	0	1021	236	0
50	BS	771	0	832	206	0
51	BT	1142	0	1202	332	0
52	BU	958	0	1015	317	0
53	BV	779	0	852	219	0
54	BW	896	0	953	173	0
55	BX	726	0	778	114	0
56	BY	776	0	870	193	0
57	BZ	1403	0	1432	371	0
58	AY	32	0	14	11	0
All	All	151017	0	103381	18971	1

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 75.

The worst 5 of 18971 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)
24:AY:111:MET:CE	24:AY:139:THR:HG23	1.18	1.62
24:AY:331:LEU:CD2	24:AY:379:PHE:HD2	1.19	1.51
24:AY:331:LEU:HD22	24:AY:379:PHE:CD2	1.46	1.47
37:BC:127:MET:SD	37:BC:127:MET:CG	2.03	1.45
24:AY:135:THR:CG2	24:AY:136:PRO:HD2	1.44	1.45

All (1) 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:62:ALA:O	37:BC:30:LYS:O[2_656]	2.18	0.02

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	110 (47%)	62 (27%)	61 (26%)	0	1
3	AC	205/239 (86%)	134 (65%)	39 (19%)	32 (16%)	0	4
4	AD	206/209 (99%)	131 (64%)	51 (25%)	24 (12%)	0	6
5	AE	149/162 (92%)	108 (72%)	31 (21%)	10 (7%)	1	19
6	AF	99/101 (98%)	67 (68%)	24 (24%)	8 (8%)	1	14
7	AG	153/156 (98%)	85 (56%)	44 (29%)	24 (16%)	0	3
8	AH	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	6
9	AI	125/128 (98%)	78 (62%)	28 (22%)	19 (15%)	0	4
10	AJ	97/105 (92%)	60 (62%)	23 (24%)	14 (14%)	0	4
11	AK	117/129 (91%)	72 (62%)	32 (27%)	13 (11%)	0	7
12	AL	123/135 (91%)	66 (54%)	33 (27%)	24 (20%)	0	2
13	AM	123/126 (98%)	63 (51%)	31 (25%)	29 (24%)	0	1
14	AN	58/61 (95%)	33 (57%)	12 (21%)	13 (22%)	0	1
15	AO	86/89 (97%)	59 (69%)	21 (24%)	6 (7%)	1	17
16	AP	82/88 (93%)	55 (67%)	17 (21%)	10 (12%)	0	6
17	AQ	98/105 (93%)	82 (84%)	10 (10%)	6 (6%)	1	20
18	AR	68/88 (77%)	37 (54%)	18 (26%)	13 (19%)	0	2
19	AS	77/93 (83%)	42 (54%)	18 (23%)	17 (22%)	0	1
20	AT	97/106 (92%)	46 (47%)	32 (33%)	19 (20%)	0	2
21	AU	23/27 (85%)	11 (48%)	8 (35%)	4 (17%)	0	3
24	AY	488/529 (92%)	314 (64%)	88 (18%)	86 (18%)	0	2
25	B0	82/85 (96%)	64 (78%)	9 (11%)	9 (11%)	0	8
26	B1	92/98 (94%)	63 (68%)	16 (17%)	13 (14%)	0	4
27	B2	69/72 (96%)	38 (55%)	22 (32%)	9 (13%)	0	5
28	B3	58/60 (97%)	38 (66%)	15 (26%)	5 (9%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	B4	43/71 (61%)	26 (60%)	9 (21%)	8 (19%)	0	2
30	B5	57/60 (95%)	34 (60%)	11 (19%)	12 (21%)	0	1
31	B6	48/54 (89%)	18 (38%)	16 (33%)	14 (29%)	0	0
32	B7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0	3
33	B8	62/65 (95%)	30 (48%)	16 (26%)	16 (26%)	0	1
34	B9	35/37 (95%)	19 (54%)	10 (29%)	6 (17%)	0	3
37	BC	226/229 (99%)	158 (70%)	39 (17%)	29 (13%)	0	5
38	BD	273/276 (99%)	195 (71%)	46 (17%)	32 (12%)	0	6
39	BE	203/206 (98%)	99 (49%)	48 (24%)	56 (28%)	0	0
40	BF	206/210 (98%)	134 (65%)	35 (17%)	37 (18%)	0	2
41	BG	179/182 (98%)	95 (53%)	47 (26%)	37 (21%)	0	2
42	BH	154/180 (86%)	111 (72%)	23 (15%)	20 (13%)	0	5
43	BJ	1/173 (1%)	1 (100%)	0	0	100	100
45	BN	137/140 (98%)	78 (57%)	28 (20%)	31 (23%)	0	1
46	BO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	8
47	BP	144/150 (96%)	70 (49%)	37 (26%)	37 (26%)	0	1
48	BQ	139/141 (99%)	79 (57%)	40 (29%)	20 (14%)	0	4
49	BR	115/118 (98%)	69 (60%)	27 (24%)	19 (16%)	0	3
50	BS	97/112 (87%)	41 (42%)	23 (24%)	33 (34%)	0	0
51	BT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0	1
52	BU	115/118 (98%)	59 (51%)	27 (24%)	29 (25%)	0	1
53	BV	99/101 (98%)	56 (57%)	21 (21%)	22 (22%)	0	1
54	BW	111/113 (98%)	72 (65%)	25 (22%)	14 (13%)	0	5
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	0	10
56	BY	99/110 (90%)	33 (33%)	36 (36%)	30 (30%)	0	0
57	BZ	174/206 (84%)	88 (51%)	48 (28%)	38 (22%)	0	1
All	All	6255/6850 (91%)	3758 (60%)	1413 (23%)	1084 (17%)	0	3

5 of 1084 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL

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Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	19	HIS
2	AB	24	TRP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	AB	202/220 (92%)	152 (75%)	50 (25%)	0 5
3	AC	160/188 (85%)	133 (83%)	27 (17%)	2 14
4	AD	180/181 (99%)	154 (86%)	26 (14%)	3 20
5	AE	115/123 (94%)	94 (82%)	21 (18%)	1 11
6	AF	90/90 (100%)	76 (84%)	14 (16%)	2 17
7	AG	126/127 (99%)	114 (90%)	12 (10%)	8 34
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3 18
9	AI	98/99 (99%)	82 (84%)	16 (16%)	2 15
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	1 10
11	AK	90/99 (91%)	73 (81%)	17 (19%)	1 10
12	AL	104/111 (94%)	86 (83%)	18 (17%)	2 13
13	AM	99/101 (98%)	79 (80%)	20 (20%)	1 9
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0 3
15	AO	79/80 (99%)	52 (66%)	27 (34%)	0 1
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6 29
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	8 34
18	AR	61/77 (79%)	54 (88%)	7 (12%)	5 27
19	AS	69/80 (86%)	58 (84%)	11 (16%)	2 16
20	AT	76/82 (93%)	69 (91%)	7 (9%)	9 35
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7 30
24	AY	427/453 (94%)	308 (72%)	119 (28%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	B0	66/67 (98%)	49 (74%)	17 (26%)	0	4
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	15
27	B2	66/67 (98%)	61 (92%)	5 (8%)	13	43
28	B3	51/52 (98%)	42 (82%)	9 (18%)	2	13
29	B4	39/63 (62%)	29 (74%)	10 (26%)	0	4
30	B5	51/52 (98%)	47 (92%)	4 (8%)	12	42
31	B6	49/52 (94%)	37 (76%)	12 (24%)	0	5
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5	25
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1	8
34	B9	34/34 (100%)	26 (76%)	8 (24%)	1	5
37	BC	180/181 (99%)	150 (83%)	30 (17%)	2	15
38	BD	217/218 (100%)	150 (69%)	67 (31%)	0	2
39	BE	165/166 (99%)	134 (81%)	31 (19%)	1	10
40	BF	165/166 (99%)	142 (86%)	23 (14%)	3	21
41	BG	155/156 (99%)	127 (82%)	28 (18%)	1	12
42	BH	128/148 (86%)	90 (70%)	38 (30%)	0	2
43	BJ	1/1 (100%)	1 (100%)	0	100	100
45	BN	117/119 (98%)	99 (85%)	18 (15%)	2	17
46	BO	100/100 (100%)	89 (89%)	11 (11%)	6	29
47	BP	112/116 (97%)	91 (81%)	21 (19%)	1	10
48	BQ	111/111 (100%)	87 (78%)	24 (22%)	1	7
49	BR	100/101 (99%)	78 (78%)	22 (22%)	1	7
50	BS	77/88 (88%)	60 (78%)	17 (22%)	1	6
51	BT	120/127 (94%)	96 (80%)	24 (20%)	1	9
52	BU	92/94 (98%)	74 (80%)	18 (20%)	1	9
53	BV	82/82 (100%)	65 (79%)	17 (21%)	1	8
54	BW	91/92 (99%)	81 (89%)	10 (11%)	6	29
55	BX	74/78 (95%)	63 (85%)	11 (15%)	3	18
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2	12
57	BZ	155/179 (87%)	117 (76%)	38 (24%)	0	5
All	All	5271/5546 (95%)	4255 (81%)	1016 (19%)	1	10

5 of 1016 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	B0	27	GLU
51	BT	24	PRO
37	BC	162	GLU
50	BS	56	LEU
54	BW	82	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 184 such sidechains are listed below:

Mol	Chain	Res	Type
38	BD	166	GLN
46	BO	5	GLN
39	BE	48	GLN
40	BF	169	ASN
48	BQ	46	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	273 (18%)	58 (3%)
22	AV	76/77 (98%)	36 (47%)	3 (3%)
23	AX	8/9 (88%)	5 (62%)	0
35	BA	2900/2915 (99%)	654 (22%)	73 (2%)
36	BB	118/122 (96%)	24 (20%)	1 (0%)
All	All	4605/4645 (99%)	992 (21%)	135 (2%)

5 of 992 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 135 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	1996	C
35	BA	2126	A

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Mol	Chain	Res	Type
35	BA	2689	U
1	AA	1285	A
1	AA	1283	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
58	GCP	AY	1000	-	27,34,34	2.58	7 (25%)	34,54,54	2.04	10 (29%)

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
58	GCP	AY	1000	-	-	10/15/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	C6-N1	8.37	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PB-O3A	5.84	1.64	1.58
58	AY	1000	GCP	C2-N1	4.88	1.44	1.35
58	AY	1000	GCP	C4-N3	4.57	1.42	1.35
58	AY	1000	GCP	PG-O2G	-2.81	1.48	1.54

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	1000	GCP	C5-C6-N1	-6.21	114.93	123.43
58	AY	1000	GCP	C2-N1-C6	4.62	123.27	115.93
58	AY	1000	GCP	N3-C2-N1	-4.35	121.42	127.22
58	AY	1000	GCP	O3G-PG-O1G	-2.67	105.32	112.39
58	AY	1000	GCP	O3G-PG-O2G	2.66	115.84	108.08

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

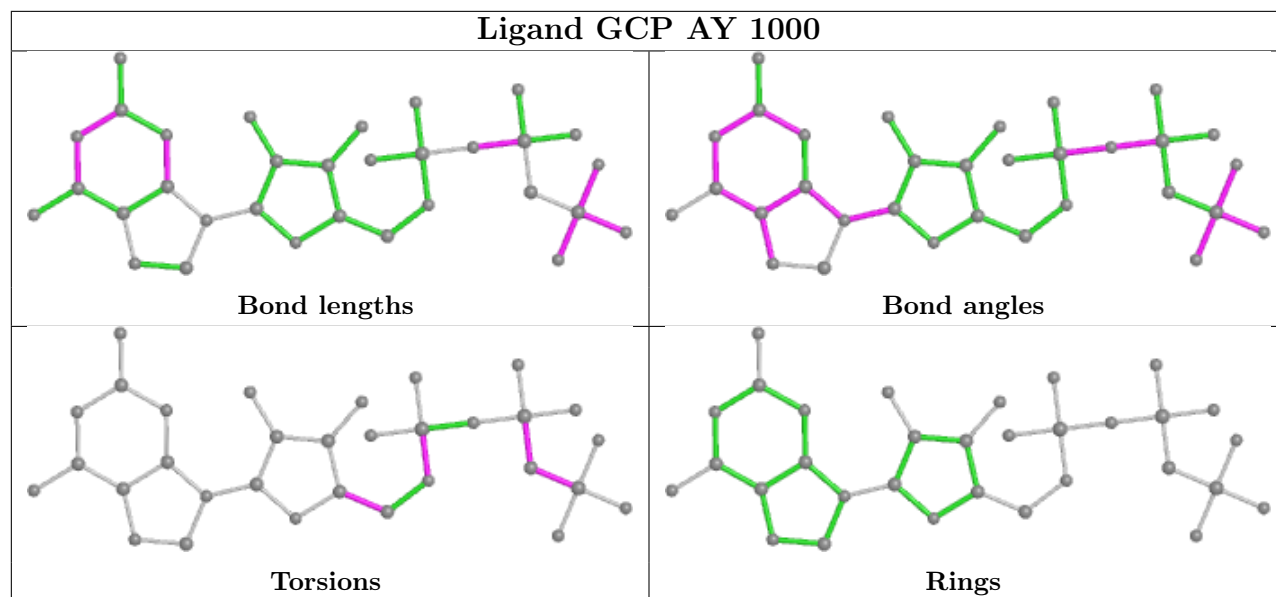
Mol	Chain	Res	Type	Atoms
58	AY	1000	GCP	PB-C3B-PG-O1G
58	AY	1000	GCP	PB-C3B-PG-O2G
58	AY	1000	GCP	PG-C3B-PB-O1B
58	AY	1000	GCP	PG-C3B-PB-O3A
58	AY	1000	GCP	C5'-O5'-PA-O3A

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AY	1000	GCP	11	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	AY	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AY	444:LEU	C	445:GLN	N	1.12
1	AY	504:ILE	C	505:ALA	N	1.11

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.14	37 (2%) 57 49	52, 140, 199, 200	0
2	AB	235/256 (91%)	-0.44	2 (0%) 84 79	40, 110, 177, 200	0
3	AC	207/239 (86%)	-0.49	2 (0%) 82 76	37, 117, 174, 200	0
4	AD	208/209 (99%)	0.22	13 (6%) 20 15	48, 158, 200, 200	0
5	AE	151/162 (93%)	-0.18	3 (1%) 65 58	38, 112, 171, 200	0
6	AF	101/101 (100%)	-0.60	0 100 100	59, 135, 188, 200	0
7	AG	155/156 (99%)	-0.37	3 (1%) 66 59	46, 128, 189, 200	0
8	AH	138/138 (100%)	-0.10	6 (4%) 35 30	36, 114, 180, 200	0
9	AI	127/128 (99%)	-0.12	2 (1%) 72 64	32, 121, 172, 200	0
10	AJ	99/105 (94%)	0.40	10 (10%) 7 6	32, 125, 191, 200	0
11	AK	119/129 (92%)	-0.10	5 (4%) 36 30	40, 116, 179, 200	0
12	AL	125/135 (92%)	0.24	5 (4%) 38 32	45, 119, 192, 200	0
13	AM	125/126 (99%)	0.29	11 (8%) 10 8	64, 127, 200, 200	0
14	AN	60/61 (98%)	-0.28	0 100 100	28, 104, 172, 200	0
15	AO	88/89 (98%)	0.04	4 (4%) 33 28	59, 130, 188, 200	0
16	AP	84/88 (95%)	1.03	18 (21%) 0 1	79, 156, 200, 200	0
17	AQ	100/105 (95%)	0.70	13 (13%) 3 4	66, 141, 200, 200	0
18	AR	70/88 (79%)	-0.01	2 (2%) 51 42	59, 124, 176, 200	0
19	AS	79/93 (84%)	0.13	4 (5%) 28 24	57, 118, 197, 200	0
20	AT	99/106 (93%)	0.55	10 (10%) 7 6	87, 153, 200, 200	0
21	AU	25/27 (92%)	0.70	4 (16%) 1 2	46, 117, 175, 185	0
22	AV	77/77 (100%)	-0.68	1 (1%) 77 70	77, 151, 189, 199	0
23	AX	9/9 (100%)	0.18	0 100 100	79, 156, 192, 199	0
24	AY	496/529 (93%)	0.42	51 (10%) 6 6	71, 170, 202, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B0	84/85 (98%)	1.13	18 (21%) 0 1	37, 118, 194, 200	0
26	B1	94/98 (95%)	0.59	8 (8%) 10 9	65, 143, 197, 200	0
27	B2	71/72 (98%)	0.13	7 (9%) 7 6	101, 153, 200, 200	0
28	B3	60/60 (100%)	0.68	6 (10%) 7 6	54, 126, 198, 200	0
29	B4	45/71 (63%)	-0.05	3 (6%) 17 14	108, 174, 200, 200	0
30	B5	59/60 (98%)	0.40	8 (13%) 3 3	62, 150, 200, 200	0
31	B6	50/54 (92%)	0.79	10 (20%) 1 1	62, 139, 186, 200	0
32	B7	49/49 (100%)	0.56	5 (10%) 6 6	78, 153, 197, 200	0
33	B8	64/65 (98%)	0.13	2 (3%) 49 40	66, 129, 179, 200	0
34	B9	37/37 (100%)	1.39	11 (29%) 0 0	71, 142, 178, 194	0
35	BA	2901/2915 (99%)	0.09	112 (3%) 39 32	51, 159, 201, 202	0
36	BB	119/122 (97%)	-0.48	0 100 100	66, 123, 172, 190	0
37	BC	228/229 (99%)	2.01	89 (39%) 0 0	87, 182, 200, 200	0
38	BD	275/276 (99%)	0.15	21 (7%) 13 11	40, 117, 175, 200	0
39	BE	205/206 (99%)	0.19	18 (8%) 10 8	51, 143, 199, 200	0
40	BF	208/210 (99%)	0.51	29 (13%) 2 3	51, 156, 200, 200	0
41	BG	181/182 (99%)	-0.08	4 (2%) 62 54	47, 134, 194, 200	0
42	BH	156/180 (86%)	0.30	12 (7%) 13 11	78, 165, 200, 200	0
43	BJ	1/173 (0%)	3.32	1 (100%) 0 0	174, 174, 174, 174	0
44	BK	0/147	-	-	-	-
45	BN	139/140 (99%)	0.01	2 (1%) 75 68	69, 131, 190, 200	0
46	BO	122/122 (100%)	0.47	15 (12%) 4 4	59, 133, 198, 200	0
47	BP	146/150 (97%)	0.86	22 (15%) 2 2	65, 147, 200, 200	0
48	BQ	141/141 (100%)	0.05	7 (4%) 28 25	20, 107, 171, 200	0
49	BR	117/118 (99%)	0.80	20 (17%) 1 1	81, 169, 200, 200	0
50	BS	99/112 (88%)	0.05	9 (9%) 9 7	49, 123, 194, 200	0
51	BT	138/146 (94%)	0.51	21 (15%) 2 2	89, 162, 200, 200	0
52	BU	117/118 (99%)	-0.05	3 (2%) 56 47	47, 121, 179, 200	0
53	BV	101/101 (100%)	0.82	17 (16%) 1 2	42, 146, 200, 200	0
54	BW	113/113 (100%)	1.30	35 (30%) 0 0	78, 165, 200, 200	0
55	BX	93/96 (96%)	1.10	23 (24%) 0 0	38, 167, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BY	101/110 (91%)	1.53	32 (31%) 0 0	86, 169, 200, 200	0
57	BZ	176/206 (85%)	-0.29	1 (0%) 89 85	43, 122, 195, 200	0
All	All	10971/11642 (94%)	0.18	777 (7%) 16 12	20, 146, 200, 202	0

The worst 5 of 777 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BC	165	ASN	14.2
37	BC	173	ALA	12.2
37	BC	216	THR	11.9
28	B3	1	MET	11.0
24	AY	349	MET	10.9

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

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

6.3 Carbohydrates [i](#)

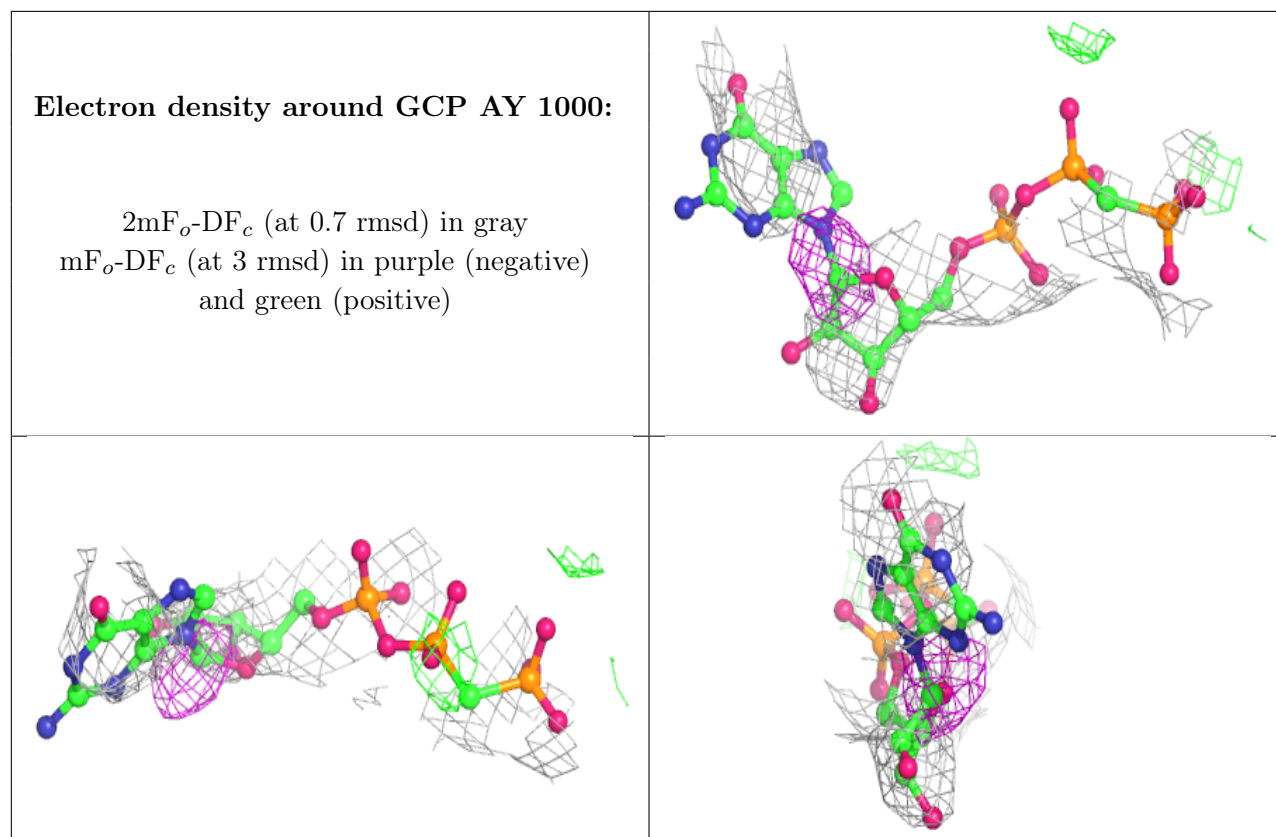
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
58	GCP	AY	1000	32/32	0.82	0.24	95,109,121,122	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.