



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 23, 2019 – 03:34 PM EDT

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

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

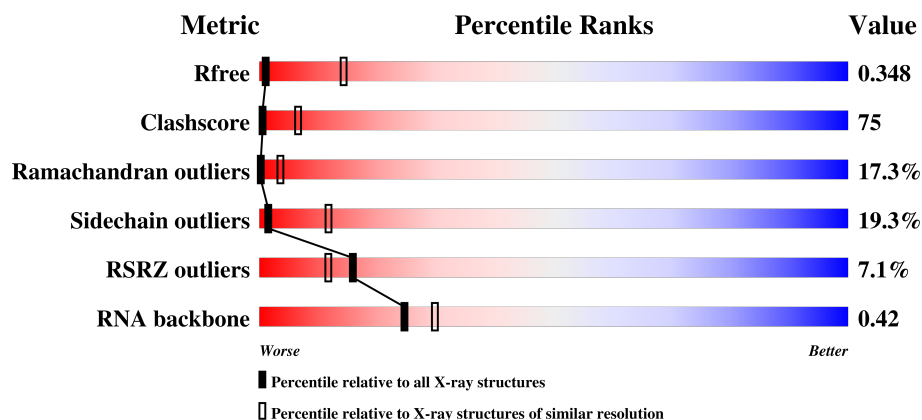
1 Overall quality at a glance

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}	111664	1028 (4.02-3.58)
Clashscore	122126	1061 (4.00-3.60)
Ramachandran outliers	120053	1025 (4.00-3.60)
Sidechain outliers	120020	1019 (4.00-3.60)
RSRZ outliers	108989	1021 (4.06-3.54)
RNA backbone	2636	1083 (4.70-2.90)

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. 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

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
1	AA	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			

- 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			

- 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			

- 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			

- 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			

- 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			

- 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			

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

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

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
10	AJ	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			

- 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			

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
13	AM	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			

- 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			

- 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			

- 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			

- 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				

- 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
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

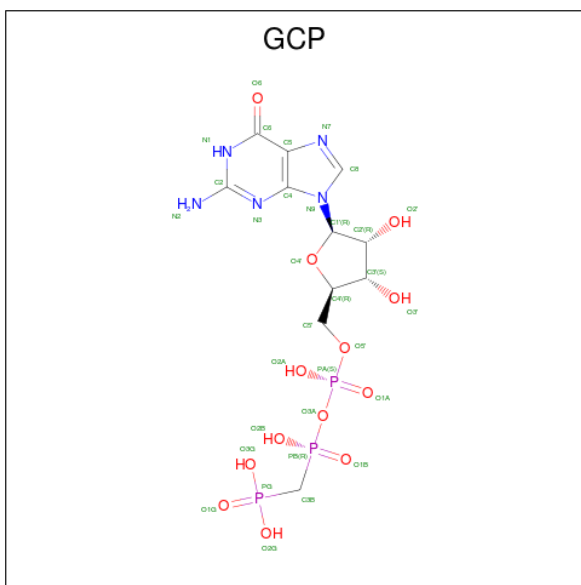
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

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

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

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

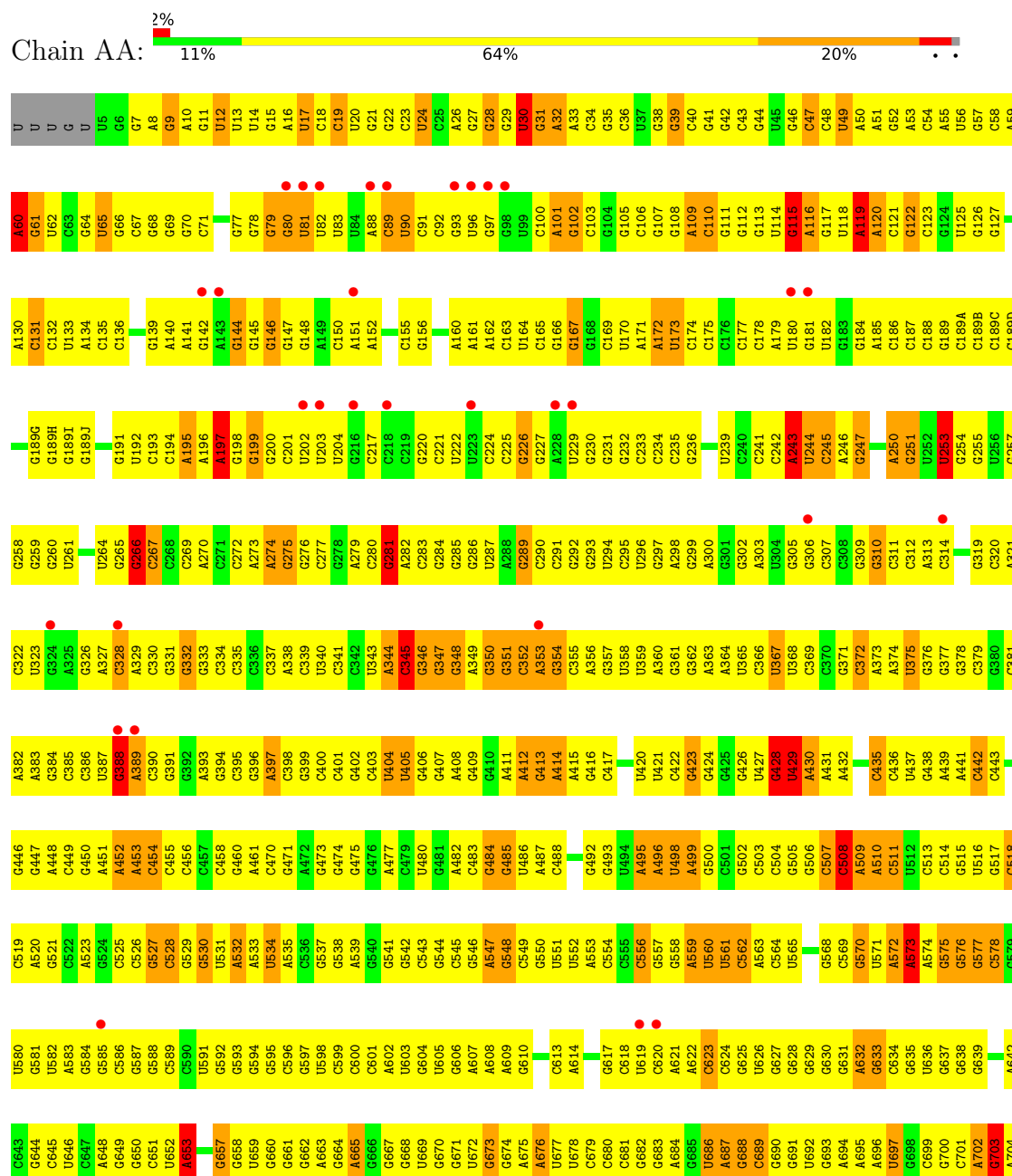


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

3 Residue-property plots

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

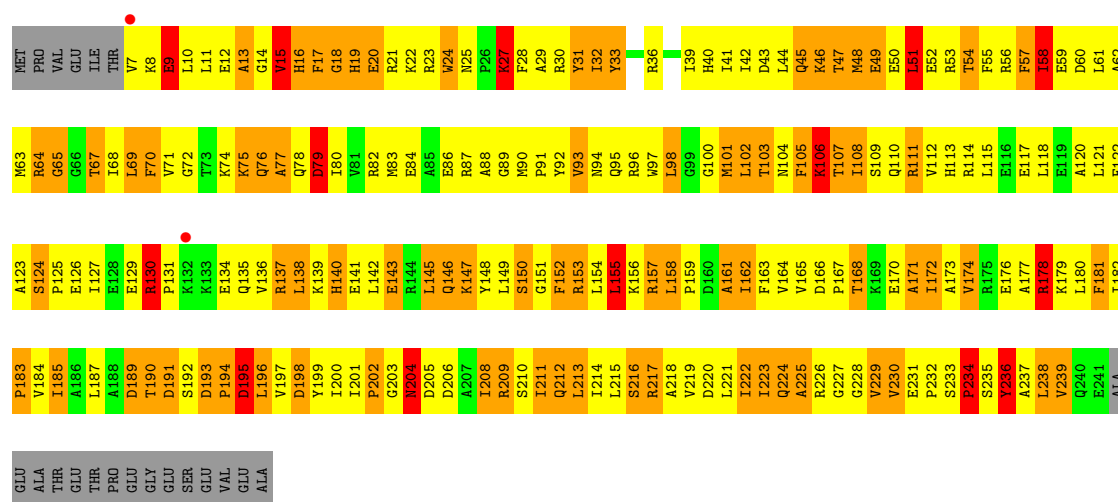
• Molecule 1: 16S rRNA



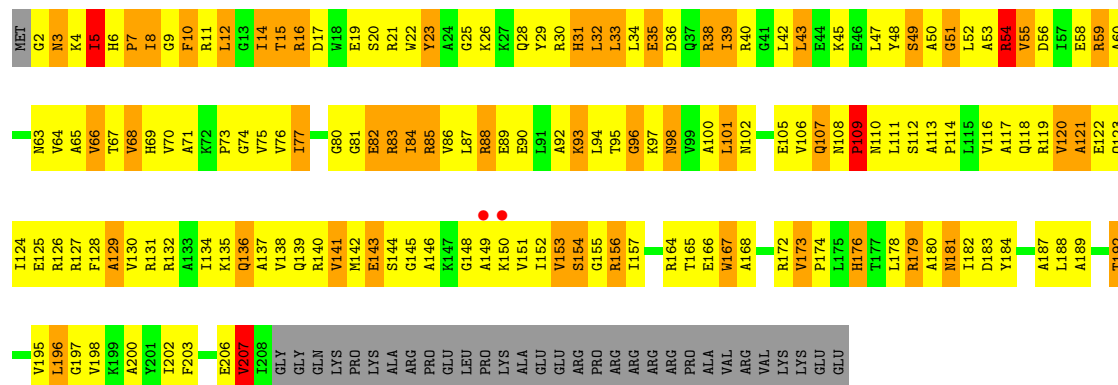
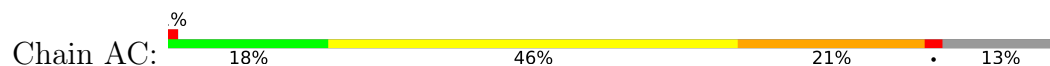
A1503	G1438	G1376	G1316	A1256	U1194	C1132	G1072	U1012	U952	A892	C826	A766	U705
G1504	C1439	U1376	C1317	U1257	C1195	G1133	U1073	G1013	G953	C893	U827	A767	A706
G1505	C1440	A1377	C1440	G1258	U1196	A1318	G1074	G1134	G954	C894	G828	A768	A707
U1506	G1441	C1378	A1319	C1259	G1197	U1135	C1075	A1015	U955	C895	A769	A769	C708
A1507	G1442	G1379	C1320	C1260	G1198	U1136	C1076	A1016	U956	C896	U830	C770	G709
G1508	U1380	U1380	C1321	A1261	U1199	C1137	G1077	G1017	U957	C897	G831	C771	G710
C1509	U1381	C1382	C1322	C1262	C1200	G1138	U1078	C1018	A958	C898	C832	U772	G711
U1510	G1443	G1383	G1323	C1263	A1201	G1139	G1079	C1019	A959	C899	U833	C773	A712
G1511	C1444	C1384	A1324	C1264	G1202	G1140	A1080	U1020	U960	A900	U834	G774	G713
U1512	C1445	G1385	C1325	G1265	C1203	C1141	G1081	U1021	U961	A901	U835	G775	G714
A1513	G1446	C1386	C1326	G1266	A1204	G1142	G1082	G1021	C962	G902	G836	G776	A715
C1514	A1447	G1387	C1327	C1267	U1205	G1143	U1083	U1025	G963	G903	G837	A777	A716
C1515	G1452	C1388	C1328	A1268	G1206	G1144	U1084	G1026	A964	C904	G838	G778	C717
G1516	G1456	C1389	A1329	A1269	G1207	C1145	U1085	C1027	A965	U965	U839	C779	G718
G1517	G1457	C1390	G1331	C1270	C1208	A1146	U1086	C1028	G966	G906	C840	A780	C719
A1519	C1459	U1391	C1332	G1272	C1209	G1147	G1087	C1029	U967	A907	U841	A781	C720
G1520	A1460	G1392	A1333	G1273	C1210	U1148	G1088	G1030	A968	A908	A782	A782	G721
G1521	G1461	U1393	C1334	G1274	C1211	C1149	G1089	G1030A	A969	A909	C849	C783	A722
U1522	G1462	A1394	C1335	A1275	U1212	U1150	U1090	C1030B	C970	C910	U850	C784	U723
G1523	C1463	C1395	C1336	G1276	A1213	A1151	U1091	G1030C	G971	U911	G851	G785	G724
G1526	G1464	A1396	G1337	C1277	C1214	A1152	A1092	A1030D	C972	C912	G852	G786	G725
C1527	G1465	C1397	G1338	U1278	G1215	G1153	A1093	G1031	A974	A914	G853	A787	C726
U1528	C1466	A1398	C1339	A1279	C1216	G1154	G1094	G1032	A975	A915	G854	U788	G727
G1529	G1467	C1399	A1340	U1280	C1217	G1155	U1095	G1033	A976	A916	G855	U789	A728
G1530	A1468	C1400	U1341	U1281	U1219	A1157	C1097	A1035	A977	G917	C857	G791	G730
A1531	G1469	G1401	C1342	C1282	G1220	U1158	C1098	G1036	A978	A918	G858	A792	G731
U	G1470	A1402	G1343	G1283	G1221	U1159	G1099	C1037	C979	A919	A859	U793	G734
C	G1471	C1403	C1344	C1284	G1222	G1160	C1100	C1038	C980	U920	A860	A794	C735
C	U1472	A1404	U1345	A1285	C1223	C1161	A1101	C1039	U981	U921	G861	C795	C736
C	A1473	G1405	A1346	A1286	G1224	C1162	A1102	U1040	U982	G922	C862	C796	C737
C	G1474	U1406	G1347	A1287	A1225	U1165	C1103	A1041	A983	A923	U863	C797	C738
U	G1475	C1407	U1348	A1288	C1226	C1166	G1104	C1042	C984	C924	A864	G798	C739
U	A1476	A1408	A1349	A1289	A1227	G1166	A1105	A1046	C985	G925	A865	G799	U740
C	C1477	G1410	A1350	G1290	C1228	A1168	G1106	C1047	A986	G926	C866	U801	G741
C	C1478	U1411	U1351	U1291	A1229	A1169	C1107	G1048	G987	G927	C867	A802	G742
U	C1479	C1412	C1352	U1292	C1230	A1170	G1108	U1049	C988	G928	C868	G803	U743
U	G1480	C1413	G1353	G1293	G1231	G1171	C1109	G1050	C989	G929	G869	U804	C744
U	U1481	A1414	C1354	G1294	U1232	C1172	A1110	C1051	C990	C930	U870	C805	C745
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A1483	G1483	G1416	G1356	C1296	C1234	G1174	C1112	G1053	U992	C932	A872	A807	C747
U1485	C1484	G1417	A1357	C1297	U1235	G1175	C1113	G1054	G993	G933	A873	C808	C748
G1486	U1485	C1418	U1358	C1298	A1236	A1176	C1114	C1055	A994	C934	C875	C809	C749
G1487	C1486	A1419	C1359	A1299	C1237	G1177	C1115	U1056	A995	G935	G876	C810	G750
G1488	G1487	U1420	A1360	G1300	A1238	G1178	C1116	U1057	A996	G936	G877	C811	U751
G1489	G1488	U1421	G1361	U1301	A1239	A1179	G1117	G1058	U997	A937	C878	C812	G752
C1490	C1489	C1424	C1362	C1302	U1240	A1180	C1118	G1059	C998	A938	G879	U813	A753
G1491	C1490	U1425	A1363	C1303	G1241	G1181	C1119	C1060	C999	G939	C880	A814	C754
A1492	G1491	C1426	U1364	G1304	C1242	G1182	C1120	U1061	A1001	C940	G881	A815	G755
A1493	U1365	U1427	G1365	G1305	C1243	A1183	U1121	U1062	G941	G941	C882	A816	G756
G1494	C1366	U1307	U1367	U1307	U1248	G1185	A1123	G1063	G942	G942	C883	C817	U757
U1495	C1367	U1308	C1368	G1309	C1249	G1186	G1124	G1064	U943	U943	C884	G818	G758
C1496	G1368	G1309	U1369	G1310	U1250	A1187	U1125	U1065	G944	G944	G885	A819	A759
G1497	G1369	G1311	A1433	G1312	A1251	A1188	U1126	C1066	G945	G945	G886	U820	G760
U1498	C1370	G1311	G1370	G1312	A1252	A1189	G1127	A1067	A946	A946	G887	G821	G761
A1499	G1371	G1312	G1371	G1313	A1253	G1190	C1128	G1068	C948	C948	G888	C822	C762
U1500	U1372	U1313	C1373	C1314	G1253	A1191	C1129	G1069	A949	A949	A889	G823	G763
C1501	U1436	C1373	C1373	C1314	G1254	A1192	C1130	U1070	U950	U950	C824	G824	C764
A1502	A1374	U1315	G1255	G1255	G1255	G1193	G1131	C1071	G1011	G951	U891	G825	G765

• Molecule 2: 30S RIBOSOMAL PROTEIN S2

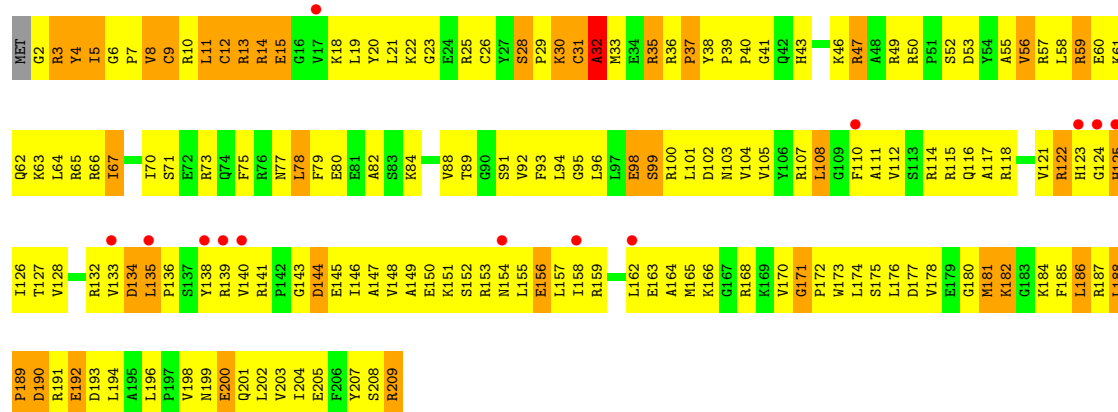




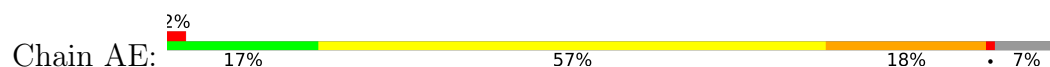
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

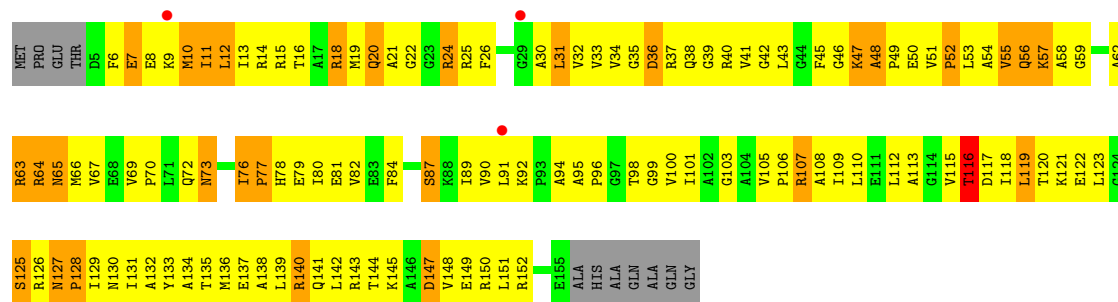


• Molecule 4: 30S RIBOSOMAL PROTEIN S4



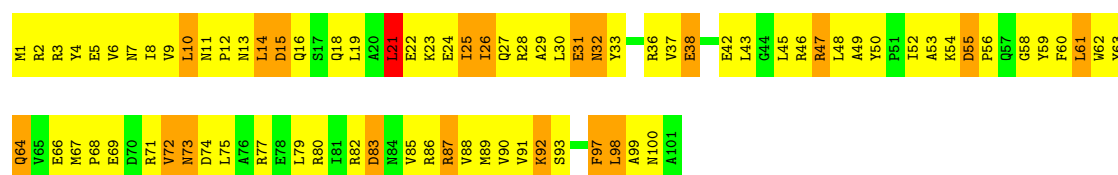
• Molecule 5: 30S RIBOSOMAL PROTEIN S5





• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF: 20% 60% 19%



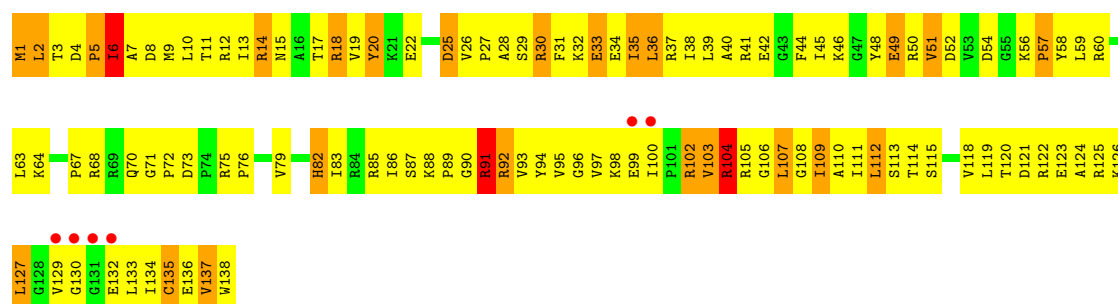
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG: 2% 18% 65% 15%



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

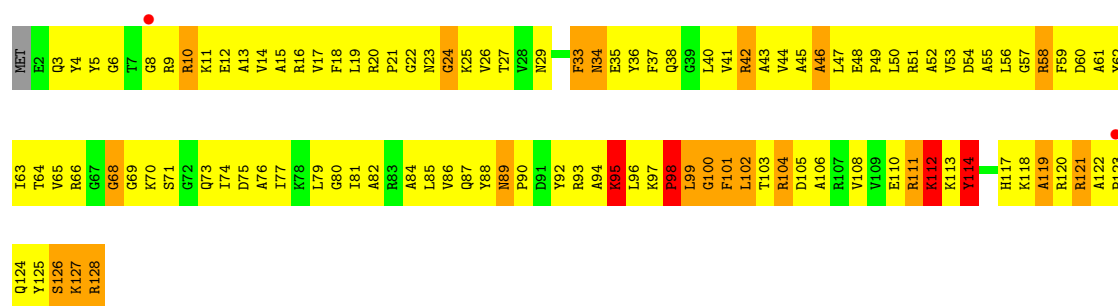
Chain AH: 4% 17% 63% 17%



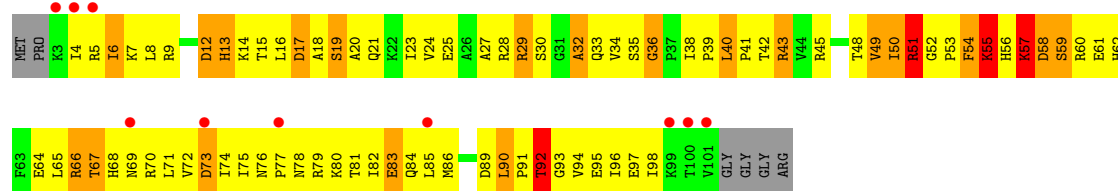
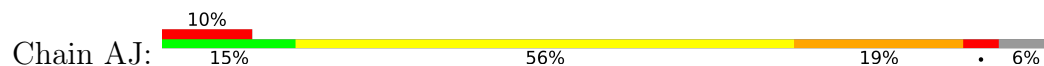
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI: 2% 13% 68% 16%





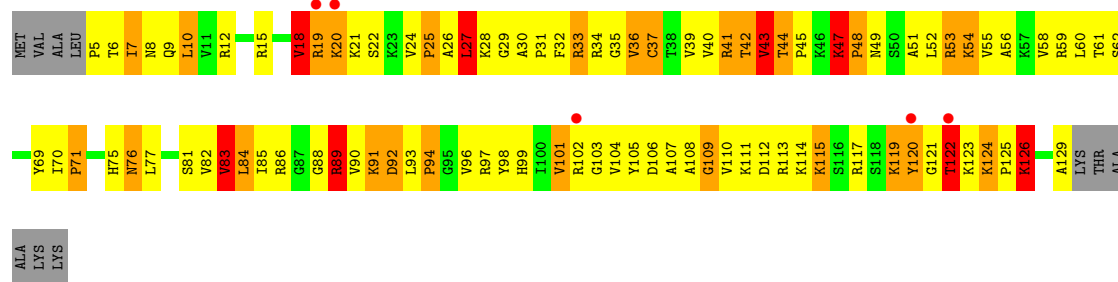
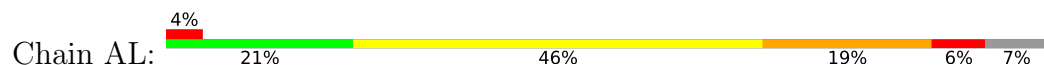
• Molecule 10: 30S RIBOSOMAL PROTEIN S10



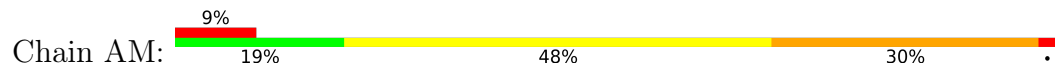
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

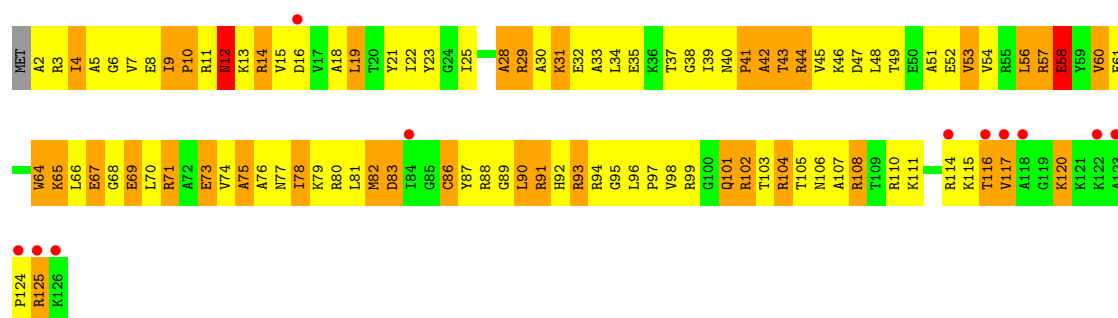


• Molecule 12: 30S RIBOSOMAL PROTEIN S12



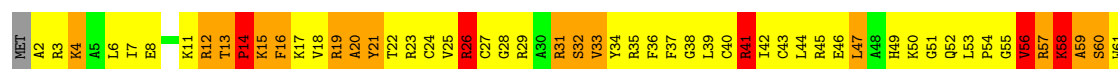
• Molecule 13: 30S RIBOSOMAL PROTEIN S13





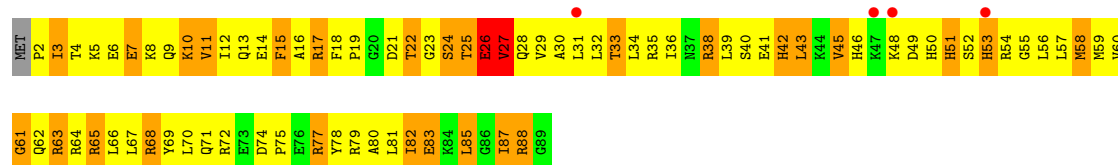
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN: 8% 57% 25% 8%



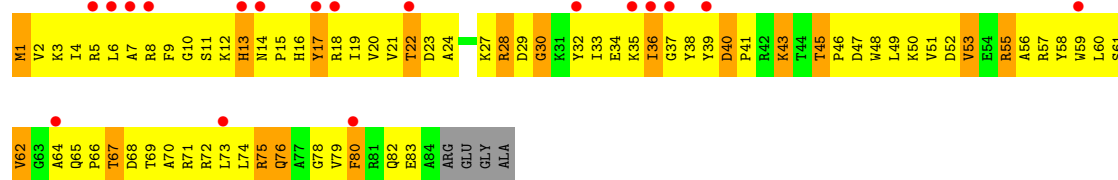
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO: 4% 10% 56% 30%



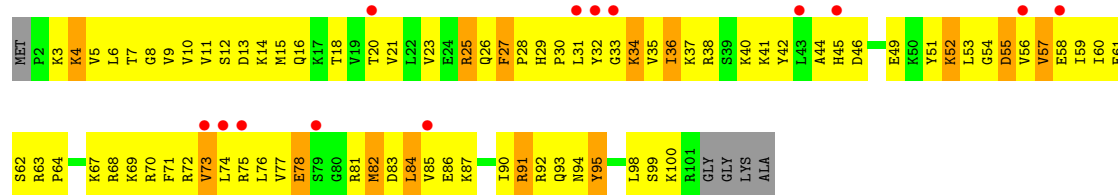
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP: 20% 11% 65% 19% 5%



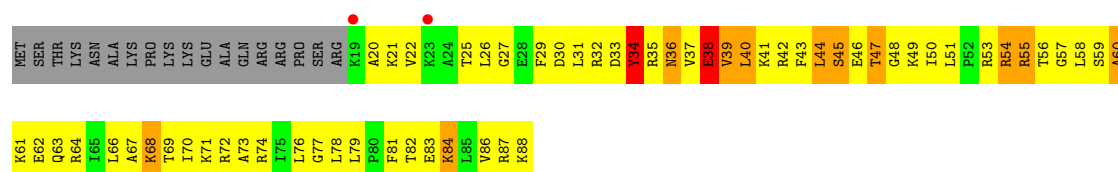
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ: 12% 18% 64% 13% 5%

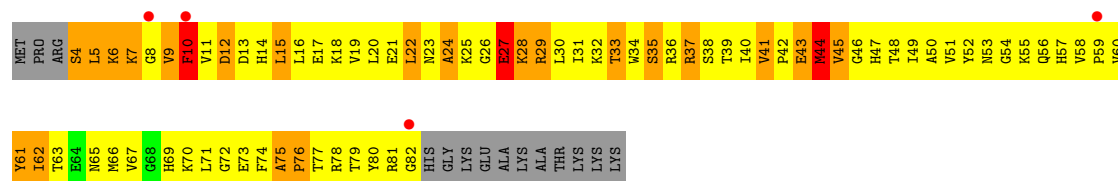


• Molecule 18: 30S RIBOSOMAL PROTEIN S18

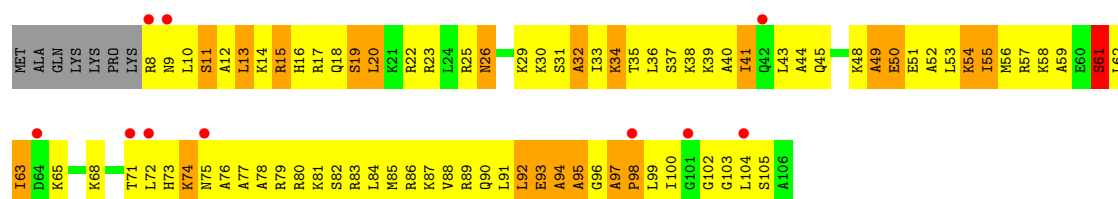
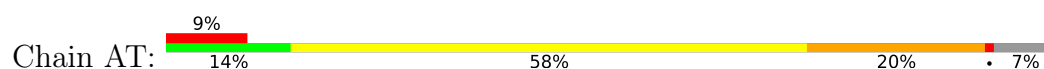
Chain AR: 2% 10% 55% 13% 20%



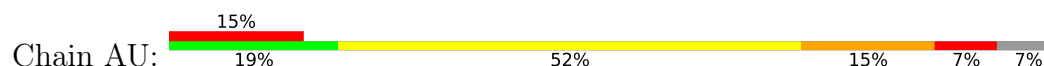
• Molecule 19: 30S RIBOSOMAL PROTEIN S19



• Molecule 20: 30S RIBOSOMAL PROTEIN S20



• Molecule 21: 30S RIBOSOMAL PROTEIN THX



• Molecule 22: PE HYBRID STATE TRNA FMET



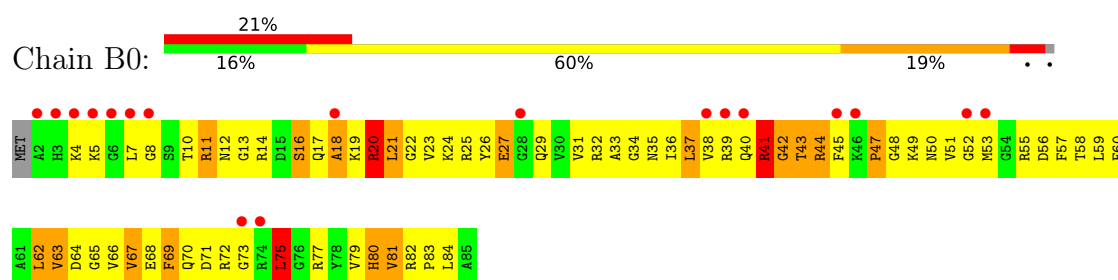
• Molecule 23: MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'



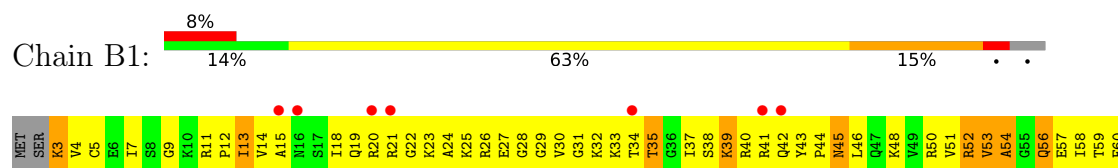
• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3

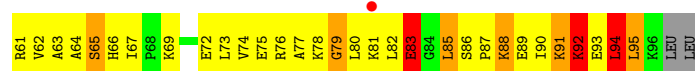


• Molecule 25: 50S RIBOSOMAL PROTEIN L27

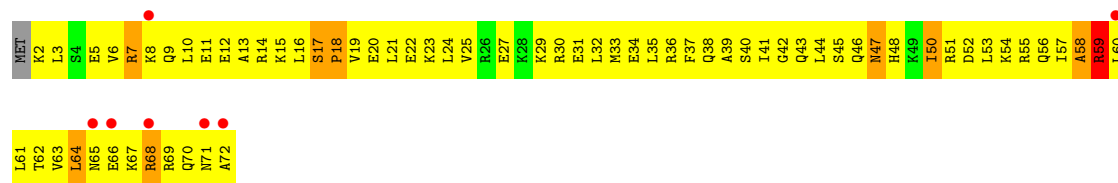


• Molecule 26: 50S RIBOSOMAL PROTEIN L28

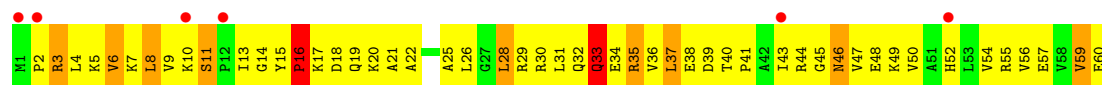




• Molecule 27: 50S RIBOSOMAL PROTEIN L29



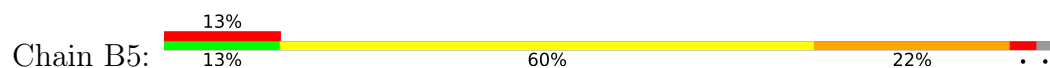
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



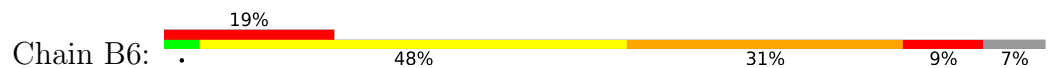
• Molecule 29: 50S RIBOSOMAL PROTEIN L31



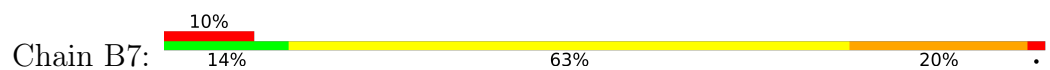
• Molecule 30: 50S RIBOSOMAL PROTEIN L32



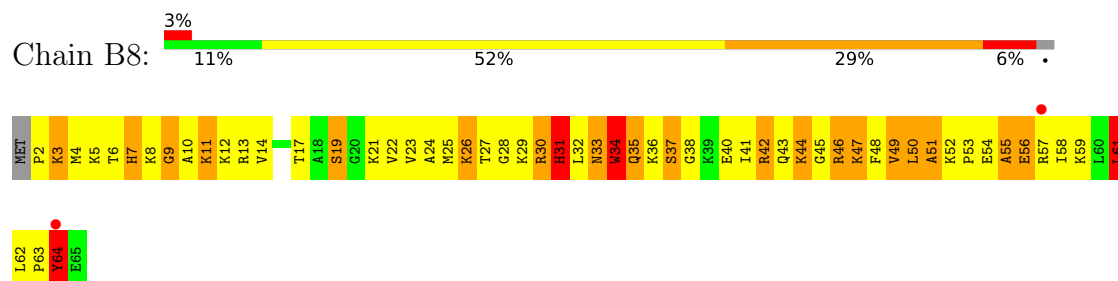
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



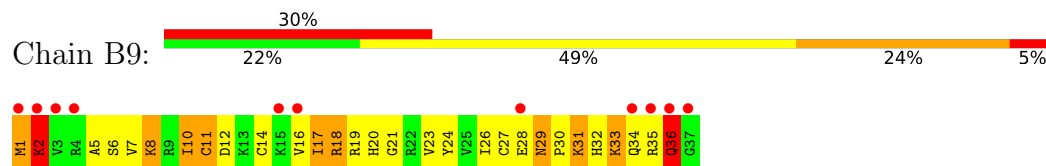
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



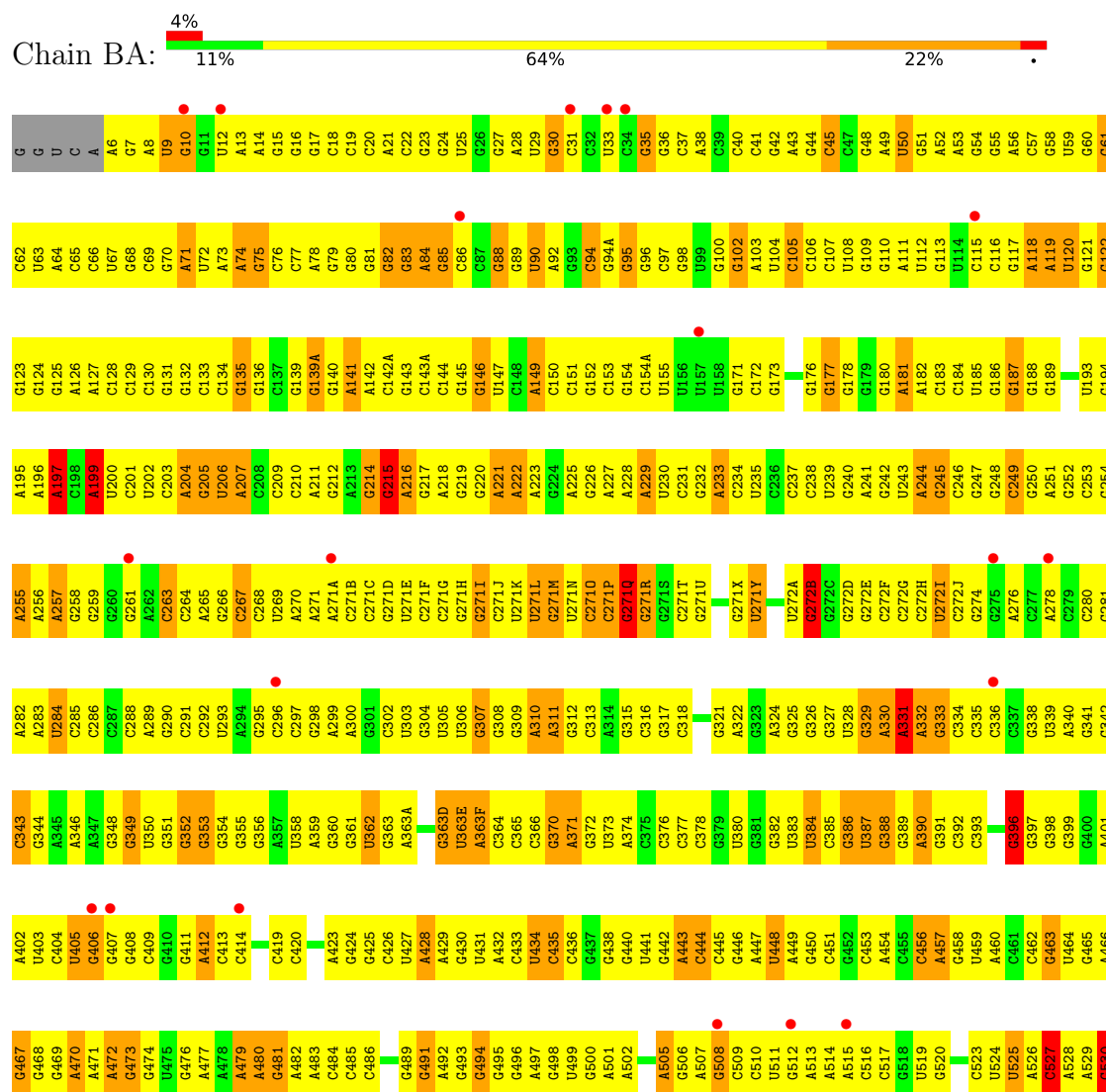
● Molecule 33: 50S RIBOSOMAL PROTEIN L35



● Molecule 34: 50S RIBOSOMAL PROTEIN L36

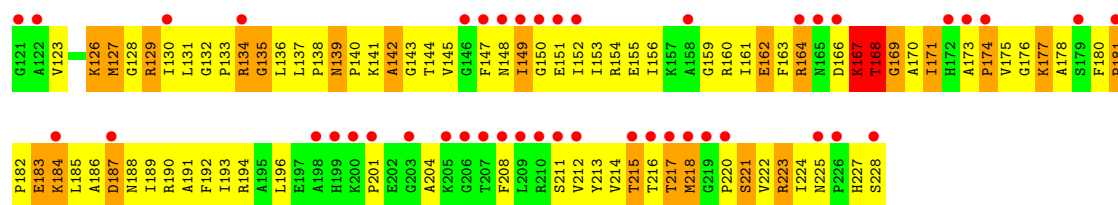


● Molecule 35: 23S RIBOSOMAL RNA

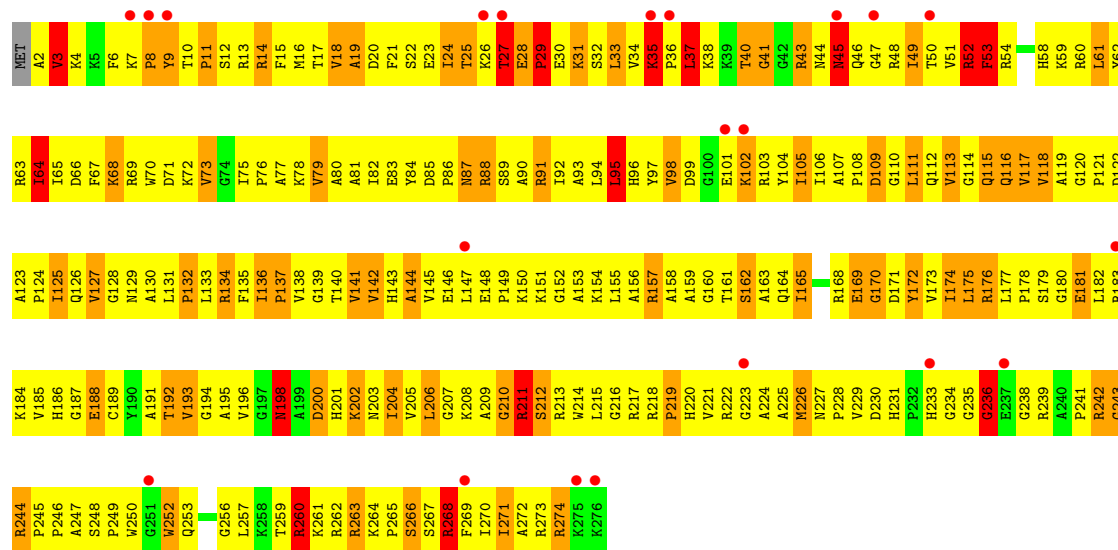
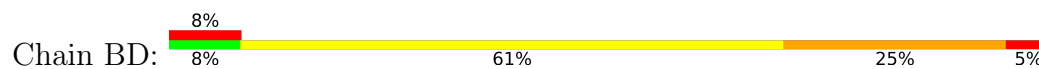




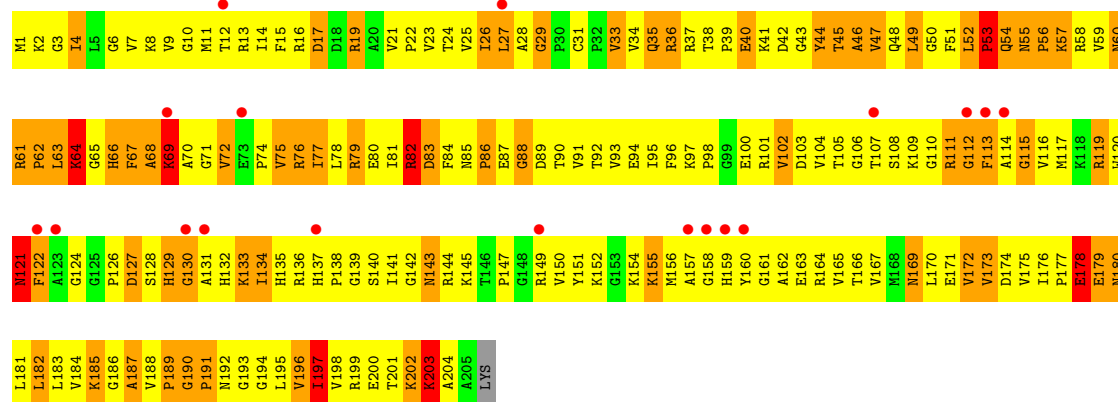
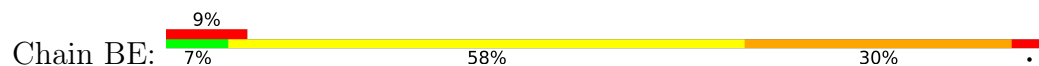
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G2323	G2190	C2127	U2067	U1944	A1884	C1754	G1674	A1614	A1614	G1552	G1492	C1430
C2324	G2191	C2128	U2068	A1885	A1815	A1755	C1675	C1615	C1615	C1553	C1493	A1431
G2325	G2192	G2129	C2069	C1947	C1886	G1756	G1756	A1616	A1616	A1554	A1494	A1432
C2326	U2130	U2130	G2010	G1948	C1887	G1817	U1757	G1617	G1617	C1555	A1495	U1433
A2327	G2131	G2131	G2071	G1949	C1888	U1818	G1758	U1678	A1618	C1556	A1496	A1434
A2328	U2132	U2132	A2071	G1950	A1889	A1819	G1759	U1679	G1619	C1557	A1497	A1435
G2329	C2133	C2133	G2072	U1951	A1890	U1820	A1759	U1680	G1620	A1558	C1498	G1436
G2330	A2134	A2134	U2074	A1952	G1891	A1821	C1761	U1681	U1621	G1559	C1499	G1437
G2331	C2137	C2137	A2015	A1953	C1892	G1822	A1762	G1682	G1622	G1560	G1500	U1438
A2332	U2138	U2138	U2076	G1954	C1893	G1823	G1763	A1662	G1623	A1562	C1501	A1439
C2333	C2139	C2139	G2018	U1955	C1894	G1824	G1764	C1684	G1624	A1563	G1502	G1440
A2334	G2140	G2140	A2019	U1956	C1895	A1825	C1765	C1684	C1625	C1564	U1503	G1441
C2335	C2141	C2141	U2079	C1957	G1896	G1826	U1766	C1684	G1626	C1565	C1504	G1442
G2336	C2142	C2142	A2080	C1958	G1897	C1827	C1767	C1684	G1627	C1566	C1505	G1443
C2337	C2143	C2143	C2021	U1959	U1898	G1827	U1768	C1684	G1628	A1567	C1506	G1444
G2338	U2144	U2144	U2022	A1960	G1899	A1829	G1769	C1684	G1629	A1568	A1507	A1445
C2339	C2145	C2145	G2023	C1961	A1900	C1830	G1770	U1692	A1631A	A1569	A1508	C1445A
G2340	G2146	G2146	G2024	C1962	A1901	G1831	C1771	U1693	A1632	A1570	C1509	G1446
C2341	C2147	C2147	C2085	U1963	C1902	G1832	G1772	U1694	A1633	A1571	A1509A	G1447
G2342	G2148	G2148	U2086	G1964	G1903	A1773	G1773	G1695	G1633	A1572	A1509B	G1448
C2343	C2149	C2149	G2087	C1965	G1904	U1833	C1774	G1696	A1634	G1573	G1510	A1449
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G2356	C2161	C2161	G2100	A1978	U1917	A1847	C1787	G1710	G1647	A1587	G1525	C1462
C2357	G2162	G2162	G2101	C1979	A1918	U1848	C1788	G1711	G1648	C1588	G1526	C1463
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C2359	C2164	C2164	C2103	A1981	C1920	G1850	C1790	G1713	G1650	U1590	A1528	G1465
A2360	U2167	U2167	C2104	C1982	G1921	U1851	A1791	G1714	G1651	G1591	A1528A	G1466
C2361	G2168	G2168	C2105	G1983	G1922	C1852	G1792	G1717	A1652	G1592	G1529	C1467
G2362	C2169	C2169	G2106	C1984	U1923	A1853	C1793	G1718	G1653	G1593	C1530	C1468
C2363	A2169	A2169	C2107	G1985	C1924	U1854	U1794	G1719	A1654	G1594	A1469	A1469
G2364	C2170	C2170	C2108	A1986	C1925	G1855	C1795	U1720	G1655	G1595	G1470	G1470
A2365	A2171	A2171	U2109	G1987	U1926	G1856	U1796	G1721	C1656	A1596	A1471	A1471
C2366	U2172	U2172	G2110	C1988	A1927	G1857	C1797	A1722	C1657	A1597	A1472	A1472
G2367	C2173	C2173	C2111	G1989	U1928	G1858	U1798	U1739	C1658	C1598	C1473	C1473
C2368	C2174	C2174	G2112	C1990	G1929	A1859	G1799	G1740	U1659	C1599	C1474	C1474
A2369	U2175	U2175	U2113	U1991	G1930	G1860	C1800	A1741	C1660	C1537	G1538	G1475
G2370	C2177	C2177	A2114	G1992	U1931	G1861	A1801	G1742	G1661	G1601	G1539	A1476
C2371	C2178	C2178	G2115	U1993	A1932	G1862	A1802	C1743	C1662	U1602	U1540	A1477
A2372	C2179	C2179	G2116	C1994	G1933	G1863	A1803	G1744	C1663	A1603	G1541	G1478
G2373	U2180	U2180	A2117	U1995	C1934	U1864	C1804	G1746	A1664	C1604	A1542	G1479
C2374	G2181	G2181	U2118	C1996	G1935	G1865	U1805	G1747	A1665	C1605	G1480	G1480
G2375	C2182	C2182	A2119	G1997	A1936	C1866	C1806	G1747	G1666	G1606	A1544	U1481
C2376	G2183	G2183	G2120	G1998	A1937	C1867	G1807	G1747A	G1667	C1607	A1545	G1482
A2377	G2184	G2184	G2121	C1999	A1938	G1878	U1808	G1748	A1668	A1608	C1546	G1484
G2378	C2185	C2185	U2122	A2000	U1939	C1879	A1809	A1749	A1669	A1609	C1547	G1485
C2379	G2186	G2186	G2123	G2001	U1940	C1880	A1810	G1750	A1670	A1610	C1548	A1486
G2380	C2187	C2187	G2124	G2002	C1941	C1881	G1811	C1751	U1671	C1611	C1549	



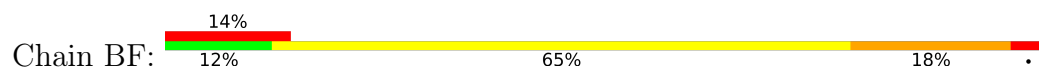
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

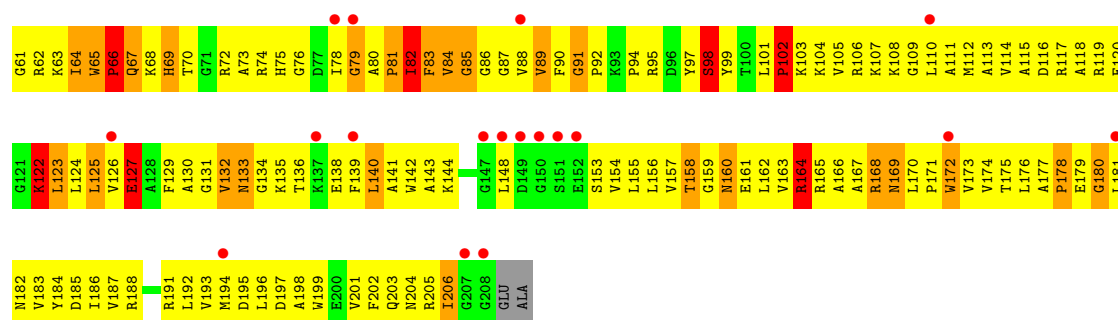


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

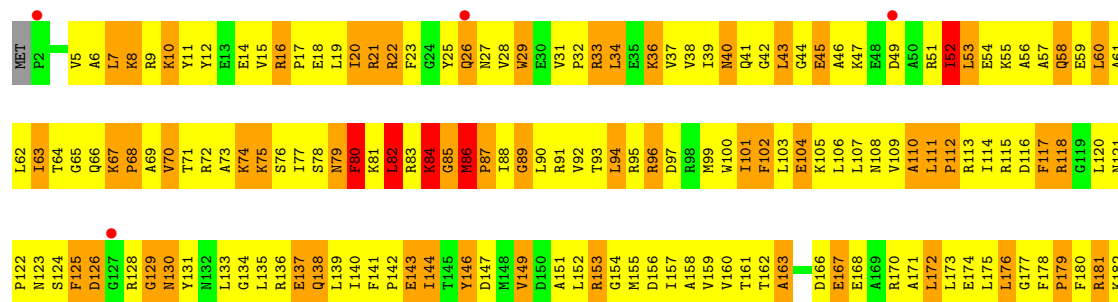
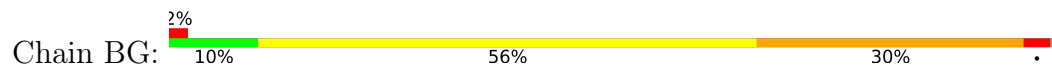


• Molecule 40: 50S RIBOSOMAL PROTEIN L4

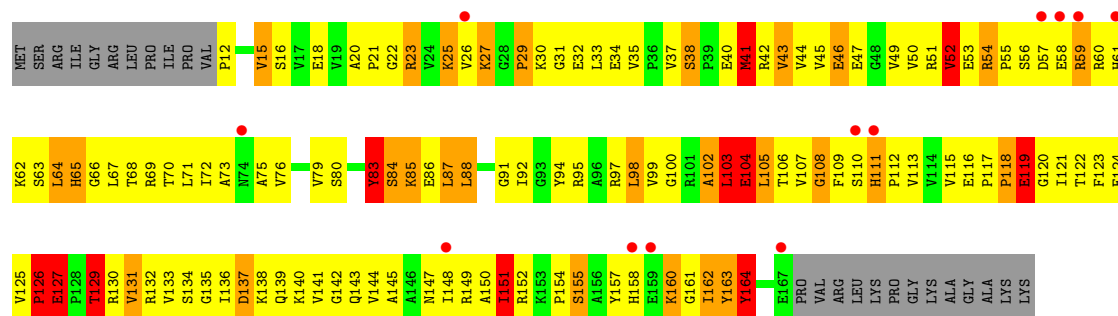
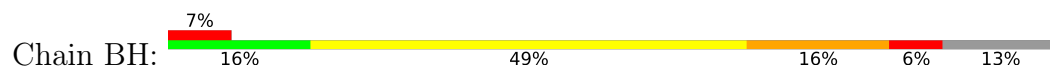




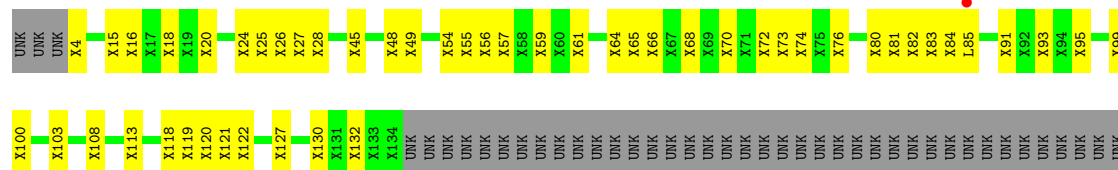
• Molecule 41: 50S RIBOSOMAL PROTEIN L5



• Molecule 42: 50S RIBOSOMAL PROTEIN L6

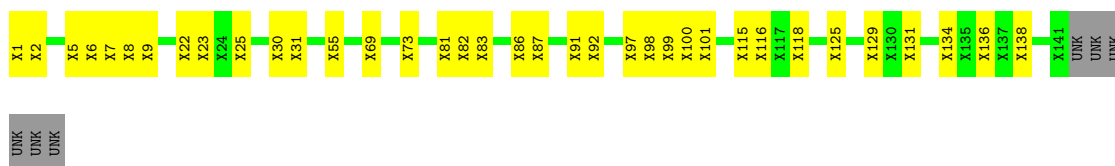


• Molecule 43: 50S RIBOSOMAL PROTEIN L10

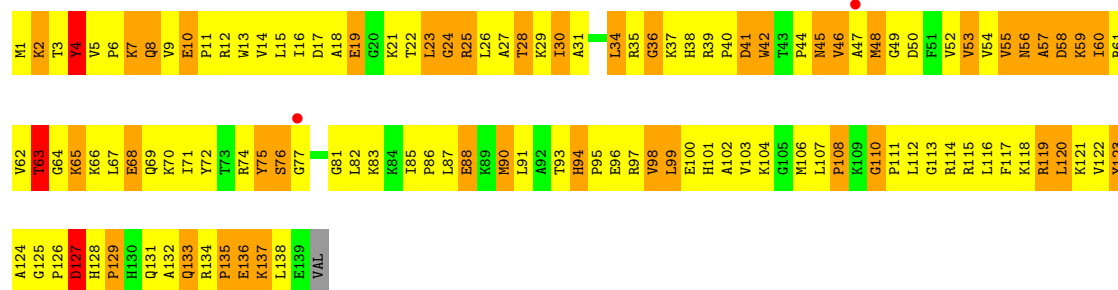
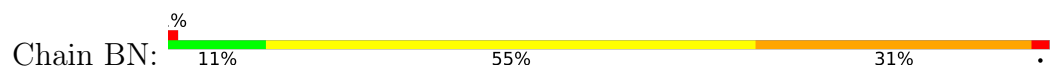


• Molecule 44: 50S RIBOSOMAL PROTEIN L11

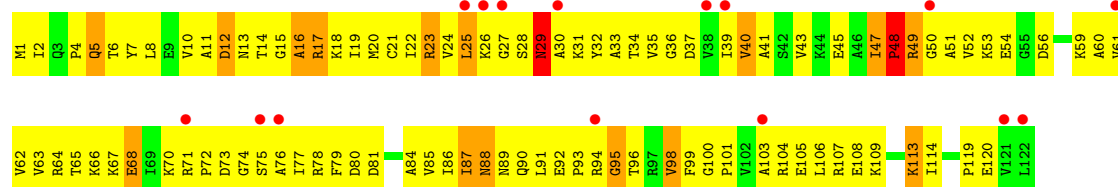




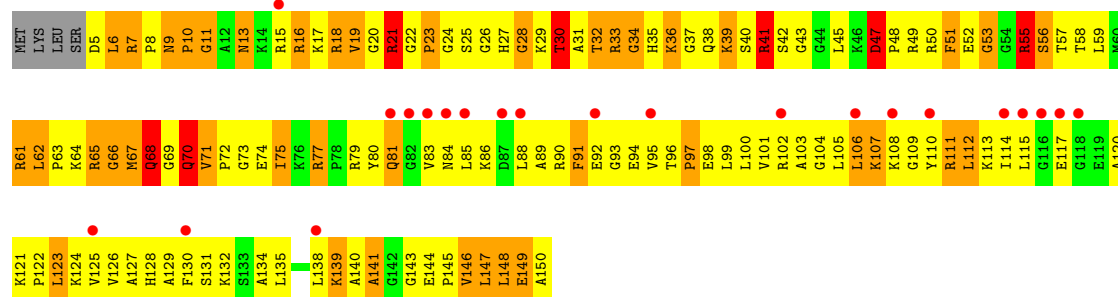
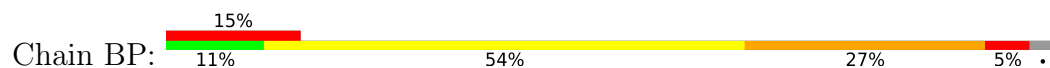
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



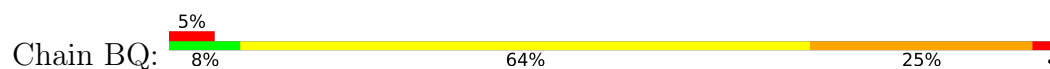
• Molecule 46: 50S RIBOSOMAL PROTEIN L14

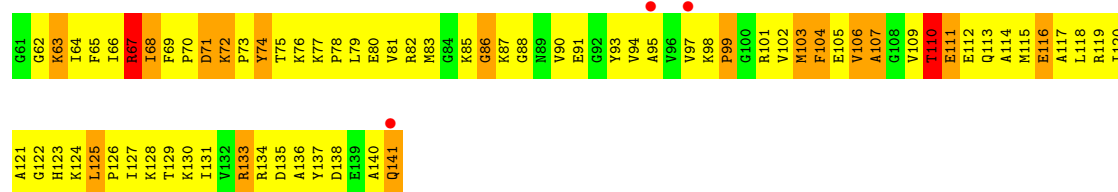


• Molecule 47: 50S RIBOSOMAL PROTEIN L15

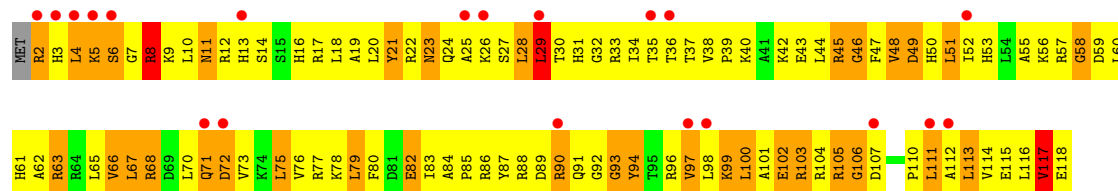
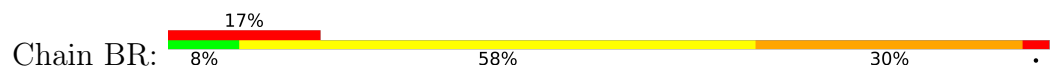


• Molecule 48: 50S RIBOSOMAL PROTEIN L16

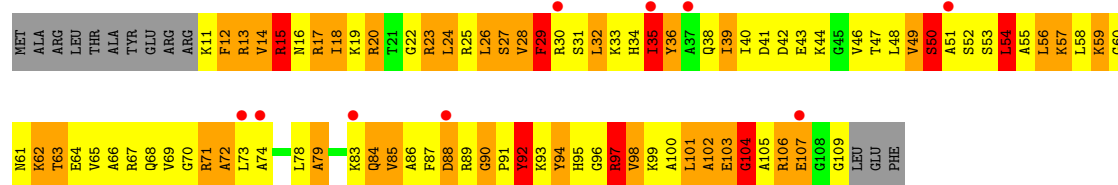




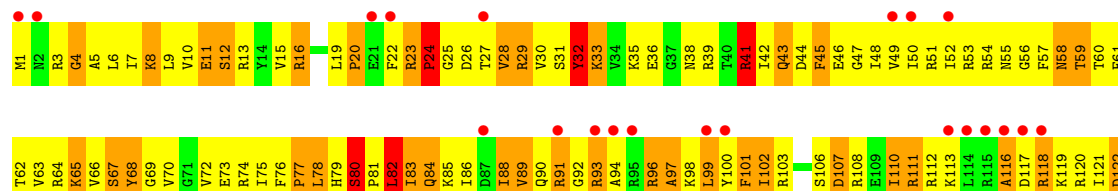
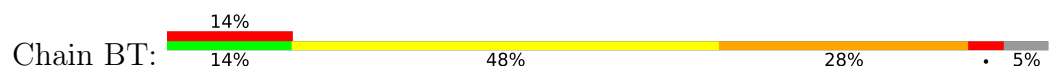
● Molecule 49: 50S RIBOSOMAL PROTEIN L17



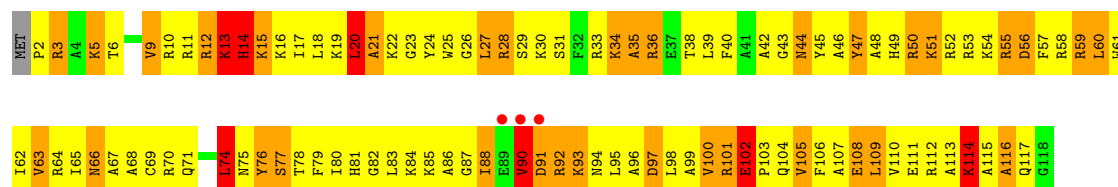
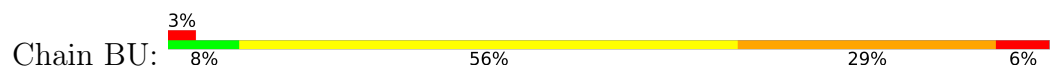
● Molecule 50: 50S RIBOSOMAL PROTEIN L18



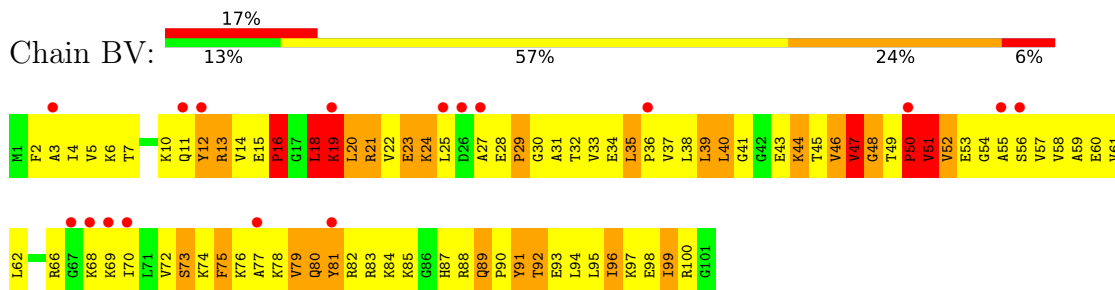
● Molecule 51: 50S RIBOSOMAL PROTEIN L19



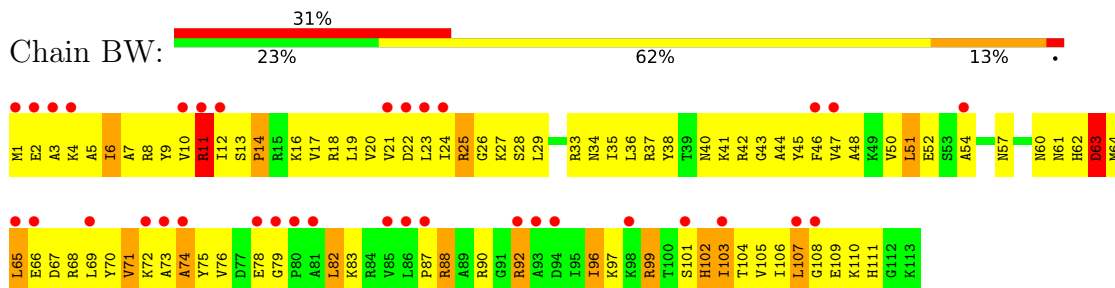
● Molecule 52: 50S RIBOSOMAL PROTEIN L20



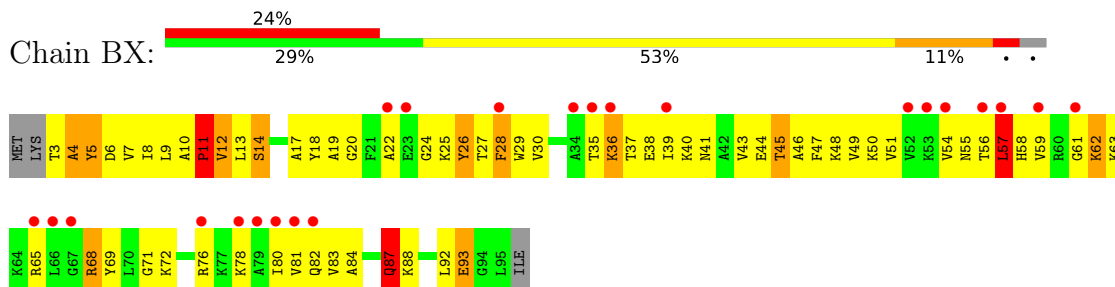
• Molecule 53: 50S RIBOSOMAL PROTEIN L21



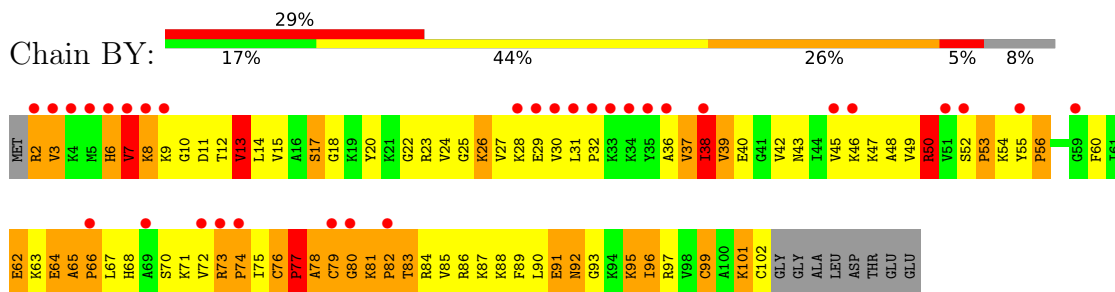
• Molecule 54: 50S RIBOSOMAL PROTEIN L22



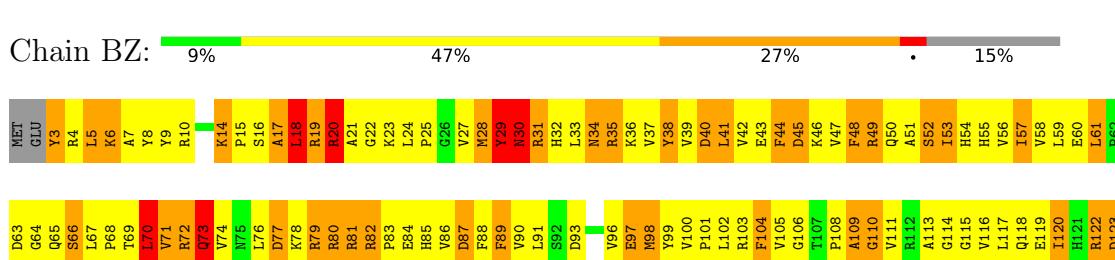
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

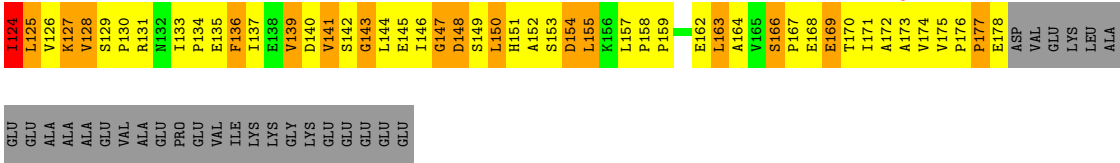


• Molecule 56: 50S RIBOSOMAL PROTEIN L24



• Molecule 57: 50S RIBOSOMAL PROTEIN L25





GLU
GLU
ALA
ALA
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ALA
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GLY
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GLU
GLU
GLU
GLU

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)	Xtriage
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	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
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

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

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 ⓘ

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%)	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	8
5	AE	149/162 (92%)	108 (72%)	31 (21%)	10 (7%)	1	22
6	AF	99/101 (98%)	67 (68%)	24 (24%)	8 (8%)	1	16
7	AG	153/156 (98%)	85 (56%)	44 (29%)	24 (16%)	0	4
8	AH	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	0	8
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	5
11	AK	117/129 (91%)	72 (62%)	32 (27%)	13 (11%)	0	9
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	21
16	AP	82/88 (93%)	55 (67%)	17 (21%)	10 (12%)	0	7
17	AQ	98/105 (93%)	82 (84%)	10 (10%)	6 (6%)	1	24
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	3
25	B0	82/85 (96%)	64 (78%)	9 (11%)	9 (11%)	0	9
26	B1	92/98 (94%)	63 (68%)	16 (17%)	13 (14%)	0	5
27	B2	69/72 (96%)	38 (55%)	22 (32%)	9 (13%)	0	6
28	B3	58/60 (97%)	38 (66%)	15 (26%)	5 (9%)	1	15

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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	2
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	4
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	4
37	BC	226/229 (99%)	158 (70%)	39 (17%)	29 (13%)	0	6
38	BD	273/276 (99%)	195 (71%)	46 (17%)	32 (12%)	0	8
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	3
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	6
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	10
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	5
49	BR	115/118 (98%)	69 (60%)	27 (24%)	19 (16%)	0	4
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	7
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	1	12
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 ⓘ

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	17
4	AD	180/181 (99%)	154 (86%)	26 (14%)	3	24
5	AE	115/123 (94%)	94 (82%)	21 (18%)	2	13
6	AF	90/90 (100%)	76 (84%)	14 (16%)	3	21
7	AG	126/127 (99%)	114 (90%)	12 (10%)	9	39
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	21
9	AI	98/99 (99%)	82 (84%)	16 (16%)	2	18
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	1	12
11	AK	90/99 (91%)	73 (81%)	17 (19%)	1	12
12	AL	104/111 (94%)	86 (83%)	18 (17%)	2	16
13	AM	99/101 (98%)	79 (80%)	20 (20%)	1	10
14	AN	49/50 (98%)	36 (74%)	13 (26%)	0	4
15	AO	79/80 (99%)	52 (66%)	27 (34%)	0	1
16	AP	72/74 (97%)	64 (89%)	8 (11%)	7	33
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	9	39
18	AR	61/77 (79%)	54 (88%)	7 (12%)	6	32
19	AS	69/80 (86%)	58 (84%)	11 (16%)	3	20
20	AT	76/82 (93%)	69 (91%)	7 (9%)	10	41
21	AU	19/22 (86%)	17 (90%)	2 (10%)	7	35
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	5
26	B1	78/83 (94%)	65 (83%)	13 (17%)	2	17
27	B2	66/67 (98%)	61 (92%)	5 (8%)	14	50
28	B3	51/52 (98%)	42 (82%)	9 (18%)	2	15
29	B4	39/63 (62%)	29 (74%)	10 (26%)	0	5
30	B5	51/52 (98%)	47 (92%)	4 (8%)	14	49
31	B6	49/52 (94%)	37 (76%)	12 (24%)	1	6
32	B7	41/42 (98%)	36 (88%)	5 (12%)	5	29
33	B8	53/55 (96%)	42 (79%)	11 (21%)	1	9
34	B9	34/34 (100%)	26 (76%)	8 (24%)	1	6
37	BC	180/181 (99%)	150 (83%)	30 (17%)	2	17
38	BD	217/218 (100%)	150 (69%)	67 (31%)	0	2
39	BE	165/166 (99%)	134 (81%)	31 (19%)	1	12
40	BF	165/166 (99%)	142 (86%)	23 (14%)	4	25
41	BG	155/156 (99%)	127 (82%)	28 (18%)	2	14
42	BH	128/148 (86%)	90 (70%)	38 (30%)	0	3
43	BJ	1/1 (100%)	1 (100%)	0	100	100
45	BN	117/119 (98%)	99 (85%)	18 (15%)	3	21
46	BO	100/100 (100%)	89 (89%)	11 (11%)	7	34
47	BP	112/116 (97%)	91 (81%)	21 (19%)	1	12
48	BQ	111/111 (100%)	87 (78%)	24 (22%)	1	8
49	BR	100/101 (99%)	78 (78%)	22 (22%)	1	8
50	BS	77/88 (88%)	60 (78%)	17 (22%)	1	8
51	BT	120/127 (94%)	96 (80%)	24 (20%)	1	11
52	BU	92/94 (98%)	74 (80%)	18 (20%)	1	11
53	BV	82/82 (100%)	65 (79%)	17 (21%)	1	9
54	BW	91/92 (99%)	81 (89%)	10 (11%)	7	34
55	BX	74/78 (95%)	63 (85%)	11 (15%)	3	22
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2	14
57	BZ	155/179 (87%)	117 (76%)	38 (24%)	1	6
All	All	5271/5546 (95%)	4255 (81%)	1016 (19%)	1	12

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

Mol	Chain	Res	Type
25	B0	5	LYS
37	BC	108	MET
53	BV	91	TYR
25	B0	80	HIS
30	B5	25	LEU

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

Mol	Chain	Res	Type
25	B0	70	GLN
33	B8	35	GLN
53	BV	89	GLN
26	B1	45	ASN
28	B3	52	HIS

5.3.3 RNA ⓘ

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	50	U
35	BA	603	A

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Mol	Chain	Res	Type
35	BA	2282	G
35	BA	71	A
35	BA	331	A

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 carbohydrates 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	-	26,34,34	2.78	7 (26%)	31,54,54	1.89	8 (25%)

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	-	-	13/18/38/38	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	8.97	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PB-O3A	5.78	1.64	1.58
58	AY	1000	GCP	C4-N9	-5.77	1.40	1.47
58	AY	1000	GCP	C5-C6	-5.15	1.43	1.52
58	AY	1000	GCP	PG-O2G	-2.73	1.48	1.54

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	1000	GCP	C4-C5-N7	6.84	111.53	102.46
58	AY	1000	GCP	C5-C6-N1	-2.80	114.93	118.27
58	AY	1000	GCP	O6-C6-C5	2.70	125.39	119.82
58	AY	1000	GCP	O3G-PG-O2G	2.63	115.84	108.18
58	AY	1000	GCP	O3G-PG-O1G	-2.62	105.32	112.29

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

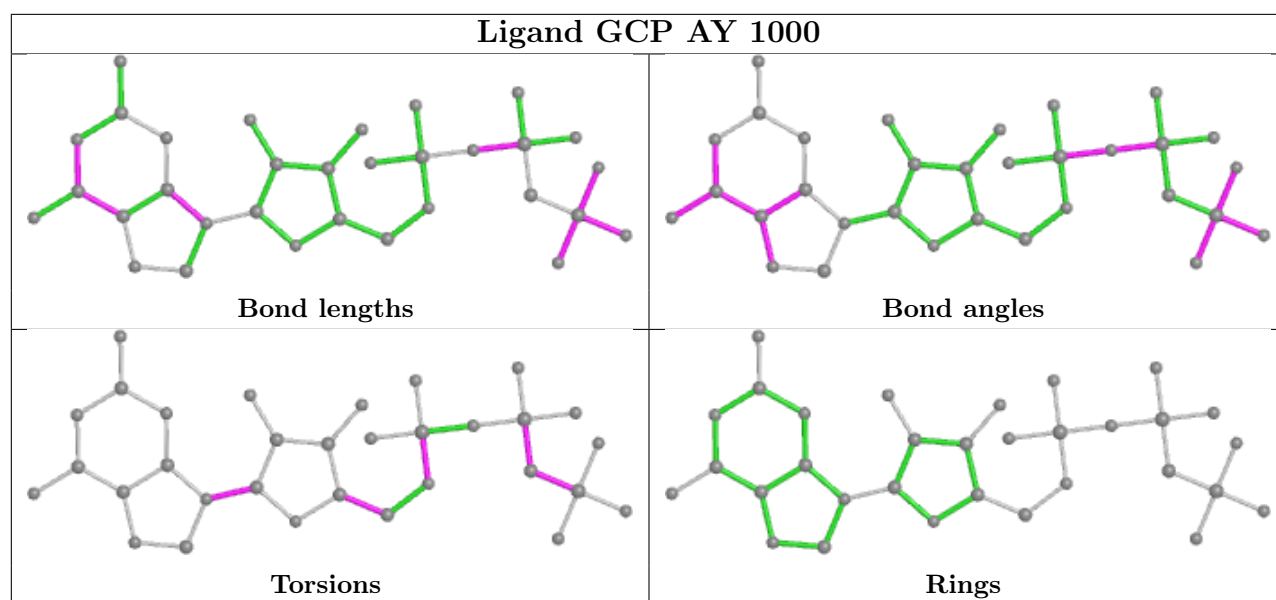
Mol	Chain	Res	Type	Atoms
58	AY	1000	GCP	PB-C3B-PG-O1G
58	AY	1000	GCP	PB-C3B-PG-O2G
58	AY	1000	GCP	PG-C3B-PB-O1B
58	AY	1000	GCP	PG-C3B-PB-O3A
58	AY	1000	GCP	C5'-O5'-PA-O3A

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 ⓘ

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%)	-0.14	37 (2%) 57 46	52, 140, 199, 200	0
2	AB	235/256 (91%)	-0.44	2 (0%) 84 77	40, 110, 177, 200	0
3	AC	207/239 (86%)	-0.49	2 (0%) 82 75	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 55	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 57	46, 128, 189, 200	0
8	AH	138/138 (100%)	-0.10	6 (4%) 35 27	36, 114, 180, 200	0
9	AI	127/128 (99%)	-0.12	2 (1%) 72 62	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 28	40, 116, 179, 200	0
12	AL	125/135 (92%)	0.24	5 (4%) 38 29	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 26	59, 130, 188, 200	0
16	AP	84/88 (95%)	1.03	18 (21%) 1 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 40	59, 124, 176, 200	0
19	AS	79/93 (84%)	0.13	4 (5%) 28 22	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 68	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 5	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%) 1 1	37, 118, 194, 200	0
26	B1	94/98 (95%)	0.59	8 (8%) 11 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%) 18 13	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%) 7 6	78, 153, 197, 200	0
33	B8	64/65 (98%)	0.13	2 (3%) 49 38	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 30	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%) 14 10	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 51	47, 134, 194, 200	0
42	BH	156/180 (86%)	0.30	12 (7%) 13 10	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 66	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%) 29 23	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 44	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 84	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 ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

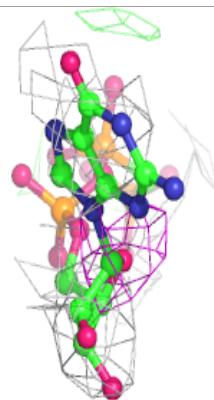
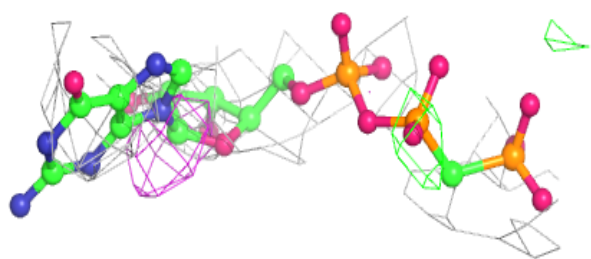
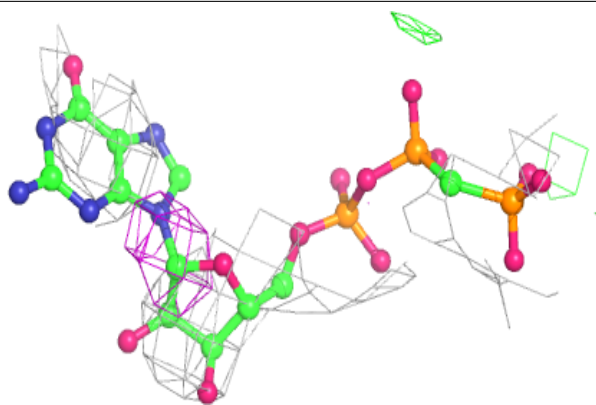
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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.

Electron density around GCP AY 1000:

$2mF_o-DF_c$ (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.