



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 04:16 pm BST

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:

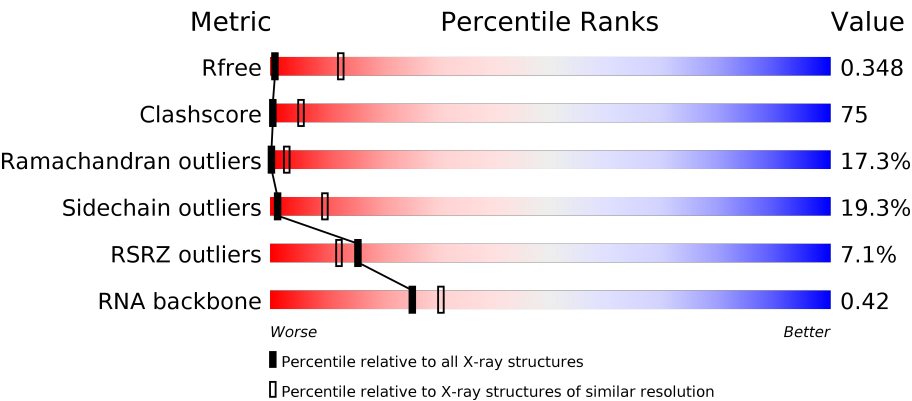
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber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

1 Overall quality at a glance i

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div><div>2%</div><div>11%64%20%</div><div></div></div>
2	AB	256	<div><div>%</div><div>9%46%31%5%8%</div><div></div></div>
3	AC	239	<div><div>%</div><div>18%46%21%13%</div><div></div></div>
4	AD	209	<div><div>6%</div><div>20%60%19%</div><div></div></div>

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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				

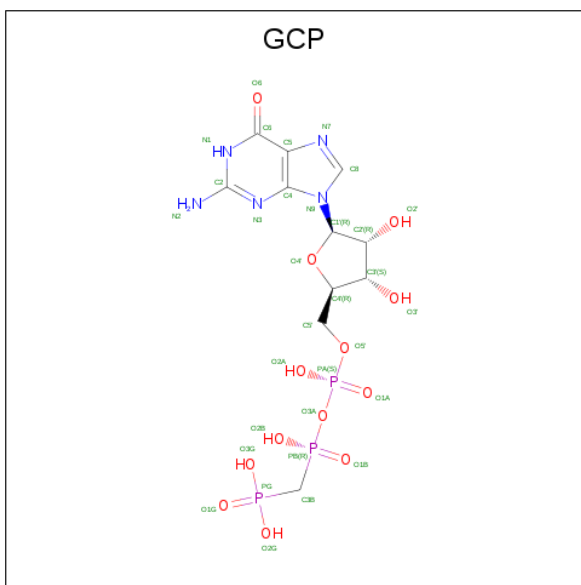
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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: C₁₁H₁₈N₅O₁₃P₃).

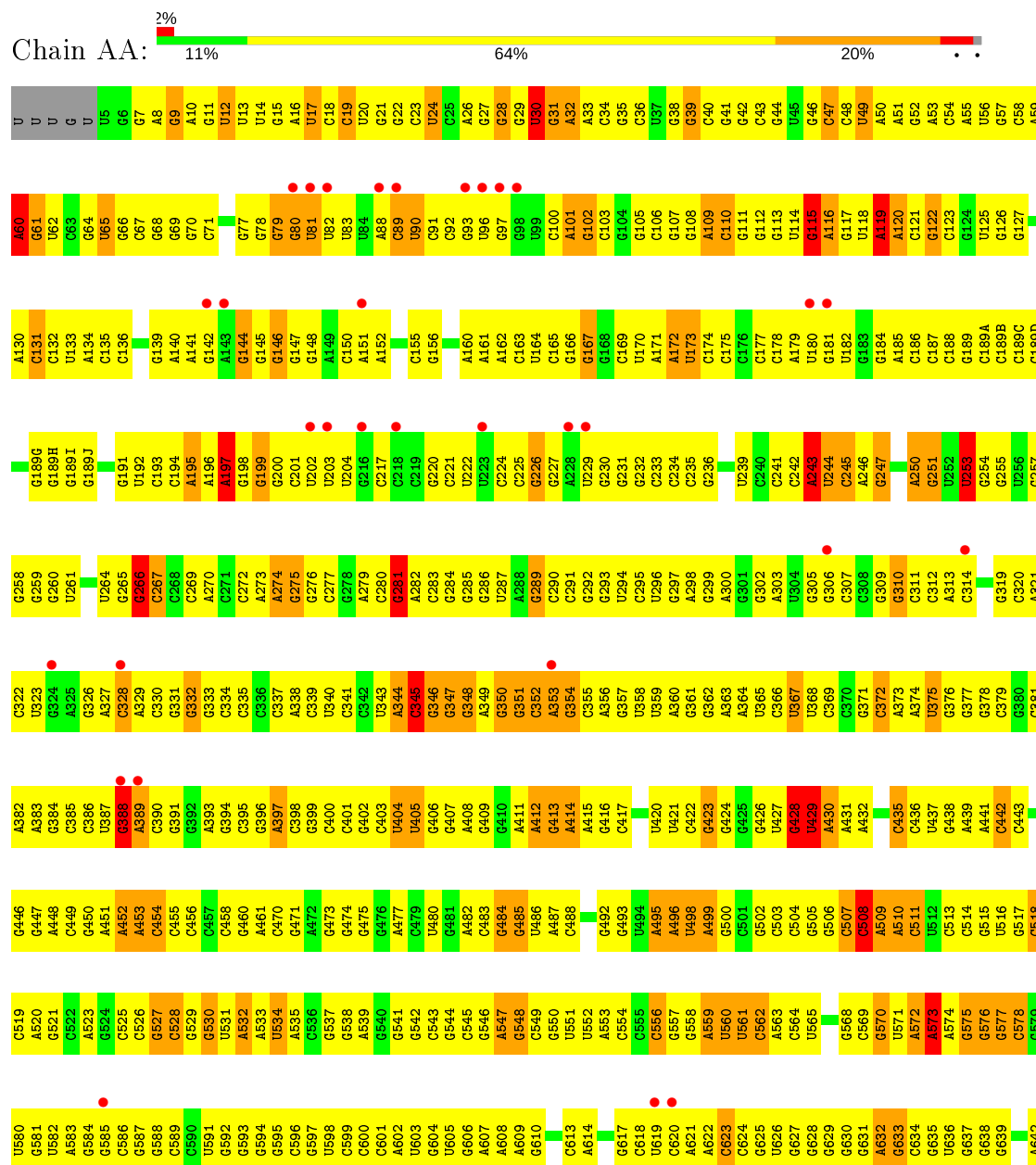


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
58	AY	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

3 Residue-property plots

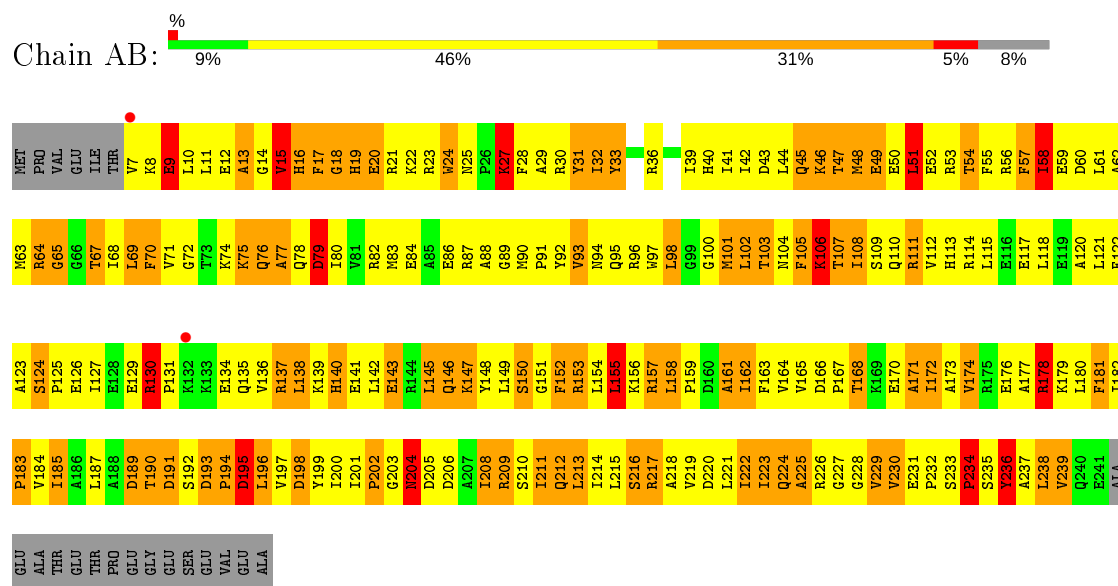
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

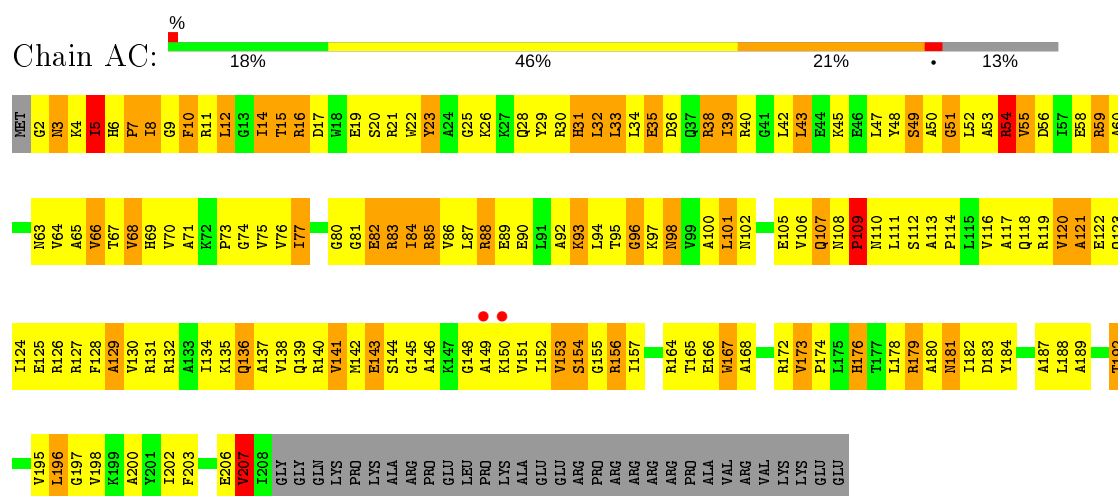


A1503	G1438	G1316	A1256	U1194	C1132	G1072	U1012	U952	A892	C826	A766	U705	C643
G1504	C1439	C1317	U1257	C1195	G1133	U1073	G1013	G993	C893	U827	A767	A706	G644
U1505	A1318	A1318	G1258	U1196	G1134	G1074	A1014	G994	A1014	A828	A768	C707	C645
U1506	A1319	A1319	C1259	G1197	U1135	G1075	A1015	U995	G895	G829	G769	C708	U646
A1507	G1379	C1260	G1260	G1198	U1136	G1076	A1016	U956	C896	G830	C770	G709	C647
U1508	G1442A	C1321	A1261	U1199	C1137	G1077	A1017	U957	C897	U831	G771	G710	A648
C1509	A1442B	C1322	C1262	C1200	G1138	U1078	C1018	A958	C898	C832	U772	C711	G649
U1510	G1443	G1323	C1263	A1201	G1139	G1079	C1019	A959	C899	U833	G773	A712	G650
G1511	C1383	A1324	G1264	G1202	C1140	A1080	U1020	U960	A900	C834	G774	G713	C651
U1512	C1384	C1325	G1265	C1203	C1141	G1081	U1021	U961	A901	U835	G775	A714	U852
A1513	G1385	C1326	G1266	A1204	G1142	G1082	U1022	C982	G902	C836	G776	G715	A653
C1514	A1447	C1327	G1267	U1205	G1143	U1083	U1023	G963	G903	G837	A777	A716	G657
U1515	C1387	C1328	A1268	C1206	G1144	G1084	G1026	G964	C904	G838	G778	C717	G658
G1516	C1388	A1329	A1269	G1207	C1145	U1085	C1027	A965	U965	U839	C779	G718	U859
U1517	G1457	U1330	C1270	C1208	A1146	U1086	C1028	G966	G906	C840	A780	C719	G660
A1518	G1458	G1331	G1271	C1209	C1147	G1087	C1029	C967	U907	U841	A781	C720	G661
U1519	C1459	A1332	G1272	C1210	U1148	G1088	G1030	A968	A968	C848	A782	G721	G662
G1520	G1460	A1333	G1273	U1211	C1149	G1089	G1030A	A969	A909	C849	C783	A722	G663
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G1522	G1461	G1335	A1275	A1213	A1151	U1091	G1030C	G971	U911	G851	G785	G724	G664
U1523	C1463	C1336	G1276	C1214	A1152	U1092	A1030D	C972	C912	G852	G786	G725	A665
G1526	G1464	G1337	U1277	G1215	C1153	G1093	G1031	G973	A913	G853	A787	G726	G666
C1527	C1465	G1338	G1278	G1216	G1154	U1094	G1032	A974	A914	G854	U788	G727	G667
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G1529	G1467	A1340	A1280	G1218	G1156	U1096	G1034	G976	C856	A790	A790	U729	U669
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A1531	G1469	C1342	C1282	G1220	U1158	U1098	G1036	A978	A918	G858	A792	G731	U671
U	G1470	G1343	G1283	G1221	U1159	G1099	C1037	C979	A919	A859	U793	G732	U672
C	G1471	C1344	C1284	C1222	C1160	C1100	C1038	C980	U920	A860	A794	G734	G673
C	G1472	U1345	A1285	C1223	C1161	A1011	C1039	U921	C861	C795	C795	G735	G674
A	A1473	A1346	A1286	G1224	C1162	A1012	U1040	U982	C922	C862	C796	G736	A675
C	G1474	G1347	A1287	A1225	C1165	C1103	A1041	A983	A923	U863	C797	A737	A676
C	G1475	U1348	A1288	C1226	C1166	G1104	G1042	C984	C924	A864	G798	C738	U677
U	C1476	A1349	A1289	A1227	A1168	G1105	A1046	C985	G925	A865	G799	U740	U678
C	C1477	A1350	G1290	C1228	C1169	C1106	G1047	A986	G926	C866	G800	C739	C679
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U	G1480	G1353	G1293	G1231	C1172	C1109	U1050	C989	G929	C869	G803	U743	G682
U	U1481	C1354	G1294	U1232	G1173	A1110	G1051	C990	C930	U870	U804	C744	G683
C	A1482	G1355	G1295	G1233	G1174	A1111	C1052	U991	C931	U871	C805	C745	A684
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A1484	G1357	A1357	C1297	U1235	G1176	C1113	G1054	G993	G933	A873	A807	C747	U686
U1485	U1358	C1298	A1298	A1236	A1177	C1114	A1054	A994	C934	C874	C808	C748	G687
C	G1359	C1299	A1299	C1237	G1177	C1115	C1055	C995	A935	C875	G809	C749	A688
U	A1360	A1238	G1300	A1238	G1178	C1116	U1056	A996	G936	G876	C810	G750	C689
U	G1361	U1239	A1239	C1240	A1179	G1117	G1057	U997	A937	C877	C811	U751	G690
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U	C1424	C1363	C1303	G1241	G1181	C1119	C1059	C999	C939	C879	U813	A753	U692
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U	U1427	G1365	A1306	C1244	G1184	U1122	U1062	A999	G942	C882	A816	C756	A695
U	C1366	U1307	U1307	A1248	G1185	A1123	G1063	G999	U943	C883	C817	U757	A696
U	C1367	G1308	U1308	C1249	G1186	U1124	G1064	U999	G944	U884	G818	G758	U697
U	G1368	U1309	G1309	U1250	G1187	U1125	U1065	A999	G945	A885	A819	A759	G698
U	C1369	G1310	G1310	A1251	A1188	U1126	C1066	A999	A946	G886	U820	G760	C699
U	G1370	G1311	G1311	A1252	C1189	U1127	A1067	A999	G947	G887	G821	G761	G700
U	G1371	G1312	G1312	A1252	G1190	C1128	G1068	A999	G948	G888	C822	C762	C701
U	U1372	U1313	G1253	G1253	G1191	C1129	G1069	A999	G949	A889	G823	G763	A702
U	G1373	C1314	C1254	C1254	A1191	A1130	U1070	G999	U950	G890	C824	C764	G703
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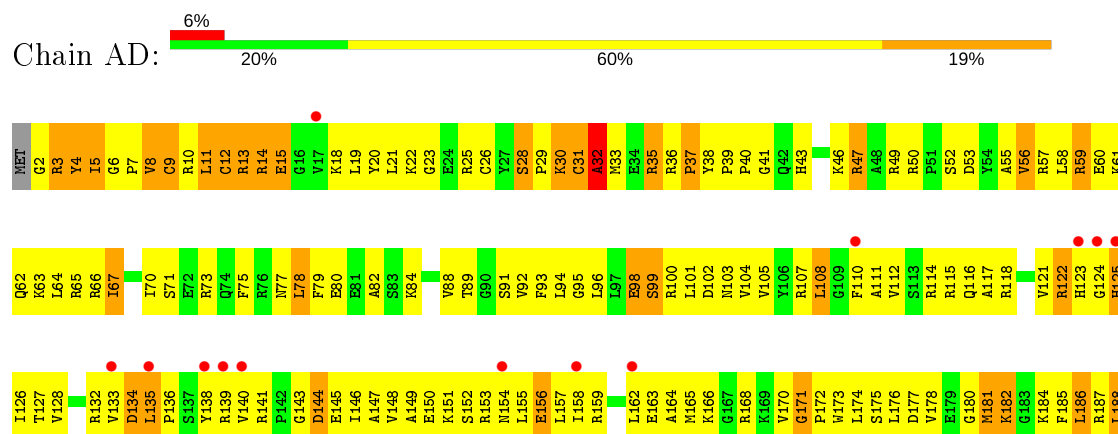
- Molecule 2: 30S RIBOSOMAL PROTEIN S2



- Molecule 3: 30S RIBOSOMAL PROTEIN S3

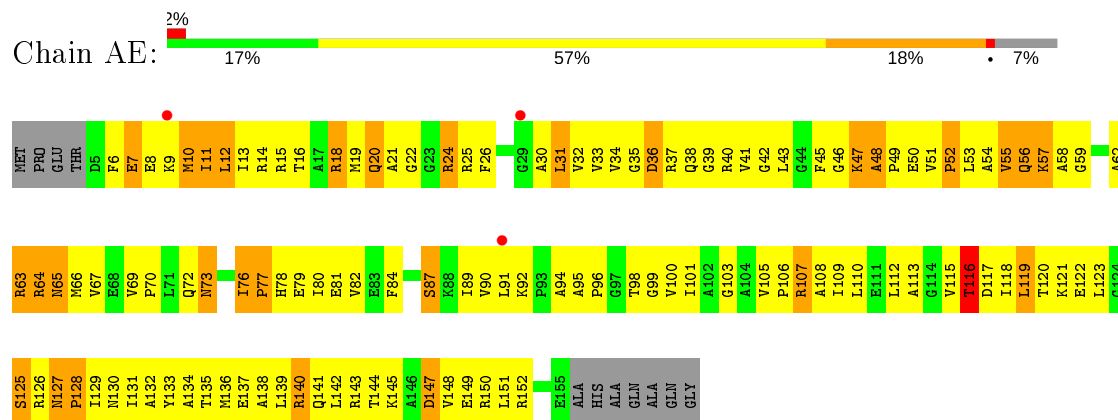


- Molecule 4: 30S RIBOSOMAL PROTEIN S4

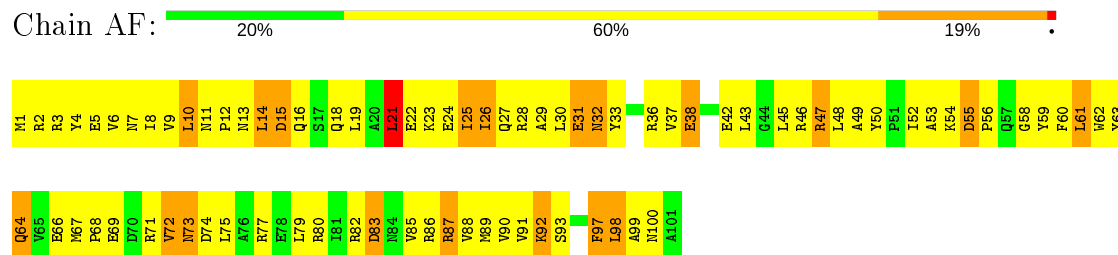


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D190
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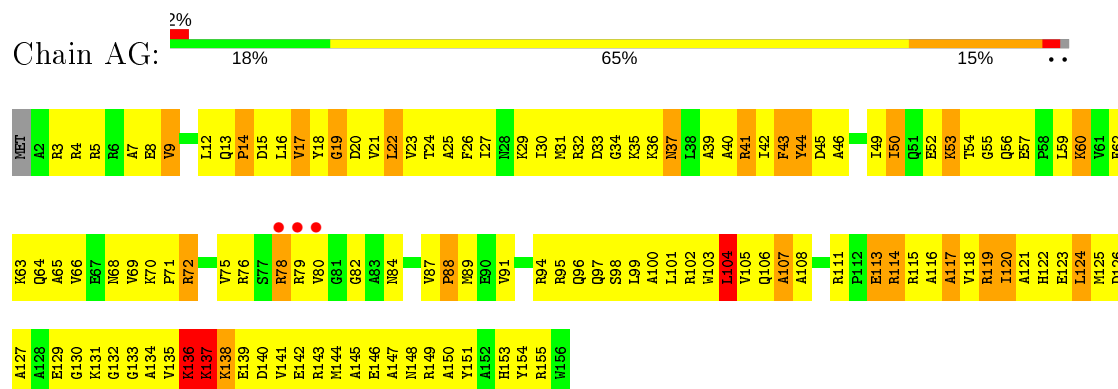
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



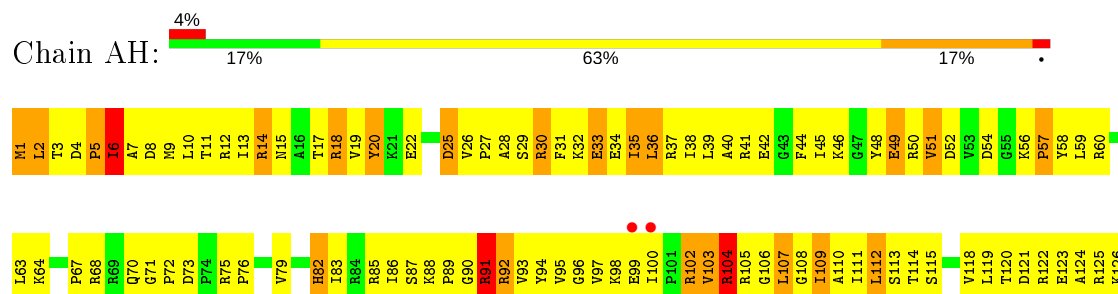
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

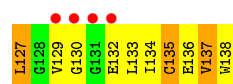


• Molecule 7: 30S RIBOSOMAL PROTEIN S7

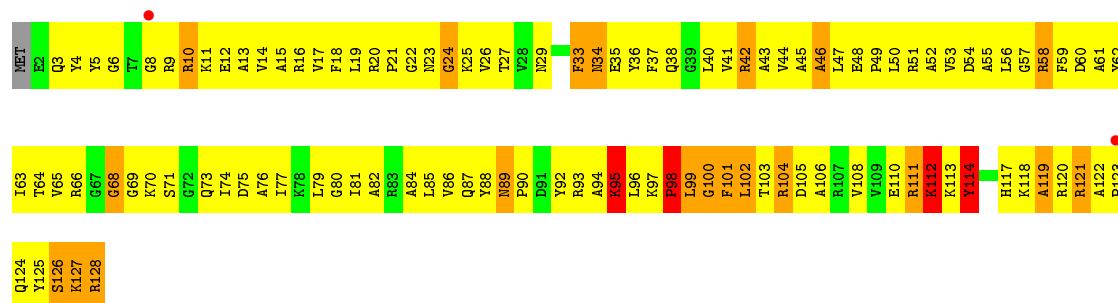


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

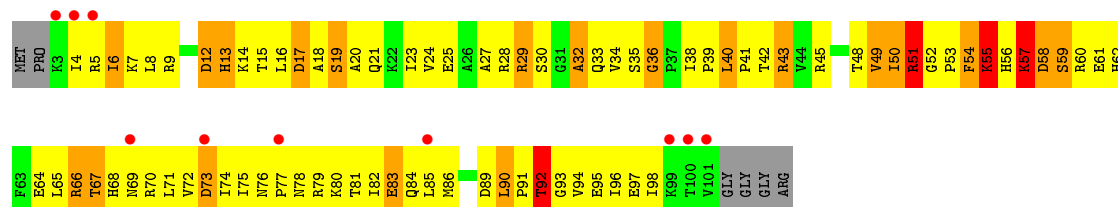
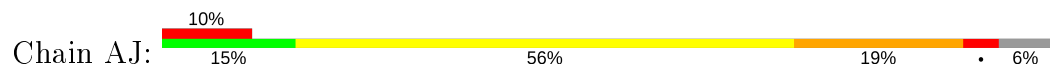




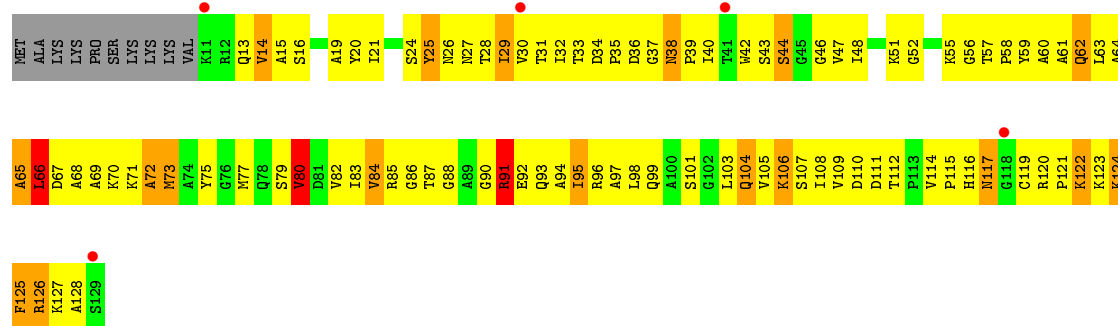
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



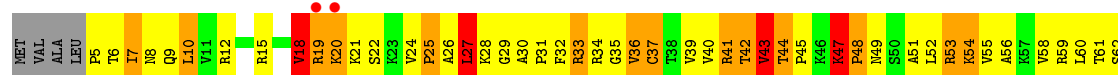
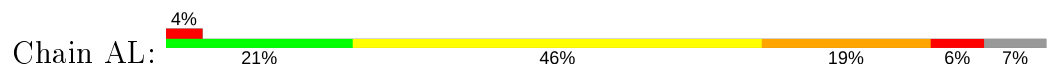
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

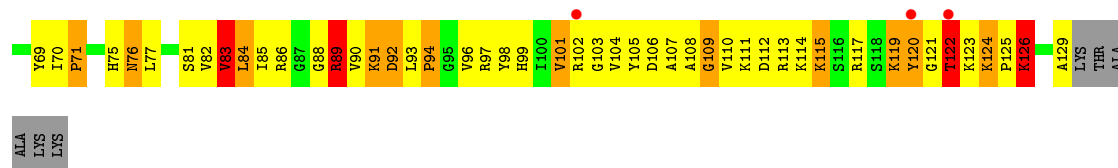


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

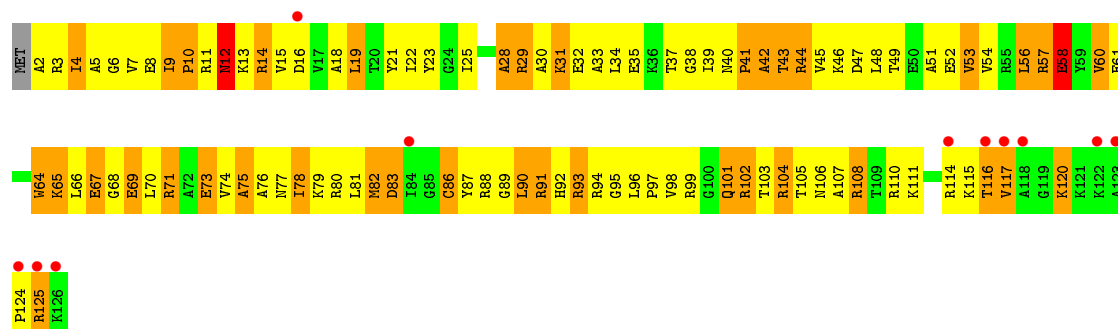


• Molecule 12: 30S RIBOSOMAL PROTEIN S12

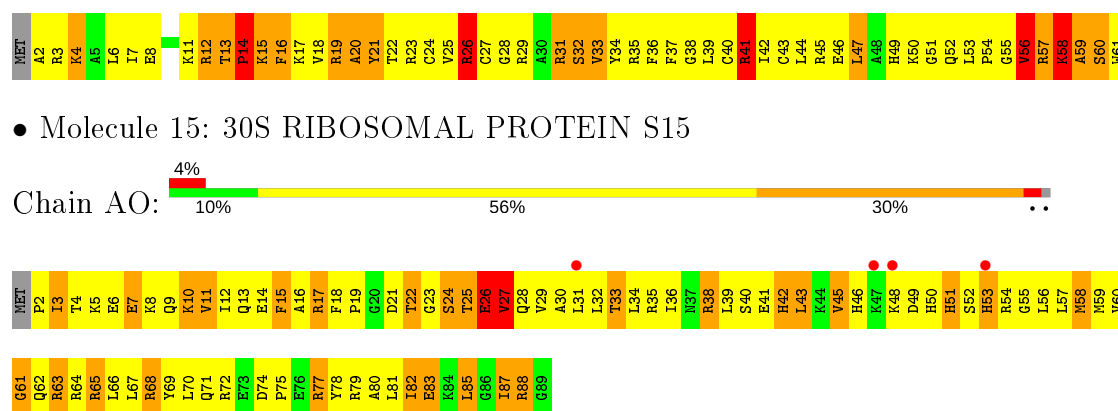
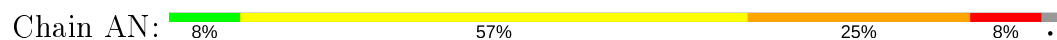




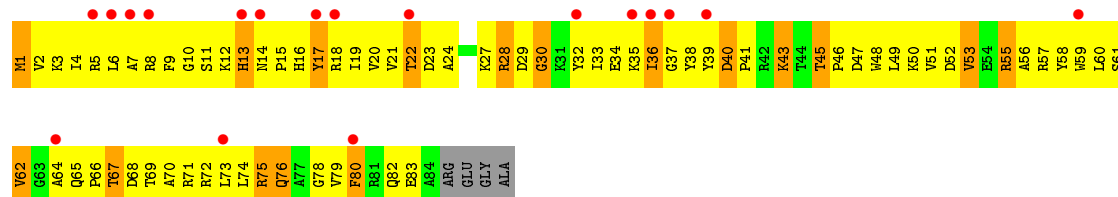
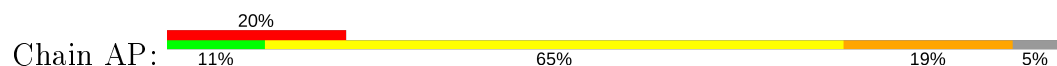
• Molecule 13: 30S RIBOSOMAL PROTEIN S13



• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z



• Molecule 15: 30S RIBOSOMAL PROTEIN S15



• Molecule 16: 30S RIBOSOMAL PROTEIN S16





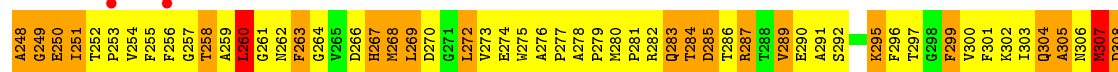
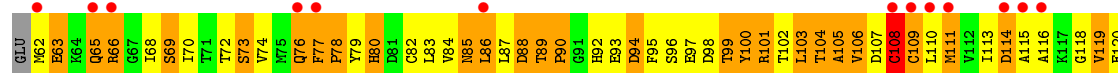
- Molecule 23: MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

Chain AX: 11% 44% 44%



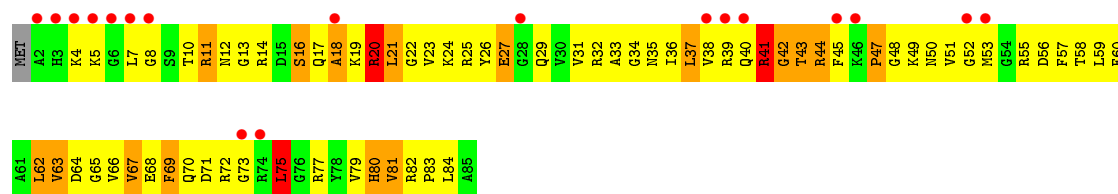
- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3

Chain AY: 10% 12% 47% 29% 5% 6%

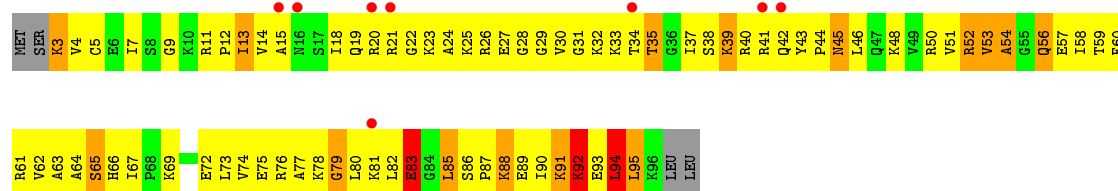


- Molecule 25: 50S RIBOSOMAL PROTEIN L27

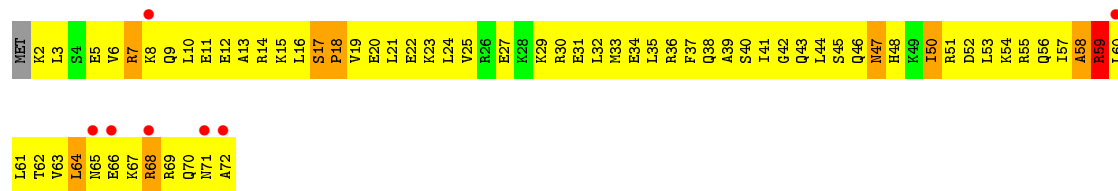
Chain B0: 21% 16% 60% 19%



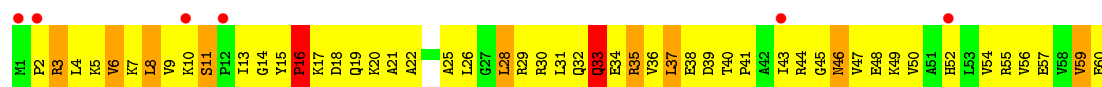
• Molecule 26: 50S RIBOSOMAL PROTEIN L28



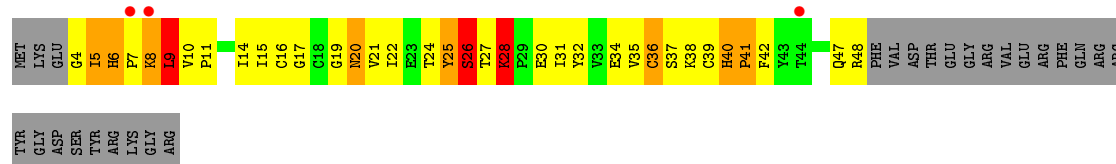
• Molecule 27: 50S RIBOSOMAL PROTEIN L29



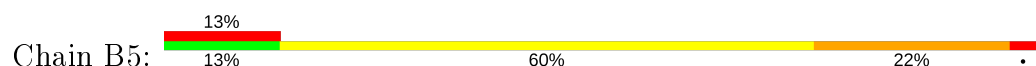
• Molecule 28: 50S RIBOSOMAL PROTEIN L30



• Molecule 29: 50S RIBOSOMAL PROTEIN L31



• Molecule 30: 50S RIBOSOMAL PROTEIN L32





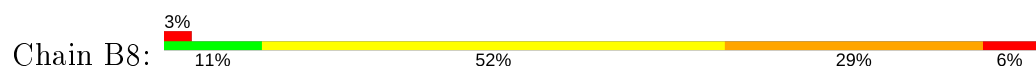
• Molecule 31: 50S RIBOSOMAL PROTEIN L33



• Molecule 32: 50S RIBOSOMAL PROTEIN L34



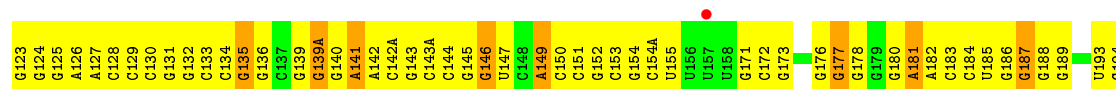
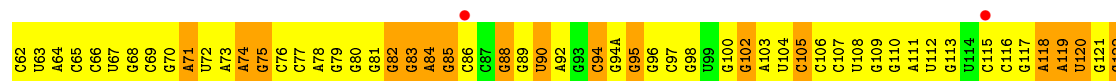
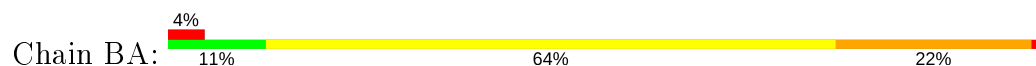
• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 34: 50S RIBOSOMAL PROTEIN L36



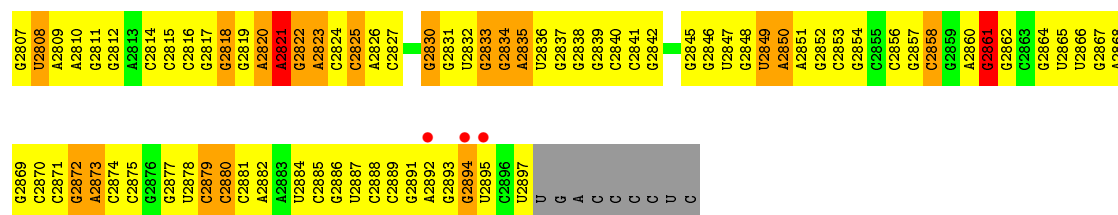
• Molecule 35: 23S RIBOSOMAL RNA



A1001	G942	A878	C817	A752	C692	A653	U594	C531	G467	A402	C343	A282	A196
G1002	U943	G879	G818	C753	C693	A654	C595	A532	G468	U403	G344	A283	A197
G1003	G944	G880	G819	C754	U694	G654C	G596	U534	G469	C404	A345	U284	C198
G1004	A945	G881	C755	G754	G695	G654D	U597	C533	C285	G258	A346	C286	C199
C1005	G946	G882	G823	C756	C696	G654E	G598	C535	A471	G406	A347	C287	A200
G1006	G947	C883	G824	A761	C698	G654F	G600	C536	A472	G407	G348	C288	C201
C1007	G948	C884	A824	U762	A699	G654G	C601	U537	G473	G408	C349	C289	C202
G1008	G949	C885	C825	U763	A699	G654H	G602	G538	U474	C409	U350	A290	C203
G950	G950	A887	U826	G763	G700	G654I	G603	C539	C286	G261	A262	G290	C204
A1010	C951	C888	U827	G764	G701	G654J	A603	C540	C291	C264	C352	C291	G205
G1011	G952	C889	U828	G765	G702	A654K	A604	C541	A277	A412	G353	C292	G206
A953	G953	A890	A829	C766	U703	G654L	C605	C542	A478	C413	G354	U293	A207
C1013	G954	G892	G830	U767	G704	G654M	U606	C543	A479	C414	A355	A294	C208
U1014	C955	C893	G831	G768	A705	C654N	U607	A547	A480	C419	G356	G295	C209
G1015	G956	C894	G832	G769	A706	G654O	A608	A548	A481	C420	A357	C296	C210
G1018	A957	U895	U833	G770	G707	G654P	A609	G549	A482	A271	U358	C297	A211
U1019	U958	A896	C834	G771	C708	G654Q	G612	G550	A483	A423	A359	G298	A212
A1020	A959	C897	A835	G772	U709	A654R	G613	G551	A484	A424	G360	A299	G212
A1021	C961	C898	G836	U773	G710	G654S	U614	G552	C485	G425	G361	A300	A213
G962	U962	A900	C837	G774	G711	G654T	U615	G553	C486	U426	U362	G301	G214
U1023	U963	A901	C838	G775	G712	C654U	U616	U554	G489	C427	G363	C302	G215
G1024	C964	C902	U839	G776	G713	A654U	G617A	U555	A491	U427	A363A	U303	A216
G965	G965	C903	C840	A777	U714	A654V	A614C	G556	A492	A428	G364	G304	G217
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A1026	G967	U905	G842	U779	A716	G656	G616	G558	A494	U431	U366	U306	A219
A1027	G968	G906	G843	G780	G717	U657	C618	G559	G495	G432	A367	G307	G220
A1028	U969	U907	C844	A781	A718	C658	G619	C560	G496	A433	C364	G308	A221
A1029	C970	A908	G845	A782	C719	C659	G620	G561	C497	A434	G365	G309	A222
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A1032	G972	A910	U847	A784	G721	C661	G622	G563	G499	C435	G367	A311	G224
U1033	A973	C912	G848	G785	A722	G662	G623	C564	U499	C436	A371	G312	A225
G1034	G974	C912	C850	G786	G723	G663	G624	C565	G500	G437	G372	C313	G226
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G1036	G975A	C914	G852	A788	G725	G665	U626	U567	A502	G440	G374	G315	A228
C1037	C976	C915	G853	G790	G726	G666	A627	U568	G442	G271G	C375	G316	A229
U1038	G977	G916	G854	C791	A727	U667	G628	U569	A505	G443	C376	G317	U230
G1039	G978	A917	G855	G792	G728	G668	G629	G570	A506	G444	C377	C318	C231
C1040	G979	A918	C856	G793	G729	G669	G630	A571	A507	C445	C378	G321	G232
G1041	A980	G919	C857	C731	C731	A670	A631	A572	G508	G446	G379	A322	A233
C1042	C981	G920	U858	C732	C732	C671	A632	G573	C509	G447	U380	G323	C234
G1043	C982	C921	U859	C733	G733	C672	A633	C574	U510	U447	G381	A324	U235
A1044	A983	U922	U860	A734	A734	C673	C634	A575	G511	U448	G382	G325	C236
A1045	C984	C923	A861	A735	A735	G674	C635	U576	G512	A449	U384	G326	C237
A1046	C985	C924	G862	C736	C736	A675	G636	G577	A513	C450	C385	G327	U239
G1047	C986	C925	A863	G737	G737	A676	A637	A578	A514	G452	G386	U328	G240
A1048	G987	A926	G864	U803	G738	C677	G638	G579	A515	C453	U387	G329	A241
C1049	A988	C927	C865	A804	G739	C678	U639	C580	C516	G454	G388	A330	G242
A1050	G989	U930	A866	G805	U740	G680	C641	C581	G517	C455	G389	A331	U243
G1051	A990	C931	G867	C806	G741	G681	G642	G582	U519	C456	A390	A332	U244
C1052	C991	G932	U868	U807	G742	G682	A643	C584	G520	A457	G391	G333	G245
A1053	G992	C932	G869	G808	G743	C683	A644	G585	C523	G458	C392	C334	C246
G1054	A993	A933	A870	U809	G744	G684	C645	A586	U524	U459	C393	C335	G247
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G1056	G995	C935	A872	U811	A746	G686	G647	U588	U526	C461	G395	C337	C249
A1057	A996	G936	G873	C812	U747	C687	G648	C589	A527	G462	G396	G338	G250
G1058	G997	G937	G874	U813	G748	U688	G649	A590	C527	G463	G397	U339	A251
G1059	C998	G938	G875	C814	G749	C689	C650	A591	U528	U464	G398	A340	G252
U1060	U999	G940	C876	A750	A750	A690	G651	C592	A529	G465	G399	G341	C253
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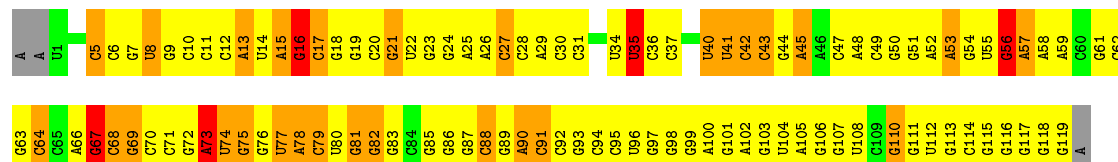
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G1823	C1683	G1623	A1562	C1501	A1439	A1379	A1317	G1256	G1135		A1073
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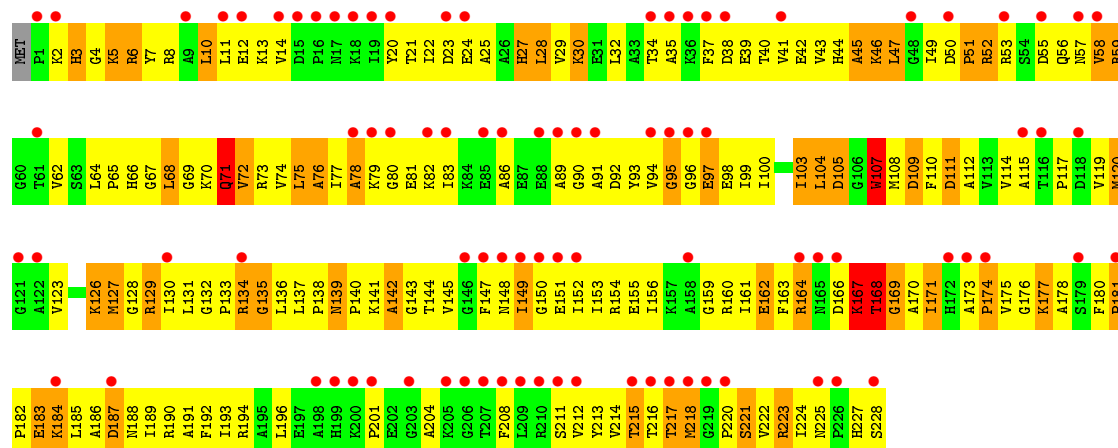
• Molecule 36: 5S RIBOSOMAL RNA

Chain BB: 11% 60% 23% . .



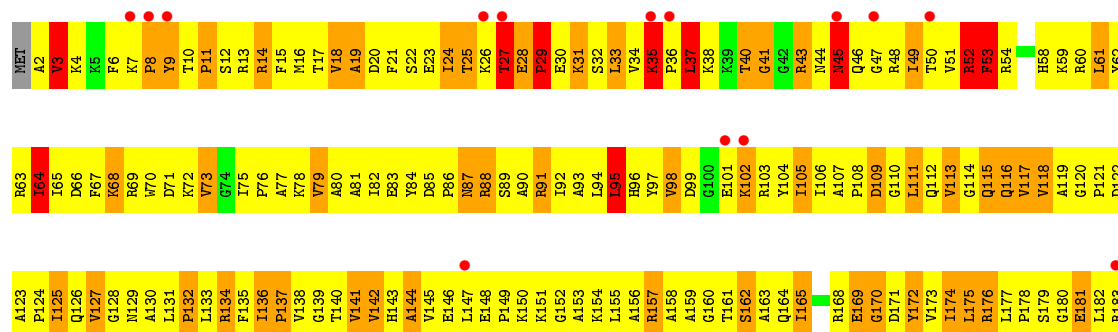
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

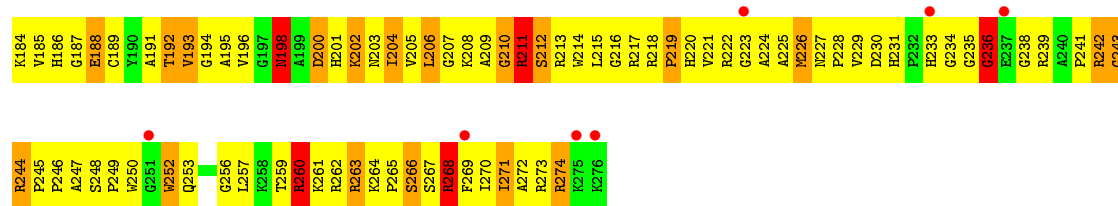
Chain BC: 22% 39% 54% 22% .



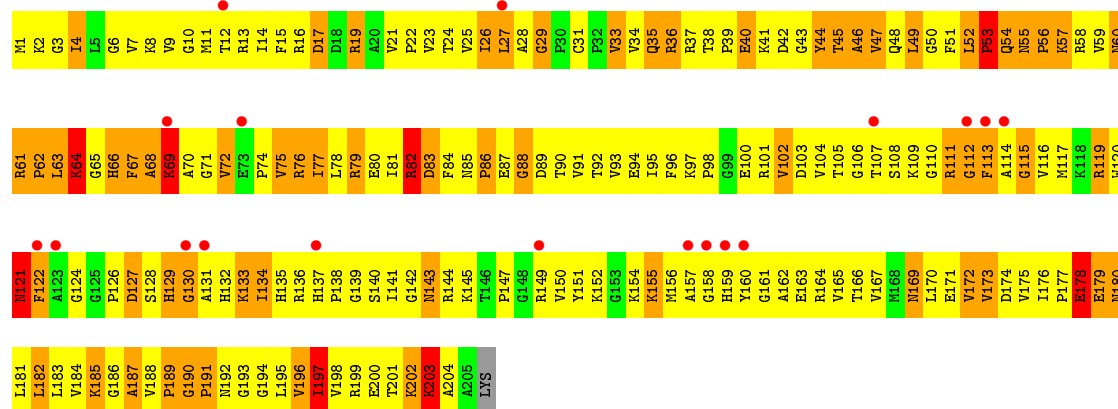
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

Chain BD: 8% 61% 25% 5%

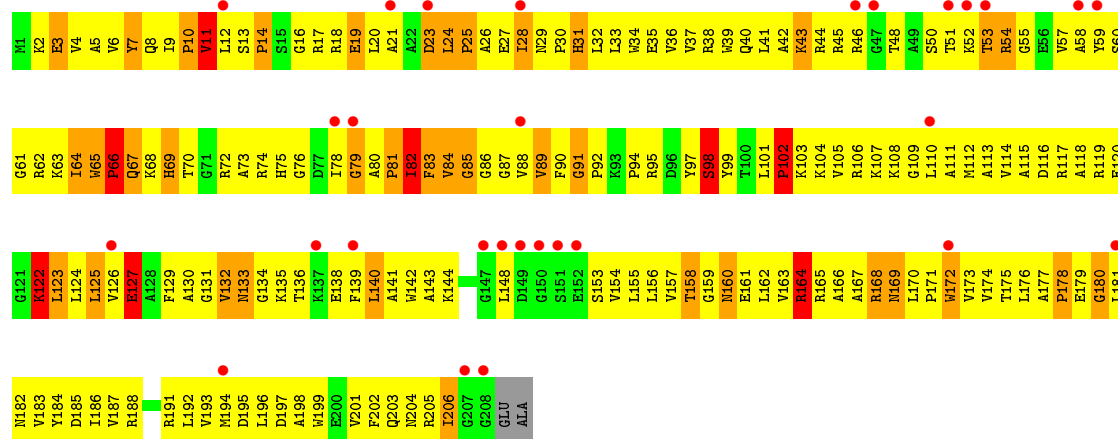
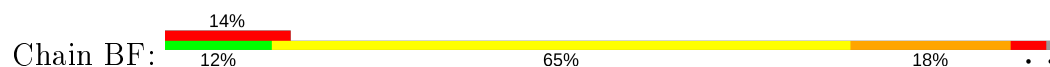




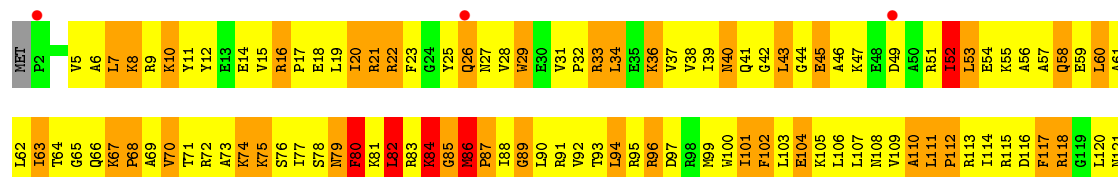
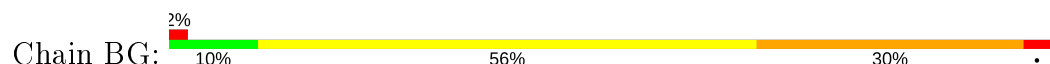
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



• Molecule 40: 50S RIBOSOMAL PROTEIN L4

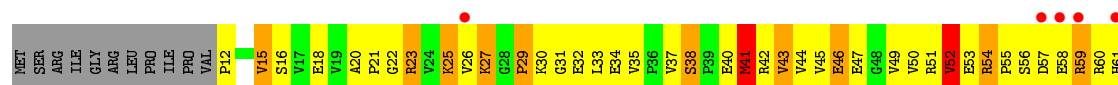
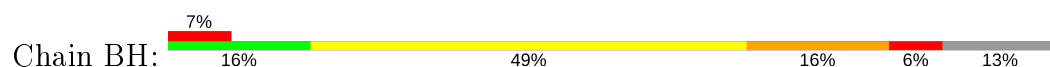


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

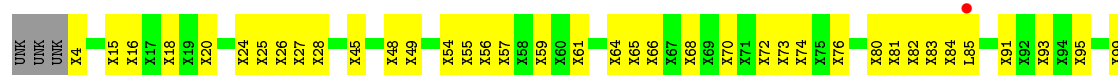




• Molecule 42: 50S RIBOSOMAL PROTEIN L6



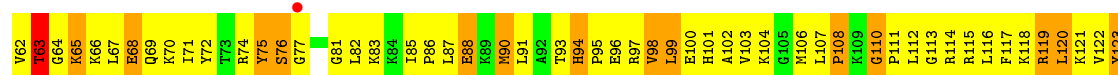
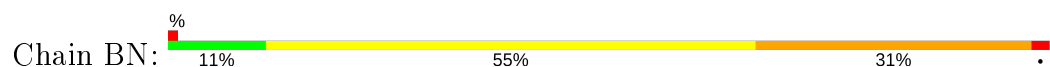
• Molecule 43: 50S RIBOSOMAL PROTEIN L10



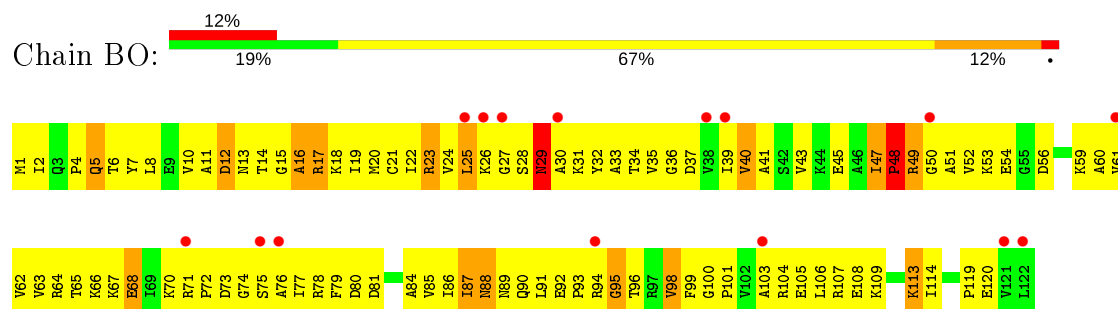
• Molecule 44: 50S RIBOSOMAL PROTEIN L11



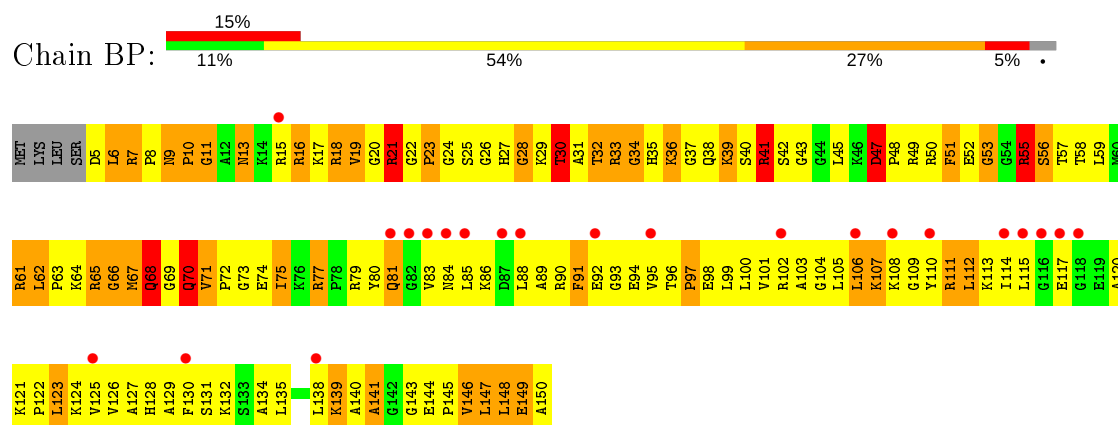
• Molecule 45: 50S RIBOSOMAL PROTEIN L13



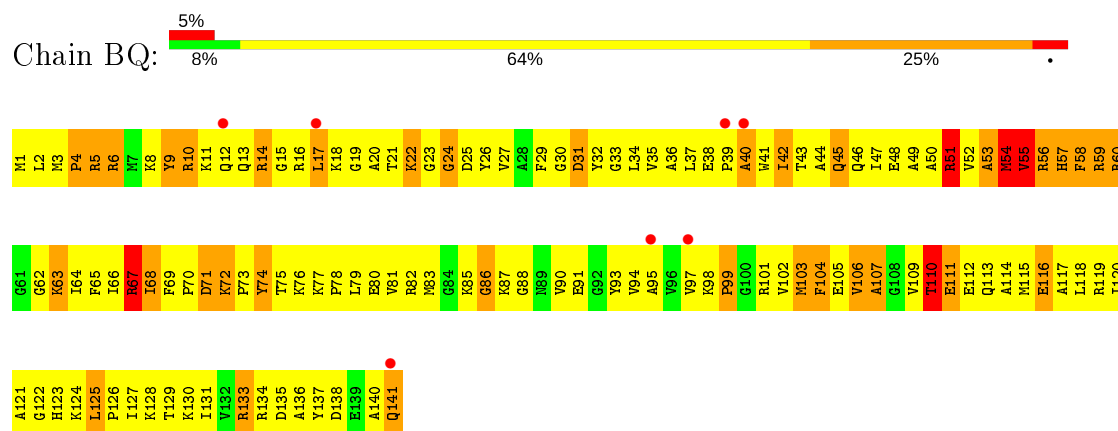
● Molecule 46: 50S RIBOSOMAL PROTEIN L14



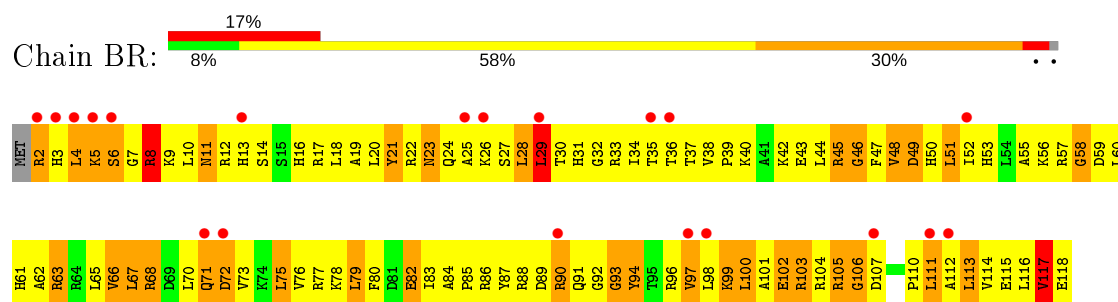
● Molecule 47: 50S RIBOSOMAL PROTEIN L15



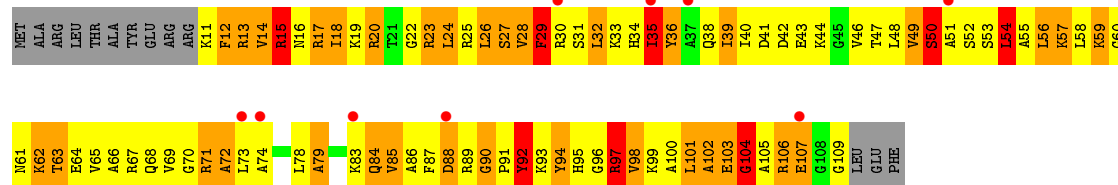
● Molecule 48: 50S RIBOSOMAL PROTEIN L16



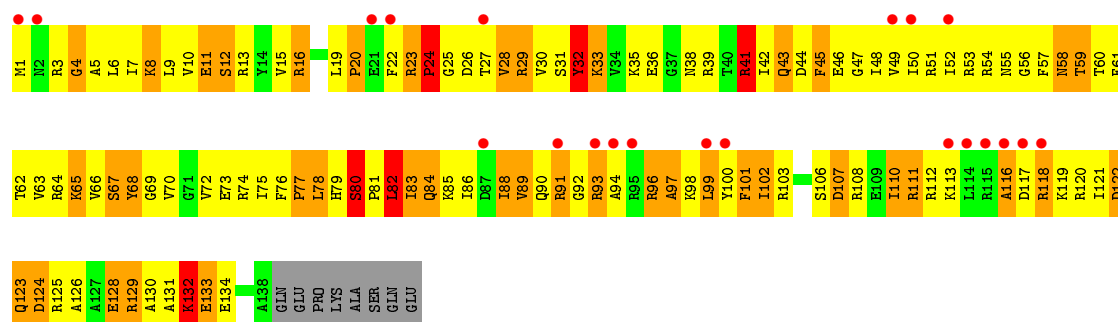
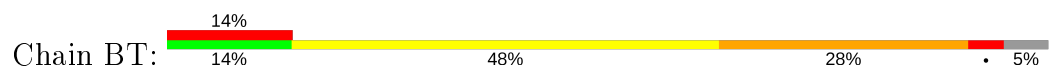
● Molecule 49: 50S RIBOSOMAL PROTEIN L17

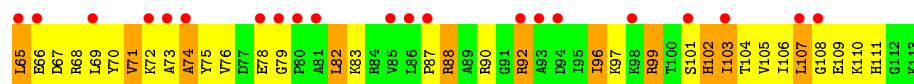


● Molecule 50: 50S RIBOSOMAL PROTEIN L18

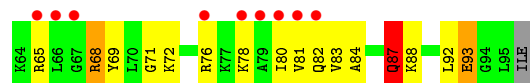
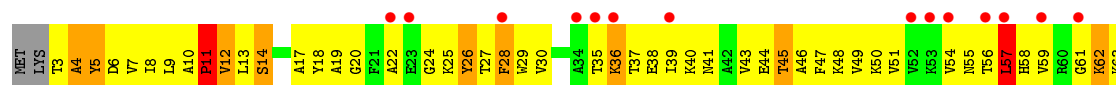


• Molecule 51: 50S RIBOSOMAL PROTEIN L19

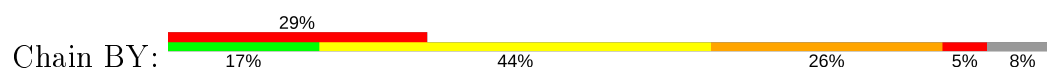




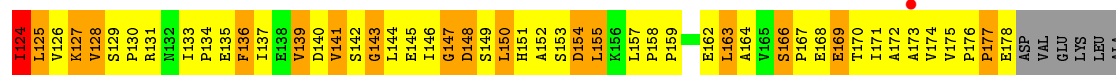
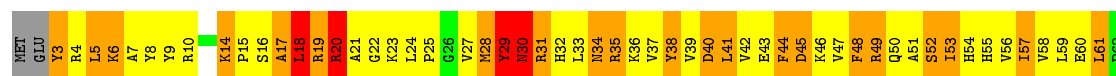
• Molecule 55: 50S RIBOSOMAL PROTEIN L23



• 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)	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	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 ⓘ

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	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	2.81	7 (26%)	31,54,54	1.90	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	9.05	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	C4-N9	-5.77	1.40	1.47
58	AY	1000	GCP	C5-C6	-5.19	1.43	1.52
58	AY	1000	GCP	PG-O2G	-2.81	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	O6-C6-C5	2.71	125.39	119.86
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
58	AY	1000	GCP	C5-C6-N1	-2.64	114.93	118.19

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

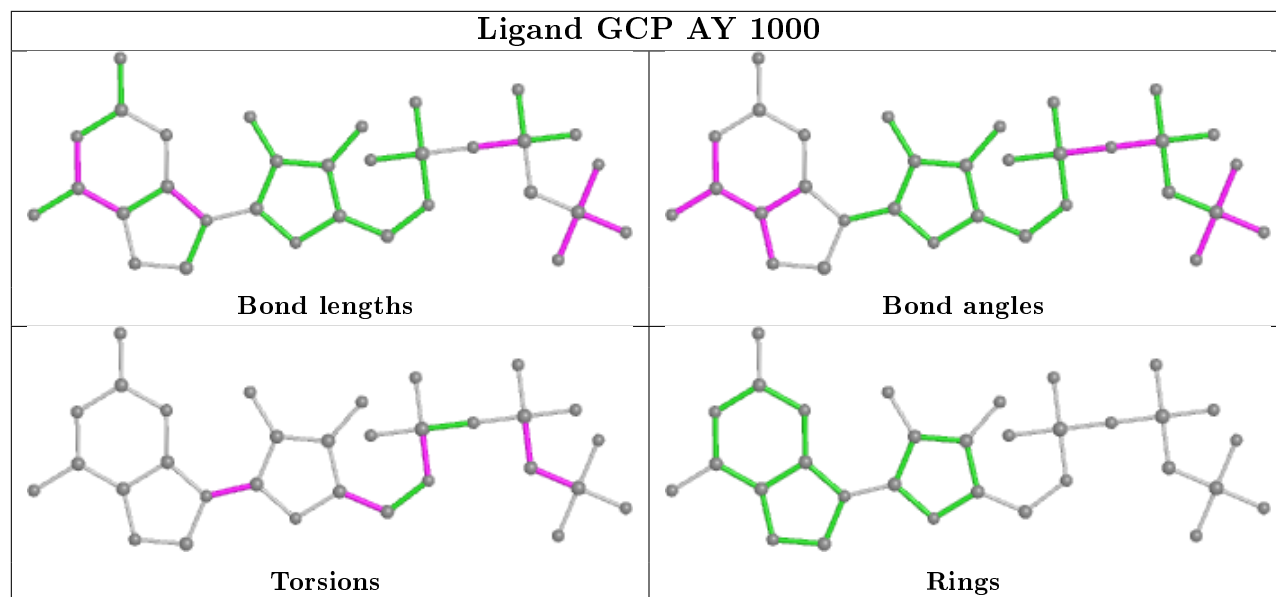
Mol	Chain	Res	Type	Atoms
58	AY	1000	GCP	PB-C3B-PG-O1G
58	AY	1000	GCP	PB-C3B-PG-O2G
58	AY	1000	GCP	PG-C3B-PB-O1B
58	AY	1000	GCP	PG-C3B-PB-O3A
58	AY	1000	GCP	C5'-O5'-PA-O3A

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 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 ⓘ

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 ⓘ

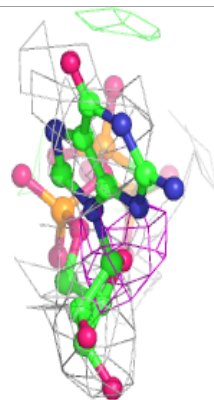
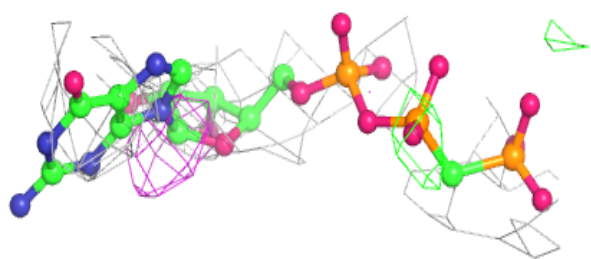
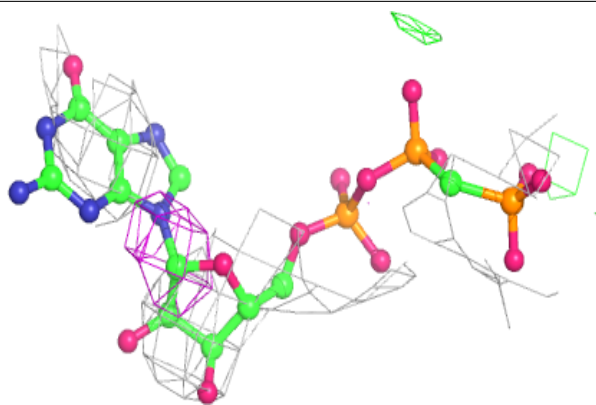
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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