



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:12 PM UTC

PDB ID : 4V89 / pdb_00004v89
Title : Crystal Structure of Release Factor RF3 Trapped in the GTP State on a Rotated Conformation of the Ribosome (without viomycin)
Authors : Zhou, J.; Lancaster, L.; Trakhanov, S.; Noller, H.F.
Deposited on : 2011-11-17
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

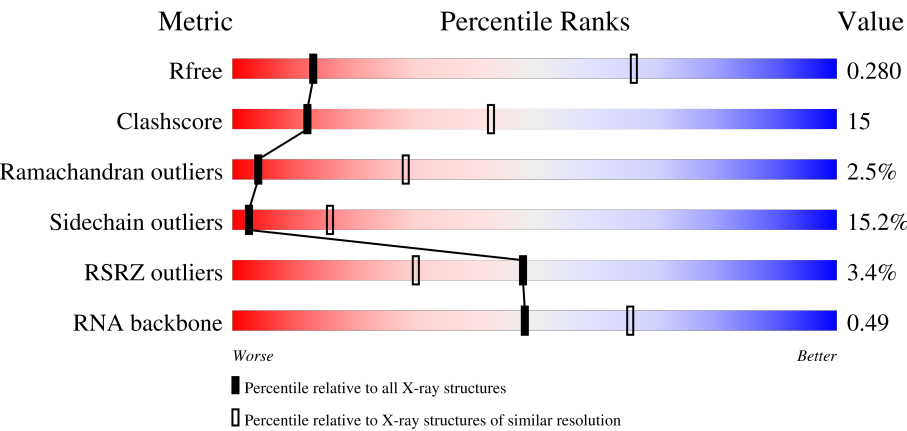
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)
RNA backbone	3983	1007 (4.30-3.08)

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

Mol	Chain	Length	Quality of chain
1	AA	1533	2% 51%40%10%
2	AB	241	3% 43%37%10%10%
3	AC	233	2% 48%31%9%12%
4	AD	206	6% 49%42%9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	AE	167	
6	AF	135	
7	AG	179	
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	27	
23	AW	534	
24	B0	85	
25	B1	78	
26	B2	63	
27	B3	59	
28	B4	57	
29	B5	55	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	B6	46	
31	B7	65	
32	B8	38	
33	BA	2903	
34	BB	118	
35	BC	273	
36	BD	209	
37	BE	201	
38	BF	179	
39	BG	177	
40	BH	165	
41	BI	142	
42	BJ	121	
42	BK	121	
42	BL	121	
42	BM	121	
43	BN	142	
44	BO	123	
45	BP	144	
46	BQ	136	
47	BR	127	
48	BS	117	
49	BT	115	
50	BU	118	
51	BV	103	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
52	BW	110	57%32%11%
53	BX	100	% 37%44%11%7%
54	BY	104	% 61%32%6%
55	BZ	94	65%31%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 146665 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	1532	Total	C	N	O	P	0	0	0
			32873	14661	6031	10649	1532			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- 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
			1022	634	206	179	3			

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- 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
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- 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	0
			637	408	120	107	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	6	Total	C	N	O	P	0	0	0
			129	58	24	41	6			

- Molecule 23 is a protein called Peptide chain release factor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	525	Total	C	N	O	S	0	0	0
			4144	2617	722	783	22			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AW	530	HIS	-	expression tag	UNP P0A7I4
AW	531	HIS	-	expression tag	UNP P0A7I4
AW	532	HIS	-	expression tag	UNP P0A7I4
AW	533	HIS	-	expression tag	UNP P0A7I4
AW	534	HIS	-	expression tag	UNP P0A7I4

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B0	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B1	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B2	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B3	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 28 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B4	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	B5	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B6	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B7	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B8	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 33 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BA	2853	Total	C	N	O	P	0	0	0
			61252	27324	11274	19801	2853			

- Molecule 34 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 36 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 37 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 38 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 39 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 40 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BH	163	Total	C	N	O	S	0	0	0
			1230	775	219	229	7			

- Molecule 41 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 42 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BJ	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
42	BK	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
42	BL	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			
42	BM	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			

- Molecule 43 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BN	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 44 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BO	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 45 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BP	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 46 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BQ	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 47 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BR	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 48 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BS	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 49 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BT	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 50 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BU	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 51 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BV	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 52 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 53 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BX	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

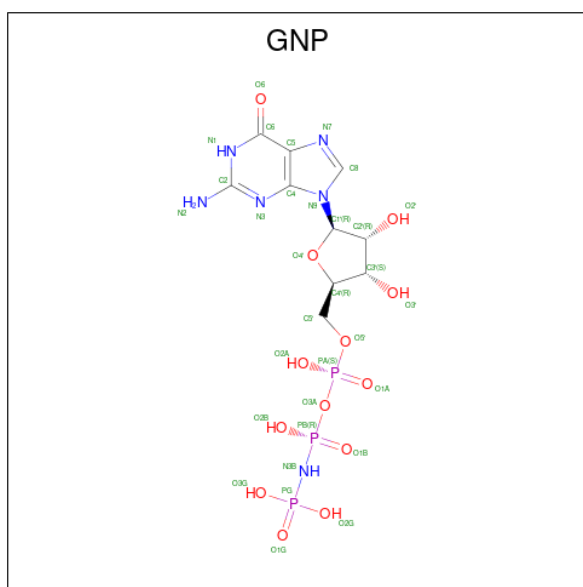
- Molecule 54 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	BY	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 55 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BZ	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

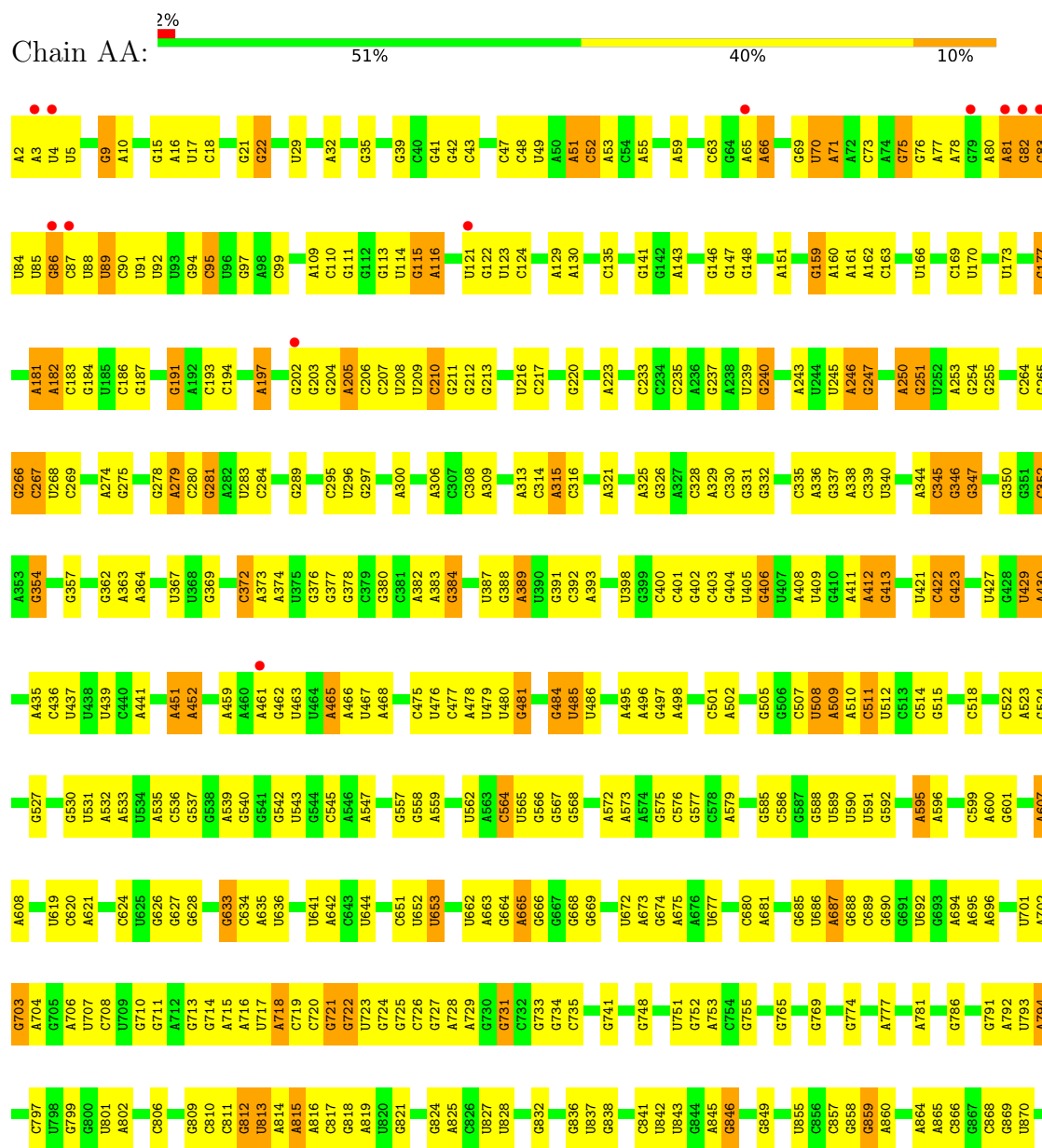
- Molecule 56 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

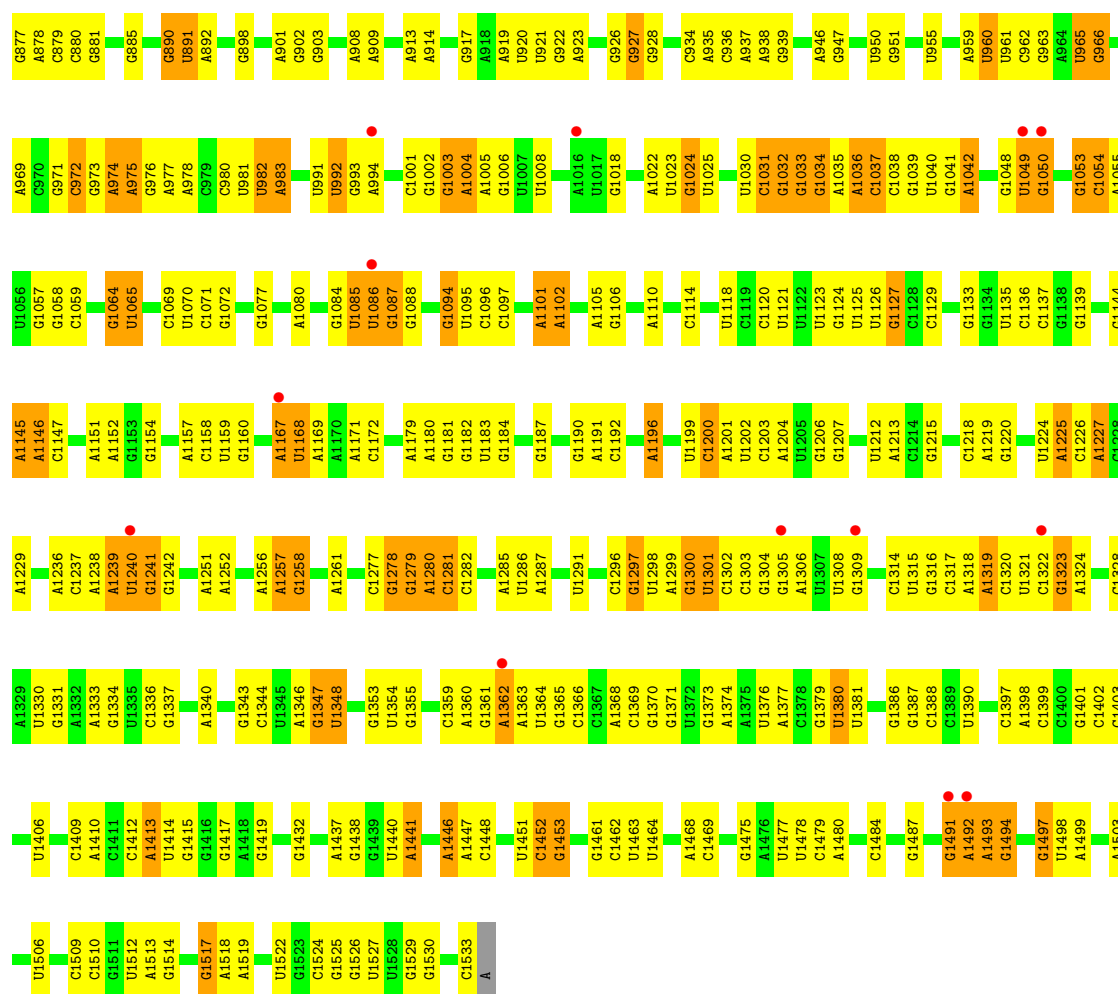


3 Residue-property plots

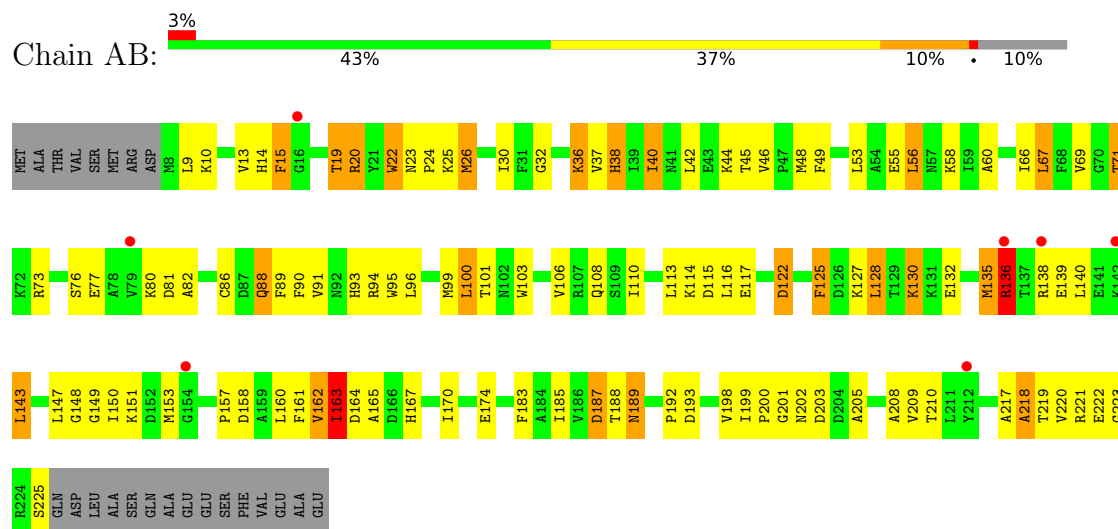
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA



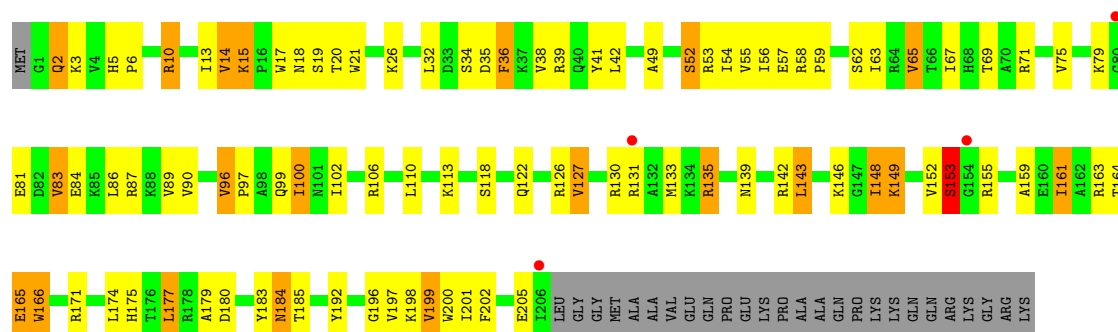


- Molecule 2: 30S ribosomal protein S2

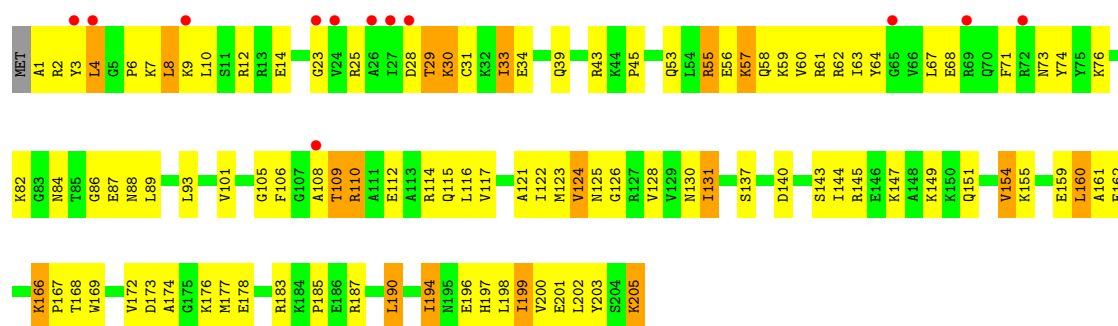


- Molecule 3: 30S ribosomal protein S3

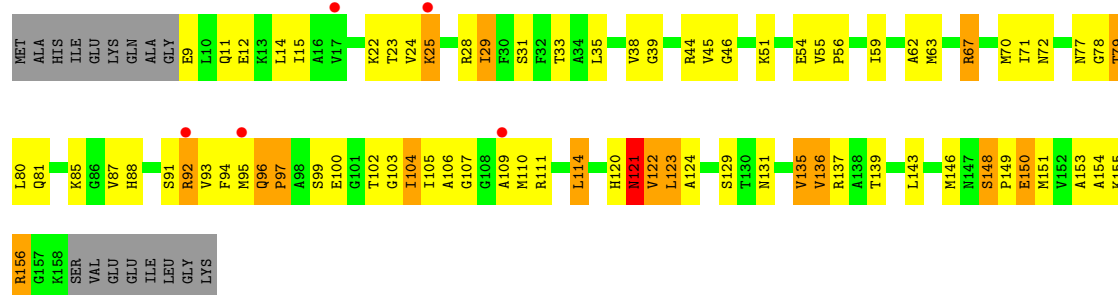
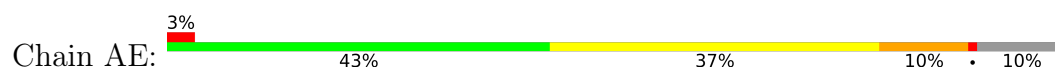




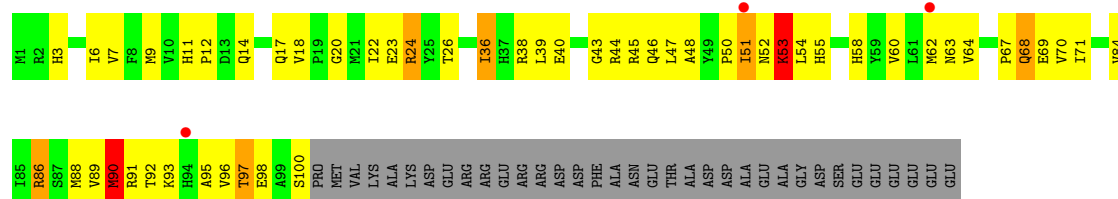
• Molecule 4: 30S ribosomal protein S4



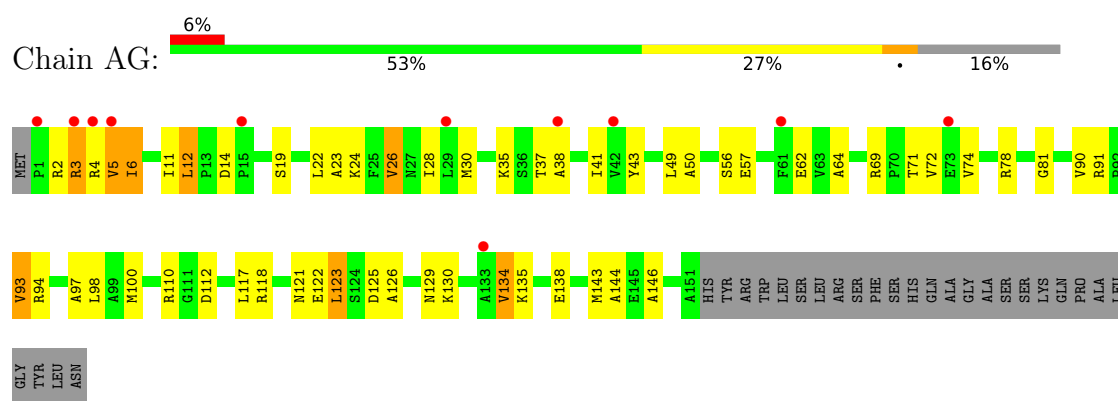
• Molecule 5: 30S ribosomal protein S5



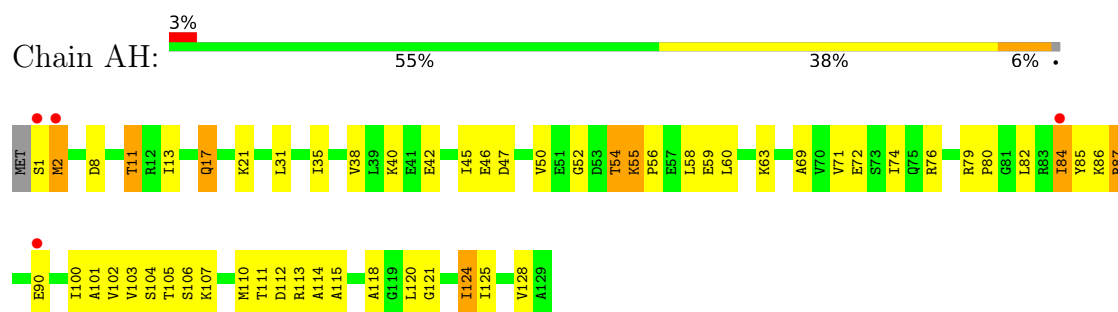
• Molecule 6: 30S ribosomal protein S6



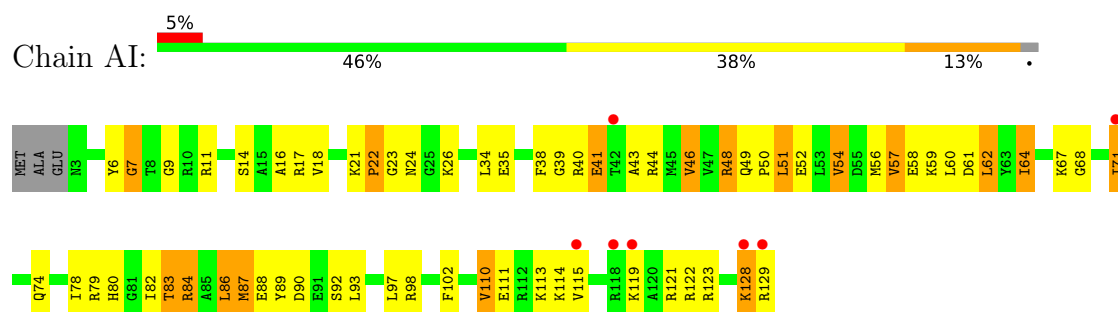
• Molecule 7: 30S ribosomal protein S7



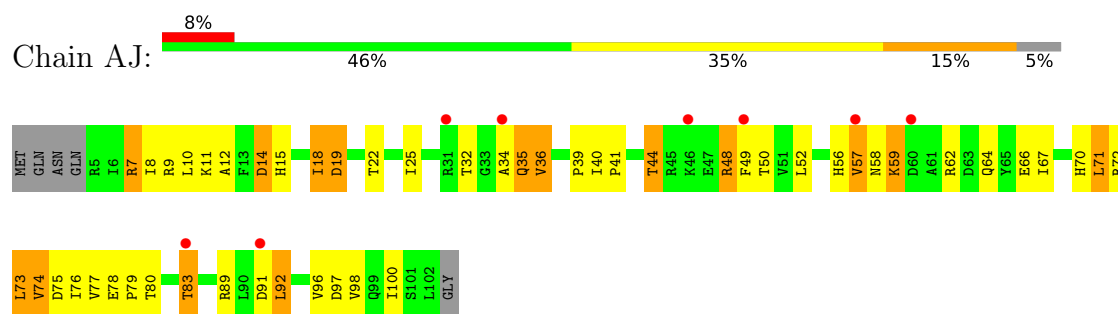
• Molecule 8: 30S ribosomal protein S8



• Molecule 9: 30S ribosomal protein S9

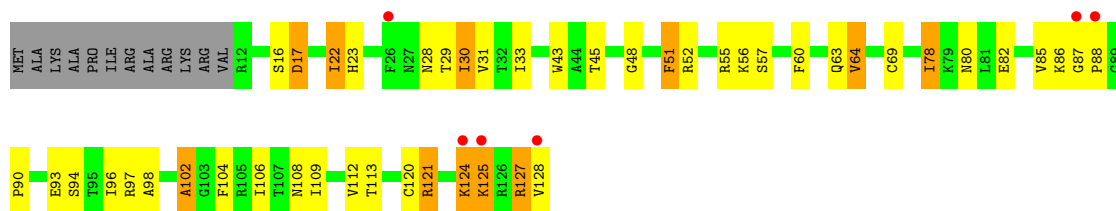


• Molecule 10: 30S ribosomal protein S10

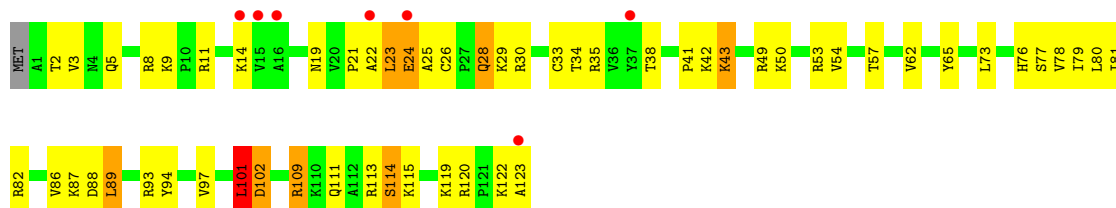


• Molecule 11: 30S ribosomal protein S11

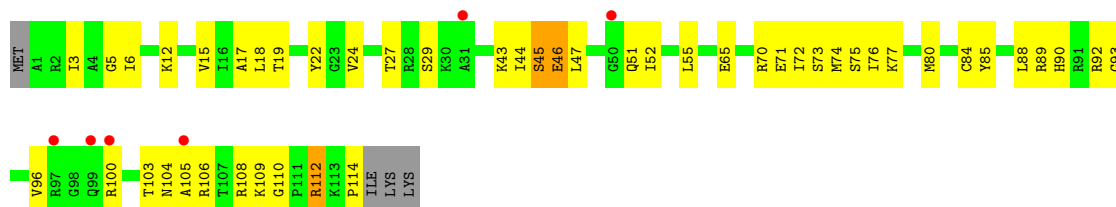




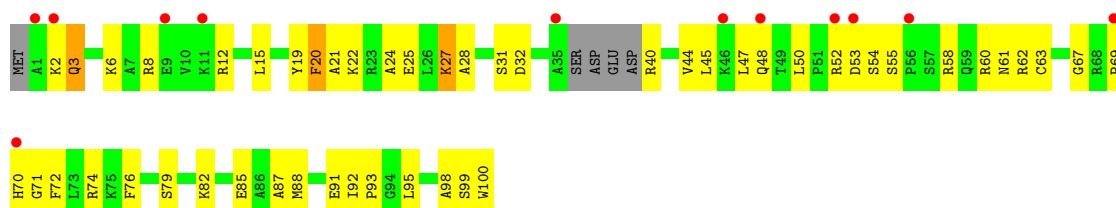
• Molecule 12: 30S ribosomal protein S12



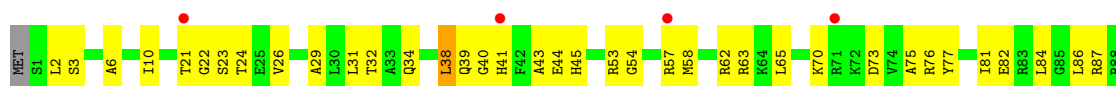
• Molecule 13: 30S ribosomal protein S13



• Molecule 14: 30S ribosomal protein S14



• Molecule 15: 30S ribosomal protein S15

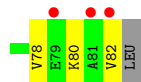
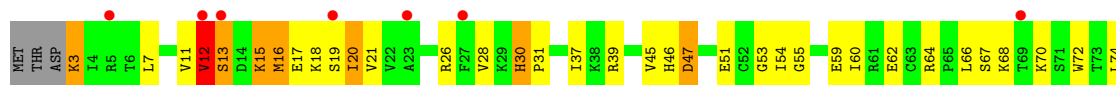


• Molecule 16: 30S ribosomal protein S16

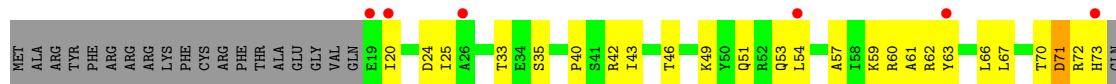




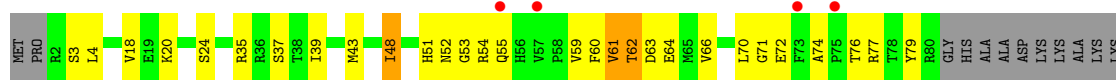
- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20

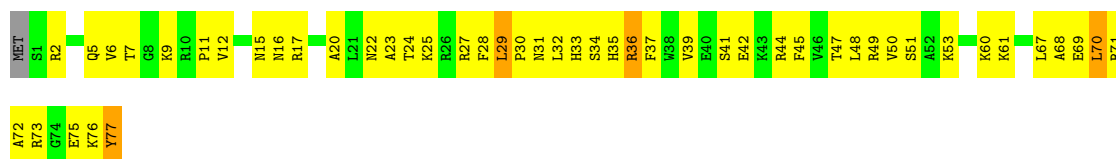


- Molecule 21: 30S ribosomal protein S21

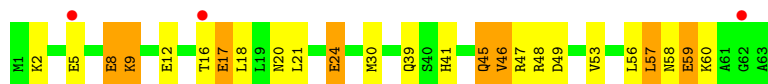


Chain AV:

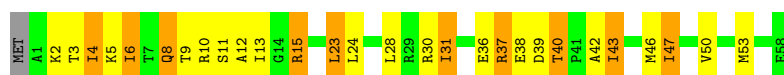




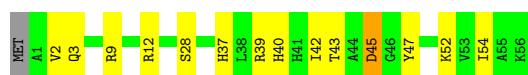
- Molecule 26: 50S ribosomal protein L29



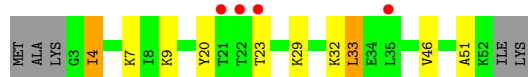
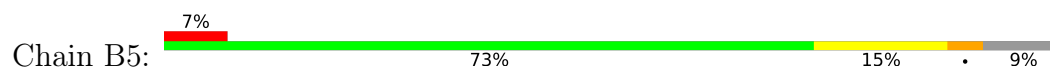
- Molecule 27: 50S ribosomal protein L30



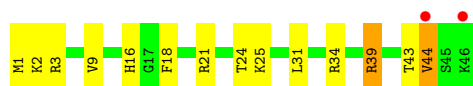
- Molecule 28: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L33



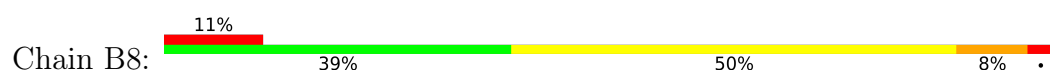
- Molecule 30: 50S ribosomal protein L34



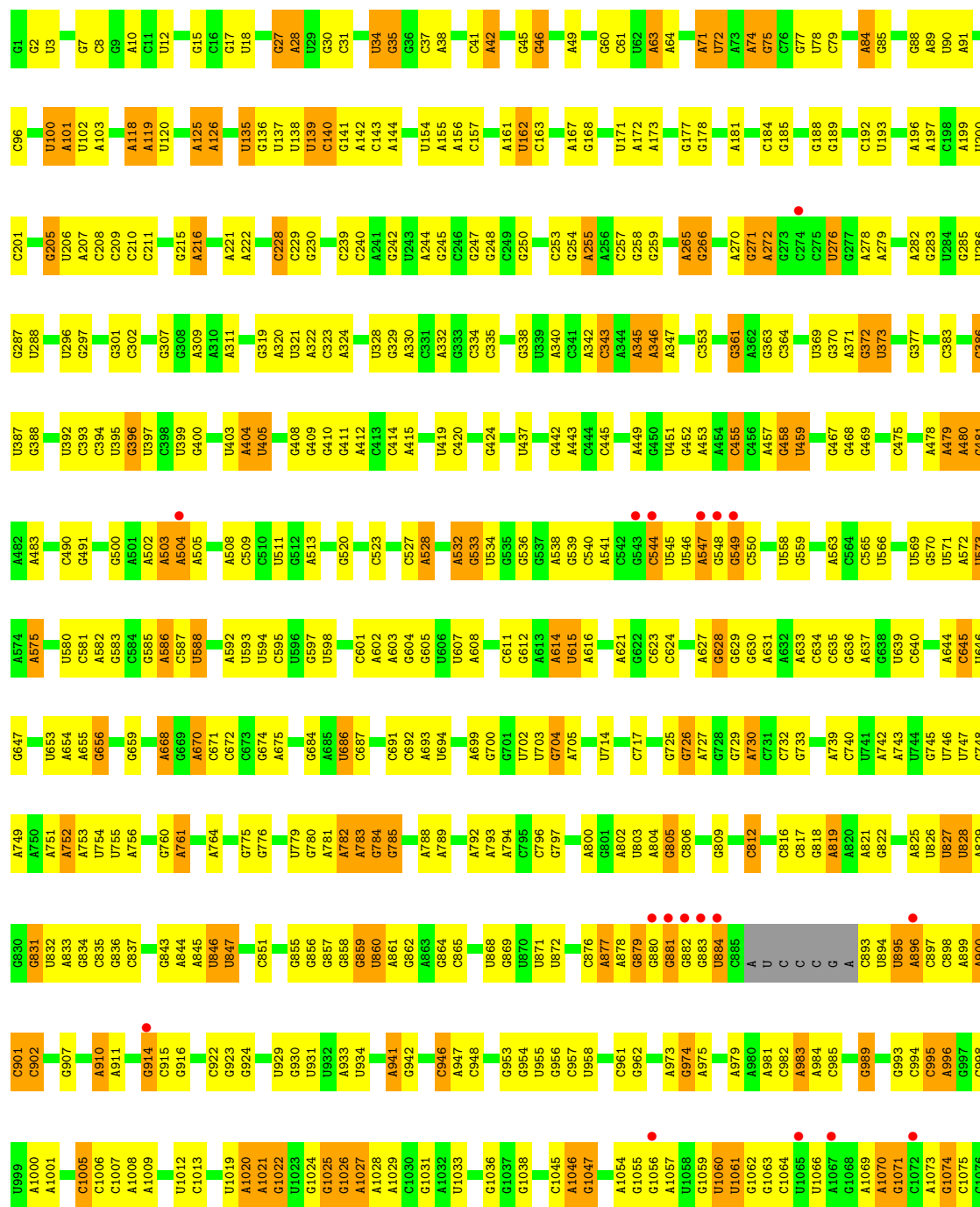
- Molecule 31: 50S ribosomal protein L35



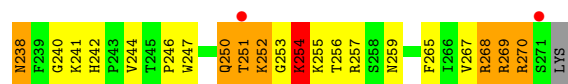
- Molecule 32: 50S ribosomal protein L36



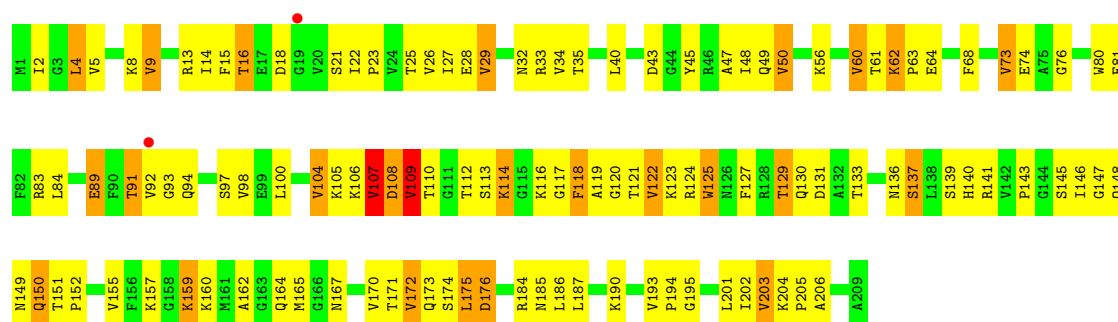
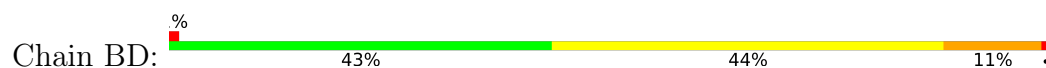
• Molecule 33: 23S rRNA



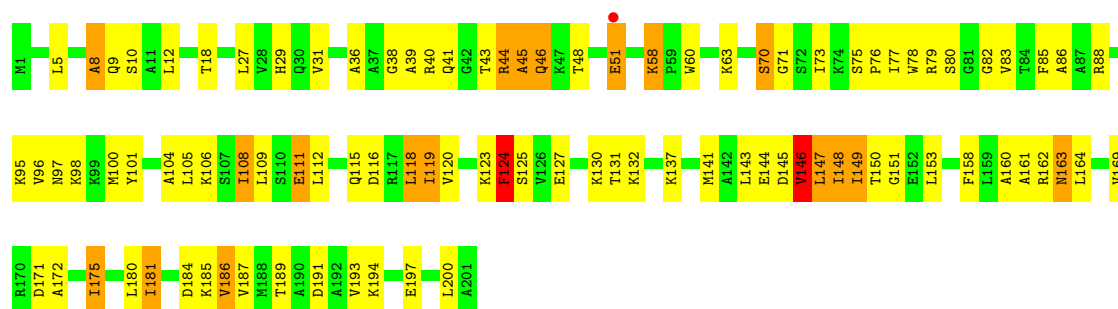
A2225	G2156	U2086	C2006	G1908	U1812	U1729	C1806	A1522	A1427	U1240	A1156	A1077
C2226	G2157	G2087	U2007	C1909	G1813	C1730	C1607	U1523	C1428	A1327	G1157	U1078
A2227	A	U2092	C2008	G1910	G1816	G1731	A1608	G1524	A1434	C1243	C1161	A1080
G2228	G	G2093	C2009	U1911	C1817	C1732	A1609	G1527	G1436	G1245	G1162	U1081
G2230	C	A1912	G2012	A1912	U1818	G1733	A1610	A1528	G1437	A1246	A1165	U1082
U2231	C	C1914	A2013	C1914	A1819	A1735	A1641	C1531	U1442	G1248	G1166	U1083
G2232	G	U1915	A2014	U1915	C1822	U1736	G1642	G1532	G1443	A1247	G1167	A1084
G2233	A	A1918	A2015	A1918	C1827	G1738	G1645	C1533	U1444	G1249	C1168	A1085
G2234	C	A1919	U2016	A1919	U1827	G1742	U1647	U1534	G1445	G1250	A1169	G1087
G2238	U	C1920	U2021	C1920	A1829	G1743	U1648	A1535	U1344	A1253	G1172	A1088
G2239	G	U1923	G2022	U1923	C1830	A1744	G1649	G1537	G1448	A1254	U1173	A1089
U2243	A	C1924	C2023	C1924	C1833	A1745	A1650	G1538	C1451	U1255	U1174	A1090
U2244	A	G1925	G2024	G1925	U1834	A1746	G1651	U1539	G1452	G1256	A1175	G1091
C2248	U	U1926	A2030	A1927	G1835	C1748	A1652	G1540	A1453	G1257	U1176	G1092
U2249	A	A1928	A2031	A1928	C1836	A1749	A1654	A1544	U1458	A1269	U1177	G1093
G2250	C	G1929	G2032	G1929	C1837	G1750	A1655	U1559	G1464	U1270	G1178	U1094
C2251	C	U1930	A2033	G1930	C1838	G1756	A1656	G1560	G1465	C1271	G1185	A1095
C2252	A	U1931	U2034	U1931	G1839	A1757	U1657	G1563	U1466	A1272	G1186	A1096
C2253	C	G1935	A2037	G1935	C1844	U1758	A1665	U1563	U1476	A1275	G1187	A1097
C2254	A	A1936	G2038	A1936	U1847	A1759	G1666	C1564	U1481	A1276	U1189	A1098
C2255	G	A1937	U2039	A1937	A1848	C1764	G1667	C1565	G1482	G1277	G1197	A1099
C2256	U	A1938	A2042	A1938	G1849	C1774	A1669	G1567	U1488	G1278	U1198	A1100
C2257	G	U1943	C2043	U1943	G1850	U1775	U1671	G1568	U1489	G1279	U1199	A1101
C2258	A	C1947	G2046	C1947	U1851	U1779	G1674	G1569	U1490	U1282	A1205	A1102
C2259	C	G1948	G2047	G1948	U1852	U1780	C1675	A1570	U1497	A1287	G1206	A1103
C2260	G	U1955	G2048	U1955	A1853	U1781	C1676	A1571	C1498	G1288	G1210	A1104
C2261	C	A1960	A2051	C1961	G1857	U1782	A1677	A1572	C1499	C1289	G1211	A1105
C2262	U	C1962	G2053	C1962	A1858	A1783	U1688	U1578	G1500	C1291	G1212	A1106
C2263	G	U1963	A2054	U1963	A1866	A1784	U1689	G1581	G1501	G1292	U1217	A1107
C2264	A	G1964	C2055	G1964	G1869	A1785	U1693	G1584	A1502	C1293	G1218	A1108
C2265	C	C1965	G2056	C1965	C1870	A1786	C1694	G1585	A1503	G1300	U1219	A1109
C2266	U	A1966	A2057	A1966	A1871	C1788	G1695	U1589	A1504	A1301	U1220	A1110
C2267	G	C1967	G2058	C1967	A1872	U1789	A1705	A1590	U1505	U1397	U1221	A1111
C2268	A	G1968	A2060	G1968	C1873	C1790	C1706	A1591	C1507	C1306	U1222	A1112
C2269	C	A1969	G2061	A1969	C1874	C1791	G1707	A1592	A1508	U1412	G1223	A1113
C2270	U	U1970	A2062	A1970	G1875	A1792	C1708	U1593	A1509	A1413	U1224	A1114
C2271	C	U1971	C2063	U1971	C1876	C1793	G1709	U1594	A1510	G1309	G1225	A1115
C2272	A	G1972	G2064	G1972	G1884	C1795	U1710	A1595	A1511	G1310	G1226	A1116
C2273	C	U1973	C2065	G1973	A1889	U1796	G1715	A1596	C1512	U1312	U1227	A1117
C2274	U	C1974	U2068	C1974	A1891	G1797	U1716	A1597	A1515	U1313	G1235	A1118
C2275	G	U1991	G2069	U1991	C1894	G1798	G1722	G1601	U1519	A1420	G1236	A1119
C2276	A	G1992	A2070	G1992	C1895	U1799	G1723	U1602	U1520	G1421	G1237	A1120
C2277	C	U1993	C2072	U1993	C1896	C1800	G1724	A1603	G1426	U1314	A1238	A1121
C2278	U	C1994	C2073	U1994	G1903	A1801	A1722	A1603	U1521	C1315	G1239	A1122
C2279	A	U1995	U2081	U1995	G1904	A1805	G1723	U1603	U1522	G1316	G1240	A1123
C2280	C	C1996	A2082	C1996	G1905	A1808	G1724	A1603	U1523	U1317	G1241	A1124
C2281	G	U1997	G2083	U1997	G1906	A1809	G1725	A1603	U1524	U1318	G1242	A1125
C2282	A	C1998	U2084	C1998	G1907	A1810	G1726	A1603	U1525	U1319	G1243	A1126
C2283	C	U1999	G2085	C1999	G1908	A1811	G1727	A1603	U1526	U1320	G1244	A1127
C2284	U	G1999	U2086	G1999	G1909	A1812	G1728	A1603	U1527	U1321	G1245	A1128
C2285	A	C1999	A2087	C1999	G1910	A1813	G1729	A1603	U1528	U1322	G1246	A1129
C2286	C	U1999	G2088	C1999	G1911	A1814	G1730	A1603	U1529	U1323	G1247	A1130
C2287	G	A1999	U2089	A1999	G1912	A1815	G1731	A1603	U1530	U1324	G1248	A1131
C2288	U	C1999	A2088	C1999	G1913	A1816	G1732	A1603	U1531	U1325	G1249	A1132
C2289	A	U1999	G2089	U1999	G1914	A1817	G1733	A1603	U1532	U1326	G1250	A1133
C2290	C	C1999	U2090	C1999	G1915	A1818	G1734	A1603	U1533	U1327	G1251	A1134
C2291	G	A1999	A2089	A1999	G1916	A1819	G1735	A1603	U1534	U1328	G1252	A1135
C2292	U	C1999	G2090	C1999	G1917	A1820	G1736	A1603	U1535	U1329	G1253	A1136
C2293	A	U1999	A2090	U1999	G1918	A1821	G1737	A1603	U1536	U1330	G1254	A1137
C2294	C	C1999	G2091	C1999	G1919	A1822	G1738	A1603	U1537	U1331	G1255	A1138
C2295	G	A1999	U2091	A1999	G1920	A1823	G1739	A1603	U1538	U1332	G1256	A1139
C2296	U	C1999	A2091	C1999	G1921	A1824	G1740	A1603	U1539	U1333	G1257	A1140
C2297	A	U1999	G2092	U1999	G1922	A1825	G1741	A1603	U1540	U1334	G1258	A1141
C2298	C	C1999	U2092	C1999	G1923	A1826	G1742	A1603	U1541	U1335	G1259	A1142
C2299	G	A1999	A2092	A1999	G1924	A1827	G1743	A1603	U1542	U1336	G1260	A1143
C2300	U	C1999	G2093	C1999	G1925	A1828	G1744	A1603	U1543	U1337	G1261	A1144
C2301	A	U1999	U2093	U1999	G1926	A1829	G1745	A1603	U1544	U1338	G1262	A1145
C2302	C	C1999	A2093	C1999	G1927	A1830	G1746	A1603	U1545	U1339	G1263	A1146
C2303	G	A1999	G2094	A1999	G1928	A1831	G1747	A1603	U1546	U1340	G1264	A1147
C2304	U	C1999	U2094	C1999	G1929	A1832	G1748	A1603	U1547	U1341	G1265	A1148
C2305	A	U1999	A2094	U1999	G1930	A1833	G1749	A1603	U1548	U1342	G1266	A1149
C2306	C	C1999	G2095	C1999	G1931	A1834	G1750	A1603	U1549	U1343	G1267	A1150
C2307	G	A1999	U2095	A1999	G1932	A1835	G1751	A1603	U1550	U1344	G1268	A1151
C2308	U	C1999	A2095	C1999	G1933	A1836	G1752	A1603	U1551	U1345	G1269	A1152
C2309	A	U1999	G2096	U1999	G1934	A1837	G1753	A1603	U1552	U1346	G1270	A1153
C2310	C	C1999	U2096	C1999	G1935	A1838	G1754	A1603	U1553	U1347	G1271	A1154
C2311	G	A1999	A2096	A1999	G1936	A1839	G1755	A1603	U1554	U1348	G1272	A1155
C2312	U	C1999	G2097	C1999	G1937	A1840	G1756	A1603	U1555	U1349	G1273	A1156
C2313	A	U1999	U2097	U1999	G1938	A1841	G1757	A1603	U1556	U1350	G1274	A1157
C2314	C	C1999	A2097	C1999	G1939	A1842	G1758	A1603	U1557	U1351	G1275	A1158
C2315	G	A1999	G2098	A1999	G1940	A1843	G1759	A1603	U1558	U1352	G1276	A1159
C2316	U	C1999	U2098	C1999	G1941	A1844	G1760	A1603	U1559	U1353	G1277	A1160
C2317	A	U1999	A2098	U1999	G1942	A1845	G1761	A1603	U1560	U1354	G1278	A1161
C2318	C	C1999	G2099	C1999	G1943	A1846	G1762	A1603	U1561	U1355	G1279	A1162
C2319	G	A1999	U2099	A1999	G1944	A1847	G1763	A1603	U1562	U1356	G1280	A1163
C2320	U	C1999	A2099	C1999	G1945	A1848	G1764	A1603	U1563	U1357	G1281	A1164
C2321	A	U1999	G2100	U1999	G1946	A1849	G1765	A1603	U1564	U1358	G1282	A1165
C2322	C	C1999	U2100	C1999	G1947	A1850	G1766	A1603	U1565	U1359	G1283	A1166
C2323	G	A1999	A2100	A1999	G1948	A1851	G1767	A1603	U1566	U1360	G1284	A1167
C2324	U	C1999	G2101	C1999	G1949	A1852	G1768	A1603	U1567	U1361	G1285	A1168
C2325	A	U1999	U2101	U1999	G1950	A1853	G1769	A1603	U1568	U1362	G1286	A1169
C2326	C	C1999	A2101	C1999	G1951	A1854	G1770	A1603	U1569	U1363	G1287	A1170
C2327	G	A1999	G2102	A1999	G1952	A1855	G1771	A1603	U1570	U1364	G1288	A1171
C2328	U	C1999	U2102	C1999	G1953	A1856	G1772	A1603	U1571	U1365	G1289	A1172
C2329	A	U1999	A2102	U1999	G1954	A1857	G1773	A1603	U1572	U1366	G1290	A1173
C2330	C	C1999	G2103	C1999	G1955	A1858	G1774	A1603	U1573	U1367	G1291	A1174
C2331	G	A1999	U2103	A1999	G1956	A1859	G1775	A1603	U1574	U1368	G1292	A1175
C2332	U	C1999	A2103	C1999	G1957	A1860	G1776	A1603	U1575	U1369	G1293	A1176
C2333	A	U1999	G2104	U1999	G1958	A1861	G1777	A1603	U1576	U1370	G1294	A1177
C2334	C	C1999	U2104	C1999	G1959	A1862	G1778	A1603	U1577	U1371	G1295	A1178
C2335	G	A1999	A2104	A1999	G1960	A1863	G1779	A1603	U1578	U1372	G1296	A1179
C2336	U	C1999	G2105	C1999	G1961	A1864	G1780	A1603	U1579	U1373	G1297	A1180
C2337												



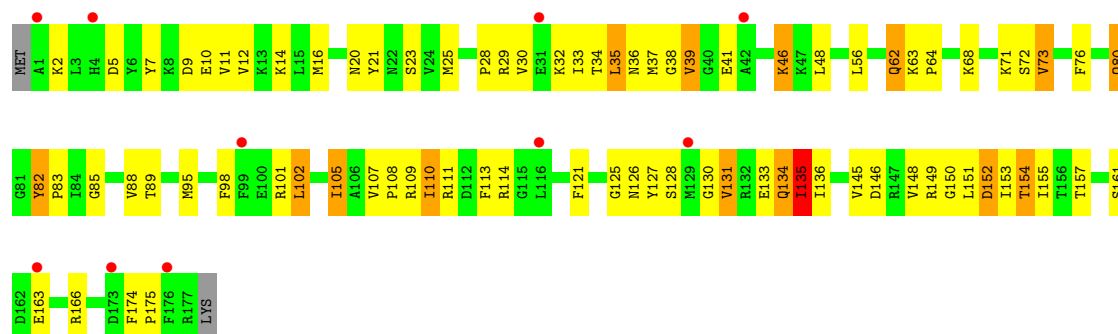
• Molecule 36: 50S ribosomal protein L3



• Molecule 37: 50S ribosomal protein L4

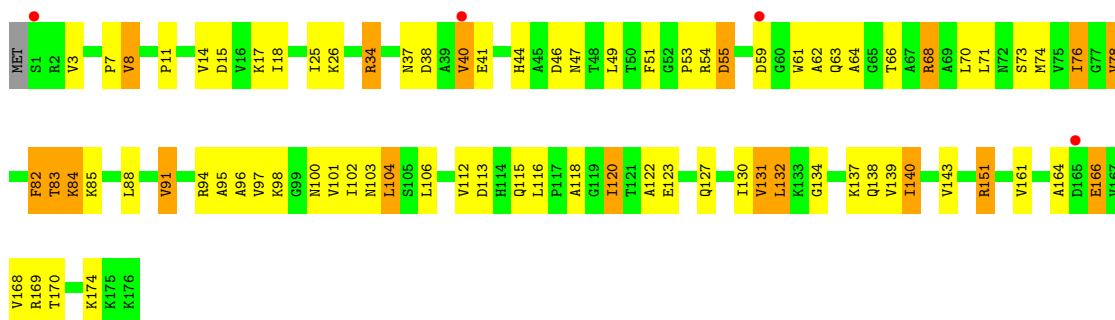


• Molecule 38: 50S ribosomal protein L5

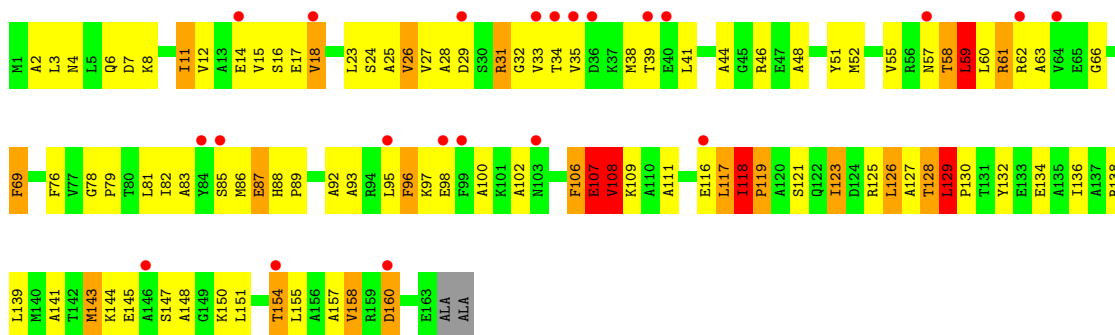


• Molecule 39: 50S ribosomal protein L6

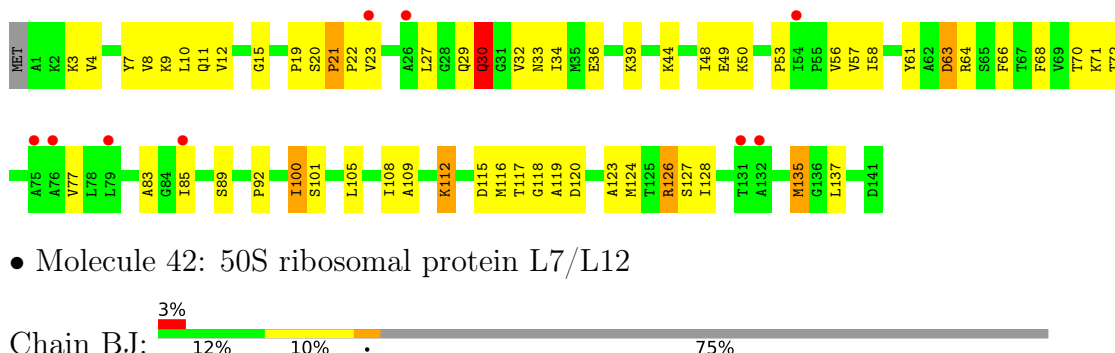




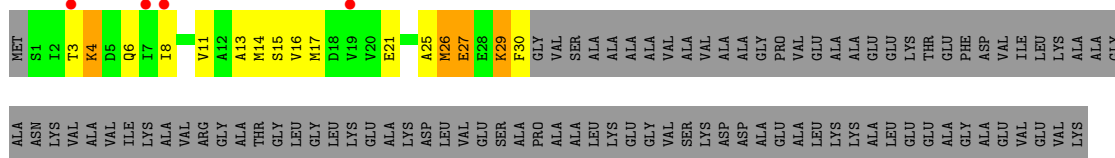
- Molecule 40: 50S ribosomal protein L10



- Molecule 41: 50S ribosomal protein L11



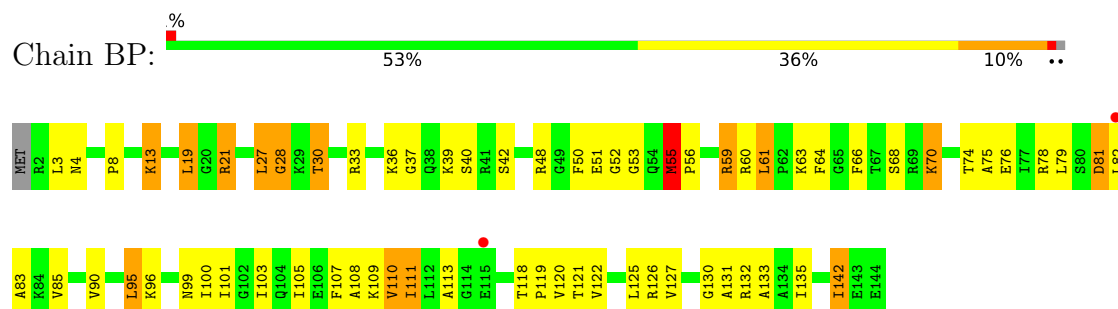
- Molecule 42: 50S ribosomal protein L7/L12



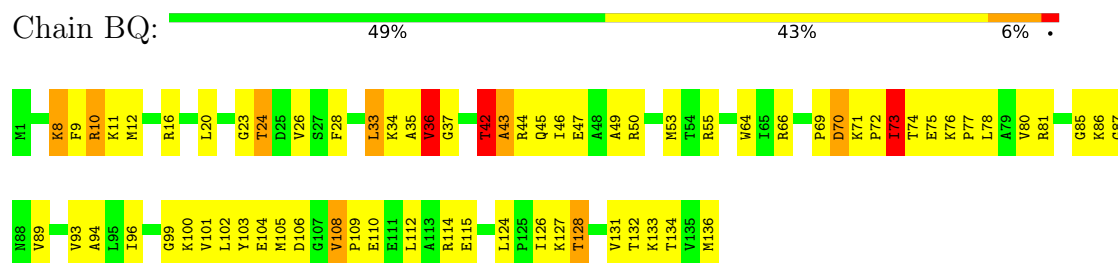
- Molecule 42: 50S ribosomal protein L7/L12



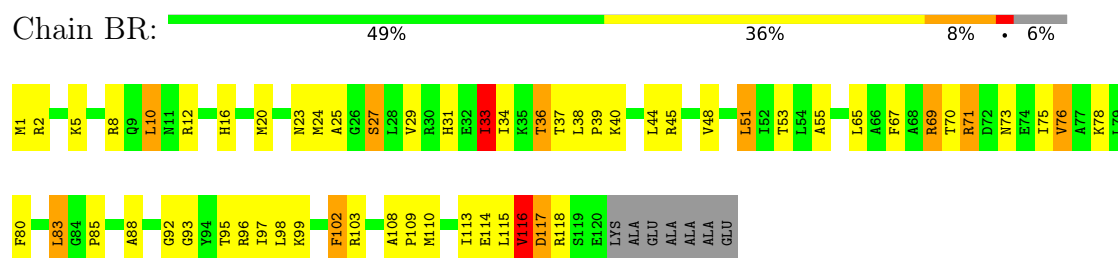
- Molecule 45: 50S ribosomal protein L15



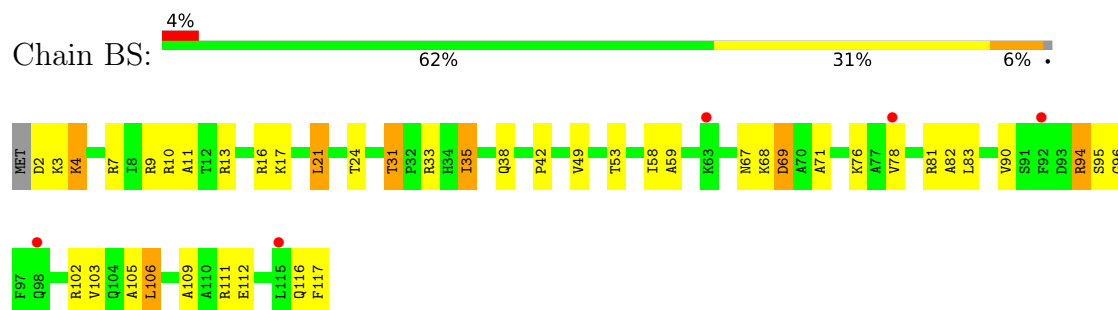
- Molecule 46: 50S ribosomal protein L16



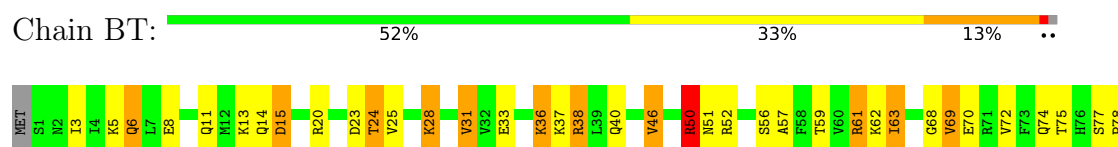
- Molecule 47: 50S ribosomal protein L17



- Molecule 48: 50S ribosomal protein L18

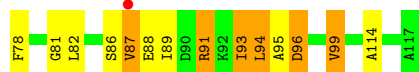
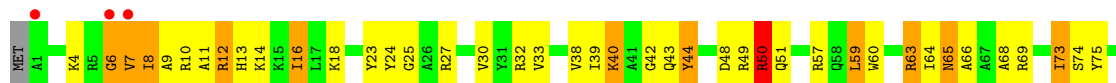


- Molecule 49: 50S ribosomal protein L19

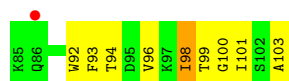
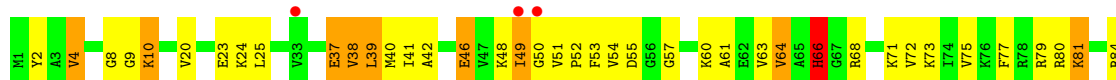




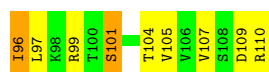
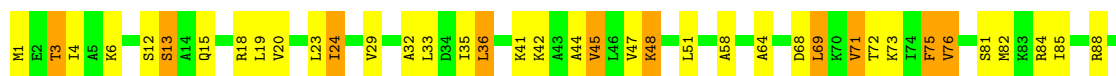
- Molecule 50: 50S ribosomal protein L20



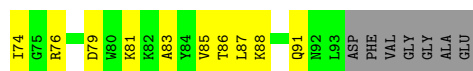
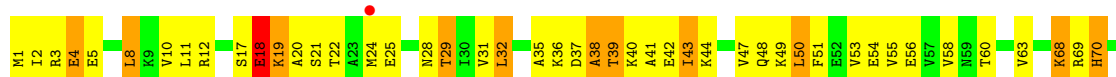
- Molecule 51: 50S ribosomal protein L21



- Molecule 52: 50S ribosomal protein L22

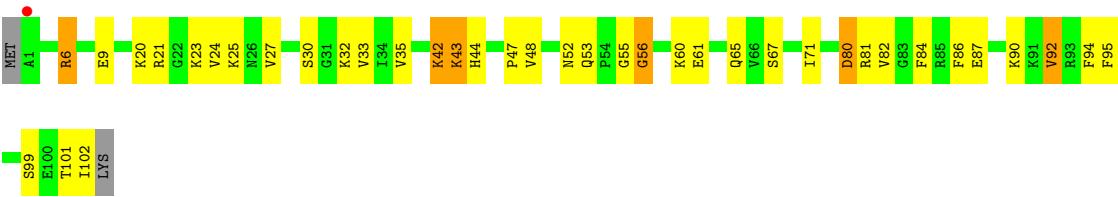


- Molecule 53: 50S ribosomal protein L23



- Molecule 54: 50S ribosomal protein L24

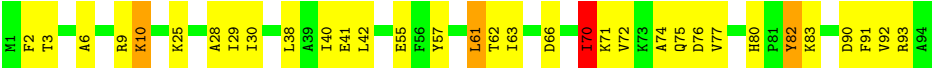




- Molecule 55: 50S ribosomal protein L25

Chain BZ:

65%31%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	258.00Å 312.00Å 333.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.70 40.00 – 3.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.70) 99.4 (40.00-3.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.49Å)	Xtriage
Refinement program	PHENIX, CNS 1.2	Depositor
R, R_{free}	0.240 , 0.290 0.234 , 0.280	Depositor DCC
R_{free} test set	16644 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 92.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	146665	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: GNP, MG

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	0.25	0/36809	0.38	0/57423
2	AB	0.47	0/1735	1.02	6/2338 (0.3%)
3	AC	0.46	0/1651	0.93	4/2225 (0.2%)
4	AD	0.48	0/1665	0.92	2/2227 (0.1%)
5	AE	0.51	0/1118	1.19	8/1504 (0.5%)
6	AF	0.53	0/835	1.04	4/1128 (0.4%)
7	AG	0.39	0/1195	0.86	0/1602
8	AH	0.40	0/989	0.88	1/1326 (0.1%)
9	AI	0.44	0/1034	0.93	2/1375 (0.1%)
10	AJ	0.49	0/796	0.91	0/1077
11	AK	0.49	0/893	1.01	3/1205 (0.2%)
12	AL	0.48	0/969	1.03	4/1300 (0.3%)
13	AM	0.43	0/892	0.95	2/1193 (0.2%)
14	AN	0.40	0/785	0.99	1/1043 (0.1%)
15	AO	0.44	0/722	0.98	1/964 (0.1%)
16	AP	0.48	0/659	1.00	2/884 (0.2%)
17	AQ	0.51	0/657	1.06	5/881 (0.6%)
18	AR	0.58	0/462	1.01	0/621
19	AS	0.38	0/652	0.82	1/877 (0.1%)
20	AT	0.57	0/671	1.05	2/888 (0.2%)
21	AU	0.49	0/430	1.03	0/570
22	AV	0.25	0/144	0.40	0/222
23	AW	0.64	7/4221 (0.2%)	1.09	27/5702 (0.5%)
24	B0	0.61	0/603	1.22	3/797 (0.4%)
25	B1	0.50	0/635	0.97	2/848 (0.2%)
26	B2	0.52	0/510	1.10	5/677 (0.7%)
27	B3	0.58	0/453	1.10	1/605 (0.2%)
28	B4	0.54	0/450	0.93	0/599
29	B5	0.57	0/416	0.87	0/554
30	B6	0.56	0/380	1.04	0/498
31	B7	0.51	0/513	1.02	0/676
32	B8	0.47	0/303	1.00	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BA	0.29	2/68601 (0.0%)	0.41	5/107017 (0.0%)
34	BB	0.25	0/2828	0.38	0/4410
35	BC	0.55	0/2121	1.14	13/2852 (0.5%)
36	BD	0.66	0/1586	1.21	13/2134 (0.6%)
37	BE	0.56	0/1571	1.14	9/2113 (0.4%)
38	BF	0.44	0/1434	0.94	3/1926 (0.2%)
39	BG	0.56	0/1343	0.97	1/1816 (0.1%)
40	BH	0.55	0/1244	1.13	11/1675 (0.7%)
41	BI	0.47	0/1046	0.97	2/1410 (0.1%)
42	BJ	0.54	0/227	0.97	0/304
42	BK	0.46	0/227	0.87	1/304 (0.3%)
42	BL	0.45	0/227	0.85	0/304
42	BM	0.59	0/227	0.99	1/304 (0.3%)
43	BN	0.67	0/1152	1.20	7/1551 (0.5%)
44	BO	0.60	0/947	1.08	2/1268 (0.2%)
45	BP	0.54	0/1054	1.19	8/1403 (0.6%)
46	BQ	0.54	0/1093	1.03	6/1460 (0.4%)
47	BR	0.58	0/973	1.19	7/1301 (0.5%)
48	BS	0.45	0/902	0.94	1/1209 (0.1%)
49	BT	0.60	0/929	1.10	3/1242 (0.2%)
50	BU	0.72	1/960 (0.1%)	1.11	3/1278 (0.2%)
51	BV	0.49	0/829	1.06	2/1107 (0.2%)
52	BW	0.66	0/864	1.19	5/1156 (0.4%)
53	BX	0.63	0/744	1.21	5/994 (0.5%)
54	BY	0.55	0/787	1.12	5/1051 (0.5%)
55	BZ	0.44	0/766	0.92	3/1025 (0.3%)
All	All	0.38	10/158929 (0.0%)	0.65	202/236840 (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
2	AB	0	3
3	AC	0	1
5	AE	0	2
6	AF	0	1
11	AK	0	1
13	AM	0	1
14	AN	0	2
23	AW	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
24	B0	0	1
37	BE	0	1
39	BG	0	1
40	BH	0	3
41	BI	0	2
43	BN	0	1
45	BP	0	1
47	BR	0	1
50	BU	0	1
53	BX	0	1
54	BY	0	1
All	All	0	28

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	22	PRO	C-N	14.76	1.55	1.33
33	BA	1914	C	O3'-P	-12.70	1.42	1.61
23	AW	72	THR	C-O	8.52	1.34	1.24
23	AW	65	GLN	C-N	-8.27	1.22	1.33
33	BA	2104	C	O3'-P	-7.07	1.50	1.61

The worst 5 of 202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	AE	96	GLN	CA-C-N	12.33	135.26	119.84
5	AE	96	GLN	C-N-CA	12.33	135.26	119.84
36	BD	172	VAL	N-CA-C	10.57	121.28	111.45
33	BA	1914	C	P-O3'-C3'	-10.35	104.68	120.20
23	AW	26	LYS	O-C-N	9.69	132.45	122.08

There are no chirality outliers.

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	135	MET	Peptide
2	AB	20	ARG	Peptide
2	AB	218	ALA	Peptide
3	AC	153	SER	Peptide
5	AE	78	GLY	Peptide

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	32873	0	16542	565	1
2	AB	1704	0	1732	88	0
3	AC	1624	0	1699	66	4
4	AD	1643	0	1710	73	1
5	AE	1105	0	1148	47	0
6	AF	817	0	808	39	0
7	AG	1181	0	1240	36	0
8	AH	979	0	1034	36	0
9	AI	1022	0	1070	54	0
10	AJ	786	0	828	43	0
11	AK	877	0	887	37	0
12	AL	955	0	1019	65	0
13	AM	883	0	944	41	0
14	AN	774	0	827	42	0
15	AO	714	0	737	22	0
16	AP	649	0	666	23	0
17	AQ	648	0	691	26	0
18	AR	455	0	478	15	0
19	AS	637	0	665	17	1
20	AT	665	0	714	26	0
21	AU	425	0	449	21	0
22	AV	129	0	65	2	0
23	AW	4144	0	4127	314	0
24	B0	596	0	610	71	0
25	B1	625	0	655	38	0
26	B2	509	0	543	17	0
27	B3	449	0	491	22	0
28	B4	444	0	461	13	0
29	B5	409	0	440	6	0
30	B6	377	0	418	8	0
31	B7	504	0	574	17	0
32	B8	302	0	340	21	0
33	BA	61252	0	30808	1112	4
34	BB	2529	0	1281	44	0
35	BC	2082	0	2157	122	0
36	BD	1565	0	1616	104	0
37	BE	1552	0	1619	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BF	1410	0	1447	64	0
39	BG	1323	0	1374	58	0
40	BH	1230	0	1282	94	0
41	BI	1032	0	1088	46	0
42	BJ	227	0	237	13	0
42	BK	227	0	237	5	0
42	BL	227	0	237	9	0
42	BM	227	0	237	16	0
43	BN	1129	0	1162	70	0
44	BO	938	0	1012	43	0
45	BP	1045	0	1117	48	0
46	BQ	1074	0	1157	51	0
47	BR	960	0	1000	43	0
48	BS	892	0	923	27	0
49	BT	917	0	965	44	0
50	BU	947	0	1022	56	0
51	BV	816	0	839	50	0
52	BW	857	0	922	28	0
53	BX	738	0	807	40	0
54	BY	779	0	834	26	0
55	BZ	753	0	780	21	1
56	AW	32	0	13	7	0
57	AW	1	0	0	0	0
All	All	146665	0	100785	3715	6

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 15.

The worst 5 of 3715 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)
1:AA:497:G:OP2	23:AW:480:LYS:HE3	1.11	1.25
1:AA:497:G:OP2	23:AW:480:LYS:CE	1.83	1.25
12:AL:101:LEU:HG	23:AW:409:GLN:NE2	1.53	1.21
33:BA:974:G:C8	33:BA:989:G:C2	2.31	1.18
40:BH:25:ALA:HB3	40:BH:85:SER:OG	1.38	1.18

The worst 5 of 6 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)
3:AC:131:ARG:NH2	33:BA:2156:G:O2'[4_445]	1.71	0.49
3:AC:135:ARG:CG	33:BA:2157:G:OP2[4_445]	1.99	0.21
3:AC:131:ARG:CB	33:BA:2157:G:OP1[4_445]	2.11	0.09
1:AA:205:A:OP2	19:AS:24:SER:OG[2_355]	2.12	0.08
3:AC:131:ARG:NE	33:BA:2157:G:O5'[4_445]	2.12	0.08

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/241 (90%)	175 (81%)	40 (18%)	1 (0%)	24	56
3	AC	204/233 (88%)	178 (87%)	24 (12%)	2 (1%)	12	43
4	AD	203/206 (98%)	170 (84%)	29 (14%)	4 (2%)	6	32
5	AE	148/167 (89%)	125 (84%)	19 (13%)	4 (3%)	4	27
6	AF	98/135 (73%)	77 (79%)	20 (20%)	1 (1%)	12	43
7	AG	149/179 (83%)	124 (83%)	25 (17%)	0	100	100
8	AH	127/130 (98%)	113 (89%)	13 (10%)	1 (1%)	16	48
9	AI	125/130 (96%)	109 (87%)	12 (10%)	4 (3%)	3	25
10	AJ	96/103 (93%)	77 (80%)	16 (17%)	3 (3%)	3	26
11	AK	115/129 (89%)	100 (87%)	15 (13%)	0	100	100
12	AL	121/124 (98%)	107 (88%)	12 (10%)	2 (2%)	7	34
13	AM	112/118 (95%)	96 (86%)	14 (12%)	2 (2%)	6	34
14	AN	92/101 (91%)	73 (79%)	19 (21%)	0	100	100
15	AO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
16	AP	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	9	38
17	AQ	78/84 (93%)	65 (83%)	12 (15%)	1 (1%)	9	38
18	AR	53/75 (71%)	46 (87%)	7 (13%)	0	100	100
19	AS	77/92 (84%)	69 (90%)	8 (10%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AT	83/87 (95%)	73 (88%)	9 (11%)	1 (1%)	10	40
21	AU	49/71 (69%)	36 (74%)	12 (24%)	1 (2%)	6	32
23	AW	523/534 (98%)	382 (73%)	82 (16%)	59 (11%)	0	4
24	B0	77/85 (91%)	49 (64%)	24 (31%)	4 (5%)	1	17
25	B1	75/78 (96%)	65 (87%)	10 (13%)	0	100	100
26	B2	61/63 (97%)	47 (77%)	12 (20%)	2 (3%)	3	25
27	B3	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
28	B4	54/57 (95%)	45 (83%)	8 (15%)	1 (2%)	6	33
29	B5	48/55 (87%)	43 (90%)	4 (8%)	1 (2%)	5	31
30	B6	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	5	30
31	B7	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	7	35
32	B8	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	4	27
35	BC	269/273 (98%)	234 (87%)	29 (11%)	6 (2%)	5	31
36	BD	207/209 (99%)	176 (85%)	26 (13%)	5 (2%)	4	29
37	BE	199/201 (99%)	170 (85%)	23 (12%)	6 (3%)	3	26
38	BF	175/179 (98%)	145 (83%)	27 (15%)	3 (2%)	7	34
39	BG	174/177 (98%)	141 (81%)	32 (18%)	1 (1%)	21	52
40	BH	161/165 (98%)	123 (76%)	31 (19%)	7 (4%)	2	19
41	BI	139/142 (98%)	113 (81%)	26 (19%)	0	100	100
42	BJ	28/121 (23%)	20 (71%)	8 (29%)	0	100	100
42	BK	28/121 (23%)	23 (82%)	5 (18%)	0	100	100
42	BL	28/121 (23%)	22 (79%)	6 (21%)	0	100	100
42	BM	28/121 (23%)	19 (68%)	7 (25%)	2 (7%)	1	12
43	BN	140/142 (99%)	118 (84%)	20 (14%)	2 (1%)	9	37
44	BO	120/123 (98%)	97 (81%)	19 (16%)	4 (3%)	3	25
45	BP	141/144 (98%)	118 (84%)	22 (16%)	1 (1%)	18	50
46	BQ	134/136 (98%)	112 (84%)	18 (13%)	4 (3%)	3	26
47	BR	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	16	48
48	BS	114/117 (97%)	99 (87%)	14 (12%)	1 (1%)	14	45
49	BT	112/115 (97%)	93 (83%)	16 (14%)	3 (3%)	4	27
50	BU	115/118 (98%)	103 (90%)	10 (9%)	2 (2%)	7	34

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BV	101/103 (98%)	88 (87%)	11 (11%)	2 (2%)	6	32
52	BW	108/110 (98%)	97 (90%)	10 (9%)	1 (1%)	14	45
53	BX	91/100 (91%)	62 (68%)	25 (28%)	4 (4%)	2	19
54	BY	100/104 (96%)	78 (78%)	21 (21%)	1 (1%)	12	43
55	BZ	92/94 (98%)	82 (89%)	10 (11%)	0	100	100
All	All	6270/7019 (89%)	5201 (83%)	915 (15%)	154 (2%)	4	29

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	14	VAL
4	AD	30	LYS
4	AD	125	ASN
13	AM	46	GLU
17	AQ	12	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/199 (90%)	150 (83%)	30 (17%)	2	14
3	AC	170/190 (90%)	141 (83%)	29 (17%)	2	13
4	AD	172/173 (99%)	149 (87%)	23 (13%)	4	20
5	AE	113/126 (90%)	94 (83%)	19 (17%)	2	13
6	AF	87/116 (75%)	73 (84%)	14 (16%)	2	14
7	AG	124/147 (84%)	113 (91%)	11 (9%)	9	33
8	AH	104/105 (99%)	90 (86%)	14 (14%)	4	20
9	AI	105/107 (98%)	87 (83%)	18 (17%)	2	13
10	AJ	86/90 (96%)	69 (80%)	17 (20%)	1	9
11	AK	90/99 (91%)	77 (86%)	13 (14%)	3	18
12	AL	103/104 (99%)	86 (84%)	17 (16%)	2	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AM	92/96 (96%)	87 (95%)	5 (5%)	20	46
14	AN	79/84 (94%)	73 (92%)	6 (8%)	12	38
15	AO	76/77 (99%)	72 (95%)	4 (5%)	20	46
16	AP	65/65 (100%)	57 (88%)	8 (12%)	4	22
17	AQ	74/78 (95%)	61 (82%)	13 (18%)	2	12
18	AR	48/65 (74%)	43 (90%)	5 (10%)	7	28
19	AS	70/79 (89%)	63 (90%)	7 (10%)	7	30
20	AT	65/66 (98%)	54 (83%)	11 (17%)	2	13
21	AU	44/61 (72%)	37 (84%)	7 (16%)	2	15
23	AW	447/458 (98%)	371 (83%)	76 (17%)	2	13
24	B0	59/63 (94%)	46 (78%)	13 (22%)	1	7
25	B1	67/68 (98%)	61 (91%)	6 (9%)	9	33
26	B2	55/55 (100%)	49 (89%)	6 (11%)	6	26
27	B3	48/49 (98%)	38 (79%)	10 (21%)	1	8
28	B4	47/48 (98%)	46 (98%)	1 (2%)	47	64
29	B5	45/49 (92%)	40 (89%)	5 (11%)	6	25
30	B6	38/38 (100%)	34 (90%)	4 (10%)	6	28
31	B7	51/52 (98%)	49 (96%)	2 (4%)	28	53
32	B8	34/34 (100%)	29 (85%)	5 (15%)	3	17
35	BC	216/218 (99%)	173 (80%)	43 (20%)	1	9
36	BD	164/164 (100%)	141 (86%)	23 (14%)	3	18
37	BE	165/165 (100%)	140 (85%)	25 (15%)	3	16
38	BF	148/150 (99%)	130 (88%)	18 (12%)	5	22
39	BG	137/138 (99%)	115 (84%)	22 (16%)	2	14
40	BH	123/123 (100%)	103 (84%)	20 (16%)	2	14
41	BI	109/110 (99%)	93 (85%)	16 (15%)	3	17
42	BJ	26/85 (31%)	21 (81%)	5 (19%)	1	9
42	BK	26/85 (31%)	25 (96%)	1 (4%)	29	53
42	BL	26/85 (31%)	25 (96%)	1 (4%)	29	53
42	BM	26/85 (31%)	23 (88%)	3 (12%)	5	24
43	BN	116/116 (100%)	93 (80%)	23 (20%)	1	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BO	103/104 (99%)	79 (77%)	24 (23%)	1	6
45	BP	102/103 (99%)	85 (83%)	17 (17%)	2	14
46	BQ	109/109 (100%)	88 (81%)	21 (19%)	1	9
47	BR	100/103 (97%)	84 (84%)	16 (16%)	2	15
48	BS	86/87 (99%)	70 (81%)	16 (19%)	1	10
49	BT	99/100 (99%)	81 (82%)	18 (18%)	2	11
50	BU	89/90 (99%)	69 (78%)	20 (22%)	1	6
51	BV	84/84 (100%)	70 (83%)	14 (17%)	2	14
52	BW	93/93 (100%)	74 (80%)	19 (20%)	1	8
53	BX	80/84 (95%)	67 (84%)	13 (16%)	2	14
54	BY	83/85 (98%)	71 (86%)	12 (14%)	3	17
55	BZ	78/78 (100%)	71 (91%)	7 (9%)	9	33
All	All	5226/5685 (92%)	4430 (85%)	796 (15%)	3	16

5 of 796 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	BD	201	LEU
42	BM	2	ILE
37	BE	118	LEU
36	BD	176	ASP
39	BG	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
40	BH	103	ASN
50	BU	65	ASN
43	BN	47	HIS
48	BS	29	HIS
53	BX	28	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1531/1533 (99%)	280 (18%)	29 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AV	5/27 (18%)	3 (60%)	0
33	BA	2849/2903 (98%)	504 (17%)	53 (1%)
34	BB	117/118 (99%)	20 (17%)	3 (2%)
All	All	4502/4581 (98%)	807 (17%)	85 (1%)

5 of 807 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	22	G
1	AA	32	A
1	AA	39	G

5 of 85 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	BA	1253	A
33	BA	2146	C
33	BA	1378	A
33	BA	1870	C
33	BA	2225	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	GNP	AW	601	57	34,34,34	1.93	6 (17%)	47,54,54	1.11	5 (10%)

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
56	GNP	AW	601	57	-	6/18/38/38	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	AW	601	GNP	PA-O3A	-6.91	1.52	1.59
56	AW	601	GNP	PB-O3A	-5.70	1.52	1.59
56	AW	601	GNP	PB-O2B	-3.40	1.47	1.56
56	AW	601	GNP	PG-O1G	3.20	1.51	1.46
56	AW	601	GNP	PG-O2G	-2.30	1.50	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	AW	601	GNP	O2B-PB-O1B	4.11	118.69	109.87
56	AW	601	GNP	O1G-PG-N3B	-3.26	106.96	111.77
56	AW	601	GNP	O3G-PG-O1G	-2.84	106.33	113.45
56	AW	601	GNP	O2G-PG-O3G	2.09	113.21	107.59
56	AW	601	GNP	C2'-C3'-C4'	2.06	106.59	102.61

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

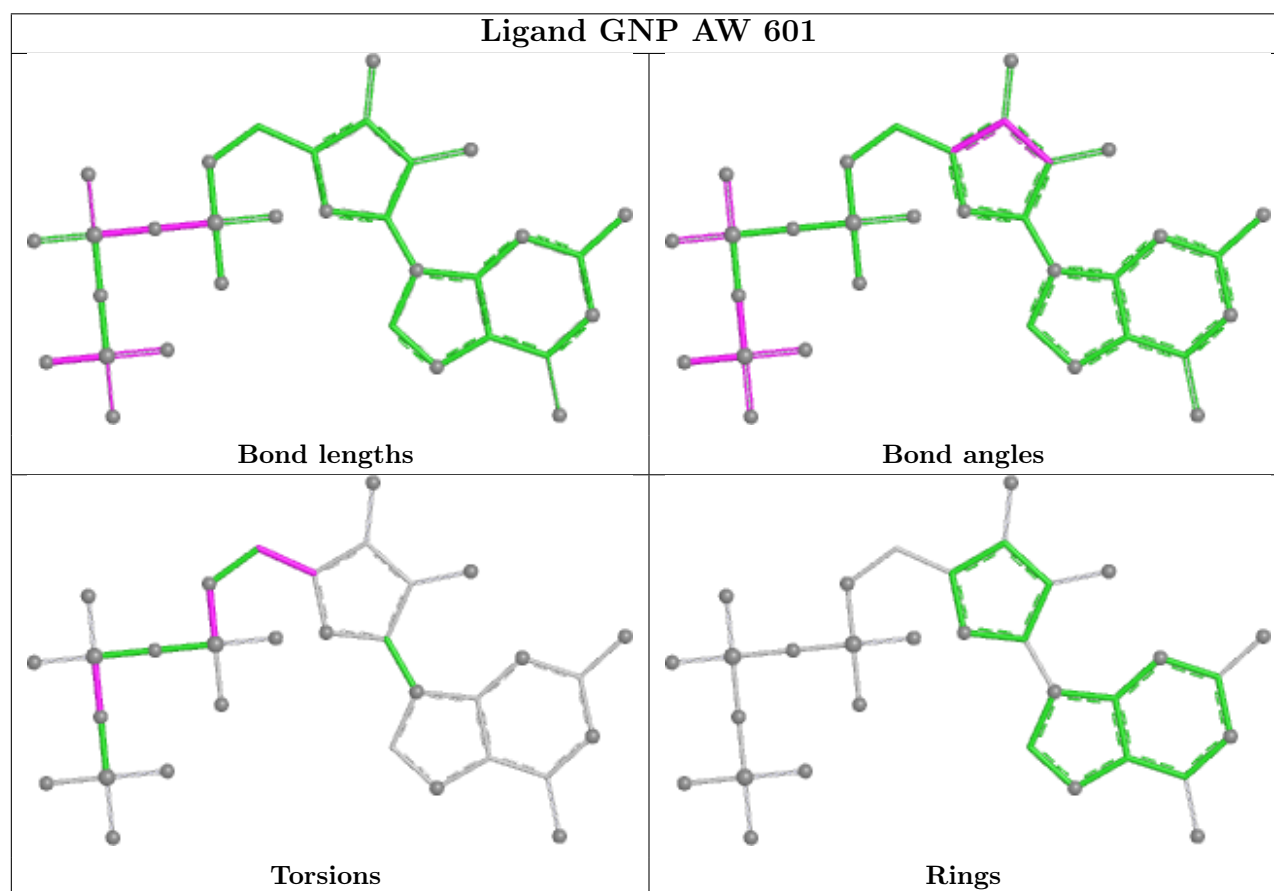
Mol	Chain	Res	Type	Atoms
56	AW	601	GNP	PG-N3B-PB-O1B
56	AW	601	GNP	C3'-C4'-C5'-O5'
56	AW	601	GNP	O4'-C4'-C5'-O5'
56	AW	601	GNP	C5'-O5'-PA-O3A
56	AW	601	GNP	C5'-O5'-PA-O1A

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	AW	601	GNP	7	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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	1532/1533 (99%)	0.23	25 (1%) 70 45	72, 119, 232, 344	0
2	AB	218/241 (90%)	0.44	7 (3%) 50 31	124, 181, 235, 328	0
3	AC	206/233 (88%)	0.19	4 (1%) 66 42	88, 129, 167, 218	0
4	AD	205/206 (99%)	0.49	12 (5%) 28 19	88, 120, 177, 250	0
5	AE	150/167 (89%)	0.38	5 (3%) 49 31	88, 123, 176, 253	0
6	AF	100/135 (74%)	0.38	3 (3%) 52 32	106, 153, 182, 204	0
7	AG	151/179 (84%)	0.58	11 (7%) 21 16	132, 178, 218, 300	0
8	AH	129/130 (99%)	0.29	4 (3%) 51 32	108, 137, 177, 228	0
9	AI	127/130 (97%)	0.58	7 (5%) 30 20	102, 145, 212, 252	0
10	AJ	98/103 (95%)	0.77	8 (8%) 17 14	95, 124, 243, 282	0
11	AK	117/129 (90%)	0.32	6 (5%) 33 22	81, 116, 155, 200	0
12	AL	123/124 (99%)	0.46	7 (5%) 29 20	83, 103, 188, 250	0
13	AM	114/118 (96%)	0.75	6 (5%) 32 21	137, 194, 233, 273	0
14	AN	96/101 (95%)	0.91	12 (12%) 8 10	93, 161, 212, 250	0
15	AO	88/89 (98%)	0.42	4 (4%) 38 24	100, 137, 190, 275	0
16	AP	82/82 (100%)	0.36	3 (3%) 45 28	78, 105, 160, 252	0
17	AQ	80/84 (95%)	0.78	10 (12%) 8 10	96, 139, 204, 301	0
18	AR	55/75 (73%)	0.56	6 (10%) 10 12	91, 119, 176, 247	0
19	AS	79/92 (85%)	0.61	4 (5%) 33 22	158, 201, 238, 282	0
20	AT	85/87 (97%)	0.81	11 (12%) 7 9	96, 126, 172, 184	0
21	AU	51/71 (71%)	1.47	11 (21%) 2 3	158, 215, 255, 264	0
22	AV	6/27 (22%)	1.36	1 (16%) 4 6	221, 256, 294, 306	0
23	AW	525/534 (98%)	0.67	22 (4%) 40 25	35, 99, 188, 267	0
24	B0	79/85 (92%)	0.92	13 (16%) 4 6	61, 105, 177, 200	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	B1	77/78 (98%)	0.05	0 100 100	68, 83, 132, 154	0
26	B2	63/63 (100%)	0.13	3 (4%) 35 23	72, 100, 145, 187	0
27	B3	58/59 (98%)	0.13	0 100 100	67, 92, 143, 174	0
28	B4	56/57 (98%)	-0.13	0 100 100	44, 65, 108, 150	0
29	B5	50/55 (90%)	0.65	4 (8%) 18 14	133, 176, 209, 228	0
30	B6	46/46 (100%)	0.10	2 (4%) 40 25	48, 60, 84, 197	0
31	B7	64/65 (98%)	0.39	2 (3%) 51 32	63, 85, 109, 128	0
32	B8	38/38 (100%)	0.97	4 (10%) 11 12	82, 104, 135, 178	0
33	BA	2853/2903 (98%)	-0.11	60 (2%) 63 40	28, 79, 260, 445	0
34	BB	118/118 (100%)	0.13	4 (3%) 48 30	71, 127, 173, 221	0
35	BC	271/273 (99%)	0.08	4 (1%) 72 46	47, 77, 100, 151	0
36	BD	209/209 (100%)	-0.01	2 (0%) 79 55	48, 64, 108, 162	0
37	BE	201/201 (100%)	0.12	1 (0%) 87 69	45, 94, 146, 200	0
38	BF	177/179 (98%)	0.54	10 (5%) 30 20	117, 157, 214, 286	0
39	BG	176/177 (99%)	0.17	4 (2%) 61 38	71, 108, 162, 189	0
40	BH	163/165 (98%)	1.05	22 (13%) 7 8	135, 263, 334, 394	0
41	BI	141/142 (99%)	0.80	9 (6%) 25 18	185, 276, 378, 452	0
42	BJ	30/121 (24%)	1.13	4 (13%) 7 9	222, 260, 328, 407	0
42	BK	30/121 (24%)	1.46	5 (16%) 4 6	222, 263, 318, 343	0
42	BL	30/121 (24%)	1.63	9 (30%) 1 1	187, 275, 348, 365	0
42	BM	30/121 (24%)	0.91	2 (6%) 24 17	206, 255, 324, 352	0
43	BN	142/142 (100%)	0.08	2 (1%) 73 48	56, 72, 105, 173	0
44	BO	122/123 (99%)	0.12	1 (0%) 82 60	48, 75, 107, 196	0
45	BP	143/144 (99%)	0.36	2 (1%) 73 48	55, 100, 149, 201	0
46	BQ	136/136 (100%)	0.03	0 100 100	65, 92, 133, 188	0
47	BR	120/127 (94%)	-0.13	0 100 100	39, 64, 85, 233	0
48	BS	116/117 (99%)	0.37	5 (4%) 40 25	91, 125, 157, 180	0
49	BT	114/115 (99%)	0.08	0 100 100	61, 83, 133, 164	0
50	BU	117/118 (99%)	0.18	4 (3%) 48 30	44, 69, 116, 219	0
51	BV	103/103 (100%)	0.14	4 (3%) 43 28	51, 93, 151, 334	0
52	BW	110/110 (100%)	-0.17	0 100 100	42, 61, 101, 181	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
53	BX	93/100 (93%)	0.28	1 (1%) 78 53	52, 88, 150, 197	0
54	BY	102/104 (98%)	0.23	1 (0%) 79 55	68, 95, 169, 203	0
55	BZ	94/94 (100%)	-0.00	0 100 100	83, 112, 151, 177	0
All	All	10889/11600 (93%)	0.24	373 (3%) 48 30	28, 105, 249, 452	0

The worst 5 of 373 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	BJ	7	ILE	7.2
7	AG	4	ARG	6.7
42	BK	21	GLU	6.3
20	AT	3	ILE	5.7
4	AD	24	VAL	5.7

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 oligosaccharides in this entry.

6.4 Ligands ⓘ

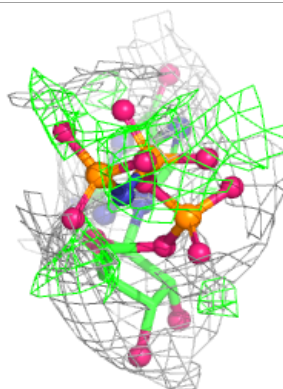
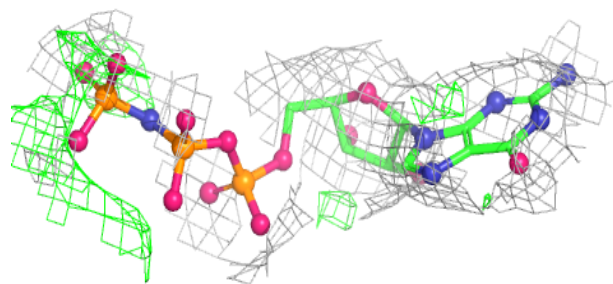
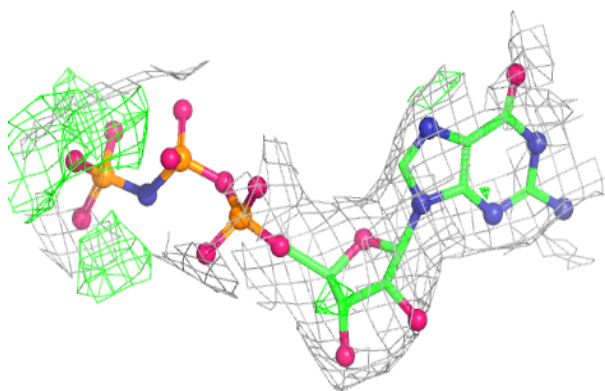
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
57	MG	AW	602	1/1	0.78	0.13	36,36,36,36	0
56	GNP	AW	601	32/32	0.88	0.11	81,97,115,121	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 GNP AW 601:

$2mF_o-DF_c$ (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.