



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 25, 2026 – 09:56 PM EDT

PDB ID : 4V9H / pdb_00004v9h
Title : Crystal structure of the ribosome bound to elongation factor G in the guanosine triphosphatase state
Authors : Tourigny, D.S.; Fernandez, I.S.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2013-03-25
Resolution : 2.86 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

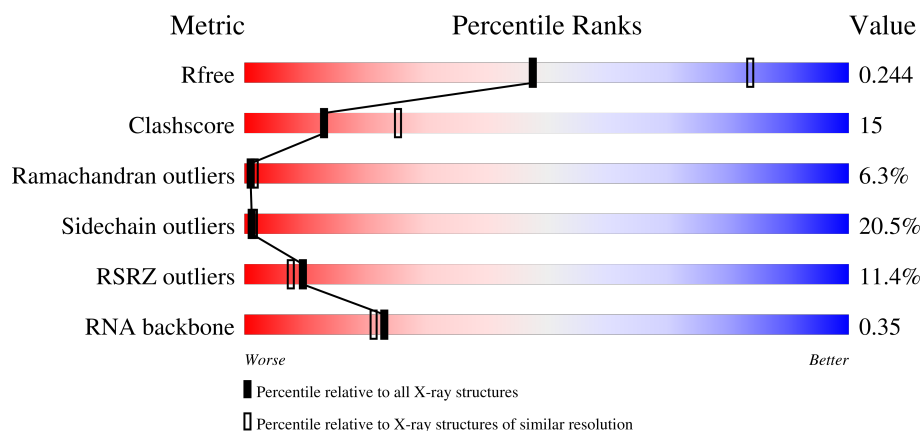
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.86 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)
RNA backbone	3983	1009 (3.06-2.66)

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	1516	3% 46% 38% 13%
2	AV	76	4% 36% 29% 22% 11%
3	AX	25	4% 12% 8% 76%
4	AJ	98	24% 56% 31% 12%

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Mol	Chain	Length	Quality of chain
5	AK	119	
6	AL	124	
7	AM	124	
8	AN	60	
9	AO	88	
10	AP	83	
11	AQ	99	
12	AR	70	
13	AS	78	
14	AT	99	
15	AB	234	
16	AC	206	
17	AD	208	
18	AE	150	
19	AF	101	
20	AG	155	
21	AH	138	
22	AI	127	
23	AY	680	
24	AU	24	
25	BA	2915	
26	BB	122	
27	BN	140	
28	BO	122	
29	BP	150	

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Mol	Chain	Length	Quality of chain
30	BQ	141	
31	BR	118	
32	BS	112	
33	BT	146	
34	BU	118	
35	BV	101	
36	BW	113	
37	BX	96	
38	BY	110	
39	BZ	206	
40	B0	85	
41	B1	98	
42	B2	72	
43	BD	276	
44	B3	60	
45	B4	71	
46	B5	60	
47	B6	54	
48	B7	49	
49	B8	65	
50	B9	37	
51	BC	229	
52	BE	206	
53	BF	210	
54	BG	182	

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Mol	Chain	Length	Quality of chain
55	BH	180	15% 46% 38% 9%
56	BK	147	81% 38% 40% 7% 14%
57	BJ	130	81% 69% 26% 5%
58	BL	125	46% 11% 42%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 151831 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1514	Total	C	N	O	P	0	0	0
			32529	14480	6018	10518	1513			

- Molecule 2 is a RNA chain called PE hybrid state tRNA Phe.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	74	Total	C	N	O	P	0	0	0
			1579	705	285	516	73			

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AX	6	Total	C	N	O	P	0	0	0
			125	56	19	44	6			

- Molecule 4 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 5 is a protein called 30S ribosomal protein S11.

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

- Molecule 6 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 7 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			

- Molecule 8 is a protein called 30S ribosomal protein S14 TYPE Z.

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

- Molecule 9 is a protein called 30S ribosomal protein S15.

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

- Molecule 10 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 11 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AQ	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			

- Molecule 12 is a protein called 30S ribosomal protein S18.

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

- Molecule 13 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 14 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 15 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 16 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 17 is a protein called 30S ribosomal protein S4.

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

- Molecule 18 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			

- Molecule 19 is a protein called 30S ribosomal protein S6.

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

- Molecule 20 is a protein called 30S ribosomal protein S7.

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

- Molecule 21 is a protein called 30S ribosomal protein S8.

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

- Molecule 22 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AI	127	Total	C	N	O		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 23 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AY	622	Total	C	N	O	S	0	0	0
			4877	3097	837	924	19			

- Molecule 24 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AU	24	Total	C	N	O		0	0	0
			209	128	50	31				

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2859	Total	C	N	O	P	0	0	0
			61580	27407	11519	19796	2858			

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BN	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 28 is a protein called 50S ribosomal protein L14.

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

- Molecule 29 is a protein called 50S ribosomal protein L15.

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

- Molecule 30 is a protein called 50S ribosomal protein L16.

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

- Molecule 31 is a protein called 50S ribosomal protein L17.

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

- Molecule 32 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
32	BS	98	Total	C	N	O	0	0	0
			770	486	154	130			

- Molecule 33 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BT	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 34 is a protein called 50S ribosomal protein L20.

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

- Molecule 35 is a protein called 50S ribosomal protein L21.

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

- Molecule 36 is a protein called 50S ribosomal protein L22.

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

- Molecule 37 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BX	92	Total	C	N	O	S	0	0	0
			725	471	131	123				

- Molecule 38 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BY	100	Total	C	N	O	S	0	0	0
			775	500	148	123	4			

- Molecule 39 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BZ	198	Total	C	N	O	S	0	0	0
			1508	960	274	272	2			

- Molecule 40 is a protein called 50S ribosomal protein L27.

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

- Molecule 41 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	B1	93	Total	C	N	O	S	0	0	0
			731	460	145	125	1			

- Molecule 42 is a protein called 50S ribosomal protein L29.

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

- Molecule 43 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BD	271	Total	C	N	O	S	0	0	0
			2104	1329	416	356	3			

- Molecule 44 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	B3	59	Total	C	N	O	S	0	0	0
			467	298	90	78	1			

- Molecule 45 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	B4	30	Total	C	N	O	S	0	0	0
			225	142	36	43	4			

- Molecule 46 is a protein called 50S ribosomal protein L32.

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

- Molecule 47 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B6	44	Total	C	N	O	S	0	0	0
			380	235	77	64	4			

- Molecule 48 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 49 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B8	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BC	225	Total	C	N	O	S	0	0	0
			1718	1085	315	316	2			

- Molecule 52 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BE	204	Total	C	N	O	S	0	0	0
			1563	988	299	270	6			

- Molecule 53 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BF	207	Total	C	N	O	S	0	0	0
			1623	1035	303	282	3			

- Molecule 54 is a protein called 50S ribosomal protein L5.

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

- Molecule 55 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BH	173	Total	C	N	O	S	0	0	0
			1303	824	244	234	1			

- Molecule 56 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	BK	127	Total	C	N	O	S	0	0	0
			936	598	161	172	5			

- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

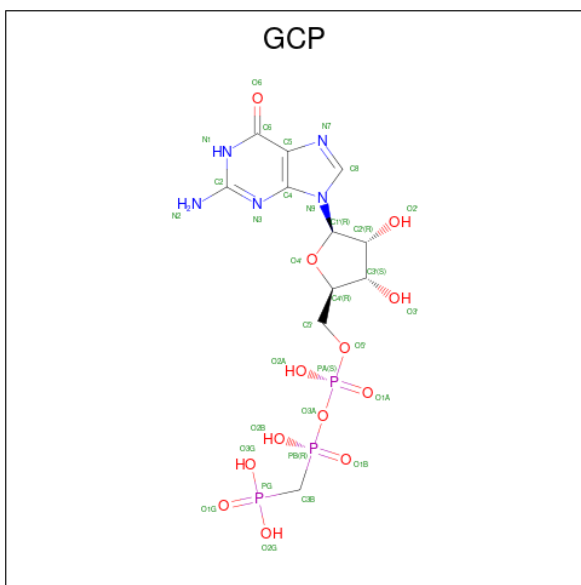
- Molecule 58 is a protein called 50S ribosomal protein L12 CTD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BL	72	Total	C	N	O		0	0	1
			356	213	72	71				

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	45	Total	Mg	0	0
			45	45		
59	AY	1	Total	Mg	0	0
			1	1		
59	BA	88	Total	Mg	0	0
			88	88		
59	BD	1	Total	Mg	0	0
			1	1		
59	B8	1	Total	Mg	0	0
			1	1		
59	BE	1	Total	Mg	0	0
			1	1		
59	BF	1	Total	Mg	0	0
			1	1		

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



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

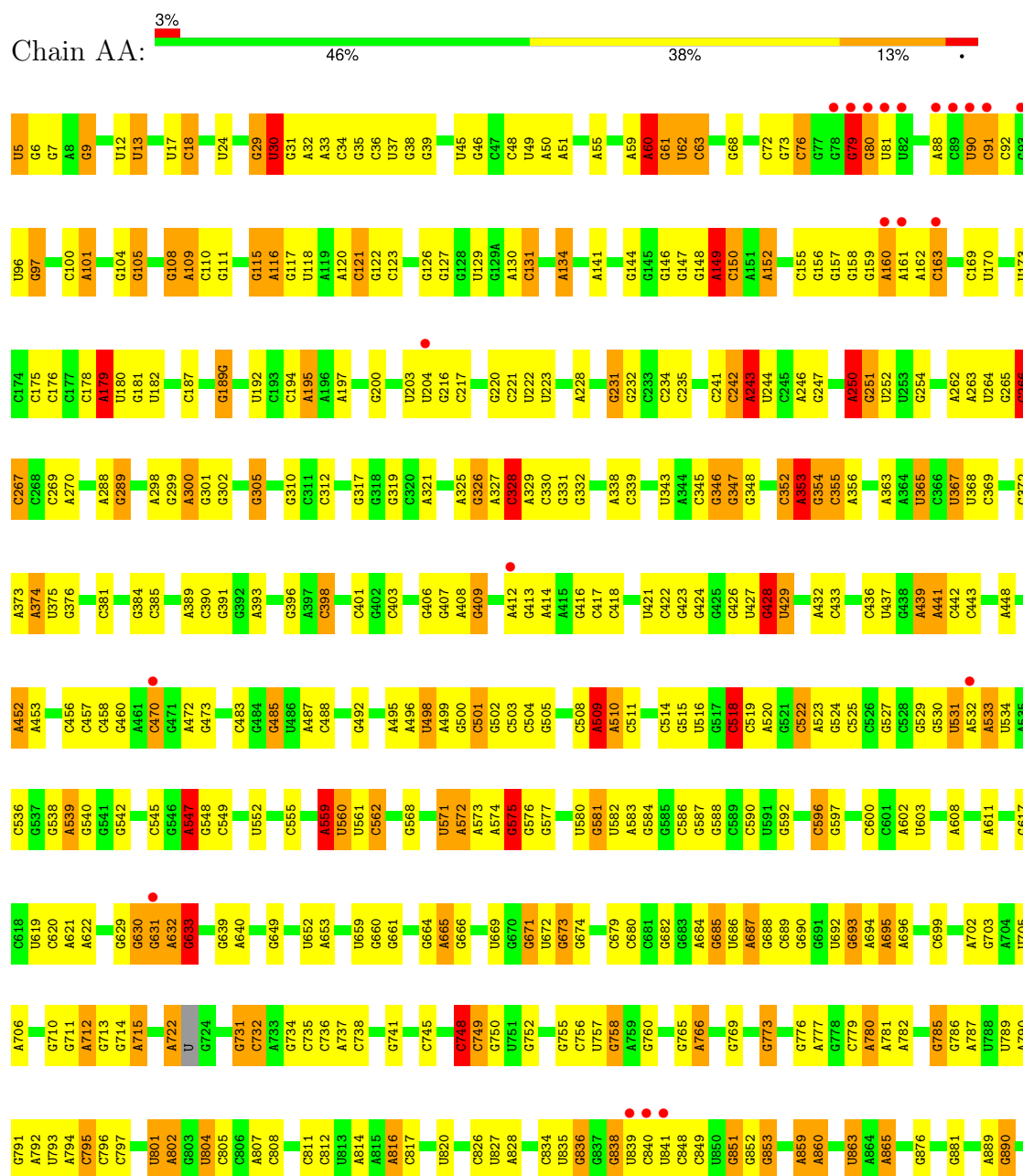
- Molecule 61 is water.

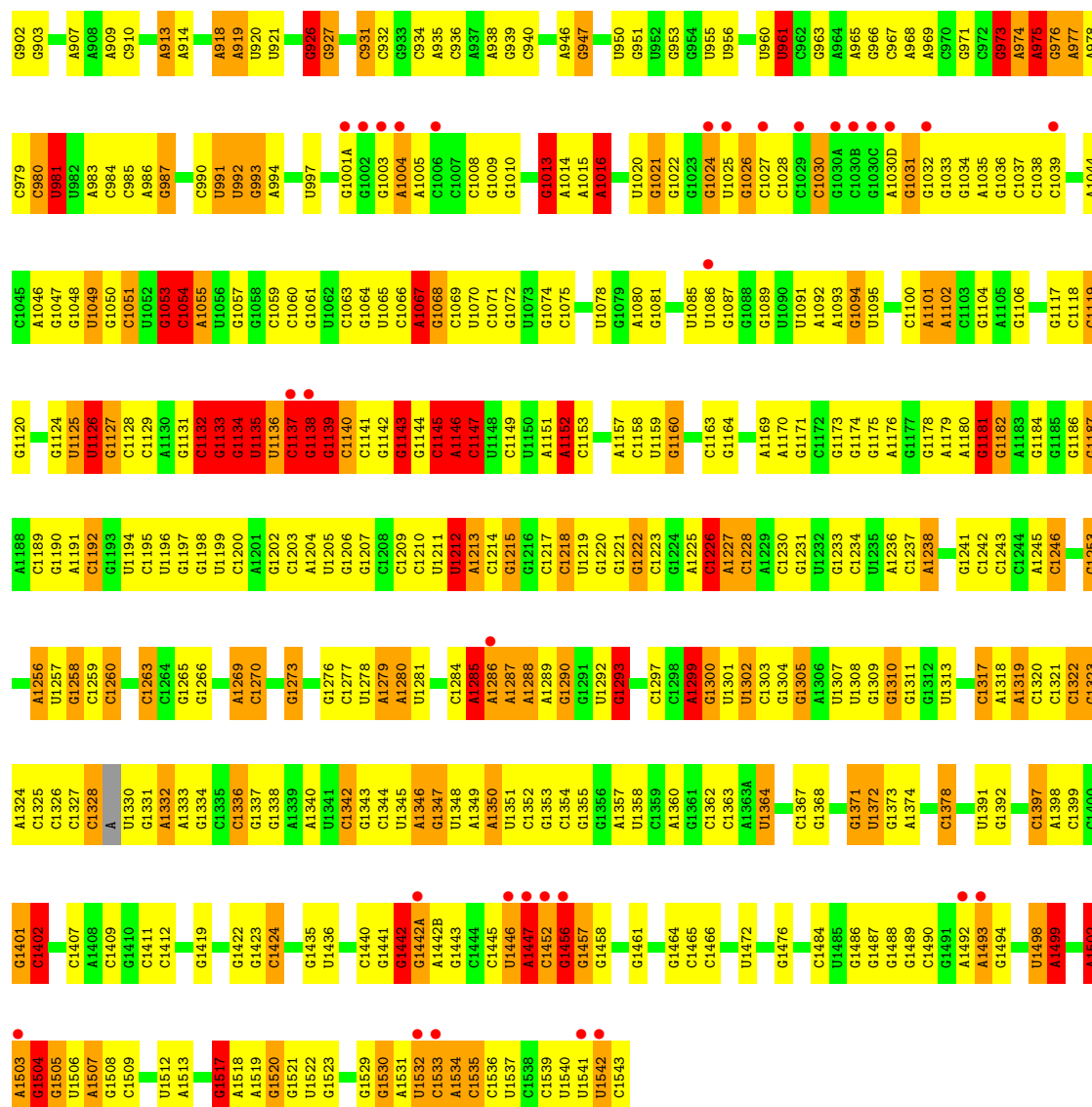
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
61	AY	4	Total O 4 4	0	0

3 Residue-property plots

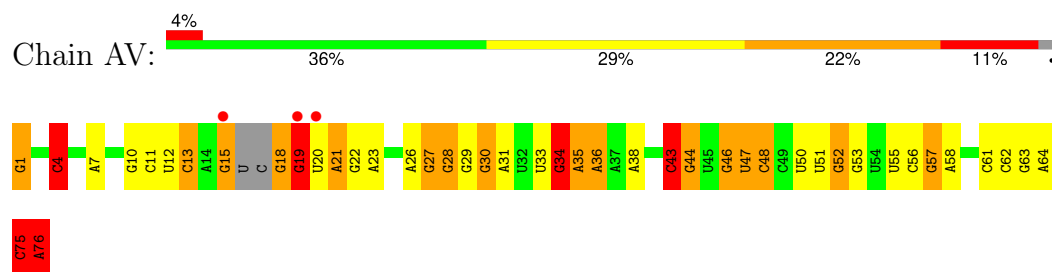
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





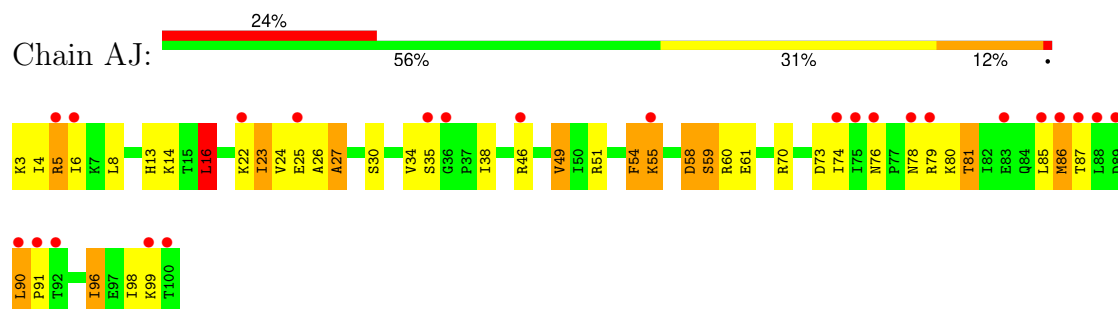
• Molecule 2: PE hybrid state tRNA Phe



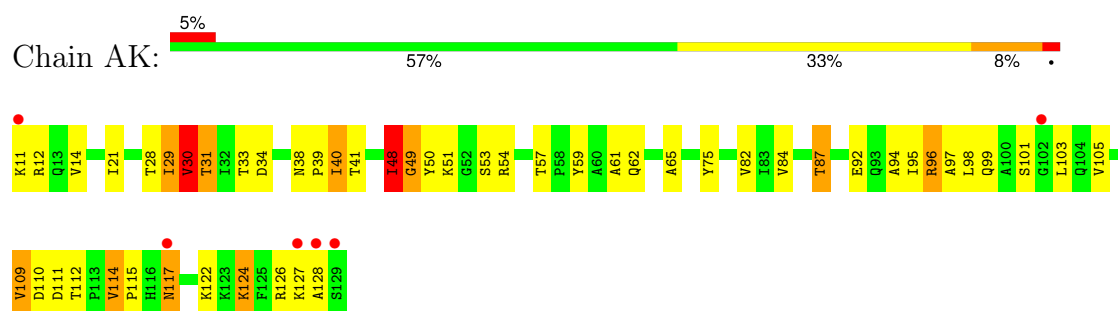
• Molecule 3: mRNA



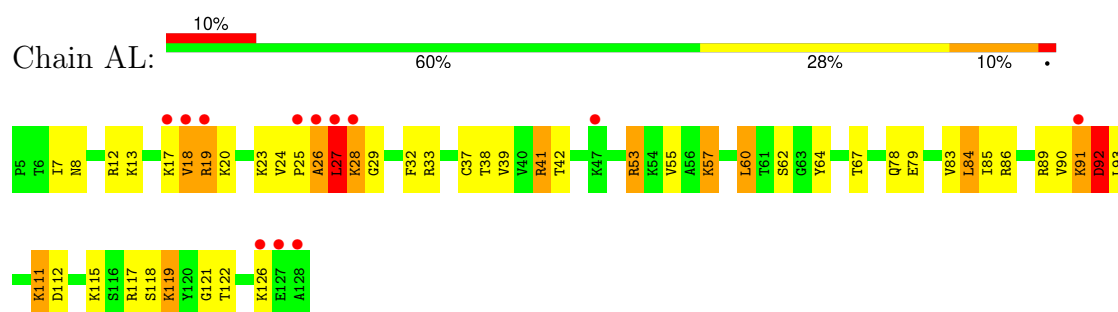
- Molecule 4: 30S ribosomal protein S10



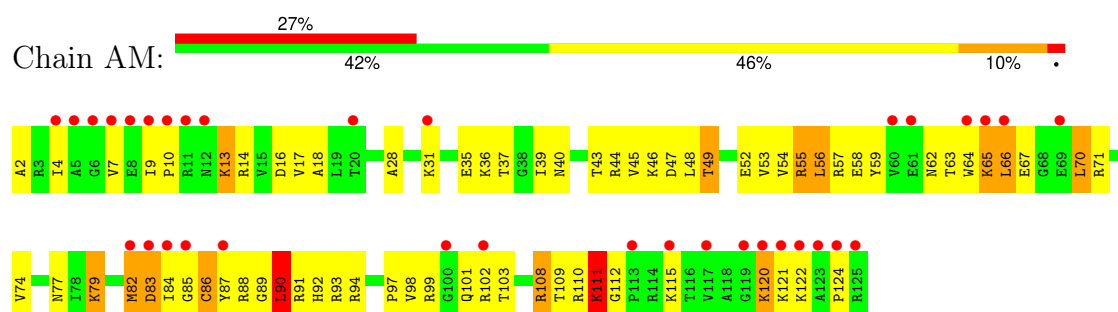
- Molecule 5: 30S ribosomal protein S11



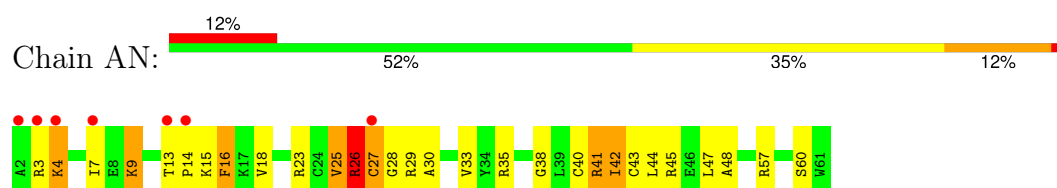
- Molecule 6: 30S ribosomal protein S12



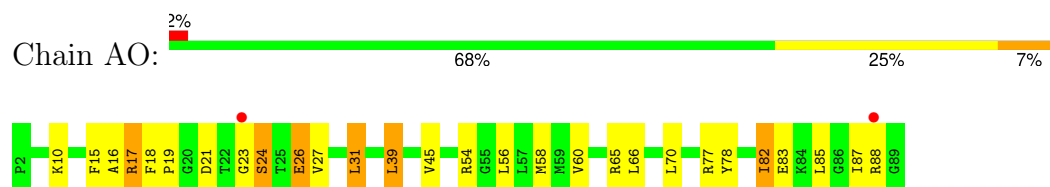
- Molecule 7: 30S ribosomal protein S13



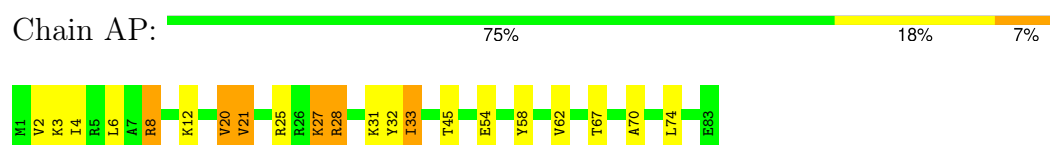
- Molecule 8: 30S ribosomal protein S14 TYPE Z



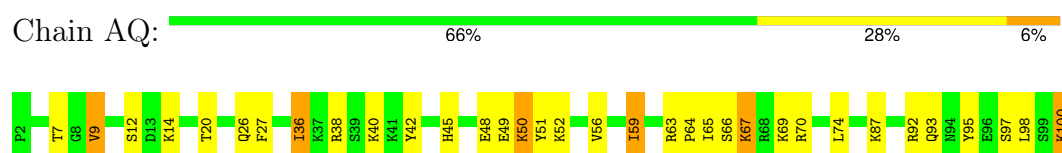
- Molecule 9: 30S ribosomal protein S15



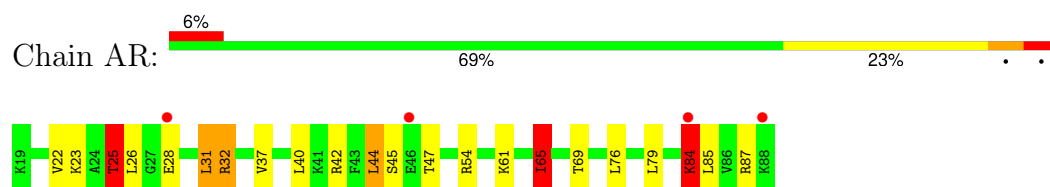
- Molecule 10: 30S ribosomal protein S16



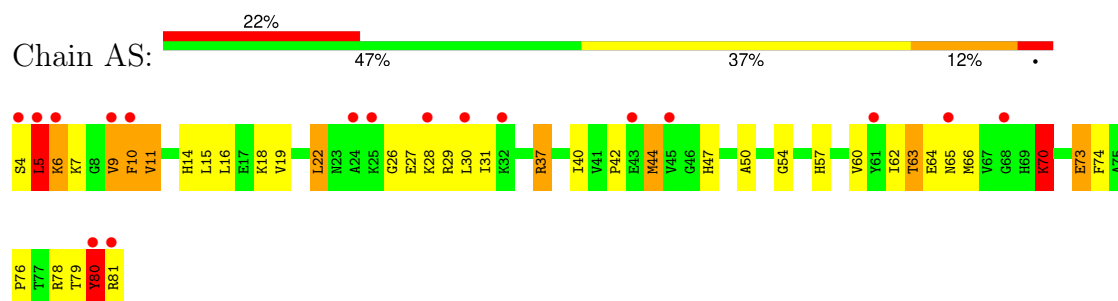
- Molecule 11: 30S ribosomal protein S17



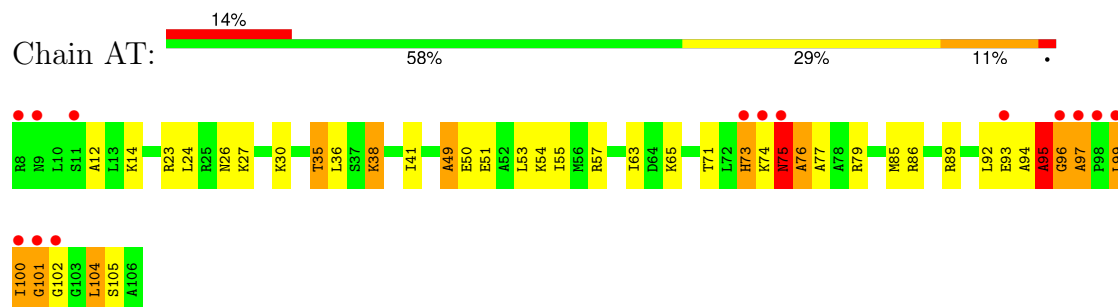
- Molecule 12: 30S ribosomal protein S18



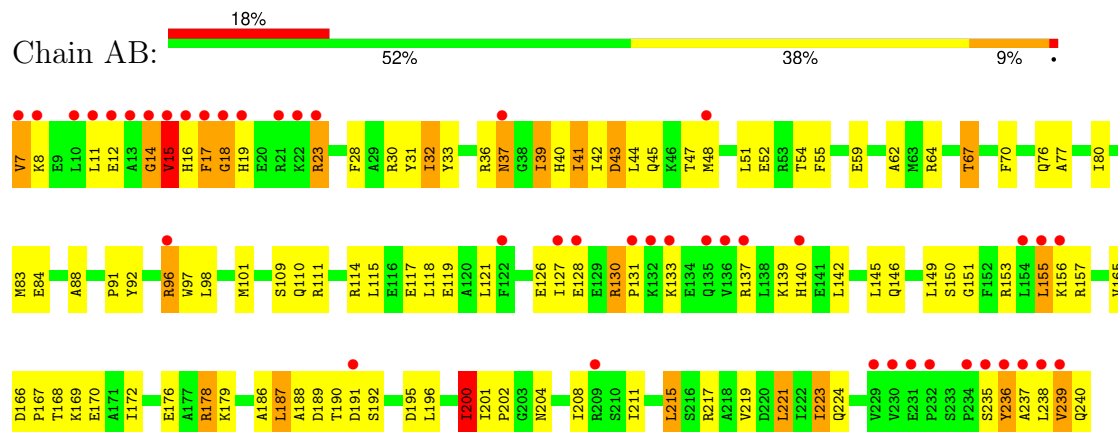
- Molecule 13: 30S ribosomal protein S19



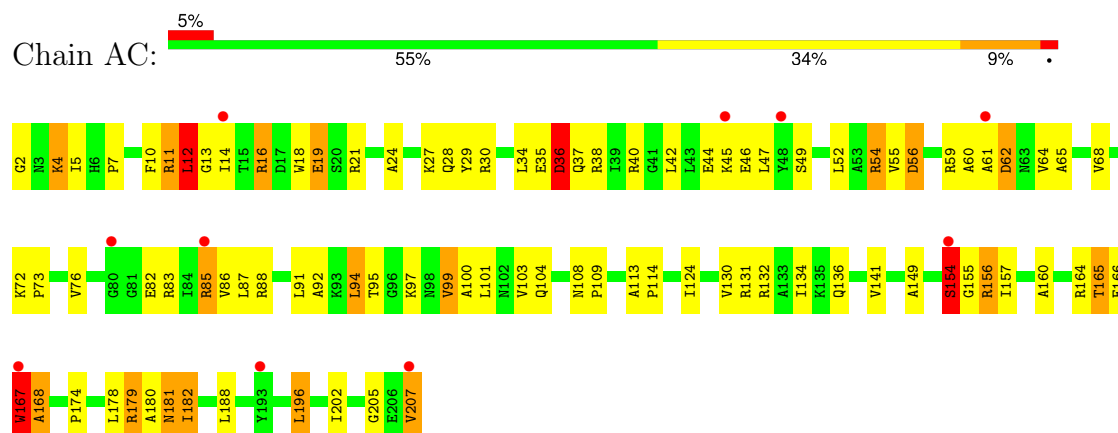
- Molecule 14: 30S ribosomal protein S20



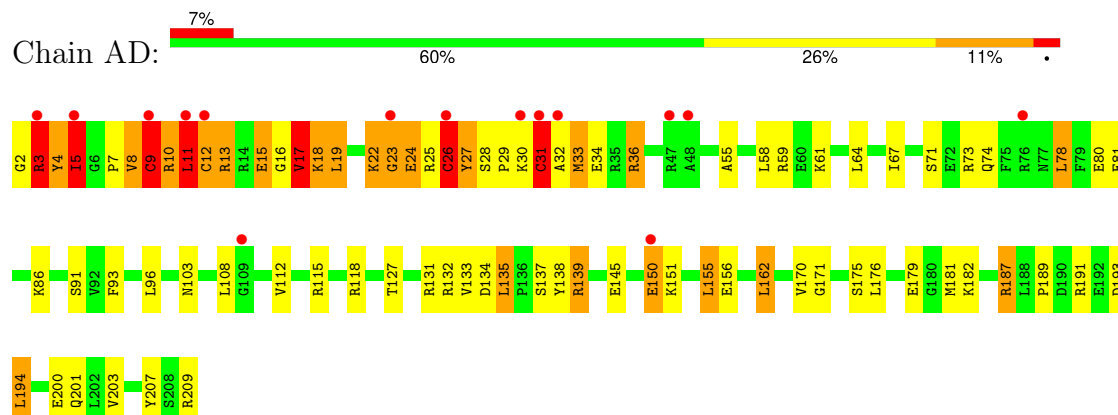
- Molecule 15: 30S ribosomal protein S2



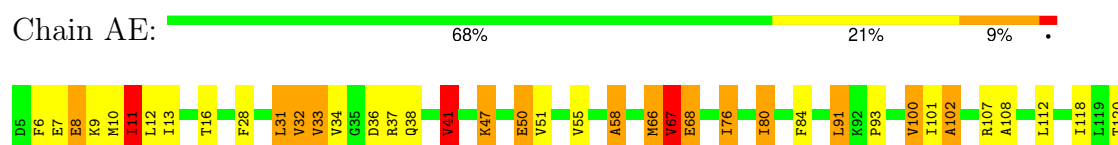
- Molecule 16: 30S ribosomal protein S3



- Molecule 17: 30S ribosomal protein S4



- Molecule 18: 30S ribosomal protein S5

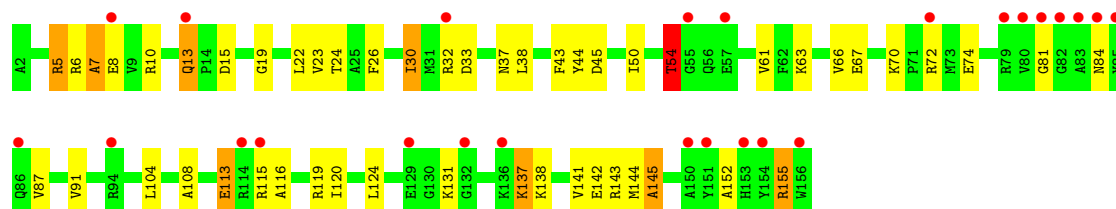




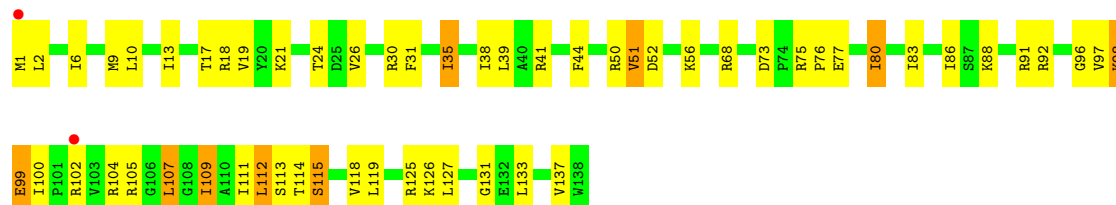
- Molecule 19: 30S ribosomal protein S6



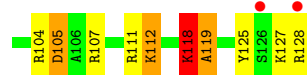
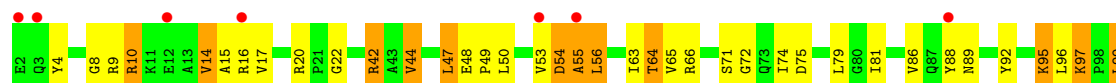
- Molecule 20: 30S ribosomal protein S7



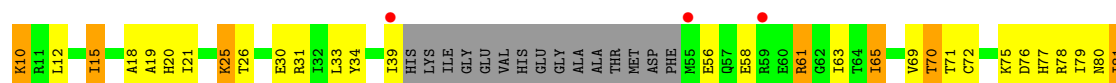
- Molecule 21: 30S ribosomal protein S8

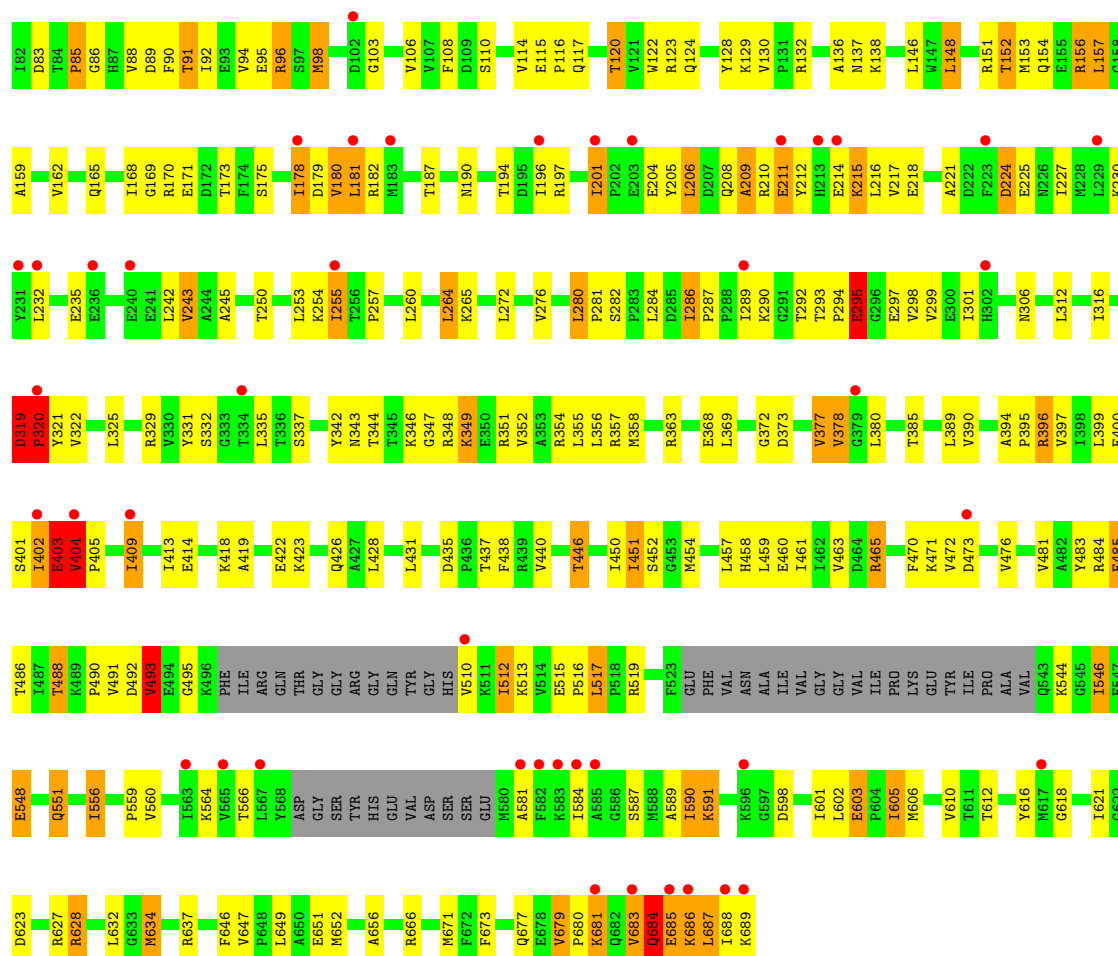


- Molecule 22: 30S ribosomal protein S9



- Molecule 23: Elongation factor G

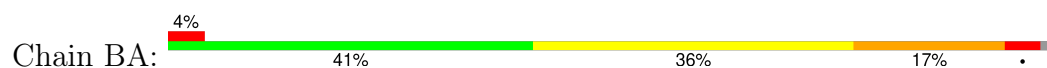




• Molecule 24: 30S ribosomal protein THX

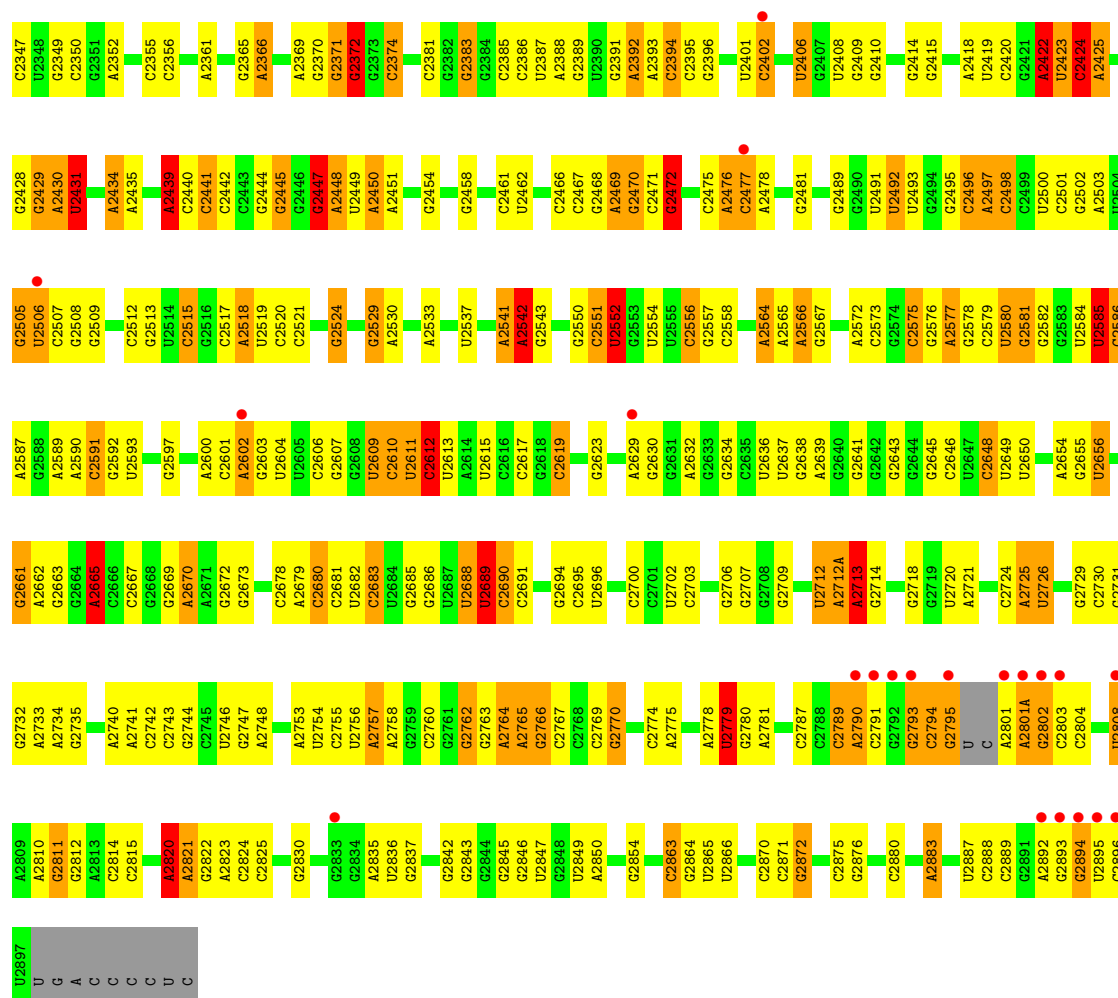


• Molecule 25: 23S ribosomal RNA

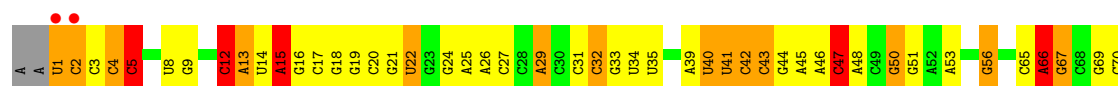




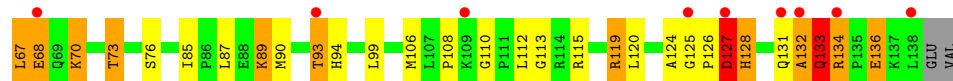
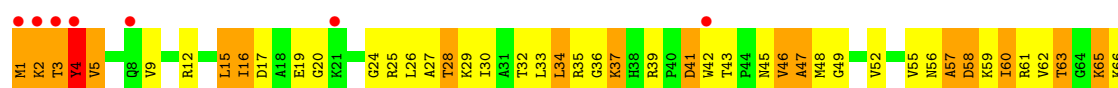
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G2285	G2191	G2126	C2055	U1976	C1905	G1814	C1743	A1652	U1576	C1505	G1435	G1358	A1275
A2286	G2192	G2127	G2056	A1977	G1906	G1815	C1745	G1653	U1577	C1506	C1437	A1359	
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			A2060	C1979	C	G1817	G1746	A1655	A1579	C1508		A1365	G1279
G2290	A2198	A2134	A2061	G1980	C1909	U1818	G1747	C1656	A1580	C1509	A1445	A1366	G1280
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	C2201	C2137	C2064	C1983	A1913	A1921	A1749	U1659	A1583	C1512	G1448	G1368	A1284
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C2297		C2139		G1987	U1915	G1923		C1663	A1588	U1514	G1450	A1371	A1286
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A2300	G2208	C2142	G2070	C1990	A1918		A1756	A1668		U1523	C1452	C1289	C1290
C2301	G2210	C2143	A2071	U1991	U1833	U1839	U1757	A1669	G1591	G1520	U1453	C1376	C1291
G2302	G2211	U2144	G2072	U1992	A1920	U1834		A1670		U1523		A1379	
G2303	G2212	C2145	C2073	U1993	G1921	G1935	A1760	U1671	G1596	G1524	G1458	G1380	G1295
G2304	C2146	C2146					C1761	C1672	A1596	G1525	G1459	G1381	G1296
A2305	A2225	G2147	A2077	C1996	C1924	C1938	A1762	U1673	A1597	G1526	A1460		
C2306	C2226	G2148	C2078	G1997	C1925	G1939	G1763	C1674	C1598	G1527	A1461		
G2307	G2226	G2149	U2079		U1926		G1764	C1675	C1599	A1528	C1462		
A2308	G2230	U2150	G2080	A2001	A1927	C1943		A1676	C1600	A1528A	C1463	A1384	G1299
G2309	C2231	G2151	C2081	G2002	A1928		G1769	A1677		G1529	G1464	G1386	U1300
A2310	U2232	G2152		G2003	G1929	G1846	G1770	G1678	A1603	C1530	G1465	C1387	A1301
A2311		G2153	U2086		U1930	A1847	C1771	U1679		C1531	G1466	G1388	A1302
U2312	G2238	G2154	G2087	G2009	A1932	G1848	G1772	U1680	G1606	C1532	C1467	G1389	C1306
C2313	G2239	G2155			G1933	G1849	A1773	G1681	C1607	G	C1468	U1390	U1307
G2314		G2156	U2092	A2013	G1933	G1950	C1774	G1682	A1608	U	A1469	A1307	A1308
G2315	U2243	G2157	G2093	U2016		G1857	U1775	C1683	A1609	A	G1470	A1392	
C2316	A2158	A2158	C2094	U2016	A1936	G1857	G1776	C1684	A1610	C	A1471	A1393	
C2317	G2159	G2160	G2095	A2019	A1937	G1858	U1777	C1685		G	C1474	A1394	U1312
G2318	A2247	G2160	U2096	A2019	A1938	G1859	U1778	C1686	C1615	G1538	G1475	U1394	U1313
A2319	G2248	C2097	C2097	A2020		G1860	U1779	C1686	A1616	G1539	C1476	A1395	C1314
A2320	U2249	C2101	U2098	C2021	U1943	G1863	G1781	U1688	C1617	U1540	A1477	U1397	C1315
G2321	G2250	G2165	U2099	U2022	G1945	U1864	C1782	A1689	G1619	G1541	G1478		
A2322	G2251	G2166	G2100	G2023	G1945	G1865	U1783	A1690	G1620	A1542	G1479	C1403	A1322
G2323	G2252	U2167	G2101	G2024	U1946	C1866	C1783	C1691	U1621	C1543	G1480	C1404	U1323
C2324	G2253	G2168	C2103	C2026	C1947	C1866	A1784	U1692	G1622	A1544	U1481	U1405	U1326
G2325	G2259	G2169	G2104	G2027	A1952	A1876	A1785	C1693	G1623	C1546	U1482	U1406	C1327
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A2328	U2262	U2171	C2107	A2031	U1956	C1880	G1789	G1696	G1630	C1549	U1415	C1330	U1329
	C2263	U2172	C2108	A2032	U1957	C1881	A1790	G1697			G1488	C1331	C1330
G2331	G2264	C2173	U2109	A2033	C1957	C1882	A1791	A1698	A1632	A1554	U1489	C1417	G1332
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G2333	A2266	C2175	G2111	U2035	G1959	A1884	C1795	U1713	A1634	A1558	G1491	A1419	G1338
G2334	A2267	A2176	C2111	G2035	A1960	A1885	U1796	G1710	G1635	G1559	C1492	U1420	
A2335	A2268	C2177	G2112	C2036	C1961	C1886	C1797		C1636		A1493	G1421	G1344
		C2178	U2113		C1962	C1887	U1798	U1713	A1637	A1562	A1494	G1422	C1345
G2337	U2272	A2114	A2114	C2039	U1963	G1888	C1799	G1714	C1638	A1563	A1495	G1426	C1346
U2338	A2273	G2115	G2115	C2040	G1964	A1889	U1799	G1714	C1639	C1564	A1496	G1347	G1346
G2340	A2274	G2181	C2116	U2041	C1965	A1889	G1799	G1714	C1640	C1565	U1497	A1427	G1348
G2341	C2275	G2182	A2117	A2042	A1966		C1800	U1720		A1566	U1498	C1428	G1349
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C2343			G2120	C2044	G1968		A1802	G1721		A1570	C1500	C1430	
U2344	G2279	G2186	G2121	C2049	A1969	G1999	A1722	G1721	G1645	A1569	G1500	C1430	A1353
G2345	G2280	C2187	U2122	G2049	A1970	A1900	U1739	U1739	G1646	A1570	C1501	C1431	
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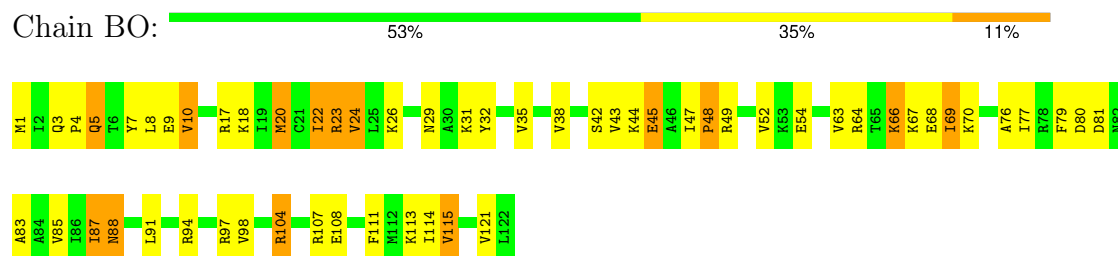
- Molecule 26: 5S ribosomal RNA



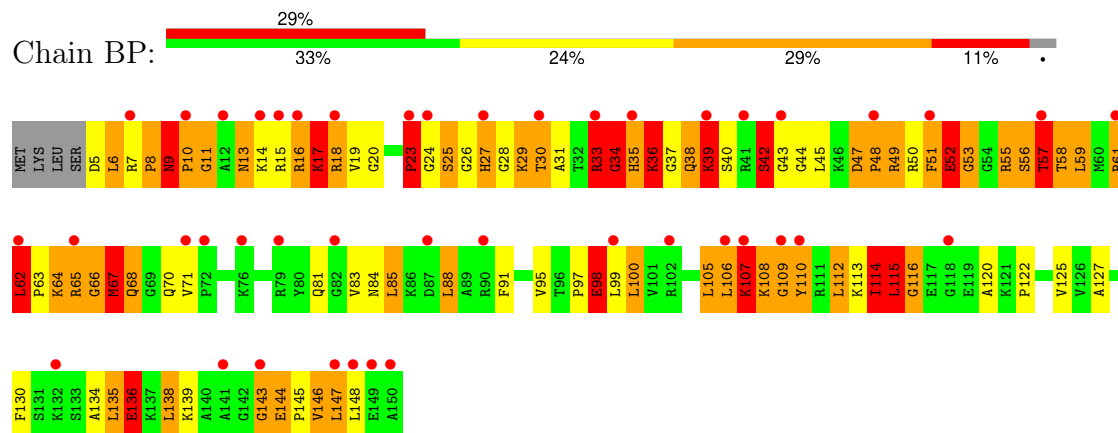
- Molecule 27: 50S ribosomal protein L13



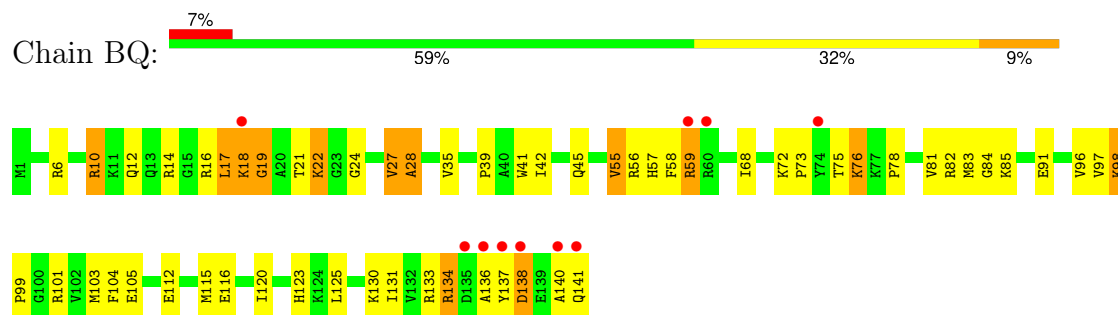
- Molecule 28: 50S ribosomal protein L14



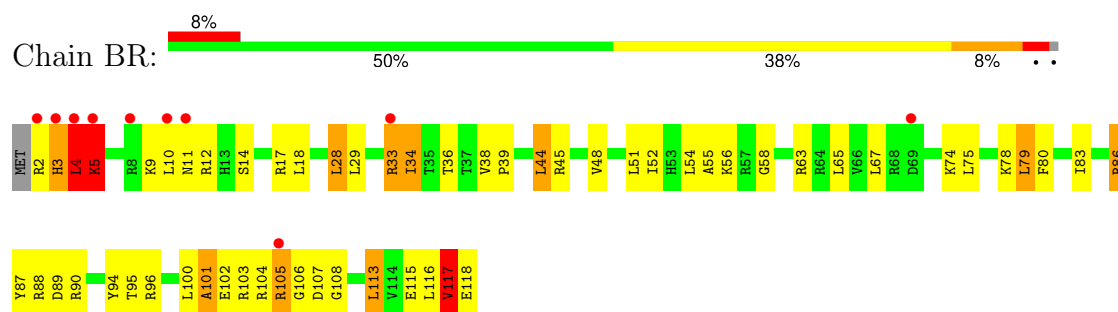
- Molecule 29: 50S ribosomal protein L15



- Molecule 30: 50S ribosomal protein L16

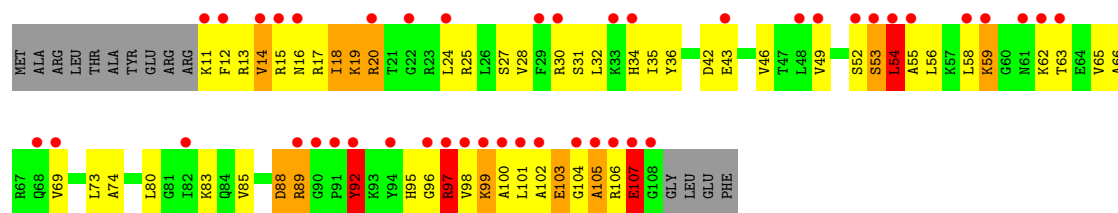


- Molecule 31: 50S ribosomal protein L17

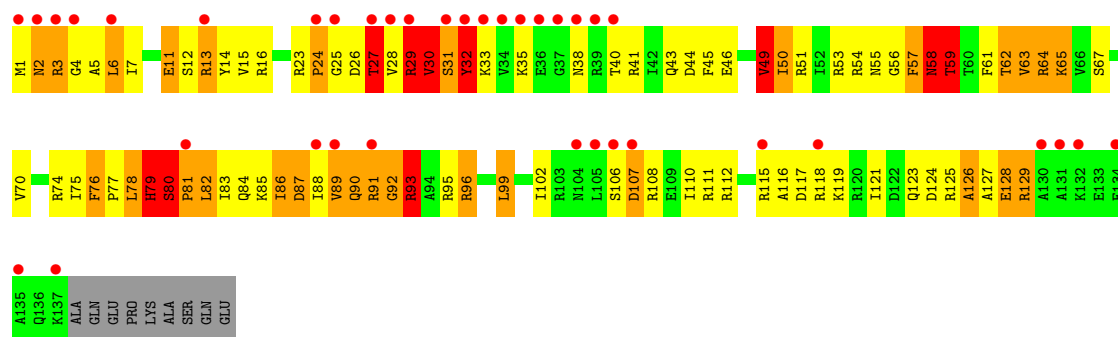


- Molecule 32: 50S ribosomal protein L18

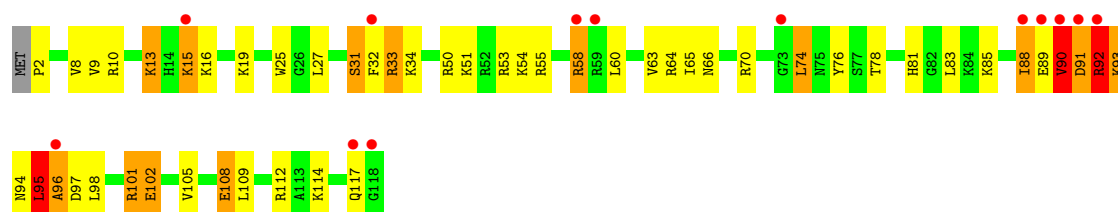




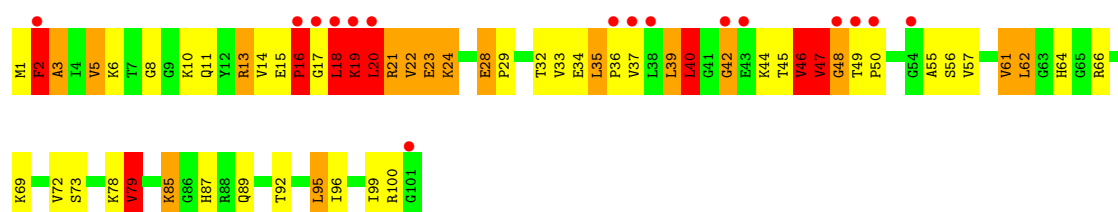
• Molecule 33: 50S ribosomal protein L19



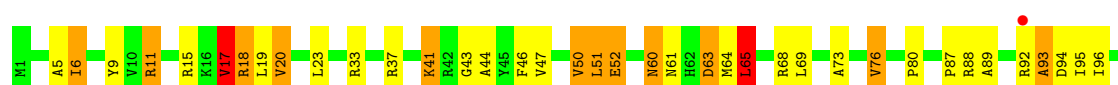
• Molecule 34: 50S ribosomal protein L20



• Molecule 35: 50S ribosomal protein L21

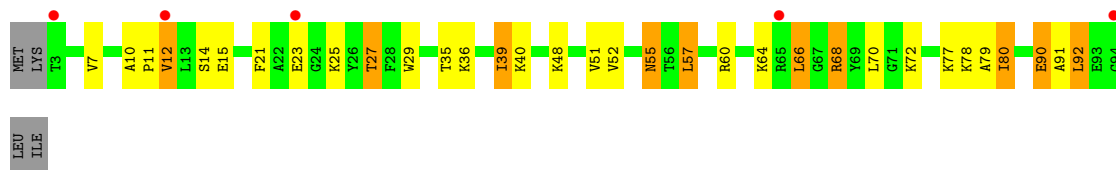


• Molecule 36: 50S ribosomal protein L22

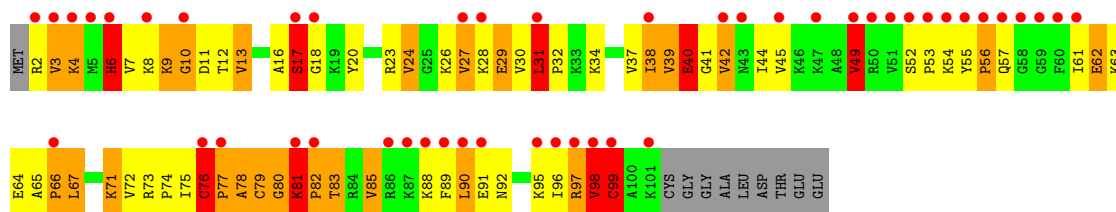
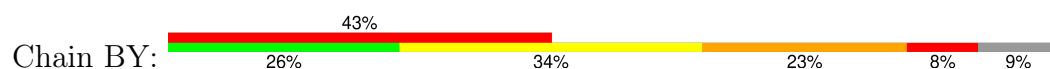




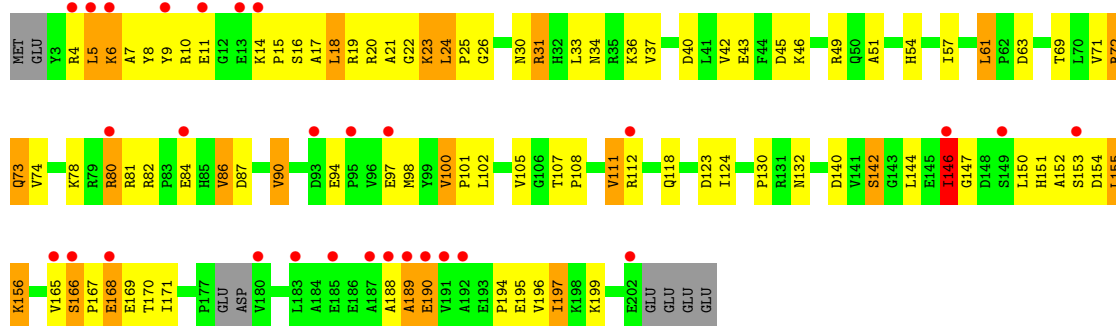
- Molecule 37: 50S ribosomal protein L23



- Molecule 38: 50S ribosomal protein L24



- Molecule 39: 50S ribosomal protein L25

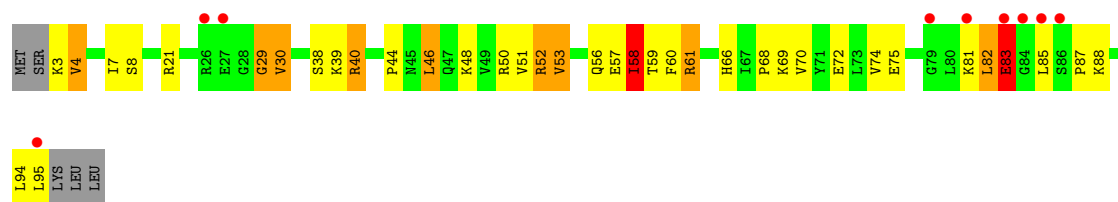


- Molecule 40: 50S ribosomal protein L27



- Molecule 41: 50S ribosomal protein L28

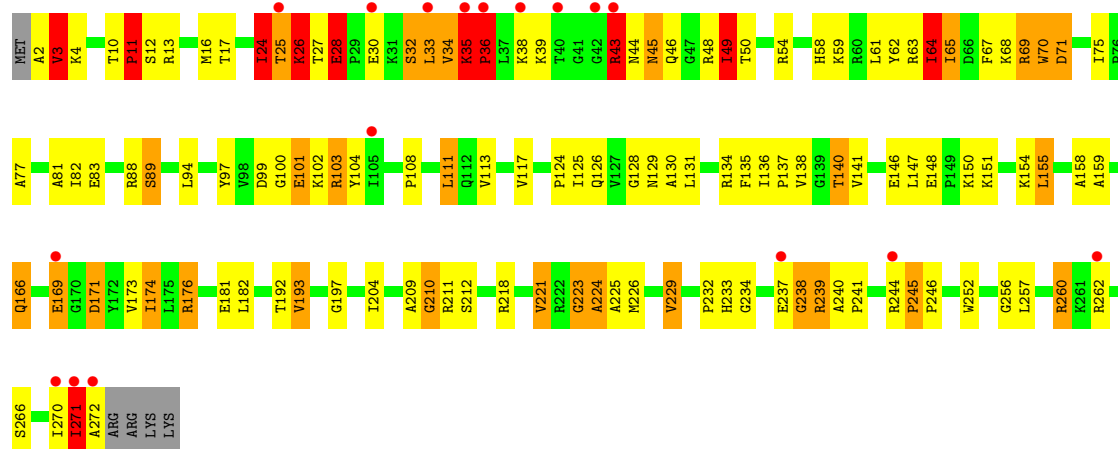




- Molecule 42: 50S ribosomal protein L29



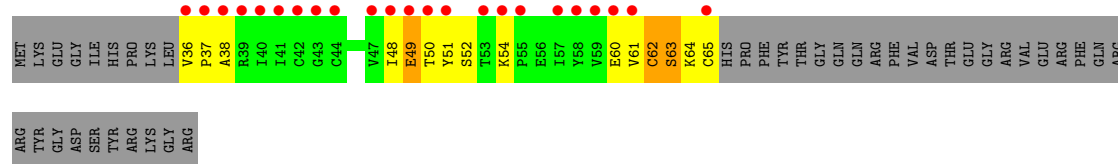
- Molecule 43: 50S ribosomal protein L2



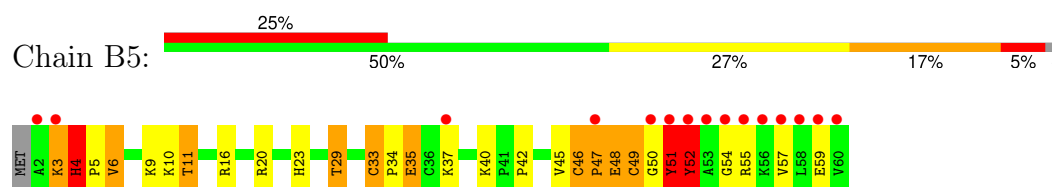
- Molecule 44: 50S ribosomal protein L30



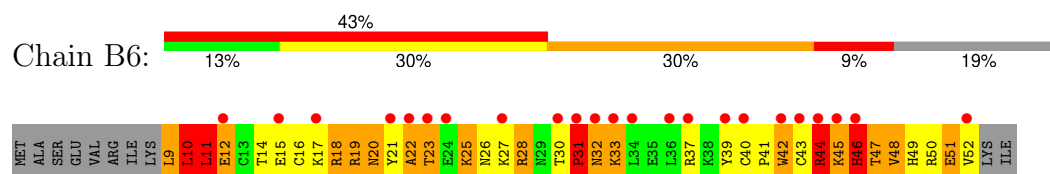
- Molecule 45: 50S ribosomal protein L31



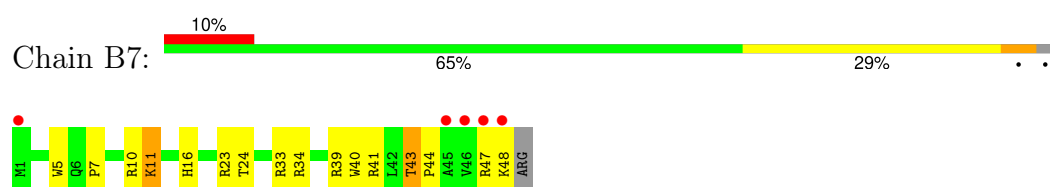
- Molecule 46: 50S ribosomal protein L32



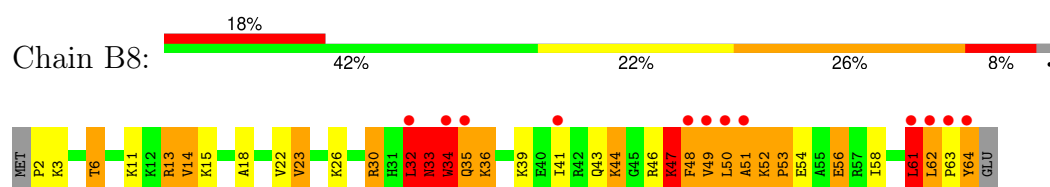
- Molecule 47: 50S ribosomal protein L33



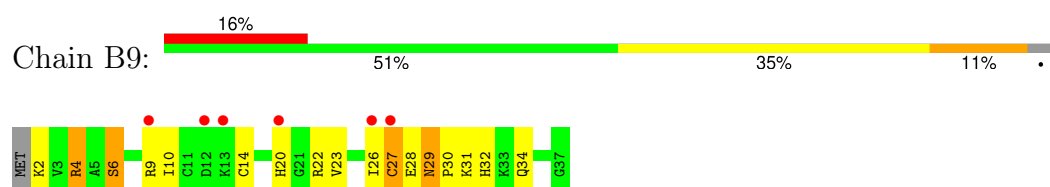
- Molecule 48: 50S ribosomal protein L34



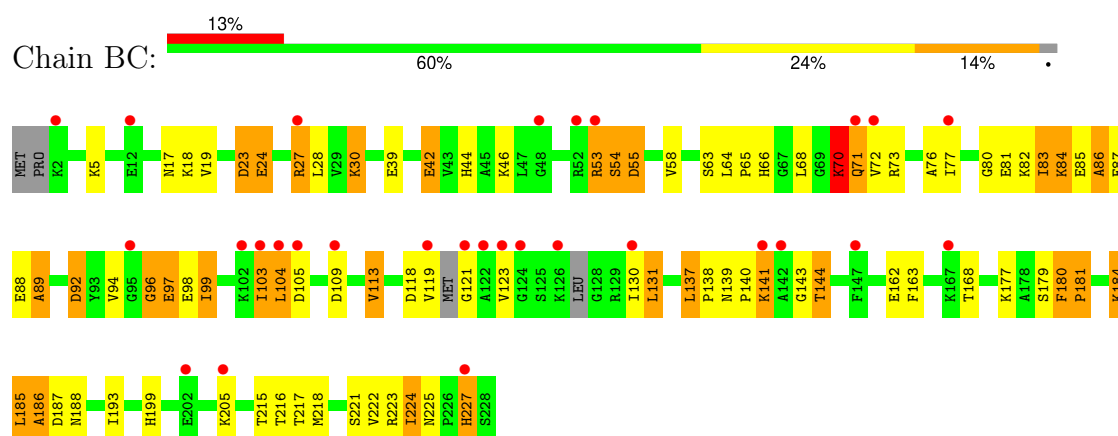
- Molecule 49: 50S ribosomal protein L35



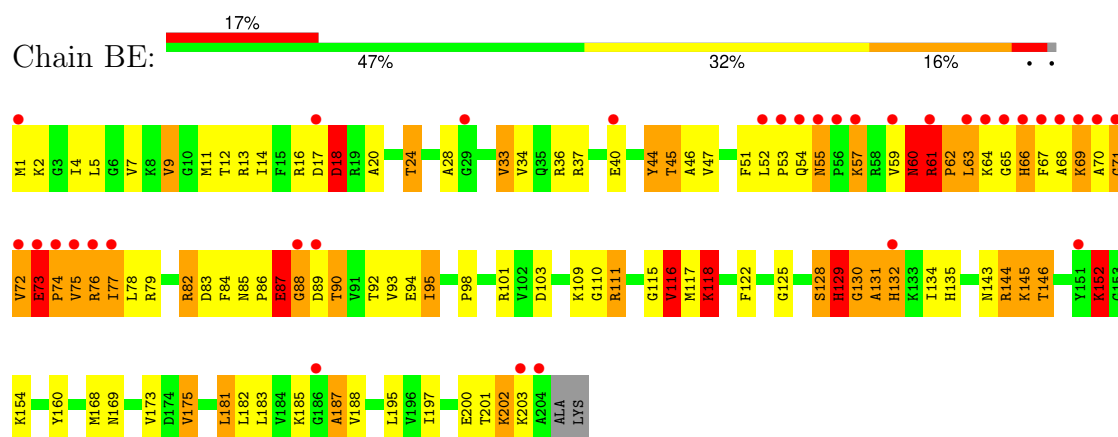
- Molecule 50: 50S ribosomal protein L36



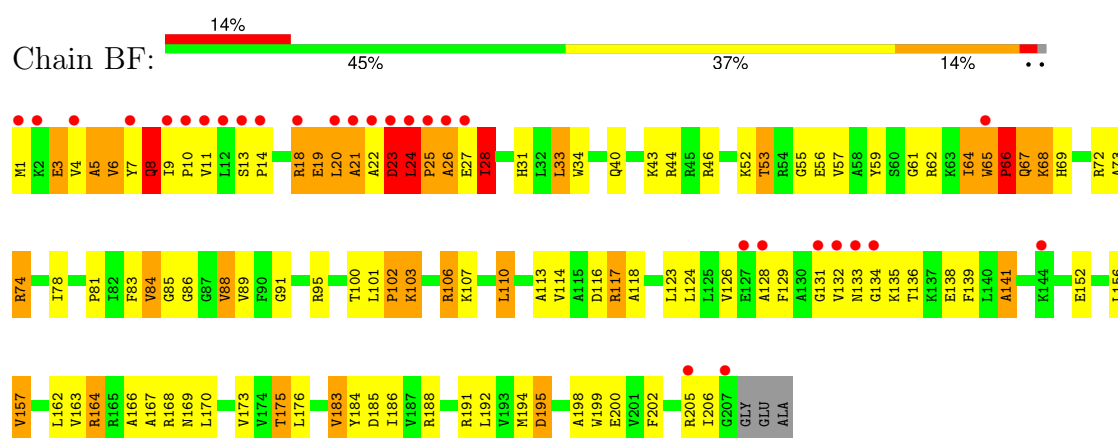
- Molecule 51: 50S ribosomal protein L1



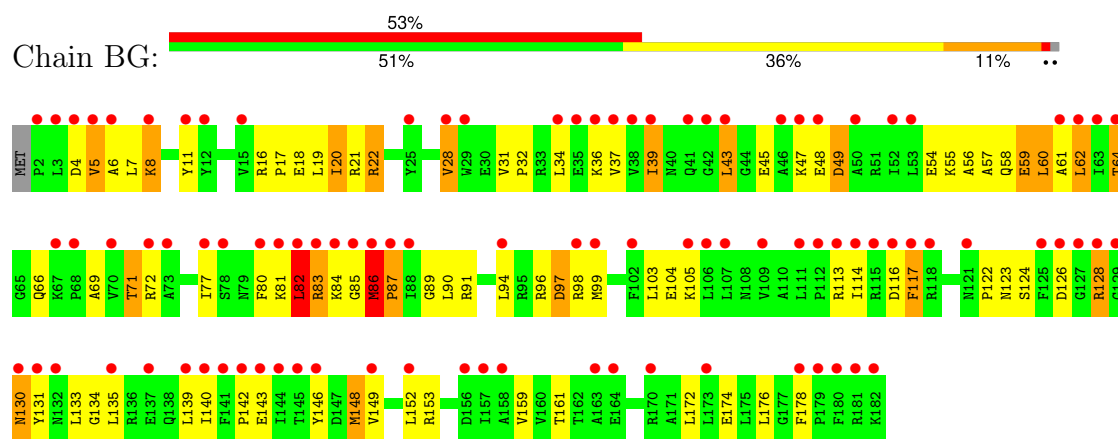
- Molecule 52: 50S ribosomal protein L3



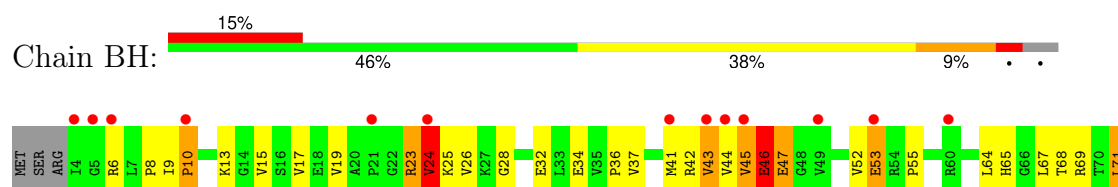
• Molecule 53: 50S ribosomal protein L4

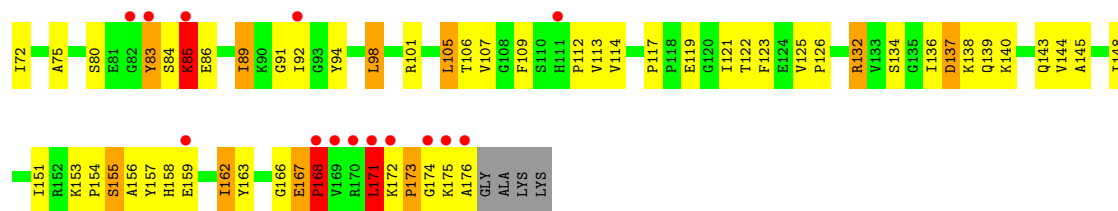


• Molecule 54: 50S ribosomal protein L5

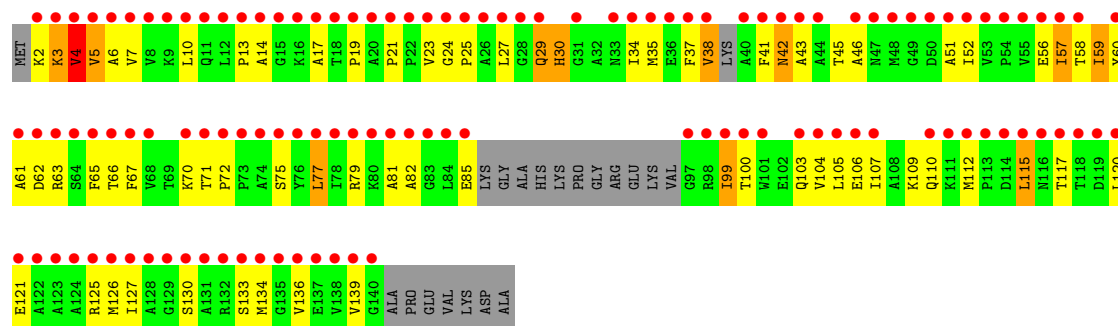
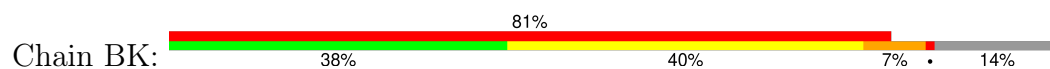


• Molecule 55: 50S ribosomal protein L6

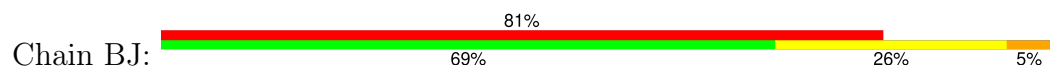




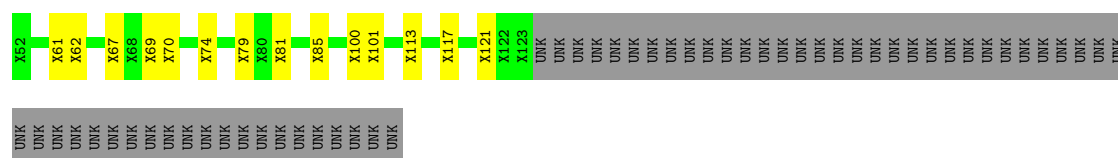
• Molecule 56: 50S ribosomal protein L11



• Molecule 57: 50S ribosomal protein L10



• Molecule 58: 50S ribosomal protein L12 CTD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	201.58Å 241.65Å 305.80Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	39.60 – 2.86 39.60 – 2.86	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.60-2.86) 98.5 (39.60-2.86)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.22	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.200 , 0.250 0.201 , 0.244	Depositor DCC
R_{free} test set	32790 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	151831	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% 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, 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	0.53	2/36408 (0.0%)	1.06	278/56818 (0.5%)
2	AV	0.50	1/1764 (0.1%)	1.18	23/2747 (0.8%)
3	AX	0.49	0/138	1.23	2/212 (0.9%)
4	AJ	0.95	0/808	1.17	4/1085 (0.4%)
5	AK	0.84	0/900	1.13	7/1213 (0.6%)
6	AL	0.95	1/987 (0.1%)	1.22	3/1320 (0.2%)
7	AM	0.78	0/999	1.14	6/1336 (0.4%)
8	AN	0.88	1/501 (0.2%)	1.29	6/664 (0.9%)
9	AO	0.88	0/745	1.08	0/992
10	AP	0.85	0/717	1.05	0/963
11	AQ	0.91	0/837	1.14	1/1117 (0.1%)
12	AR	0.81	0/579	1.08	2/768 (0.3%)
13	AS	0.81	0/643	1.10	2/865 (0.2%)
14	AT	0.90	1/765 (0.1%)	1.21	4/1007 (0.4%)
15	AB	0.76	0/1936	1.05	3/2609 (0.1%)
16	AC	0.90	2/1637 (0.1%)	1.12	2/2205 (0.1%)
17	AD	0.89	7/1733 (0.4%)	1.13	13/2318 (0.6%)
18	AE	0.94	0/1163	1.23	10/1564 (0.6%)
19	AF	0.79	0/856	1.00	1/1154 (0.1%)
20	AG	0.75	0/1276	1.04	2/1709 (0.1%)
21	AH	0.90	0/1136	1.13	3/1527 (0.2%)
22	AI	0.76	0/1029	1.09	3/1378 (0.2%)
23	AY	0.73	1/4961 (0.0%)	1.06	16/6710 (0.2%)
24	AU	0.77	0/213	0.98	0/277
25	BA	0.57	8/68964 (0.0%)	1.11	627/107644 (0.6%)
26	BB	0.46	0/2853	1.02	19/4451 (0.4%)
27	BN	0.99	3/1131 (0.3%)	1.31	9/1525 (0.6%)
28	BO	0.91	0/943	1.24	3/1269 (0.2%)
29	BP	1.21	8/1131 (0.7%)	1.53	13/1504 (0.9%)
30	BQ	0.87	0/1143	1.18	9/1527 (0.6%)
31	BR	1.03	3/974 (0.3%)	1.21	6/1302 (0.5%)
32	BS	0.76	0/778	1.05	1/1036 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BT	0.99	1/1155 (0.1%)	1.43	17/1542 (1.1%)
34	BU	1.02	1/975 (0.1%)	1.28	6/1297 (0.5%)
35	BV	0.97	0/790	1.23	6/1057 (0.6%)
36	BW	0.96	0/907	1.19	2/1216 (0.2%)
37	BX	0.93	0/739	1.20	2/993 (0.2%)
38	BY	1.23	3/788 (0.4%)	1.51	12/1051 (1.1%)
39	BZ	0.80	0/1539	1.09	5/2093 (0.2%)
40	B0	0.78	0/671	0.99	0/892
41	B1	0.97	0/738	1.24	5/981 (0.5%)
42	B2	0.81	0/600	1.12	0/793
43	BD	1.16	3/2154 (0.1%)	1.33	19/2905 (0.7%)
44	B3	0.81	0/472	1.02	0/634
45	B4	0.81	0/228	0.92	0/309
46	B5	1.22	3/473 (0.6%)	1.69	15/639 (2.3%)
47	B6	1.31	2/387 (0.5%)	1.61	6/518 (1.2%)
48	B7	1.03	0/426	1.02	0/561
49	B8	1.08	2/515 (0.4%)	1.44	8/679 (1.2%)
50	B9	0.98	0/302	1.30	5/397 (1.3%)
51	BC	0.75	2/1747 (0.1%)	1.17	12/2351 (0.5%)
52	BE	1.06	4/1596 (0.3%)	1.32	15/2153 (0.7%)
53	BF	0.91	0/1658	1.21	10/2244 (0.4%)
54	BG	0.71	1/1499 (0.1%)	0.95	3/2016 (0.1%)
55	BH	0.83	0/1327	1.24	10/1794 (0.6%)
56	BK	0.65	0/951	0.88	0/1290
57	BJ	0.91	1/650 (0.2%)	1.07	4/907 (0.4%)
All	All	0.69	61/163935 (0.0%)	1.12	1240/244128 (0.5%)

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
4	AJ	0	1
6	AL	0	1
8	AN	0	1
14	AT	0	2
17	AD	0	2
23	AY	0	4
27	BN	0	2
29	BP	0	15
30	BQ	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	BR	0	2
32	BS	0	1
33	BT	0	6
34	BU	0	3
35	BV	0	3
38	BY	0	6
41	B1	0	2
43	BD	0	4
46	B5	0	2
47	B6	0	3
51	BC	0	2
52	BE	0	5
53	BF	0	1
55	BH	0	1
58	BL	0	1
All	All	0	72

The worst 5 of 61 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	2506	U	O3'-P	10.11	1.76	1.61
17	AD	26	CYS	CA-C	9.30	1.65	1.52
31	BR	5	LYS	CA-C	8.74	1.60	1.52
17	AD	26	CYS	CA-CB	7.62	1.66	1.53
29	BP	27	HIS	CA-C	7.58	1.62	1.52

The worst 5 of 1240 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1498	U	C2'-C3'-O3'	18.14	136.71	109.50
1	AA	1067	A	C2'-C3'-O3'	16.92	134.88	109.50
1	AA	328	C	C2'-C3'-O3'	15.30	132.44	109.50
25	BA	1799	G	C2'-C3'-O3'	15.14	132.21	109.50
25	BA	2506	U	C2'-C3'-O3'	14.89	131.84	109.50

There are no chirality outliers.

5 of 72 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AJ	54	PHE	Peptide
6	AL	28	LYS	Peptide

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Mol	Chain	Res	Type	Group
8	AN	13	THR	Peptide
14	AT	73	HIS	Peptide
14	AT	95	ALA	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	32529	0	16426	527	0
2	AV	1579	0	802	43	0
3	AX	125	0	64	2	0
4	AJ	795	0	840	30	0
5	AK	885	0	904	29	0
6	AL	971	0	1057	30	0
7	AM	988	0	1059	44	0
8	AN	492	0	529	21	0
9	AO	734	0	771	16	0
10	AP	701	0	720	15	0
11	AQ	824	0	891	19	0
12	AR	574	0	644	11	0
13	AS	630	0	652	30	0
14	AT	763	0	861	32	0
15	AB	1901	0	1951	90	0
16	AC	1613	0	1677	50	0
17	AD	1703	0	1763	73	0
18	AE	1147	0	1207	34	0
19	AF	843	0	857	20	0
20	AG	1257	0	1296	26	0
21	AH	1116	0	1177	27	0
22	AI	1011	0	1043	35	0
23	AY	4877	0	4964	176	0
24	AU	209	0	221	8	0
25	BA	61580	0	31049	1166	0
26	BB	2551	0	1295	57	0
27	BN	1104	0	1180	67	0
28	BO	933	0	996	38	0
29	BP	1114	0	1187	146	0
30	BQ	1122	0	1179	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BR	960	0	1021	41	0
32	BS	770	0	832	43	0
33	BT	1141	0	1202	119	0
34	BU	958	0	1015	54	0
35	BV	779	0	852	49	0
36	BW	896	0	953	28	0
37	BX	725	0	778	17	0
38	BY	775	0	870	74	0
39	BZ	1508	0	1486	63	0
40	B0	662	0	688	23	0
41	B1	731	0	808	35	0
42	B2	598	0	653	33	0
43	BD	2104	0	2182	109	0
44	B3	467	0	523	6	0
45	B4	225	0	229	9	0
46	B5	459	0	477	32	0
47	B6	380	0	390	59	0
48	B7	418	0	467	12	0
49	B8	507	0	576	58	0
50	B9	299	0	323	10	0
51	BC	1718	0	1766	55	0
52	BE	1563	0	1629	91	0
53	BF	1623	0	1677	89	0
54	BG	1474	0	1535	61	0
55	BH	1303	0	1348	59	0
56	BK	936	0	970	67	0
57	BJ	651	0	649	17	0
58	BL	356	0	75	7	0
59	AA	45	0	0	0	0
59	AY	1	0	0	0	0
59	B8	1	0	0	0	0
59	BA	88	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	1	0	0	0	0
60	AY	32	0	14	5	0
61	AY	4	0	0	1	0
All	All	151831	0	105250	3794	0

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 3794 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:2111:C:N3	25:BA:2147:G:N2	1.74	1.36
25:BA:1332:G:N2	25:BA:1609:A:O2'	1.62	1.26
47:B6:40:CYS:SG	47:B6:45:LYS:NZ	1.02	1.24
25:BA:90:U:O2'	25:BA:92:A:OP2	1.54	1.24
25:BA:1332:G:N2	25:BA:1609:A:HO2'	1.30	1.23

There are no symmetry-related clashes.

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	
4	AJ	96/98 (98%)	80 (83%)	10 (10%)	6 (6%)	1	2
5	AK	117/119 (98%)	105 (90%)	9 (8%)	3 (3%)	4	9
6	AL	122/124 (98%)	107 (88%)	10 (8%)	5 (4%)	2	4
7	AM	122/124 (98%)	82 (67%)	32 (26%)	8 (7%)	1	1
8	AN	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	3	6
9	AO	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	10	22
10	AP	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
11	AQ	97/99 (98%)	92 (95%)	4 (4%)	1 (1%)	12	25
12	AR	68/70 (97%)	60 (88%)	5 (7%)	3 (4%)	2	3
13	AS	76/78 (97%)	60 (79%)	8 (10%)	8 (10%)	0	0
14	AT	97/99 (98%)	86 (89%)	5 (5%)	6 (6%)	1	2
15	AB	232/234 (99%)	191 (82%)	32 (14%)	9 (4%)	2	4
16	AC	204/206 (99%)	173 (85%)	22 (11%)	9 (4%)	2	3
17	AD	206/208 (99%)	171 (83%)	25 (12%)	10 (5%)	1	3
18	AE	148/150 (99%)	141 (95%)	5 (3%)	2 (1%)	9	19
19	AF	99/101 (98%)	91 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	AG	153/155 (99%)	132 (86%)	17 (11%)	4 (3%)	4	9
21	AH	136/138 (99%)	127 (93%)	6 (4%)	3 (2%)	5	12
22	AI	125/127 (98%)	99 (79%)	17 (14%)	9 (7%)	1	1
23	AY	612/680 (90%)	520 (85%)	72 (12%)	20 (3%)	3	7
24	AU	22/24 (92%)	17 (77%)	5 (23%)	0	100	100
27	BN	136/140 (97%)	113 (83%)	17 (12%)	6 (4%)	2	3
28	BO	120/122 (98%)	113 (94%)	3 (2%)	4 (3%)	3	7
29	BP	144/150 (96%)	90 (62%)	21 (15%)	33 (23%)	0	0
30	BQ	139/141 (99%)	117 (84%)	17 (12%)	5 (4%)	2	5
31	BR	115/118 (98%)	101 (88%)	9 (8%)	5 (4%)	2	4
32	BS	96/112 (86%)	61 (64%)	20 (21%)	15 (16%)	0	0
33	BT	135/146 (92%)	96 (71%)	24 (18%)	15 (11%)	0	0
34	BU	115/118 (98%)	101 (88%)	10 (9%)	4 (4%)	3	6
35	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	0
36	BW	111/113 (98%)	101 (91%)	4 (4%)	6 (5%)	1	2
37	BX	90/96 (94%)	83 (92%)	7 (8%)	0	100	100
38	BY	98/110 (89%)	58 (59%)	18 (18%)	22 (22%)	0	0
39	BZ	194/206 (94%)	146 (75%)	32 (16%)	16 (8%)	0	1
40	B0	82/85 (96%)	71 (87%)	8 (10%)	3 (4%)	2	5
41	B1	91/98 (93%)	76 (84%)	12 (13%)	3 (3%)	3	7
42	B2	69/72 (96%)	58 (84%)	4 (6%)	7 (10%)	0	0
43	BD	269/276 (98%)	231 (86%)	24 (9%)	14 (5%)	1	2
44	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	6	15
45	B4	28/71 (39%)	21 (75%)	4 (14%)	3 (11%)	0	0
46	B5	57/60 (95%)	47 (82%)	4 (7%)	6 (10%)	0	0
47	B6	42/54 (78%)	20 (48%)	15 (36%)	7 (17%)	0	0
48	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	5	12
49	B8	61/65 (94%)	45 (74%)	11 (18%)	5 (8%)	0	1
50	B9	34/37 (92%)	32 (94%)	2 (6%)	0	100	100
51	BC	219/229 (96%)	166 (76%)	35 (16%)	18 (8%)	0	1
52	BE	202/206 (98%)	145 (72%)	30 (15%)	27 (13%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BF	205/210 (98%)	165 (80%)	24 (12%)	16 (8%)	1	1
54	BG	179/182 (98%)	123 (69%)	44 (25%)	12 (7%)	1	1
55	BH	171/180 (95%)	128 (75%)	26 (15%)	17 (10%)	0	0
56	BK	121/147 (82%)	84 (69%)	30 (25%)	7 (6%)	1	2
57	BJ	128/130 (98%)	84 (66%)	31 (24%)	13 (10%)	0	0
All	All	6610/6949 (95%)	5383 (81%)	812 (12%)	415 (6%)	1	2

5 of 415 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AJ	23	ILE
4	AJ	59	SER
4	AJ	86	MET
5	AK	117	ASN
5	AK	128	ALA

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	
4	AJ	88/88 (100%)	70 (80%)	18 (20%)	1	1
5	AK	90/90 (100%)	69 (77%)	21 (23%)	1	0
6	AL	104/104 (100%)	80 (77%)	24 (23%)	1	0
7	AM	99/99 (100%)	80 (81%)	19 (19%)	1	2
8	AN	49/49 (100%)	37 (76%)	12 (24%)	1	0
9	AO	79/79 (100%)	67 (85%)	12 (15%)	3	5
10	AP	72/72 (100%)	61 (85%)	11 (15%)	3	5
11	AQ	94/94 (100%)	79 (84%)	15 (16%)	2	4
12	AR	61/61 (100%)	49 (80%)	12 (20%)	1	2
13	AS	69/69 (100%)	51 (74%)	18 (26%)	0	0
14	AT	76/76 (100%)	64 (84%)	12 (16%)	2	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles		
15	AB	202/202 (100%)	168 (83%)	34 (17%)	2	3	
16	AC	160/160 (100%)	121 (76%)	39 (24%)	1	0	
17	AD	180/180 (100%)	143 (79%)	37 (21%)	1	1	
18	AE	115/115 (100%)	102 (89%)	13 (11%)	5	11	
19	AF	90/90 (100%)	76 (84%)	14 (16%)	2	4	
20	AG	126/126 (100%)	110 (87%)	16 (13%)	4	8	
21	AH	119/119 (100%)	94 (79%)	25 (21%)	1	1	
22	AI	98/98 (100%)	79 (81%)	19 (19%)	1	2	
23	AY	528/573 (92%)	412 (78%)	116 (22%)	1	1	
24	AU	19/19 (100%)	12 (63%)	7 (37%)	0	0	
27	BN	117/119 (98%)	83 (71%)	34 (29%)	0	0	
28	BO	100/100 (100%)	79 (79%)	21 (21%)	1	1	
29	BP	112/116 (97%)	79 (70%)	33 (30%)	0	0	
30	BQ	111/111 (100%)	97 (87%)	14 (13%)	4	8	
31	BR	100/101 (99%)	77 (77%)	23 (23%)	1	0	
32	BS	77/88 (88%)	63 (82%)	14 (18%)	2	2	
33	BT	120/127 (94%)	90 (75%)	30 (25%)	0	0	
34	BU	92/94 (98%)	75 (82%)	17 (18%)	1	2	
35	BV	82/82 (100%)	56 (68%)	26 (32%)	0	0	
36	BW	91/92 (99%)	72 (79%)	19 (21%)	1	1	
37	BX	74/78 (95%)	58 (78%)	16 (22%)	1	1	
38	BY	84/91 (92%)	63 (75%)	21 (25%)	0	0	
39	BZ	154/179 (86%)	125 (81%)	29 (19%)	1	2	
40	B0	66/67 (98%)	56 (85%)	10 (15%)	3	5	
41	B1	78/83 (94%)	62 (80%)	16 (20%)	1	1	
42	B2	66/67 (98%)	52 (79%)	14 (21%)	1	1	
43	BD	213/218 (98%)	168 (79%)	45 (21%)	1	1	
44	B3	51/52 (98%)	38 (74%)	13 (26%)	0	0	
45	B4	27/63 (43%)	23 (85%)	4 (15%)	3	5	
46	B5	51/52 (98%)	43 (84%)	8 (16%)	2	4	
47	B6	43/52 (83%)	31 (72%)	12 (28%)	0	0	

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	B7	41/42 (98%)	35 (85%)	6 (15%)	3	5
49	B8	53/55 (96%)	34 (64%)	19 (36%)	0	0
50	B9	33/34 (97%)	24 (73%)	9 (27%)	0	0
51	BC	177/181 (98%)	149 (84%)	28 (16%)	2	4
52	BE	165/166 (99%)	132 (80%)	33 (20%)	1	2
53	BF	165/166 (99%)	129 (78%)	36 (22%)	1	1
54	BG	155/156 (99%)	126 (81%)	29 (19%)	1	2
55	BH	136/148 (92%)	106 (78%)	30 (22%)	1	1
56	BK	96/111 (86%)	82 (85%)	14 (15%)	3	5
All	All	5448/5654 (96%)	4331 (80%)	1117 (20%)	1	1

5 of 1117 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	B8	32	LEU
51	BC	53	ARG
49	B8	30	ARG
53	BF	183	VAL
23	AY	120	THR

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

Mol	Chain	Res	Type
43	BD	116	GLN
53	BF	169	ASN
47	B6	26	ASN
51	BC	66	HIS
56	BK	29	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1512/1516 (99%)	322 (21%)	65 (4%)
2	AV	73/76 (96%)	29 (39%)	9 (12%)
25	BA	2850/2915 (97%)	770 (27%)	130 (4%)
26	BB	119/122 (97%)	34 (28%)	4 (3%)
3	AX	5/25 (20%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	4559/4654 (97%)	1155 (25%)	208 (4%)

5 of 1155 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	9	G
1	AA	13	U
1	AA	30	U
1	AA	31	G

5 of 208 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	933	A
25	BA	1396	U
25	BA	2655	G
25	BA	1026	U
25	BA	1128	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 139 ligands modelled in this entry, 138 are 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
60	GCP	AY	702	59	32,34,34	2.04	10 (31%)	49,54,54	2.10	19 (38%)

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
60	GCP	AY	702	59	-	2/19/38/38	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	AY	702	GCP	PA-O3A	4.15	1.64	1.59
60	AY	702	GCP	PB-O2B	-4.07	1.46	1.56
60	AY	702	GCP	C2'-C3'	-4.02	1.42	1.53
60	AY	702	GCP	PG-O2G	-3.66	1.46	1.55
60	AY	702	GCP	PG-O3G	-3.29	1.47	1.55

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AY	702	GCP	O4'-C4'-C5'	-4.85	93.80	109.33
60	AY	702	GCP	C2-N3-C4	4.79	120.56	112.30
60	AY	702	GCP	O1G-PG-C3B	-3.82	103.03	111.37
60	AY	702	GCP	C5-C4-N3	-3.67	122.55	128.39
60	AY	702	GCP	C2'-C3'-C4'	-3.67	95.53	102.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

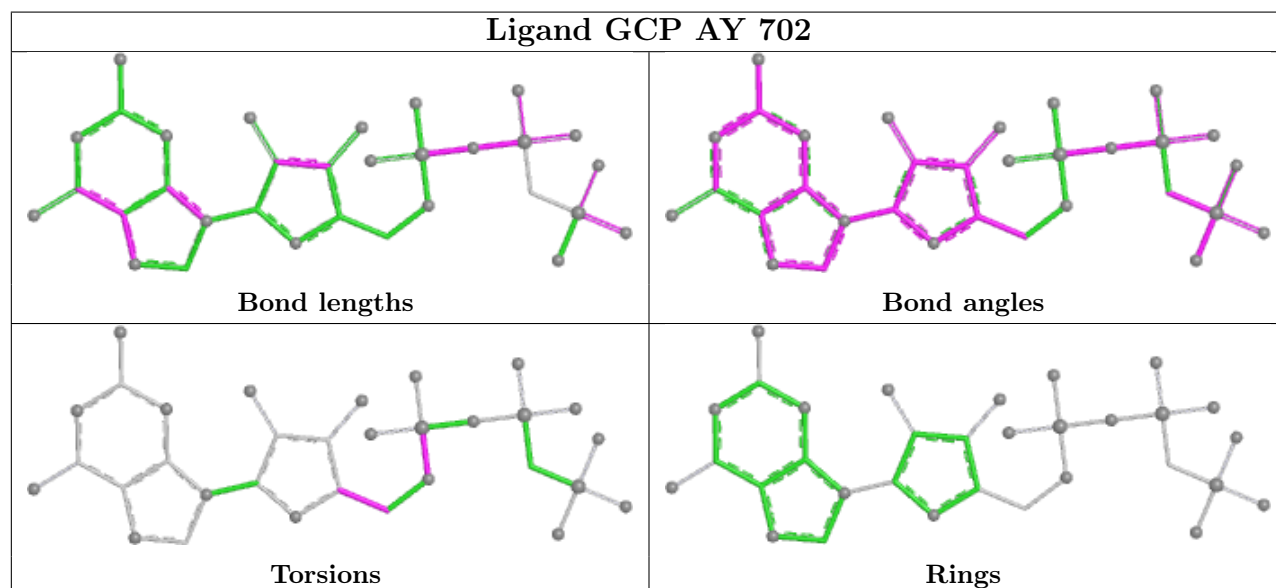
Mol	Chain	Res	Type	Atoms
60	AY	702	GCP	C5'-O5'-PA-O1A
60	AY	702	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	AY	702	GCP	5	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
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2506:U	O3'	2507:C	P	1.76

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	1514/1516 (99%)	-0.28	52 (3%) 48 38	9, 32, 113, 247	0
2	AV	74/76 (97%)	0.23	3 (4%) 41 32	23, 54, 91, 134	0
3	AX	6/25 (24%)	0.09	1 (16%) 4 3	18, 22, 53, 75	0
4	AJ	98/98 (100%)	1.09	24 (24%) 2 1	22, 49, 98, 108	0
5	AK	119/119 (100%)	0.46	6 (5%) 34 27	18, 41, 65, 104	0
6	AL	124/124 (100%)	0.37	12 (9%) 13 10	16, 32, 64, 107	0
7	AM	124/124 (100%)	1.56	34 (27%) 1 1	31, 69, 118, 161	0
8	AN	60/60 (100%)	0.49	7 (11%) 9 7	21, 33, 69, 83	0
9	AO	88/88 (100%)	0.26	2 (2%) 61 52	24, 41, 67, 73	0
10	AP	83/83 (100%)	0.35	0 100 100	29, 40, 60, 112	0
11	AQ	99/99 (100%)	-0.03	0 100 100	20, 34, 53, 59	0
12	AR	70/70 (100%)	0.26	4 (5%) 29 22	23, 41, 75, 92	0
13	AS	78/78 (100%)	1.29	17 (21%) 2 2	39, 69, 107, 121	0
14	AT	99/99 (100%)	0.63	14 (14%) 6 4	24, 39, 78, 90	0
15	AB	234/234 (100%)	0.89	43 (18%) 3 3	21, 55, 117, 134	0
16	AC	206/206 (100%)	0.27	10 (4%) 35 27	22, 41, 67, 103	0
17	AD	208/208 (100%)	0.64	15 (7%) 21 15	26, 49, 75, 90	0
18	AE	150/150 (100%)	-0.10	0 100 100	19, 30, 54, 81	0
19	AF	101/101 (100%)	0.41	5 (4%) 34 27	28, 52, 75, 87	0
20	AG	155/155 (100%)	0.90	25 (16%) 4 4	31, 53, 104, 148	0
21	AH	138/138 (100%)	-0.08	2 (1%) 73 67	19, 32, 55, 84	0
22	AI	127/127 (100%)	0.67	9 (7%) 22 16	21, 51, 82, 108	0
23	AY	622/680 (91%)	0.60	46 (7%) 20 14	30, 55, 97, 131	0
24	AU	24/24 (100%)	1.24	4 (16%) 4 3	33, 48, 65, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BA	2859/2915 (98%)	-0.35	107 (3%) 45 35	7, 27, 90, 267	0
26	BB	119/122 (97%)	0.42	3 (2%) 58 49	26, 63, 95, 134	0
27	BN	138/140 (98%)	0.53	16 (11%) 9 7	18, 35, 66, 80	0
28	BO	122/122 (100%)	-0.08	0 100 100	18, 31, 49, 60	0
29	BP	146/150 (97%)	1.71	43 (29%) 1 1	18, 55, 94, 127	0
30	BQ	141/141 (100%)	0.32	10 (7%) 22 16	23, 35, 64, 112	0
31	BR	117/118 (99%)	0.35	10 (8%) 16 12	15, 33, 58, 75	0
32	BS	98/112 (87%)	2.10	44 (44%) 0 0	50, 80, 106, 125	0
33	BT	137/146 (93%)	1.27	37 (27%) 1 1	23, 50, 135, 151	0
34	BU	117/118 (99%)	0.36	13 (11%) 10 8	16, 29, 58, 85	0
35	BV	101/101 (100%)	0.85	16 (15%) 5 4	15, 49, 77, 97	0
36	BW	113/113 (100%)	0.17	5 (4%) 39 30	18, 29, 67, 122	0
37	BX	92/96 (95%)	0.23	5 (5%) 31 23	20, 34, 54, 61	0
38	BY	100/110 (90%)	2.24	47 (47%) 0 0	29, 56, 122, 168	0
39	BZ	198/206 (96%)	1.00	29 (14%) 6 4	33, 59, 92, 103	0
40	B0	84/85 (98%)	0.69	10 (11%) 9 7	26, 41, 96, 133	0
41	B1	93/98 (94%)	0.52	9 (9%) 13 10	18, 33, 72, 121	0
42	B2	71/72 (98%)	0.55	5 (7%) 22 16	30, 49, 82, 100	0
43	BD	271/276 (98%)	0.02	17 (6%) 26 19	9, 20, 46, 89	0
44	B3	59/60 (98%)	0.39	4 (6%) 23 17	24, 40, 76, 137	0
45	B4	30/71 (42%)	2.87	23 (76%) 0 0	102, 130, 156, 174	0
46	B5	59/60 (98%)	1.12	15 (25%) 1 1	10, 35, 98, 134	0
47	B6	44/54 (81%)	2.55	23 (52%) 0 0	34, 59, 99, 109	0
48	B7	48/49 (97%)	0.17	5 (10%) 11 9	10, 19, 59, 101	0
49	B8	63/65 (96%)	1.27	12 (19%) 3 3	22, 37, 61, 118	0
50	B9	36/37 (97%)	1.06	6 (16%) 4 3	26, 44, 69, 77	0
51	BC	225/229 (98%)	0.96	29 (12%) 7 5	36, 64, 111, 132	0
52	BE	204/206 (99%)	0.57	34 (16%) 4 3	14, 32, 85, 109	0
53	BF	207/210 (98%)	0.68	29 (14%) 6 5	15, 37, 103, 187	0
54	BG	181/182 (99%)	2.23	96 (53%) 0 0	67, 101, 130, 147	0
55	BH	173/180 (96%)	1.22	27 (15%) 5 4	35, 60, 95, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BK	127/147 (86%)	3.74	119 (93%) 0 0	127, 181, 237, 263	0
57	BJ	130/130 (100%)	3.08	105 (80%) 0 0	74, 106, 140, 195	0
58	BL	0/125	-	-	-	-
All	All	11304/11728 (96%)	0.37	1288 (11%) 10 8	7, 40, 108, 267	0

The worst 5 of 1288 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
38	BY	3	VAL	11.3
56	BK	74	ALA	10.9
7	AM	123	ALA	10.6
53	BF	12	LEU	10.3
55	BH	44	VAL	10.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	AA	1636	1/1	0.79	0.16	24,24,24,24	0
59	MG	BA	3004	1/1	0.80	0.17	46,46,46,46	0
59	MG	BA	3011	1/1	0.85	0.23	30,30,30,30	0
59	MG	BA	3039	1/1	0.85	0.26	24,24,24,24	0
59	MG	BF	301	1/1	0.85	0.11	27,27,27,27	0
59	MG	AA	1644	1/1	0.86	0.30	33,33,33,33	0
59	MG	BA	3012	1/1	0.87	0.09	10,10,10,10	0
59	MG	AA	1640	1/1	0.88	0.22	21,21,21,21	0
59	MG	BA	3065	1/1	0.88	0.31	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3073	1/1	0.88	0.23	14,14,14,14	0
59	MG	AA	1642	1/1	0.88	0.24	30,30,30,30	0
59	MG	BA	3059	1/1	0.89	0.18	9,9,9,9	0
59	MG	AA	1635	1/1	0.89	0.15	24,24,24,24	0
59	MG	AA	1645	1/1	0.89	0.33	35,35,35,35	0
59	MG	BA	3052	1/1	0.89	0.22	19,19,19,19	0
59	MG	BA	3027	1/1	0.90	0.24	30,30,30,30	0
59	MG	BA	3056	1/1	0.90	0.15	18,18,18,18	0
59	MG	BA	3086	1/1	0.90	0.20	26,26,26,26	0
59	MG	BA	3051	1/1	0.90	0.27	24,24,24,24	0
59	MG	BA	3029	1/1	0.91	0.23	28,28,28,28	0
59	MG	BA	3060	1/1	0.91	0.24	22,22,22,22	0
59	MG	BA	3008	1/1	0.91	0.24	13,13,13,13	0
59	MG	BA	3072	1/1	0.91	0.19	19,19,19,19	0
59	MG	AA	1619	1/1	0.91	0.20	27,27,27,27	0
59	MG	BA	3001	1/1	0.91	0.34	32,32,32,32	0
59	MG	B8	101	1/1	0.91	0.09	15,15,15,15	0
59	MG	AA	1641	1/1	0.91	0.15	25,25,25,25	0
59	MG	BA	3071	1/1	0.92	0.29	29,29,29,29	0
59	MG	BA	3013	1/1	0.92	0.26	26,26,26,26	0
59	MG	AA	1643	1/1	0.92	0.17	31,31,31,31	0
59	MG	BA	3080	1/1	0.92	0.19	16,16,16,16	0
59	MG	BA	3082	1/1	0.92	0.21	21,21,21,21	0
59	MG	AA	1633	1/1	0.92	0.15	27,27,27,27	0
59	MG	BA	3087	1/1	0.92	0.22	26,26,26,26	0
59	MG	AA	1618	1/1	0.92	0.20	22,22,22,22	0
59	MG	AA	1603	1/1	0.92	0.23	23,23,23,23	0
59	MG	BA	3017	1/1	0.93	0.21	16,16,16,16	0
59	MG	BA	3020	1/1	0.93	0.20	6,6,6,6	0
59	MG	BA	3074	1/1	0.93	0.17	16,16,16,16	0
59	MG	AA	1626	1/1	0.93	0.19	19,19,19,19	0
59	MG	AA	1637	1/1	0.93	0.20	34,34,34,34	0
59	MG	BA	3030	1/1	0.93	0.25	12,12,12,12	0
59	MG	BA	3033	1/1	0.93	0.20	12,12,12,12	0
59	MG	BA	3067	1/1	0.93	0.18	16,16,16,16	0
59	MG	BE	301	1/1	0.93	0.21	16,16,16,16	0
59	MG	BA	3014	1/1	0.93	0.30	27,27,27,27	0
59	MG	BA	3078	1/1	0.94	0.15	15,15,15,15	0
59	MG	AA	1638	1/1	0.94	0.18	22,22,22,22	0
59	MG	BA	3081	1/1	0.94	0.18	17,17,17,17	0
59	MG	BA	3023	1/1	0.94	0.19	9,9,9,9	0
59	MG	BA	3070	1/1	0.94	0.23	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1617	1/1	0.94	0.20	21,21,21,21	0
59	MG	AA	1625	1/1	0.94	0.26	25,25,25,25	0
59	MG	AA	1601	1/1	0.94	0.21	13,13,13,13	0
59	MG	AA	1629	1/1	0.94	0.19	38,38,38,38	0
59	MG	BA	3048	1/1	0.95	0.17	9,9,9,9	0
59	MG	AA	1622	1/1	0.95	0.17	25,25,25,25	0
59	MG	BA	3002	1/1	0.95	0.16	17,17,17,17	0
59	MG	BA	3054	1/1	0.95	0.15	9,9,9,9	0
59	MG	BA	3075	1/1	0.95	0.17	12,12,12,12	0
59	MG	BA	3076	1/1	0.95	0.17	8,8,8,8	0
59	MG	BA	3032	1/1	0.95	0.16	21,21,21,21	0
59	MG	BA	3079	1/1	0.95	0.18	14,14,14,14	0
59	MG	AA	1610	1/1	0.95	0.24	14,14,14,14	0
59	MG	AA	1605	1/1	0.95	0.11	25,25,25,25	0
59	MG	BA	3063	1/1	0.95	0.24	22,22,22,22	0
59	MG	BA	3041	1/1	0.95	0.19	11,11,11,11	0
59	MG	BA	3066	1/1	0.95	0.16	15,15,15,15	0
59	MG	BA	3043	1/1	0.95	0.20	7,7,7,7	0
59	MG	BA	3069	1/1	0.95	0.19	14,14,14,14	0
59	MG	BA	3045	1/1	0.95	0.19	16,16,16,16	0
59	MG	BA	3061	1/1	0.96	0.18	8,8,8,8	0
59	MG	BA	3031	1/1	0.96	0.19	16,16,16,16	0
59	MG	AA	1624	1/1	0.96	0.14	14,14,14,14	0
59	MG	AA	1609	1/1	0.96	0.23	16,16,16,16	0
59	MG	BA	3034	1/1	0.96	0.18	5,5,5,5	0
59	MG	BA	3068	1/1	0.96	0.15	7,7,7,7	0
59	MG	BA	3035	1/1	0.96	0.27	18,18,18,18	0
59	MG	BA	3037	1/1	0.96	0.19	7,7,7,7	0
59	MG	AA	1602	1/1	0.96	0.30	16,16,16,16	0
59	MG	BA	3040	1/1	0.96	0.20	10,10,10,10	0
59	MG	AA	1611	1/1	0.96	0.23	7,7,7,7	0
59	MG	BA	3018	1/1	0.96	0.15	12,12,12,12	0
59	MG	BA	3044	1/1	0.96	0.17	15,15,15,15	0
59	MG	BA	3019	1/1	0.96	0.24	16,16,16,16	0
59	MG	BA	3077	1/1	0.96	0.17	17,17,17,17	0
59	MG	BA	3047	1/1	0.96	0.35	27,27,27,27	0
59	MG	AA	1639	1/1	0.96	0.14	20,20,20,20	0
59	MG	AA	1630	1/1	0.96	0.29	29,29,29,29	0
59	MG	BA	3025	1/1	0.96	0.18	16,16,16,16	0
59	MG	BA	3053	1/1	0.96	0.19	7,7,7,7	0
59	MG	BA	3083	1/1	0.96	0.21	37,37,37,37	0
59	MG	BA	3084	1/1	0.96	0.20	22,22,22,22	0

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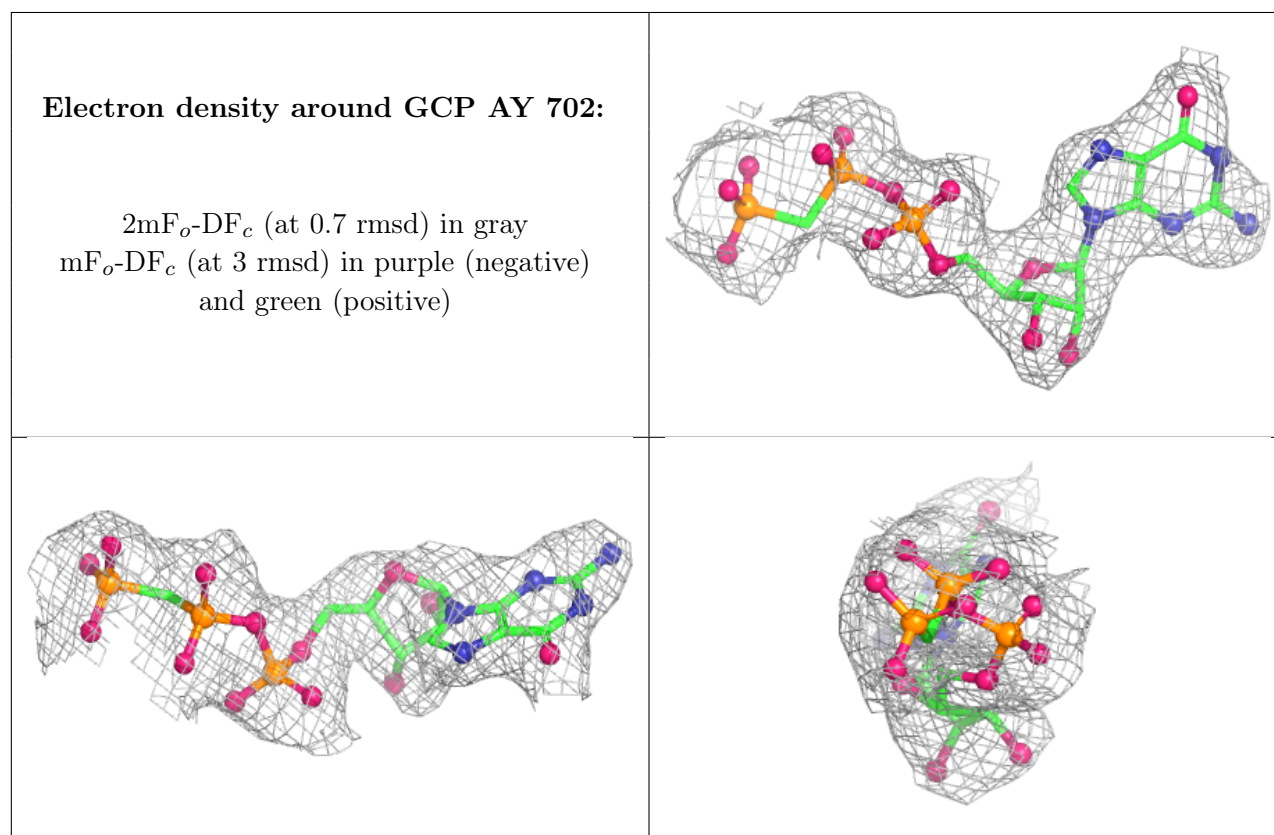
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3085	1/1	0.96	0.18	18,18,18,18	0
59	MG	BA	3026	1/1	0.96	0.18	19,19,19,19	0
59	MG	AA	1632	1/1	0.96	0.19	22,22,22,22	0
59	MG	BA	3088	1/1	0.96	0.23	26,26,26,26	0
59	MG	BD	301	1/1	0.96	0.19	7,7,7,7	0
59	MG	BA	3057	1/1	0.96	0.14	8,8,8,8	0
59	MG	BA	3009	1/1	0.96	0.28	31,31,31,31	0
59	MG	AA	1613	1/1	0.96	0.15	6,6,6,6	0
59	MG	BA	3024	1/1	0.97	0.18	2,2,2,2	0
59	MG	AA	1615	1/1	0.97	0.21	24,24,24,24	0
59	MG	BA	3010	1/1	0.97	0.24	14,14,14,14	0
59	MG	BA	3064	1/1	0.97	0.21	22,22,22,22	0
59	MG	AA	1621	1/1	0.97	0.18	14,14,14,14	0
59	MG	AA	1616	1/1	0.97	0.14	5,5,5,5	0
59	MG	AA	1631	1/1	0.97	0.19	13,13,13,13	0
59	MG	AA	1623	1/1	0.97	0.17	15,15,15,15	0
59	MG	BA	3003	1/1	0.97	0.19	2,2,2,2	0
59	MG	AA	1606	1/1	0.97	0.23	15,15,15,15	0
59	MG	BA	3005	1/1	0.97	0.25	12,12,12,12	0
59	MG	BA	3007	1/1	0.97	0.21	4,4,4,4	0
59	MG	BA	3055	1/1	0.97	0.16	5,5,5,5	0
59	MG	BA	3036	1/1	0.97	0.26	20,20,20,20	0
59	MG	BA	3021	1/1	0.97	0.25	25,25,25,25	0
59	MG	AA	1607	1/1	0.97	0.11	24,24,24,24	0
60	GCP	AY	702	32/32	0.97	0.07	27,42,47,49	0
59	MG	AA	1628	1/1	0.98	0.09	18,18,18,18	0
59	MG	AA	1634	1/1	0.98	0.08	6,6,6,6	0
59	MG	BA	3016	1/1	0.98	0.07	15,15,15,15	0
59	MG	BA	3042	1/1	0.98	0.23	11,11,11,11	0
59	MG	AA	1604	1/1	0.98	0.08	3,3,3,3	0
59	MG	AA	1620	1/1	0.98	0.25	18,18,18,18	0
59	MG	BA	3058	1/1	0.98	0.09	3,3,3,3	0
59	MG	AA	1614	1/1	0.98	0.19	11,11,11,11	0
59	MG	BA	3046	1/1	0.98	0.18	14,14,14,14	0
59	MG	BA	3028	1/1	0.98	0.23	23,23,23,23	0
59	MG	BA	3062	1/1	0.98	0.19	18,18,18,18	0
59	MG	AA	1612	1/1	0.98	0.14	14,14,14,14	0
59	MG	BA	3050	1/1	0.98	0.18	10,10,10,10	0
59	MG	BA	3038	1/1	0.98	0.25	19,19,19,19	0
59	MG	AY	701	1/1	0.99	0.03	41,41,41,41	0
59	MG	BA	3022	1/1	0.99	0.22	13,13,13,13	0
59	MG	AA	1608	1/1	0.99	0.29	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1627	1/1	0.99	0.17	15,15,15,15	0
59	MG	BA	3049	1/1	0.99	0.17	2,2,2,2	0
59	MG	BA	3006	1/1	0.99	0.25	13,13,13,13	0
59	MG	BA	3015	1/1	0.99	0.19	10,10,10,10	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.