



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 09:45 PM GMT

PDB ID : 4V4T
Title : Crystal structure of the whole ribosomal complex with a stop codon in the A-site.
Authors : Petry, S.; Brodersen, D.E.; Murphy IV, F.V.; Dunham, C.M.; Selmer, M.; Tarry, M.J.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2005-10-12
Resolution : 6.46 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

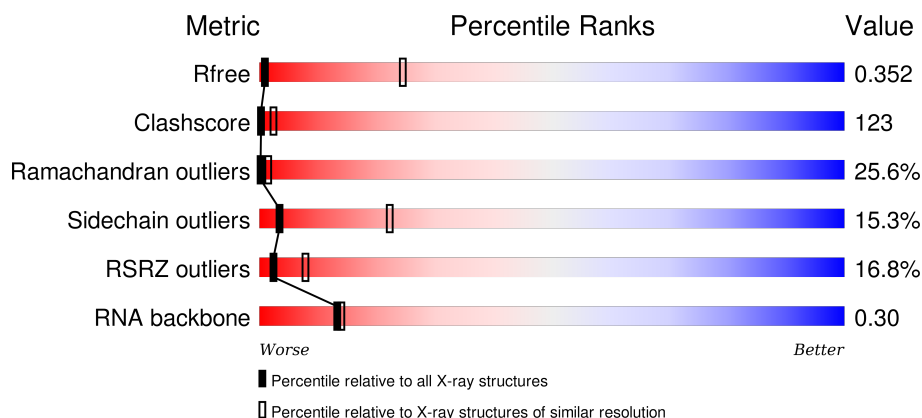
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.46 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}	91344	1012 (9.00-3.66)
Clashscore	102246	1060 (9.00-3.70)
Ramachandran outliers	100387	1033 (9.00-3.66)
Sidechain outliers	100360	1004 (9.00-3.66)
RSRZ outliers	91569	1011 (9.00-3.66)
RNA backbone	2183	1105 (10.00-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>13%</div> <div>24% 42% 24% 9%</div> </div>
2	AV	76	<div> <div>14%</div> <div>17% 61% 22%</div> </div>
3	AW	76	<div> <div>14%</div> <div>30% 39% 21% 9%</div> </div>
4	AX	18	<div> <div>28%</div> <div>61% 33% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
5	AB	256	
6	AC	239	
7	AD	209	
8	AE	162	
9	AF	101	
10	AG	156	
11	AH	138	
12	AI	128	
13	AJ	105	
14	AK	129	
15	AL	135	
16	AM	126	
17	AN	61	
18	AO	89	
19	AP	88	
20	AQ	105	
21	AR	88	
22	AS	93	
23	AT	106	
24	AU	27	
25	BB	123	
26	BA	2916	
27	BD	173	
28	BE	338	
29	BF	246	

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Mol	Chain	Length	Quality of chain
30	BG	176	
31	BH	177	
32	BI	149	
33	BN	145	
34	BO	122	
35	BP	164	
36	BQ	138	
37	BS	186	
38	BT	66	
39	BW	113	
40	BX	84	
41	BY	119	
42	BZ	253	
43	BR	118	
44	BU	118	
45	BV	100	
46	B2	70	
47	B3	60	
48	B0	91	
49	B4	73	
50	B5	60	
51	B6	82	
52	B7	47	
53	B8	64	
54	B9	36	

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Mol	Chain	Length	Quality of chain
55	BK	141	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	YYG	AW	37	X	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 142447 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	1515	Total	C	N	O	P	0	0	0
			32551	14490	6022	10525	1514			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	416	G	-	INSERTION	GB 155076
AA	905	U	-	INSERTION	GB 155076
AA	1395	C	-	INSERTION	GB 155076

- Molecule 2 is a RNA chain called P-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AV	76	Total	C	N	O	P	0	0	0
			1622	725	293	529	75			

- Molecule 3 is a RNA chain called E-site tRNA (Phe).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AW	76	Total	C	N	O	P	0	0	0
			1638	736	294	533	75			

- Molecule 4 is a RNA chain called 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*C
P*AP*AP*UP*AP*AP*U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AX	17	Total	C	N	O	P	0	0	11
			136	56	19	44	17			

- Molecule 5 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AB	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 6 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AC	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AE	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AJ	98	Total	C	N	O	S			
			794	499	156	138	1	0	0	0

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AL	124	Total	C	N	O	S			
			970	611	195	163	1	0	0	0

- Molecule 16 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AM	125	Total	C	N	O	S			
			997	617	207	171	2	0	0	0

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AP	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 20 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AQ	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 21 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AR	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 22 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AS	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 23 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AT	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- 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
			208	128	50	30				

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	123	Total	C	N	O	P	0	0	0
			2637	1175	488	852	122			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	INSERTION	GB 48271

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2814	Total	C	N	O	P	0	0	0
			60600	26974	11331	19482	2813			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	INSERTION	GB 48268

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BI	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

- Molecule 33 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BN	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BO	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	BP	84	Total	C	N	O	0	0	0
			639	391	109	139			

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BQ	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

- Molecule 37 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BS	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

- Molecule 38 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BT	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

- Molecule 39 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BW	108	Total	C	N	O	0	0	0
			860	542	169	149			

- Molecule 40 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BX	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 41 is a protein called 50S ribosomal protein 24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BY	110	Total	C	N	O	0	0	0
			879	531	166	182			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BZ	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 43 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BR	105	Total	C	N	O	0	0	0
			855	536	174	145			

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BU	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 45 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BV	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B2	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	B3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B0	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

- Molecule 49 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

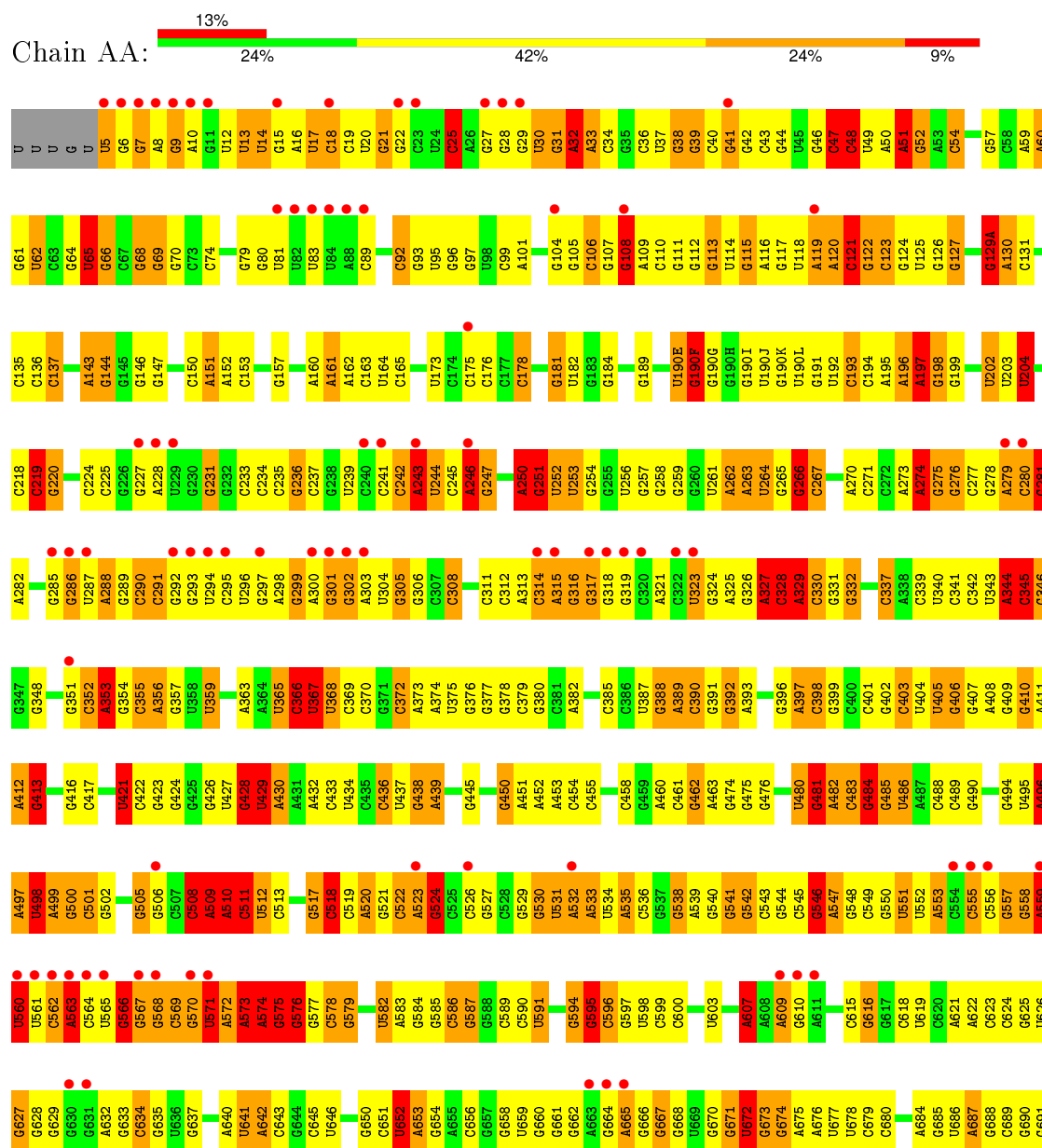
- Molecule 55 is a protein called 50S ribosomal protein L11.

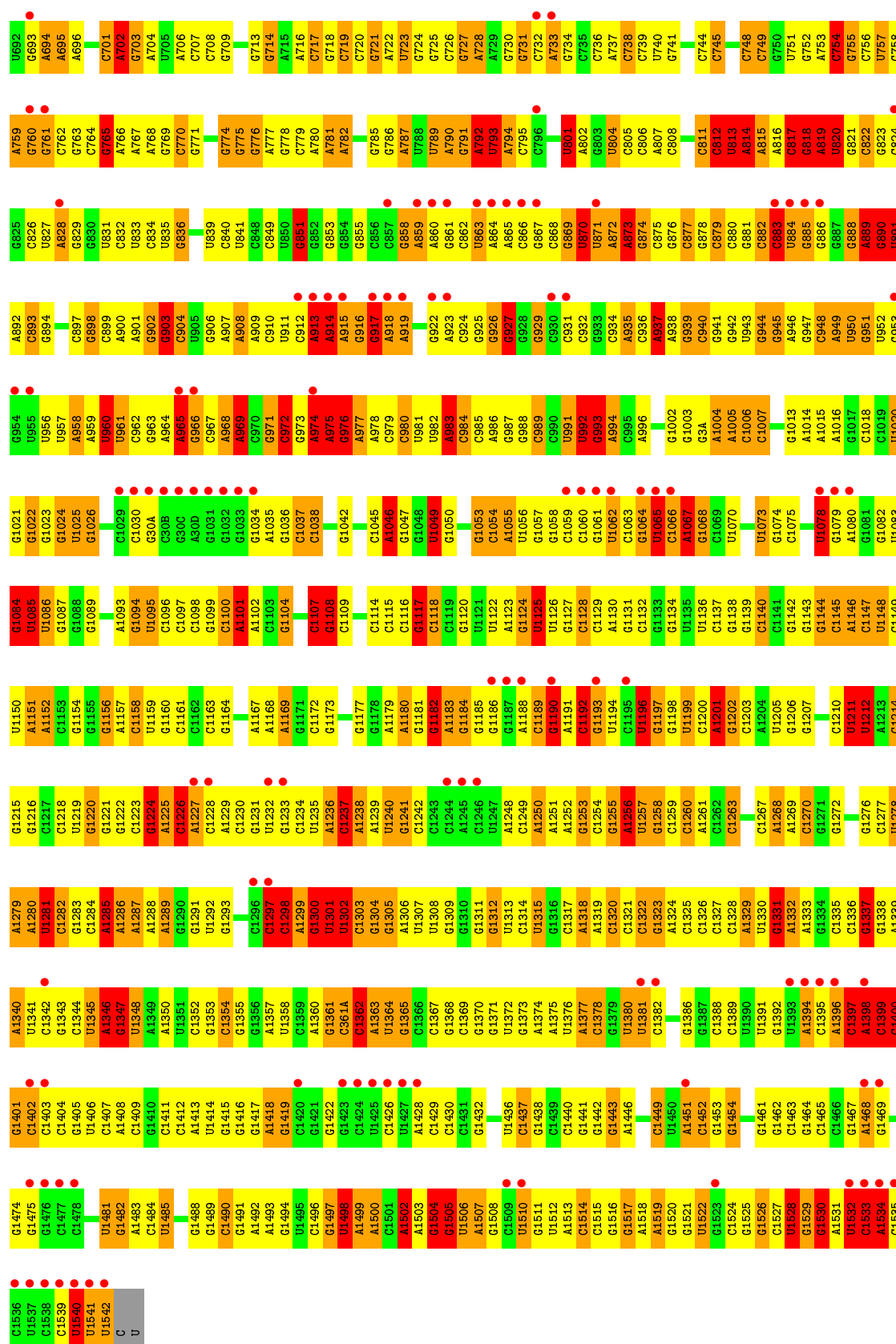
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BK	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

3 Residue-property plots

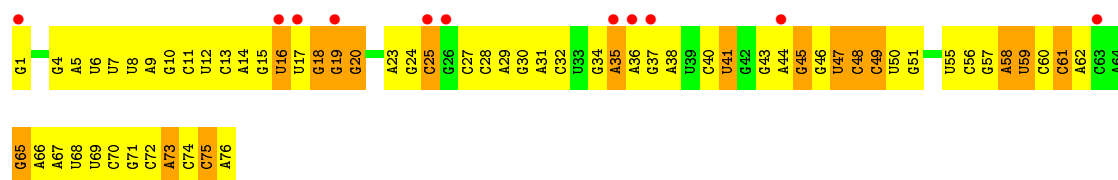
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

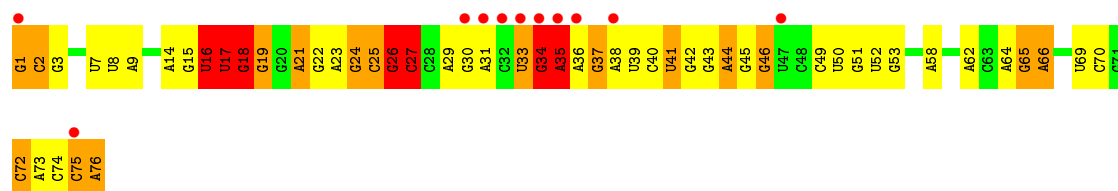




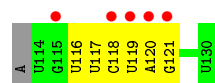
• Molecule 2: P-site tRNA (Phe)



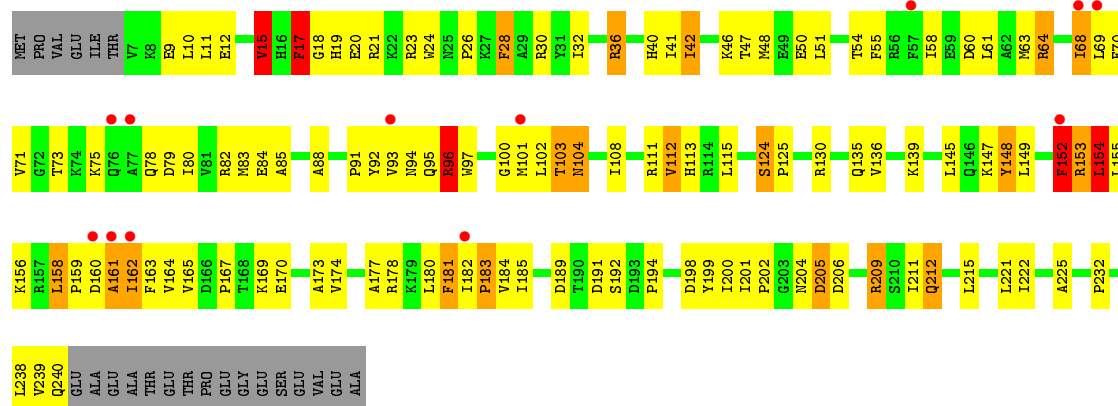
• Molecule 3: E-site tRNA (Phe)



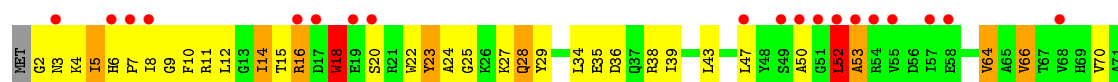
• Molecule 4: 5'-D(*AP*UP*GP*UP*UP*CP*UP*AP*GP*UP*AP*CP*AP*AP*UP*AP*AP*U)-3'

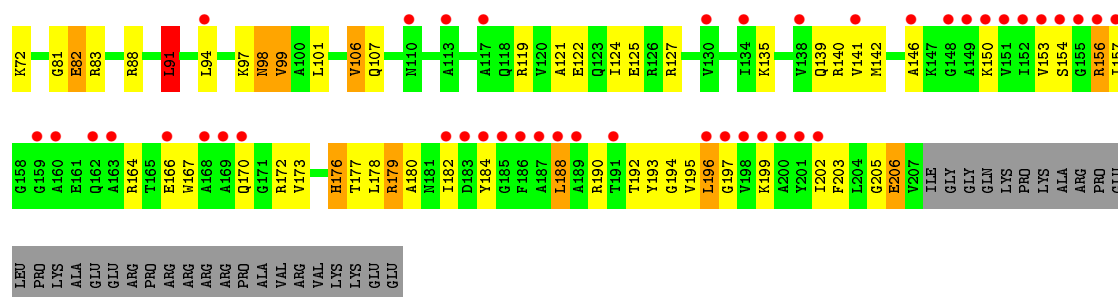


• Molecule 5: 30S ribosomal protein S2

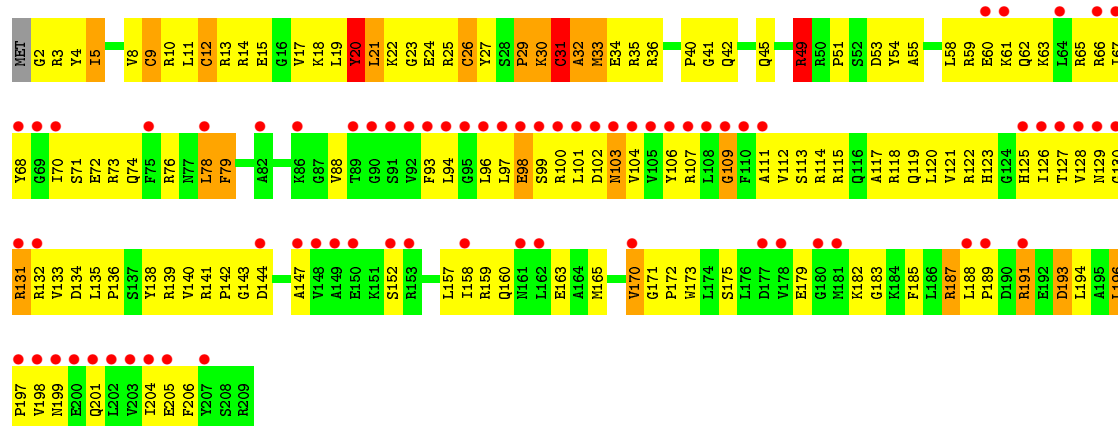


• Molecule 6: 30S ribosomal protein S3

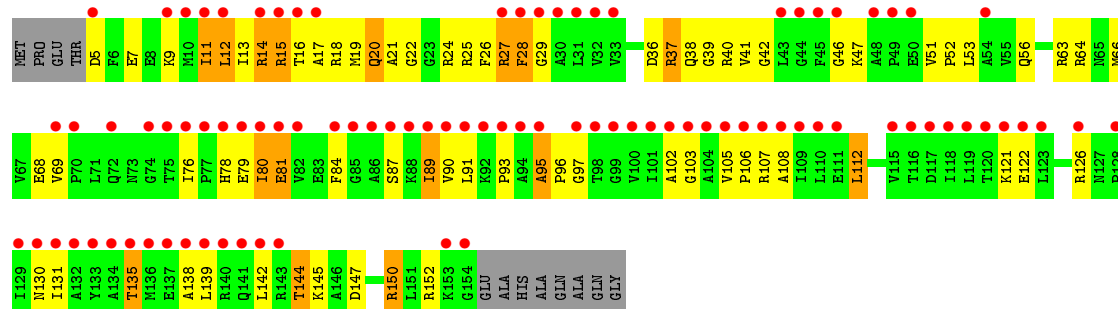




• Molecule 7: 30S ribosomal protein S4



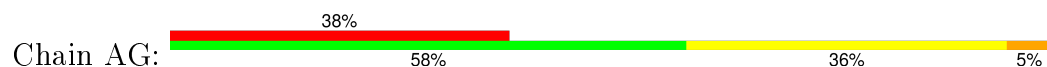
• Molecule 8: 30S ribosomal protein S5

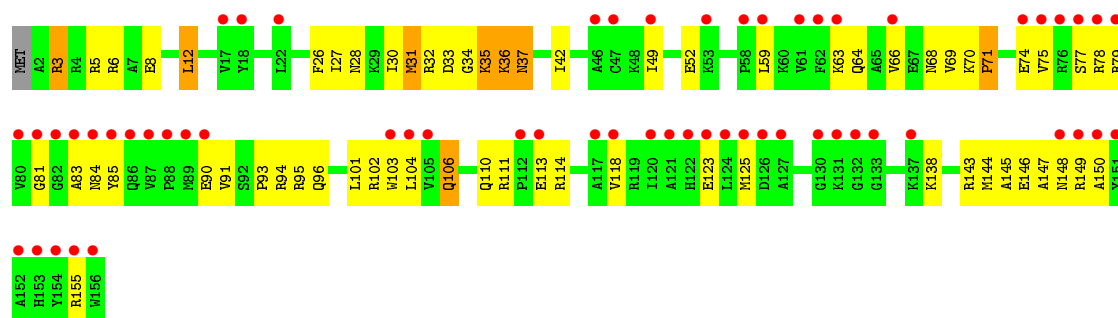


• Molecule 9: 30S ribosomal protein S6

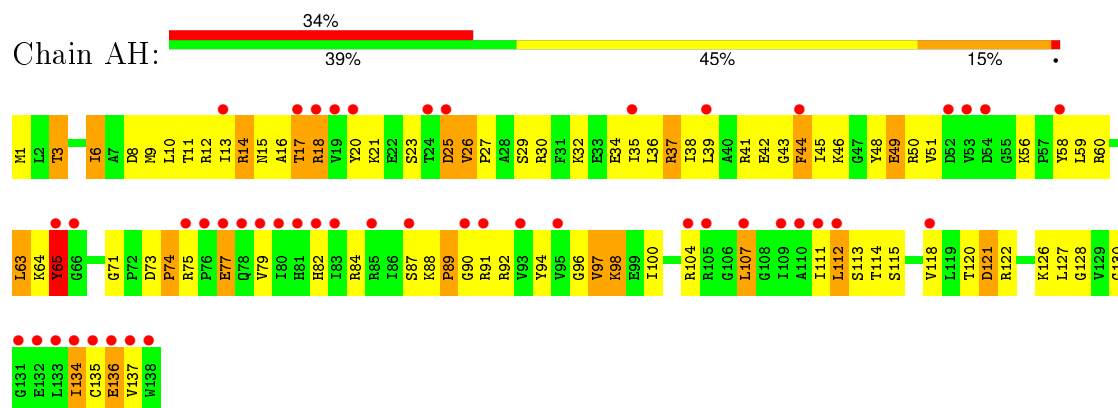


• Molecule 10: 30S ribosomal protein S7

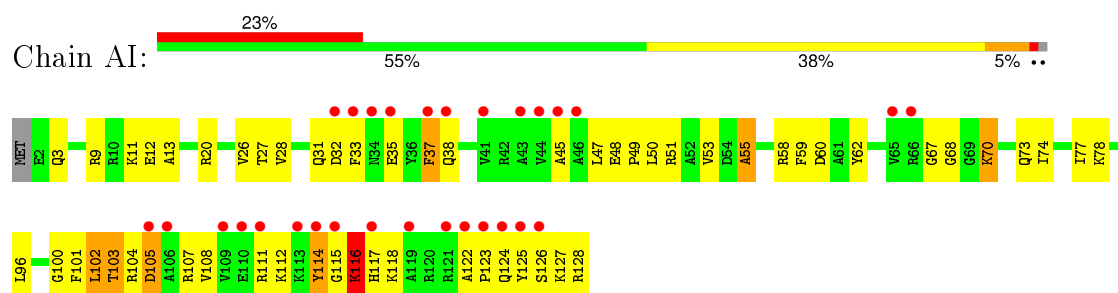




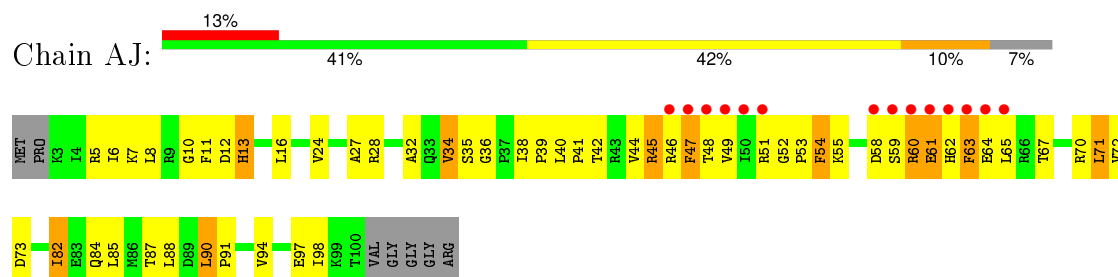
- Molecule 11: 30S ribosomal protein S8



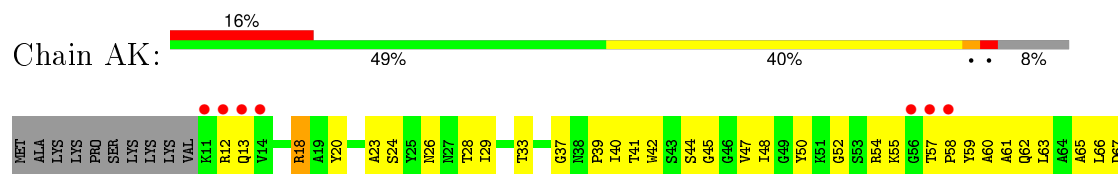
- Molecule 12: 30S ribosomal protein S9

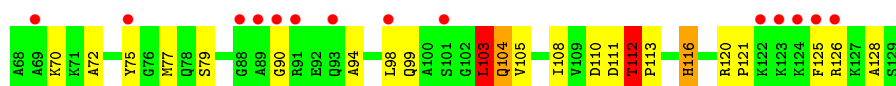


- Molecule 13: 30S ribosomal protein S10

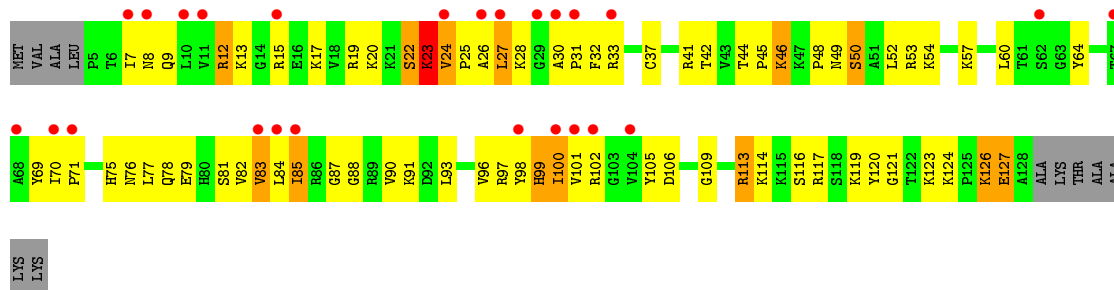


- Molecule 14: 30S ribosomal protein S11

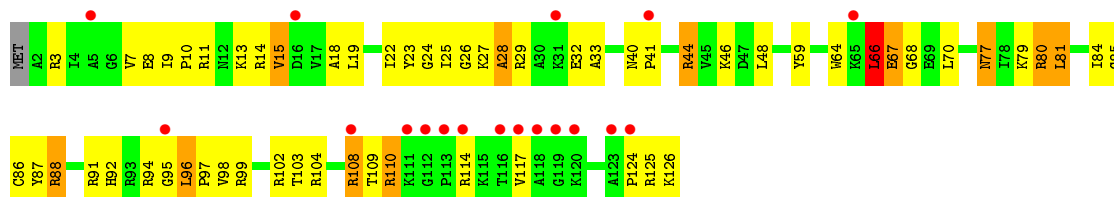




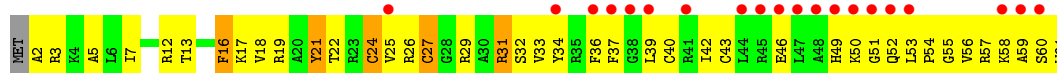
• Molecule 15: 30S ribosomal protein S12



• Molecule 16: 30S ribosomal protein S13



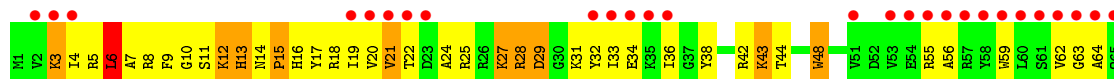
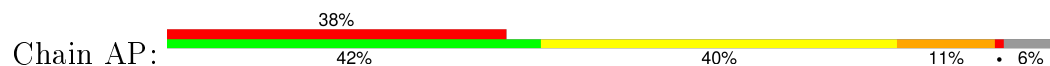
• Molecule 17: 30S ribosomal protein S14

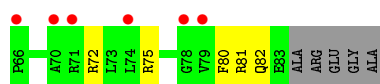


• Molecule 18: 30S ribosomal protein S15

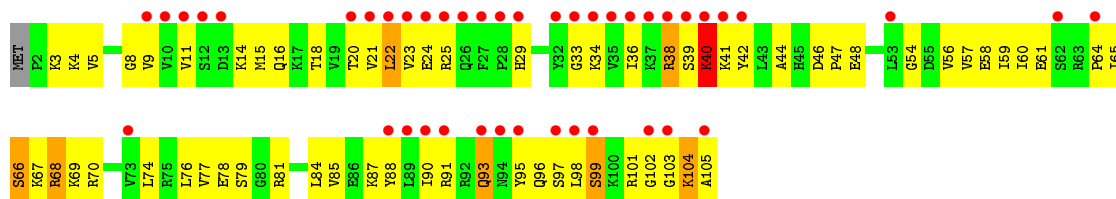
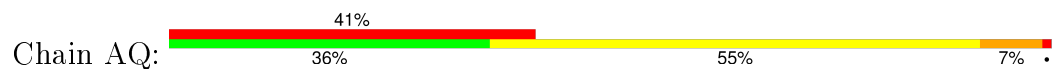


• Molecule 19: 30S ribosomal protein S16

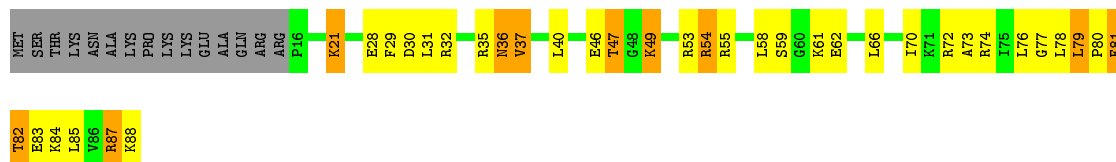




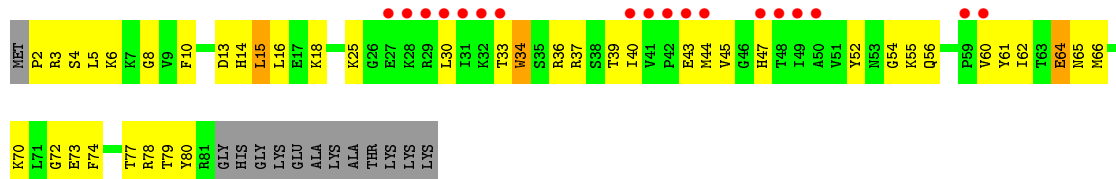
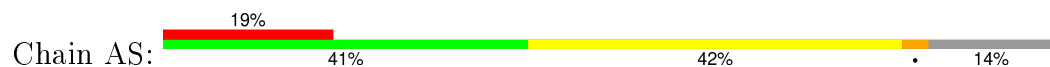
- Molecule 20: 30S ribosomal protein S17



- Molecule 21: 30S ribosomal protein S18



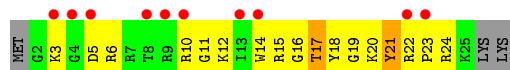
- Molecule 22: 30S ribosomal protein S19



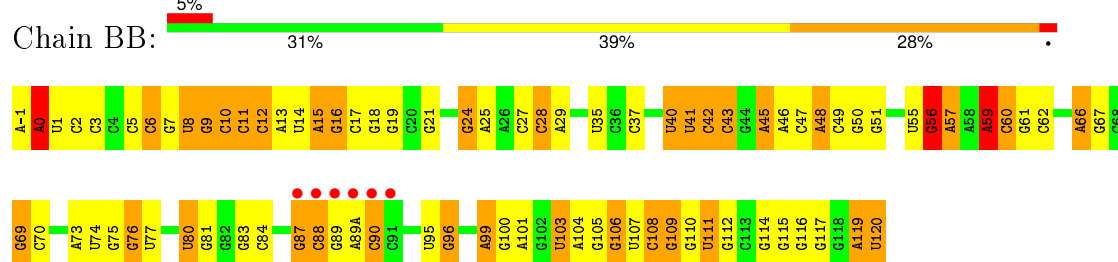
- Molecule 23: 30S ribosomal protein S20



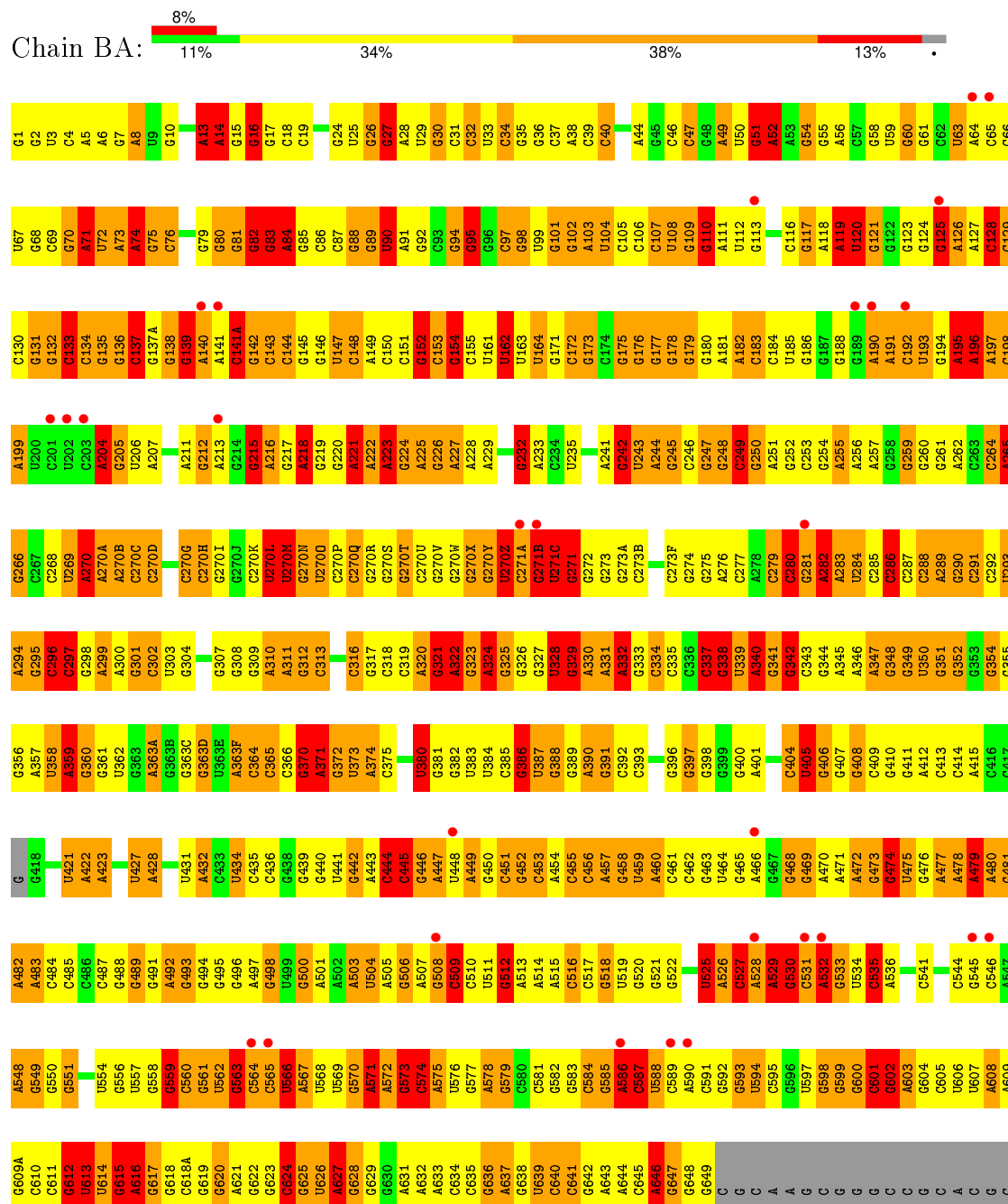
- Molecule 24: 30S ribosomal protein Thx



• Molecule 25: 5S ribosomal RNA

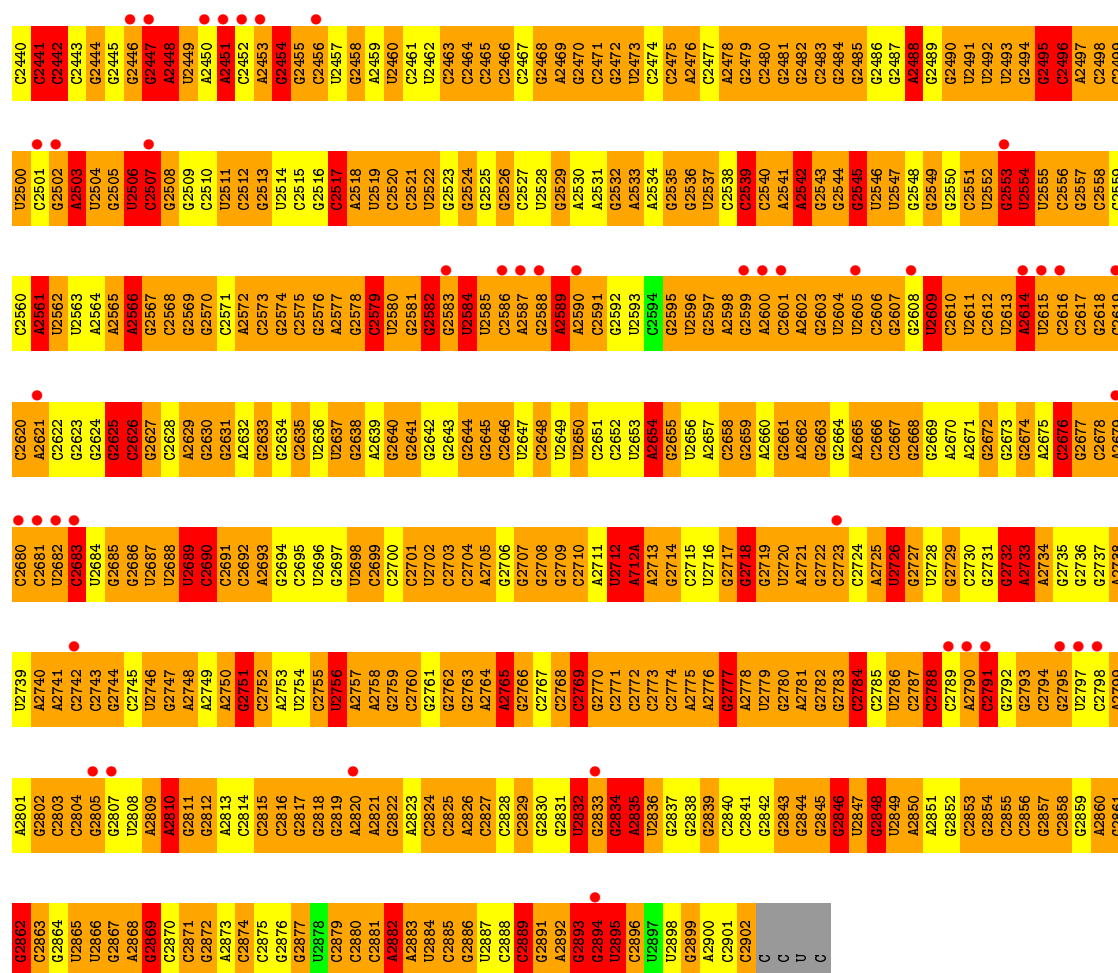


• Molecule 26: 23S ribosomal RNA

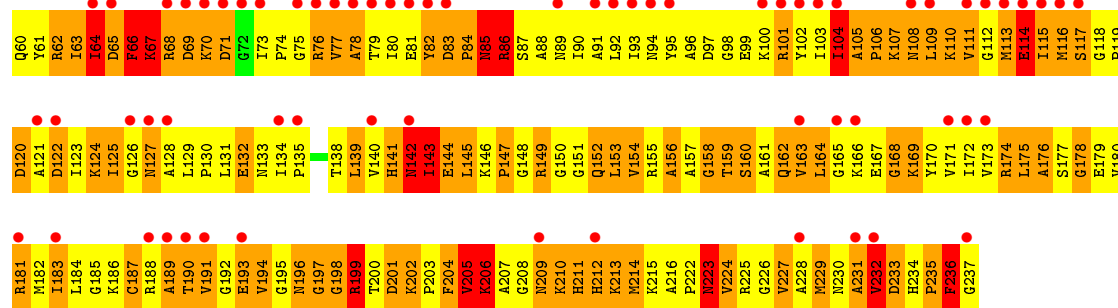




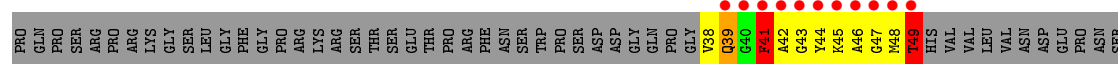
C2380	A2320	G2190	G2070	G1947	A1884	G1811	C1751	A1668	A1608	U1541
C2381	G2321	G2191	A2071	G1948	A1885	A1812	C1752	A1669	A1609	G1542
G2382	A2322	G2192	G2072	G1949	A1886	G1813	C1753	A1670	A1610	G1543
G2383	G2323	G2193	G2073	G1950	C1887	G1814	C1754	U1671	C1611	C1544
G2384	C2264	G2194	U2074	U1951	A1888	A1815	A1754	C1672	G1612	A1545
C2385	G2325	C2195	U2075	A1952	A1889	G1816	C1755	U1673	G1613	A545A
C2386	A2266	G2196	U2076	A1953	A1890	G1817	G1756	C1674	A1614	C1546
U2387	A2267	U2197	A2077	G1954	G1891	U1818	U1757	C1675	C1615	C1548
A2388	A2328	C2208	C2078	U1955	C1895	A1819	G1758	A1676	A1616	G1552
G2389	G2329	C2209	U2079	U1956	A1896	U1820	A1759	C1677	C1617	G1553
U2390	G2330	C2210	G2080	C1957	A1897	A1821	A1760	C1678	A1618	A1553
G2391	G2331	C2206	C2081	C1958	C1898	G1822	G1761	U1679	G1619	G1620
C2392	U2332	U2207	A2082	C1959	G1899	G1823	U1762	U1680	A1554	G1555
A2393	A2333	C2208	C2083	A1960	A1900	G1824	G1763	G1681	U1621	G1556
C2394	A2274	C2209	C2084	C1961	A1901	A1825	G1764	C1682	G1624	G1557
C2395	C2275	G2210	C2085	C1962	C1902	G1826	C1683	C1683	C1625	C1557
G2396	G2276	C2211	U2086	G1963	G1903	A1827	U1766	C1684	G1626	A1558
G2397	G2277	A2212	G2087	G1964	G1904	G1828	G1767	C1685	G1627	G1559
G2398	G2278	U2213	U2088	C1965	C1905	A1829	U1768	C1686	G1628	G1560
G2399	G2279	G2215	U2089	A1866	G1906	C1830	G1769	G1687	U1629	G1561
G2400	G2340	G2216	G2090	C1967	G1907	C1831	G1770	C1688	A1562	A1562
U2401	G2341	G2217	U2091	G1968	C1908	U1832	C1771	A1689	G1563	G1563
C2402	G2342	G2282	U2092	A1969	C1909	U1833	G1772	A1690	C630A	C1564
C2403	C2343	G2283	G2093	C1970	G1910	U1834	A1773	A1631	A1631	G1565
C2404	U2344	G2284	G2094	A1971	U1911	G1835	C1774	C1632	C1566	G1566
G2405	G2285	C2285	C2095	A1972	A1912	C1836	U1775	G1633	A1567	A1567
A2406	A2346	C2226	U2096	G1973	A1913	C1837	G1776	G1695	G1568	G1568
G2407	C2347	A2227	G2097	G1974	C1914	C1838	U1777	G1696	A1569	A1569
U2408	U2348	G2228	U2098	G1975	U1915	A1839	U1778	G1697	C1635	C1635
G2409	G2349	G2229	U2099	U1976	A1916	G1840	U1779	A1698	C1636	A1570
G2410	G2350	G2230	G2100	A1977	U1917	U1841	U1780	G1699	C1637	A1571
A2411	G2351	U2291	G2101	A1978	A1918	G1842	C1781	A1780	C1638	A1572
A2412	A2352	U2292	U2102	C1979	A1919	U1843	C1782	U1701	U1639	G1573
G2413	G2353	U2293	C2103	G1980	C1920	C1844	A1783	C1640	C1574	C1574
G2414	G2354	C2294	G2104	A1981	G1921	C1844	G1702	G1642	U1575	U1575
G2415	C2355	G2295	G2105	G1982	G1922	A1847	A1785	G1643	U1577	U1577
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U2419	G2359	G2239	C2099	G1989	U1926	C1852	C1789	C1647	A1581	A1581
C2420	A2360	G2240	C2050	U1990	A1927	A1853	C1790	C1648	C1582	C1582
G2421	A2361	A2241	A2051	C1991	A1928	A1854	A1791	G1649	A1583	A1583
A2422	G2362	G2242	U2052	U1992	G1929	G1855	G1792	C1650	C1585	C1585
C2423	C2363	U2243	G2053	G1992	G1930	G1856	C1793	C1651	A1586	A1586
C2424	C2364	U2244	A2054	U1993	U1931	G1857	C1795	A1652	A1587	A1587
A2425	G2365	U2245	C2055	C1994	A1932	U1858	U1796	G1653	C1588	C1588
A2426	C2366	G2246	G2056	U1995	G1933	A1859	C1797	G1654	G1596	G1596
C2427	G2367	A2247	A2057	C1996	C1934	G1860	U1798	C1655	A1597	A1597
G2428	G2368	C2248	U2058	G1997	G1935	G1861	G1799	C1656	C1598	C1598
G2429	A2369	U2249	C2059	G1998	A1936	G1862	C1800	C1657	C1599	C1599
A2430	G2370	G2250	A2060	C1999	A1937	C1870	G1801	C1658	C1600	C1600
U2431	A2371	G2251	G2061	G2000	A1938	C1871	A1732	U1659	G1601	G1601
A2432	G2372	G2252	A2062	A2001	U1939	A1872	A1803	C1660	C1602	C1602
A2433	G2373	G2253	C2183	G2002	U1940	A1873	C1733	G1661	U1602	U1602
A2434	C2374	G2254	C2063	G2003	C1941	G1878	G1735	C1662	A1603	A1603
A2435	G2375	G2255	G2065	C1942	C1942	C1879	C1741	C1663	C1604	C1604
G2436	A2376	G2256	C2066	C2006	U1943	C1880	G1742	A1664	G1605	G1605
U2437	A2377	U2257	G2067	C2007	U1944	C1881	G1743	G1665	C1606	C1606
U2438	G2378	C2258	U2068	C2008	C1882	C1882	G1746	G1666	G1607	G1607
A2439	G2379	G2259	G2069	G2009	U1946	G1883	A1810	G1667		

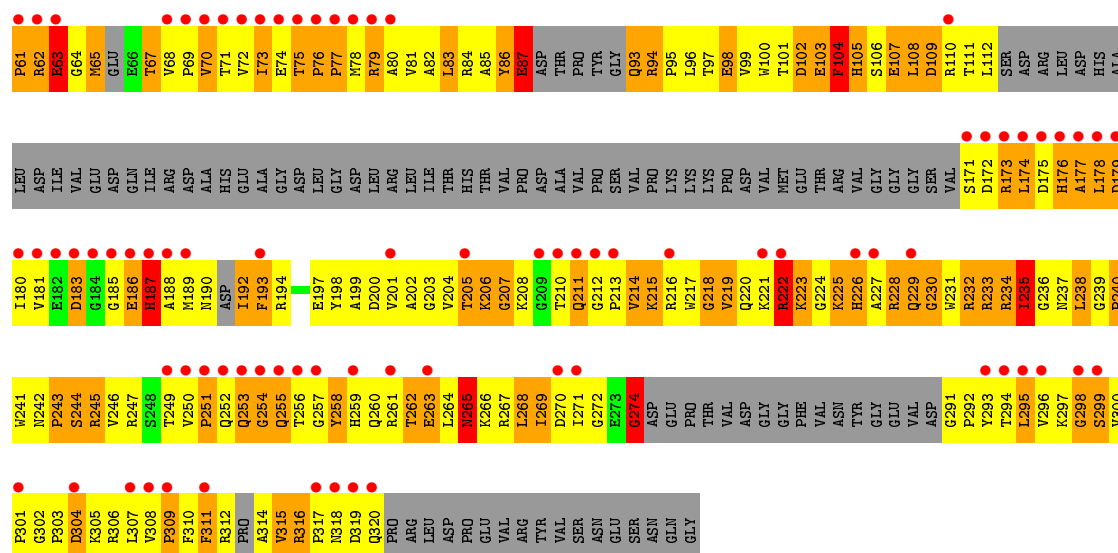


• Molecule 27: 50S ribosomal protein L2

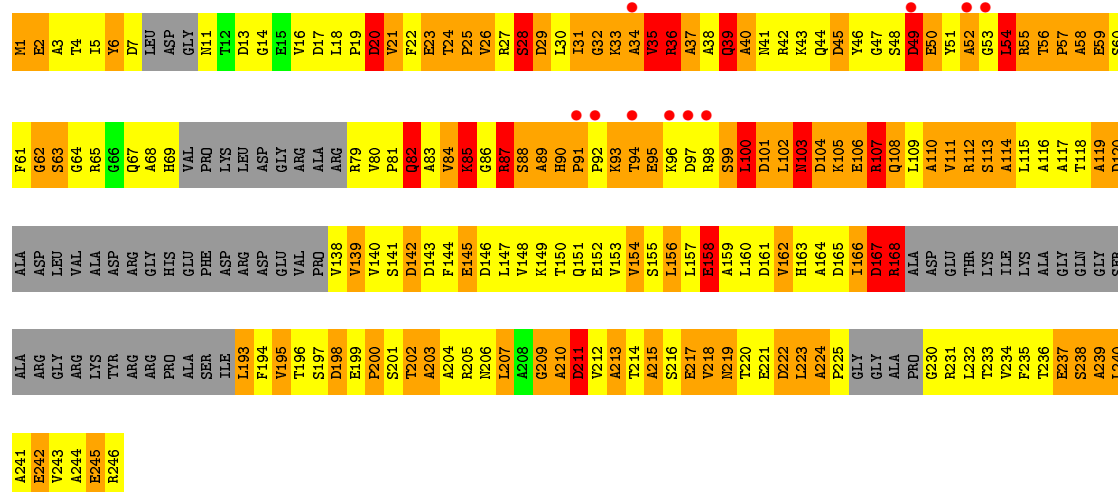


• Molecule 28: 50S ribosomal protein L3

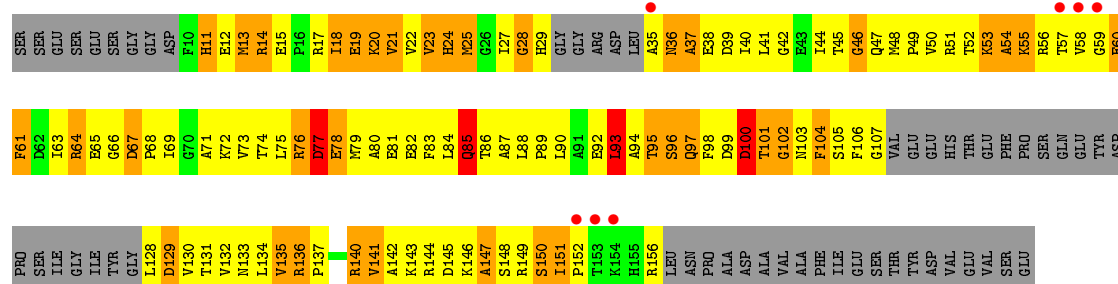




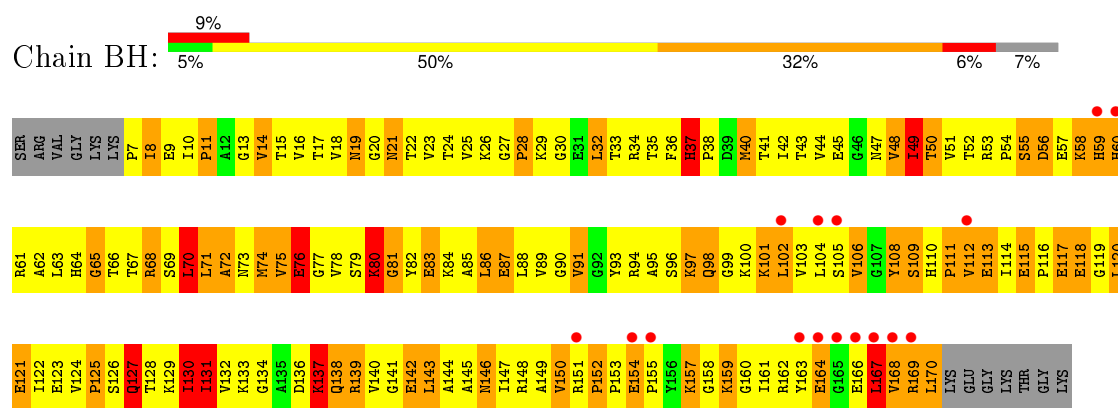
• Molecule 29: 50S ribosomal protein L4



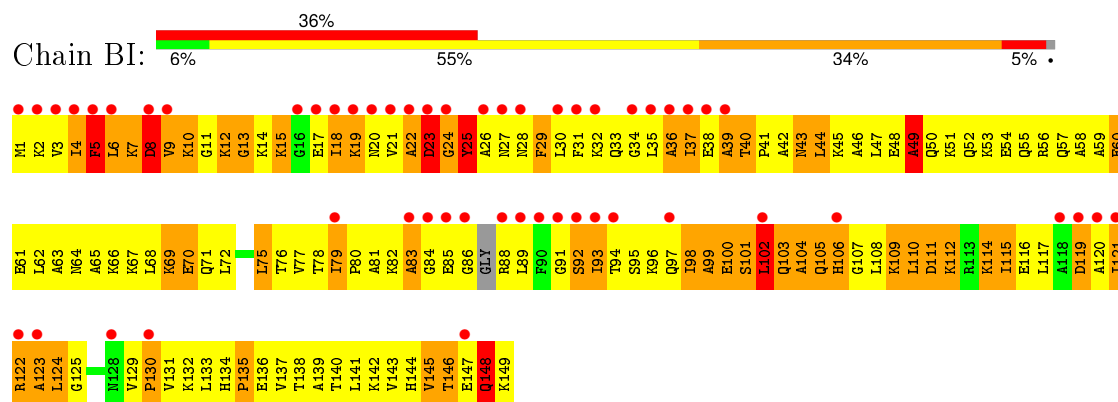
• Molecule 30: 50S ribosomal protein L5



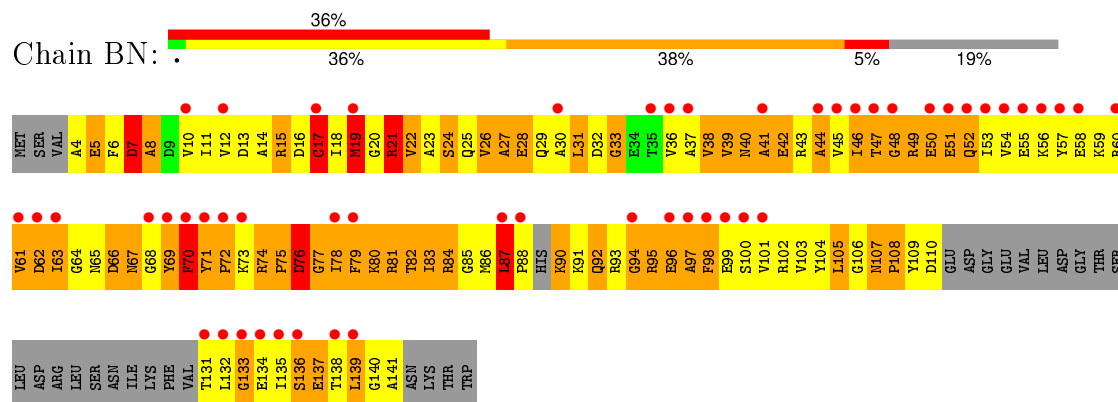
• Molecule 31: 50S ribosomal protein L6



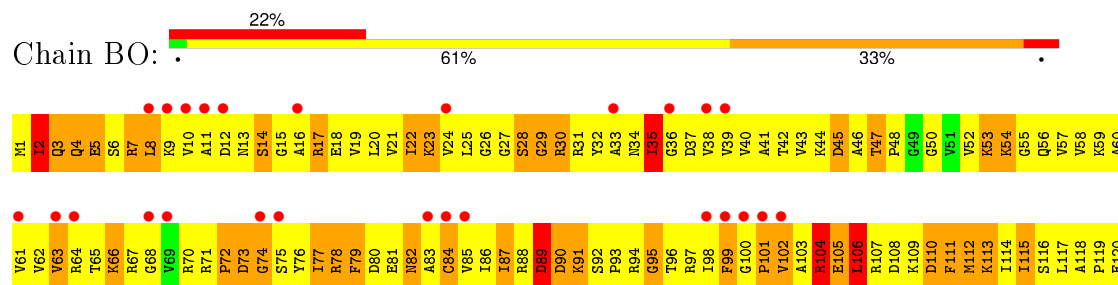
• Molecule 32: 50S ribosomal protein L9

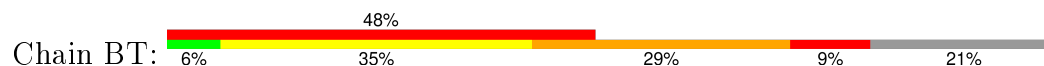


• Molecule 33: 50S ribosomal protein L13

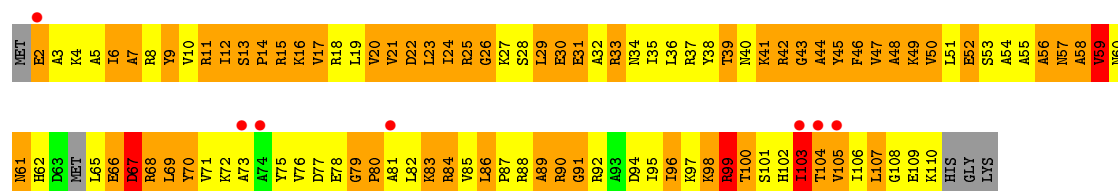


• Molecule 34: 50S ribosomal protein L14

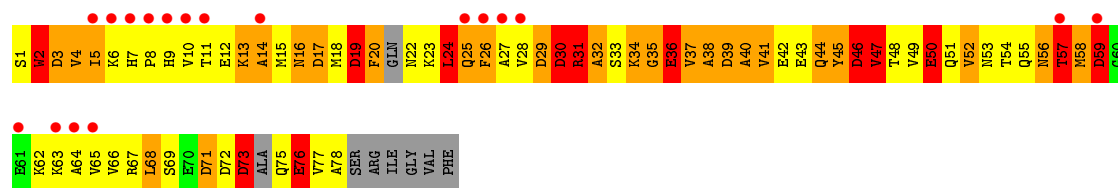




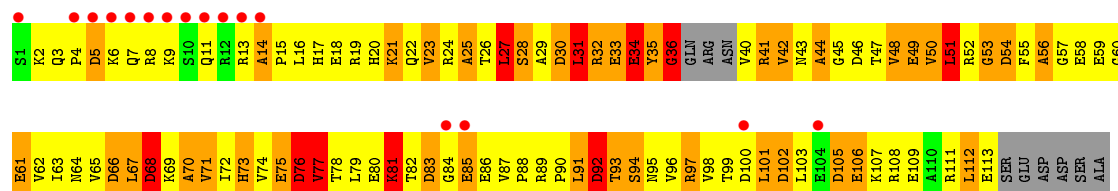
- Molecule 39: 50S ribosomal protein L22



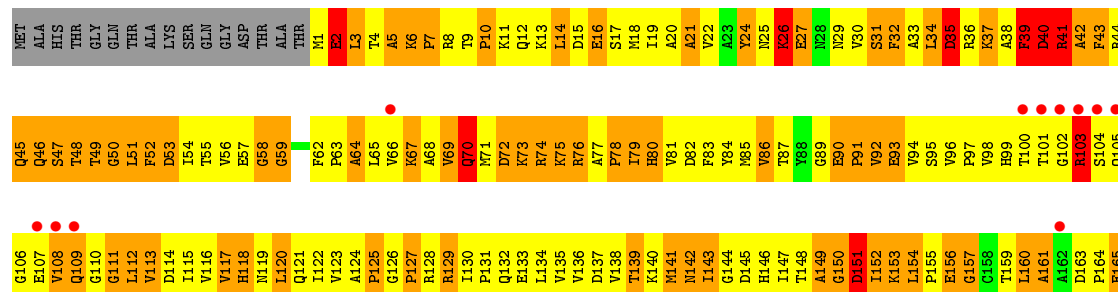
- Molecule 40: 50S ribosomal protein L23

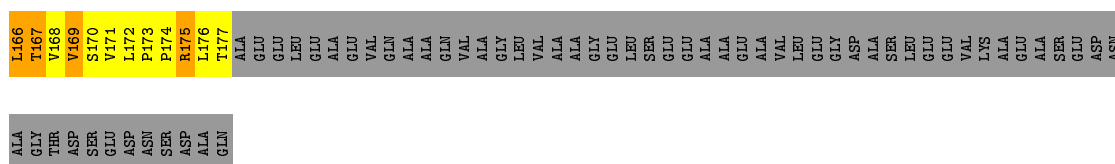


- Molecule 41: 50S ribosomal protein 24

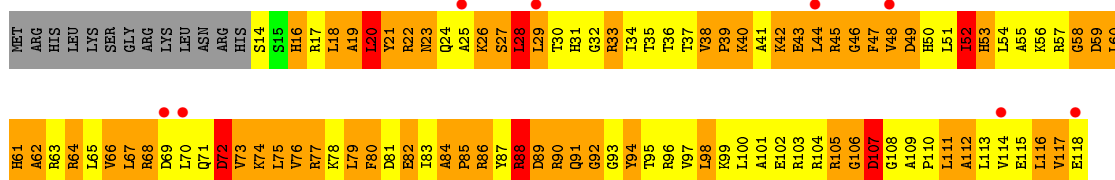


- Molecule 42: 50S ribosomal protein CTC

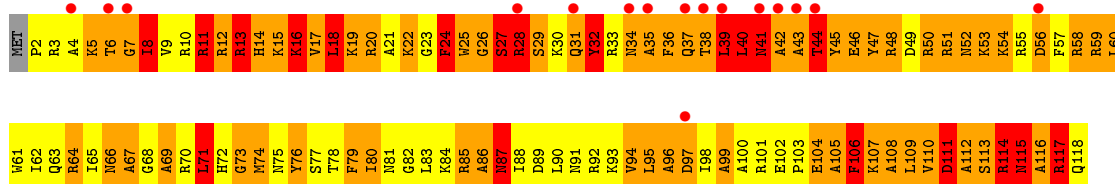




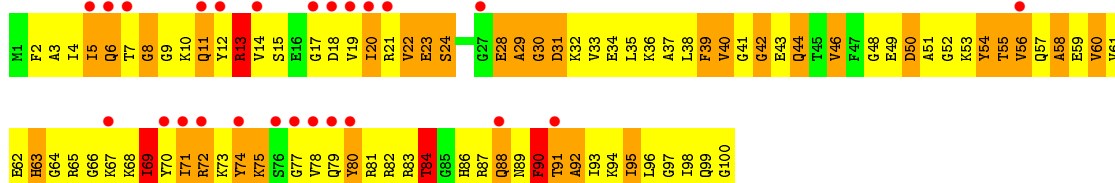
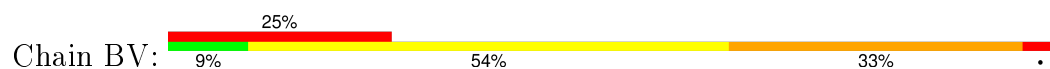
• Molecule 43: 50S ribosomal protein L17



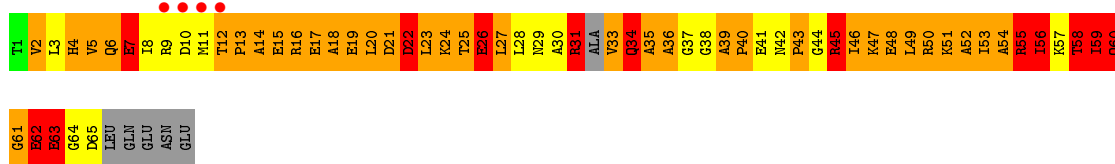
• Molecule 44: 50S ribosomal protein L20



• Molecule 45: 50S ribosomal protein L21



• Molecule 46: 50S ribosomal protein L29

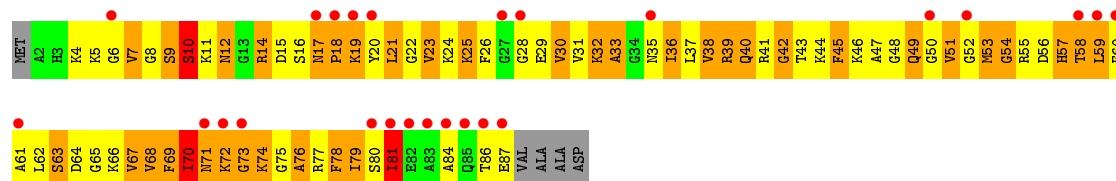


• Molecule 47: 50S ribosomal protein L30

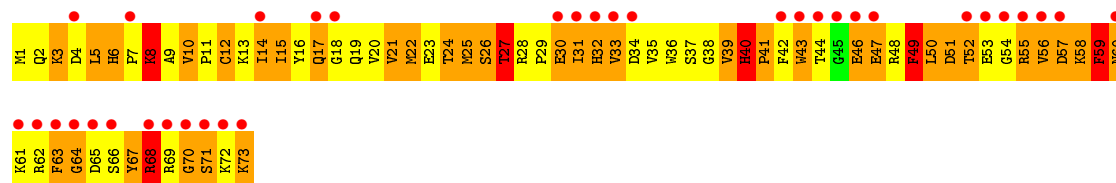




- Molecule 48: 50S ribosomal protein L27



- Molecule 49: 50S ribosomal protein L31



- Molecule 50: 50S ribosomal protein L32



- Molecule 51: 50S ribosomal protein L33

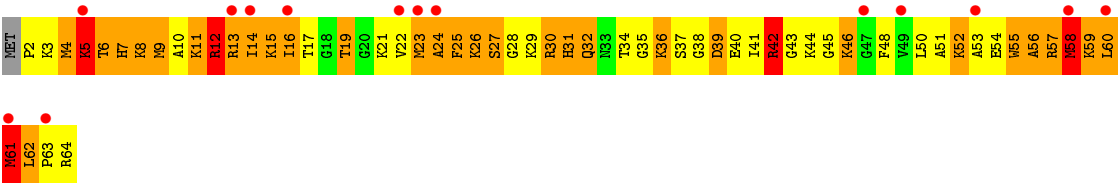


- Molecule 52: 50S ribosomal protein L34

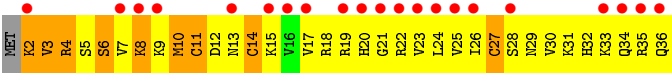
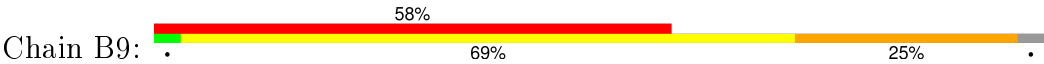


- Molecule 53: 50S ribosomal protein L35

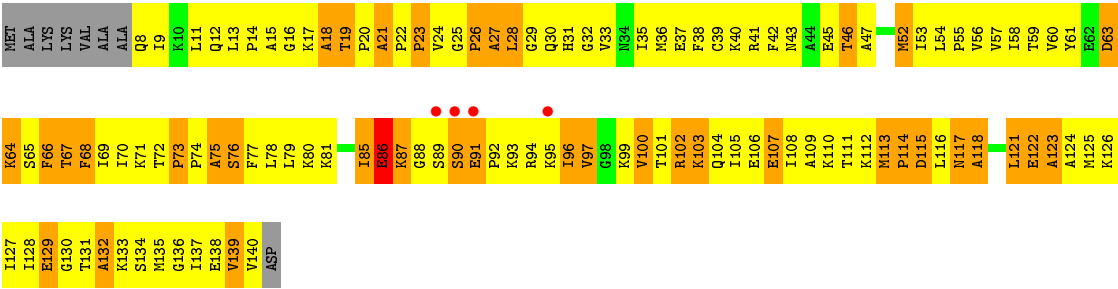
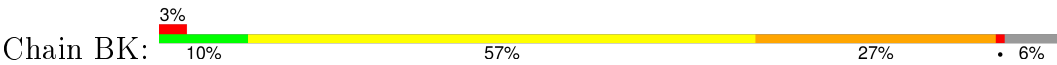




● Molecule 54: 50S ribosomal protein L36



● Molecule 55: 50S ribosomal protein L11



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	517.41Å 517.41Å 365.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 6.46 99.57 – 6.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.00-6.46) 99.7 (99.57-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 6.19Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.354 , 0.361 0.340 , 0.352	Depositor DCC
R_{free} test set	4886 reflections (5.21%)	DCC
Wilson B-factor (Å ²)	240.8	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.10 , 90.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 123103 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	142447	wwPDB-VP
Average B, all atoms (Å ²)	314.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: YYG, PSU

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	1.32	68/36413 (0.2%)	1.49	439/56777 (0.8%)
2	AV	0.74	3/1812 (0.2%)	1.20	8/2819 (0.3%)
3	AW	1.81	19/1739 (1.1%)	2.15	47/2698 (1.7%)
4	AX	0.18	0/139	0.67	0/213
5	AB	0.60	2/1935 (0.1%)	0.61	0/2609
6	AC	0.73	2/1636 (0.1%)	0.61	4/2205 (0.2%)
7	AD	0.70	4/1733 (0.2%)	1.03	11/2318 (0.5%)
8	AE	0.83	1/1162 (0.1%)	0.63	1/1564 (0.1%)
9	AF	0.35	0/856	0.54	0/1154
10	AG	0.34	0/1276	0.59	3/1709 (0.2%)
11	AH	0.41	0/1136	0.66	0/1527
12	AI	0.34	0/1029	0.54	0/1378
13	AJ	0.35	0/807	0.56	0/1085
14	AK	0.59	1/900 (0.1%)	0.54	0/1213
15	AL	1.33	1/986 (0.1%)	1.11	3/1320 (0.2%)
16	AM	0.92	1/1007 (0.1%)	0.59	1/1344 (0.1%)
17	AN	0.49	1/501 (0.2%)	0.65	1/664 (0.2%)
18	AO	0.32	0/745	0.54	0/992
19	AP	0.40	0/716	0.59	1/963 (0.1%)
20	AQ	1.23	2/870 (0.2%)	1.38	6/1159 (0.5%)
21	AR	0.40	0/603	0.70	0/799
22	AS	0.34	0/661	0.53	0/890
23	AT	0.32	0/764	0.57	1/1006 (0.1%)
24	AU	0.33	0/212	0.49	0/277
25	BB	1.25	6/2950 (0.2%)	1.44	25/4602 (0.5%)
26	BA	1.17	153/67839 (0.2%)	1.46	906/105818 (0.9%)
27	BD	0.38	0/1328	0.60	0/1783
28	BE	0.65	4/1540 (0.3%)	1.07	7/2078 (0.3%)
29	BF	0.76	3/1444 (0.2%)	0.83	1/1954 (0.1%)
30	BG	0.25	0/971	0.46	0/1304
31	BH	0.54	1/1272 (0.1%)	0.80	3/1721 (0.2%)
32	BI	0.32	0/1156	0.71	3/1544 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BN	0.35	0/927	0.55	0/1245
34	BO	0.32	0/946	0.57	0/1269
35	BP	1.59	3/643 (0.5%)	1.31	5/870 (0.6%)
36	BQ	0.32	0/1106	0.53	0/1490
37	BS	1.13	3/877 (0.3%)	0.69	1/1179 (0.1%)
38	BT	0.39	0/412	0.70	0/554
39	BW	0.75	3/869 (0.3%)	0.75	4/1166 (0.3%)
40	BX	0.49	1/608 (0.2%)	1.04	3/820 (0.4%)
41	BY	0.26	0/887	0.83	3/1195 (0.3%)
42	BZ	0.32	1/1385 (0.1%)	0.62	3/1883 (0.2%)
43	BR	0.30	0/867	0.50	0/1162
44	BU	0.64	1/994 (0.1%)	0.74	3/1323 (0.2%)
45	BV	0.82	1/796 (0.1%)	0.91	3/1058 (0.3%)
46	B2	0.37	0/497	1.00	2/668 (0.3%)
47	B3	0.31	0/482	0.50	0/646
48	B0	0.38	1/649 (0.2%)	0.87	3/860 (0.3%)
49	B4	0.89	2/620 (0.3%)	0.54	0/831
50	B5	0.36	0/469	0.90	3/629 (0.5%)
51	B6	0.32	0/438	0.55	1/583 (0.2%)
52	B7	0.38	0/387	0.64	0/509
53	B8	0.91	2/503 (0.4%)	0.92	3/657 (0.5%)
54	B9	0.33	0/286	0.59	0/375
55	BK	0.27	1/1014 (0.1%)	0.44	0/1363
All	All	1.09	291/154800 (0.2%)	1.33	1508/231822 (0.7%)

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
3	AW	1	5
5	AB	0	1
6	AC	0	1
7	AD	0	1
14	AK	0	1
15	AL	0	1
20	AQ	0	1
27	BD	0	1
28	BE	0	3
29	BF	0	4
31	BH	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	BI	0	1
35	BP	0	1
37	BS	0	1
40	BX	0	1
41	BY	0	1
46	B2	0	1
50	B5	0	1
55	BK	0	1
All	All	1	28

The worst 5 of 291 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	2199	A	O3'-P	-71.04	0.75	1.61
1	AA	1278	U	O3'-P	-56.53	0.93	1.61
1	AA	1337	G	O3'-P	-53.91	0.96	1.61
26	BA	1546	C	O3'-P	-51.62	0.99	1.61
1	AA	1004	A	O3'-P	48.18	2.19	1.61

The worst 5 of 1508 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	65	G	P-O3'-C3'	-50.68	58.88	119.70
26	BA	712(A)	A	P-O3'-C3'	-43.62	67.36	119.70
26	BA	2199	A	O3'-P-O5'	-43.07	22.17	104.00
2	AV	65	G	P-O3'-C3'	39.88	167.56	119.70
1	AA	1255	G	P-O3'-C3'	-38.36	73.67	119.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

5 of 28 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AW	16	U	Sidechain
3	AW	17	U	Sidechain
3	AW	18	G	Sidechain
3	AW	19	G	Sidechain
3	AW	62	A	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32551	0	16459	2042	3
2	AV	1622	0	821	231	0
3	AW	1638	0	836	243	0
4	AX	136	0	63	26	0
5	AB	1900	0	1950	97	0
6	AC	1612	0	1675	99	0
7	AD	1703	0	1761	289	0
8	AE	1146	0	1206	68	0
9	AF	843	0	857	30	0
10	AG	1257	0	1295	102	0
11	AH	1116	0	1177	100	0
12	AI	1011	0	1040	80	0
13	AJ	794	0	840	81	0
14	AK	885	0	904	53	0
15	AL	970	0	1056	72	0
16	AM	997	0	1070	149	0
17	AN	492	0	529	82	0
18	AO	734	0	771	28	0
19	AP	700	0	720	70	0
20	AQ	857	0	928	80	0
21	AR	597	0	668	40	0
22	AS	647	0	673	155	0
23	AT	762	0	859	37	0
24	AU	208	0	221	84	0
25	BB	2637	0	1339	219	1
26	BA	60600	0	30514	11060	138
27	BD	1308	0	1346	1086	0
28	BE	1507	0	1478	1144	3
29	BF	1430	0	1357	1085	0
30	BG	957	0	952	692	0
31	BH	1251	0	1291	754	0
32	BI	1145	0	1225	625	3
33	BN	917	0	896	771	2
34	BO	937	0	992	613	0
35	BP	639	0	605	482	0
36	BQ	1081	0	1047	932	0
37	BS	866	0	866	677	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	BT	406	0	359	167	0
39	BW	860	0	909	557	0
40	BX	602	0	558	460	0
41	BY	879	0	860	755	0
42	BZ	1360	0	1378	902	0
43	BR	855	0	904	579	0
44	BU	978	0	996	895	0
45	BV	787	0	782	635	0
46	B2	494	0	504	393	0
47	B3	477	0	527	460	0
48	B0	641	0	661	531	0
49	B4	604	0	587	489	0
50	B5	457	0	456	279	0
51	B6	431	0	454	289	0
52	B7	383	0	409	382	0
53	B8	496	0	539	349	0
54	B9	285	0	312	195	0
55	BK	999	0	1064	573	0
All	All	142447	0	94546	28969	145

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 123.

The worst 5 of 28969 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)
50:B5:33:CYS:SG	50:B5:36:CYS:HB2	1.24	1.69
26:BA:2470:G:C2	26:BA:2471:C:C5	1.81	1.68
52:B7:30:ILE:HA	52:B7:33:ARG:CD	1.21	1.67
26:BA:2712:U:C6	26:BA:712(A):A:C8	1.77	1.67
26:BA:2580:U:C6	26:BA:2581:G:C8	1.82	1.66

The worst 5 of 145 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)
26:BA:6:A:O4'	26:BA:2902:C:C2'[8_554]	0.72	1.48
26:BA:2899:G:N1	26:BA:2901:C:C4[8_554]	0.79	1.41
26:BA:6:A:C4'	26:BA:2902:C:C2'[8_554]	0.97	1.23
26:BA:2900:A:N7	26:BA:2900:A:N6[8_554]	1.03	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:BA:3:U:O4	26:BA:2899:G:O2'[8_554]	1.09	1.11

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	
5	AB	232/256 (91%)	183 (79%)	33 (14%)	16 (7%)	1	22
6	AC	204/239 (85%)	166 (81%)	24 (12%)	14 (7%)	1	22
7	AD	206/209 (99%)	157 (76%)	33 (16%)	16 (8%)	1	20
8	AE	148/162 (91%)	116 (78%)	29 (20%)	3 (2%)	9	51
9	AF	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	4	35
10	AG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	7	45
11	AH	136/138 (99%)	101 (74%)	25 (18%)	10 (7%)	1	21
12	AI	125/128 (98%)	86 (69%)	31 (25%)	8 (6%)	2	25
13	AJ	96/105 (91%)	73 (76%)	14 (15%)	9 (9%)	1	16
14	AK	117/129 (91%)	88 (75%)	22 (19%)	7 (6%)	2	26
15	AL	122/135 (90%)	90 (74%)	13 (11%)	19 (16%)	0	5
16	AM	121/126 (96%)	95 (78%)	20 (16%)	6 (5%)	3	31
17	AN	58/61 (95%)	42 (72%)	12 (21%)	4 (7%)	1	22
18	AO	86/89 (97%)	76 (88%)	9 (10%)	1 (1%)	16	61
19	AP	81/88 (92%)	64 (79%)	11 (14%)	6 (7%)	1	21
20	AQ	102/105 (97%)	78 (76%)	18 (18%)	6 (6%)	2	26
21	AR	71/88 (81%)	54 (76%)	11 (16%)	6 (8%)	1	18
22	AS	78/93 (84%)	60 (77%)	15 (19%)	3 (4%)	4	37
23	AT	97/106 (92%)	79 (81%)	12 (12%)	6 (6%)	2	25
24	AU	22/27 (82%)	17 (77%)	3 (14%)	2 (9%)	1	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BD	169/173 (98%)	60 (36%)	34 (20%)	75 (44%)	0	0
28	BE	183/338 (54%)	89 (49%)	34 (19%)	60 (33%)	0	0
29	BF	179/246 (73%)	51 (28%)	47 (26%)	81 (45%)	0	0
30	BG	116/176 (66%)	46 (40%)	31 (27%)	39 (34%)	0	0
31	BH	162/177 (92%)	74 (46%)	39 (24%)	49 (30%)	0	0
32	BI	144/149 (97%)	71 (49%)	29 (20%)	44 (31%)	0	0
33	BN	111/145 (77%)	34 (31%)	21 (19%)	56 (50%)	0	0
34	BO	120/122 (98%)	61 (51%)	27 (22%)	32 (27%)	0	1
35	BP	82/164 (50%)	28 (34%)	21 (26%)	33 (40%)	0	0
36	BQ	130/138 (94%)	38 (29%)	35 (27%)	57 (44%)	0	0
37	BS	105/186 (56%)	36 (34%)	20 (19%)	49 (47%)	0	0
38	BT	48/66 (73%)	17 (35%)	13 (27%)	18 (38%)	0	0
39	BW	104/113 (92%)	41 (39%)	16 (15%)	47 (45%)	0	0
40	BX	72/84 (86%)	26 (36%)	18 (25%)	28 (39%)	0	0
41	BY	108/119 (91%)	49 (45%)	20 (18%)	39 (36%)	0	0
42	BZ	175/253 (69%)	52 (30%)	53 (30%)	70 (40%)	0	0
43	BR	103/118 (87%)	35 (34%)	20 (19%)	48 (47%)	0	0
44	BU	115/118 (98%)	22 (19%)	23 (20%)	70 (61%)	0	0
45	BV	96/100 (96%)	39 (41%)	25 (26%)	32 (33%)	0	0
46	B2	62/70 (89%)	8 (13%)	9 (14%)	45 (73%)	0	0
47	B3	58/60 (97%)	24 (41%)	13 (22%)	21 (36%)	0	0
48	B0	84/91 (92%)	32 (38%)	17 (20%)	35 (42%)	0	0
49	B4	71/73 (97%)	21 (30%)	16 (22%)	34 (48%)	0	0
50	B5	56/60 (93%)	16 (29%)	18 (32%)	22 (39%)	0	0
51	B6	51/82 (62%)	21 (41%)	9 (18%)	21 (41%)	0	0
52	B7	44/47 (94%)	4 (9%)	7 (16%)	33 (75%)	0	0
53	B8	61/64 (95%)	22 (36%)	10 (16%)	29 (48%)	0	0
54	B9	33/36 (92%)	14 (42%)	9 (27%)	10 (30%)	0	0
55	BK	129/141 (92%)	73 (57%)	18 (14%)	38 (30%)	0	0
All	All	5325/6250 (85%)	2945 (55%)	1015 (19%)	1365 (26%)	0	1

5 of 1365 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AB	24	TRP
5	AB	104	ASN
5	AB	153	ARG
5	AB	154	LEU
5	AB	161	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	
5	AB	202/220 (92%)	173 (86%)	29 (14%)	4	25
6	AC	160/188 (85%)	146 (91%)	14 (9%)	12	45
7	AD	180/181 (99%)	162 (90%)	18 (10%)	9	38
8	AE	115/123 (94%)	94 (82%)	21 (18%)	2	14
9	AF	90/90 (100%)	83 (92%)	7 (8%)	16	51
10	AG	126/127 (99%)	116 (92%)	10 (8%)	15	51
11	AH	119/119 (100%)	92 (77%)	27 (23%)	1	8
12	AI	98/99 (99%)	90 (92%)	8 (8%)	14	49
13	AJ	88/92 (96%)	77 (88%)	11 (12%)	6	30
14	AK	90/99 (91%)	85 (94%)	5 (6%)	26	62
15	AL	104/111 (94%)	93 (89%)	11 (11%)	8	36
16	AM	100/101 (99%)	87 (87%)	13 (13%)	5	28
17	AN	49/50 (98%)	43 (88%)	6 (12%)	6	31
18	AO	79/80 (99%)	70 (89%)	9 (11%)	7	32
19	AP	72/74 (97%)	62 (86%)	10 (14%)	4	26
20	AQ	96/97 (99%)	87 (91%)	9 (9%)	11	42
21	AR	64/77 (83%)	57 (89%)	7 (11%)	8	35
22	AS	71/80 (89%)	64 (90%)	7 (10%)	10	39
23	AT	76/82 (93%)	68 (90%)	8 (10%)	8	36
24	AU	19/22 (86%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	BD	135/135 (100%)	99 (73%)	36 (27%)	0	5
28	BE	156/284 (55%)	128 (82%)	28 (18%)	2	15
29	BF	152/193 (79%)	124 (82%)	28 (18%)	2	14
30	BG	102/147 (69%)	93 (91%)	9 (9%)	12	45
31	BH	137/147 (93%)	111 (81%)	26 (19%)	2	13
32	BI	119/119 (100%)	98 (82%)	21 (18%)	2	16
33	BN	95/121 (78%)	80 (84%)	15 (16%)	3	21
34	BO	101/101 (100%)	81 (80%)	20 (20%)	1	12
35	BP	67/126 (53%)	56 (84%)	11 (16%)	3	20
36	BQ	110/110 (100%)	83 (76%)	27 (24%)	1	6
37	BS	89/149 (60%)	73 (82%)	16 (18%)	2	15
38	BT	44/52 (85%)	30 (68%)	14 (32%)	0	2
39	BW	88/92 (96%)	74 (84%)	14 (16%)	3	21
40	BX	67/73 (92%)	44 (66%)	23 (34%)	0	2
41	BY	97/105 (92%)	80 (82%)	17 (18%)	2	16
42	BZ	151/203 (74%)	130 (86%)	21 (14%)	4	26
43	BR	89/101 (88%)	71 (80%)	18 (20%)	1	11
44	BU	96/97 (99%)	68 (71%)	28 (29%)	0	3
45	BV	79/79 (100%)	69 (87%)	10 (13%)	5	29
46	B2	51/56 (91%)	37 (72%)	14 (28%)	0	4
47	B3	52/52 (100%)	47 (90%)	5 (10%)	10	40
48	B0	64/67 (96%)	57 (89%)	7 (11%)	8	35
49	B4	66/66 (100%)	54 (82%)	12 (18%)	2	15
50	B5	51/53 (96%)	43 (84%)	8 (16%)	3	21
51	B6	46/69 (67%)	39 (85%)	7 (15%)	3	23
52	B7	39/40 (98%)	31 (80%)	8 (20%)	1	10
53	B8	50/51 (98%)	39 (78%)	11 (22%)	1	9
54	B9	34/35 (97%)	30 (88%)	4 (12%)	6	31
55	BK	108/113 (96%)	104 (96%)	4 (4%)	41	73
All	All	4533/5148 (88%)	3841 (85%)	692 (15%)	3	22

5 of 692 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BF	120	ASP
33	BN	87	LEU
49	B4	15	ILE
30	BG	13	MET
31	BH	137	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 129 such sidechains are listed below:

Mol	Chain	Res	Type
28	BE	242	ASN
32	BI	64	ASN
48	B0	71	ASN
28	BE	260	GLN
29	BF	219	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1497/1522 (98%)	520 (34%)	164 (10%)
2	AV	73/76 (96%)	16 (21%)	1 (1%)
25	BB	122/123 (99%)	45 (36%)	3 (2%)
26	BA	2780/2916 (95%)	1487 (53%)	360 (12%)
3	AW	70/76 (92%)	16 (22%)	3 (4%)
4	AX	5/18 (27%)	0	0
All	All	4547/4731 (96%)	2084 (45%)	531 (11%)

5 of 2084 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	12	U

5 of 531 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	646	A
26	BA	1126	A
26	BA	2612	C

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Mol	Chain	Res	Type
26	BA	704	G
26	BA	827	U

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	YYG	AW	37	10,3	27,42,43	1.03	2 (7%)	29,62,65	2.22	8 (27%)
3	PSU	AW	39	3	13,21,22	1.32	2 (15%)	18,30,33	6.12	4 (22%)
3	PSU	AW	55	3	13,21,22	1.52	2 (15%)	18,30,33	6.00	6 (33%)

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
3	YYG	AW	37	10,3	1/1/8/9	0/20/42/43	0/4/4/4
3	PSU	AW	39	3	-	0/7/25/26	0/2/2/2
3	PSU	AW	55	3	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	AW	39	PSU	C6-C5	-3.30	1.33	1.38
3	AW	55	PSU	C6-C5	-2.85	1.34	1.38
3	AW	37	YYG	C2-N2	2.05	1.38	1.35
3	AW	37	YYG	C6-N1	2.86	1.42	1.37
3	AW	39	PSU	C4-N3	2.96	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AW	39	PSU	N1-C2-N3	-21.95	114.33	128.33
3	AW	55	PSU	N1-C2-N3	-21.67	114.51	128.33
3	AW	37	YYG	C13-C12-C11	-4.15	123.52	130.59
3	AW	37	YYG	O23-C21-O22	-3.81	119.73	124.70
3	AW	55	PSU	C4-C5-C1'	-2.42	116.81	121.23

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	AW	37	YYG	C15

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	AW	37	YYG	38	0
3	AW	39	PSU	4	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
26	BA	58
1	AA	45
3	AW	6

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Mol	Chain	Number of breaks
36	BQ	3
25	BB	2
2	AV	2
6	AC	2
45	BV	2
16	AM	2
44	BU	1
20	AQ	1
5	AB	1
8	AE	1
29	BF	1
27	BD	1
37	BS	1
55	BK	1
35	BP	1
7	AD	1
31	BH	1
15	AL	1

The worst 5 of 134 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AA	30(D):A	O3'	1031:G	P	5.01
1	BA	142(A):A	O3'	1143:A	P	4.98
1	AW	73:A	O3'	74:C	P	4.88
1	BA	1171:G	O3'	1173:G	P	4.41
1	AA	440:A	O3'	442:C	P	4.34

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	1515/1522 (99%)	0.61	193 (12%) 5 11	188, 339, 400, 400	0
2	AV	76/76 (100%)	1.07	11 (14%) 3 9	242, 299, 394, 394	0
3	AW	73/76 (96%)	0.56	11 (15%) 3 9	253, 400, 400, 400	0
4	AX	17/18 (94%)	1.52	5 (29%) 1 5	400, 400, 400, 400	0
5	AB	234/256 (91%)	0.15	12 (5%) 32 32	395, 395, 400, 400	0
6	AC	206/239 (86%)	1.74	62 (30%) 1 5	393, 398, 398, 398	0
7	AD	208/209 (99%)	1.73	71 (34%) 0 4	257, 391, 400, 400	0
8	AE	150/162 (92%)	3.37	91 (60%) 0 3	371, 400, 400, 400	0
9	AF	101/101 (100%)	-0.39	1 (0%) 84 79	400, 400, 400, 400	0
10	AG	155/156 (99%)	2.02	59 (38%) 0 4	358, 400, 400, 400	0
11	AH	138/138 (100%)	1.50	47 (34%) 0 4	396, 396, 396, 396	0
12	AI	127/128 (99%)	0.77	29 (22%) 1 6	395, 395, 395, 395	0
13	AJ	98/105 (93%)	1.34	14 (14%) 4 9	400, 400, 400, 400	0
14	AK	119/129 (92%)	0.90	21 (17%) 2 7	202, 202, 400, 400	0
15	AL	124/135 (91%)	1.06	25 (20%) 1 7	399, 399, 400, 400	0
16	AM	125/126 (99%)	0.54	18 (14%) 3 9	348, 400, 400, 400	0
17	AN	60/61 (98%)	1.61	20 (33%) 0 4	400, 400, 400, 400	0
18	AO	88/89 (98%)	-0.08	4 (4%) 37 36	400, 400, 400, 400	0
19	AP	83/88 (94%)	1.90	33 (39%) 0 4	400, 400, 400, 400	0
20	AQ	104/105 (99%)	1.96	43 (41%) 0 4	400, 400, 400, 400	0
21	AR	73/88 (82%)	-0.35	0 100 100	400, 400, 400, 400	0
22	AS	80/93 (86%)	0.75	18 (22%) 1 6	400, 400, 400, 400	0
23	AT	99/106 (93%)	-0.03	8 (8%) 15 18	400, 400, 400, 400	0
24	AU	24/27 (88%)	2.03	10 (41%) 0 4	400, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	BB	123/123 (100%)	-0.09	6 (4%) 33 33	267, 323, 388, 388	0
26	BA	2814/2916 (96%)	0.46	220 (7%) 16 19	65, 238, 393, 400	0
27	BD	173/173 (100%)	1.67	65 (37%) 0 4	392, 392, 400, 400	0
28	BE	191/338 (56%)	2.17	91 (47%) 0 4	400, 400, 400, 400	0
29	BF	189/246 (76%)	-0.30	10 (5%) 30 31	393, 396, 396, 396	0
30	BG	122/176 (69%)	0.10	7 (5%) 27 28	400, 400, 400, 400	0
31	BH	164/177 (92%)	0.32	16 (9%) 10 14	400, 400, 400, 400	0
32	BI	148/149 (99%)	1.53	53 (35%) 0 4	400, 400, 400, 400	0
33	BN	117/145 (80%)	1.84	52 (44%) 0 4	400, 400, 400, 400	0
34	BO	122/122 (100%)	1.20	27 (22%) 1 6	400, 400, 400, 400	0
35	BP	84/164 (51%)	1.11	20 (23%) 1 5	395, 395, 400, 400	0
36	BQ	138/138 (100%)	2.54	73 (52%) 0 3	393, 393, 393, 393	0
37	BS	113/186 (60%)	-0.08	2 (1%) 71 66	278, 400, 400, 400	0
38	BT	52/66 (78%)	3.18	32 (61%) 0 3	400, 400, 400, 400	0
39	BW	108/113 (95%)	0.24	7 (6%) 22 23	278, 395, 400, 400	0
40	BX	76/84 (90%)	0.89	18 (23%) 1 5	400, 400, 400, 400	0
41	BY	110/119 (92%)	0.77	16 (14%) 3 9	400, 400, 400, 400	0
42	BZ	177/253 (69%)	0.34	11 (6%) 24 25	396, 398, 398, 398	0
43	BR	105/118 (88%)	0.42	8 (7%) 17 19	400, 400, 400, 400	0
44	BU	117/118 (99%)	0.51	16 (13%) 4 9	391, 391, 400, 400	0
45	BV	100/100 (100%)	1.20	25 (25%) 1 5	400, 400, 400, 400	0
46	B2	64/70 (91%)	0.07	4 (6%) 23 24	400, 400, 400, 400	0
47	B3	60/60 (100%)	0.34	4 (6%) 21 23	398, 398, 398, 398	0
48	B0	86/91 (94%)	1.55	25 (29%) 1 5	396, 400, 400, 400	0
49	B4	73/73 (100%)	2.04	35 (47%) 0 4	396, 397, 397, 397	0
50	B5	58/60 (96%)	-0.10	0 100 100	400, 400, 400, 400	0
51	B6	53/82 (64%)	-0.04	2 (3%) 44 42	400, 400, 400, 400	0
52	B7	46/47 (97%)	0.88	4 (8%) 13 17	396, 396, 396, 396	0
53	B8	63/64 (98%)	1.11	14 (22%) 1 6	400, 400, 400, 400	0
54	B9	35/36 (97%)	3.82	21 (60%) 0 3	400, 400, 400, 400	0
55	BK	133/141 (94%)	0.10	4 (3%) 54 49	392, 400, 400, 400	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	10091/10981 (91%)	0.80	1694 (16%) 2 8	65, 395, 400, 400	0

The worst 5 of 1694 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AJ	61	GLU	18.0
13	AJ	62	HIS	16.7
13	AJ	48	THR	15.4
8	AE	134	ALA	15.0
54	B9	24	LEU	14.2

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
3	PSU	AW	39	20/21	0.58	0.44	-	399,399,399,399	0
3	YYG	AW	37	39/40	0.17	0.79	-	399,399,399,399	0
3	PSU	AW	55	20/21	0.94	0.09	-	400,400,400,400	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.