



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 10:36 PM BST

PDB ID : 4V8O
Title : Crystal structure of the hybrid state of ribosome in complex with the guanosine triphosphatase release factor 3
Authors : Jin, H.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2011-07-26
Resolution : 3.80 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

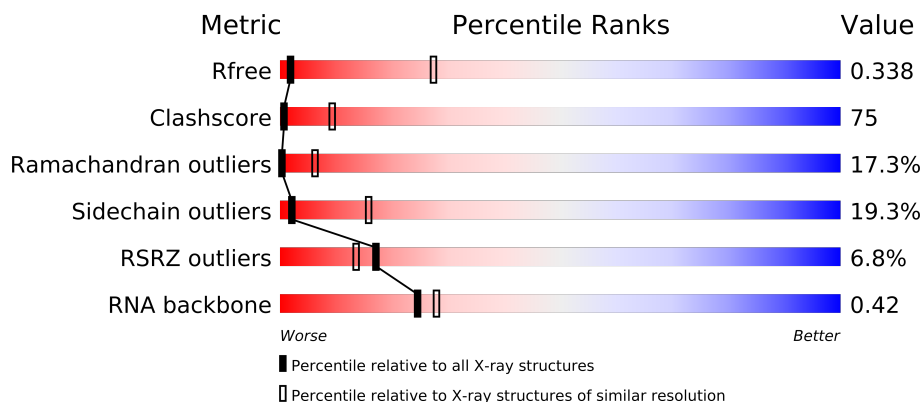
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : stable23397
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23397

1 Overall quality at a glance

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)
RNA backbone	1838	1009 (4.76-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1522	
2	AB	256	
3	AC	239	
4	AD	209	
5	AE	162	
6	AF	101	
7	AG	156	
8	AH	138	
9	AI	128	
10	AJ	105	
11	AK	129	
12	AL	135	

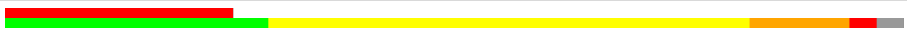
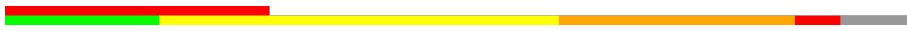

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Mol	Chain	Length	Quality of chain
13	AM	126	
14	AN	61	
15	AO	89	
16	AP	88	
17	AQ	105	
18	AR	88	
19	AS	93	
20	AT	106	
21	AU	27	
22	AV	77	
23	AX	9	
24	AY	529	
25	B0	85	
26	B1	98	
27	B2	72	
28	B3	60	
29	B4	71	
30	B5	60	
31	B6	54	
32	B7	49	
33	B8	65	
34	B9	37	
35	BA	2915	
36	BB	122	
37	BC	229	
38	BD	276	
39	BE	206	
40	BF	210	
41	BG	182	
42	BH	180	
43	BJ	173	
44	BK	147	
45	BN	140	
46	BO	122	
47	BP	150	
48	BQ	141	
49	BR	118	
50	BS	112	
51	BT	146	
52	BU	118	
53	BV	101	
54	BW	113	

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Mol	Chain	Length	Quality of chain
55	BX	96	
56	BY	110	
57	BZ	206	

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 151017 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	1	MET	-	EXPRESSION TAG	UNP P17293
AL	2	VAL	-	EXPRESSION TAG	UNP P17293
AL	3	ALA	-	EXPRESSION TAG	UNP P17293
AL	4	LEU	-	EXPRESSION TAG	UNP P17293

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called PE HYBRID STATE TRNA FMET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	9	Total	C	N	O	P	0	0	0
			192	88	39	57	8			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	496	Total	C	N	O	S	0	0	0
			3934	2492	677	744	21			

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BC	19	ILE	VAL	CONFLICT	UNP Q5SLP7
BC	27	HIS	ARG	CONFLICT	UNP Q5SLP7
BC	127	MET	LEU	CONFLICT	UNP Q5SLP7

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

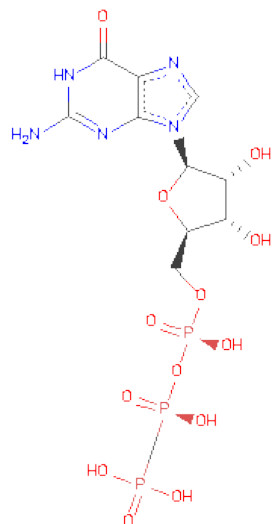
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

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

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

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

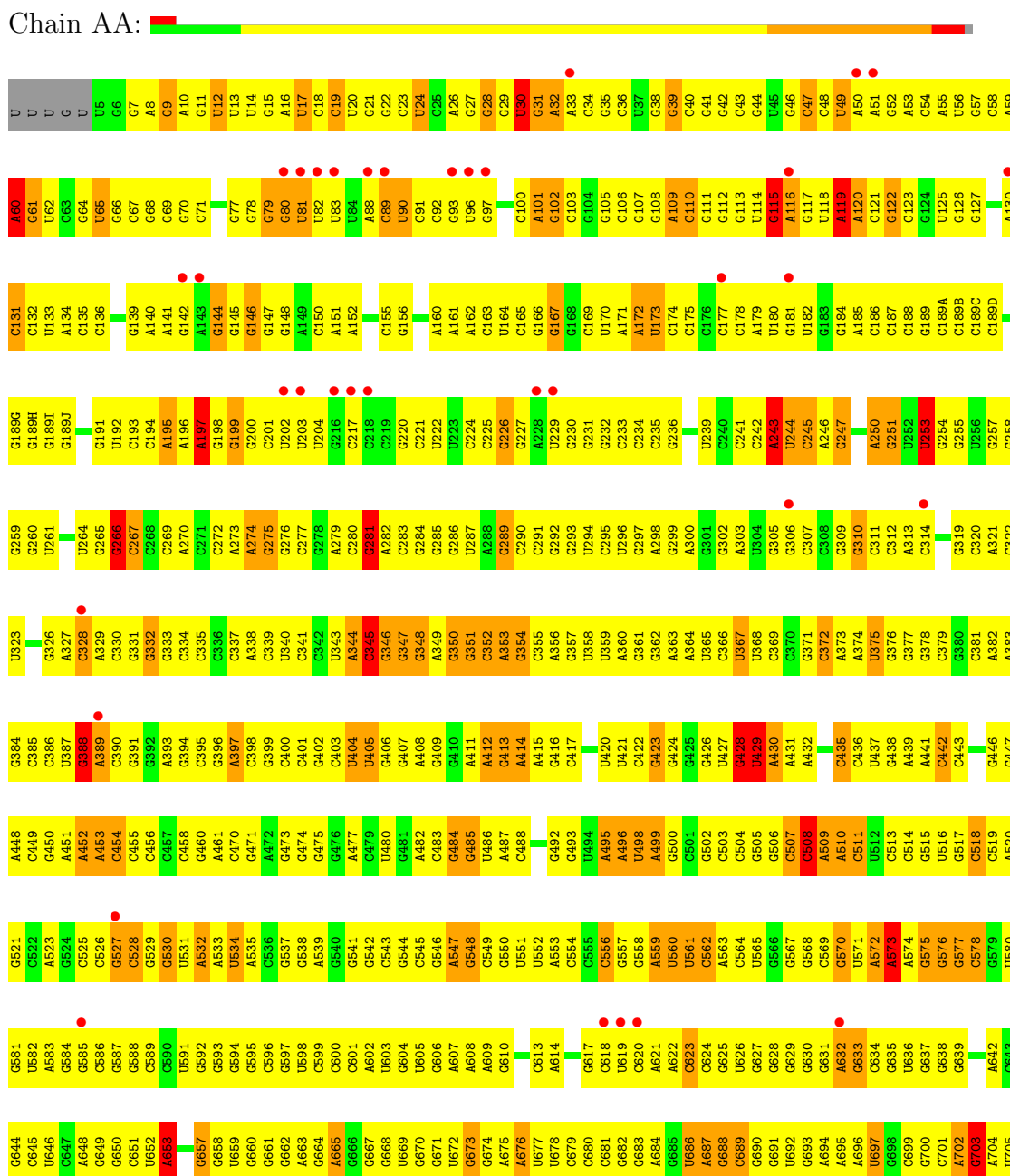


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
58	AY	1	32	11	5	13	3	0	0

3 Residue-property plots

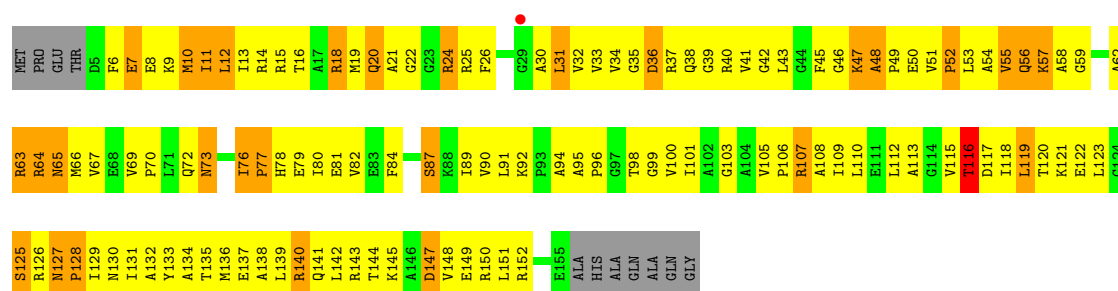
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



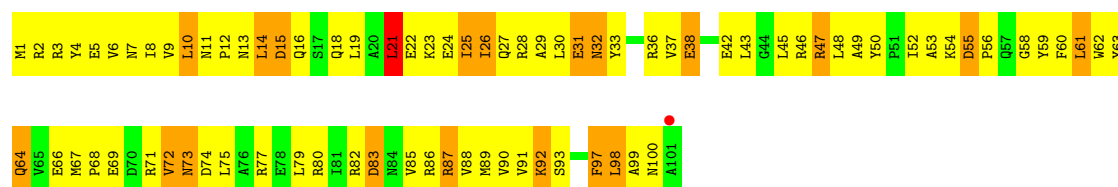
Chain AB:





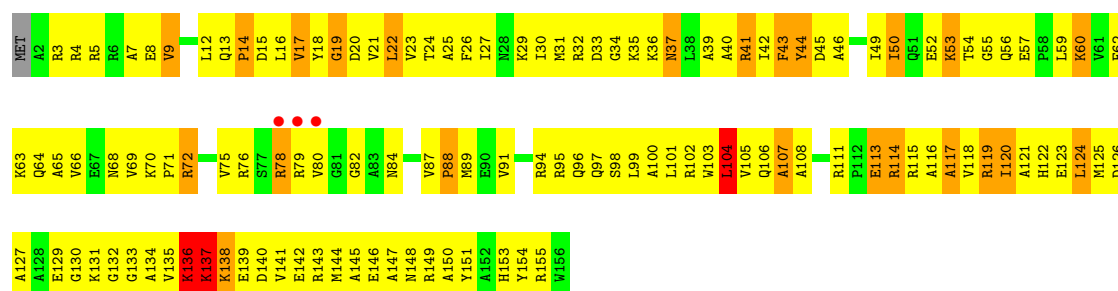
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



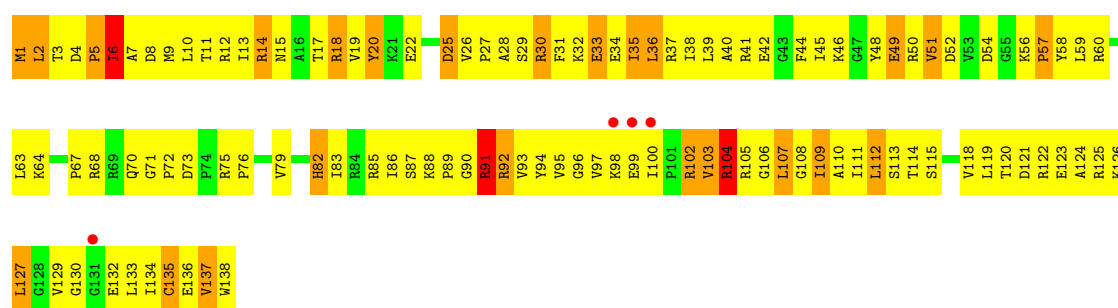
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

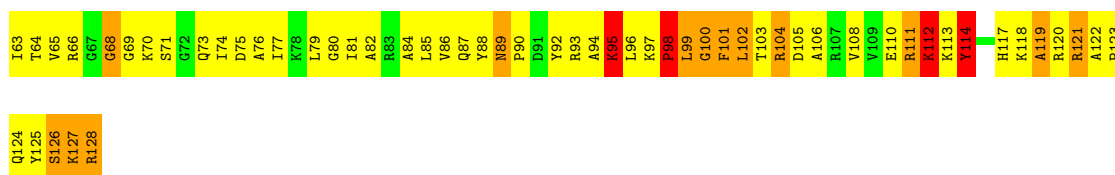
Chain AH:



• Molecule 9: 30S RIBOSOMAL PROTEIN S9

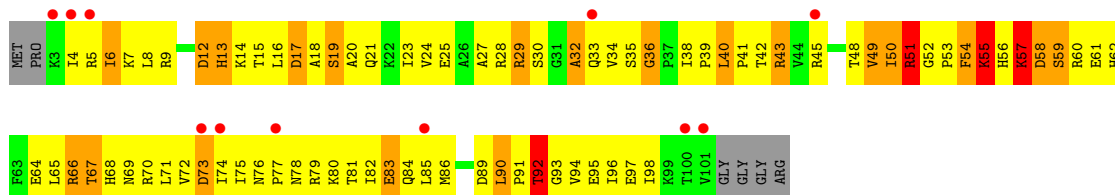
Chain AI:





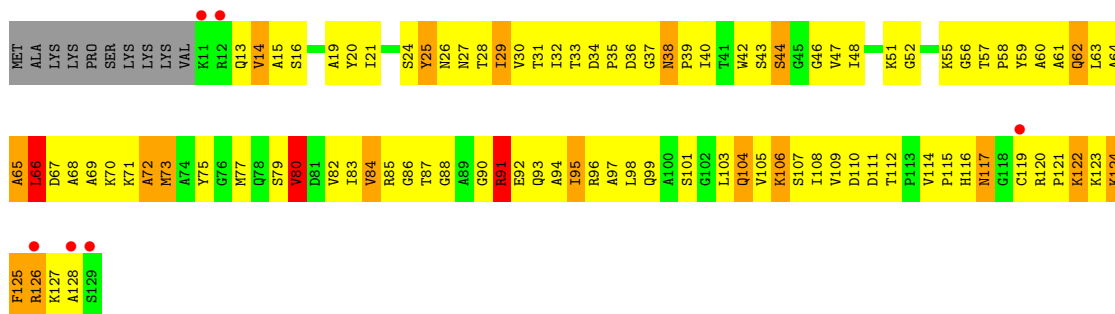
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



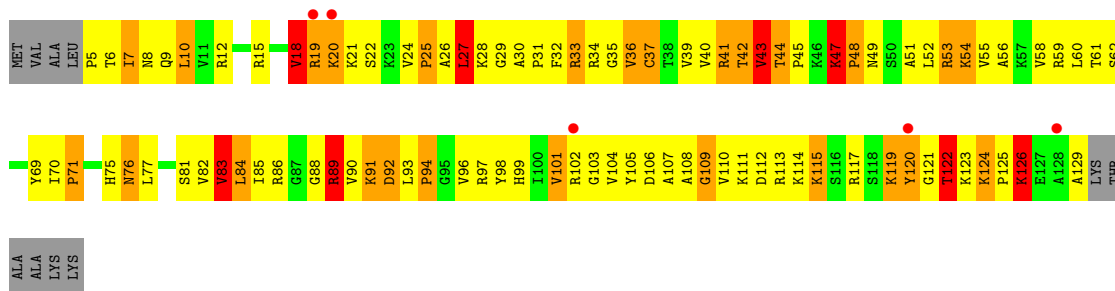
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



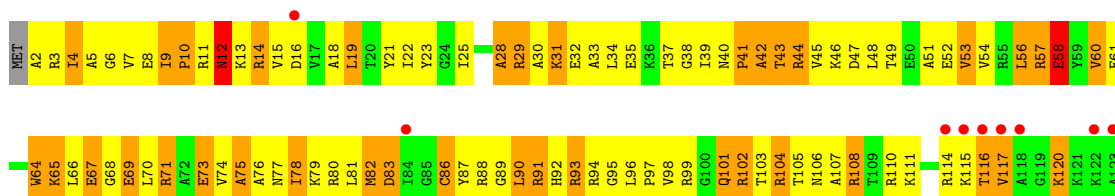
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:





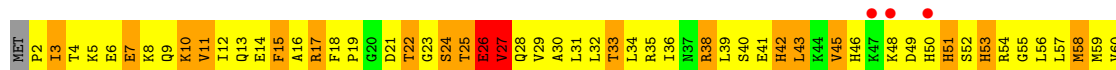
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



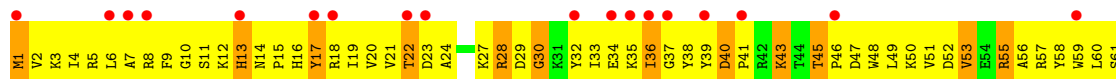
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



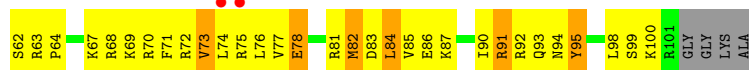
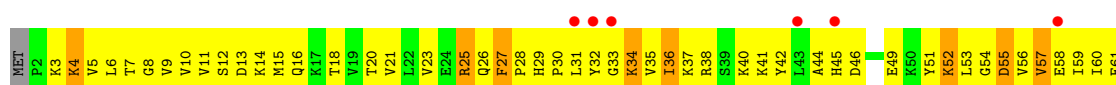
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

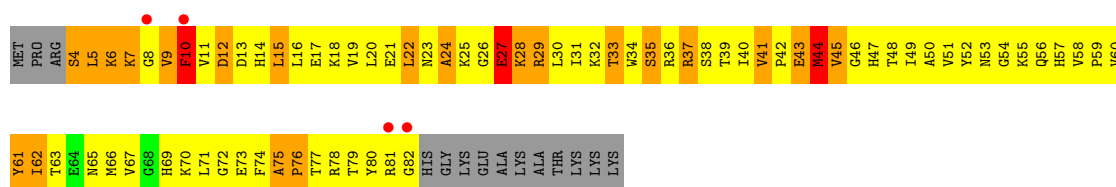
Chain AR:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

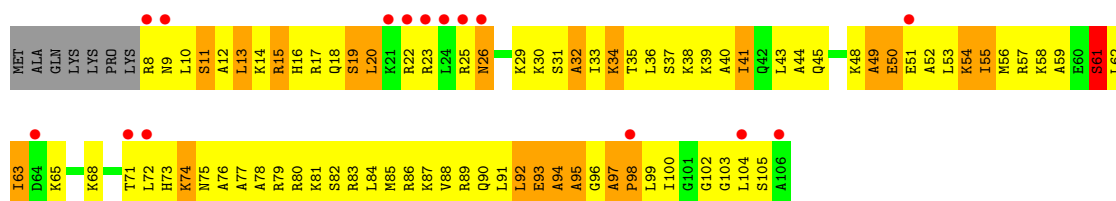
Chain AS:





• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain AT:



• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



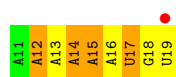
• Molecule 22: PE HYBRID STATE TRNA FMET

Chain AV:



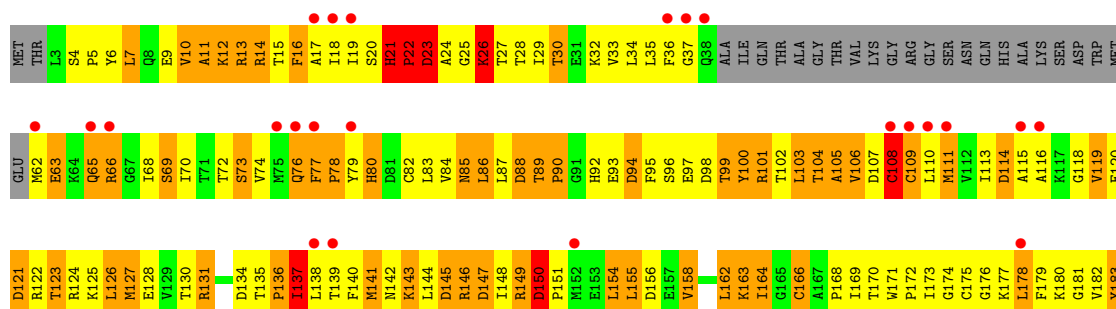
• Molecule 23: MRNA 5'-R(*AP*AP*AP*AP*AP*AP*UP*GP*UP)-3'

Chain AX:

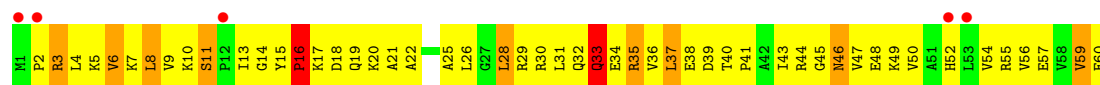


• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 3

Chain AY:

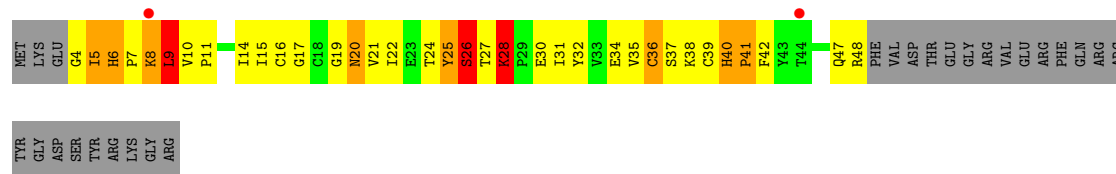


Chain B3:



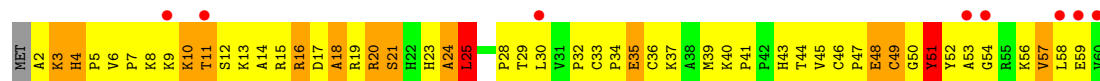
- Molecule 29: 50S RIBOSOMAL PROTEIN L31

Chain B4:



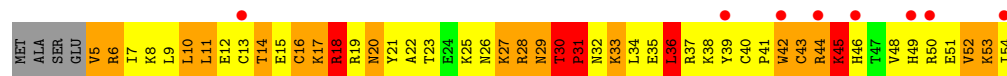
- Molecule 30: 50S RIBOSOMAL PROTEIN L32

Chain B5:



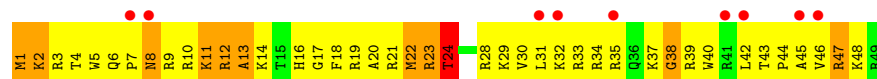
- Molecule 31: 50S RIBOSOMAL PROTEIN L33

Chain B6:



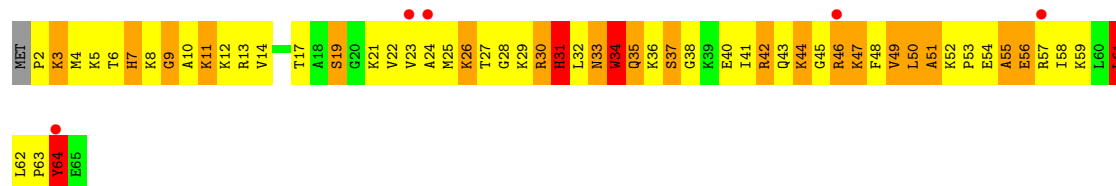
- Molecule 32: 50S RIBOSOMAL PROTEIN L34

Chain B7:



- Molecule 33: 50S RIBOSOMAL PROTEIN L35

Chain B8:



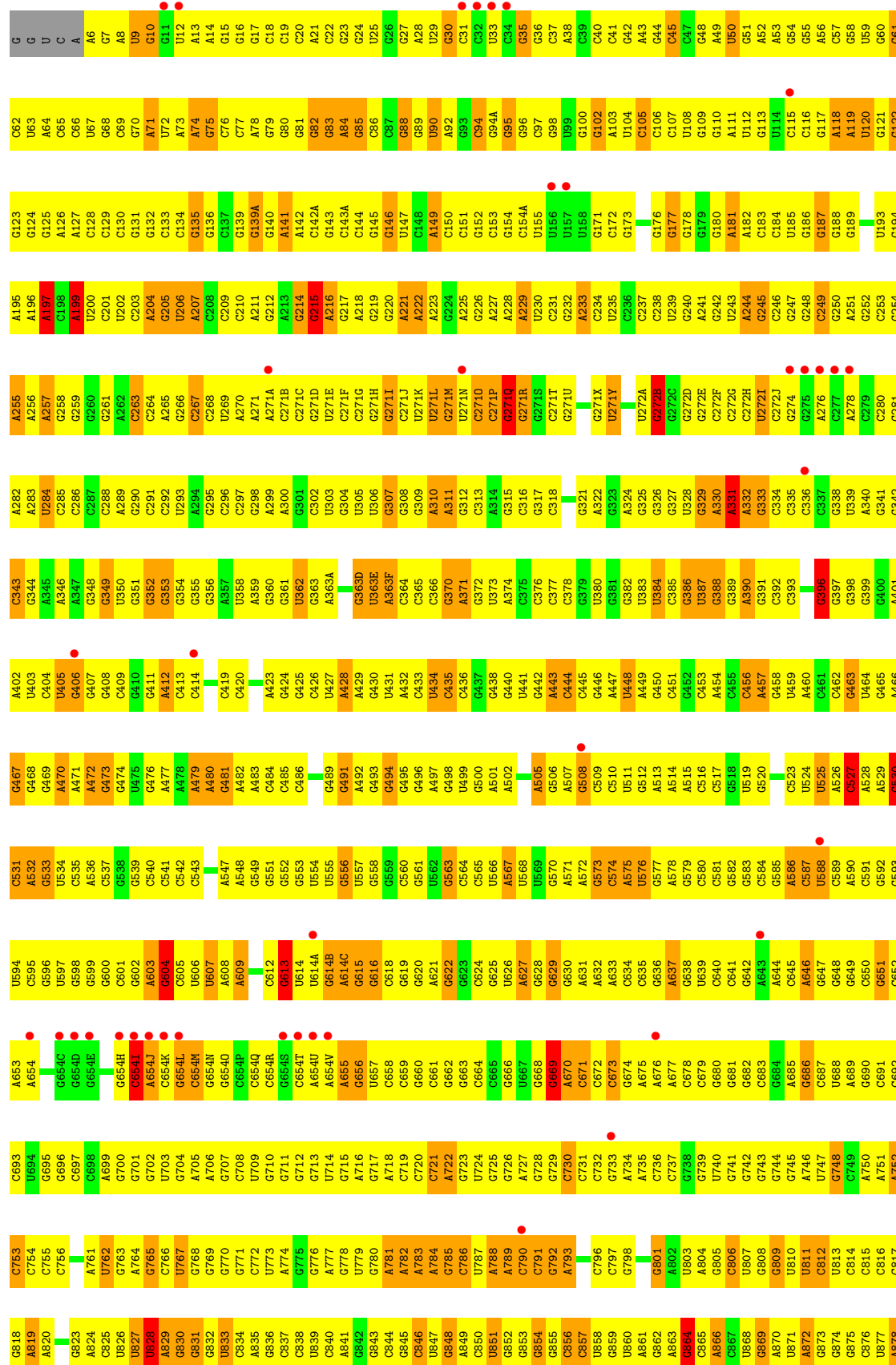
- Molecule 34: 50S RIBOSOMAL PROTEIN L36

Chain B9:



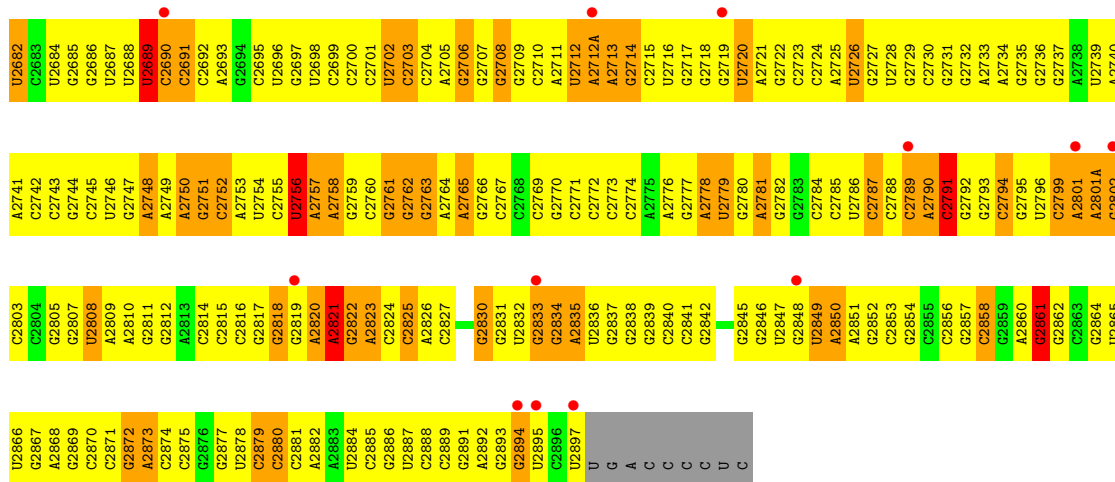
- Molecule 35: 23S RIBOSOMAL RNA

Chain BA:



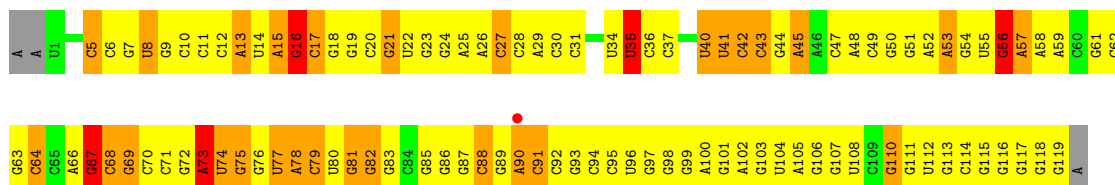


C2619	C2559	C2438	A2378	G2318	C2258	C2185	U2122	A2062	A2001	C1980	G1810	G1750
C2620	C2560	A2439	G2379	G2319	G2259	G2186	G2123	C2063	G2002	C1881	G1811	C1751
A2621	A2561	C2440	C2380	A2320	C2260	C2187	G2124	C2064	G2003	C1882	A1812	C1752
G2624	G2562	C2441	G2381	G2321	C2261	G2188	G2125	C2065	C2006	G1883	G1813	G1753
G2625	G2563	C2442	G2382	A2322	C2262	U2189	A2126	G2066	G2007	A1884	G1814	C1754
G2626	A2564	C2443	G2383	G2323	C2263	G2190	G2127	G2067	G2008	A1885	A1815	G1755
G2627	A2565	G2444	G2384	C2324	C2264	G2191	C2128	U2068	C2009	C1886	G1816	G1756
G2628	G2566	G2445	C2385	G2325	U2265	G2192	C2129	G2069	G2010	C1887	G1817	U1757
A2629	G2568	G2446	A2386	G2326	A2266	G2193	U2130	G2070	G1949	C1888	G1818	G1758
G2630	G2569	A2448	U2387	A2327	A2267	G2194	G2131	A2071	A1950	A1889	A1819	A1759
G2631	G2570	U2449	G2388	A2328	A2268	C2195	U2132	G2072	G2012	A1900	U1820	A1760
A2632	U2510	U2450	G2389	G2329	A2269	C2196	G2133	C2073	A2013	G1891	A1821	C1761
G2633	C2512	A2451	G2391	G2331	G2271	U2197	A2134	U2074	G2014	C1892	G1822	G1762
G2634	G2513	C2452	A2392	U2332	U2272	A2198		U2075	A2015	C1893	G1823	G1763
G2635	G2514	A2453	A2393	A2333	U2273	A2199	C2137	U2076	U2016	C1894	G1824	G1764
G2636	C2515	G2454	C2394	G2334	A2274	C2200	C2138	A2077	U2017	C1895	A1825	C1765
U2637	G2516	G2455	C2395	A2335	C2275	G2206	C2139	C2078	G2018	G1896	G1826	G1766
G2638	G2517	U2456	G2396	A2336	G2276	G2207	G2141	U2079	A2019	G1897	C1827	C1767
A2639	U2518	U2457	C2397	G2337	G2277	A2208	C2142	C2081	A2020	U1898	G1828	U1768
G2640	G2519	G2458	U2398	G2338	A2278	U2218		C2082	C2022	G1899	A1829	G1769
G2641	C2520	A2459	G2399	G2339	G2279	G2219	U2144	A2082	U2021	A1900	C1830	G1770
G2642	U2521	U2460	G2400	G2340	G2280	G2220	C2145	C2083	G2024	A1901	G1831	C1771
G2643	U2522	C2461	U2401	G2341	C2281	G2221	G2146	U2091	U1963	C1902	G1832	G1772
G2644	G2523	U2462	C2402	C2342	G2282	G2222	C2147	U2092	C2025	G1903	U1833	A1773
G2645	G2524	C2463	C2403	C2343	C2283	G2223	G2148	G2093	G2027	G1904	U1834	C1774
U2646	G2525	C2464	G2404	U2344	C2284	G2224		G2100	A1972	C1905	G1835	U1775
U2647	G2526	U2465	G2405	G2345	C2285	G2225	G2150	G2101	U2032	G1906	C1836	G1776
A2648	C2527	C2466	U2406	A2346	A2286	C2226	G2151	C2102	A2030	G1907	C1837	G1777
U2649	U2528	C2467	G2407	C2347	A2287	G2227	C2152	U2096	C2031	C1908	C1838	U1778
U2650	G2529	G2468	U2408	U2348	A2288	G2228	G2153	U2097	G1970	C1909	G1839	U1779
A2651	A2530	A2469	G2409	C2349	G2289	C2229	G2154	U2098	G2032	G1910	G1840	A1780
C2652	A2531	G2470	G2410	C2350	G2290	G2230	G2155	G2099	U2033	U1911	U1841	C1781
G2653	G2532	C2471	A2411	G2351	U2291	C2231	G2156	C2095	G2035	A1912	G1842	C1782
A2654	A2533	G2472	A2412	A2352	C2292	U2232	C2157	U2096	C2036	C1913	C1843	A1783
G2655	C2534	U2473	G2413	C2353	C2293	G2233	A2158	U2097	G2037	G1914	C1844	A1784
U2656	G2535	C2474	G2414	G2354	C2294	G2234	G2159	U2098	G2038	U1915	G1845	A1785
A2657	G2536	G2475	G2415	C2355	C2295	G2235	G2160	U2099	C2039	A1916	G1846	A1786
C2658	U2537	A2476	C2416	C2356	U2296	C2236		G2100	C2040	U1917	A1847	A1787
	C2538	C2477	C2417	U2357	C2297	G2237	C2161	G1980	C2041	A1918	A1848	C1788
G2661	C2539	A2478	A2418	G2358	A2298	G2238	G2162	U1981	U2041	A1789	A1849	A1789
A2662	G2540	G2479	U2419	C2359	G2299	C2239	C2163	A1982	C1920	C1790	G1850	C1790
G2663	A2541	C2480	G2420	A2360	G2300	C2240	C2164	C1983	G1921	U1951	C1852	G1792
A2665	G2542	G2481	A2421	G2362	C2301	A2241		G2105	C2044	C1922	A1853	C1793
G2666	G2543	G2482	A2422	C2363	G2302	G2242	G2167	G2106	G2045	C1924	A1854	U1794
C2667	G2544	C2483	U2423	C2364	G2303	U2243	A2169	A1986	C2046	C1925	G1855	C1795
G2668	G2545	G2484	C2424	G2365	G2304	U2244	A2170	G1987	U2047	U1926	G1856	U1796
	U2546		A2425	G2366	A2305	G2245	A2171	C1988	G2049	A1927	G1857	C1797
G2669	U2547	G2487	G2426	A2367	C2306	G2246	U2172	G1989	C2050	A1928	G1858	U1798
	G2548	A2488	C2427	G2367	G2307	A2247	A2173	C1990	G1929	A1929	A1859	G1799
U2672	G2549	G2489	G2428	C2368	G2308	C2248	C2174	U1991	G1930	C1800	G1860	C1800
G2673	C2550	G2490	A2429	A2369	U2309	U2249		G1992	U1931	G1801	G1861	G1801
A2674	U2551	U2491	A2430	G2370	A2310	G2250	C2177	U1993	C2053	A1802	G1862	A1802
A2675	U2552	U2492	U2431	G2371	G2311	G2251	G2178	C1994	G1933	A1803	G1863	A1803
G2676	G2553	U2493	A2432	G2372	U2312	G2252	C2179	U1995	G2056	C1804	U1864	C1804
A2677	U2554	G2494	A2433	G2373	G2313	G2253	U2180	G1996	G1935	U1805	G1865	U1805
G2678	U2555	G2495	A2434	C2374	C2314	C2254	G2181	G1997	A1936	C1806	C1866	C1806
A2679	G2556	C2496	A2435	C2375	G2315	G2255	G2182	G1998	A1937	U1807	G1878	U1807
C2680	G2557	G2497	G2436	A2376	C2316	G2256	C2183	C1999	A2060	G1879	G1879	A1809
C2681	C2558	C2498	U2437	A2377	C2317	U2257	G2184	G2000	G2061	U1939	C1879	



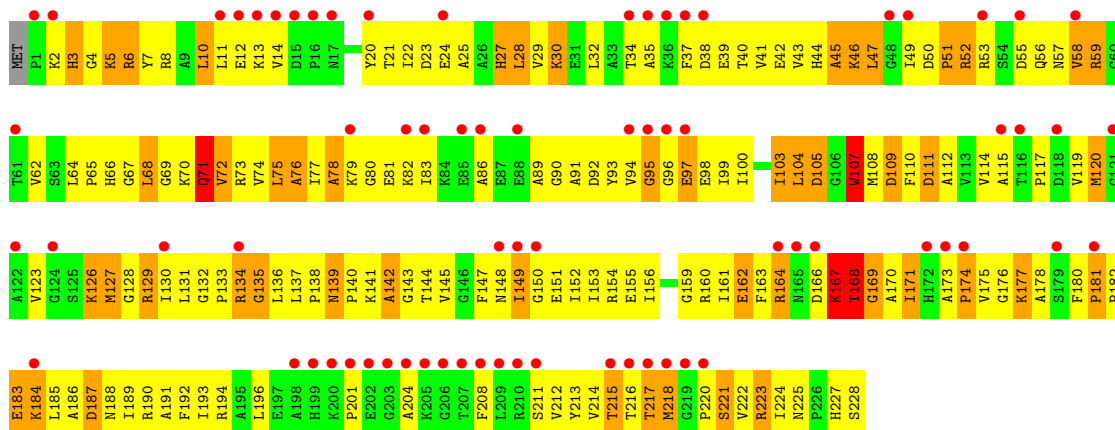
• Molecule 36: 5S RIBOSOMAL RNA

Chain BB:



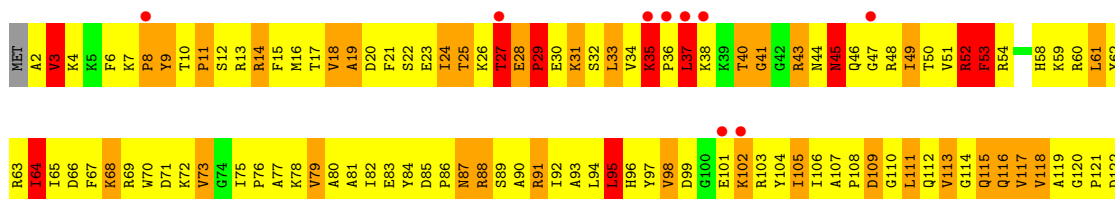
• Molecule 37: 50S RIBOSOMAL PROTEIN L1

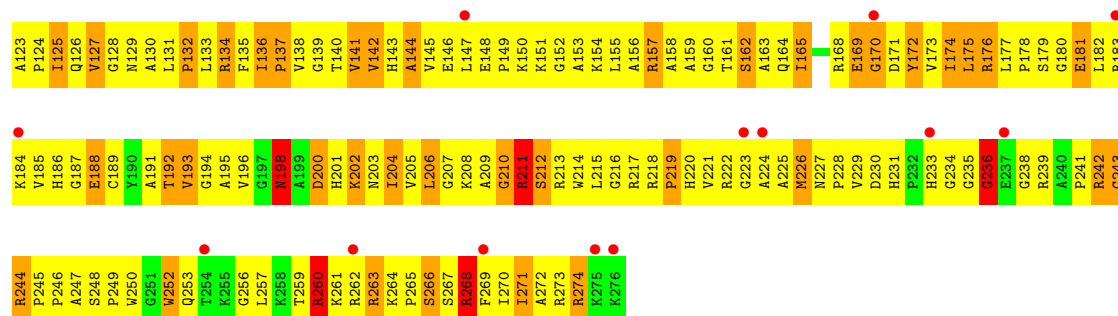
Chain BC:



• Molecule 38: 50S RIBOSOMAL PROTEIN L2

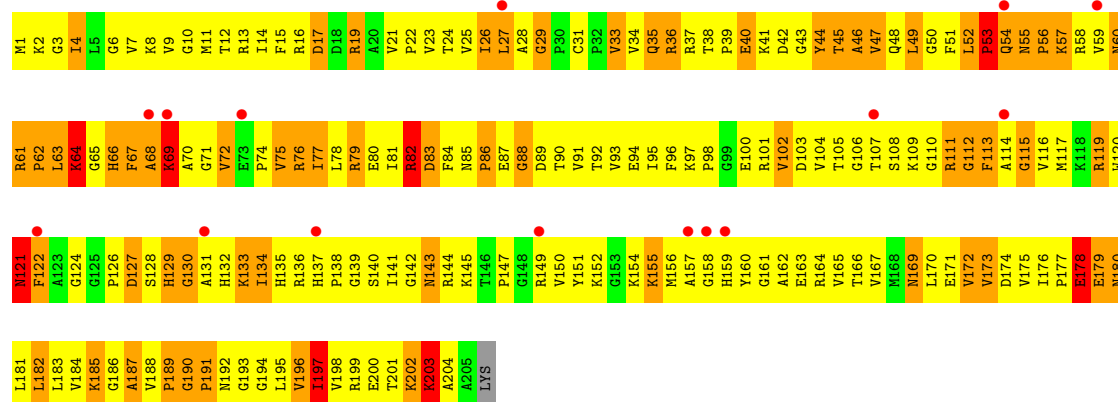
Chain BD:





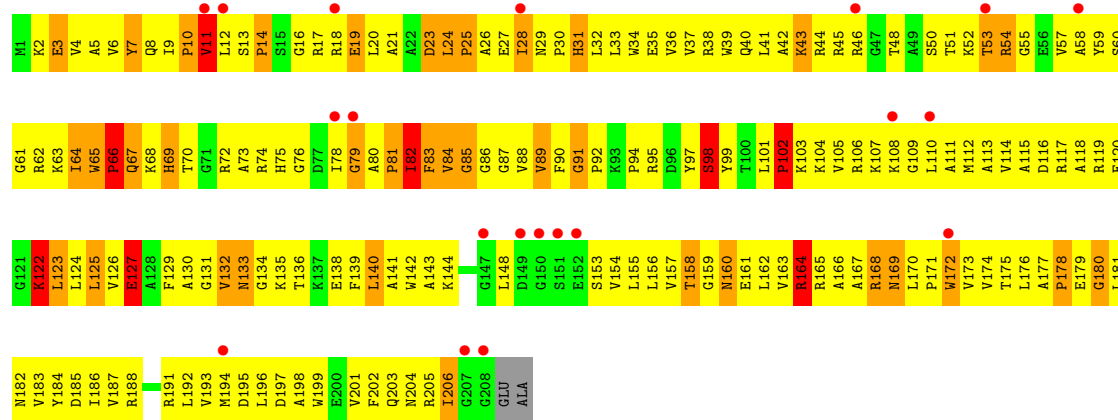
• Molecule 39: 50S RIBOSOMAL PROTEIN L3

Chain BE:



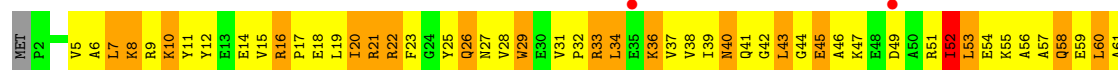
• Molecule 40: 50S RIBOSOMAL PROTEIN L4

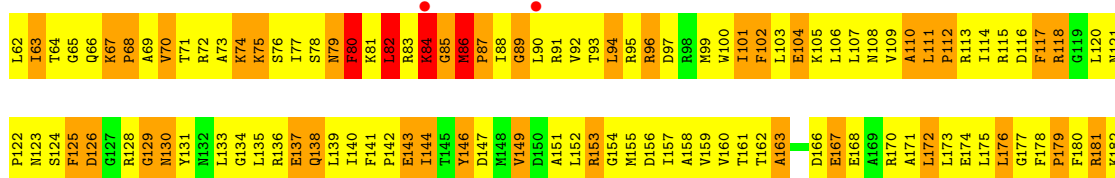
Chain BF:



• Molecule 41: 50S RIBOSOMAL PROTEIN L5

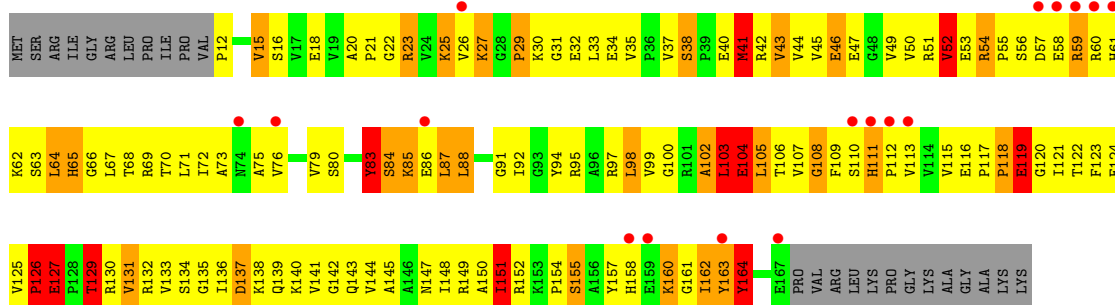
Chain BG:





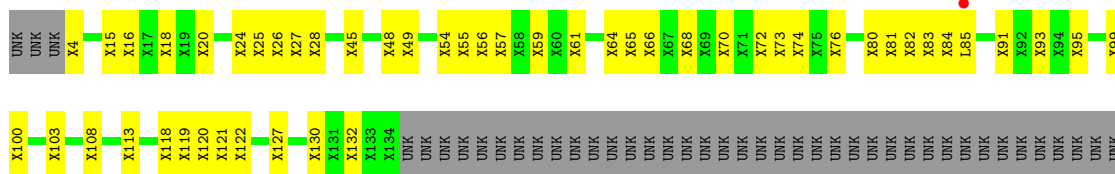
• Molecule 42: 50S RIBOSOMAL PROTEIN L6

Chain BH:



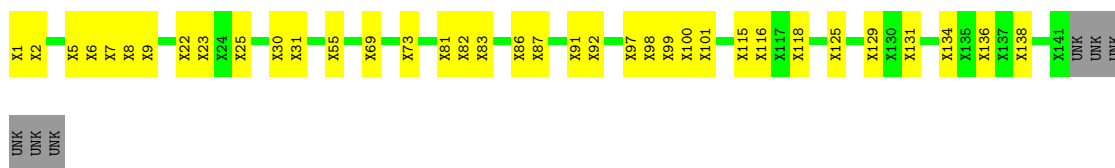
• Molecule 43: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



• Molecule 44: 50S RIBOSOMAL PROTEIN L11

Chain BK:



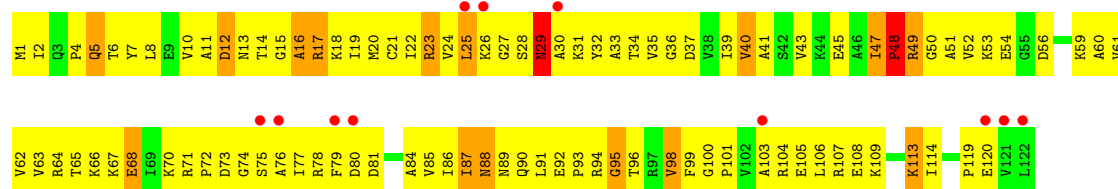
• Molecule 45: 50S RIBOSOMAL PROTEIN L13

Chain BN:



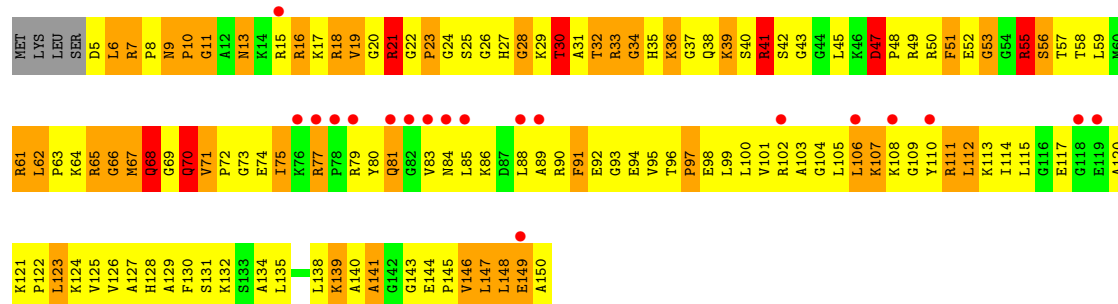
- Molecule 46: 50S RIBOSOMAL PROTEIN L14

Chain BO:



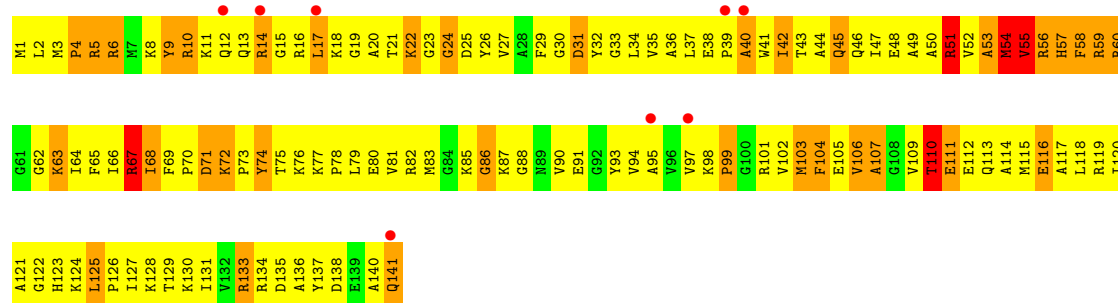
- Molecule 47: 50S RIBOSOMAL PROTEIN L15

Chain BP:



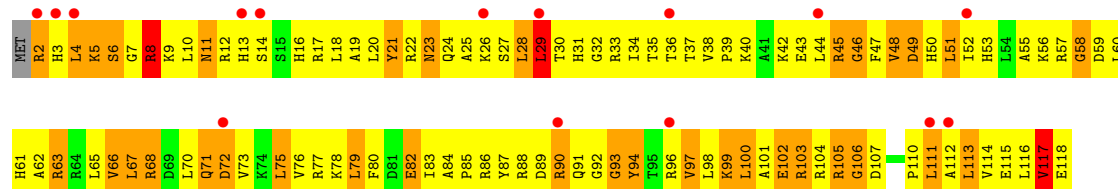
- Molecule 48: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



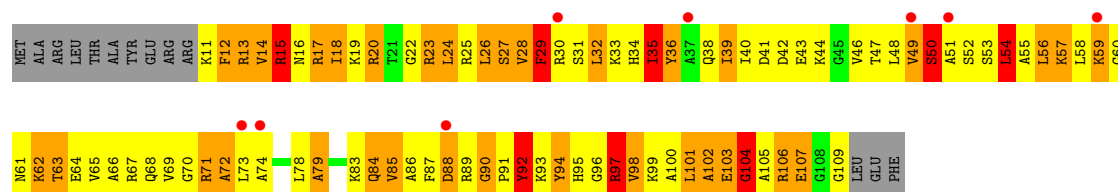
- Molecule 49: 50S RIBOSOMAL PROTEIN L17

Chain BR:



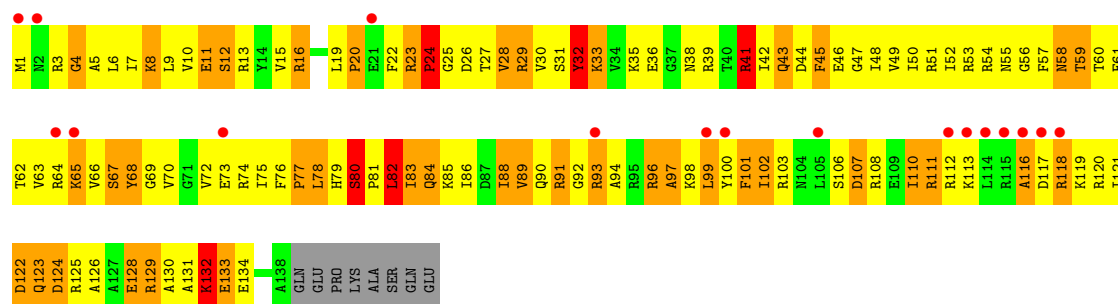
- Molecule 50: 50S RIBOSOMAL PROTEIN L18

Chain BS:



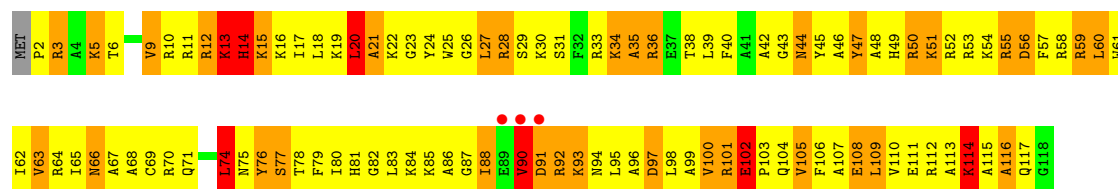
• Molecule 51: 50S RIBOSOMAL PROTEIN L19

Chain BT:



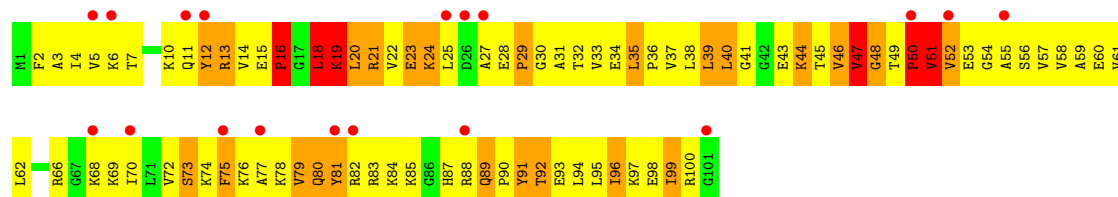
• Molecule 52: 50S RIBOSOMAL PROTEIN L20

Chain BU:



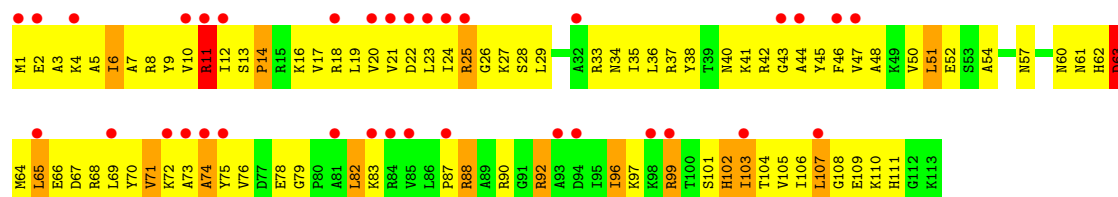
• Molecule 53: 50S RIBOSOMAL PROTEIN L21

Chain BV:



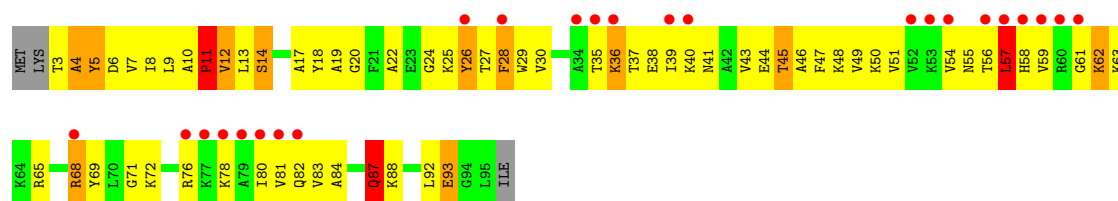
• Molecule 54: 50S RIBOSOMAL PROTEIN L22

Chain BW:



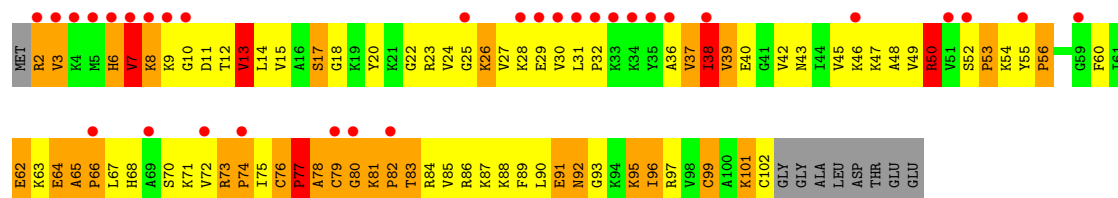
• Molecule 55: 50S RIBOSOMAL PROTEIN L23

Chain BX:



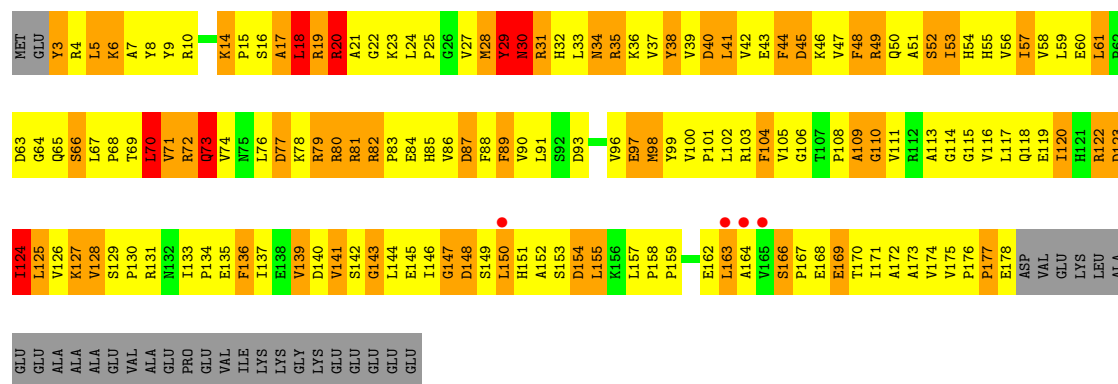
• Molecule 56: 50S RIBOSOMAL PROTEIN L24

Chain BY:



• Molecule 57: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	204.70Å 229.30Å 307.00Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	44.90 – 3.80 44.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.7 (44.90-3.80) 96.6 (44.91-3.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 3.57Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.293 , 0.351 0.287 , 0.338	Depositor DCC
R_{free} test set	6543 reflections (2.07%)	DCC
Wilson B-factor (Å ²)	110.2	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.16 , -3.9	EDS
Estimated twinning fraction	0.166 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	6 of 2273458 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	151017	wwPDB-VP
Average B, all atoms (Å ²)	147.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GCP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.79	12/36190 (0.0%)	0.89	56/56486 (0.1%)
2	AB	0.62	0/1936	0.96	1/2611 (0.0%)
3	AC	0.60	0/1637	0.93	3/2207 (0.1%)
4	AD	0.50	0/1733	0.86	2/2318 (0.1%)
5	AE	0.63	0/1163	0.94	1/1566 (0.1%)
6	AF	0.56	0/856	0.88	0/1154
7	AG	0.59	0/1276	0.85	0/1709
8	AH	0.56	0/1136	0.91	1/1527 (0.1%)
9	AI	0.56	0/1029	0.83	0/1378
10	AJ	0.59	0/808	0.88	0/1087
11	AK	0.57	0/900	0.89	0/1213
12	AL	0.59	0/987	1.01	2/1322 (0.2%)
13	AM	0.59	0/999	0.95	0/1338
14	AN	0.71	0/501	1.03	1/664 (0.2%)
15	AO	0.65	0/745	0.86	0/992
16	AP	0.53	0/717	0.88	0/965
17	AQ	0.61	0/837	0.92	1/1119 (0.1%)
18	AR	0.60	0/579	0.89	1/768 (0.1%)
19	AS	0.68	0/643	0.91	1/867 (0.1%)
20	AT	0.54	0/765	0.80	0/1007
21	AU	0.70	0/213	0.95	1/279 (0.4%)
22	AV	0.65	0/1832	0.82	0/2855
23	AX	0.66	0/216	0.77	0/335
24	AY	1.05	19/4005 (0.5%)	1.16	32/5407 (0.6%)
25	B0	0.61	0/671	0.98	2/892 (0.2%)
26	B1	0.49	0/739	0.85	0/983
27	B2	0.51	0/600	0.82	0/793
28	B3	0.57	0/473	0.93	0/636
29	B4	0.69	0/350	0.80	0/476
30	B5	0.64	0/473	0.89	0/639
31	B6	0.79	0/440	1.09	2/586 (0.3%)
32	B7	0.53	0/427	0.79	0/563

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	B8	0.68	0/516	0.92	0/681
34	B9	0.53	0/310	0.85	0/407
35	BA	0.76	16/69976 (0.0%)	0.86	82/109244 (0.1%)
36	BB	0.76	1/2853 (0.0%)	0.89	5/4451 (0.1%)
37	BC	0.81	4/1775 (0.2%)	0.94	4/2392 (0.2%)
38	BD	0.69	0/2195	1.07	9/2955 (0.3%)
39	BE	0.59	0/1597	0.95	1/2155 (0.0%)
40	BF	0.61	0/1659	0.88	0/2246
41	BG	0.58	0/1499	0.92	3/2016 (0.1%)
42	BH	0.66	0/1211	0.88	0/1636
43	BJ	0.53	0/7	0.70	0/8
45	BN	0.57	0/1132	0.91	1/1527 (0.1%)
46	BO	0.60	0/943	0.90	0/1269
47	BP	0.57	0/1131	1.08	6/1504 (0.4%)
48	BQ	0.63	0/1143	1.00	3/1527 (0.2%)
49	BR	0.49	0/974	0.92	1/1302 (0.1%)
50	BS	0.66	0/779	1.12	6/1038 (0.6%)
51	BT	0.60	0/1156	0.92	3/1544 (0.2%)
52	BU	0.63	0/975	0.91	1/1297 (0.1%)
53	BV	0.54	0/790	0.97	2/1057 (0.2%)
54	BW	0.59	0/907	0.82	0/1216
55	BX	0.63	0/740	0.83	1/995 (0.1%)
56	BY	0.61	0/789	0.90	0/1053
57	BZ	0.62	0/1435	0.95	0/1949
All	All	0.73	52/162368 (0.0%)	0.89	235/242211 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	3	125
9	AI	0	1
11	AK	0	1
17	AQ	0	1
21	AU	0	1
22	AV	0	5
24	AY	0	5
30	B5	0	1
35	BA	3	160
36	BB	0	12

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Mol	Chain	#Chirality outliers	#Planarity outliers
42	BH	0	1
45	BN	0	1
48	BQ	0	1
53	BV	0	1
All	All	6	316

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	191	TYR	CE2-CZ	11.85	1.53	1.38
24	AY	189	GLU	CG-CD	-10.57	1.36	1.51
24	AY	191	TYR	CD1-CE1	10.46	1.55	1.39
24	AY	504	ILE	C-N	-9.62	1.11	1.34
24	AY	444	LEU	C-N	-9.54	1.12	1.34

The worst 5 of 235 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AY	191	TYR	CB-CG-CD1	-18.01	110.19	121.00
24	AY	307	MET	CG-SD-CE	13.35	121.55	100.20
24	AY	319	ARG	NE-CZ-NH1	12.45	126.52	120.30
24	AY	504	ILE	C-N-CA	-12.18	91.26	121.70
1	AA	1498	U	C2'-C3'-O3'	11.78	135.42	109.50

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1049	U	C3'
1	AA	1399	C	C3'
1	AA	1498	U	C3'
35	BA	1300	U	C3'
35	BA	1799	G	C3'

5 of 316 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	19	C	Sidechain
1	AA	28	G	Sidechain
1	AA	96	U	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	2581	0
2	AB	1901	0	1951	513	1
3	AC	1613	0	1677	306	0
4	AD	1703	0	1767	335	0
5	AE	1147	0	1207	231	0
6	AF	843	0	857	144	0
7	AG	1257	0	1296	177	0
8	AH	1116	0	1177	205	0
9	AI	1011	0	1043	205	0
10	AJ	795	0	840	196	0
11	AK	885	0	904	152	0
12	AL	971	0	1057	217	0
13	AM	988	0	1059	192	0
14	AN	492	0	533	153	0
15	AO	734	0	771	229	0
16	AP	701	0	720	131	0
17	AQ	824	0	891	158	0
18	AR	574	0	644	122	0
19	AS	630	0	652	209	0
20	AT	763	0	861	150	0
21	AU	209	0	221	48	0
22	AV	1640	0	837	194	0
23	AX	192	0	99	22	0
24	AY	3934	0	3922	1256	0
25	B0	662	0	688	138	0
26	B1	732	0	808	131	0
27	B2	598	0	653	126	0
28	B3	468	0	523	108	0
29	B4	341	0	339	89	0
30	B5	459	0	480	131	0
31	B6	433	0	461	109	0
32	B7	419	0	467	110	0
33	B8	508	0	576	154	0
34	B9	307	0	338	70	0
35	BA	62477	0	31497	5291	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BB	2551	0	1295	230	0
37	BC	1742	0	1794	377	1
38	BD	2145	0	2234	780	0
39	BE	1564	0	1629	448	0
40	BF	1624	0	1677	415	0
41	BG	1474	0	1535	340	0
42	BH	1189	0	1247	282	0
43	BJ	654	0	157	36	0
44	BK	701	0	168	41	0
45	BN	1105	0	1180	270	0
46	BO	933	0	996	182	0
47	BP	1114	0	1187	361	0
48	BQ	1122	0	1179	291	0
49	BR	960	0	1021	236	0
50	BS	771	0	832	206	0
51	BT	1142	0	1202	332	0
52	BU	958	0	1015	317	0
53	BV	779	0	852	219	0
54	BW	896	0	953	173	0
55	BX	726	0	778	114	0
56	BY	776	0	870	193	0
57	BZ	1403	0	1432	371	0
58	AY	32	0	14	11	0
All	All	151017	0	103381	18980	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 75.

The worst 5 of 18980 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:AY:111:MET:CE	24:AY:139:THR:HG23	1.18	1.62
24:AY:331:LEU:CD2	24:AY:379:PHE:HD2	1.19	1.51
24:AY:331:LEU:HD22	24:AY:379:PHE:CD2	1.46	1.47
37:BC:127:MET:SD	37:BC:127:MET:CG	2.03	1.45
24:AY:135:THR:CG2	24:AY:136:PRO:HD2	1.44	1.45

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:AB:62:ALA:O	37:BC:30:LYS:O[2.656]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	110 (47%)	62 (27%)	61 (26%)	0	2
3	AC	205/239 (86%)	134 (65%)	39 (19%)	32 (16%)	0	8
4	AD	206/209 (99%)	131 (64%)	51 (25%)	24 (12%)	1	15
5	AE	149/162 (92%)	108 (72%)	31 (21%)	10 (7%)	2	36
6	AF	99/101 (98%)	67 (68%)	24 (24%)	8 (8%)	1	28
7	AG	153/156 (98%)	85 (56%)	44 (29%)	24 (16%)	0	8
8	AH	136/138 (99%)	94 (69%)	26 (19%)	16 (12%)	1	15
9	AI	125/128 (98%)	78 (62%)	28 (22%)	19 (15%)	0	8
10	AJ	97/105 (92%)	60 (62%)	23 (24%)	14 (14%)	0	10
11	AK	117/129 (91%)	72 (62%)	32 (27%)	13 (11%)	1	17
12	AL	123/135 (91%)	66 (54%)	33 (27%)	24 (20%)	0	4
13	AM	123/126 (98%)	63 (51%)	31 (25%)	29 (24%)	0	2
14	AN	58/61 (95%)	33 (57%)	12 (21%)	13 (22%)	0	2
15	AO	86/89 (97%)	59 (69%)	21 (24%)	6 (7%)	2	34
16	AP	82/88 (93%)	55 (67%)	17 (21%)	10 (12%)	1	14
17	AQ	98/105 (93%)	82 (84%)	10 (10%)	6 (6%)	2	38
18	AR	68/88 (77%)	37 (54%)	18 (26%)	13 (19%)	0	4
19	AS	77/93 (83%)	42 (54%)	18 (23%)	17 (22%)	0	3
20	AT	97/106 (92%)	46 (47%)	32 (33%)	19 (20%)	0	4
21	AU	23/27 (85%)	11 (48%)	8 (35%)	4 (17%)	0	6
24	AY	488/529 (92%)	314 (64%)	88 (18%)	86 (18%)	0	6
25	B0	82/85 (96%)	64 (78%)	9 (11%)	9 (11%)	1	17
26	B1	92/98 (94%)	63 (68%)	16 (17%)	13 (14%)	0	10
27	B2	69/72 (96%)	38 (55%)	22 (32%)	9 (13%)	0	13
28	B3	58/60 (97%)	38 (66%)	15 (26%)	5 (9%)	1	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	B4	43/71 (61%)	26 (60%)	9 (21%)	8 (19%)	0	5
30	B5	57/60 (95%)	34 (60%)	11 (19%)	12 (21%)	0	3
31	B6	48/54 (89%)	18 (38%)	16 (33%)	14 (29%)	0	1
32	B7	47/49 (96%)	29 (62%)	10 (21%)	8 (17%)	0	6
33	B8	62/65 (95%)	30 (48%)	16 (26%)	16 (26%)	0	2
34	B9	35/37 (95%)	19 (54%)	10 (29%)	6 (17%)	0	6
37	BC	226/229 (99%)	158 (70%)	39 (17%)	29 (13%)	0	13
38	BD	273/276 (99%)	195 (71%)	46 (17%)	32 (12%)	1	15
39	BE	203/206 (98%)	99 (49%)	48 (24%)	56 (28%)	0	1
40	BF	206/210 (98%)	134 (65%)	35 (17%)	37 (18%)	0	5
41	BG	179/182 (98%)	95 (53%)	47 (26%)	37 (21%)	0	4
42	BH	154/180 (86%)	111 (72%)	23 (15%)	20 (13%)	0	13
43	BJ	1/173 (1%)	1 (100%)	0	0	100	100
45	BN	137/140 (98%)	78 (57%)	28 (20%)	31 (23%)	0	2
46	BO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	1	18
47	BP	144/150 (96%)	70 (49%)	37 (26%)	37 (26%)	0	2
48	BQ	139/141 (99%)	79 (57%)	40 (29%)	20 (14%)	0	10
49	BR	115/118 (98%)	69 (60%)	27 (24%)	19 (16%)	0	7
50	BS	97/112 (87%)	41 (42%)	23 (24%)	33 (34%)	0	0
51	BT	136/146 (93%)	75 (55%)	31 (23%)	30 (22%)	0	3
52	BU	115/118 (98%)	59 (51%)	27 (24%)	29 (25%)	0	2
53	BV	99/101 (98%)	56 (57%)	21 (21%)	22 (22%)	0	3
54	BW	111/113 (98%)	72 (65%)	25 (22%)	14 (13%)	0	14
55	BX	91/96 (95%)	55 (60%)	27 (30%)	9 (10%)	1	21
56	BY	99/110 (90%)	33 (33%)	36 (36%)	30 (30%)	0	1
57	BZ	174/206 (84%)	88 (51%)	48 (28%)	38 (22%)	0	3
All	All	6255/6850 (91%)	3758 (60%)	1413 (23%)	1084 (17%)	0	6

5 of 1084 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL

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Mol	Chain	Res	Type
2	AB	18	GLY
2	AB	19	HIS
2	AB	24	TRP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	152 (75%)	50 (25%)	1	8
3	AC	160/188 (85%)	133 (83%)	27 (17%)	3	24
4	AD	180/181 (99%)	154 (86%)	26 (14%)	5	32
5	AE	115/123 (94%)	94 (82%)	21 (18%)	2	18
6	AF	90/90 (100%)	76 (84%)	14 (16%)	4	28
7	AG	126/127 (99%)	114 (90%)	12 (10%)	12	55
8	AH	119/119 (100%)	101 (85%)	18 (15%)	4	30
9	AI	98/99 (99%)	82 (84%)	16 (16%)	3	26
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	2	16
11	AK	90/99 (91%)	73 (81%)	17 (19%)	2	17
12	AL	104/111 (94%)	86 (83%)	18 (17%)	3	22
13	AM	99/101 (98%)	79 (80%)	20 (20%)	2	14
14	AN	49/50 (98%)	36 (74%)	13 (26%)	1	7
15	AO	79/80 (99%)	52 (66%)	27 (34%)	0	3
16	AP	72/74 (97%)	64 (89%)	8 (11%)	9	47
17	AQ	94/97 (97%)	85 (90%)	9 (10%)	12	55
18	AR	61/77 (79%)	54 (88%)	7 (12%)	8	44
19	AS	69/80 (86%)	58 (84%)	11 (16%)	4	28
20	AT	76/82 (93%)	69 (91%)	7 (9%)	13	57
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	50
24	AY	427/453 (94%)	308 (72%)	119 (28%)	0	6
25	B0	66/67 (98%)	49 (74%)	17 (26%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	B1	78/83 (94%)	65 (83%)	13 (17%)	3	24
27	B2	66/67 (98%)	61 (92%)	5 (8%)	19	67
28	B3	51/52 (98%)	42 (82%)	9 (18%)	3	21
29	B4	39/63 (62%)	29 (74%)	10 (26%)	1	8
30	B5	51/52 (98%)	47 (92%)	4 (8%)	18	65
31	B6	49/52 (94%)	37 (76%)	12 (24%)	1	8
32	B7	41/42 (98%)	36 (88%)	5 (12%)	7	42
33	B8	53/55 (96%)	42 (79%)	11 (21%)	2	13
34	B9	34/34 (100%)	26 (76%)	8 (24%)	1	9
37	BC	180/181 (99%)	150 (83%)	30 (17%)	3	24
38	BD	217/218 (100%)	150 (69%)	67 (31%)	0	5
39	BE	165/166 (99%)	134 (81%)	31 (19%)	2	17
40	BF	165/166 (99%)	142 (86%)	23 (14%)	5	35
41	BG	155/156 (99%)	127 (82%)	28 (18%)	2	19
42	BH	128/148 (86%)	90 (70%)	38 (30%)	0	5
43	BJ	1/1 (100%)	1 (100%)	0	100	100
45	BN	117/119 (98%)	99 (85%)	18 (15%)	4	29
46	BO	100/100 (100%)	89 (89%)	11 (11%)	9	48
47	BP	112/116 (97%)	91 (81%)	21 (19%)	2	17
48	BQ	111/111 (100%)	87 (78%)	24 (22%)	1	12
49	BR	100/101 (99%)	78 (78%)	22 (22%)	1	11
50	BS	77/88 (88%)	60 (78%)	17 (22%)	1	11
51	BT	120/127 (94%)	96 (80%)	24 (20%)	2	15
52	BU	92/94 (98%)	74 (80%)	18 (20%)	2	15
53	BV	82/82 (100%)	65 (79%)	17 (21%)	2	13
54	BW	91/92 (99%)	81 (89%)	10 (11%)	9	48
55	BX	74/78 (95%)	63 (85%)	11 (15%)	4	31
56	BY	84/91 (92%)	69 (82%)	15 (18%)	2	20
57	BZ	155/179 (87%)	117 (76%)	38 (24%)	1	8
All	All	5271/5546 (95%)	4255 (81%)	1016 (19%)	2	16

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

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

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

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

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	273 (18%)	58 (3%)
22	AV	76/77 (98%)	36 (47%)	3 (3%)
23	AX	8/9 (88%)	5 (62%)	0
35	BA	2900/2915 (99%)	654 (22%)	73 (2%)
36	BB	118/122 (96%)	24 (20%)	1 (0%)
All	All	4605/4645 (99%)	992 (21%)	135 (2%)

5 of 992 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 135 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	BA	50	U
35	BA	603	A
35	BA	2282	G
35	BA	71	A

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Mol	Chain	Res	Type
35	BA	331	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	GCP	AY	1000	-	34,34,34	3.69	11 (32%)	52,54,54	4.66	10 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	GCP	AY	1000	-	-	0/20/38/38	0/3/3/3

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PG-C3B	13.87	1.93	1.79
58	AY	1000	GCP	C6-N1	7.62	1.47	1.36
58	AY	1000	GCP	C2-N3	6.74	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AY	1000	GCP	PB-C3B	6.31	1.85	1.79
58	AY	1000	GCP	PB-O3A	5.67	1.64	1.58

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AY	1000	GCP	C6-C5-N7	-32.00	129.83	134.14
58	AY	1000	GCP	C6-N1-C2	5.43	123.27	120.20
58	AY	1000	GCP	O3G-PG-O1G	-2.71	105.32	112.49
58	AY	1000	GCP	C8-N9-C1'	2.63	131.11	126.15
58	AY	1000	GCP	PA-O3A-PB	-2.42	124.74	132.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	-0.08	39 (2%) 53 35	52, 140, 199, 200	0
2	AB	235/256 (91%)	-0.13	2 (0%) 81 62	40, 110, 177, 200	0
3	AC	207/239 (86%)	-0.18	2 (0%) 79 59	37, 117, 174, 200	0
4	AD	208/209 (99%)	0.37	7 (3%) 43 29	48, 158, 200, 200	0
5	AE	151/162 (93%)	0.09	1 (0%) 84 67	38, 112, 171, 200	0
6	AF	101/101 (100%)	-0.21	1 (0%) 79 59	59, 135, 188, 200	0
7	AG	155/156 (99%)	-0.03	3 (1%) 64 42	46, 128, 189, 200	0
8	AH	138/138 (100%)	0.13	4 (2%) 49 32	36, 114, 180, 200	0
9	AI	127/128 (99%)	0.25	1 (0%) 83 64	32, 121, 172, 200	0
10	AJ	99/105 (94%)	0.62	11 (11%) 6 7	32, 125, 191, 200	0
11	AK	119/129 (92%)	0.20	6 (5%) 28 19	40, 116, 179, 200	0
12	AL	125/135 (92%)	0.39	5 (4%) 36 25	45, 119, 192, 200	0
13	AM	125/126 (99%)	0.54	12 (9%) 8 8	64, 127, 200, 200	0
14	AN	60/61 (98%)	0.07	0 100 100	28, 104, 172, 200	0
15	AO	88/89 (98%)	0.32	5 (5%) 23 16	59, 130, 188, 200	0
16	AP	84/88 (95%)	1.36	21 (25%) 1 2	79, 156, 200, 200	0
17	AQ	100/105 (95%)	0.80	8 (8%) 12 11	66, 141, 200, 200	0
18	AR	70/88 (79%)	0.31	2 (2%) 49 32	59, 124, 176, 200	0
19	AS	79/93 (84%)	0.34	4 (5%) 27 19	57, 118, 197, 200	0
20	AT	99/106 (93%)	0.75	15 (15%) 3 4	87, 153, 200, 200	0
21	AU	25/27 (92%)	0.98	4 (16%) 3 4	46, 117, 175, 185	0
22	AV	77/77 (100%)	-0.62	1 (1%) 74 52	77, 151, 189, 199	0
23	AX	9/9 (100%)	0.51	1 (11%) 6 7	79, 156, 192, 199	0
24	AY	496/529 (93%)	0.52	46 (9%) 9 9	71, 170, 202, 202	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
25	B0	84/85 (98%)	1.10	13 (15%)	3 4	37, 118, 194, 200	0
26	B1	94/98 (95%)	0.84	11 (11%)	5 6	65, 143, 197, 200	0
27	B2	71/72 (98%)	0.24	4 (5%)	24 17	101, 153, 200, 200	0
28	B3	60/60 (100%)	0.75	5 (8%)	11 10	54, 126, 198, 200	0
29	B4	45/71 (63%)	0.15	2 (4%)	33 23	108, 174, 200, 200	0
30	B5	59/60 (98%)	0.54	8 (13%)	4 4	62, 150, 200, 200	0
31	B6	50/54 (92%)	0.86	8 (16%)	3 4	62, 139, 186, 200	0
32	B7	49/49 (100%)	0.99	9 (18%)	2 3	78, 153, 197, 200	0
33	B8	64/65 (98%)	0.57	5 (7%)	13 11	66, 129, 179, 200	0
34	B9	37/37 (100%)	1.61	10 (27%)	1 2	71, 142, 178, 194	0
35	BA	2901/2915 (99%)	0.14	116 (3%)	36 25	51, 159, 201, 202	0
36	BB	119/122 (97%)	-0.30	1 (0%)	83 64	66, 123, 172, 190	0
37	BC	228/229 (99%)	1.73	72 (31%)	1 2	87, 182, 200, 200	0
38	BD	275/276 (99%)	0.44	22 (8%)	12 11	40, 117, 175, 200	0
39	BE	205/206 (99%)	0.40	15 (7%)	15 12	51, 143, 199, 200	0
40	BF	208/210 (99%)	0.59	20 (9%)	8 8	51, 156, 200, 200	0
41	BG	181/182 (99%)	0.12	4 (2%)	59 39	47, 134, 194, 200	0
42	BH	156/180 (86%)	0.59	17 (10%)	6 7	78, 165, 200, 200	0
43	BJ	1/173 (0%)	3.21	1 (100%)	0 0	174, 174, 174, 174	0
44	BK	0/147	-	-	-	-	-
45	BN	139/140 (99%)	0.42	5 (3%)	41 28	69, 131, 190, 200	0
46	BO	122/122 (100%)	0.66	11 (9%)	10 9	59, 133, 198, 200	0
47	BP	146/150 (97%)	0.71	19 (13%)	4 5	65, 147, 200, 200	0
48	BQ	141/141 (100%)	0.26	8 (5%)	23 16	20, 107, 171, 200	0
49	BR	117/118 (99%)	1.01	15 (12%)	4 5	81, 169, 200, 200	0
50	BS	99/112 (88%)	0.30	8 (8%)	12 11	49, 123, 194, 200	0
51	BT	138/146 (94%)	0.63	17 (12%)	5 5	89, 162, 200, 200	0
52	BU	117/118 (99%)	0.30	3 (2%)	53 35	47, 121, 179, 200	0
53	BV	101/101 (100%)	0.91	18 (17%)	2 3	42, 146, 200, 200	0
54	BW	113/113 (100%)	1.47	35 (30%)	1 2	78, 165, 200, 200	0
55	BX	93/96 (96%)	1.23	24 (25%)	1 2	38, 167, 200, 200	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
56	BY	101/110 (91%)	1.64	32 (31%) 1 2	86, 169, 200, 200	0
57	BZ	176/206 (85%)	0.05	4 (2%) 57 38	43, 122, 195, 200	0
All	All	10971/11642 (94%)	0.32	743 (6%) 17 13	20, 146, 200, 202	0

The worst 5 of 743 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	AM	126	LYS	13.2
35	BA	654(K)	C	11.7
37	BC	173	ALA	9.5
37	BC	216	THR	9.3
37	BC	36	LYS	8.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	GCP	AY	1000	32/32	0.24	-	95,109,121,122	0

6.5 Other polymers ⓘ

There are no such residues in this entry.