



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 07:13 PM UTC

PDB ID : 2QA4 / pdb\_00002qa4  
Title : A more complete structure of the the L7/L12 stalk of the Haloarcula marismortui 50S large ribosomal subunit  
Authors : Steitz, T.A.; Kavran, J.M.  
Deposited on : 2007-06-14  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

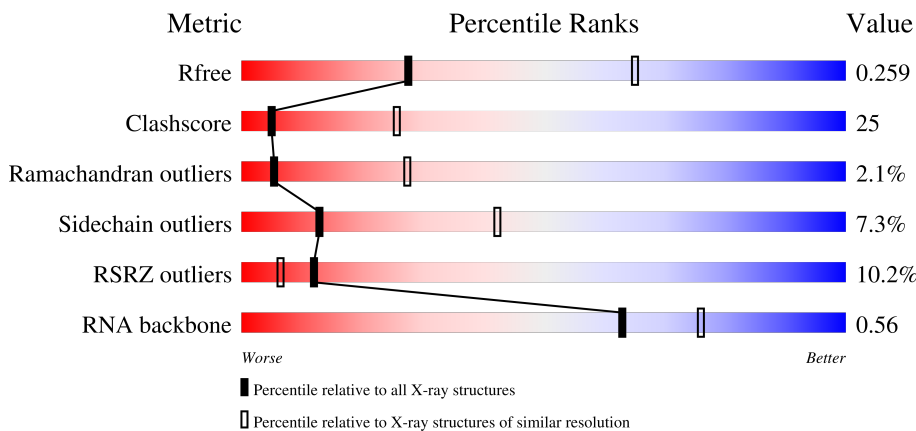
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	A	240	
4	B	338	

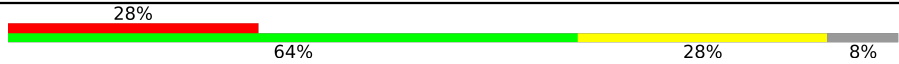

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	171	
11	I	162	
12	J	145	
13	K	132	
14	L	165	
15	M	196	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	67	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	92	
29	1	57	

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Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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
32	MG	0	2946	-	-	-	X
32	MG	0	2971	-	-	-	X
32	MG	0	2998	-	-	-	X
32	MG	0	3014	-	-	-	X
32	MG	0	3022	-	-	-	X
32	MG	0	3026	-	-	-	X
32	MG	0	3029	-	-	-	X
34	NA	0	3050	-	-	-	X
34	NA	0	3057	-	-	-	X
34	NA	0	3075	-	-	-	X
34	NA	0	3093	-	-	-	X
34	NA	0	3103	-	-	-	X
35	CL	0	3109	-	-	-	X
35	CL	3	95	-	-	X	-
35	CL	J	147	-	-	X	-
35	CL	J	149	-	-	X	-
35	CL	O	117	-	-	-	X

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 92248 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 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	0	2753	58979	26332	10869	19036	2742	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779

- Molecule 2 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	9	122	2600	1160	472	847	121	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	237	1753	1072	352	324	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	337	2625	1616	493	511	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	246	1859	1131	344	383	1	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	73	LEU	GLN	conflict	UNP P12735

- Molecule 6 is a protein called 50S ribosomal protein L5P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	140	1094	685	195	210	4	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	E	172	1357	840	224	289	4	0	0	0

- Molecule 8 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	F	119	890	551	141	197	1	0	0	0

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	G	125	959	592	162	203	2	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	248	ASP	ALA	conflict	UNP P15825

- Molecule 10 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	H	160	1266	785	237	238	6	0	0	0

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ASP	-	insertion	UNP P60617
H	165	SER	LYS	conflict	UNP P60617
H	166	SER	VAL	conflict	UNP P60617
H	167	PRO	GLU	conflict	UNP P60617
H	168	ALA	ARG	conflict	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	GLU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	?	-	LEU	deletion	UNP P60617
H	170	ASN	ILE	conflict	UNP P60617

- Molecule 11 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	I	118	876	548	135	192	1	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L13P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	J	142	1120	696	199	222	3	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	K	132	992	609	187	192	4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	conflict	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	L	145	1118	670	222	226	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	M	194	1559	943	332	283	1	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	UNP P60618
M	194	ALA	GLY	conflict	UNP P60618

- Molecule 16 is a protein called 50S ribosomal protein L18P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	N	186	1445	895	262	286	2	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
17	O	115	865	529	161	175	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	P	143	1136	683	229	224	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
19	Q	95	735	450	141	144	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	R	150	1149	713	209	223	4	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	S	81	641	389	111	138	3	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L24P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	T	119	950	568	180	202		0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
23	U	53	410	244	75	86	5	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	V	65	499	304	94	100	1	0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	W	154	1196	737	209	244	6	0	0	0

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L31E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	X	82	654	402	129	122	1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	Y	142	1130	686	228	216		0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	Z	73	578	346	116	111	5	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	UNP P60619

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	1	56	431	258	86	83	4	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	2	46	396	239	89	67	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	3	92	755	458	153	137	7	0	0	0

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	108	Total	Mg	0	0
			108	108		
32	9	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	1	Total	K	0	0
			1	1		
33	M	1	Total	K	0	0
			1	1		

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	73	Total	Na	0	0
			73	73		
34	9	3	Total	Na	0	0
			3	3		
34	A	1	Total	Na	0	0
			1	1		
34	C	1	Total	Na	0	0
			1	1		
34	H	1	Total	Na	0	0
			1	1		
34	J	1	Total	Na	0	0
			1	1		
34	L	1	Total	Na	0	0
			1	1		
34	M	1	Total	Na	0	0
			1	1		
34	Q	1	Total	Na	0	0
			1	1		
34	R	2	Total	Na	0	0
			2	2		
34	S	1	Total	Na	0	0
			1	1		

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	8	Total	Cl	0	0
			8	8		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	Q	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	3	1	Total Cl 1 1	0	0

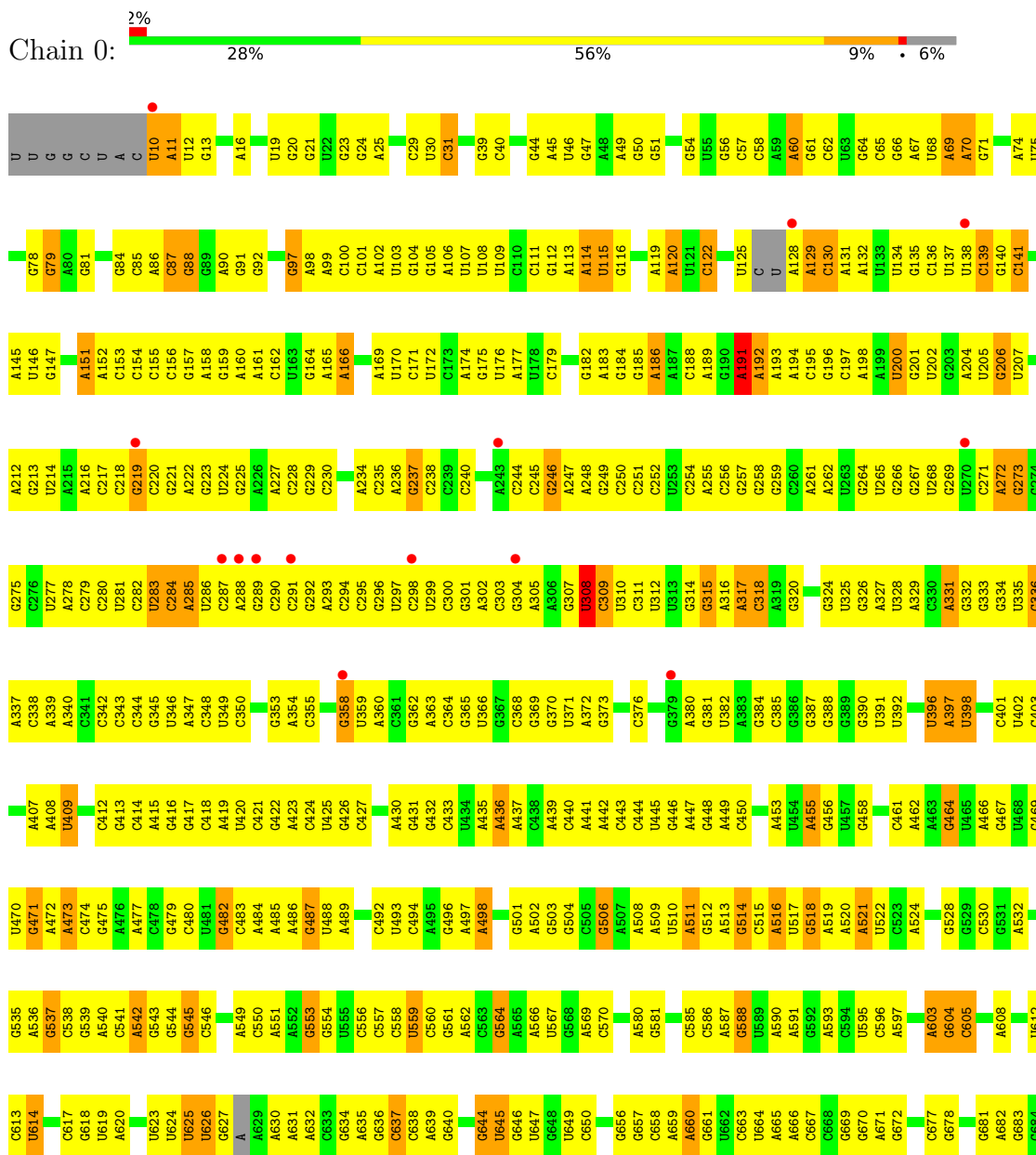
- Molecule 36 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	O	1	Total Cd 1 1	0	0
36	U	1	Total Cd 1 1	0	0
36	Z	1	Total Cd 1 1	0	0
36	1	1	Total Cd 1 1	0	0
36	3	1	Total Cd 1 1	0	0

### 3 Residue-property plots [i](#)

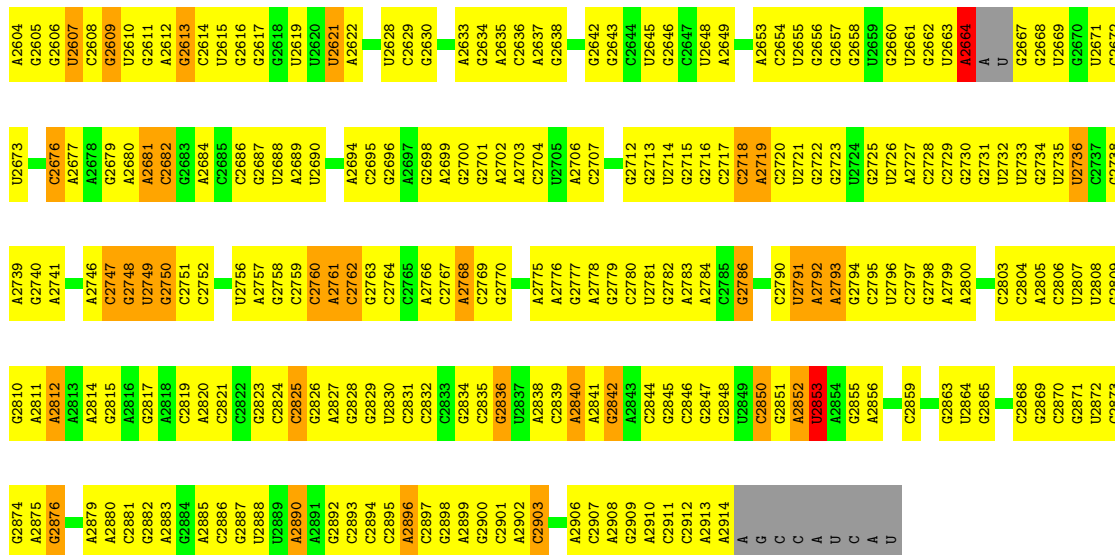
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S RIBOSOMAL RNA

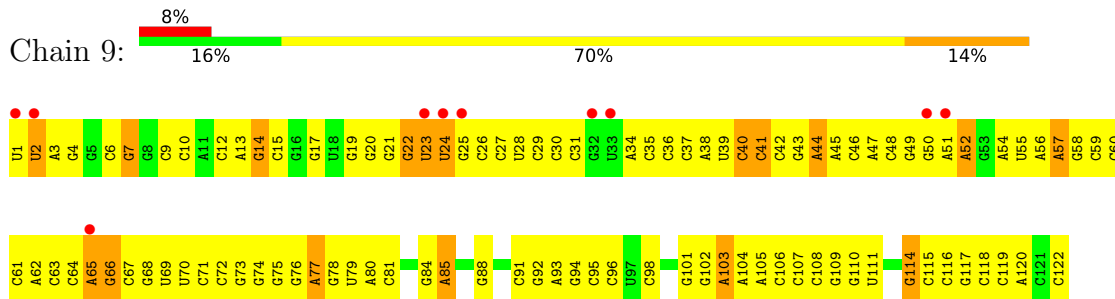




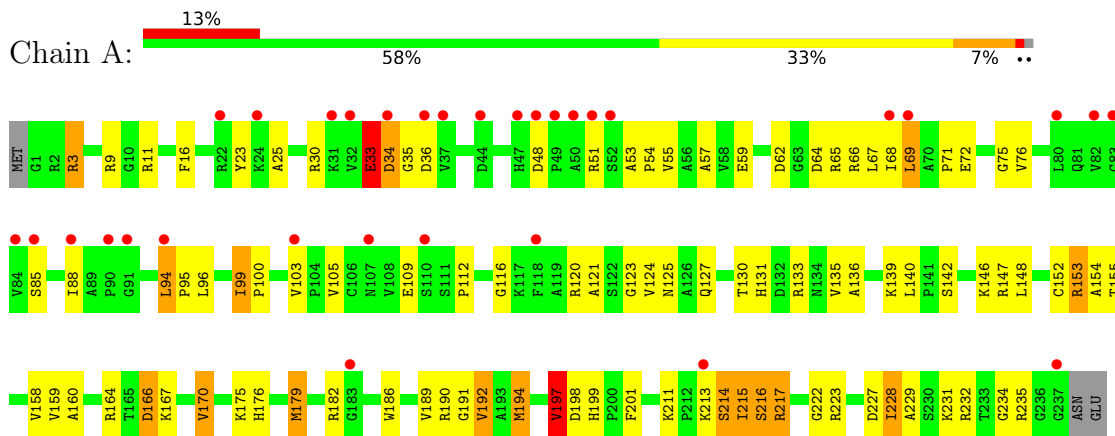
A2532	C1675	G1752	G1814	G1877	A1842	U2003	G2070	U2133	G2254	G2334	U2386	A2465	A2532
C2553	G1676	C1753	A1815	G1878	C1943	U2004	C2071	G2134	A2255	C2325	U2387	A2466	C2553
U2535	U1677	A1754	C1816	U1879	G1944	G2005	G2072	A2136	G2256	U2326	C2387	G2466	U2535
G2536	C1680	A1755	U1817	C1880	G1945	C2006	G2073	G2136	G2257	A2327	U2388	A2467	G2536
A2538	G1681	U1757	G1818	A1881	G1946	A2007	A2074	C	A2258	U2328	C2389	A2468	C2537
U2539	A1682	U1758	G1820	C1882	G1947	U2008	G2075	C	C2262	C2329	G2393	A2469	G2537
G2540	G1683	U1759	G1820	U1883	G1948	G2009	U2076	C	A2263	U2330	A2398	C2472	A2538
U2541	A1684	A1759	A1821	U1884	G1949	A2010	A2077	C	G2264	C2331	G2399	U2473	A2538
G2542	C1685	G1760	A1822	A1885	G1950	A2011	U2078	G	A2265	A2332	G2399	U2474	G2540
U2543	C1686	U1761	G1823	A1886	G1951	U2012	G2079	U	U2266	G2333	G2400	A2474	U2541
G2544	C1687	G1762	A1824	U1887	U	G2013	G2080	G	A2267	C2334	A2401	C2475	C2542
U2545	G1688	G1763	U1825	C1888	A	G2014	A2081	C	G2268	C2335	G2405	C2476	G2543
G2546	C1692	G1765	G1827	C1889	C	C2020	G2082	C	C2269	G2336	U2406	G2477	U2544
U2547	A1693	U1766	A1828	U1890	U	C2021	A2085	C	C2270	G2337	U2407	U2478	U2545
C2548	G1694	A1767	A1829	C1894	U	C2022	C2086	A	G2271	A	G2407	A2479	U2546
U2549	U1696	C1768	C1830	A1895	C	G2025	C2087	G	U2272	C	A2408	A2480	C2547
G2550	U1697	C1769	U1831	A1896	U	G2026	G2088	U	C2273	A	G2409	C2548	C2548
U2551	U1771	U1770	G1832	U1897	A	U2027	A2089	G	A2274	G	G2410	G2482	C2549
U2552	U1698	U1771	U1833	G1898	C	U2028	G2090	U	G2275	A	C2411	A2483	U2550
C2553	C1772	C1772	C1834	C1899	C	C2029	G2091	G	U2276	G2344	G2412	C2477	C2551
U2554	G1773	G1773	U1835	A1900	C	A2030	G2092	C	U2277	A2345	A2415	U2478	C2552
G2555	C1700	G1774	A1836	G1901	U	C2031	G2093	A	U2278	C2346	G2416	A2490	A2553
C2556	A1775	A1775	G1837	G1902	C	G2032	G2094	G	U2279	C2347	G2417	U2492	U2554
A2569	U1702	A1776	U1838	U1903	U	U2033	A2095	C	C2281	C2348	G2418	U2492	U2554
C2575	G1703	G1777	A1839	U1904	C	U2034	A2096	A	U2282	G2349	U2419	C2493	U2555
A2577	G1704	A1778	A1840	C1905	U	C2035	G2097	C	G2283	G2350	G2420	A2497	C2556
G2578	C1705	A1779	C1841	U1906	U	C2036	C2098	U	G2284	C2351	G2421	U2499	A2566
U2579	G1706	G1783	C1844	U1907	C	U2037	G2099	G	U2285	G2352	U2422	U2499	C2566
G2580	G1707	U1784	U1845	G1908	U	A2038	A2100	A	G2286	A2353	A2425	C2500	A2566
U2581	C1708	U1785	A1846	A1909	C	C2040	A2101	U	U2287	U2354	G2425	G2501	A2569
G2582	G1709	C1786	U1847	A1910	C	G2041	G2103	G	C2288	G2355	G2426	C2502	A2569
U2583	A1710	C1787	A1847	U1915	U	G2042	A2104	G	U2289	C2356	U2428	C2502	A2569
C2584	A1711	U1788	U1850	C1916	C	U2043	C2105	U	U2290	U2357	C2432	A2504	A2577
U2585	G1713	G1789	G1851	G1917	U	G2044	C2106	G	C2291	U2358	A2432	G2505	A2577
U2587	U1722	U1791	A1852	U1918	C	G2045	U2107	C	G2292	C2359	A2433	A2506	G2579
U2588	G1723	C1792	C1853	A1919	U	G2046	U2107	C	U2293	C2360	U2434	G2507	G2579
U2589	U1724	C1793	C1854	C1920	U	C2047	G2110	A	C2294	A2361	U2435	C2508	U2581
C2590	C1725	G1794	G1855	A1921	C	C2048	G2111	C	U2307	A2362	U2436	A2509	G2582
U2591	G1730	G1795	C1856	A1922	U	C2049	A2112	U	U2308	G2363	C2437	C2510	A2583
G2592	C1731	A1796	A1857	C1923	C	C2050	G2113	A	C2309	A2364	G2443	C2511	C2584
C2593	A1732	U1797	U1858	A1924	U	G2051	C2114	C	G2310	G2365	U2444	C2512	C2584
U2594	U1733	C1798	A1859	G1925	C	U2052	U2115	A	G2311	A2366	G2445	A2513	U2587
U2595	A1734	G1800	U1860	G1926	U	G2053	U2116	C	U2312	A2367	G2446	U2514	G2588
G2596	G1739	A1801	G1867	A1927	U	A2054	U2117	A	U2313	A2368	G2447	U2515	U2589
U2597	U1740	C1803	U1868	C1928	C	A2055	U2118	G	U2314	A2369	C2448	C2516	U2590
C2598	A1746	A1804	G1868	G1929	U	C2056	C2119	G	G2315	G2370	U2449	C2517	U2590
U2599	U1747	C1805	G1868	C1930	C	U2059	U2120	U	U2316	A2371	G2450	C2518	C2591
A2600	A1748	G1806	U1868	A1931	U	A2060	C2121	A	U2317	G2372	G2451	C2519	G2592
G2601	U1749	A1807	G1868	G1932	C	C2061	C2122	C	U2318	U2373	G2452	G2520	C2593
C2603	U1750	U1808	U1868	G1933	U	C2062	A2123	C	U2319	C2374	U2453	A2600	C2593
						U2063	G2124	G	U2320	U2375	G2454	U2461	U2594
						U2064	C2125	C	U2321	U2376	G2455	G2462	U2595
						C2065	U2126	C	U2322	U2377	G2456		U2596
						C2066	G2128	C	U2323	U2378	G2457		U2597
						A2067	U2129	U	U2324	U2379	G2458		U2598
						G2068	C2132	G	U2325	U2380	G2459		U2599
						G2069	C2132	C	U2326	U2381	G2460		A2601
						G2070	C2132	U	U2327	U2382	G2461		C2603
						C2071	C2132	G	U2328	U2383	G2462		G2603
						U2003	C2132	C	U2329	U2384	G2463		
						U2004	C2132	C	U2330	U2385	G2464		
						G2005	C2132	C	U2331	U2386	G2465		
						C2006	C2132	C	U2332	U2387	G2466		
						A2007	C2132	C	U2333	U2388	G2467		
						U2008	C2132	C	U2334	U2389	G2468		
						G2009	C2132	C	U2335	U2390	G2469		
						A2010	C2132	C	U2336	U2391	G2470		
						A2011	C2132	C	U2337	U2392	G2471		
						U2012	C2132	C	U2338	U2393	G2472		
						G2013	C2132	C	U2339	U2394	G2473		
						A2014	C2132	C	U2340	U2395	G2474		
						C2020	C2132	C	U2341	U2396	G2475		
						C2021	C2132	C	U2342	U2397	G2476		
						C1894	C2132	C	U2343	U2398	G2477		
						A1895	C2132	C	U2344	U2399	G2478		
						G1896	C2132	C	U2345	U2400	G2479		
						U1897	C2132	C	U2346	U2401	G2480		
						G1898	C2132	C	U2347	U2402	G2481		
						C1899	C2132	C	U2348	U2403	G2482		
						A1900	C2132	C	U2349	U2404	G2483		
						G1901	C2132	C	U2350	U2405	G2484		
						U1902	C2132	C	U2351	U2406	G2485		
						C1965	C2132	C	U2352	U2407	G2486		
						U1966	C2132	C	U2353	U2408	G2487		
						U1967	C2132	C	U2354	U2409	G2488		
						A1968	C2132	C	U2355	U2410	G2489		
						U1969	C2132	C	U2356	U2411	G2490		
						G1970	C2132	C	U2357	U2412	G2491		
						U1971	C2132	C	U2358	U2413	G2492		
						U1972	C2132	C	U2359	U2414	G2493		
						A1973	C2132	C	U2360	U2415	G2494		
						U1974	C2132	C	U2361	U2416	G2495		
						C1975	C2132	C	U2362	U2417	G2496		
						U1976	C2132	C	U2363	U2418	G2497		
						U1977	C2132	C	U2364	U2419	G2498		
						A1978	C2132	C	U2365	U2420	G2499		
						G1979	C2132	C	U2366	U2421	G2500		
						U1980	C2132	C	U2367	U2422	G2501		
						A1981	C2132	C	U2368	U2423	G2502		
						C1982	C2132	C	U2369	U2424	G2503		
						C1983	C2132	C	U2370	U2425	G2504		
						U1984	C2132	C	U2371	U2426	G2505		
						U1985	C2132	C	U2372	U2427	G2506		
						G1986	C2132	C	U2373	U2428	G2507		
						C1987	C2132	C	U2374	U2429	G2508		
						U1988	C2132	C	U2375	U2430	G2509		
						G1989	C2132	C	U2376	U2431	G2510		
						C1990	C2132	C	U2377	U2432	G2511		
						A1991	C2132	C	U2378	U2433	G2512		
						U1992	C2132	C	U2379	U2434	G2513		
						C1993	C2132	C	U2380	U2435	G2514		
						A1994	C2132	C	U2381	U2436	G2515		
						U1995	C2132	C	U2382	U2437	G2516		
						C1996	C2132	C	U2383	U2438	G2517		
						U1997	C2132	C	U2384	U2439	G		



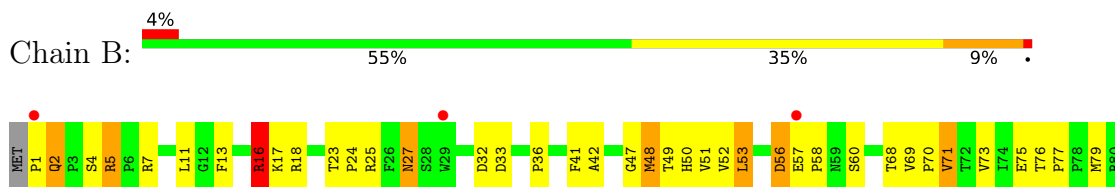
• Molecule 2: 5S RIBOSOMAL RNA

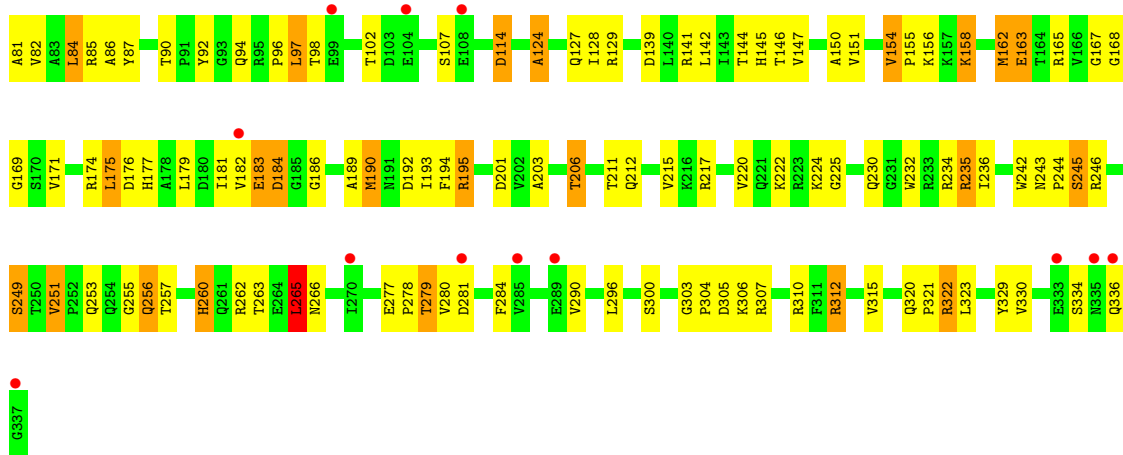


• Molecule 3: 50S ribosomal protein L2P

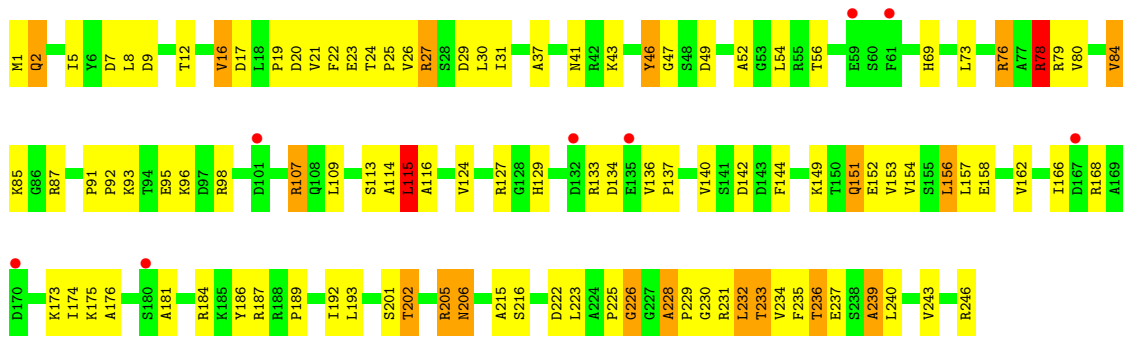


• Molecule 4: 50S ribosomal protein L3P

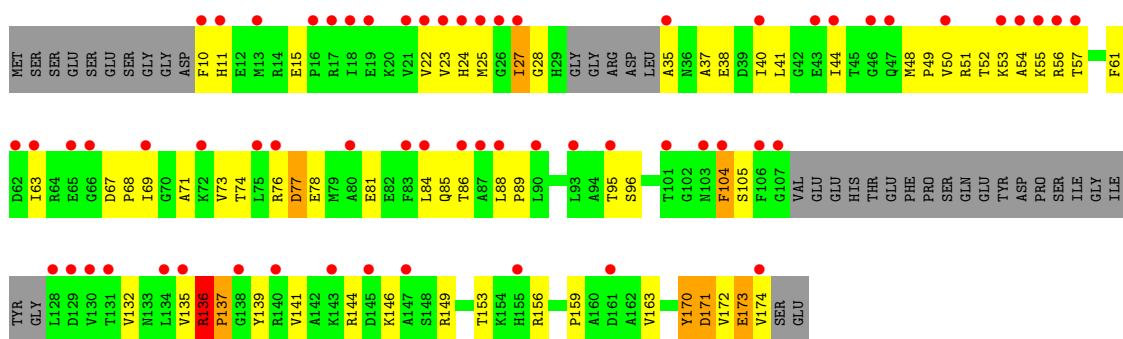
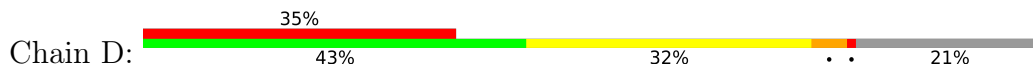




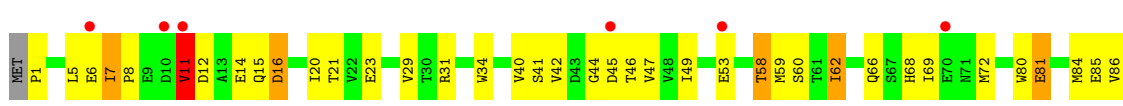
• Molecule 5: 50S ribosomal protein L4P

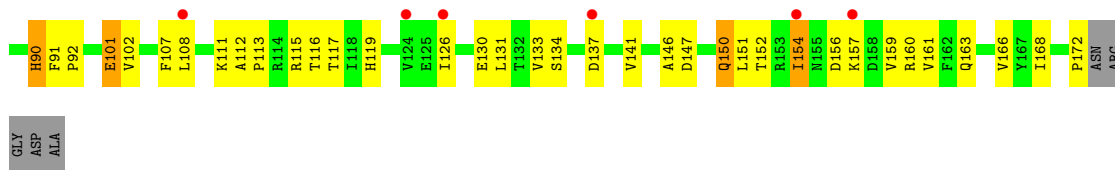


• Molecule 6: 50S ribosomal protein L5P

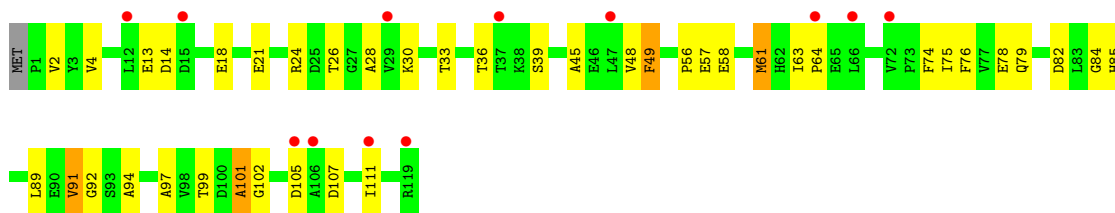


• Molecule 7: 50S ribosomal protein L6P

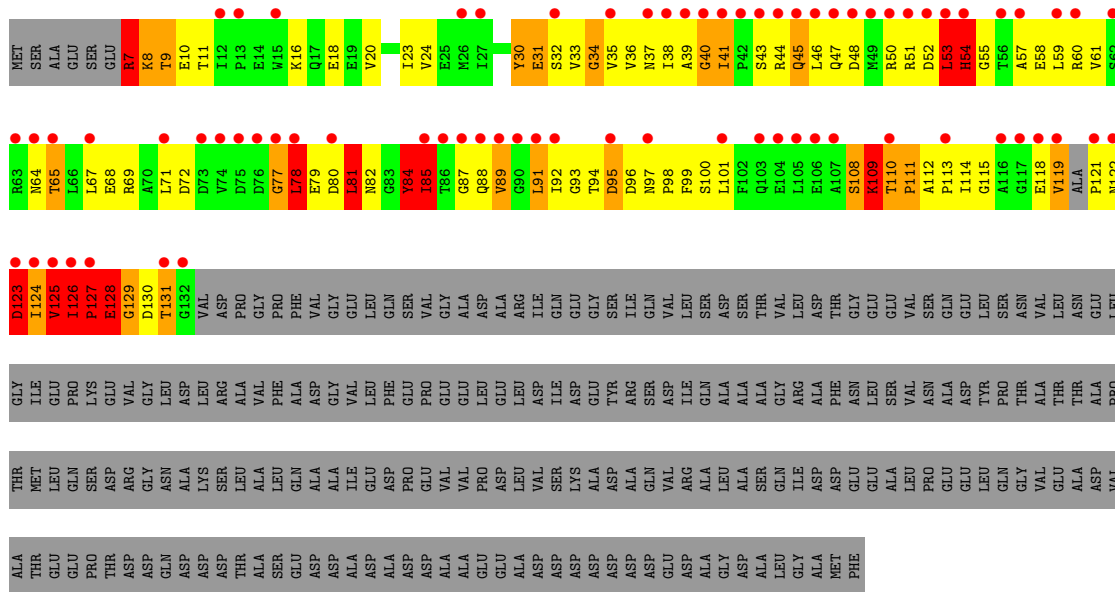




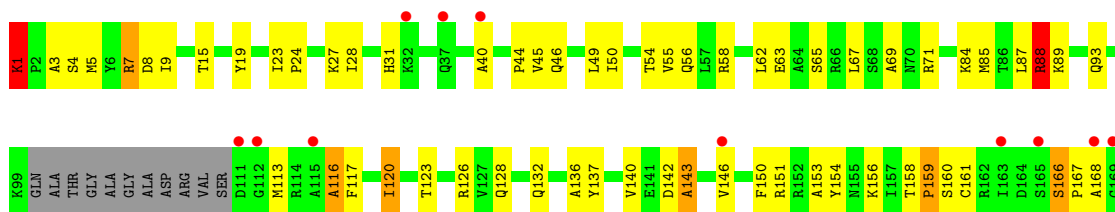
• Molecule 8: 50S ribosomal protein L7Ae



• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMO

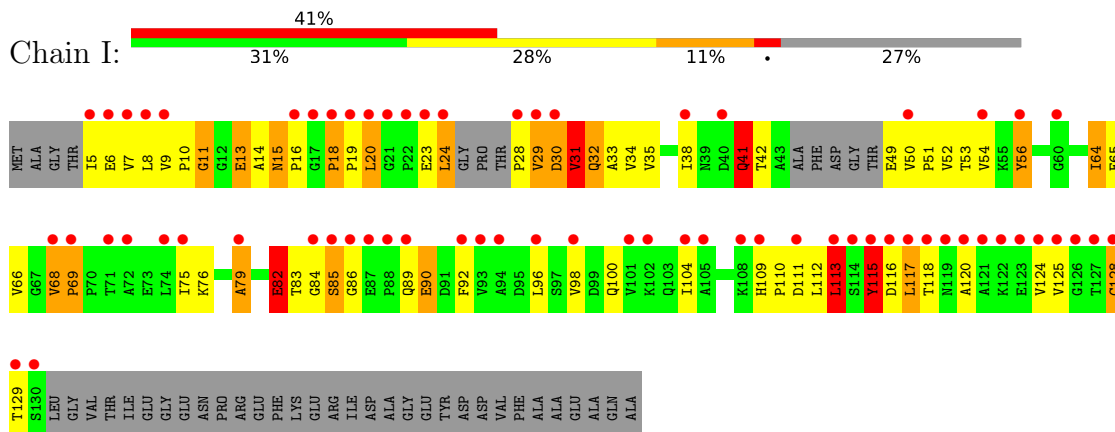


• Molecule 10: 50S ribosomal protein L10e

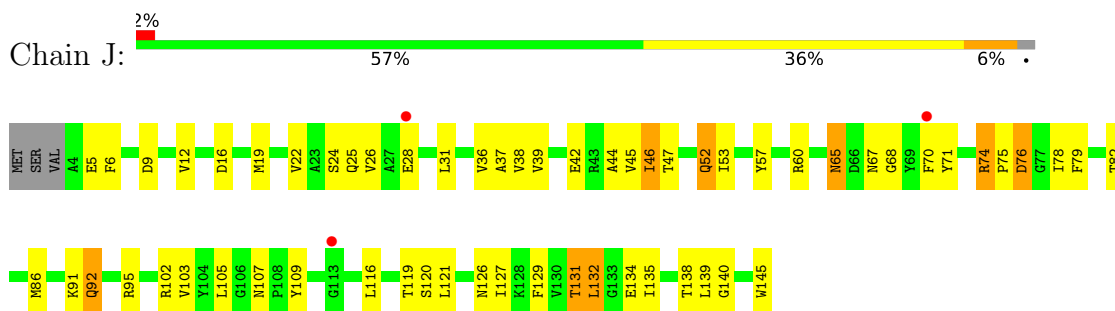


●  
H170  
A171

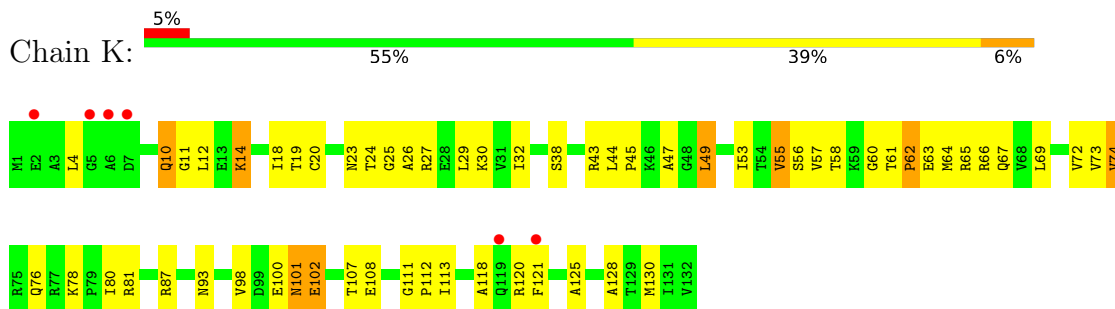
● Molecule 11: 50S ribosomal protein L11P



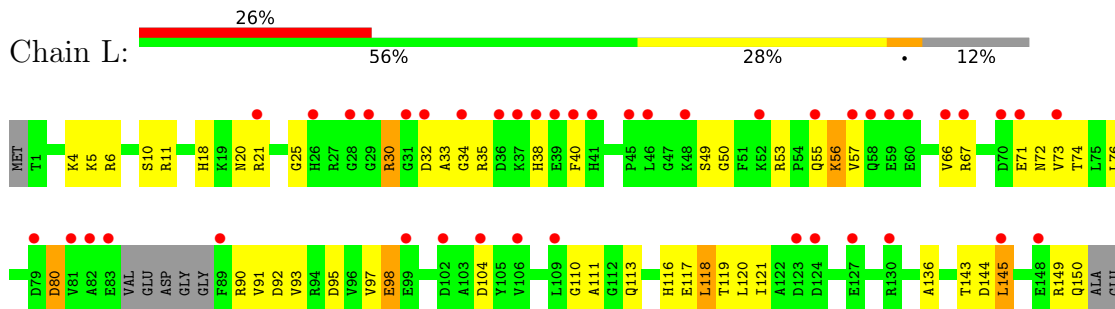
● Molecule 12: 50S ribosomal protein L13P



● Molecule 13: 50S ribosomal protein L14P

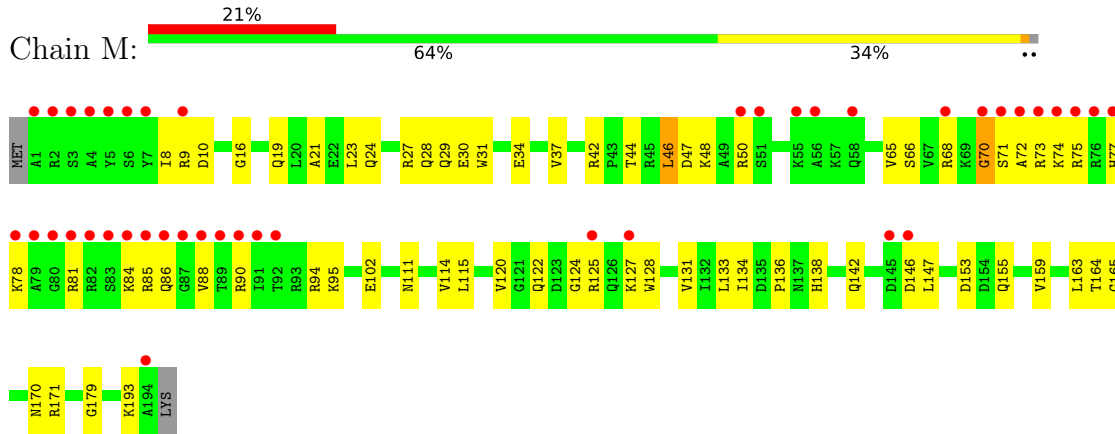


● Molecule 14: 50S ribosomal protein L15P

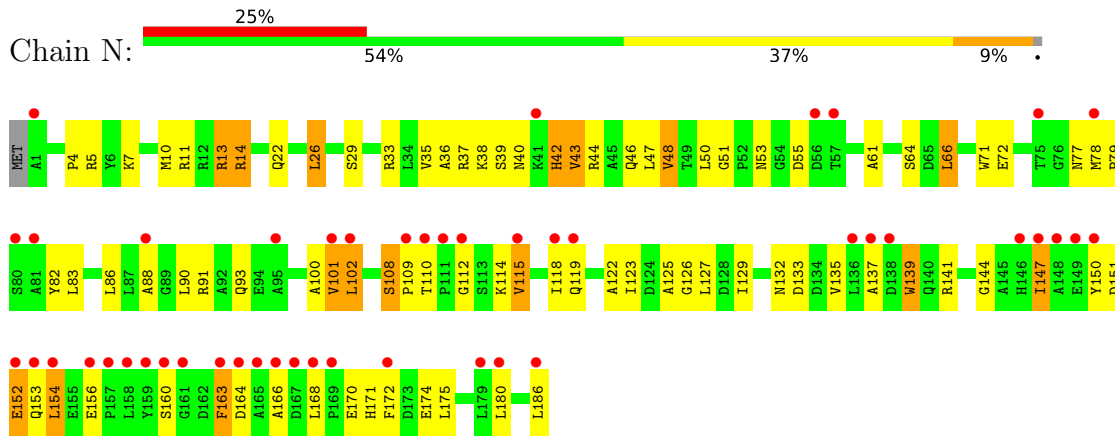


ALA  
GLU  
GLU  
THR  
GLU  
GLU  
ASP  
ASP  
ALA  
ALA  
ASP  
ASP  
GLU  
GLU

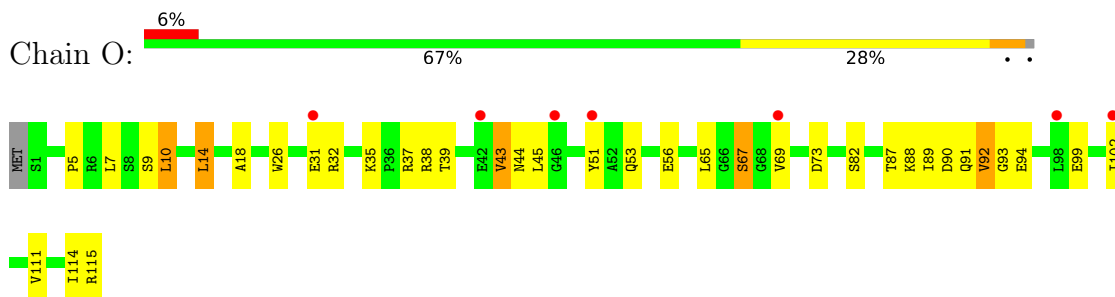
• Molecule 15: 50S ribosomal protein L15e



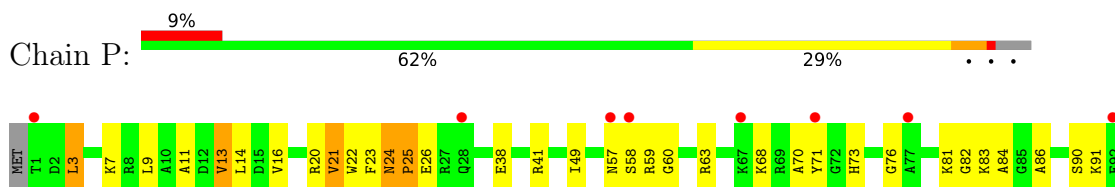
• Molecule 16: 50S ribosomal protein L18P



• Molecule 17: 50S ribosomal protein L18e

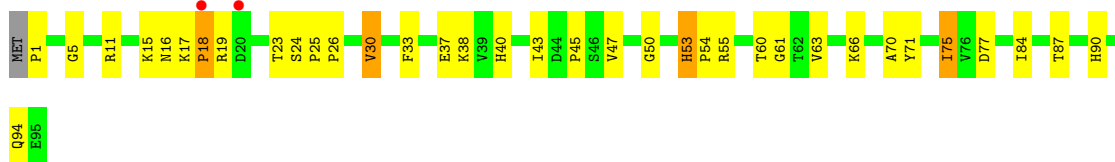


• Molecule 18: 50S ribosomal protein L19e

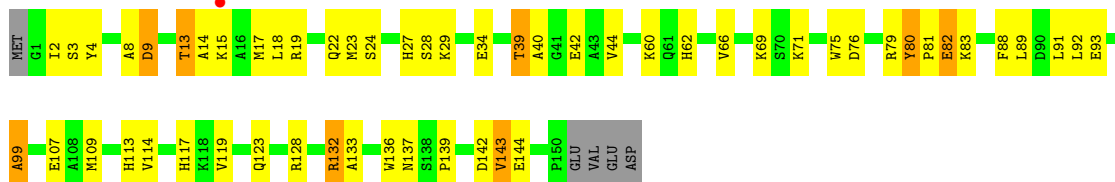




- Molecule 19: 50S ribosomal protein L21e



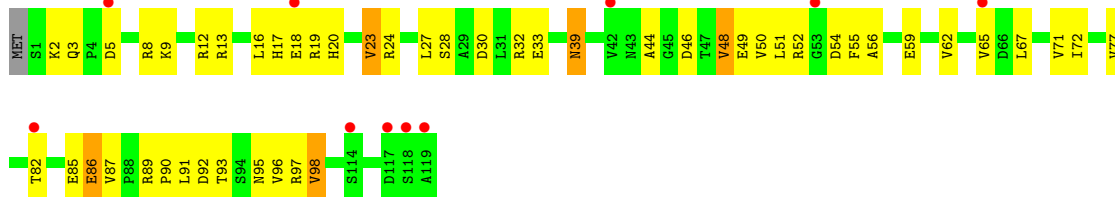
- Molecule 20: 50S ribosomal protein L22P



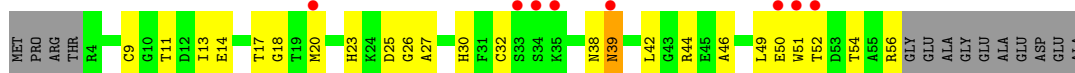
- Molecule 21: 50S ribosomal protein L23P



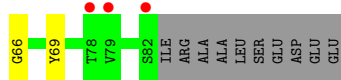
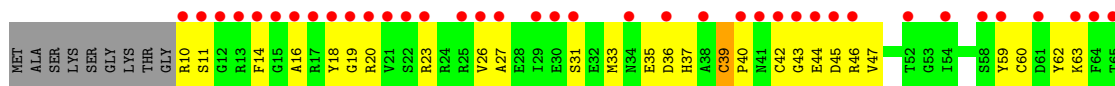
- Molecule 22: 50S ribosomal protein L24P



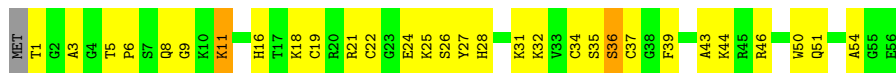
- Molecule 23: 50S ribosomal protein L24e



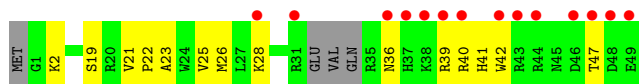




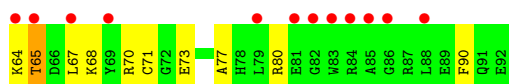
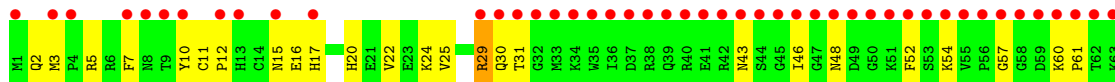
• Molecule 29: 50S ribosomal protein L37e



• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	214.49Å 302.43Å 578.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-3.00) 96.8 (50.00-3.01)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 3.01Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.241 , 0.288 0.259 , 0.259	Depositor DCC
$R_{free}$ test set	18014 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	69.6	Xtrriage
Anisotropy	0.307	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 60.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	92248	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	71.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CD, MG, OMG, K, PSU, OMU, NA, UR3

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	0	0.48	0/65932	0.72	46/102817 (0.0%)
2	9	0.43	0/2905	0.65	0/4528
3	A	0.54	0/1786	1.11	15/2408 (0.6%)
4	B	0.59	1/2690 (0.0%)	1.20	27/3652 (0.7%)
5	C	0.60	0/1884	1.15	16/2551 (0.6%)
6	D	0.45	0/1111	1.01	5/1498 (0.3%)
7	E	0.56	0/1382	1.07	8/1880 (0.4%)
8	F	0.45	0/901	0.97	0/1224
9	G	1.82	8/971 (0.8%)	2.11	36/1317 (2.7%)
10	H	0.54	0/1287	1.08	12/1725 (0.7%)
11	I	4.68	5/890 (0.6%)	2.25	18/1216 (1.5%)
12	J	0.62	0/1136	1.12	6/1530 (0.4%)
13	K	0.55	0/1001	1.20	12/1347 (0.9%)
14	L	0.47	0/1130	1.06	12/1509 (0.8%)
15	M	0.52	0/1583	1.05	3/2119 (0.1%)
16	N	0.45	0/1474	1.11	13/1999 (0.7%)
17	O	0.57	0/874	1.08	6/1181 (0.5%)
18	P	0.50	0/1147	0.97	5/1528 (0.3%)
19	Q	0.44	0/749	1.11	7/1005 (0.7%)
20	R	0.66	0/1172	1.13	9/1578 (0.6%)
21	S	0.47	0/648	0.99	3/875 (0.3%)
22	T	0.51	0/958	1.08	3/1289 (0.2%)
23	U	0.46	0/417	0.98	2/562 (0.4%)
24	V	0.50	0/502	1.15	4/675 (0.6%)
25	W	0.61	0/1219	1.18	11/1655 (0.7%)
26	X	0.66	0/664	1.20	7/895 (0.8%)
27	Y	0.61	0/1146	1.08	6/1536 (0.4%)
28	Z	0.47	0/589	0.98	2/787 (0.3%)
29	1	0.61	0/438	1.05	3/578 (0.5%)
30	2	0.51	0/401	0.98	2/529 (0.4%)
31	3	0.50	0/771	0.93	3/1024 (0.3%)
All	All	0.69	14/99758 (0.0%)	0.87	302/149017 (0.2%)

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	0	6	93
2	9	0	1
9	G	0	8
11	I	2	4
All	All	8	106

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	I	24	LEU	CA-CB	95.57	3.44	1.53
11	I	24	LEU	CG-CD2	64.38	3.65	1.52
11	I	24	LEU	CG-CD1	56.39	3.38	1.52
11	I	24	LEU	CB-CG	49.83	2.53	1.53
9	G	54	HIS	CB-CG	36.77	2.01	1.50

The worst 5 of 302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	24	LEU	CD1-CG-CD2	-41.20	20.15	110.80
11	I	24	LEU	CB-CA-C	-36.41	40.91	110.10
9	G	54	HIS	O-C-N	-24.21	90.39	122.59
11	I	24	LEU	N-CA-CB	23.28	150.08	110.50
9	G	54	HIS	CA-C-N	22.77	166.04	121.41

5 of 8 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1161	A	C1'
1	0	1167	G	C3',C1'
1	0	1193	A	C4',C3',C1'
11	I	24	LEU	CA
11	I	30	ASP	CA

5 of 106 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	116	G	Sidechain
1	0	191	A	Sidechain

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Group
1	0	206	G	Sidechain
1	0	49	A	Sidechain
1	0	79	G	Sidechain

## 5.2 Too-close contacts [i](#)

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	0	58979	0	29793	2510	0
2	9	2600	0	1326	158	0
3	A	1753	0	1766	73	0
4	B	2625	0	2533	112	0
5	C	1859	0	1816	87	0
6	D	1094	0	1085	54	0
7	E	1357	0	1266	48	0
8	F	890	0	843	31	0
9	G	959	0	928	162	0
10	H	1266	0	1268	50	0
11	I	876	0	835	60	0
12	J	1120	0	1098	53	0
13	K	992	0	1031	47	0
14	L	1118	0	1076	35	0
15	M	1559	0	1567	66	0
16	N	1445	0	1401	77	0
17	O	865	0	873	29	0
18	P	1136	0	1123	43	0
19	Q	735	0	728	28	0
20	R	1149	0	1122	53	0
21	S	641	0	605	13	0
22	T	950	0	924	50	0
23	U	410	0	367	16	0
24	V	499	0	511	21	0
25	W	1196	0	1137	78	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	53	0
28	Z	578	0	543	36	0
29	1	431	0	427	25	0
30	2	396	0	413	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	3	755	0	732	34	0
32	0	108	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
33	M	1	0	0	0	0
34	0	73	0	0	0	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	8	0	0	1	0
35	3	1	0	0	5	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	4	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	1	0
35	Q	1	0	0	1	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	1	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
All	All	92248	0	60923	3773	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 25.

The worst 5 of 3773 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)
9:G:54:HIS:CG	9:G:54:HIS:CB	2.01	1.43
9:G:33:VAL:C	9:G:123:ASP:OD2	1.72	1.31
9:G:108:SER:O	9:G:109:LYS:HE3	1.32	1.30
1:O:1167:G:H5'	1:O:1168:C:OP2	1.34	1.28
9:G:35:VAL:HG21	9:G:122:ASN:OD1	1.37	1.25

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	5	27
4	B	335/338 (99%)	287 (86%)	38 (11%)	10 (3%)	3	19
5	C	244/246 (99%)	209 (86%)	28 (12%)	7 (3%)	3	20
6	D	134/177 (76%)	95 (71%)	34 (25%)	5 (4%)	2	15
7	E	170/178 (96%)	156 (92%)	12 (7%)	2 (1%)	10	40
8	F	117/120 (98%)	101 (86%)	13 (11%)	3 (3%)	4	23
9	G	121/348 (35%)	79 (65%)	29 (24%)	13 (11%)	0	2
10	H	156/171 (91%)	141 (90%)	11 (7%)	4 (3%)	4	23
11	I	112/162 (69%)	76 (68%)	28 (25%)	8 (7%)	1	4
12	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	9	36
13	K	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	8	35
14	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	18	53
15	M	192/196 (98%)	161 (84%)	31 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	N	184/187 (98%)	162 (88%)	19 (10%)	3 (2%)	7	34
17	O	113/116 (97%)	103 (91%)	9 (8%)	1 (1%)	14	48
18	P	141/149 (95%)	129 (92%)	11 (8%)	1 (1%)	18	53
19	Q	93/96 (97%)	85 (91%)	5 (5%)	3 (3%)	3	18
20	R	148/155 (96%)	129 (87%)	18 (12%)	1 (1%)	18	53
21	S	79/85 (93%)	65 (82%)	14 (18%)	0	100	100
22	T	117/120 (98%)	105 (90%)	11 (9%)	1 (1%)	14	48
23	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	7	34
25	W	152/154 (99%)	134 (88%)	17 (11%)	1 (1%)	18	53
26	X	80/92 (87%)	66 (82%)	13 (16%)	1 (1%)	9	38
27	Y	140/241 (58%)	130 (93%)	7 (5%)	3 (2%)	5	27
28	Z	71/92 (77%)	64 (90%)	7 (10%)	0	100	100
29	1	54/57 (95%)	45 (83%)	8 (15%)	1 (2%)	6	30
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	11	43
All	All	3845/4442 (87%)	3329 (87%)	436 (11%)	80 (2%)	5	27

5 of 80 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	16	ARG
6	D	27	ILE
8	F	91	VAL
9	G	127	PRO
11	I	11	GLY

### 5.3.2 Protein sidechains [i](#)

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	
3	A	179/182 (98%)	161 (90%)	18 (10%)	7	29
4	B	282/283 (100%)	256 (91%)	26 (9%)	8	33
5	C	193/193 (100%)	170 (88%)	23 (12%)	5	22
6	D	117/148 (79%)	109 (93%)	8 (7%)	14	45
7	E	152/156 (97%)	138 (91%)	14 (9%)	8	33
8	F	93/94 (99%)	92 (99%)	1 (1%)	65	83
9	G	106/283 (38%)	92 (87%)	14 (13%)	4	18
10	H	132/138 (96%)	125 (95%)	7 (5%)	20	54
11	I	99/130 (76%)	81 (82%)	18 (18%)	2	9
12	J	118/121 (98%)	108 (92%)	10 (8%)	10	36
13	K	106/106 (100%)	98 (92%)	8 (8%)	12	41
14	L	113/127 (89%)	109 (96%)	4 (4%)	32	65
15	M	158/160 (99%)	153 (97%)	5 (3%)	34	67
16	N	149/150 (99%)	140 (94%)	9 (6%)	17	50
17	O	93/94 (99%)	87 (94%)	6 (6%)	15	47
18	P	113/117 (97%)	107 (95%)	6 (5%)	20	54
19	Q	79/80 (99%)	76 (96%)	3 (4%)	29	63
20	R	117/122 (96%)	111 (95%)	6 (5%)	21	55
21	S	71/74 (96%)	66 (93%)	5 (7%)	14	44
22	T	105/106 (99%)	97 (92%)	8 (8%)	12	41
23	U	44/53 (83%)	43 (98%)	1 (2%)	44	74
24	V	51/57 (90%)	48 (94%)	3 (6%)	18	50
25	W	130/130 (100%)	116 (89%)	14 (11%)	6	26
26	X	66/74 (89%)	60 (91%)	6 (9%)	9	33
27	Y	120/196 (61%)	110 (92%)	10 (8%)	10	37
28	Z	60/74 (81%)	60 (100%)	0	100	100
29	1	46/47 (98%)	45 (98%)	1 (2%)	45	74
30	2	42/46 (91%)	42 (100%)	0	100	100
31	3	79/79 (100%)	77 (98%)	2 (2%)	42	72
All	All	3213/3620 (89%)	2977 (93%)	236 (7%)	13	42

5 of 236 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	I	24	LEU
26	X	84	ILE
13	K	74	VAL
26	X	21	PRO
23	U	39	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
18	P	57	ASN
21	S	51	GLN
18	P	73	HIS
20	R	62	HIS
24	V	4	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2742/2922 (93%)	292 (10%)	35 (1%)
2	9	121/122 (99%)	17 (14%)	4 (3%)
All	All	2863/3044 (94%)	309 (10%)	39 (1%)

5 of 309 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2467	A
2	9	14	G
1	0	2536	C
1	0	2791	U
2	9	65	A

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

4 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
1	UR3	0	2619	1	19,22,23	0.49	0	26,32,35	0.69	1 (3%)
1	PSU	0	2621	1	18,21,22	1.57	2 (11%)	21,30,33	1.46	4 (19%)
1	OMG	0	2588	1	23,26,27	0.34	0	32,38,41	0.48	0
1	OMU	0	2587	1	19,22,23	0.41	0	25,31,34	0.54	0

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
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	1/9/27/28	0/3/3/3
1	OMU	0	2587	1	-	0/9/27/28	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	5.45	1.43	1.36
1	0	2621	PSU	C6-C5	2.39	1.37	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.66	120.65	118.17
1	0	2621	PSU	C6-N1-C2	-2.97	119.93	122.69
1	0	2621	PSU	O2-C2-N1	2.89	125.76	122.79
1	0	2619	UR3	C4-N3-C2	2.65	126.71	124.58
1	0	2621	PSU	O2'-C2'-C1'	-2.47	105.35	111.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2621	PSU	1	0
1	0	2588	OMG	3	0
1	0	2587	OMU	5	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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
9	G	2

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Mol	Chain	Number of breaks
1	0	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	0	1207:A	O3'	1208:C	P	2.51
1	G	53:LEU	C	54:HIS	N	1.63
1	G	54:HIS	C	55:GLY	N	0.99

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	0.02	69 (2%) 58 35	17, 56, 120, 184	0
2	9	122/122 (100%)	0.62	10 (8%) 17 9	41, 89, 136, 181	0
3	A	237/240 (98%)	0.99	32 (13%) 7 4	34, 90, 133, 148	0
4	B	337/338 (99%)	0.46	15 (4%) 38 20	25, 60, 100, 112	0
5	C	246/246 (100%)	0.39	8 (3%) 49 28	29, 58, 91, 106	0
6	D	140/177 (79%)	2.05	62 (44%) 0 1	89, 146, 170, 178	0
7	E	172/178 (96%)	0.66	12 (6%) 22 12	46, 73, 100, 109	0
8	F	119/120 (99%)	1.00	12 (10%) 12 7	74, 110, 150, 166	0
9	G	125/348 (35%)	2.49	73 (58%) 0 0	100, 133, 165, 168	0
10	H	160/171 (93%)	0.84	12 (7%) 20 10	51, 76, 109, 120	0
11	I	118/162 (72%)	2.65	66 (55%) 0 0	20, 181, 199, 200	0
12	J	142/145 (97%)	0.29	3 (2%) 63 40	31, 54, 83, 99	0
13	K	132/132 (100%)	0.57	6 (4%) 38 20	33, 61, 98, 103	0
14	L	145/165 (87%)	1.66	43 (29%) 1 1	49, 111, 158, 162	0
15	M	194/196 (98%)	1.40	42 (21%) 2 2	2, 62, 161, 180	0
16	N	186/187 (99%)	1.53	47 (25%) 1 1	62, 106, 176, 189	0
17	O	115/116 (99%)	0.62	7 (6%) 27 14	48, 70, 88, 91	0
18	P	143/149 (95%)	0.80	14 (9%) 13 7	44, 68, 103, 109	0
19	Q	95/96 (98%)	0.62	2 (2%) 63 40	52, 74, 87, 100	0
20	R	150/155 (96%)	0.06	1 (0%) 84 66	30, 48, 74, 81	0
21	S	81/85 (95%)	0.78	5 (6%) 26 14	56, 87, 108, 123	0
22	T	119/120 (99%)	0.78	10 (8%) 17 9	51, 74, 106, 139	0
23	U	53/67 (79%)	1.27	8 (15%) 5 3	96, 108, 126, 133	0
24	V	65/71 (91%)	1.33	14 (21%) 2 1	66, 105, 145, 148	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.36	2 (1%) 75 53	38, 55, 81, 95	0
26	X	82/92 (89%)	0.54	4 (4%) 35 18	43, 63, 84, 95	0
27	Y	142/241 (58%)	0.36	0 100 100	23, 51, 87, 106	0
28	Z	73/92 (79%)	3.14	41 (56%) 0 0	164, 174, 200, 200	0
29	1	56/57 (98%)	0.04	0 100 100	28, 43, 56, 65	0
30	2	46/50 (92%)	1.55	14 (30%) 1 1	48, 87, 150, 152	0
31	3	92/92 (100%)	3.16	58 (63%) 0 0	184, 198, 200, 200	0
All	All	6790/7486 (90%)	0.61	692 (10%) 12 6	2, 67, 162, 200	0

The worst 5 of 692 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	Z	11	SER	13.1
31	3	84	ARG	12.3
31	3	83	TRP	11.8
11	I	24	LEU	10.6
1	0	1181	A	10.5

## 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. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	OMU	0	2587	21/22	0.95	0.11	33,36,42,43	0
1	OMG	0	2588	24/25	0.95	0.10	38,42,48,49	0
1	UR3	0	2619	21/22	0.95	0.09	34,42,44,47	0
1	PSU	0	2621	20/21	0.95	0.08	35,37,44,44	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands i

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	3100	1/1	0.39	0.26	56,56,56,56	0
34	NA	0	3078	1/1	0.42	0.35	78,78,78,78	0
32	MG	0	2971	1/1	0.42	0.76	200,200,200,200	0
34	NA	0	3046	1/1	0.44	0.14	26,26,26,26	0
34	NA	S	85	1/1	0.44	0.18	64,64,64,64	0
32	MG	0	3017	1/1	0.49	0.26	166,166,166,166	0
34	NA	0	3041	1/1	0.49	0.34	70,70,70,70	0
34	NA	0	3103	1/1	0.50	0.52	198,198,198,198	0
32	MG	0	3027	1/1	0.51	0.25	110,110,110,110	0
36	CD	3	94	1/1	0.53	0.35	200,200,200,200	0
32	MG	0	2998	1/1	0.54	0.51	73,73,73,73	0
35	CL	3	95	1/1	0.55	0.13	124,124,124,124	0
34	NA	0	3057	1/1	0.55	0.54	124,124,124,124	0
34	NA	0	3050	1/1	0.56	1.04	137,137,137,137	0
32	MG	A	241	1/1	0.59	0.32	142,142,142,142	0
35	CL	O	117	1/1	0.60	0.45	127,127,127,127	0
34	NA	0	3033	1/1	0.61	0.24	60,60,60,60	0
34	NA	0	3093	1/1	0.63	0.76	116,116,116,116	0
32	MG	0	3018	1/1	0.64	0.37	78,78,78,78	0
32	MG	0	3014	1/1	0.64	0.54	87,87,87,87	0
32	MG	0	2962	1/1	0.64	0.29	60,60,60,60	0
34	NA	Q	96	1/1	0.64	0.17	64,64,64,64	0
32	MG	0	2946	1/1	0.65	0.73	200,200,200,200	0
34	NA	0	3051	1/1	0.65	0.24	49,49,49,49	0
34	NA	0	3059	1/1	0.66	0.19	53,53,53,53	0
34	NA	0	3075	1/1	0.67	0.41	41,41,41,41	0
32	MG	0	2981	1/1	0.67	0.32	44,44,44,44	0
34	NA	0	3047	1/1	0.69	0.21	53,53,53,53	0
32	MG	0	3025	1/1	0.69	0.31	57,57,57,57	0
32	MG	0	2938	1/1	0.69	0.19	42,42,42,42	0
35	CL	0	3106	1/1	0.70	0.21	120,120,120,120	0
35	CL	0	3109	1/1	0.71	0.49	135,135,135,135	0
34	NA	0	3060	1/1	0.71	0.22	101,101,101,101	0
34	NA	0	3052	1/1	0.72	0.16	72,72,72,72	0
34	NA	9	124	1/1	0.72	0.09	34,34,34,34	0
34	NA	0	3082	1/1	0.72	0.16	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	3094	1/1	0.73	0.30	116,116,116,116	0
32	MG	0	3026	1/1	0.74	1.06	79,79,79,79	0
33	K	M	196	1/1	0.74	0.36	127,127,127,127	0
32	MG	0	3007	1/1	0.74	0.23	54,54,54,54	0
34	NA	0	3065	1/1	0.74	0.12	27,27,27,27	0
34	NA	0	3068	1/1	0.74	0.28	68,68,68,68	0
32	MG	Y	241	1/1	0.75	0.16	68,68,68,68	0
34	NA	0	3038	1/1	0.75	0.30	67,67,67,67	0
34	NA	0	3067	1/1	0.76	0.15	47,47,47,47	0
32	MG	0	2988	1/1	0.76	0.10	52,52,52,52	0
34	NA	0	3101	1/1	0.76	0.20	43,43,43,43	0
32	MG	0	3022	1/1	0.76	0.44	44,44,44,44	0
34	NA	C	247	1/1	0.77	0.10	41,41,41,41	0
35	CL	L	166	1/1	0.77	0.14	68,68,68,68	0
32	MG	0	3028	1/1	0.77	0.19	66,66,66,66	0
32	MG	0	2949	1/1	0.77	0.19	45,45,45,45	0
34	NA	0	3040	1/1	0.77	0.15	29,29,29,29	0
32	MG	0	3019	1/1	0.78	0.10	41,41,41,41	0
32	MG	0	3001	1/1	0.78	0.10	38,38,38,38	0
32	MG	0	3029	1/1	0.78	0.45	69,69,69,69	0
32	MG	0	2980	1/1	0.79	0.35	48,48,48,48	0
34	NA	0	3064	1/1	0.79	0.26	60,60,60,60	0
34	NA	0	3099	1/1	0.79	0.35	56,56,56,56	0
35	CL	A	243	1/1	0.79	0.28	90,90,90,90	0
32	MG	0	2959	1/1	0.80	0.23	39,39,39,39	0
34	NA	0	3048	1/1	0.80	0.26	46,46,46,46	0
34	NA	9	125	1/1	0.80	0.35	78,78,78,78	0
34	NA	9	126	1/1	0.80	0.21	91,91,91,91	0
32	MG	A	240	1/1	0.80	0.18	56,56,56,56	0
34	NA	H	172	1/1	0.80	0.08	43,43,43,43	0
33	K	0	3031	1/1	0.80	0.39	153,153,153,153	0
34	NA	R	156	1/1	0.80	0.19	53,53,53,53	0
34	NA	0	3098	1/1	0.81	0.36	62,62,62,62	0
32	MG	0	2999	1/1	0.81	0.16	25,25,25,25	0
32	MG	0	3011	1/1	0.81	0.24	71,71,71,71	0
32	MG	0	2973	1/1	0.81	0.18	51,51,51,51	0
34	NA	0	3054	1/1	0.81	0.21	63,63,63,63	0
34	NA	0	3072	1/1	0.82	0.20	65,65,65,65	0
34	NA	0	3044	1/1	0.82	0.35	46,46,46,46	0
32	MG	0	2941	1/1	0.82	0.18	15,15,15,15	0
32	MG	0	2947	1/1	0.82	0.13	15,15,15,15	0
34	NA	J	146	1/1	0.82	0.15	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	M	198	1/1	0.82	0.17	77,77,77,77	0
32	MG	0	2945	1/1	0.82	0.18	27,27,27,27	0
34	NA	R	155	1/1	0.82	0.15	31,31,31,31	0
36	CD	O	116	1/1	0.82	0.19	200,200,200,200	0
36	CD	Z	93	1/1	0.82	0.23	200,200,200,200	0
32	MG	0	2972	1/1	0.82	0.13	109,109,109,109	0
34	NA	0	3053	1/1	0.83	0.12	19,19,19,19	0
32	MG	0	2987	1/1	0.83	0.18	35,35,35,35	0
32	MG	0	3020	1/1	0.83	0.25	84,84,84,84	0
34	NA	A	242	1/1	0.83	0.16	55,55,55,55	0
35	CL	J	149	1/1	0.83	0.09	45,45,45,45	0
32	MG	0	2944	1/1	0.83	0.13	25,25,25,25	0
34	NA	0	3074	1/1	0.84	0.16	66,66,66,66	0
32	MG	0	2974	1/1	0.84	0.22	51,51,51,51	0
32	MG	0	2964	1/1	0.84	0.24	50,50,50,50	0
32	MG	0	2967	1/1	0.84	0.20	50,50,50,50	0
34	NA	0	3104	1/1	0.84	0.31	34,34,34,34	0
34	NA	0	3090	1/1	0.84	0.30	81,81,81,81	0
34	NA	0	3034	1/1	0.84	0.20	91,91,91,91	0
32	MG	0	2969	1/1	0.84	0.27	38,38,38,38	0
32	MG	3	93	1/1	0.84	0.21	69,69,69,69	0
32	MG	0	2985	1/1	0.85	0.10	34,34,34,34	0
32	MG	0	3016	1/1	0.85	0.10	43,43,43,43	0
32	MG	0	2936	1/1	0.85	0.09	17,17,17,17	0
34	NA	0	3058	1/1	0.85	0.11	61,61,61,61	0
34	NA	0	3095	1/1	0.85	0.32	126,126,126,126	0
32	MG	0	2968	1/1	0.85	0.15	60,60,60,60	0
32	MG	0	3009	1/1	0.85	0.09	40,40,40,40	0
32	MG	0	2937	1/1	0.85	0.26	14,14,14,14	0
35	CL	0	3112	1/1	0.85	0.22	96,96,96,96	0
32	MG	0	2993	1/1	0.86	0.27	78,78,78,78	0
32	MG	0	3013	1/1	0.86	0.15	41,41,41,41	0
32	MG	0	2954	1/1	0.86	0.12	29,29,29,29	0
32	MG	0	2961	1/1	0.86	0.28	41,41,41,41	0
34	NA	0	3077	1/1	0.86	0.33	119,119,119,119	0
32	MG	0	3030	1/1	0.86	0.13	46,46,46,46	0
34	NA	0	3045	1/1	0.86	0.12	33,33,33,33	0
32	MG	0	3010	1/1	0.86	0.19	56,56,56,56	0
34	NA	0	3089	1/1	0.87	0.10	51,51,51,51	0
32	MG	0	2982	1/1	0.87	0.16	14,14,14,14	0
32	MG	0	2984	1/1	0.87	0.28	59,59,59,59	0
32	MG	B	338	1/1	0.87	0.23	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	3063	1/1	0.87	0.35	162,162,162,162	0
34	NA	0	3032	1/1	0.87	0.20	30,30,30,30	0
34	NA	0	3056	1/1	0.87	0.20	42,42,42,42	0
35	CL	0	3108	1/1	0.87	0.18	72,72,72,72	0
32	MG	0	2963	1/1	0.87	0.11	72,72,72,72	0
35	CL	0	3111	1/1	0.87	0.17	54,54,54,54	0
32	MG	0	2957	1/1	0.88	0.19	37,37,37,37	0
32	MG	0	2983	1/1	0.88	0.18	43,43,43,43	0
34	NA	0	3083	1/1	0.88	0.28	27,27,27,27	0
35	CL	N	187	1/1	0.88	0.13	64,64,64,64	0
34	NA	0	3085	1/1	0.88	0.24	15,15,15,15	0
34	NA	0	3073	1/1	0.88	0.11	25,25,25,25	0
32	MG	0	2986	1/1	0.88	0.09	53,53,53,53	0
32	MG	0	3003	1/1	0.88	0.11	26,26,26,26	0
32	MG	0	3004	1/1	0.88	0.29	27,27,27,27	0
32	MG	0	2989	1/1	0.89	0.55	56,56,56,56	0
35	CL	K	134	1/1	0.89	0.12	55,55,55,55	0
32	MG	0	3006	1/1	0.89	0.17	49,49,49,49	0
34	NA	0	3055	1/1	0.89	0.08	36,36,36,36	0
34	NA	0	3081	1/1	0.89	0.19	49,49,49,49	0
34	NA	0	3069	1/1	0.89	0.19	58,58,58,58	0
34	NA	0	3061	1/1	0.89	0.14	39,39,39,39	0
34	NA	0	3084	1/1	0.89	0.17	62,62,62,62	0
32	MG	0	2951	1/1	0.89	0.18	11,11,11,11	0
34	NA	0	3042	1/1	0.89	0.32	32,32,32,32	0
32	MG	0	2997	1/1	0.90	0.11	59,59,59,59	0
32	MG	0	2977	1/1	0.90	0.21	43,43,43,43	0
32	MG	0	2935	1/1	0.90	0.23	28,28,28,28	0
34	NA	0	3102	1/1	0.90	0.16	47,47,47,47	0
34	NA	0	3076	1/1	0.90	0.15	51,51,51,51	0
34	NA	0	3043	1/1	0.90	0.26	115,115,115,115	0
34	NA	0	3092	1/1	0.90	0.22	45,45,45,45	0
32	MG	K	133	1/1	0.90	0.26	35,35,35,35	0
34	NA	0	3079	1/1	0.90	0.12	53,53,53,53	0
32	MG	0	2965	1/1	0.90	0.16	47,47,47,47	0
32	MG	0	2943	1/1	0.90	0.17	23,23,23,23	0
35	CL	J	148	1/1	0.91	0.07	49,49,49,49	0
32	MG	0	3015	1/1	0.91	0.45	53,53,53,53	0
34	NA	0	3039	1/1	0.91	0.12	29,29,29,29	0
34	NA	0	3080	1/1	0.91	0.16	57,57,57,57	0
32	MG	0	2924	1/1	0.91	0.15	35,35,35,35	0
32	MG	0	2956	1/1	0.91	0.10	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	3005	1/1	0.91	0.10	47,47,47,47	0
32	MG	0	2934	1/1	0.91	0.21	22,22,22,22	0
32	MG	0	2970	1/1	0.91	0.14	32,32,32,32	0
34	NA	0	3086	1/1	0.91	0.14	26,26,26,26	0
34	NA	0	3088	1/1	0.91	0.12	33,33,33,33	0
32	MG	0	3024	1/1	0.92	0.32	1,1,1,1	0
32	MG	0	2950	1/1	0.92	0.09	17,17,17,17	0
32	MG	0	2996	1/1	0.92	0.17	21,21,21,21	0
34	NA	0	3035	1/1	0.92	0.09	17,17,17,17	0
32	MG	0	3012	1/1	0.92	0.06	39,39,39,39	0
32	MG	0	1	1/1	0.92	0.16	26,26,26,26	0
35	CL	Q	97	1/1	0.92	0.19	93,93,93,93	0
34	NA	M	197	1/1	0.92	0.06	28,28,28,28	0
34	NA	0	3087	1/1	0.92	0.06	22,22,22,22	0
35	CL	B	339	1/1	0.92	0.15	61,61,61,61	0
34	NA	0	3097	1/1	0.92	0.19	50,50,50,50	0
32	MG	0	2976	1/1	0.93	0.07	19,19,19,19	0
32	MG	0	2939	1/1	0.93	0.28	20,20,20,20	0
32	MG	0	2979	1/1	0.93	0.10	20,20,20,20	0
34	NA	0	3096	1/1	0.93	0.07	47,47,47,47	0
34	NA	0	3071	1/1	0.93	0.05	27,27,27,27	0
32	MG	0	2940	1/1	0.93	0.16	24,24,24,24	0
32	MG	0	2930	1/1	0.93	0.07	55,55,55,55	0
32	MG	0	2990	1/1	0.93	0.06	31,31,31,31	0
32	MG	0	2991	1/1	0.93	0.16	20,20,20,20	0
32	MG	0	2992	1/1	0.93	0.40	52,52,52,52	0
32	MG	0	2966	1/1	0.93	0.09	46,46,46,46	0
35	CL	Y	242	1/1	0.93	0.08	27,27,27,27	0
32	MG	0	2953	1/1	0.93	0.09	8,8,8,8	0
34	NA	0	3091	1/1	0.93	0.15	31,31,31,31	0
35	CL	0	3110	1/1	0.93	0.10	56,56,56,56	0
32	MG	0	2928	1/1	0.93	0.13	32,32,32,32	0
32	MG	0	3021	1/1	0.94	0.17	20,20,20,20	0
32	MG	0	2975	1/1	0.94	0.17	45,45,45,45	0
32	MG	0	3023	1/1	0.94	0.24	29,29,29,29	0
32	MG	0	2948	1/1	0.94	0.18	18,18,18,18	0
34	NA	0	3070	1/1	0.94	0.06	27,27,27,27	0
32	MG	9	123	1/1	0.94	0.14	37,37,37,37	0
34	NA	0	3062	1/1	0.94	0.11	38,38,38,38	0
32	MG	0	2929	1/1	0.94	0.09	14,14,14,14	0
32	MG	0	2958	1/1	0.94	0.22	33,33,33,33	0
32	MG	0	2942	1/1	0.95	0.21	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	0	3105	1/1	0.95	0.09	59,59,59,59	0
32	MG	0	2994	1/1	0.95	0.14	14,14,14,14	0
35	CL	R	157	1/1	0.95	0.12	55,55,55,55	0
35	CL	0	3107	1/1	0.95	0.09	55,55,55,55	0
34	NA	0	3049	1/1	0.95	0.21	28,28,28,28	0
34	NA	0	3037	1/1	0.95	0.06	61,61,61,61	0
34	NA	0	3066	1/1	0.95	0.05	9,9,9,9	0
32	MG	0	3008	1/1	0.95	0.10	52,52,52,52	0
32	MG	0	2932	1/1	0.96	0.09	10,10,10,10	0
35	CL	J	147	1/1	0.96	0.09	69,69,69,69	0
32	MG	0	3000	1/1	0.96	0.08	7,7,7,7	0
32	MG	0	2960	1/1	0.96	0.21	11,11,11,11	0
32	MG	0	2927	1/1	0.96	0.11	18,18,18,18	0
32	MG	0	2926	1/1	0.96	0.11	17,17,17,17	0
32	MG	0	2978	1/1	0.96	0.06	46,46,46,46	0
32	MG	0	2931	1/1	0.96	0.06	27,27,27,27	0
32	MG	0	2952	1/1	0.97	0.10	4,4,4,4	0
32	MG	T	120	1/1	0.97	0.05	38,38,38,38	0
32	MG	0	2925	1/1	0.97	0.07	5,5,5,5	0
32	MG	0	2995	1/1	0.97	0.05	13,13,13,13	0
36	CD	U	67	1/1	0.97	0.11	134,134,134,134	0
32	MG	0	3002	1/1	0.97	0.13	20,20,20,20	0
34	NA	L	165	1/1	0.97	0.09	42,42,42,42	0
34	NA	0	3036	1/1	0.98	0.15	49,49,49,49	0
32	MG	0	2933	1/1	0.98	0.21	1,1,1,1	0
36	CD	1	57	1/1	0.99	0.07	76,76,76,76	0
32	MG	0	2955	1/1	0.99	0.13	11,11,11,11	0

## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.