



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:38 AM GMT

PDB ID : 3OW2
Title : Crystal Structure of Enhanced Macrolide Bound to 50S Ribosomal Subunit
Authors : Kanyo, Z.F.
Deposited on : 2010-09-17
Resolution : 2.70 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

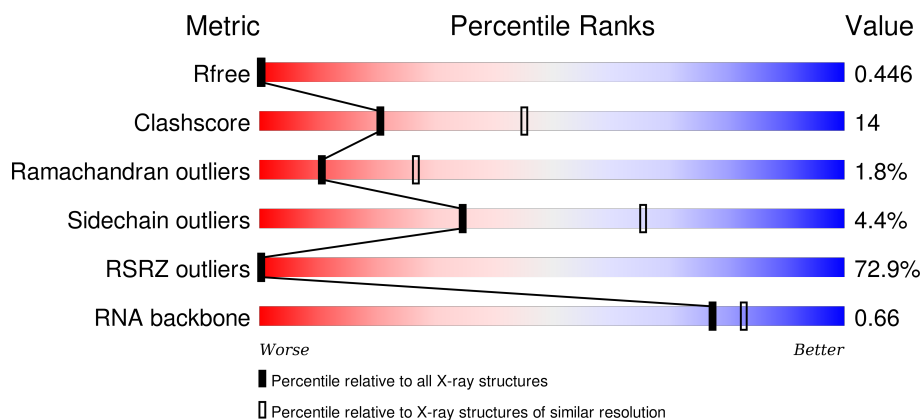
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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

Mol	Chain	Length	Quality of chain
1	0	2902	<div> <div>68%</div> <div>55% 35% 5% 5%</div> </div>
2	9	122	<div> <div>67%</div> <div>51% 39% 9% .</div> </div>
3	A	237	<div> <div>87%</div> <div>67% 28% 5%</div> </div>
4	B	337	<div> <div>75%</div> <div>62% 34% .</div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	165	
7	E	172	
8	F	119	
9	G	62	
10	H	167	
11	I	142	
12	J	132	
13	K	150	
14	L	194	
15	M	186	
16	N	115	
17	O	143	
18	P	95	
19	Q	150	
20	R	81	
21	S	119	
22	T	53	
23	U	65	
24	V	154	
25	W	82	
26	X	142	
27	Y	73	
28	Z	56	
29	1	48	

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Mol	Chain	Length	Quality of chain
30	2	92	<div> <div>75%</div> <div>76%</div> <div>24%</div> </div>

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
31	MG	0	8001	-	-	-	X
31	MG	0	8003	-	-	-	X
31	MG	0	8009	-	-	-	X
31	MG	0	8011	-	-	-	X
31	MG	0	8012	-	-	-	X
31	MG	0	8018	-	-	-	X
31	MG	0	8021	-	-	-	X
31	MG	0	8024	-	-	-	X
31	MG	0	8028	-	-	-	X
31	MG	0	8032	-	-	-	X
31	MG	0	8033	-	-	-	X
31	MG	0	8034	-	-	-	X
31	MG	0	8037	-	-	-	X
31	MG	0	8038	-	-	-	X
31	MG	0	8043	-	-	-	X
31	MG	0	8047	-	-	-	X
31	MG	0	8053	-	-	-	X
31	MG	J	201	-	-	-	X
31	MG	X	301	-	-	-	X
32	K	0	8056	-	-	-	X
33	NA	0	8057	-	-	-	X
33	NA	0	8059	-	-	-	X
33	NA	0	8061	-	-	-	X
33	NA	0	8062	-	-	-	X
33	NA	0	8064	-	-	-	X
33	NA	0	8067	-	-	-	X
33	NA	0	8070	-	-	-	X
33	NA	0	8072	-	-	-	X
33	NA	0	8073	-	-	-	X
33	NA	0	8074	-	-	-	X
33	NA	0	8075	-	-	-	X
33	NA	9	3202	-	-	-	X
33	NA	C	301	-	-	-	X
33	NA	I	201	-	-	-	X
33	NA	L	201	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	NA	P	101	-	-	-	X
33	NA	Q	201	-	-	-	X
33	NA	Q	202	-	-	-	X
34	CL	I	203	-	-	-	X
34	CL	L	202	-	-	-	X
34	CL	N	201	-	-	-	X
35	SR	0	8138	-	-	-	X
35	SR	0	8141	-	-	-	X
35	SR	A	305	-	-	-	X
35	SR	B	402	-	-	-	X
36	EMK	0	8163	-	-	X	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 90725 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
1	0	2754	Total	C	N	O	P	0	0	0
			59016	26346	10878	19047	2745			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	?	-	U	DELETION	GB 3377779
0	?	-	C	DELETION	GB 3377779
0	560	C	U	CONFLICT	GB 3377779
0	2099	A	G	CONFLICT	GB 3377779

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1755	1072	352	326	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	140	Total	C	N	O	S	0	0	0
			1095	685	195	211	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 9 is a protein called 50S ribosomal protein L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	29	Total	C	N	O	S	0	0	0
			241	149	39	52	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	145	Total	C	N	O		0	0	0
			1119	670	222	227				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	143	Total	C	N	O		0	0	0
			1134	680	230	224				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	Q	150	Total	C	N	O	S		
			1150	713	209	224	4	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	81	Total	C	N	O	S		
			642	389	111	139	3	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	53	Total	C	N	O	S		
			411	244	75	87	5	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	65	Total	C	N	O	S		
			500	304	94	101	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	W	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	X	142	Total	C	N	O		0	0	0
			1131	686	228	217				

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

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

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	0	55	Total	Mg	0	0
			55	55		
31	J	1	Total	Mg	0	0
			1	1		
31	K	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
31	B	1	Total 1	Mg 1	0	0
31	X	1	Total 1	Mg 1	0	0
31	9	1	Total 1	Mg 1	0	0
31	S	1	Total 1	Mg 1	0	0

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	1	Total 1	K 1	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	19	Total 19	Na 19	0	0
33	P	1	Total 1	Na 1	0	0
33	Q	2	Total 2	Na 2	0	0
33	I	1	Total 1	Na 1	0	0
33	C	1	Total 1	Na 1	0	0
33	9	1	Total 1	Na 1	0	0
33	L	1	Total 1	Na 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	5	Total 5	Cl 5	0	0
34	Q	1	Total 1	Cl 1	0	0
34	D	1	Total 1	Cl 1	0	0

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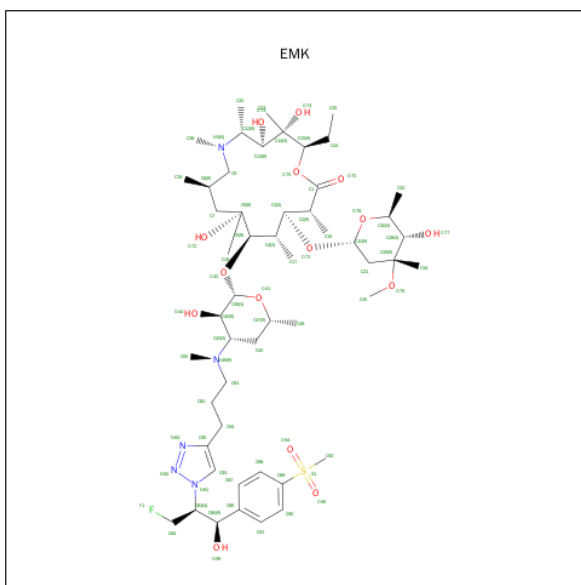
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	I	2	Total 2	Cl 2	0	0
34	A	1	Total 1	Cl 1	0	0
34	N	1	Total 1	Cl 1	0	0
34	X	1	Total 1	Cl 1	0	0
34	L	1	Total 1	Cl 1	0	0

- Molecule 35 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	82	Total 82	Sr 82	0	0
35	Q	1	Total 1	Sr 1	0	0
35	B	2	Total 2	Sr 2	0	0
35	Z	2	Total 2	Sr 2	0	0
35	A	4	Total 4	Sr 4	0	0
35	R	1	Total 1	Sr 1	0	0
35	9	3	Total 3	Sr 3	0	0
35	2	2	Total 2	Sr 2	0	0
35	F	1	Total 1	Sr 1	0	0

- Molecule 36 is (2R,3S,4R,5R,8R,10R,11R,12S,13S,14R)-2-ETHYL-3,4,10-TRIHYDROXY-3,5,6,8,10,12,14-HEPTAMETHYL-15-OXO-11-[(3,4,6-TRIDEOXY-3-{[3-(1-{(1S,2R)-1-(FLUOROMETHYL)-2-HYDROXY-2-[4-(METHYLSULFONYL)PHENYL]ETHYL}-1H-1,2,3-TRIAZOL-4-YL)PROPYL](METHYL)AMINO}-BETA-D-XYLO-HEXOPYRANOSYL)OXY]-1-OXA-6-AZACYCLOPENTADECAN-13-YL 2,6-DIDEOXY-3-C-METHYL-3-O-METHYL-ALPHA-L-RIBO-HEXOPYRANOSIDE (three-letter code: EMK) (formula: C₅₂H₈₈FN₅O₁₅S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
36	0	1	Total	C	F	N	O	S	0	0
			74	52	1	5	15	1		

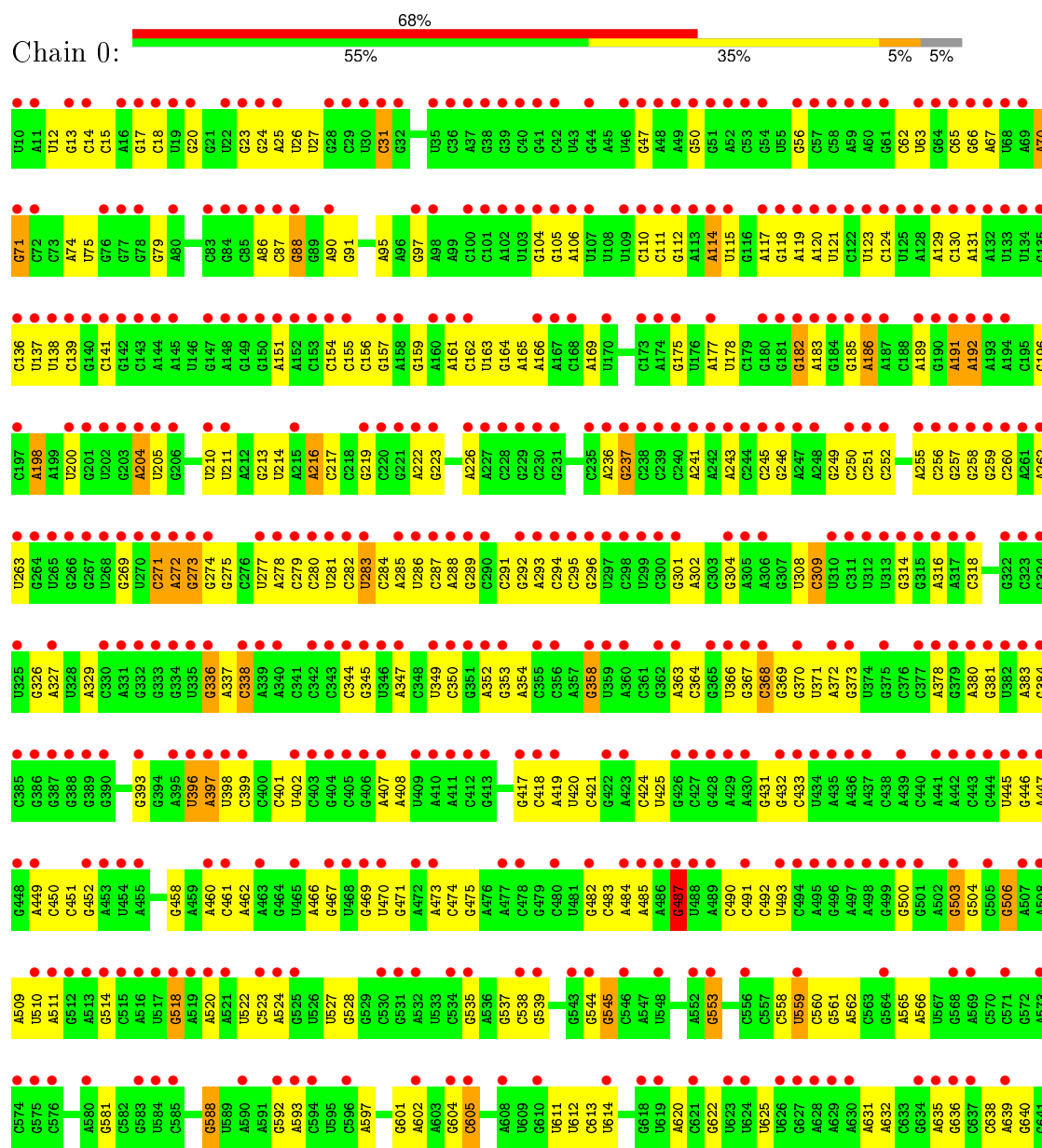
- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	Z	1	Total Cd 1 1	0	0
37	Y	1	Total Cd 1 1	0	0
37	T	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0

3 Residue-property plots [i](#)

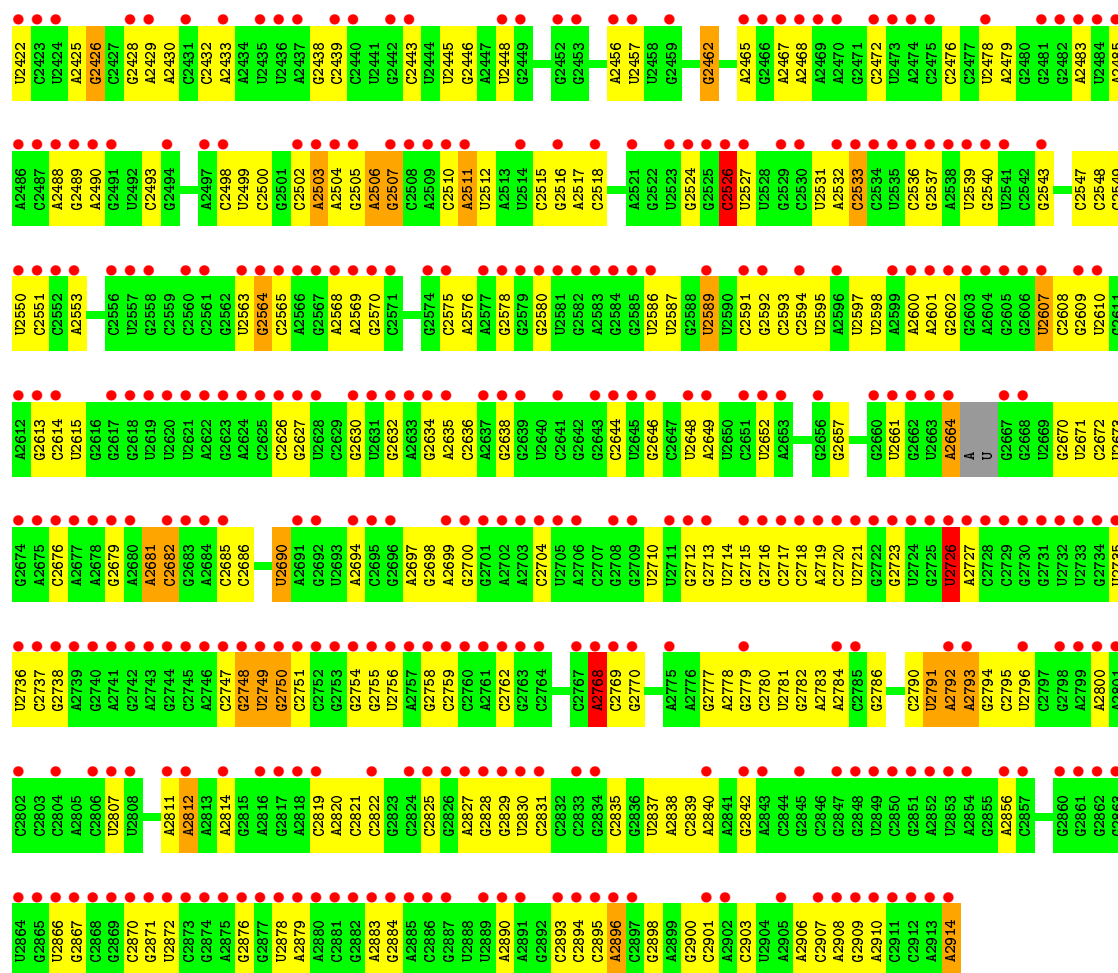
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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

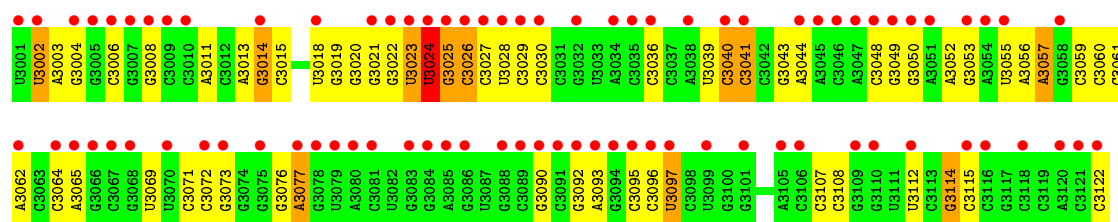




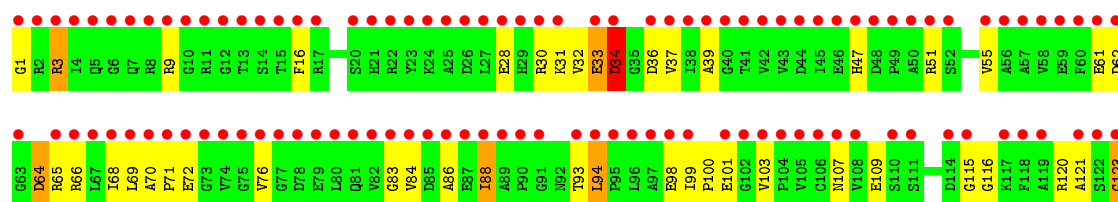
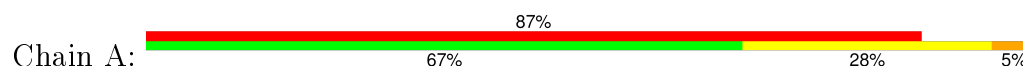
A2356	U2290	G	A	G2110	C2040	U1980	A1919	A1858	C1798	A1737	U1677	G1617	C1557
G2357	A2291	U	C	G2111	G2041	A1981	C1920	A1859	G1799	C1738	A1678	G1618	C1558
C2360	G2292	G	A	A2112	U2042	C1982	A1921	C1860	G1800	G1739	A1679	G1619	A1559
A2361	G2293	A	C	C2113	U2043	C1983	A1922	C1861	A1801	U1740	C1680	C1620	U
A2362	G2294	C	U	G2114	G2044	U1984	G1923	C1862	G1802	U1741	G1681	G1621	C1561
C2363	G2295	U	A	C2115	C2045	U1985	A1924	G1863	C1803	A1742	A1682	G1622	C1562
A2364	C2296	C	C	U2116	G2046	C1986	G1925	C1864	A1804	G1743	G1683	C1623	C1563
A2367	G2297	C	C	U2117	C2047	C1987	G1926	A1865	G1805	G1744	A1684	C1624	C1564
A2368	A2300	A	C	A2118	C2048	C1988	A1927	A1866	G1806	G1745	A1685	U1625	C1565
A2369	A2301	G	A	C2119	G2049	C1989	G1928	G1867	G1807	A1746	C1686	G1626	C1566
A2370	A2302	U	G	U2120	G2050	C1990	G1929	G1868	C1808	A1747	C1687	A1627	U1567
G2371	A2303	U	U	G2121	G2051	A1991	A1930	A1869	G1809	U1748	G1688	G1628	U1568
A2372	G2304	A	A	C2122	U2052	U1992	A1931	C1870	C1810	U1749	A1689	A1629	U1569
U2373	G2310	C	C	G2123	G2053	C1993	G1932	U1871	A1811	C1750	C1690	A1630	C1570
A2374	A2311	C	C	G2124	A2054	A1994	G1933	C1872	G1812	G1751	C1691	A1631	G1571
G2375	A2312	C	C	G2125	U2055	U1996	A1934	G1873	U1813	G1752	C1692	A1632	A1572
C2376	G2313	C	C	C2126	U2056	C1997	U1937	A1874	G1814	C1753	G1693	G1633	A1573
U2377	G2314	C	C	U2127	G2057	C1998	G1938	G1875	A1815	A1754	G1694	G1634	C1574
U2378	G2315	C	C	G2128	G2058	G1999	U1939	G1876	C1816	A1755	G1695	U1635	C1575
A2379	G2316	C	C	U2129	U2063	G2000	U1940	G1877	U1817	G1756	U1696	G1636	U1576
G2380	G2317	U	A	C2130	U2064	G2001	C1941	U1878	G1818	U1757	G1697	A1637	U1577
C2381	G2318	C	A	G2131	C2065	C2002	A1942	C1880	G1819	U1758	C1698	U1638	C1578
C2382	C2319	C	G	C2132	C2066	U2003	G1943	A1881	G1820	A1759	C1699	U1639	C1579
U2383	U2320	C	C	U2133	U2069	U2004	G1944	A1882	A1821	G1760	C1700	C1640	A1580
G2384	A2321	G	G	G2134	U2070	G2005	G1945	U1883	A1822	U1761	A1641	C1641	A1581
U2385	G2324	G	G	A2135	G2070	C2006	C1946	A1884	G1823	C1762	U1702	A1642	C1582
U2386	G2325	C	C	G2136	C2071	A2007	G1947	A1885	U1824	C1763	C1643	C1643	C1583
U2387	G2326	C	C	C	G2072	U2008	G1948	A1886	U1825	G1764	G1704	U1644	C1584
C2388	U2326	C	C	C	G2073	G2009	G1949	U1887	G1826	U1765	G1705	U1645	C1585
U2389	U2327	C	C	U	A2074	A2010	G1950	A1889	G1827	U1766	G1646	G1586	C1586
U2390	U2328	C	C	U	C2077	A2011	G1951	U1890	A1828	A1767	G1707	G1647	U1587
C2391	U2329	C	C	G	U2078	U2012	U	G1891	A1829	C1768	C1708	G1648	U1588
A2395	U2330	C	A	U	G2079	G2013	A	C1892	U1831	U1770	A1710	G1649	C1589
C2396	C2331	C	A	C	G2080	G2014	A	C1893	G1832	U1771	C1651	C1650	A1590
C2397	A2332	U	U	G	A2081	A2015	C	A1894	U1833	G1772	A1712	C1652	C1592
C2398	C2333	C	C	C	G2082	U2016	U	G1895	C1834	G1773	G1713	A1653	C1593
C2399	C2334	C	C	C	A2083	U2017	A	G1896	U1835	G1774	C1714	U1654	C1594
G2400	C2335	C	A	C	A2084	A2018	U	U1897	A1836	A1775	C1715	G1655	C1595
A2401	C2336	C	A	C	A2085	A2019	G	G1898	G1837	A1776	G1716	G1656	U1596
A2402	G2337	C	A	U	C2086	C2020	A	C1899	U1838	G1777	A1657	A1657	A1597
C2405	G2338	C	C	U	A2089	C2021	C	A1900	A1839	A1778	G1718	A1658	U1598
U2406	A	U	U	U	G2090	A2022	C	G1901	A1840	A1779	G1719	A1659	U1599
G2407	C	U	U	G	G2091	G2023	U1964	U1902	C1841	G1780	C1720	G1660	U1600
A2408	G	C	G	C	G2092	A2024	C1965	U1903	A1842	U1781	C1721	A1661	G1601
C2409	A	A	A	A	G2093	G2025	U1966	A1904	A1843	U1782	U1722	C1662	C1602
G2410	G2344	U	U	C	G2094	C2026	U1967	U1905	C1844	U1783	G1723	G1663	A1603
C2411	A2345	U	U	C	A2095	U2027	A1968	C1906	A1845	G1784	U1724	A1664	G1604
G2412	C2346	C	C	A	A2096	U2028	A1969	U1907	U1846	G1785	G1725	G1665	C1605
A2413	C2347	C	C	U	U2097	G2029	G1970	G1908	A1847	C1787	G1726	C1666	A1606
A2414	C2348	U	U	A	A2099	A2030	G1971	A1909	G1848	U1788	G1727	A1667	U1607
G2415	G2349	C	C	G	U2100	G2031	U1972	U1910	G1849	G1789	G1728	U1668	A1608
G2416	G2350	C	C	G	A2101	U2032	A1973	A1911	U1850	C1790	A1729	A1669	C1609
G2417	C2351	C	U	A	G2102	G2033	G1974	A1912	G1851	U1791	G1730	G1670	G1610
G2418	G2352	C	C	U	A2103	U2034	C1975	C1913	A1852	C1792	G1731	U1671	A1611
U2419	A2353	G	G	G	C2104	C2035	G1976	U1914	C1853	G1793	A1732	G1672	A1612
G2420	G2354	U	U	G	C2105	C2036	G1977	U1915	C1854	G1794	A1733	U1673	C1613
A2421	G2355	C	C	G	C2106	C2037	A1978	C1916	G1855	G1795	C1734	U1674	G1614
		G	G	G	U2107	A2038	G1979	G1917	C1856	A1796	C1735	C1675	A1615
			G	G		A2039	G1979	U1918	A1857	A1797	A1736	G1676	A1616

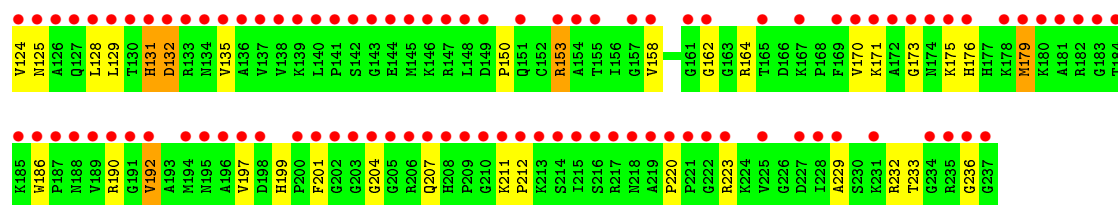


• Molecule 2: 5S RIBOSOMAL RNA

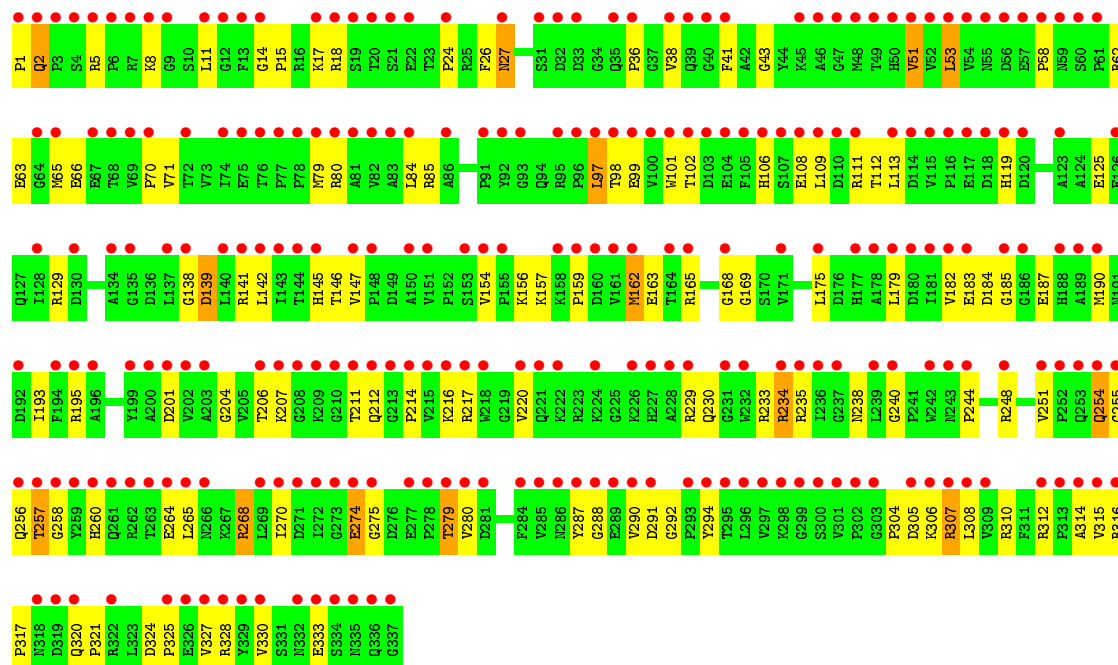
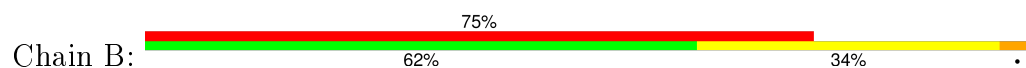


• Molecule 3: 50S ribosomal protein L2P

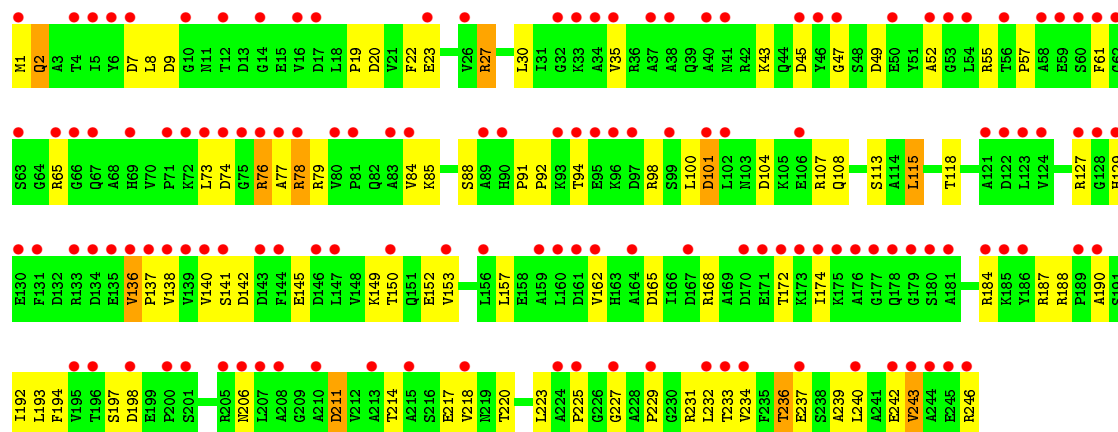




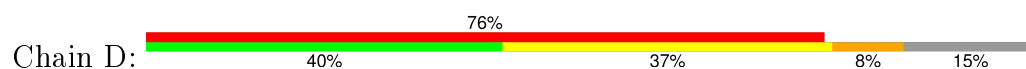
• Molecule 4: 50S ribosomal protein L3P

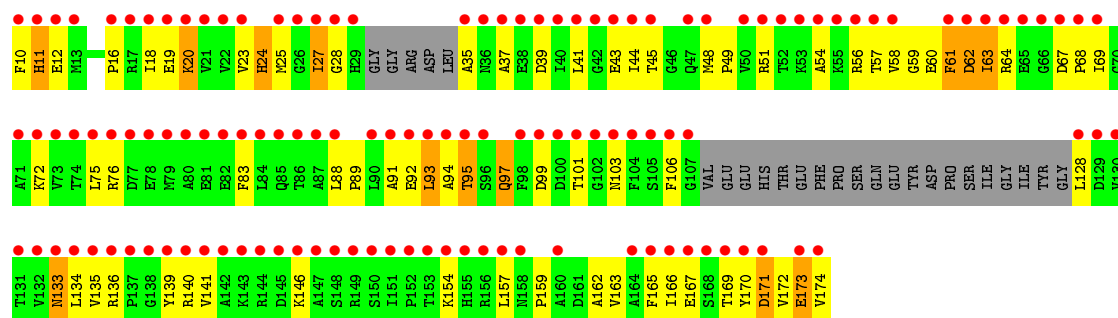


• Molecule 5: 50S ribosomal protein L4P

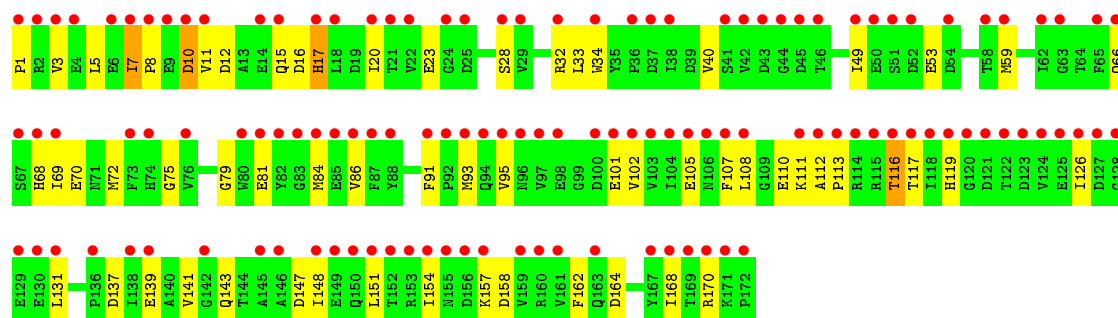


• Molecule 6: 50S ribosomal protein L5P

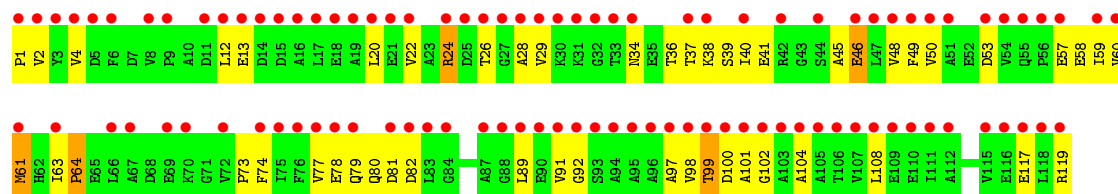
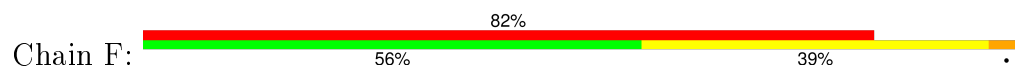




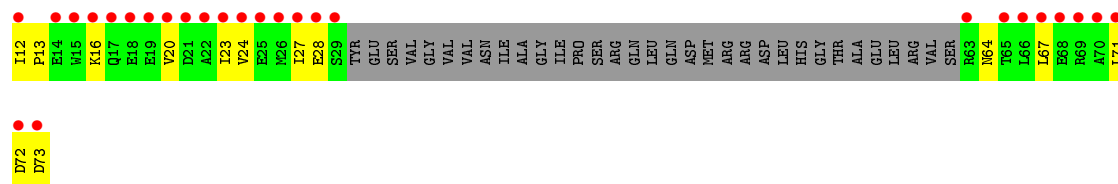
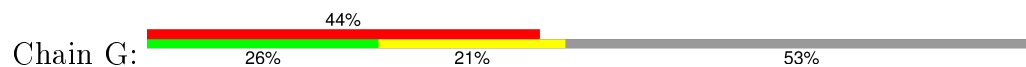
• Molecule 7: 50S ribosomal protein L6P



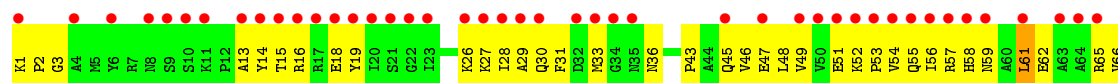
• Molecule 8: 50S ribosomal protein L7Ae

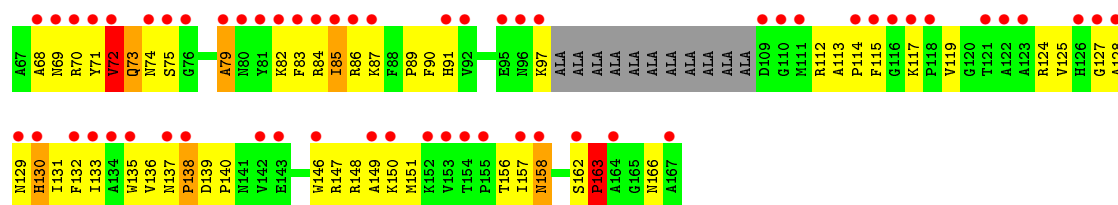


• Molecule 9: 50S ribosomal protein L10E

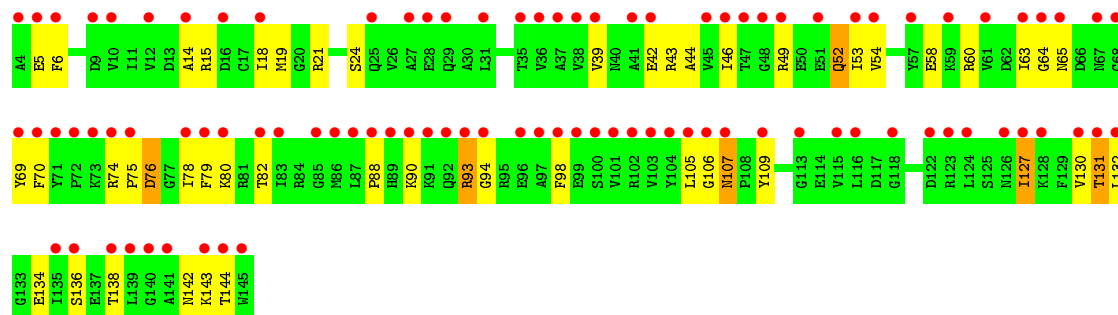


• Molecule 10: 50S ribosomal protein L10e

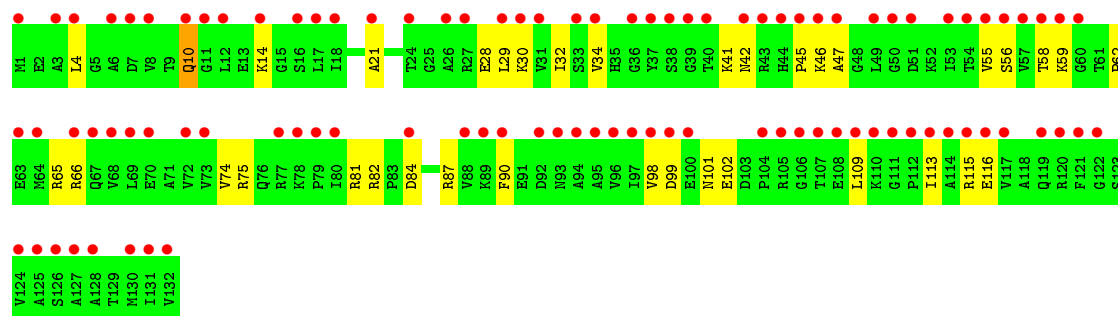




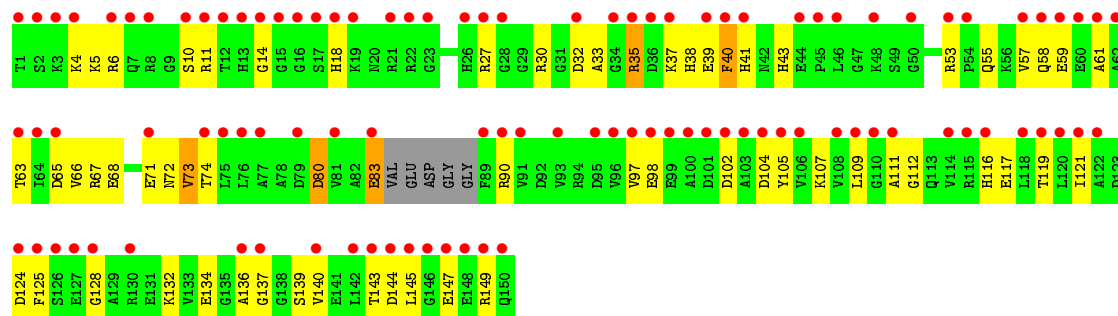
• Molecule 11: 50S ribosomal protein L13P



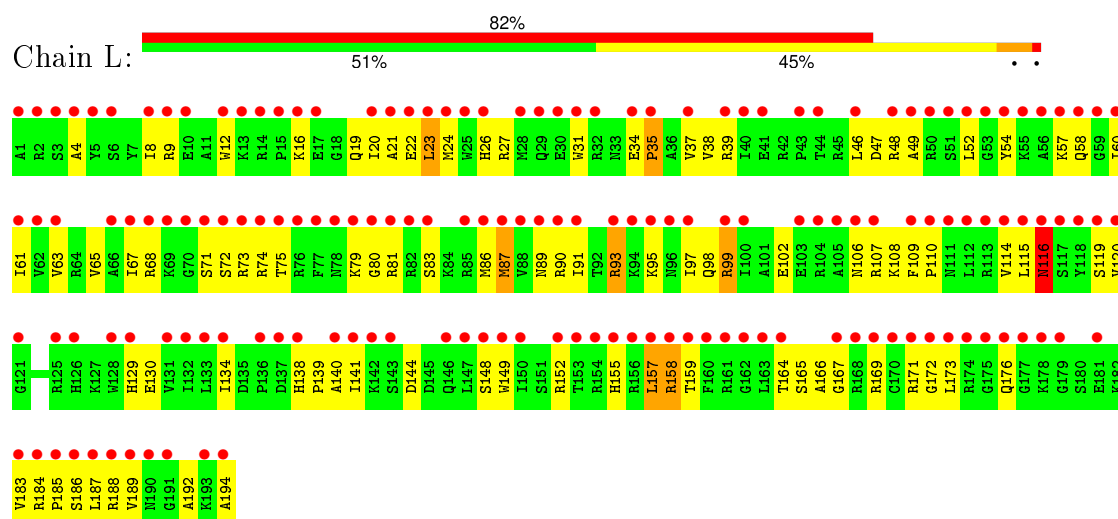
• Molecule 12: 50S ribosomal protein L14P



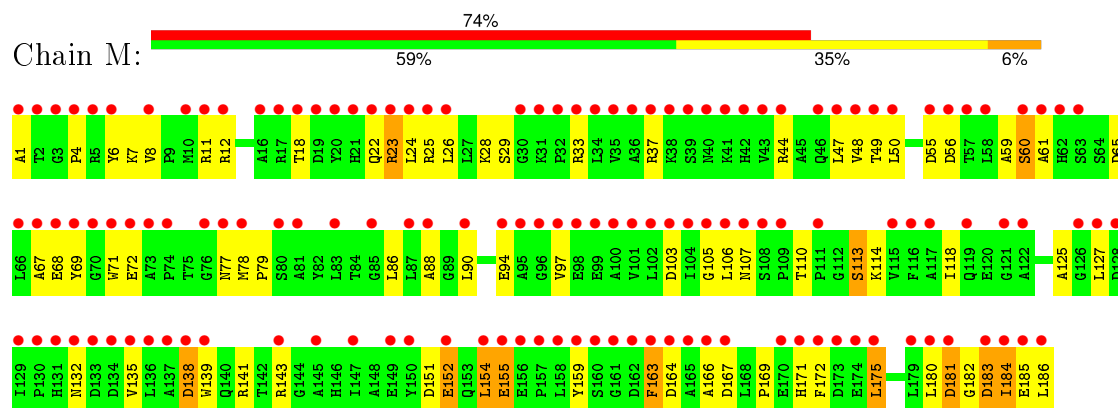
• Molecule 13: 50S ribosomal protein L15P



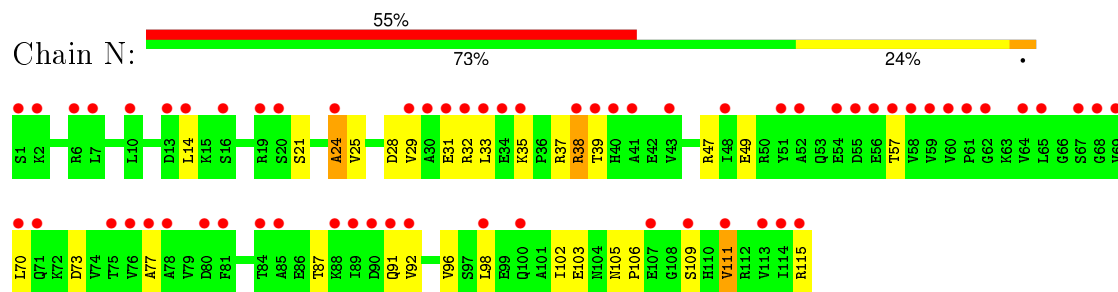
• Molecule 14: 50S ribosomal protein L15e



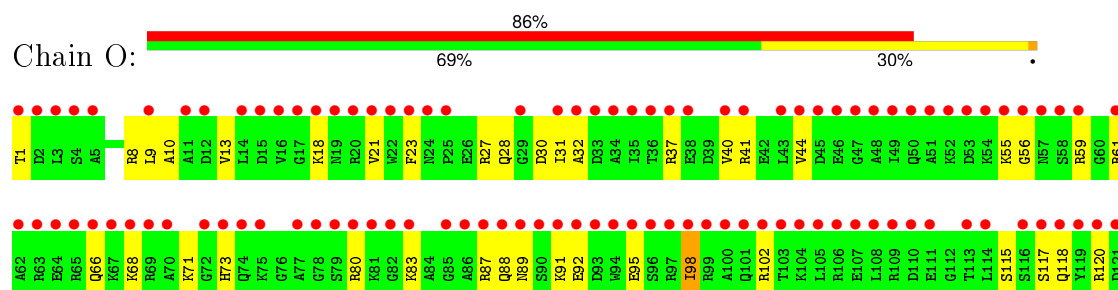
• Molecule 15: 50S ribosomal protein L18P

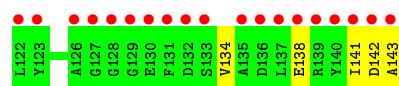


• Molecule 16: 50S ribosomal protein L18e

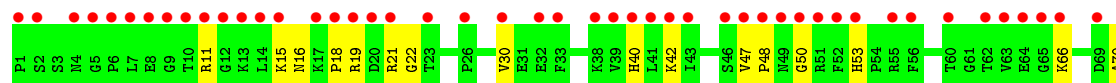
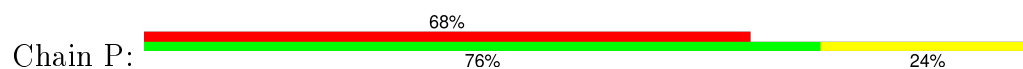


• Molecule 17: 50S ribosomal protein L19e

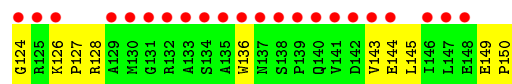
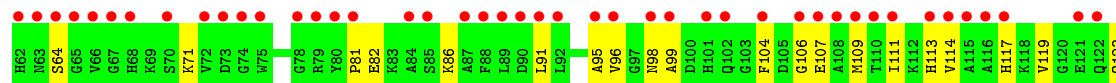
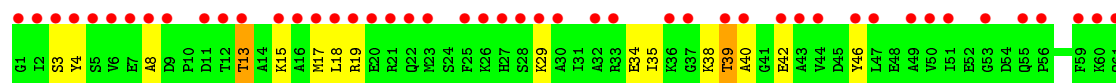
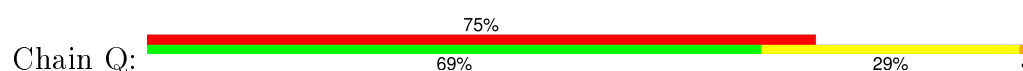




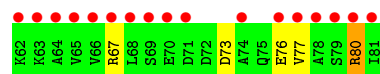
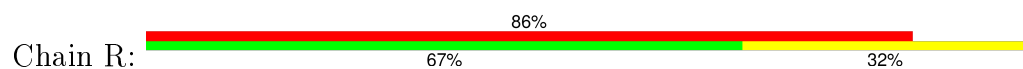
• Molecule 18: 50S ribosomal protein L21e



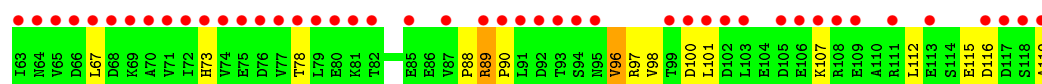
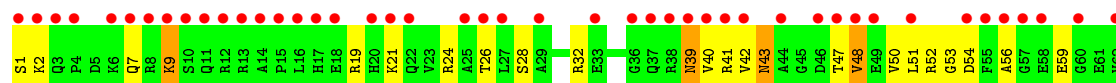
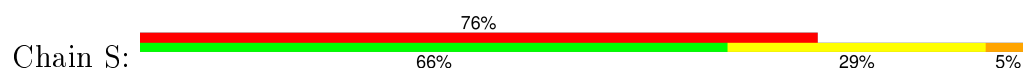
• Molecule 19: 50S ribosomal protein L22P



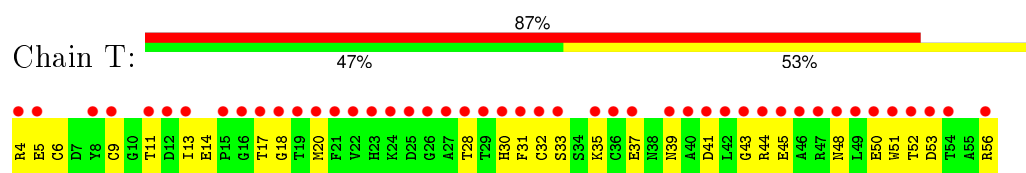
• Molecule 20: 50S ribosomal protein L23P



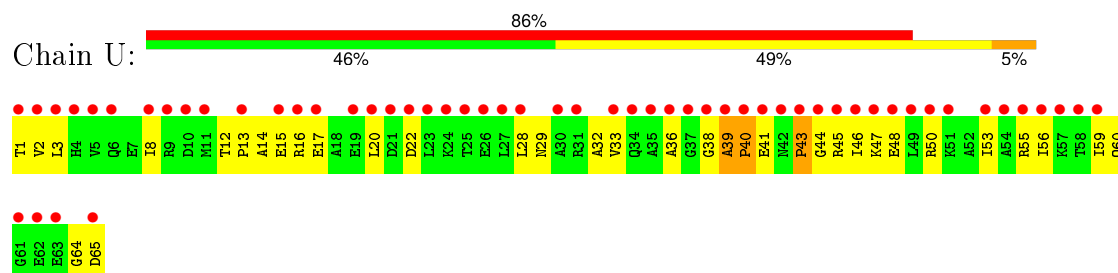
• Molecule 21: 50S ribosomal protein L24P



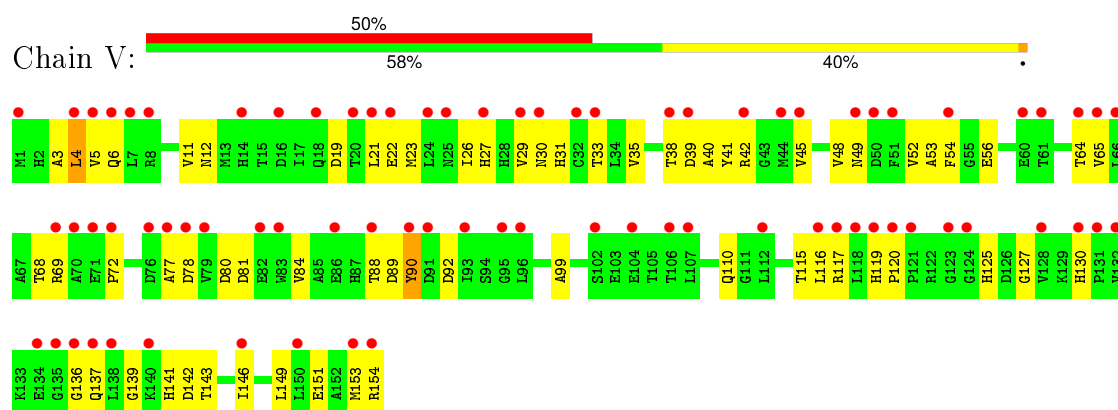
• Molecule 22: 50S ribosomal protein L24e



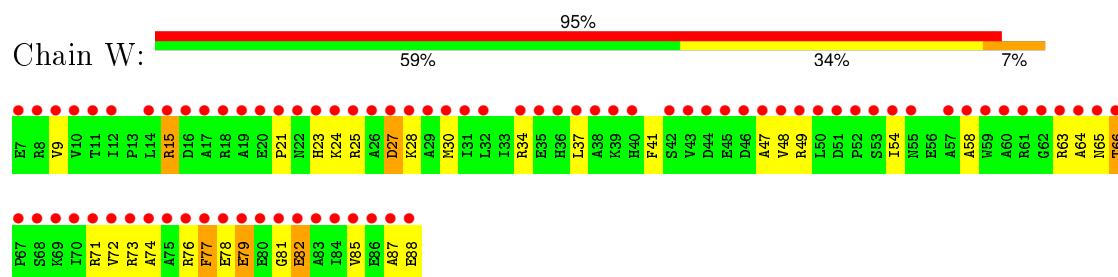
• Molecule 23: 50S ribosomal protein L29P



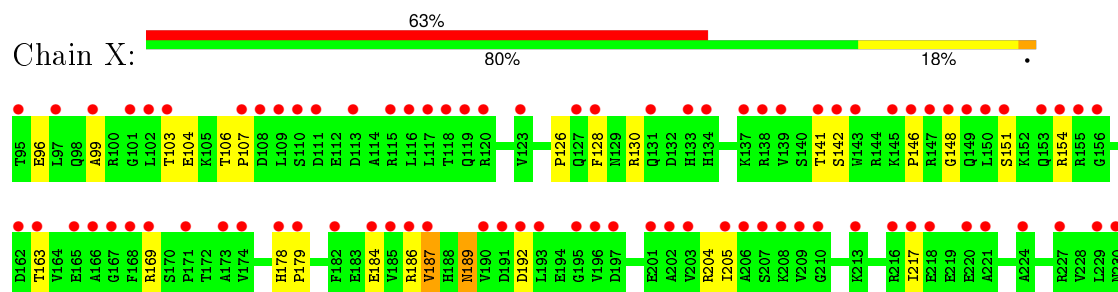
• Molecule 24: 50S ribosomal protein L30P

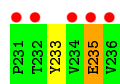


• Molecule 25: 50S ribosomal protein L31e

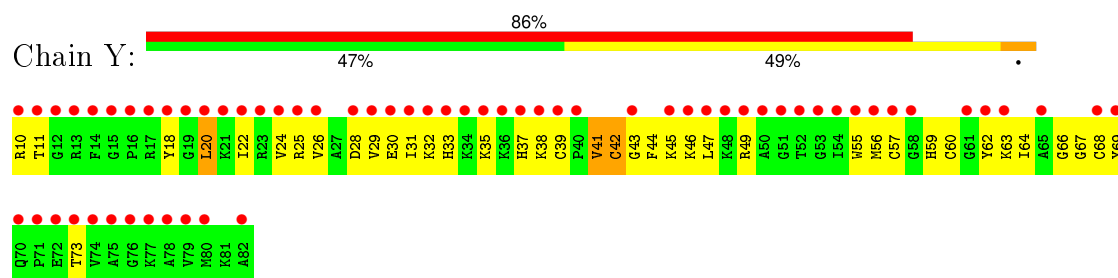


• Molecule 26: 50S ribosomal protein L32e

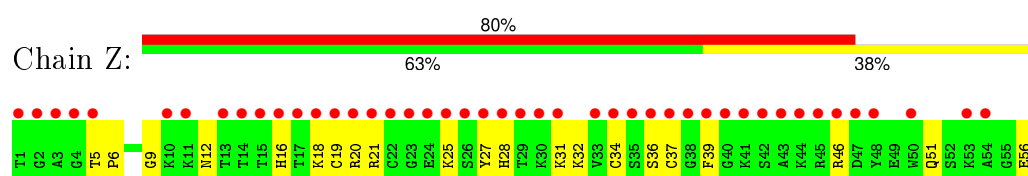




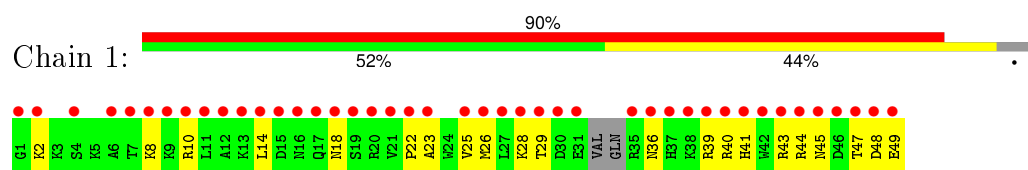
- Molecule 27: 50S ribosomal protein L37Ae



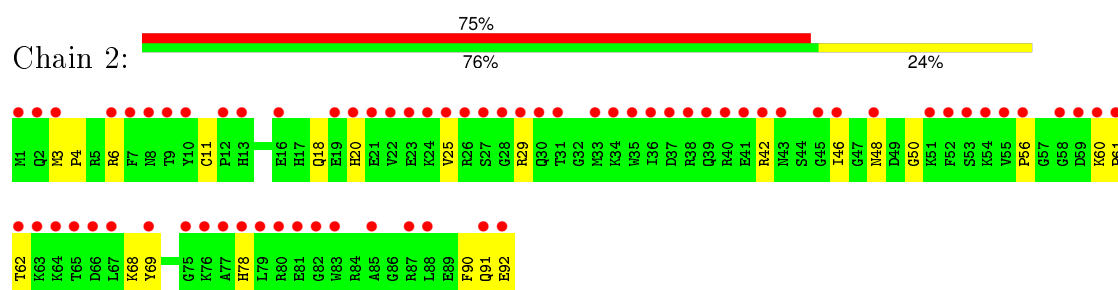
- Molecule 28: 50S ribosomal protein L37e



- Molecule 29: 50S ribosomal protein L39e



- Molecule 30: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.85Å 298.00Å 574.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 49.90 – 2.72	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-2.70) 90.9 (49.90-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.73Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.222 , 0.253 0.456 , 0.446	Depositor DCC
R_{free} test set	3128 reflections (0.71%)	DCC
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 454618 reflections	Xtriage
F_o, F_c correlation	0.58	EDS
Total number of atoms	90725	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.02% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, EMK, CD, SR

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	0.41	0/66075	0.69	18/103050 (0.0%)
2	9	0.37	0/2905	0.72	2/4528 (0.0%)
3	A	0.36	0/1788	0.66	0/2409
4	B	0.39	0/2690	0.67	0/3652
5	C	0.39	0/1884	0.65	0/2551
6	D	0.32	0/1112	0.58	0/1498
7	E	0.35	0/1383	0.59	0/1880
8	F	0.37	0/897	0.58	0/1219
9	G	0.30	0/242	0.45	0/324
10	H	0.40	0/1247	0.74	1/1686 (0.1%)
11	I	0.38	0/1136	0.63	0/1530
12	J	0.39	0/1004	0.70	0/1351
13	K	0.39	0/1131	0.68	0/1509
14	L	0.39	0/1634	0.69	1/2180 (0.0%)
15	M	0.32	0/1474	0.61	0/1999
16	N	0.33	0/874	0.62	0/1181
17	O	0.37	0/1144	0.57	0/1521
18	P	0.38	0/749	0.72	0/1005
19	Q	0.36	0/1173	0.63	0/1578
20	R	0.36	0/649	0.58	0/875
21	S	0.35	0/958	0.65	0/1289
22	T	0.39	0/418	0.59	0/562
23	U	0.31	0/503	0.52	0/675
24	V	0.36	0/1219	0.65	0/1655
25	W	0.36	0/665	0.60	0/895
26	X	0.38	0/1147	0.66	0/1536
27	Y	0.40	0/576	0.71	0/763
28	Z	0.49	0/438	0.70	0/578
29	1	0.37	0/399	0.60	0/527
30	2	0.41	0/771	0.60	0/1024
All	All	0.40	0/98285	0.68	22/147030 (0.0%)

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	0	75
2	9	1	2
24	V	0	1
All	All	1	78

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	9.36	130.09	109.50
1	0	1559	A	C2'-C3'-O3'	8.36	127.88	109.50
1	0	2338	G	C2'-C3'-O3'	7.19	125.32	109.50
1	0	1120	U	C5'-C4'-C3'	-6.74	105.22	116.00
1	0	777	U	O4'-C1'-N1	6.46	113.37	108.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	9	3024	U	C3'

5 of 78 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	216	A	Sidechain
1	0	314	G	Sidechain
1	0	396	U	Sidechain
1	0	50	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59016	0	29808	892	0
2	9	2600	0	1326	67	0
3	A	1755	0	1763	77	0
4	B	2625	0	2533	124	0
5	C	1859	0	1816	85	0
6	D	1095	0	1085	84	0
7	E	1358	0	1266	53	0
8	F	886	0	854	50	0
9	G	241	0	231	8	0
10	H	1216	0	1215	132	0
11	I	1120	0	1098	57	0
12	J	994	0	1027	37	0
13	K	1119	0	1076	57	0
14	L	1606	0	1676	123	0
15	M	1445	0	1401	69	0
16	N	865	0	873	23	0
17	O	1134	0	1127	42	0
18	P	735	0	729	17	0
19	Q	1150	0	1122	53	0
20	R	642	0	605	25	0
21	S	950	0	924	31	0
22	T	411	0	364	22	0
23	U	500	0	511	32	0
24	V	1196	0	1137	69	0
25	W	655	0	653	35	0
26	X	1131	0	1133	26	0
27	Y	564	0	598	46	0
28	Z	431	0	426	24	0
29	1	394	0	406	24	0
30	2	755	0	729	22	0
31	0	55	0	0	0	0
31	9	1	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	K	1	0	0	0	0
31	S	1	0	0	0	0
31	X	1	0	0	0	0
32	0	1	0	0	0	0
33	0	19	0	0	0	0
33	9	1	0	0	0	0
33	C	1	0	0	0	0
33	I	1	0	0	0	0
33	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	P	1	0	0	0	0
33	Q	2	0	0	0	0
34	0	5	0	0	0	0
34	A	1	0	0	0	0
34	D	1	0	0	0	0
34	I	2	0	0	0	0
34	L	1	0	0	1	0
34	N	1	0	0	0	0
34	Q	1	0	0	0	0
34	X	1	0	0	0	0
35	0	82	0	0	0	0
35	2	2	0	0	0	0
35	9	3	0	0	0	0
35	A	4	0	0	0	0
35	B	2	0	0	0	0
35	F	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	Z	2	0	0	0	0
36	0	74	0	88	30	0
37	2	1	0	0	0	0
37	T	1	0	0	0	0
37	Y	1	0	0	0	0
37	Z	1	0	0	0	0
All	All	90725	0	59600	2169	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 14.

The worst 5 of 2169 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)
36:0:8163:EMK:C15	36:0:8163:EMK:C14	1.75	1.63
36:0:8163:EMK:C20	36:0:8163:EMK:C12	1.76	1.58
36:0:8163:EMK:C13	36:0:8163:EMK:C14	1.78	1.58
36:0:8163:EMK:C8	36:0:8163:EMK:C9	1.75	1.57
36:0:8163:EMK:N9	36:0:8163:EMK:C12	1.71	1.49

There are no symmetry-related clashes.

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	
3	A	235/237 (99%)	209 (89%)	21 (9%)	5 (2%)	9	23
4	B	335/337 (99%)	309 (92%)	20 (6%)	6 (2%)	11	27
5	C	244/246 (99%)	229 (94%)	13 (5%)	2 (1%)	24	51
6	D	134/165 (81%)	103 (77%)	20 (15%)	11 (8%)	1	1
7	E	170/172 (99%)	160 (94%)	9 (5%)	1 (1%)	30	59
8	F	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	11	29
9	G	25/62 (40%)	23 (92%)	1 (4%)	1 (4%)	4	8
10	H	152/167 (91%)	134 (88%)	13 (9%)	5 (3%)	5	11
11	I	140/142 (99%)	130 (93%)	7 (5%)	3 (2%)	9	23
12	J	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	24	51
13	K	141/150 (94%)	117 (83%)	22 (16%)	2 (1%)	14	35
14	L	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	19	45
15	M	184/186 (99%)	159 (86%)	17 (9%)	8 (4%)	3	7
16	N	113/115 (98%)	107 (95%)	5 (4%)	1 (1%)	21	49
17	O	141/143 (99%)	137 (97%)	4 (3%)	0	100	100
18	P	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	17	42
19	Q	148/150 (99%)	138 (93%)	9 (6%)	1 (1%)	26	55
20	R	79/81 (98%)	74 (94%)	5 (6%)	0	100	100
21	S	117/119 (98%)	111 (95%)	4 (3%)	2 (2%)	11	29
22	T	51/53 (96%)	47 (92%)	4 (8%)	0	100	100
23	U	63/65 (97%)	58 (92%)	1 (2%)	4 (6%)	2	2
24	V	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	26	55
25	W	80/82 (98%)	71 (89%)	5 (6%)	4 (5%)	3	5
26	X	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
27	Y	71/73 (97%)	63 (89%)	5 (7%)	3 (4%)	3	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Z	54/56 (96%)	46 (85%)	8 (15%)	0	100	100
29	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
30	2	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	17	42
All	All	3633/3777 (96%)	3317 (91%)	249 (7%)	67 (2%)	11	27

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	63	ILE
6	D	93	LEU
6	D	95	THR
6	D	173	GLU

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	
3	A	179/179 (100%)	168 (94%)	11 (6%)	23	49
4	B	282/282 (100%)	264 (94%)	18 (6%)	22	47
5	C	193/193 (100%)	179 (93%)	14 (7%)	17	39
6	D	117/138 (85%)	113 (97%)	4 (3%)	44	75
7	E	152/152 (100%)	148 (97%)	4 (3%)	54	83
8	F	92/92 (100%)	88 (96%)	4 (4%)	35	66
9	G	27/55 (49%)	27 (100%)	0	100	100
10	H	122/122 (100%)	113 (93%)	9 (7%)	17	39
11	I	118/118 (100%)	110 (93%)	8 (7%)	20	43
12	J	106/106 (100%)	104 (98%)	2 (2%)	65	88
13	K	113/116 (97%)	106 (94%)	7 (6%)	23	49
14	L	166/166 (100%)	158 (95%)	8 (5%)	31	62
15	M	149/149 (100%)	142 (95%)	7 (5%)	32	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	93/93 (100%)	89 (96%)	4 (4%)	35	66
17	O	113/113 (100%)	112 (99%)	1 (1%)	84	95
18	P	79/79 (100%)	77 (98%)	2 (2%)	55	84
19	Q	117/117 (100%)	114 (97%)	3 (3%)	54	83
20	R	71/71 (100%)	70 (99%)	1 (1%)	74	92
21	S	105/105 (100%)	98 (93%)	7 (7%)	20	44
22	T	44/44 (100%)	44 (100%)	0	100	100
23	U	51/51 (100%)	50 (98%)	1 (2%)	63	87
24	V	130/130 (100%)	126 (97%)	4 (3%)	47	78
25	W	66/66 (100%)	61 (92%)	5 (8%)	16	37
26	X	120/120 (100%)	115 (96%)	5 (4%)	36	68
27	Y	56/56 (100%)	55 (98%)	1 (2%)	66	89
28	Z	46/46 (100%)	46 (100%)	0	100	100
29	1	42/44 (96%)	41 (98%)	1 (2%)	57	85
30	2	79/79 (100%)	78 (99%)	1 (1%)	76	92
All	All	3028/3082 (98%)	2896 (96%)	132 (4%)	35	65

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	85	ILE
12	J	84	ASP
25	W	49	ARG
10	H	138	PRO
11	I	79	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
14	L	89	ASN
19	Q	61	GLN
28	Z	16	HIS
15	M	93	GLN
17	O	73	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2902 (94%)	233 (8%)	22 (0%)
2	9	121/122 (99%)	14 (11%)	2 (1%)
All	All	2866/3024 (94%)	247 (8%)	24 (0%)

5 of 247 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	70	A
1	0	71	G
1	0	86	A

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1237	U
1	0	1752	G
2	9	3024	U
1	0	1352	A
1	0	1684	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 ⓘ

Of 204 ligands modelled in this entry, 203 are monoatomic - leaving 1 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	EMK	0	8163	-	76,78,78	5.74	57 (75%)	103,118,118	3.39	39 (37%)

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
36	EMK	0	8163	-	-	0/92/133/133	0/5/5/5

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	0	8163	EMK	O42-C5	-11.11	1.13	1.44
36	0	8163	EMK	O73-C13	2.00	1.47	1.42
36	0	8163	EMK	N82-N81	2.06	1.38	1.34
36	0	8163	EMK	C93-N81	2.16	1.38	1.35
36	0	8163	EMK	O76-C35	2.47	1.51	1.43

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	8163	EMK	C7-C8-C9	-14.23	91.72	112.39
36	0	8163	EMK	C81-N46-C43	-8.91	96.03	112.72
36	0	8163	EMK	C6-C7-C8	-7.80	100.28	117.42
36	0	8163	EMK	O73-C13-C14	-6.79	95.36	106.79
36	0	8163	EMK	C15-O75-C1	-5.75	108.43	118.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	0	8163	EMK	30	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	0	2754/2902 (94%)	2.74	1966 (71%) 0 0	18, 37, 79, 130	0
2	9	122/122 (100%)	2.40	82 (67%) 0 0	30, 54, 76, 135	0
3	A	237/237 (100%)	3.85	206 (86%) 0 0	21, 41, 70, 88	0
4	B	337/337 (100%)	3.18	252 (74%) 0 0	21, 42, 67, 79	0
5	C	246/246 (100%)	2.33	136 (55%) 0 0	20, 37, 59, 70	0
6	D	140/165 (84%)	4.35	125 (89%) 0 0	49, 82, 103, 111	0
7	E	172/172 (100%)	2.98	122 (70%) 0 0	37, 55, 72, 78	0
8	F	119/119 (100%)	3.98	97 (81%) 0 0	39, 60, 86, 91	0
9	G	29/62 (46%)	4.18	27 (93%) 0 0	65, 81, 86, 91	0
10	H	156/167 (93%)	2.71	102 (65%) 0 0	28, 47, 72, 78	0
11	I	142/142 (100%)	2.92	94 (66%) 0 0	29, 40, 56, 75	0
12	J	132/132 (100%)	3.14	96 (72%) 0 0	26, 38, 60, 71	0
13	K	145/150 (96%)	2.94	101 (69%) 0 0	21, 52, 89, 104	0
14	L	194/194 (100%)	3.34	160 (82%) 0 0	27, 37, 51, 58	0
15	M	186/186 (100%)	3.09	138 (74%) 0 0	34, 52, 93, 104	0
16	N	115/115 (100%)	2.30	63 (54%) 0 0	33, 45, 60, 65	0
17	O	143/143 (100%)	4.04	123 (86%) 0 0	29, 42, 54, 64	0
18	P	95/95 (100%)	2.73	65 (68%) 0 0	29, 38, 53, 66	0
19	Q	150/150 (100%)	3.15	113 (75%) 0 0	24, 35, 52, 60	0
20	R	81/81 (100%)	3.89	70 (86%) 0 0	35, 49, 69, 77	0
21	S	119/119 (100%)	3.20	90 (75%) 0 0	33, 44, 66, 91	0
22	T	53/53 (100%)	3.94	46 (86%) 0 0	34, 42, 60, 70	0
23	U	65/65 (100%)	4.32	56 (86%) 0 0	44, 64, 98, 105	0
24	V	154/154 (100%)	2.23	77 (50%) 0 0	28, 39, 56, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å²)	Q<0.9	
25	W	82/82 (100%)	4.67	78 (95%)	0 0	34, 46, 69, 87	0
26	X	142/142 (100%)	2.65	89 (62%)	0 0	22, 34, 55, 73	0
27	Y	73/73 (100%)	4.57	63 (86%)	0 0	39, 52, 64, 74	0
28	Z	56/56 (100%)	2.78	45 (80%)	0 0	21, 27, 32, 42	0
29	1	46/48 (95%)	4.28	43 (93%)	0 0	27, 45, 63, 80	0
30	2	92/92 (100%)	3.14	69 (75%)	0 0	25, 44, 55, 66	0
All	All	6577/6801 (96%)	3.02	4794 (72%)	0 0	18, 41, 80, 135	0

The worst 5 of 4794 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	W	58	ALA	16.2
25	W	10	VAL	15.0
25	W	85	VAL	14.6
8	F	20	LEU	13.7
27	Y	19	GLY	13.7

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
32	K	0	8056	1/1	0.29	2.09	54.47	88,88,88,88	0
33	NA	0	8064	1/1	-0.30	1.23	24.81	61,61,61,61	0
33	NA	0	8075	1/1	0.35	0.96	22.55	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	9	3202	1/1	0.00	1.04	21.40	93,93,93,93	0
33	NA	0	8057	1/1	0.56	0.84	19.62	46,46,46,46	0
33	NA	0	8072	1/1	0.10	0.84	19.23	61,61,61,61	0
31	MG	0	8028	1/1	0.34	0.97	10.08	48,48,48,48	0
31	MG	0	8033	1/1	0.42	0.72	9.77	62,62,62,62	0
33	NA	0	8070	1/1	0.56	0.65	8.94	69,69,69,69	0
31	MG	0	8047	1/1	0.30	0.63	7.61	49,49,49,49	0
31	MG	0	8003	1/1	0.43	0.56	7.47	43,43,43,43	0
31	MG	0	8043	1/1	0.34	0.67	6.75	63,63,63,63	0
35	SR	0	8141	1/1	0.38	0.59	6.59	160,160,160,160	0
35	SR	B	402	1/1	0.66	0.58	6.46	90,90,90,90	0
33	NA	0	8074	1/1	0.15	0.67	6.36	60,60,60,60	0
31	MG	0	8018	1/1	0.15	0.56	5.89	47,47,47,47	0
33	NA	Q	201	1/1	0.63	0.54	5.50	57,57,57,57	0
34	CL	N	201	1/1	0.36	0.65	5.39	74,74,74,74	0
31	MG	0	8024	1/1	0.72	0.44	5.23	20,20,20,20	0
31	MG	0	8009	1/1	0.57	0.55	5.21	35,35,35,35	0
33	NA	0	8061	1/1	0.40	0.56	5.16	56,56,56,56	0
31	MG	0	8034	1/1	0.37	0.69	4.80	60,60,60,60	0
31	MG	0	8012	1/1	0.15	0.51	4.63	53,53,53,53	0
31	MG	0	8053	1/1	0.58	0.63	4.38	52,52,52,52	0
31	MG	J	201	1/1	0.59	0.51	4.35	32,32,32,32	0
35	SR	0	8138	1/1	0.85	0.63	3.92	137,137,137,137	0
36	EMK	0	8163	74/74	0.68	0.50	3.81	40,48,59,62	0
33	NA	0	8067	1/1	0.48	0.57	3.73	57,57,57,57	0
31	MG	0	8001	1/1	0.24	0.45	3.60	27,27,27,27	0
31	MG	0	8032	1/1	0.68	0.36	3.49	46,46,46,46	0
33	NA	L	201	1/1	0.34	0.78	3.22	62,62,62,62	0
33	NA	I	201	1/1	0.29	0.60	3.09	54,54,54,54	0
31	MG	0	8021	1/1	0.70	0.63	2.84	42,42,42,42	0
31	MG	0	8037	1/1	0.66	0.55	2.26	58,58,58,58	0
31	MG	0	8011	1/1	0.74	0.33	2.23	40,40,40,40	0
33	NA	0	8062	1/1	0.52	0.57	2.07	39,39,39,39	0
33	NA	0	8059	1/1	0.34	0.42	1.99	39,39,39,39	0
31	MG	0	8038	1/1	0.43	0.41	1.63	54,54,54,54	0
34	CL	I	203	1/1	0.76	0.51	1.53	62,62,62,62	0
33	NA	0	8073	1/1	0.57	0.58	1.51	54,54,54,54	0
31	MG	0	8052	1/1	0.54	0.37	1.36	56,56,56,56	0
31	MG	0	8013	1/1	0.64	0.36	1.35	34,34,34,34	0
33	NA	P	101	1/1	0.28	0.54	1.32	45,45,45,45	0
33	NA	Q	202	1/1	0.85	0.41	1.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	CL	L	202	1/1	0.74	0.61	1.21	51,51,51,51	0
33	NA	C	301	1/1	0.39	0.47	1.08	35,35,35,35	0
31	MG	X	301	1/1	0.53	0.45	1.06	39,39,39,39	0
31	MG	0	8040	1/1	0.88	0.35	0.84	21,21,21,21	0
35	SR	0	8147	1/1	0.24	0.35	0.81	105,105,105,105	0
35	SR	A	305	1/1	-0.21	0.44	0.64	133,133,133,133	0
31	MG	0	8008	1/1	0.91	0.36	0.57	35,35,35,35	0
33	NA	0	8069	1/1	0.48	0.34	0.50	37,37,37,37	0
35	SR	0	8132	1/1	0.08	0.28	0.26	100,100,100,100	0
31	MG	0	8017	1/1	0.44	0.36	0.17	36,36,36,36	0
34	CL	0	8076	1/1	0.54	0.37	-0.15	58,58,58,58	0
35	SR	0	8154	1/1	0.77	0.30	-0.16	147,147,147,147	0
35	SR	0	8162	1/1	0.26	0.28	-0.30	103,103,103,103	0
31	MG	0	8010	1/1	0.61	0.34	-0.33	42,42,42,42	0
31	MG	K	201	1/1	0.71	0.29	-0.37	3,3,3,3	0
33	NA	0	8066	1/1	0.63	0.33	-0.65	42,42,42,42	0
31	MG	0	8044	1/1	0.57	0.30	-0.65	51,51,51,51	0
31	MG	0	8004	1/1	0.80	0.25	-0.91	38,38,38,38	0
37	CD	2	101	1/1	0.61	0.13	-1.13	87,87,87,87	0
37	CD	T	8701	1/1	0.22	0.20	-1.16	118,118,118,118	0
35	SR	0	8119	1/1	0.83	0.25	-1.48	106,106,106,106	0
35	SR	F	201	1/1	0.75	0.15	-1.61	102,102,102,102	0
31	MG	S	201	1/1	0.76	0.19	-1.71	59,59,59,59	0
35	SR	A	302	1/1	0.68	0.30	-2.13	86,86,86,86	0
35	SR	A	303	1/1	0.09	0.19	-2.15	89,89,89,89	0
31	MG	0	8039	1/1	0.78	0.19	-2.15	36,36,36,36	0
35	SR	0	8148	1/1	0.13	0.26	-2.19	132,132,132,132	0
35	SR	0	8082	1/1	0.51	0.15	-2.27	64,64,64,64	0
37	CD	Y	101	1/1	0.25	0.14	-2.34	112,112,112,112	0
37	CD	Z	101	1/1	0.77	0.20	-2.45	141,141,141,141	0
35	SR	2	102	1/1	0.92	0.14	-2.50	67,67,67,67	0
35	SR	0	8083	1/1	0.82	0.13	-3.05	46,46,46,46	0
35	SR	0	8108	1/1	0.54	0.14	-3.17	63,63,63,63	0
35	SR	0	8115	1/1	0.57	0.16	-3.22	101,101,101,101	0
31	MG	0	8006	1/1	0.86	0.14	-3.30	26,26,26,26	0
35	SR	Q	204	1/1	0.83	0.11	-3.31	70,70,70,70	0
35	SR	0	8097	1/1	0.81	0.20	-3.44	85,85,85,85	0
35	SR	0	8120	1/1	0.46	0.13	-3.69	82,82,82,82	0
35	SR	0	8107	1/1	0.86	0.13	-3.75	62,62,62,62	0
35	SR	0	8153	1/1	0.38	0.17	-4.05	130,130,130,130	0
35	SR	0	8136	1/1	0.75	0.13	-4.07	80,80,80,80	0
35	SR	Z	102	1/1	0.92	0.10	-4.15	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	SR	0	8121	1/1	0.56	0.15	-6.01	79,79,79,79	0
35	SR	0	8117	1/1	0.78	0.19	-6.11	104,104,104,104	0
35	SR	0	8088	1/1	0.82	0.12	-6.63	62,62,62,62	0
35	SR	0	8084	1/1	0.81	0.11	-	49,49,49,49	0
35	SR	0	8152	1/1	0.68	0.17	-	89,89,89,89	0
35	SR	0	8093	1/1	0.54	0.13	-	57,57,57,57	0
33	NA	0	8068	1/1	0.27	0.76	-	42,42,42,42	0
35	SR	0	8159	1/1	0.56	0.24	-	118,118,118,118	0
31	MG	0	8045	1/1	-0.52	1.51	-	75,75,75,75	0
35	SR	0	8150	1/1	0.13	0.34	-	128,128,128,128	0
31	MG	0	8055	1/1	0.61	0.42	-	45,45,45,45	0
35	SR	0	8127	1/1	0.68	0.38	-	96,96,96,96	0
35	SR	0	8089	1/1	0.73	0.13	-	69,69,69,69	0
35	SR	0	8103	1/1	0.59	0.22	-	84,84,84,84	0
34	CL	0	8077	1/1	0.92	0.34	-	55,55,55,55	0
35	SR	0	8126	1/1	0.41	0.17	-	118,118,118,118	0
31	MG	0	8029	1/1	-0.24	0.99	-	54,54,54,54	0
35	SR	0	8096	1/1	0.79	0.14	-	63,63,63,63	0
35	SR	0	8105	1/1	0.51	0.12	-	85,85,85,85	0
35	SR	0	8098	1/1	0.44	0.21	-	71,71,71,71	0
31	MG	0	8002	1/1	-0.40	1.42	-	57,57,57,57	0
31	MG	0	8022	1/1	0.32	0.39	-	43,43,43,43	0
34	CL	D	201	1/1	0.39	0.50	-	49,49,49,49	0
35	SR	0	8128	1/1	0.58	0.15	-	92,92,92,92	0
35	SR	0	8145	1/1	0.56	0.32	-	126,126,126,126	0
35	SR	0	8104	1/1	0.77	0.18	-	77,77,77,77	0
35	SR	0	8114	1/1	0.58	0.19	-	101,101,101,101	0
35	SR	0	8151	1/1	0.57	0.25	-	122,122,122,122	0
33	NA	0	8058	1/1	0.65	0.37	-	62,62,62,62	0
35	SR	0	8095	1/1	0.35	0.16	-	92,92,92,92	0
31	MG	0	8030	1/1	0.39	0.28	-	49,49,49,49	0
31	MG	0	8025	1/1	0.27	0.61	-	56,56,56,56	0
35	SR	0	8133	1/1	0.04	0.52	-	102,102,102,102	0
31	MG	0	8005	1/1	0.77	0.31	-	32,32,32,32	0
35	SR	0	8158	1/1	-0.15	1.00	-	128,128,128,128	0
35	SR	0	8137	1/1	-0.29	0.54	-	151,151,151,151	0
35	SR	0	8122	1/1	0.58	0.23	-	113,113,113,113	0
35	SR	0	8116	1/1	0.69	0.42	-	117,117,117,117	0
31	MG	0	8050	1/1	0.52	0.63	-	78,78,78,78	0
33	NA	0	8065	1/1	-0.17	2.31	-	48,48,48,48	0
31	MG	0	8023	1/1	0.39	0.69	-	56,56,56,56	0
35	SR	0	8125	1/1	0.65	0.35	-	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	SR	0	8155	1/1	0.52	0.26	-	135,135,135,135	0
35	SR	0	8092	1/1	0.66	0.12	-	75,75,75,75	0
31	MG	0	8015	1/1	0.75	0.46	-	39,39,39,39	0
35	SR	0	8101	1/1	0.90	0.10	-	75,75,75,75	0
35	SR	0	8091	1/1	0.81	0.08	-	81,81,81,81	0
31	MG	0	8048	1/1	0.71	0.59	-	38,38,38,38	0
31	MG	0	8054	1/1	0.32	1.02	-	53,53,53,53	0
31	MG	0	8049	1/1	0.63	0.38	-	51,51,51,51	0
35	SR	0	8099	1/1	0.52	0.17	-	94,94,94,94	0
35	SR	0	8157	1/1	-0.05	1.09	-	125,125,125,125	0
35	SR	B	403	1/1	0.85	0.17	-	106,106,106,106	0
34	CL	I	202	1/1	0.28	0.33	-	58,58,58,58	0
35	SR	A	304	1/1	0.20	0.20	-	95,95,95,95	0
35	SR	0	8129	1/1	0.29	0.20	-	107,107,107,107	0
33	NA	0	8060	1/1	-0.18	0.94	-	46,46,46,46	0
31	MG	B	401	1/1	-0.61	1.23	-	66,66,66,66	0
35	SR	9	3203	1/1	0.07	0.62	-	110,110,110,110	0
35	SR	0	8130	1/1	0.69	0.32	-	106,106,106,106	0
31	MG	0	8007	1/1	0.66	0.32	-	28,28,28,28	0
35	SR	0	8124	1/1	0.24	0.23	-	84,84,84,84	0
31	MG	0	8026	1/1	0.70	0.66	-	56,56,56,56	0
34	CL	A	301	1/1	0.27	0.78	-	74,74,74,74	0
35	SR	9	3205	1/1	-0.41	0.44	-	141,141,141,141	0
31	MG	0	8041	1/1	0.63	0.40	-	52,52,52,52	0
35	SR	0	8142	1/1	-0.13	0.70	-	138,138,138,138	0
35	SR	0	8161	1/1	0.52	0.92	-	137,137,137,137	0
35	SR	0	8144	1/1	0.34	0.23	-	126,126,126,126	0
35	SR	0	8087	1/1	0.81	0.17	-	77,77,77,77	0
35	SR	0	8113	1/1	0.62	0.27	-	75,75,75,75	0
35	SR	R	101	1/1	0.02	0.43	-	119,119,119,119	0
34	CL	Q	203	1/1	0.81	0.72	-	55,55,55,55	0
31	MG	0	8014	1/1	0.49	0.62	-	50,50,50,50	0
35	SR	0	8140	1/1	0.53	0.49	-	108,108,108,108	0
33	NA	0	8071	1/1	0.60	0.40	-	51,51,51,51	0
31	MG	0	8031	1/1	0.84	0.24	-	50,50,50,50	0
35	SR	0	8143	1/1	0.76	0.17	-	63,63,63,63	0
31	MG	0	8019	1/1	0.30	0.36	-	37,37,37,37	0
35	SR	0	8100	1/1	0.87	0.08	-	68,68,68,68	0
31	MG	9	3201	1/1	0.58	0.34	-	46,46,46,46	0
35	SR	0	8102	1/1	0.69	0.15	-	72,72,72,72	0
34	CL	0	8080	1/1	0.47	0.94	-	51,51,51,51	0
35	SR	0	8106	1/1	0.32	0.32	-	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	SR	0	8146	1/1	0.22	0.29	-	156,156,156,156	0
31	MG	0	8051	1/1	0.04	0.80	-	54,54,54,54	0
35	SR	0	8135	1/1	0.38	0.15	-	99,99,99,99	0
35	SR	0	8111	1/1	0.76	0.21	-	75,75,75,75	0
35	SR	0	8131	1/1	0.07	0.24	-	104,104,104,104	0
35	SR	0	8123	1/1	0.58	0.30	-	96,96,96,96	0
31	MG	0	8042	1/1	0.48	0.44	-	28,28,28,28	0
31	MG	0	8036	1/1	0.74	0.43	-	52,52,52,52	0
35	SR	0	8149	1/1	0.75	0.58	-	200,200,200,200	0
31	MG	0	8035	1/1	0.08	0.60	-	85,85,85,85	0
34	CL	X	302	1/1	0.93	0.17	-	44,44,44,44	0
35	SR	0	8090	1/1	0.52	0.14	-	72,72,72,72	0
35	SR	0	8094	1/1	0.64	0.24	-	56,56,56,56	0
35	SR	0	8112	1/1	0.70	0.15	-	75,75,75,75	0
31	MG	0	8020	1/1	0.74	0.38	-	44,44,44,44	0
31	MG	0	8016	1/1	0.88	0.38	-	40,40,40,40	0
35	SR	2	103	1/1	0.48	0.27	-	74,74,74,74	0
35	SR	9	3204	1/1	-0.29	0.20	-	122,122,122,122	0
35	SR	0	8139	1/1	0.71	0.17	-	101,101,101,101	0
35	SR	0	8156	1/1	0.35	0.47	-	137,137,137,137	0
35	SR	Z	103	1/1	0.83	0.31	-	140,140,140,140	0
31	MG	0	8027	1/1	0.19	0.82	-	51,51,51,51	0
35	SR	0	8109	1/1	0.28	0.31	-	88,88,88,88	0
35	SR	0	8086	1/1	0.84	0.10	-	46,46,46,46	0
35	SR	0	8134	1/1	0.41	0.18	-	94,94,94,94	0
34	CL	0	8079	1/1	0.51	0.45	-	56,56,56,56	0
35	SR	0	8110	1/1	0.73	0.12	-	89,89,89,89	0
33	NA	0	8063	1/1	-0.03	0.91	-	48,48,48,48	0
34	CL	0	8078	1/1	0.87	0.99	-	63,63,63,63	0
35	SR	0	8160	1/1	0.90	0.08	-	59,59,59,59	0
31	MG	0	8046	1/1	0.47	0.42	-	47,47,47,47	0
35	SR	0	8081	1/1	0.16	0.21	-	91,91,91,91	0
35	SR	0	8118	1/1	0.57	0.33	-	96,96,96,96	0
35	SR	0	8085	1/1	0.45	0.16	-	50,50,50,50	0

6.5 Other polymers ⓘ

There are no such residues in this entry.