



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:34 PM GMT

PDB ID : 1K9M
Title : Co-crystal structure of tylosin bound to the 50S ribosomal subunit of *Haloarcula marismortui*
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-10-29
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
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

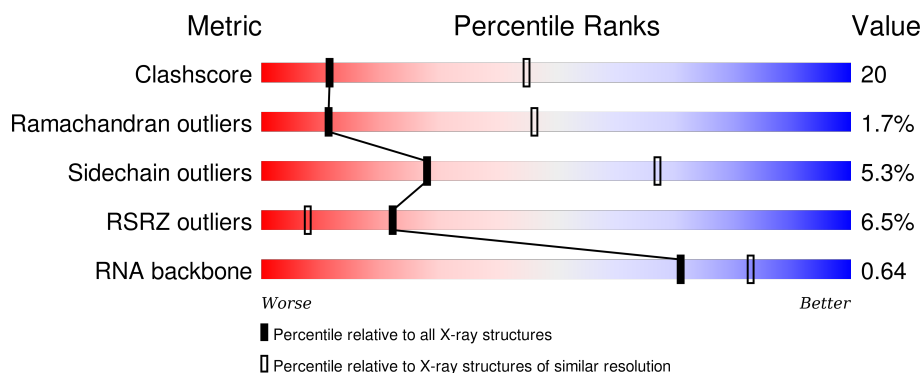
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

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	A	2922	 2% 50% 36% 7% • 6%
2	B	122	 4% 45% 39% 10% 6%
3	C	239	 7% 54% 38% 7% •
4	D	337	 50% 44% 6%
5	E	246	 61% 34% 6%

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Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	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
31	TYK	A	9000	-	-	-	X
32	MG	4	8078	-	-	-	X
32	MG	A	8067	-	-	-	X
33	NA	A	8303	-	-	-	X
33	NA	A	8321	-	-	-	X
33	NA	A	8323	-	-	-	X
33	NA	A	8340	-	-	-	X
33	NA	A	8350	-	-	-	X
33	NA	A	8355	-	-	-	X
33	NA	A	8356	-	-	-	X
33	NA	A	8359	-	-	-	X
33	NA	A	8362	-	-	-	X
33	NA	A	8364	-	-	-	X
33	NA	A	8365	-	-	-	X
33	NA	A	8366	-	-	-	X
33	NA	A	8371	-	-	-	X
33	NA	A	8372	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8374	-	-	-	X
33	NA	A	8376	-	-	-	X
33	NA	A	8378	-	-	-	X
33	NA	A	8382	-	-	-	X
33	NA	S	8337	-	-	-	X
33	NA	S	8386	-	-	-	X
34	CL	4	8504	-	-	-	X
34	CL	A	8505	-	-	-	X
34	CL	A	8515	-	-	-	X
34	CL	D	8519	-	-	-	X
34	CL	O	8507	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98593 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	? 3377779

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	29	Total	C	N	O	S	0	0	0
			240	149	39	51	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

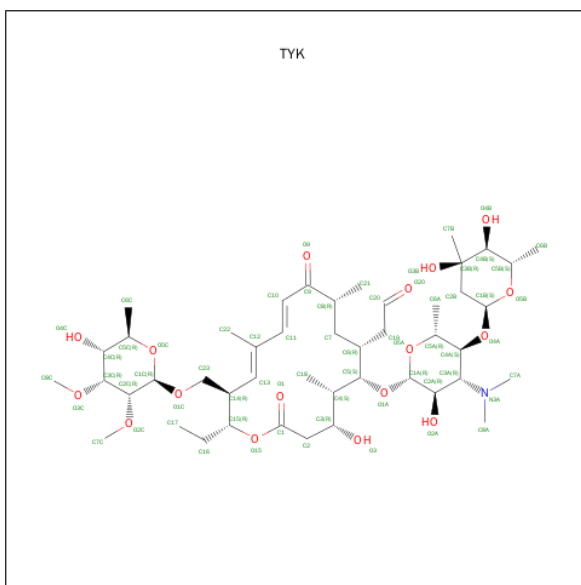
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is TYLOSIN (three-letter code: TYK) (formula: C₄₆H₇₇NO₁₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			64	46	1	17		

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	1	1	Total 1 Mg 1	0	0
32	D	1	Total 1 Mg 1	0	0
32	B	1	Total 1 Mg 1	0	0
32	C	1	Total 1 Mg 1	0	0
32	Z	1	Total 1 Mg 1	0	0
32	A	111	Total 111 Mg 111	0	0
32	4	1	Total 1 Mg 1	0	0
32	U	1	Total 1 Mg 1	0	0
32	L	1	Total 1 Mg 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	E	1	Total Na 1 1	0	0
33	B	2	Total Na 2 2	0	0
33	C	1	Total Na 1 1	0	0
33	A	72	Total Na 72 72	0	0
33	T	1	Total Na 1 1	0	0
33	N	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0
33	S	2	Total Na 2 2	0	0
33	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	P	1	Total Cl 1 1	0	0
34	D	1	Total Cl 1 1	0	0
34	K	4	Total Cl 4 4	0	0
34	C	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	A	8	Total Cl 8 8	0	0
34	4	1	Total Cl 1 1	0	0
34	N	1	Total Cl 1 1	0	0
34	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Cl 1	0	0
34	S	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	3	Total 3	K 3	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5921	Total 5921	O 5921	0	0
37	B	142	Total 142	O 142	0	0
37	C	126	Total 126	O 126	0	0
37	D	146	Total 146	O 146	0	0
37	E	174	Total 174	O 174	0	0
37	F	51	Total 51	O 51	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	26	Total 26	O 26	0	0
37	I	22	Total 22	O 22	0	0
37	J	79	Total 79	O 79	0	0
37	K	54	Total 54	O 54	0	0
37	L	60	Total 60	O 60	0	0
37	M	84	Total 84	O 84	0	0
37	N	127	Total 127	O 127	0	0
37	O	64	Total 64	O 64	0	0
37	P	42	Total 42	O 42	0	0
37	Q	66	Total 66	O 66	0	0
37	R	53	Total 53	O 53	0	0
37	S	84	Total 84	O 84	0	0
37	T	34	Total 34	O 34	0	0
37	U	39	Total 39	O 39	0	0
37	V	26	Total 26	O 26	0	0
37	W	12	Total 12	O 12	0	0
37	X	70	Total 70	O 70	0	0
37	Y	29	Total 29	O 29	0	0
37	Z	96	Total 96	O 96	0	0
37	1	37	Total 37	O 37	0	0

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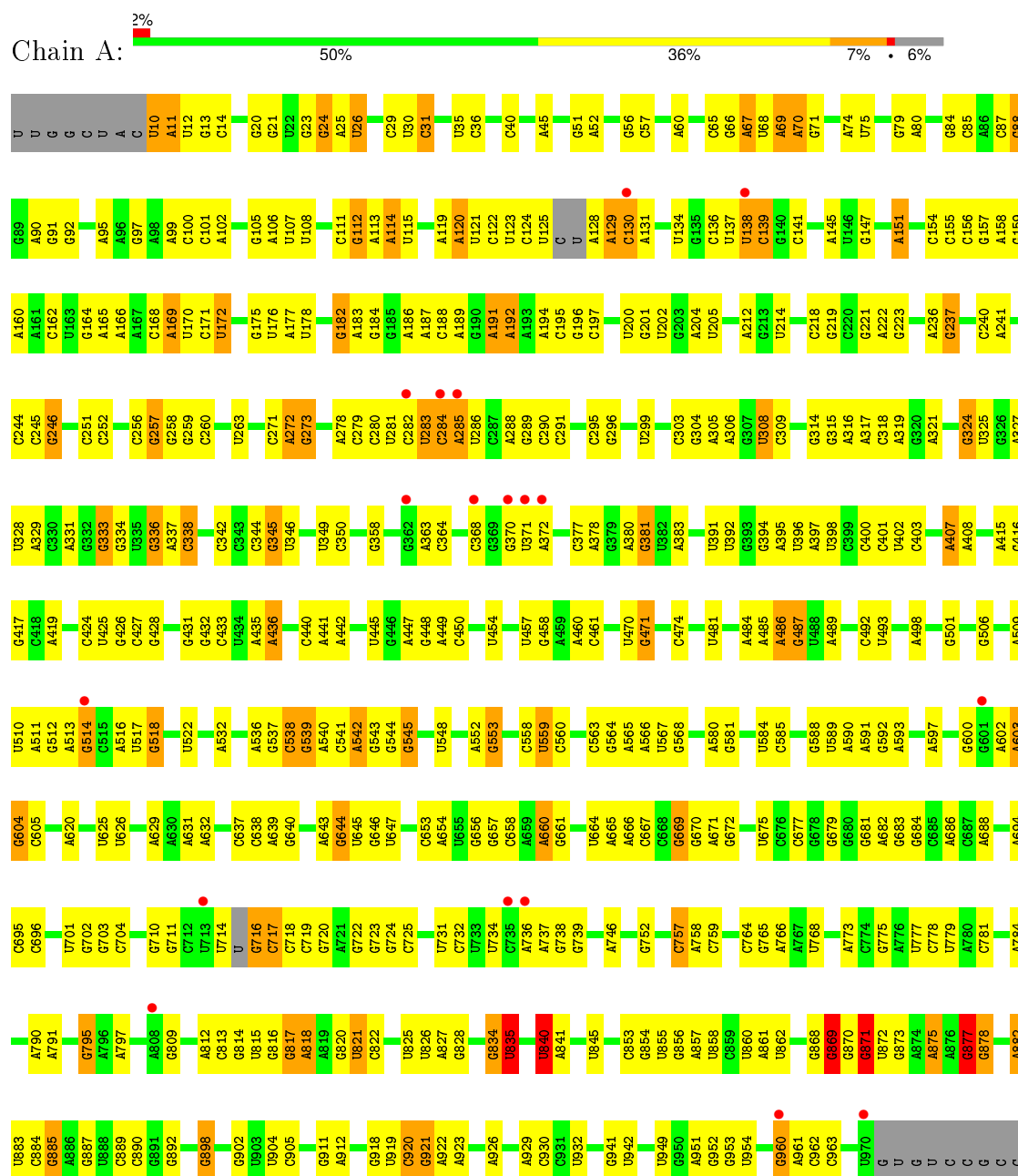
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	56	Total 56	O 56	0	0
37	3	43	Total 43	O 43	0	0
37	4	72	Total 72	O 72	0	0

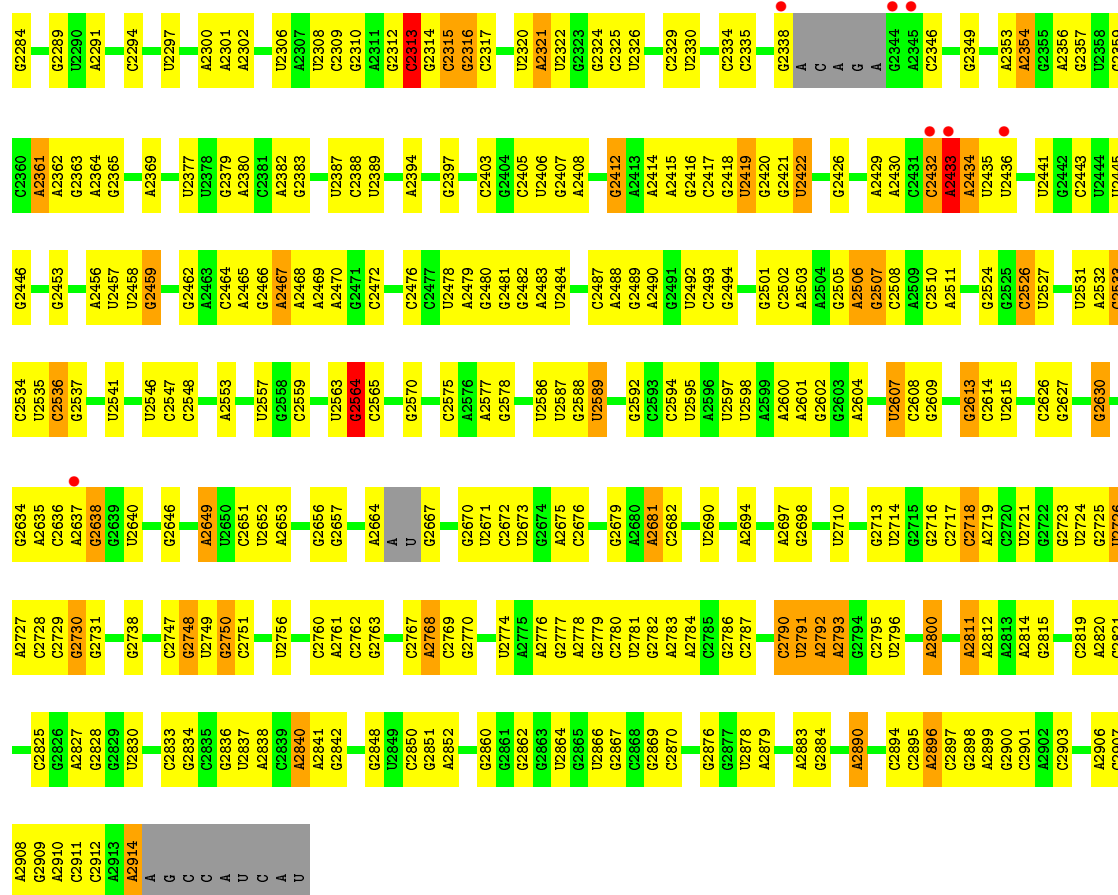
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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.

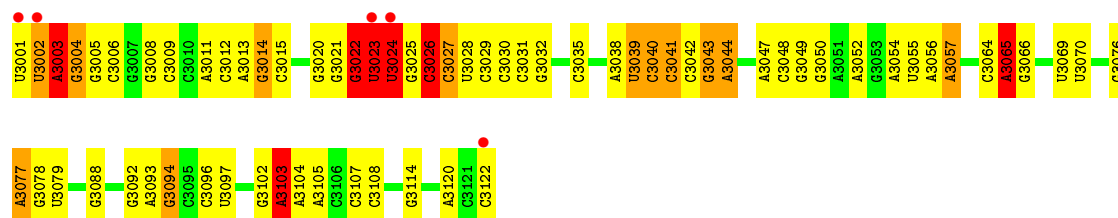
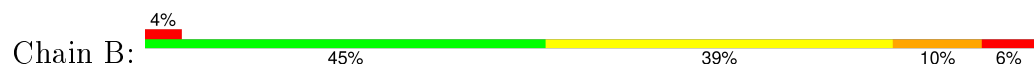
• Molecule 1: 23S rRNA



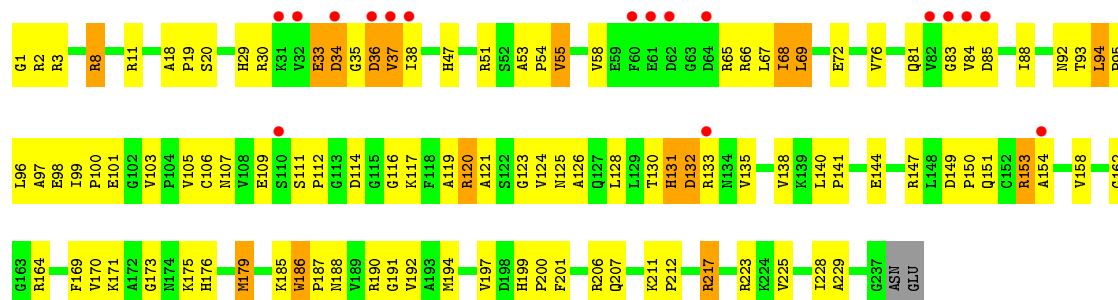
G	A2083	A1991	G1819	G1725	G1633	G1532	G1441	U1333	A1242	A1166	G1072	U
U	C2087	U1992	G1820	G1730	C1634	A1533	A1442	C1334	A1243	G1167	A1073	C
G	A2088	C1993	U1825	U1731	U1635	C1534	G1443	C1335	U1244	C1168		C
A	A2090	G1995	C1826	A1732	G1636	G1535	G1444	U1336	A1245	U1169		G
A	G2091	U1996	G1827	A1733	A1637	G1536	U1446	A1337	G1246	U1170	A1079	A
U	G2092	A1997	G1828	C1734			U1447			A1171	A1080	G
A	G2093	G1998	A1829	C1735	A1641	G1543		C1342	U1249	A1172	A1081	A
C	G2094	C1999	A1830	A1736	A1642	U1544	C1450	A1348	U1250	A1173	A1082	G
U	G2095	G2001	U1833	A1737	C1647	G1545	C1451	G1349	C1251	A1174		A
A	A2096	A1924	U1834	C1738	G1647	G1546	C1452	U1350	A1252	G1175	A1086	G
C	G2097	G2002	G1835	U1741	U1654	C1549		G1351	C1253	A1177	A1087	U
C	C2098	U2004	U1835	A1742	G1655		C1456	A1352			A1088	C
C	G2099	G2005		G1743	A1656	G1552	U1457	C1353	C1257	U1180		G
G	A2100	U2008	A1839	G1743	A1657	G1553	A1458	G1354	G1258	A1181	U1096	G
U	A2101	C1841	A1840	A1746	A1658	U1554	A1459			C1182	U1097	C
C	G2102	U1939	A1842	A1747	A1659	G1555		C1360	A1261	C1183	A1098	A
G	A2103			U1748	G1660		C1462	C1366	U1264	C1184	G1099	C
A	C2104	A1942	A1845	G1751	C1666	A1559	C1469	U1372	G1265	U1185		A
C	G2105	C1943	U1846	G1752	A1667	U	U1470	A1375	U1266	C1186	C1103	C2999
U	C2106	G1947	A1847	C1753	U1668	C1562	A1471	A1376	C1267	A1187	U1099	U1003
A	U2107			A1754	A1669	G1563	C1472	G1376	C1268	A1188	C1004	A1005
U	A2108	G1948	U1850	G1754	G1670	C1564	U1473	C1377	U1270	A1189	A1006	A1007
G	U2109	G1949	U1851				C1474			A1191	A1114	
C	G2110	G1950		U1758		A1573		U1380	C1273	A1192	U1115	
A	A2111	U	G1855	U1766	C1675	A1574	C1477			A1193	U1116	C1008
C	G2112	C2031	C1856	G1767	U1676	C1574	U1478	G1391	U1279		A1117	U1009
G	G2113	U2032	A1857	A1768	A1677	A1580		G1392		U1197	A1118	C1010
G	G2114	G2033	U1860	C1769	C1679	G1589	C1483	A1393	C1289	U1198	G1119	A1014
U	U2115	U2034	C1861	U1770	C1680		G1484	C1394	G1290	A1199	U1120	C1015
A	U2116	C2035	C1862	U1771	G1681	G1592			A1291	A1200	G1121	U1016
C	C2119	C2036	C1863	C1772	A1682	C1593	U1487	G1398	U1292	C1201	A1122	
C	U2120	A	G1864	G1773	G1683	C1594	U1488	A1399	U1293	A1202	A1123	G1021
C	G2121	G2037	G	G1774	A1684	C1595	A1494	C1400	A1294	C1203	G1127	A1022
G	A2122	A	G1868	G1774	A1685	G1596	C1495	G1401	G1295	C1204	U1128	C1023
G	A2123	C	U1874	A1778	C1686	U1596			A1296	U1205	U1129	G1024
U	U2127	G2044	U1877	A1779	C1687	A1597	U1500	A1407		U1206	U1130	C1025
A	G2128	G2045	G1878	U1779	G1688	A1598	A1501	U1408	G1299	A1207	G1131	U1029
G	U2133	G2046	U1879	A1783	A1689	G1601	A1502	G1409	G1300	C1208	A1132	
C	A2134	A2054	C1882	U1784	A1690	G1602	U1503		C1301	C1209	A1133	G1038
G	A2135	A2055	G1883	C1787	A1691	A1603	A1504	U1412		G1211	G1134	G1039
G	G2136	U2059	G1884	U1788	C1692	G1604	U1505	G1417	U1304	C1212	G1135	
C	A	U2064	A1885	C1789	C1699	G1605	U1506	U1418	C1305	C1213	U1136	C1044
C	C	U2065	G1886	C1790	C1700	A1606		U1419	U1306	G1214	G1137	G1045
A	G	G2066	U1887	U1791	A1701	A1607	C1513	C1420	A1307	A1215	G1138	
U	U	G2067	U1888	C1792	U1702	G1608	G1514	U1421	A1308	G1216	U1139	
C	G	C1975	U1889	G1798	A1703	C1609	A1515	U1422	U1309	G1217	G1140	G1053
C	U	G1976	U1890		A1704	G1610	U1516	C1423	U1310	U1218		
G	G	U1977	C1894	A1711	A1710	C1613	A1522	A1424	G1311	U1219	G1151	U1056
A	U	A1978	G1805	A1712	A1712	G1614	U1523	G1430	G1312	C1229	G1158	A1057
U	G	G1979	G1806	A1717	A1615	U1524	U1525			G1159	A1160	A1058
U	U	U1980	C1810		U1625	A1626	A1526	G1433	A1328	U1234	A1161	G1059
C	C	A1981	U1903	C1721	U1626	U1627	A1527	A1434	A1329	G1235	G1162	C1060
A	C	C1982	A1904	A1815	U1628	U1629	A1528	A1435	A1330	U1237	U1163	U1062
A	G	G1989	G1908	C1816	U1723	U1724	A1529	C1436	G1332	U1238	U1164	U1066
C	U	C1990	A1909		U1724	A1630	G1529			G1239	G1165	A1067



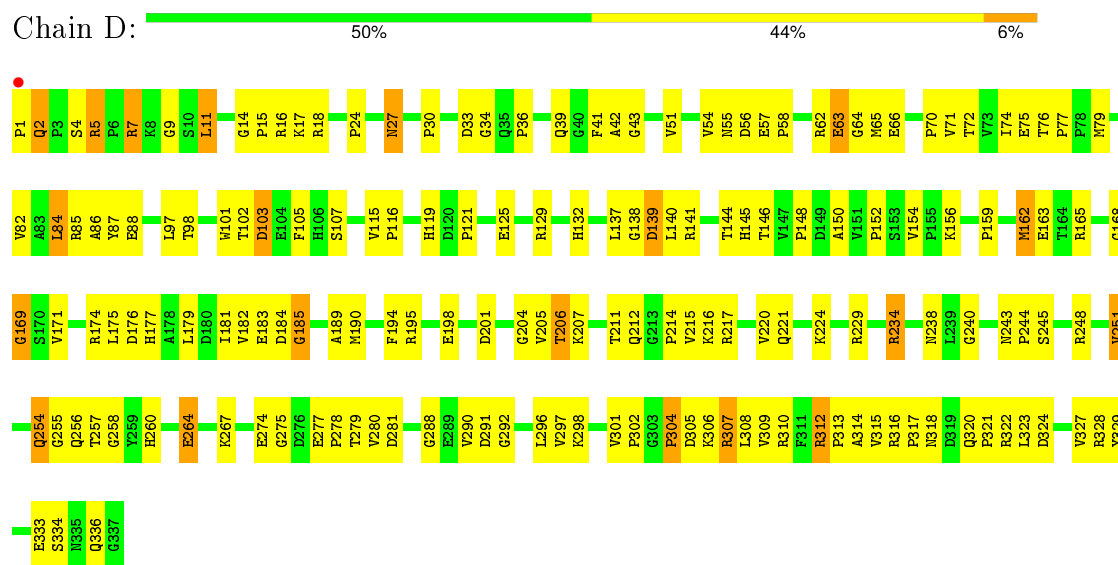
• Molecule 2: 5S rRNA



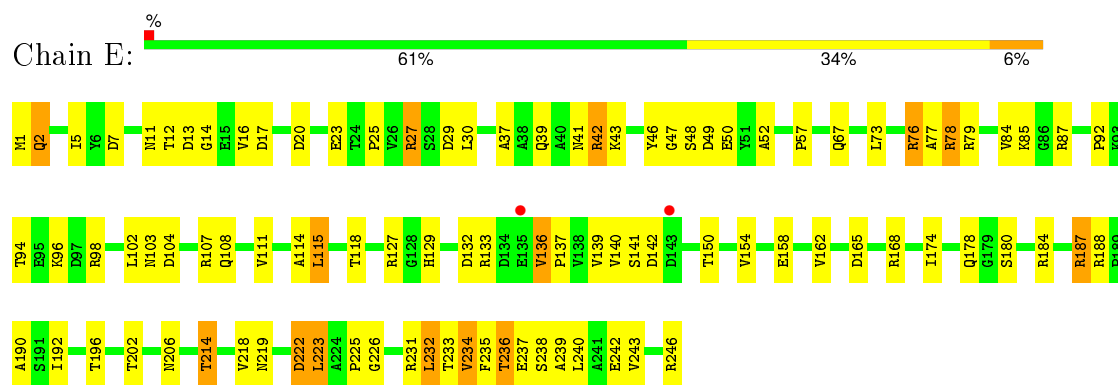
• Molecule 3: RIBOSOMAL PROTEIN L2



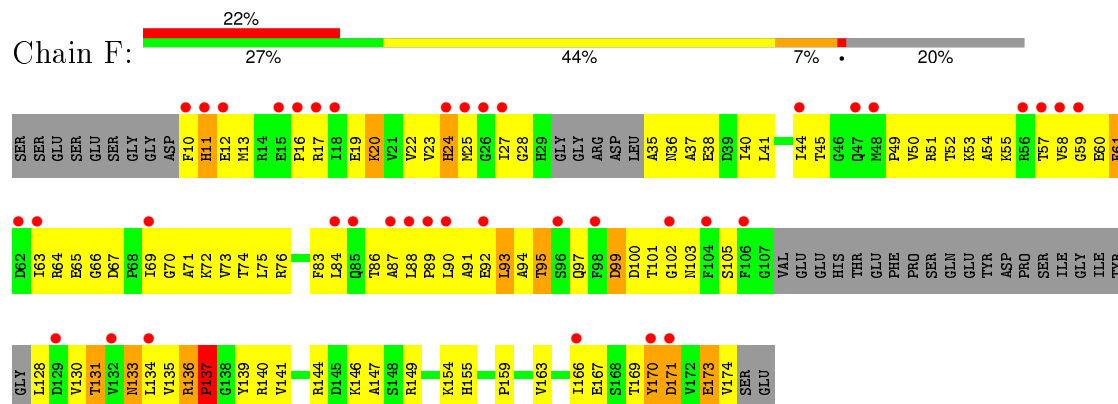
• Molecule 4: RIBOSOMAL PROTEIN L3



• Molecule 5: RIBOSOMAL PROTEIN L4



• Molecule 6: RIBOSOMAL PROTEIN L5



• Molecule 7: RIBOSOMAL PROTEIN L6

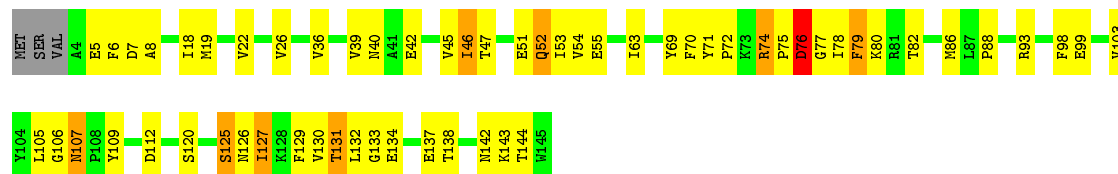






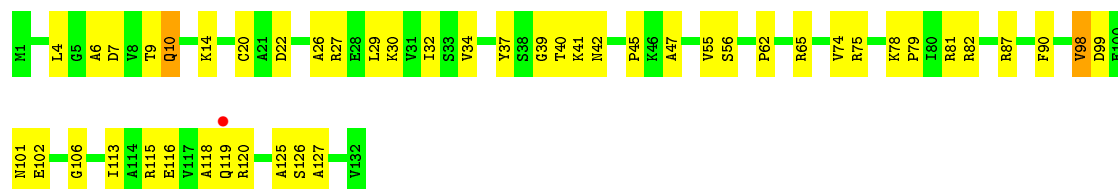
- Molecule 11: RIBOSOMAL PROTEIN L13

Chain K: 57% 34% 6% ...



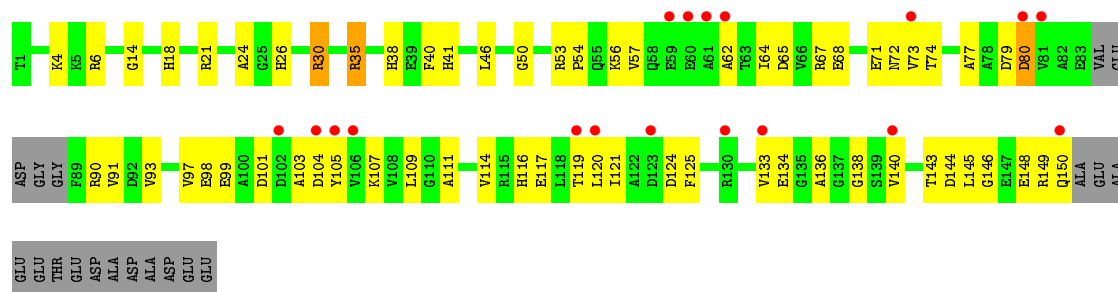
- Molecule 12: RIBOSOMAL PROTEIN L14

Chain L:  64% 34%



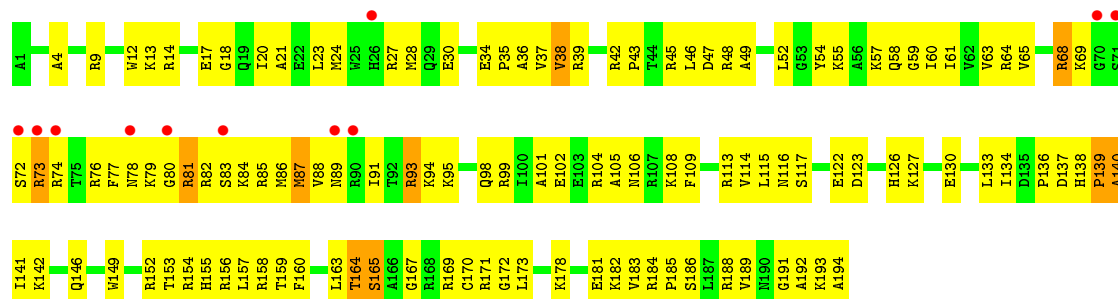
- Molecule 13: RIBOSOMAL PROTEIN L15

Chain M: 

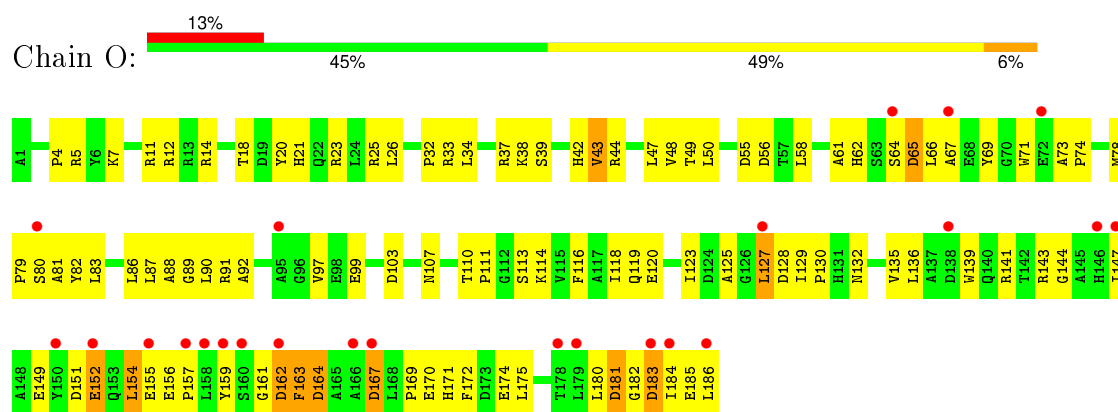


- Molecule 14: RIBOSOMAL PROTEIN L15E

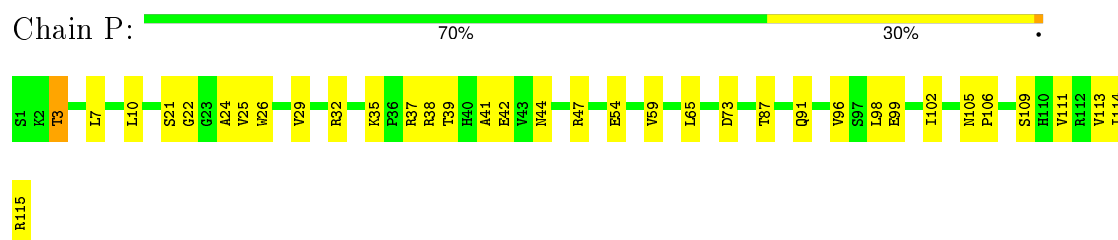
Chain N: 



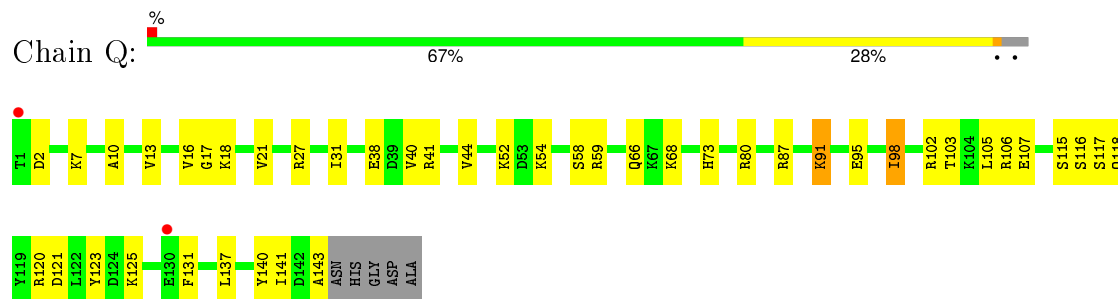
- Molecule 15: RIBOSOMAL PROTEIN L18



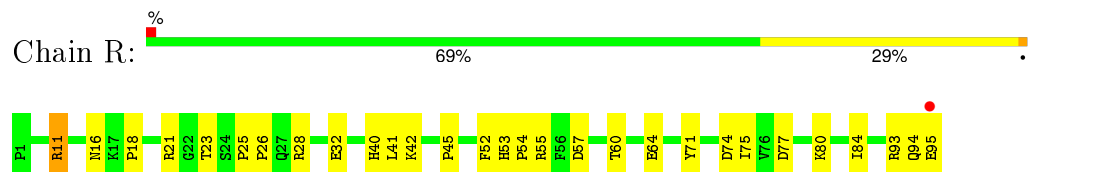
• Molecule 16: RIBOSOMAL PROTEIN L18E



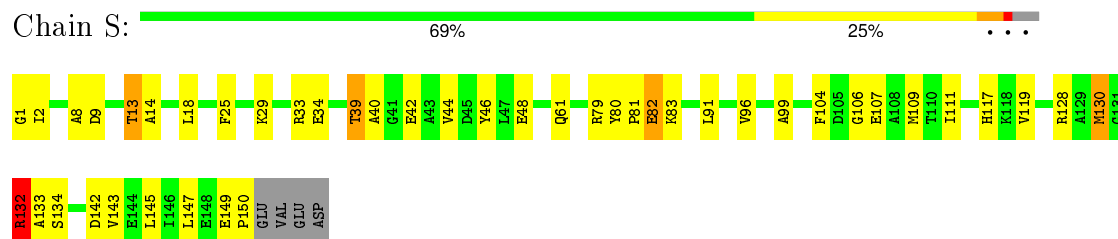
• Molecule 17: RIBOSOMAL PROTEIN L19E



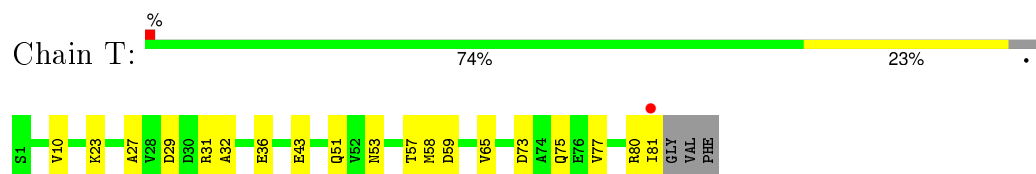
• Molecule 18: RIBOSOMAL PROTEIN L21E



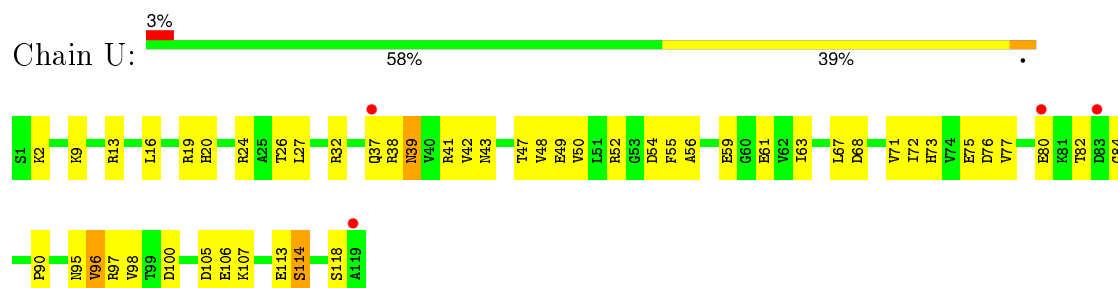
• Molecule 19: RIBOSOMAL PROTEIN L22



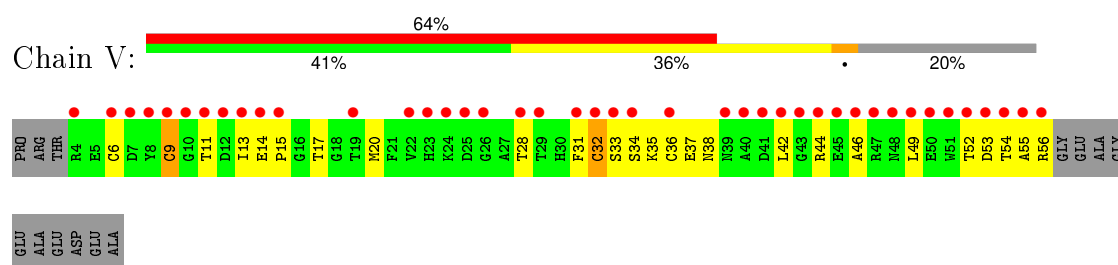
• Molecule 20: RIBOSOMAL PROTEIN L23



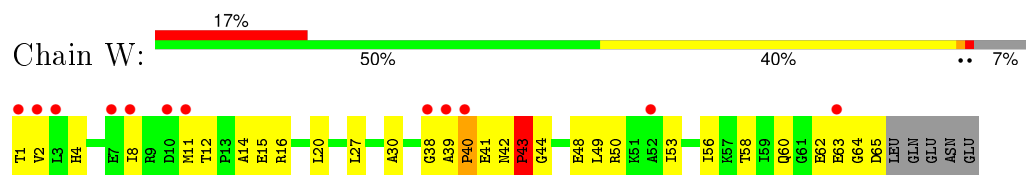
- Molecule 21: RIBOSOMAL PROTEIN L24



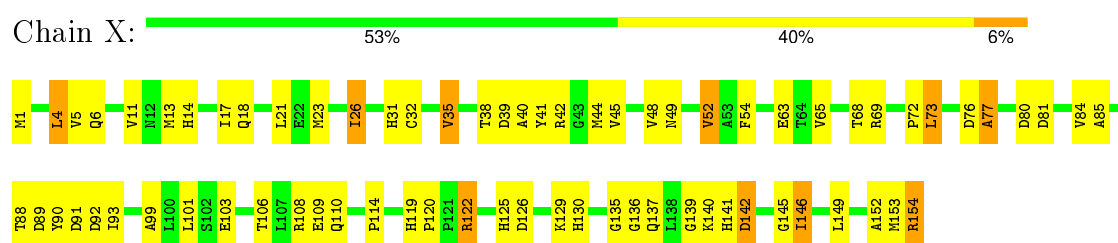
- Molecule 22: RIBOSOMAL PROTEIN L24E



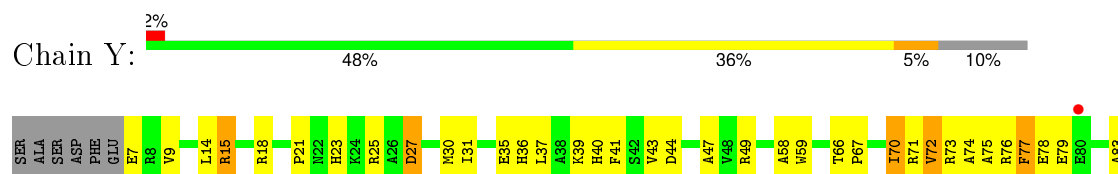
- Molecule 23: RIBOSOMAL PROTEIN L29

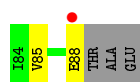


- Molecule 24: RIBOSOMAL PROTEIN L30

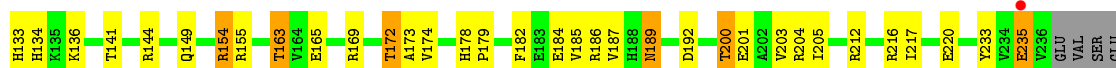
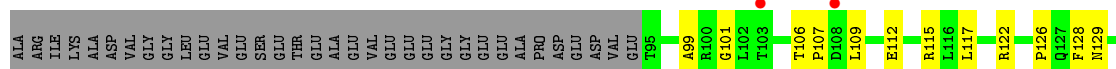


- Molecule 25: RIBOSOMAL PROTEIN L31E

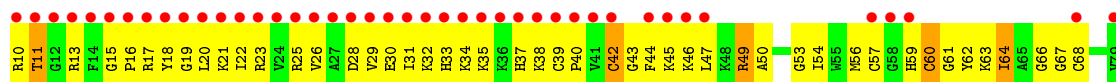




• Molecule 26: RIBOSOMAL PROTEIN L32E



• Molecule 27: RIBOSOMAL PROTEIN L37Ae



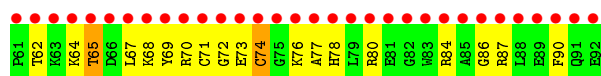
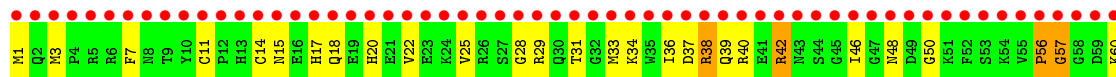
• Molecule 28: RIBOSOMAL PROTEIN L37E



• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: 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	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 49.92 – 2.99	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.99-3.00) 92.3 (49.92-2.99)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.262 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 359798 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.47% 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, TYK, NA, K, CL, CD

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	A	0.59	13/66076 (0.0%)	0.77	38/103052 (0.0%)
2	B	0.89	17/2905 (0.6%)	0.91	16/4528 (0.4%)
3	C	0.57	3/1787 (0.2%)	0.78	1/2409 (0.0%)
4	D	0.48	0/2689	0.73	0/3652
5	E	0.51	0/1883	0.74	0/2551
6	F	0.41	0/1111	0.65	0/1498
7	G	0.44	0/1382	0.63	0/1880
8	H	0.43	0/896	0.65	0/1219
9	I	0.48	0/241	0.60	0/324
10	J	0.51	0/1246	0.80	2/1686 (0.1%)
11	K	0.49	0/1135	0.68	0/1530
12	L	0.48	0/1003	0.75	0/1351
13	M	0.46	0/1126	0.74	0/1504
14	N	0.59	0/1633	0.83	2/2180 (0.1%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.50	0/873	0.73	0/1181
17	Q	0.48	0/1143	0.64	0/1521
18	R	0.49	0/748	0.76	0/1005
19	S	0.63	1/1172 (0.1%)	0.82	2/1578 (0.1%)
20	T	0.46	0/648	0.68	1/875 (0.1%)
21	U	0.44	0/957	0.72	0/1289
22	V	0.70	0/417	0.81	1/562 (0.2%)
23	W	0.41	0/502	0.62	0/675
24	X	0.49	0/1218	0.73	0/1655
25	Y	0.48	0/664	0.68	0/895
26	Z	0.47	0/1146	0.72	0/1536
27	1	0.74	0/575	0.81	0/763
28	2	0.47	0/437	0.80	0/578
29	3	0.45	0/398	0.59	0/527
30	4	0.95	0/771	0.80	0/1024
All	All	0.58	34/98255 (0.0%)	0.76	63/147027 (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	A	1	150
2	B	0	4
All	All	1	154

The worst 5 of 34 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2104	C	O5'-C5'	-12.61	1.22	1.42
2	B	3023	U	C2'-O2'	12.28	1.57	1.41
1	A	2103	A	C6-N1	9.66	1.42	1.35
2	B	3025	G	O3'-P	9.21	1.72	1.61
1	A	2103	A	C5-C6	8.57	1.48	1.41

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.07	63.25	105.20
1	A	1164	U	OP2-P-O3'	-17.80	66.05	105.20
1	A	1165	G	O5'-P-OP1	-13.80	93.28	105.70
1	A	2104	C	O5'-P-OP1	-13.33	93.70	105.70
1	A	2103	A	C5'-C4'-O4'	10.96	122.25	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 154 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	G	Sidechain
1	A	138	U	Sidechain
1	A	162	C	Sidechain
1	A	24	G	Sidechain
1	A	26	U	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	A	59017	0	29798	1175	0
2	B	2600	0	1326	79	0
3	C	1754	0	1763	134	0
4	D	2624	0	2533	189	0
5	E	1858	0	1816	121	0
6	F	1094	0	1085	137	0
7	G	1357	0	1266	76	0
8	H	885	0	854	62	0
9	I	240	0	231	20	0
10	J	1215	0	1215	160	0
11	K	1119	0	1098	67	0
12	L	993	0	1027	53	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	173	0
15	O	1444	0	1401	134	0
16	P	864	0	873	38	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	24	0
19	S	1149	0	1122	57	0
20	T	641	0	605	22	0
21	U	949	0	923	56	0
22	V	410	0	368	37	0
23	W	499	0	511	31	0
24	X	1195	0	1137	98	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	62	0
27	1	563	0	601	76	0
28	2	430	0	426	26	0
29	3	393	0	406	26	0
30	4	755	0	732	59	0
31	A	64	0	76	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	72	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	2	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
34	4	1	0	0	0	0
34	A	8	0	0	1	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	4	0	0	2	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	2	0
34	P	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
34	Z	1	0	0	0	0
35	A	3	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	37	0	0	10	0
37	2	56	0	0	4	0
37	3	43	0	0	4	0
37	4	72	0	0	4	0
37	A	5921	0	0	271	0
37	B	142	0	0	14	0
37	C	126	0	0	20	0
37	D	146	0	0	27	0
37	E	174	0	0	34	0
37	F	51	0	0	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	42	0	0	9	0
37	H	26	0	0	11	0
37	I	22	0	0	5	0
37	J	79	0	0	19	0
37	K	54	0	0	5	0
37	L	60	0	0	11	0
37	M	84	0	0	18	0
37	N	127	0	0	29	0
37	O	64	0	0	18	0
37	P	42	0	0	12	0
37	Q	66	0	0	5	0
37	R	53	0	0	3	0
37	S	84	0	0	7	0
37	T	34	0	0	4	0
37	U	39	0	0	4	0
37	V	26	0	0	5	0
37	W	12	0	0	1	0
37	X	70	0	0	10	0
37	Y	29	0	0	12	0
37	Z	96	0	0	17	0
All	All	98593	0	59582	3067	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 20.

The worst 5 of 3067 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)
1:A:1160:G:H5'	1:A:1161:A:H5'	1.25	1.15
23:W:12:THR:HG22	23:W:15:GLU:HG3	1.30	1.13
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.13
14:N:87:MET:HG2	30:4:46:ILE:HG21	1.14	1.10
14:N:87:MET:CG	30:4:46:ILE:HG21	1.84	1.08

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	C	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	11	46
4	D	335/337 (99%)	304 (91%)	22 (7%)	9 (3%)	6	32
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	39	80
6	F	134/176 (76%)	93 (69%)	30 (22%)	11 (8%)	1	5
7	G	170/177 (96%)	159 (94%)	11 (6%)	0	100	100
8	H	117/119 (98%)	102 (87%)	13 (11%)	2 (2%)	11	46
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	131 (86%)	14 (9%)	7 (5%)	3	18
11	K	140/145 (97%)	128 (91%)	8 (6%)	4 (3%)	6	29
12	L	130/132 (98%)	119 (92%)	9 (7%)	2 (2%)	13	50
13	M	141/164 (86%)	120 (85%)	20 (14%)	1 (1%)	26	70
14	N	192/194 (99%)	173 (90%)	17 (9%)	2 (1%)	19	61
15	O	184/186 (99%)	166 (90%)	11 (6%)	7 (4%)	4	22
16	P	113/115 (98%)	106 (94%)	7 (6%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	26	70
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	17	58
19	S	148/154 (96%)	139 (94%)	9 (6%)	0	100	100
20	T	79/84 (94%)	73 (92%)	6 (8%)	0	100	100
21	U	117/119 (98%)	110 (94%)	6 (5%)	1 (1%)	21	64
22	V	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	27
24	X	152/154 (99%)	145 (95%)	5 (3%)	2 (1%)	15	53
25	Y	80/91 (88%)	72 (90%)	6 (8%)	2 (2%)	7	34
26	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	14	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	8	38
All	All	3633/4235 (86%)	3300 (91%)	271 (8%)	62 (2%)	11	46

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	17	52
4	D	282/282 (100%)	265 (94%)	17 (6%)	24	62
5	E	193/193 (100%)	176 (91%)	17 (9%)	12	42
6	F	117/147 (80%)	108 (92%)	9 (8%)	16	50
7	G	152/155 (98%)	147 (97%)	5 (3%)	45	82
8	H	92/92 (100%)	91 (99%)	1 (1%)	80	94
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	110 (90%)	12 (10%)	10	36
11	K	118/121 (98%)	107 (91%)	11 (9%)	11	39
12	L	106/106 (100%)	103 (97%)	3 (3%)	51	84
13	M	112/126 (89%)	108 (96%)	4 (4%)	42	79
14	N	166/166 (100%)	158 (95%)	8 (5%)	31	71
15	O	149/149 (100%)	143 (96%)	6 (4%)	38	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	92 (99%)	1 (1%)	80	94
17	Q	113/116 (97%)	110 (97%)	3 (3%)	52	85
18	R	79/79 (100%)	75 (95%)	4 (5%)	29	69
19	S	117/121 (97%)	112 (96%)	5 (4%)	35	75
20	T	71/73 (97%)	70 (99%)	1 (1%)	74	93
21	U	105/105 (100%)	102 (97%)	3 (3%)	50	84
22	V	44/52 (85%)	42 (96%)	2 (4%)	34	74
23	W	51/56 (91%)	50 (98%)	1 (2%)	63	89
24	X	130/130 (100%)	121 (93%)	9 (7%)	19	56
25	Y	66/73 (90%)	62 (94%)	4 (6%)	23	61
26	Z	120/195 (62%)	113 (94%)	7 (6%)	25	63
27	1	56/56 (100%)	50 (89%)	6 (11%)	8	31
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	57	87
30	4	79/79 (100%)	73 (92%)	6 (8%)	16	51
All	All	3027/3441 (88%)	2868 (95%)	159 (5%)	28	67

5 of 159 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	142	VAL
13	M	35	ARG
27	1	11	THR
11	K	46	ILE
11	K	112	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	18	HIS
15	O	153	GLN
28	2	16	HIS
13	M	41	HIS
14	N	89	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	33 (1%)
2	B	121/122 (99%)	16 (13%)	6 (4%)
All	All	2868/3044 (94%)	260 (9%)	39 (1%)

5 of 260 RNA backbone outliers are listed below:

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

5 of 39 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1450	C
1	A	1942	A
2	B	3043	G
1	A	1506	U
1	A	1563	G

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 235 ligands modelled in this entry, 234 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	$\# Z > 2$
31	TYK	A	9000	1	66,67,67	3.30	29 (43%)	73,97,97	2.36	23 (31%)

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
31	TYK	A	9000	1	-	0/67/126/126	0/3/4/4

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	TYK	C4-C3	-6.43	1.41	1.54
31	A	9000	TYK	C4C-C5C	-3.40	1.45	1.52
31	A	9000	TYK	C2-C3	-3.20	1.48	1.53
31	A	9000	TYK	C6A-C5A	-2.86	1.44	1.51
31	A	9000	TYK	O5A-C5A	-2.85	1.37	1.44

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9000	TYK	O20-C20-C19	-8.82	93.06	125.24
31	A	9000	TYK	O15-C15-C16	-6.16	96.12	106.59
31	A	9000	TYK	C6C-C5C-C4C	-5.73	101.81	113.08
31	A	9000	TYK	C15-C14-C13	-5.59	98.98	110.69
31	A	9000	TYK	C10-C11-C12	-4.41	119.50	126.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9000	TYK	2	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	A	2754/2922 (94%)	-0.02	67 (2%) 62 32	20, 47, 93, 139	0
2	B	122/122 (100%)	0.26	5 (4%) 41 16	31, 65, 95, 145	0
3	C	237/239 (99%)	0.20	17 (7%) 18 7	27, 61, 90, 109	0
4	D	337/337 (100%)	-0.07	1 (0%) 94 84	20, 54, 81, 90	0
5	E	246/246 (100%)	-0.15	2 (0%) 87 67	19, 49, 72, 81	0
6	F	140/176 (79%)	1.47	39 (27%) 1 0	54, 101, 118, 126	0
7	G	172/177 (97%)	0.57	7 (4%) 41 16	39, 65, 88, 94	0
8	H	119/119 (100%)	0.80	11 (9%) 11 4	56, 78, 99, 103	0
9	I	29/348 (8%)	2.07	14 (48%) 0 0	68, 91, 100, 101	0
10	J	156/167 (93%)	0.21	7 (4%) 37 15	32, 55, 79, 88	0
11	K	142/145 (97%)	-0.12	0 100 100	32, 47, 71, 82	0
12	L	132/132 (100%)	-0.01	1 (0%) 87 67	30, 53, 76, 82	0
13	M	145/164 (88%)	0.57	18 (12%) 5 2	23, 72, 105, 115	0
14	N	194/194 (100%)	0.12	11 (5%) 27 10	34, 53, 83, 88	0
15	O	186/186 (100%)	0.70	24 (12%) 5 2	41, 69, 107, 119	0
16	P	115/115 (100%)	-0.06	0 100 100	38, 57, 76, 80	0
17	Q	143/148 (96%)	0.06	2 (1%) 78 51	33, 58, 73, 81	0
18	R	95/95 (100%)	-0.20	1 (1%) 82 58	33, 48, 59, 73	0
19	S	150/154 (97%)	-0.13	0 100 100	27, 42, 66, 74	0
20	T	81/84 (96%)	0.13	1 (1%) 81 55	47, 62, 80, 84	0
21	U	119/119 (100%)	0.38	4 (3%) 49 21	37, 58, 81, 91	0
22	V	53/66 (80%)	3.16	42 (79%) 0 0	81, 91, 97, 105	0
23	W	65/70 (92%)	1.13	12 (18%) 2 1	52, 77, 106, 113	0
24	X	154/154 (100%)	-0.31	0 100 100	31, 46, 66, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.30	2 (2%) 62 32	39, 55, 81, 93	0
26	Z	142/240 (59%)	-0.01	3 (2%) 67 36	25, 45, 69, 85	0
27	1	73/73 (100%)	3.06	43 (58%) 0 0	79, 92, 98, 99	0
28	2	56/56 (100%)	-0.50	0 100 100	26, 34, 41, 47	0
29	3	46/48 (95%)	0.14	2 (4%) 39 16	33, 59, 85, 97	0
30	4	92/92 (100%)	6.12	92 (100%) 0 0	90, 101, 105, 107	0
All	All	6577/7279 (90%)	0.25	428 (6%) 22 8	19, 54, 99, 145	0

The worst 5 of 428 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	14.2
30	4	62	THR	13.6
30	4	82	GLY	12.6
27	1	11	THR	11.4
30	4	38	ARG	11.3

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
33	NA	A	8356	1/1	0.78	0.73	68.78	57,57,57,57	0
33	NA	A	8362	1/1	0.85	0.32	23.74	63,63,63,63	0
34	CL	A	8515	1/1	0.91	0.49	23.11	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	A	8323	1/1	0.88	0.31	15.37	38,38,38,38	0
34	CL	A	8505	1/1	0.78	0.54	12.56	83,83,83,83	0
33	NA	A	8321	1/1	0.87	0.28	12.04	45,45,45,45	0
33	NA	A	8376	1/1	0.89	0.33	10.80	80,80,80,80	0
33	NA	A	8340	1/1	0.93	0.37	10.77	31,31,31,31	0
33	NA	A	8382	1/1	0.81	0.29	10.44	41,41,41,41	0
33	NA	S	8386	1/1	0.64	0.54	10.34	75,75,75,75	0
33	NA	A	8355	1/1	0.91	0.65	9.50	55,55,55,55	0
33	NA	A	8372	1/1	0.89	0.48	9.43	53,53,53,53	0
33	NA	A	8359	1/1	0.93	0.43	9.42	52,52,52,52	0
33	NA	A	8303	1/1	0.84	0.26	8.44	53,53,53,53	0
34	CL	D	8519	1/1	0.96	0.47	8.29	59,59,59,59	0
33	NA	A	8371	1/1	0.87	0.21	7.22	31,31,31,31	0
33	NA	A	8364	1/1	0.87	0.23	6.76	39,39,39,39	0
33	NA	A	8374	1/1	0.90	0.30	6.68	41,41,41,41	0
33	NA	A	8373	1/1	0.77	0.48	6.45	37,37,37,37	0
33	NA	A	8350	1/1	0.93	0.21	6.08	24,24,24,24	0
33	NA	A	8378	1/1	0.92	0.28	6.04	30,30,30,30	0
32	MG	A	8067	1/1	0.94	0.26	6.04	49,49,49,49	0
33	NA	A	8365	1/1	0.91	0.33	4.01	41,41,41,41	0
31	TYK	A	9000	64/64	0.94	0.22	3.39	33,43,48,51	0
33	NA	S	8337	1/1	0.47	0.34	3.34	34,34,34,34	0
33	NA	A	8366	1/1	0.88	0.29	2.97	43,43,43,43	0
34	CL	4	8504	1/1	0.47	1.21	2.36	112,112,112,112	0
32	MG	A	8044	1/1	0.95	0.17	1.73	44,44,44,44	0
33	NA	M	8380	1/1	0.93	0.26	1.64	49,49,49,49	0
33	NA	A	8331	1/1	0.91	0.18	1.57	46,46,46,46	0
32	MG	A	8013	1/1	0.99	0.18	1.34	42,42,42,42	0
34	CL	K	8521	1/1	0.95	0.21	1.32	50,50,50,50	0
33	NA	A	8326	1/1	0.80	0.26	1.08	56,56,56,56	0
33	NA	A	8335	1/1	0.97	0.18	1.07	45,45,45,45	0
34	CL	M	8510	1/1	0.86	0.32	0.99	75,75,75,75	0
33	NA	A	8325	1/1	0.95	0.15	0.75	47,47,47,47	0
33	NA	A	8368	1/1	0.91	0.17	0.74	43,43,43,43	0
33	NA	A	8379	1/1	0.96	0.15	0.59	32,32,32,32	0
34	CL	P	8508	1/1	0.96	0.22	0.39	83,83,83,83	0
33	NA	A	8332	1/1	0.79	0.18	0.31	34,34,34,34	0
33	NA	A	8339	1/1	0.97	0.16	0.00	22,22,22,22	0
32	MG	A	8064	1/1	0.92	0.15	-0.04	18,18,18,18	0
33	NA	B	8383	1/1	0.81	0.20	-0.15	54,54,54,54	0
32	MG	A	8112	1/1	0.74	0.18	-0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	A	8327	1/1	0.93	0.15	-0.32	28,28,28,28	0
33	NA	A	8333	1/1	0.92	0.16	-0.42	26,26,26,26	0
32	MG	4	8078	1/1	0.92	0.42	-0.65	91,91,91,91	0
32	MG	A	8057	1/1	0.95	0.18	-0.67	34,34,34,34	0
32	MG	1	8105	1/1	0.96	0.17	-0.70	42,42,42,42	0
35	K	A	8602	1/1	0.89	0.13	-0.75	56,56,56,56	0
33	NA	J	8309	1/1	0.98	0.13	-0.76	25,25,25,25	0
33	NA	A	8314	1/1	0.96	0.14	-0.80	45,45,45,45	0
33	NA	A	8361	1/1	0.96	0.13	-0.80	48,48,48,48	0
32	MG	D	8055	1/1	0.85	0.16	-0.89	84,84,84,84	0
33	NA	A	8324	1/1	0.92	0.12	-1.06	42,42,42,42	0
33	NA	A	8338	1/1	0.93	0.12	-1.16	59,59,59,59	0
32	MG	A	8086	1/1	0.98	0.10	-1.30	40,40,40,40	0
34	CL	A	8512	1/1	0.94	0.15	-1.33	32,32,32,32	0
32	MG	Z	8109	1/1	0.92	0.14	-1.54	39,39,39,39	0
32	MG	A	8107	1/1	0.97	0.06	-1.79	51,51,51,51	0
32	MG	A	8074	1/1	0.98	0.07	-1.81	12,12,12,12	0
32	MG	U	8073	1/1	0.94	0.12	-1.84	38,38,38,38	0
36	CD	V	8401	1/1	0.68	0.40	-1.86	142,142,142,142	0
36	CD	1	8403	1/1	0.93	0.21	-1.90	139,139,139,139	0
34	CL	N	8518	1/1	0.94	0.17	-1.93	38,38,38,38	0
33	NA	A	8317	1/1	0.96	0.11	-2.19	9,9,9,9	0
33	NA	A	8305	1/1	0.92	0.13	-2.20	33,33,33,33	0
32	MG	A	8003	1/1	0.97	0.12	-2.30	19,19,19,19	0
33	NA	K	8346	1/1	0.96	0.11	-2.32	17,17,17,17	0
35	K	A	8601	1/1	0.94	0.12	-2.44	62,62,62,62	0
36	CD	2	8402	1/1	0.98	0.08	-2.47	52,52,52,52	0
32	MG	A	8062	1/1	0.94	0.11	-2.58	46,46,46,46	0
33	NA	A	8381	1/1	0.98	0.09	-2.64	33,33,33,33	0
32	MG	A	8002	1/1	0.96	0.12	-2.74	42,42,42,42	0
33	NA	A	8320	1/1	0.95	0.11	-2.89	32,32,32,32	0
33	NA	A	8353	1/1	0.99	0.09	-2.99	16,16,16,16	0
32	MG	A	8008	1/1	0.98	0.08	-3.10	41,41,41,41	0
32	MG	C	8065	1/1	0.97	0.07	-3.11	52,52,52,52	0
32	MG	A	8071	1/1	0.81	0.11	-3.16	84,84,84,84	0
32	MG	A	8110	1/1	0.95	0.11	-3.24	23,23,23,23	0
32	MG	A	8058	1/1	0.98	0.11	-3.58	34,34,34,34	0
32	MG	A	8018	1/1	0.94	0.08	-3.66	32,32,32,32	0
32	MG	A	8033	1/1	0.98	0.09	-3.91	22,22,22,22	0
33	NA	N	8347	1/1	0.95	0.11	-3.96	24,24,24,24	0
32	MG	A	8053	1/1	0.92	0.10	-3.98	52,52,52,52	0
32	MG	A	8108	1/1	0.93	0.11	-3.99	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	C	8345	1/1	0.98	0.10	-4.05	34,34,34,34	0
33	NA	A	8343	1/1	0.94	0.08	-4.08	11,11,11,11	0
32	MG	A	8015	1/1	0.98	0.08	-4.11	46,46,46,46	0
33	NA	R	8348	1/1	0.98	0.06	-4.17	15,15,15,15	0
32	MG	A	8001	1/1	0.82	0.11	-4.21	38,38,38,38	0
32	MG	A	8056	1/1	0.98	0.07	-4.44	41,41,41,41	0
32	MG	A	8004	1/1	0.97	0.11	-4.61	35,35,35,35	0
33	NA	A	8344	1/1	0.96	0.07	-4.65	16,16,16,16	0
32	MG	A	8012	1/1	0.99	0.11	-4.73	34,34,34,34	0
32	MG	A	8096	1/1	0.95	0.10	-5.02	54,54,54,54	0
32	MG	A	8039	1/1	0.97	0.09	-5.07	54,54,54,54	0
32	MG	A	8059	1/1	0.90	0.09	-5.10	33,33,33,33	0
32	MG	A	8088	1/1	0.93	0.08	-5.24	28,28,28,28	0
32	MG	A	8032	1/1	0.97	0.10	-5.42	29,29,29,29	0
32	MG	A	8017	1/1	0.98	0.05	-5.68	28,28,28,28	0
32	MG	A	8035	1/1	0.98	0.06	-5.99	48,48,48,48	0
32	MG	A	8038	1/1	0.98	0.05	-6.90	14,14,14,14	0
32	MG	A	8084	1/1	0.94	0.09	-7.17	40,40,40,40	0
32	MG	A	8052	1/1	0.96	0.05	-7.23	36,36,36,36	0
32	MG	A	8020	1/1	0.99	0.05	-7.27	34,34,34,34	0
32	MG	A	8060	1/1	0.97	0.10	-7.27	48,48,48,48	0
32	MG	A	8080	1/1	0.99	0.06	-7.48	35,35,35,35	0
32	MG	A	8028	1/1	0.97	0.07	-7.56	43,43,43,43	0
32	MG	A	8006	1/1	0.95	0.06	-7.94	48,48,48,48	0
32	MG	A	8010	1/1	0.99	0.07	-8.28	29,29,29,29	0
32	MG	A	8077	1/1	0.97	0.09	-8.31	28,28,28,28	0
32	MG	A	8054	1/1	0.97	0.08	-8.87	50,50,50,50	0
32	MG	A	8019	1/1	1.00	0.05	-9.13	27,27,27,27	0
32	MG	A	8027	1/1	0.92	0.06	-9.19	51,51,51,51	0
32	MG	A	8007	1/1	0.96	0.06	-12.51	24,24,24,24	0
32	MG	A	8014	1/1	0.98	0.05	-13.61	13,13,13,13	0
34	CL	S	8506	1/1	0.97	0.14	-	42,42,42,42	0
32	MG	A	8049	1/1	0.94	0.16	-	62,62,62,62	0
32	MG	A	8092	1/1	0.92	0.17	-	83,83,83,83	0
32	MG	A	8022	1/1	0.94	0.19	-	39,39,39,39	0
32	MG	A	8111	1/1	0.95	0.06	-	54,54,54,54	0
32	MG	A	8117	1/1	0.99	0.15	-	19,19,19,19	0
36	CD	4	8404	1/1	0.73	0.51	-	148,148,148,148	0
33	NA	A	8306	1/1	0.96	0.37	-	36,36,36,36	0
33	NA	A	8363	1/1	0.93	0.19	-	49,49,49,49	0
34	CL	A	8522	1/1	0.88	0.75	-	80,80,80,80	0
32	MG	A	8048	1/1	0.95	0.15	-	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	A	8063	1/1	0.98	0.08	-	73,73,73,73	0
32	MG	A	8093	1/1	0.95	0.12	-	38,38,38,38	0
34	CL	K	8501	1/1	0.98	0.20	-	58,58,58,58	0
33	NA	A	8307	1/1	0.91	0.10	-	20,20,20,20	0
32	MG	A	8040	1/1	0.93	0.11	-	84,84,84,84	0
32	MG	A	8026	1/1	0.99	0.05	-	15,15,15,15	0
33	NA	B	8351	1/1	0.77	0.18	-	58,58,58,58	0
32	MG	A	8030	1/1	0.99	0.09	-	29,29,29,29	0
32	MG	A	8085	1/1	0.94	0.12	-	79,79,79,79	0
33	NA	A	8301	1/1	0.88	0.16	-	20,20,20,20	0
32	MG	A	8029	1/1	0.98	0.12	-	51,51,51,51	0
33	NA	A	8302	1/1	0.92	0.16	-	24,24,24,24	0
33	NA	E	8304	1/1	0.61	0.16	-	32,32,32,32	0
32	MG	A	8021	1/1	0.97	0.08	-	27,27,27,27	0
32	MG	A	8089	1/1	0.94	0.10	-	64,64,64,64	0
32	MG	A	8099	1/1	0.97	0.10	-	46,46,46,46	0
33	NA	A	8367	1/1	0.94	0.15	-	37,37,37,37	0
34	CL	A	8513	1/1	0.89	0.19	-	64,64,64,64	0
32	MG	A	8091	1/1	0.98	0.07	-	45,45,45,45	0
32	MG	A	8082	1/1	0.90	0.23	-	59,59,59,59	0
32	MG	A	8076	1/1	0.97	0.12	-	61,61,61,61	0
33	NA	A	8334	1/1	0.95	0.05	-	26,26,26,26	0
32	MG	A	8114	1/1	0.94	0.23	-	82,82,82,82	0
32	MG	A	8009	1/1	0.99	0.04	-	19,19,19,19	0
33	NA	A	8342	1/1	0.92	0.17	-	39,39,39,39	0
32	MG	A	8103	1/1	0.93	0.20	-	69,69,69,69	0
33	NA	A	8328	1/1	0.96	0.14	-	24,24,24,24	0
32	MG	A	8090	1/1	0.87	0.21	-	11,11,11,11	0
34	CL	R	8511	1/1	0.92	0.13	-	57,57,57,57	0
33	NA	A	8354	1/1	0.85	0.20	-	40,40,40,40	0
34	CL	K	8516	1/1	0.93	0.19	-	40,40,40,40	0
32	MG	A	8023	1/1	0.86	0.10	-	42,42,42,42	0
32	MG	A	8100	1/1	0.90	0.15	-	48,48,48,48	0
34	CL	K	8502	1/1	0.90	0.12	-	56,56,56,56	0
32	MG	A	8051	1/1	0.97	0.07	-	66,66,66,66	0
32	MG	A	8016	1/1	0.97	0.08	-	43,43,43,43	0
33	NA	A	8313	1/1	0.97	0.17	-	64,64,64,64	0
33	NA	A	8319	1/1	0.94	0.14	-	39,39,39,39	0
32	MG	A	8068	1/1	0.97	0.12	-	40,40,40,40	0
32	MG	L	8069	1/1	0.97	0.10	-	72,72,72,72	0
33	NA	A	8330	1/1	0.91	0.18	-	46,46,46,46	0
33	NA	A	8316	1/1	0.96	0.12	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	NA	A	8357	1/1	0.78	0.10	-	53,53,53,53	0
32	MG	A	8098	1/1	0.99	0.20	-	43,43,43,43	0
32	MG	A	8043	1/1	0.97	0.06	-	58,58,58,58	0
32	MG	A	8115	1/1	0.91	0.10	-	46,46,46,46	0
32	MG	A	8024	1/1	0.88	0.56	-	99,99,99,99	0
32	MG	A	8031	1/1	0.96	0.04	-	14,14,14,14	0
33	NA	A	8385	1/1	0.95	0.25	-	28,28,28,28	0
32	MG	A	8081	1/1	0.85	0.18	-	64,64,64,64	0
35	K	A	8603	1/1	0.91	0.43	-	76,76,76,76	0
33	NA	A	8375	1/1	0.94	0.25	-	53,53,53,53	0
33	NA	A	8384	1/1	0.27	1.12	-	106,106,106,106	0
32	MG	A	8036	1/1	0.99	0.06	-	41,41,41,41	0
32	MG	A	8011	1/1	0.97	0.07	-	25,25,25,25	0
32	MG	A	8070	1/1	0.82	0.81	-	70,70,70,70	0
32	MG	A	8066	1/1	0.90	0.07	-	70,70,70,70	0
32	MG	A	8083	1/1	0.98	0.07	-	47,47,47,47	0
33	NA	A	8318	1/1	0.96	0.14	-	37,37,37,37	0
32	MG	A	8050	1/1	0.81	0.22	-	77,77,77,77	0
32	MG	A	8118	1/1	0.84	0.33	-	31,31,31,31	0
32	MG	A	8101	1/1	0.85	0.16	-	38,38,38,38	0
33	NA	A	8377	1/1	0.84	0.32	-	77,77,77,77	0
32	MG	A	8119	1/1	0.96	0.10	-	30,30,30,30	0
36	CD	P	8405	1/1	0.72	0.19	-	154,154,154,154	0
32	MG	A	8042	1/1	0.96	0.13	-	31,31,31,31	0
32	MG	A	8005	1/1	0.98	0.14	-	47,47,47,47	0
33	NA	A	8329	1/1	0.97	0.09	-	33,33,33,33	0
32	MG	A	8072	1/1	0.96	0.15	-	88,88,88,88	0
33	NA	A	8341	1/1	0.88	0.10	-	17,17,17,17	0
34	CL	A	8514	1/1	0.96	0.12	-	51,51,51,51	0
32	MG	A	8097	1/1	0.96	0.23	-	37,37,37,37	0
32	MG	A	8094	1/1	0.98	0.05	-	60,60,60,60	0
32	MG	A	8104	1/1	0.75	0.38	-	51,51,51,51	0
32	MG	A	8106	1/1	0.93	0.13	-	62,62,62,62	0
33	NA	A	8369	1/1	0.85	0.23	-	53,53,53,53	0
33	NA	A	8308	1/1	0.91	0.12	-	50,50,50,50	0
33	NA	A	8311	1/1	0.87	0.22	-	50,50,50,50	0
32	MG	A	8079	1/1	0.96	0.09	-	24,24,24,24	0
32	MG	B	8095	1/1	0.89	0.06	-	68,68,68,68	0
33	NA	J	8322	1/1	0.64	0.45	-	56,56,56,56	0
33	NA	A	8360	1/1	0.96	0.55	-	38,38,38,38	0
34	CL	A	8517	1/1	0.93	0.24	-	49,49,49,49	0
33	NA	T	8312	1/1	0.70	0.76	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	CL	O	8507	1/1	0.95	0.14	-	54,54,54,54	0
32	MG	A	8045	1/1	0.91	0.12	-	61,61,61,61	0
32	MG	A	8061	1/1	0.91	0.06	-	35,35,35,35	0
32	MG	A	8037	1/1	0.98	0.12	-	45,45,45,45	0
33	NA	A	8315	1/1	0.99	0.11	-	27,27,27,27	0
32	MG	A	8025	1/1	0.97	0.09	-	54,54,54,54	0
32	MG	A	8046	1/1	0.89	0.07	-	62,62,62,62	0
32	MG	A	8113	1/1	0.94	0.13	-	40,40,40,40	0
32	MG	A	8041	1/1	0.91	0.36	-	62,62,62,62	0
34	CL	C	8509	1/1	0.97	0.34	-	74,74,74,74	0
32	MG	A	8116	1/1	0.88	0.20	-	80,80,80,80	0
32	MG	A	8087	1/1	0.86	0.18	-	52,52,52,52	0
32	MG	A	8034	1/1	0.98	0.05	-	32,32,32,32	0
33	NA	A	8349	1/1	0.97	0.29	-	33,33,33,33	0
32	MG	A	8102	1/1	0.95	0.84	-	82,82,82,82	0
33	NA	A	8310	1/1	0.84	0.21	-	31,31,31,31	0
33	NA	A	8336	1/1	0.92	0.15	-	46,46,46,46	0
34	CL	Z	8520	1/1	0.91	0.14	-	30,30,30,30	0
32	MG	A	8075	1/1	0.94	0.11	-	38,38,38,38	0
34	CL	A	8503	1/1	0.86	0.27	-	55,55,55,55	0
33	NA	A	8352	1/1	0.93	0.47	-	37,37,37,37	0
32	MG	A	8047	1/1	0.98	0.14	-	45,45,45,45	0
33	NA	A	8370	1/1	0.88	0.37	-	55,55,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.