



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 12, 2021 – 11:30 AM EDT

PDB ID : 1YJW
Title : Crystal Structure Of Quinupristin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2005-01-15
Resolution : 2.90 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

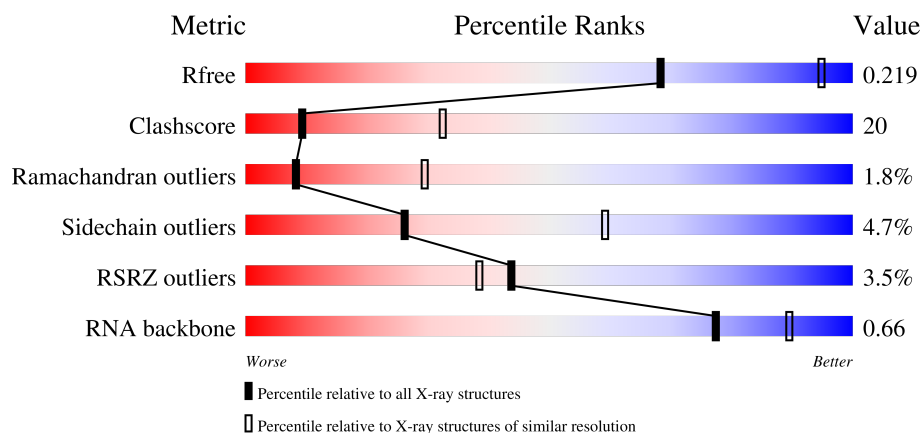
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>53%</div> <div>35%</div> <div>6%</div> <div>6%</div> </div>
2	1	57	<div> <div>65%</div> <div>33%</div> <div>.</div> </div>
3	2	50	<div> <div>4%</div> <div>46%</div> <div>46%</div> <div>8%</div> </div>
4	3	92	<div> <div>55%</div> <div>45%</div> </div>

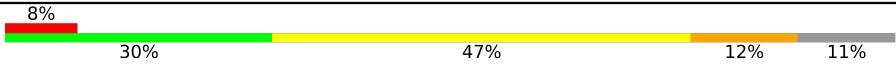


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Mol	Chain	Length	Quality of chain
5	4	8	
6	9	122	
7	A	240	
8	B	338	
9	C	246	
10	D	177	
11	E	178	
12	F	120	
13	G	348	
14	H	177	
15	I	162	
16	J	145	
17	K	132	
18	L	165	
19	M	195	
20	N	187	
21	O	116	
22	P	149	
23	Q	96	
24	R	155	
25	S	85	
26	T	120	
27	U	66	
28	V	71	
29	W	154	

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Mol	Chain	Length	Quality of chain
30	X	92	
31	Y	241	
32	Z	83	

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
35	NA	0	3120	-	-	-	X
35	NA	0	3134	-	-	-	X
35	NA	0	3174	-	-	-	X
35	NA	0	3175	-	-	-	X
35	NA	0	3183	-	-	-	X
35	NA	9	203	-	-	-	X
35	NA	R	202	-	-	-	X
36	CL	0	3189	-	-	X	-
36	CL	N	201	-	-	X	-

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99111 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
			59020	26349	10873	19053	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	2099	A	G	engineered mutation	GB 55229667

- Molecule 2 is a protein called 50S RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 3 is a protein called 50S RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 4 is a protein called 50S RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 5 is a protein called QUINUPRISTIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	4	7	Total	C	N	O	0	0	0
			63	45	8	10			

- Molecule 6 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L2P.

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

- Molecule 8 is a protein called 50S RIBOSOMAL PROTEIN L3P.

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

- Molecule 9 is a protein called 50S RIBOSOMAL PROTEIN L4E.

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

- Molecule 10 is a protein called 50S RIBOSOMAL PROTEIN L5P.

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L6P.

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

- Molecule 12 is a protein called 50S RIBOSOMAL PROTEIN L7AE.

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

- Molecule 13 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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

- Molecule 14 is a protein called 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 15 is a protein called 50S RIBOSOMAL PROTEIN L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 16 is a protein called 50S RIBOSOMAL PROTEIN L13P.

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

- Molecule 17 is a protein called 50S RIBOSOMAL PROTEIN L14P.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called 50S RIBOSOMAL PROTEIN L15P.

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

- Molecule 19 is a protein called 50S RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	M	194	Total	C	N	O	S	0	0	0
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	conflict	GB 55231501

- Molecule 20 is a protein called 50S RIBOSOMAL PROTEIN L18P.

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

- Molecule 21 is a protein called 50S RIBOSOMAL PROTEIN L18E.

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

- Molecule 22 is a protein called 50S RIBOSOMAL PROTEIN L19E.

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

- Molecule 23 is a protein called 50S RIBOSOMAL PROTEIN L21E.

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

- Molecule 24 is a protein called 50S RIBOSOMAL PROTEIN L22P.

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

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L23P.

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

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L24P.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L24E.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29P.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30P.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31E.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32E.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L37AE.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	conflict	GB 55231162

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	109	Total	Mg	0	0
			109	109		
33	3	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	Y	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	74	Total	Na	0	0
			74	74		
35	9	2	Total	Na	0	0
			2	2		

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

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total 10	Cl 10	0	0
36	3	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	J	3	Total 3	Cl 3	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0

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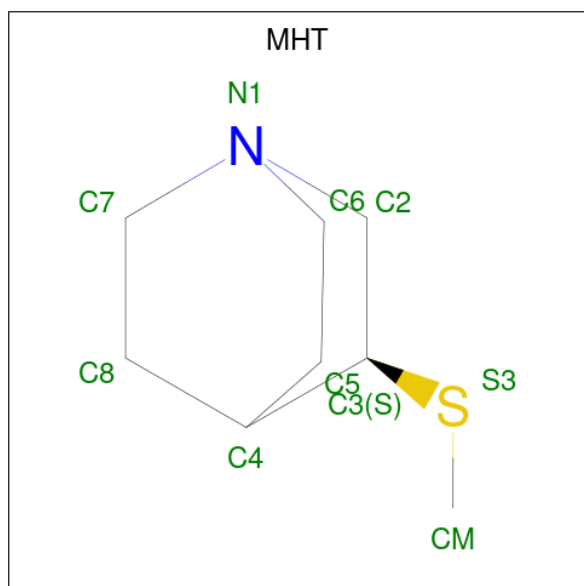
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	Y	1	Total	Cl	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	1	1	Total	Cd	0	0
			1	1		
37	3	1	Total	Cd	0	0
			1	1		
37	O	1	Total	Cd	0	0
			1	1		
37	U	1	Total	Cd	0	0
			1	1		
37	Z	1	Total	Cd	0	0
			1	1		

- Molecule 38 is (3S)-3-(methylsulfanyl)-1-azabicyclo[2.2.2]octane (three-letter code: MHT) (formula: C₈H₁₅NS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	4	1	Total	C	N	S	0	0
			10	8	1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5842	Total 5842	O 5842	0	0
39	1	60	Total 60	O 60	0	0
39	2	49	Total 49	O 49	0	0
39	3	69	Total 69	O 69	0	0
39	4	2	Total 2	O 2	0	0
39	9	143	Total 143	O 143	0	0
39	A	123	Total 123	O 123	0	0
39	B	146	Total 146	O 146	0	0
39	C	185	Total 185	O 185	0	0
39	D	49	Total 49	O 49	0	0
39	E	42	Total 42	O 42	0	0
39	F	26	Total 26	O 26	0	0
39	G	20	Total 20	O 20	0	0
39	H	69	Total 69	O 69	0	0
39	I	9	Total 9	O 9	0	0
39	J	55	Total 55	O 55	0	0
39	K	59	Total 59	O 59	0	0
39	L	82	Total 82	O 82	0	0
39	M	129	Total 129	O 129	0	0
39	N	60	Total 60	O 60	0	0
39	O	42	Total 42	O 42	0	0
39	P	72	Total 72	O 72	0	0

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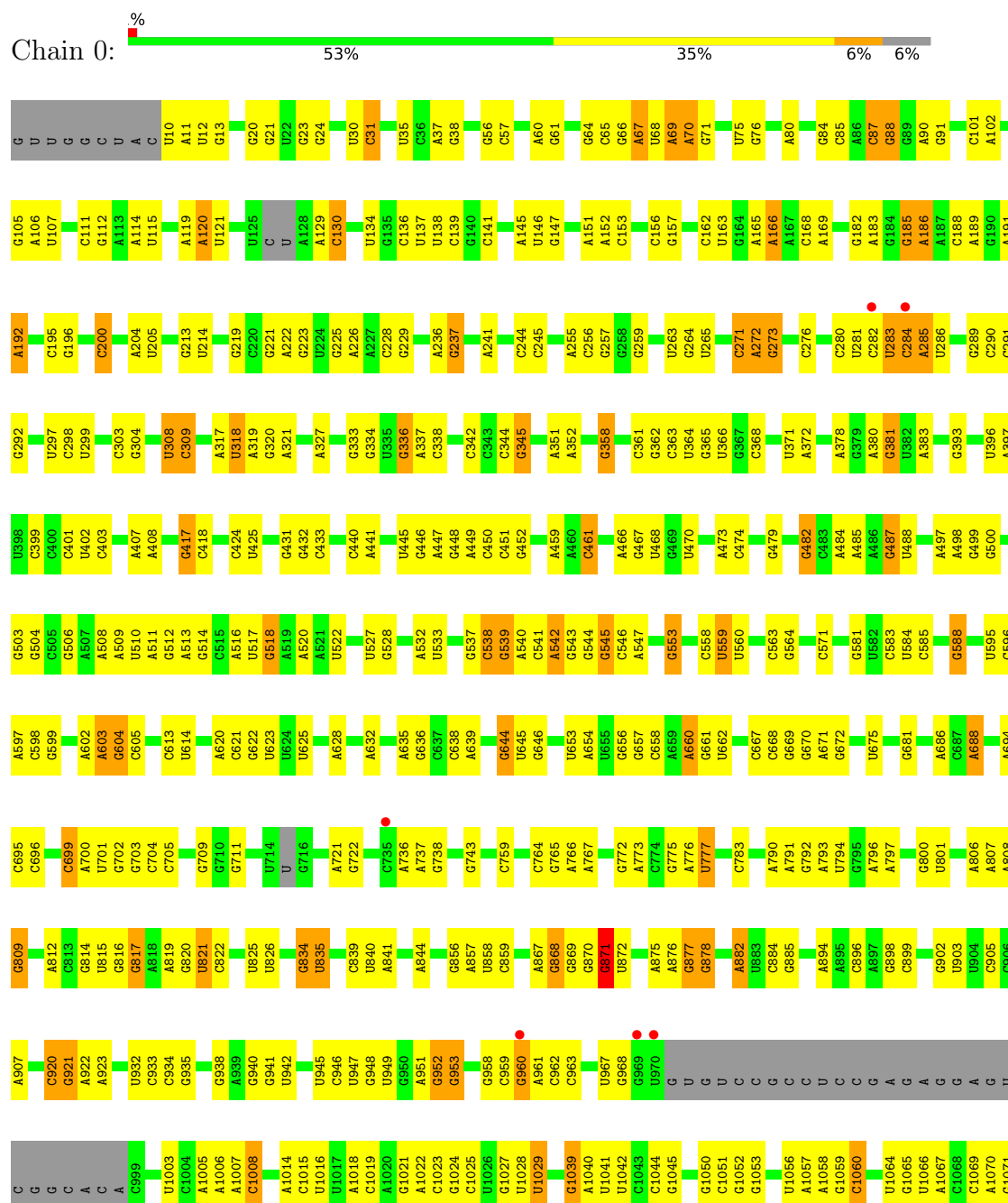
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	Q	48	Total 48	O 48	0	0
39	R	85	Total 85	O 85	0	0
39	S	30	Total 30	O 30	0	0
39	T	39	Total 39	O 39	0	0
39	U	29	Total 29	O 29	0	0
39	V	13	Total 13	O 13	0	0
39	W	69	Total 69	O 69	0	0
39	X	26	Total 26	O 26	0	0
39	Y	101	Total 101	O 101	0	0
39	Z	37	Total 37	O 37	0	0

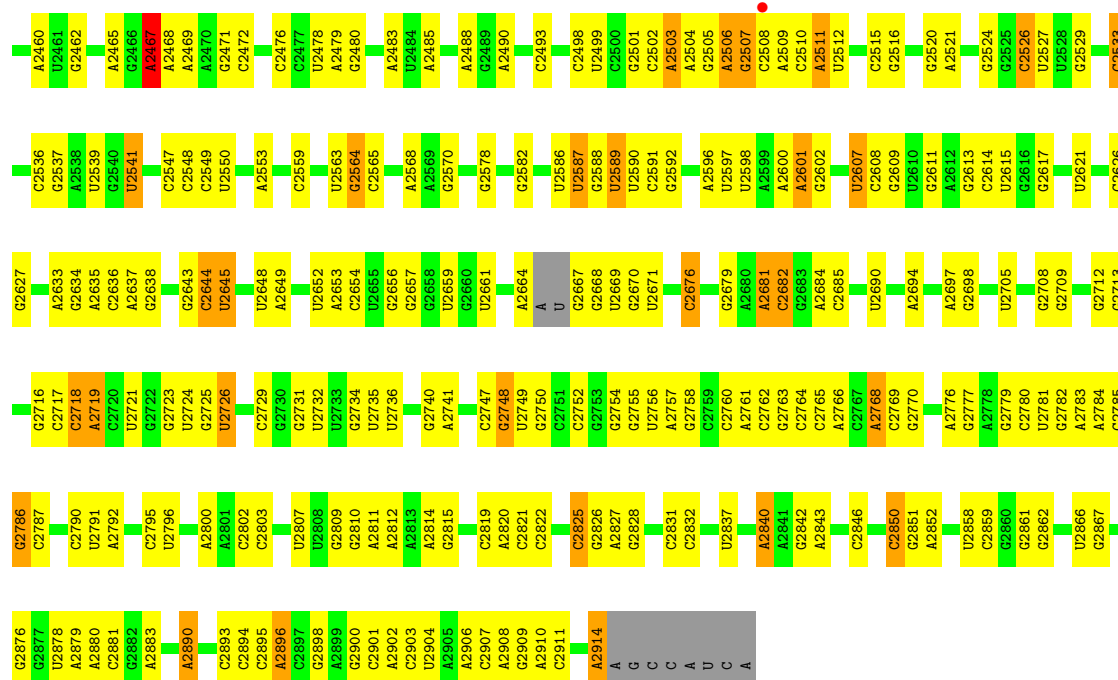
3 Residue-property plots

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

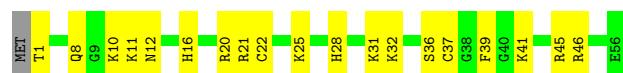
• Molecule 1: 23S RIBOSOMAL RNA



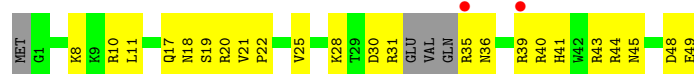
A2364	G2270	C	G1823	A1733	G1834	A1533	A1437	C1343	G1239	G1072
G2365	G2271	C	G1824	C1734	U1635	C1534	G1438	A1348	G1242	A1073
A2369	C2272	C	U1825	C1735	G1636	G1535	C1439	A1349	C1243	G1074
G2370	C2273	G	C2036	A1736	A1637	C1536	G1537	A1352	C1244	A1081
A2371	G2274	C	A1942	U1741	A1641	G1543	U1446	G1354	A1246	A1086
G2372	G2275	A	A1943	A1742	A1642	U1544	U1446	A1355	C1250	G1087
A2373	U2276	C	C1830	G1743	C1643	C1545	C1451	C1360	C1251	A1088
U2377	U2277	A	A1929	G1744	A1643	U1546	C1451	C1361	C1252	G1089
U2377	C2281	A	C1834	U1748	A1653	A1559	C1451	C1362	C1253	A1097
U2378	U2282	C	U1835	G1749	A1654	U1559	C1451	C1363	C1254	A1098
G2379	G2283	U	U1836	C1750	G1655	U1560	C1451	C1364	C1255	G1099
A2380	A2284	G	U1837	U1751	G1656	C1562	U1461	C1365	C1256	C1102
C2381	A2285	A	A1838	G1752	A1657	G1563	A1470	C1366	C1257	U1109
A2382	U2297	A	A1839	C1753	A1658	C1564	A1471	C1367	C1258	G1110
G2383	G2298	C	A1840	G1754	A1659	G1565	A1472	C1368	C1259	U1111
U2384	A2300	C	C1841	A1755	G1660	G1571	C1473	C1369	C1260	G1112
A2385	A2301	C	A1845	A1756	C1661	A1572	C1474	C1370	C1261	U1113
U2386	A2302	A	G1849	U1757	A1662	A1573	C1475	C1371	C1262	U1114
U2387	A2303	U	C1853	C1758	A1663	C1574	C1476	C1372	C1263	U1115
U2388	C2309	C	C1854	G1759	U1664	A1575	C1477	C1373	C1264	U1116
U2389	C2310	C	G1855	C1760	U1665	A1576	C1478	C1374	C1265	A1117
C2392	G2312	C	C1856	U1766	A1670	A1581	C1479	C1375	C1266	A1118
A2401	C2313	G	C1862	C1768	C1674	G1584	C1483	C1376	C1267	G1119
A2402	G2314	C	G1863	C1769	U1677	C1585	G1484	C1377	C1268	U1120
C2411	C2315	C	G1864	U1770	U1678	G1586	C1485	C1378	C1269	G1121
G2412	G2316	G	G1865	A1771	A1679	U1587	U1488	C1379	C1270	U1122
A2413	C2317	G	C1866	C1772	C1679	G1588	G1489	C1380	C1271	A1123
U2414	U2320	U	C1867	G1773	A1682	G1589	G1490	C1381	C1272	C1129
A2415	A2321	C	U1874	U1778	G1683	G1592	A1493	C1382	C1273	U1130
U2419	G2324	C	G1877	A1779	A1684	C1593	A1494	C1383	C1274	G1131
G2420	U2325	U	G1878	U1784	A1685	C1594	C1495	C1384	C1275	A1132
G2421	C2326	C	U1879	U1785	C1692	G1595	A1496	C1385	C1276	G1133
U2422	C2327	C	C1882	G1786	A1701	U1596	G1497	C1386	C1277	U1134
U2423	U2242	G	G1883	C1787	U1702	A1597	U1500	C1387	C1278	G1135
U2424	C2243	A	G1884	U1788	U1703	U1598	A1501	C1388	C1279	U1136
G2425	C2244	C	U1903	G1789	A1710	G1600	U1502	C1389	C1280	C1140
G2426	C2245	C	A1904	C1790	A1711	A1603	A1503	C1390	C1281	A1150
C2431	G2336	C	U1905	U1791	A1712	G1604	U1504	C1391	C1282	G1151
G2432	A2433	C	U1906	A1797	G1713	G1605	U1505	C1392	C1283	A1154
A2434	C2434	C	A1997	C1798	C1714	G1614	U1506	C1393	C1284	G1155
U2435	C2435	C	G2000	U1799	C1715	A1615	C1513	C1394	C1285	C1156
U2441	G2442	C	G2001	G1799	A1716	A1616	C1514	C1395	C1286	G1157
G2443	C2443	C	C2002	G1799	A1717	A1617	A1515	C1396	C1287	G1158
U2444	A2454	C	U2003	A1804	G1718	C1618	U1516	C1397	C1288	G1159
G2445	C2454	C	A1919	G1805	G1719	G1619	C1517	C1398	C1289	A1161
U2446	C2455	C	G1925	G1806	U1722	C1620	A1518	C1399	C1290	G1162
G2453	U2285	G	G1926	C1810	U1723	A1624	U1524	C1400	C1291	U1163
C2454	A2286	C	A1927	A1811	U1724	U1625	G1525	C1401	C1292	G1164
A2455	G2287	C	G1928	G1819	C1725	A1626	A1526	C1402	C1293	G1165
G2456	C2288	C	A1930	G1820	G1730	G1627	A1527	C1403	C1294	G1166
	C2289	A	A1931	A1821	C1731	C1628	G1529	C1404	C1295	G1167
			C1935	A1822	A1732	C1633		C1405	C1296	U1170



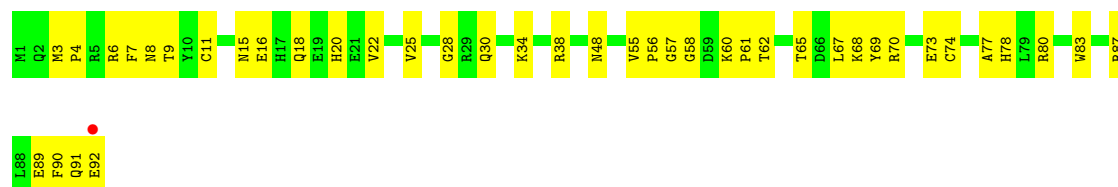
• Molecule 2: 50S RIBOSOMAL PROBLEM L37E



• Molecule 3: 50S RIBOSOMAL PROBLEM L39E



• Molecule 4: 50S RIBOSOMAL PROBLEM L44E

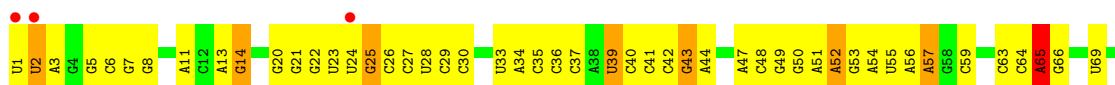


• Molecule 5: QUINUPRISTIN

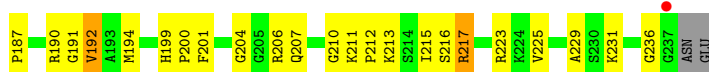




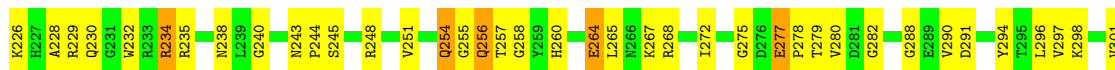
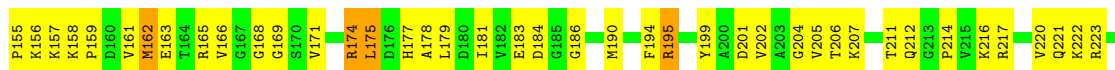
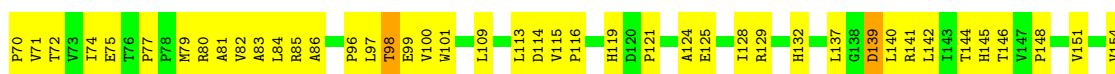
• Molecule 6: 5S RIBOSOMAL RNA



• Molecule 7: 50S RIBOSOMAL PROTEIN L2P

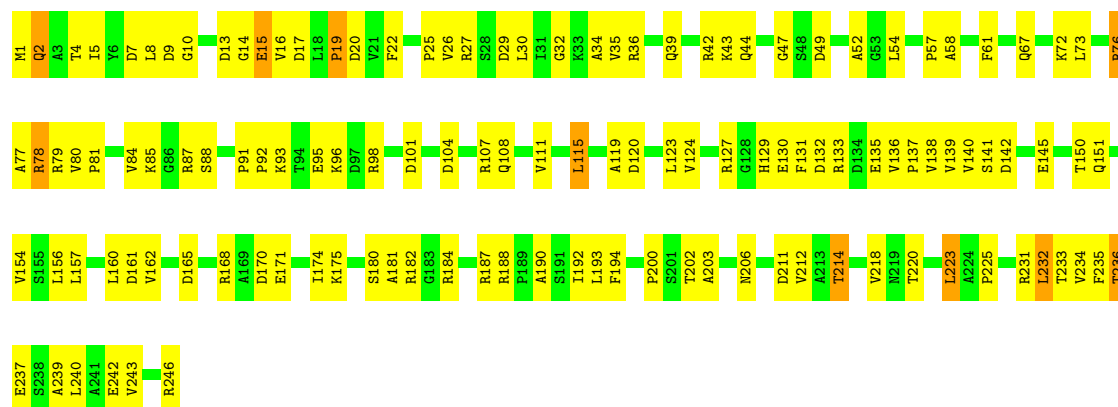


• Molecule 8: 50S RIBOSOMAL PROTEIN L3P

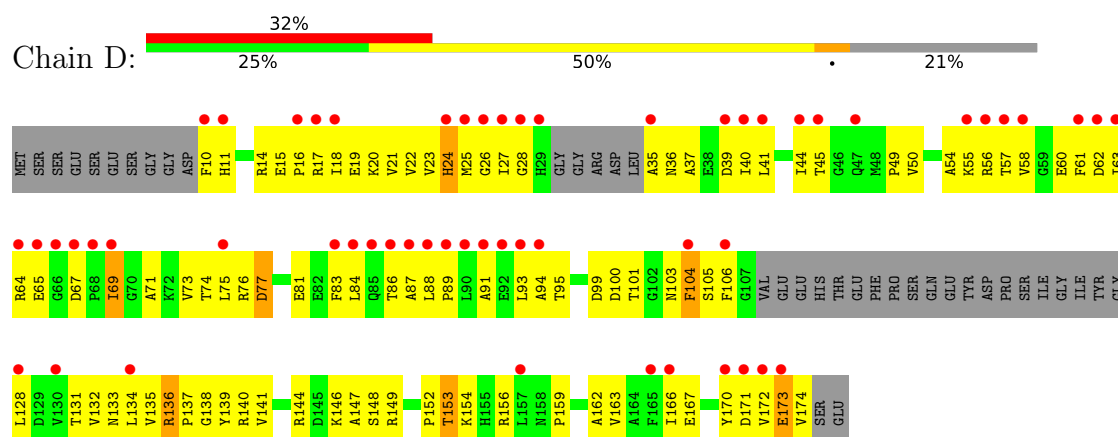


• Molecule 9: 50S RIBOSOMAL PROTEIN L4E

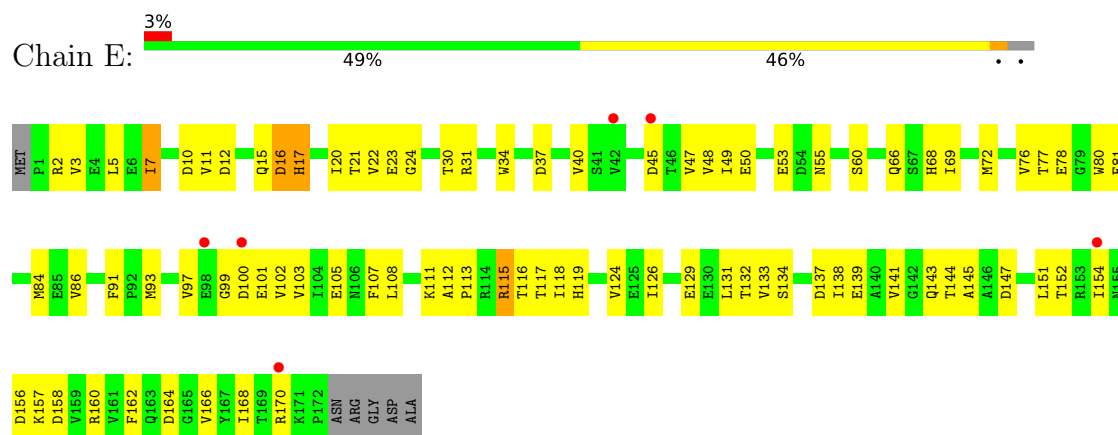




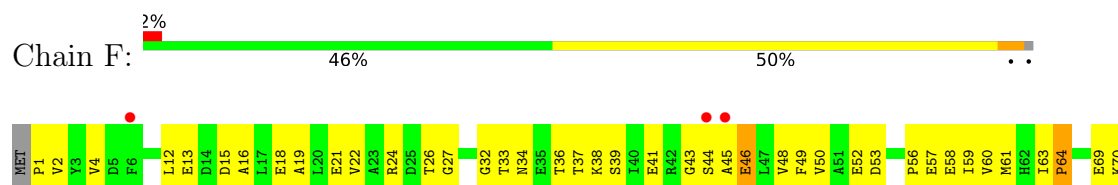
• Molecule 10: 50S RIBOSOMAL PROTEIN L5P



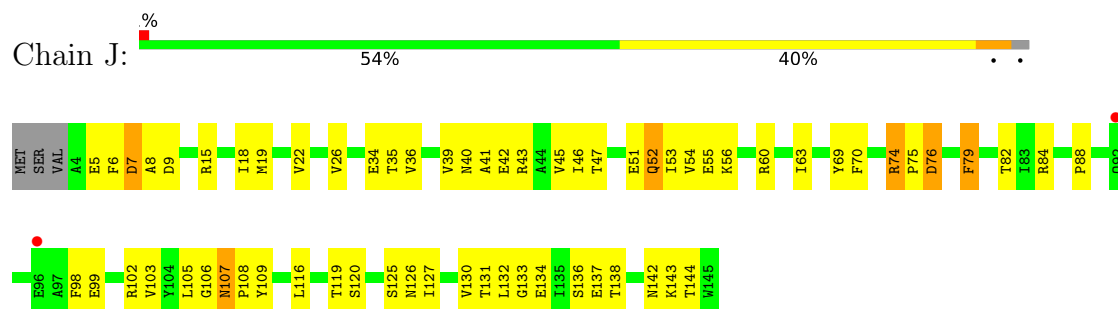
• Molecule 11: 50S RIBOSOMAL PROTEIN L6P



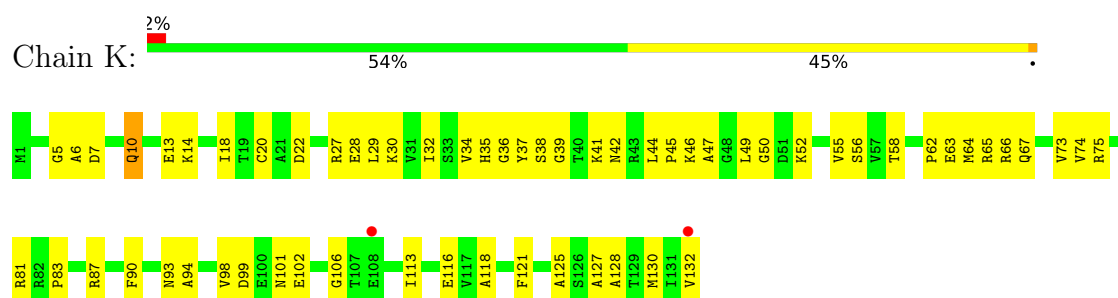
• Molecule 12: 50S RIBOSOMAL PROTEIN L7AE



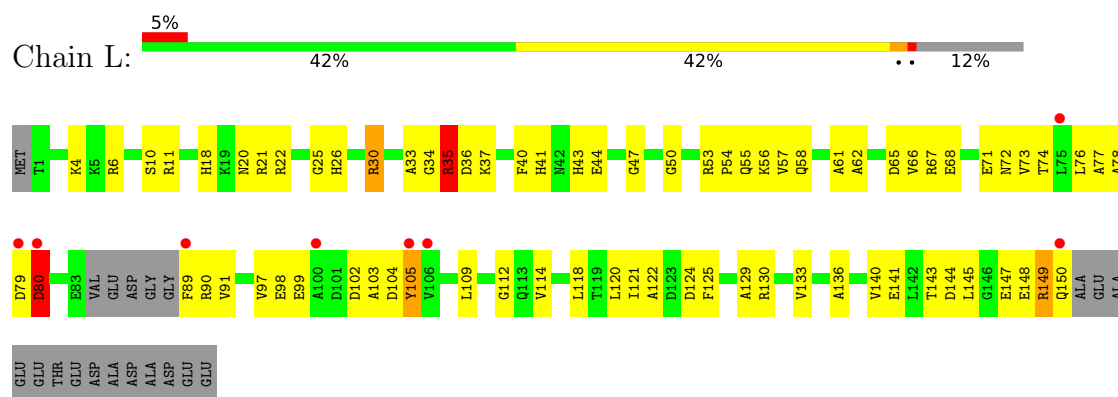
- Molecule 16: 50S RIBOSOMAL PROTEIN L13P



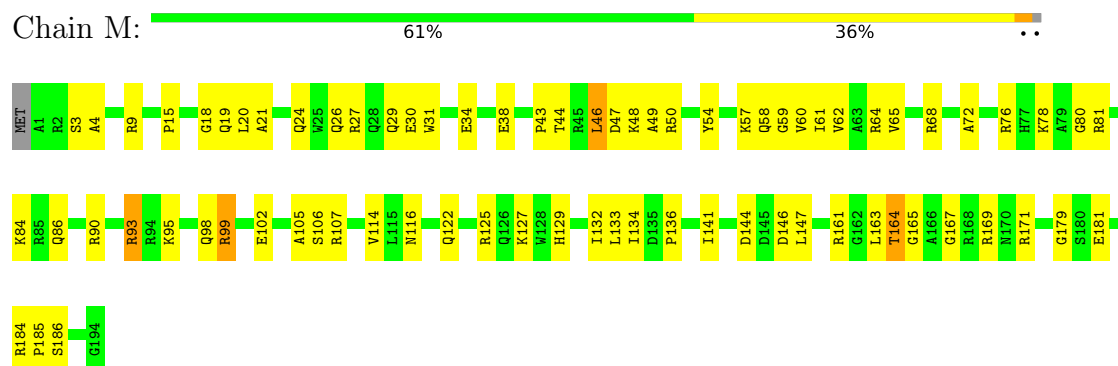
- Molecule 17: 50S RIBOSOMAL PROTEIN L14P



- Molecule 18: 50S RIBOSOMAL PROTEIN L15P

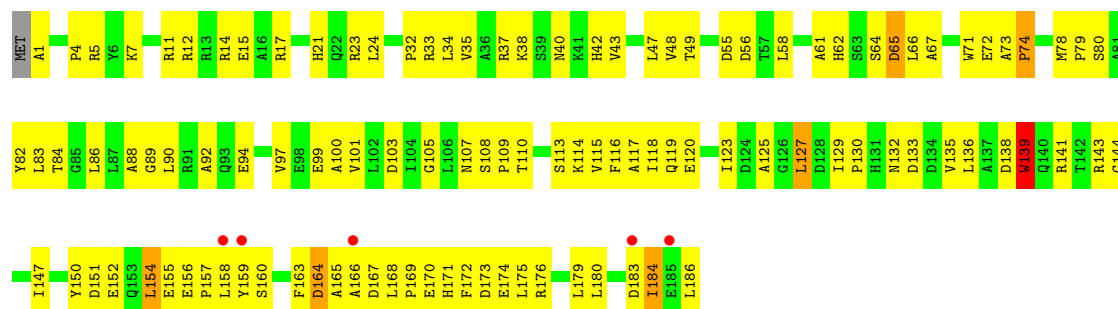


- Molecule 19: 50S RIBOSOMAL PROTEIN L15E



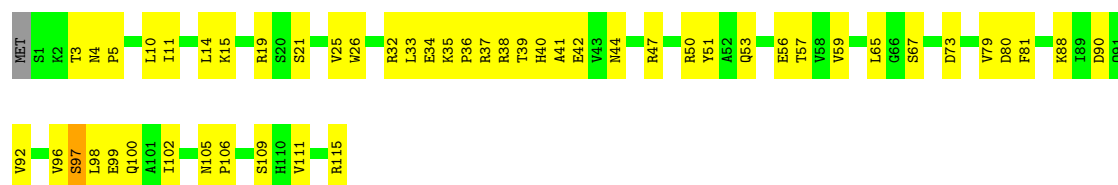
- Molecule 20: 50S RIBOSOMAL PROTEIN L18P





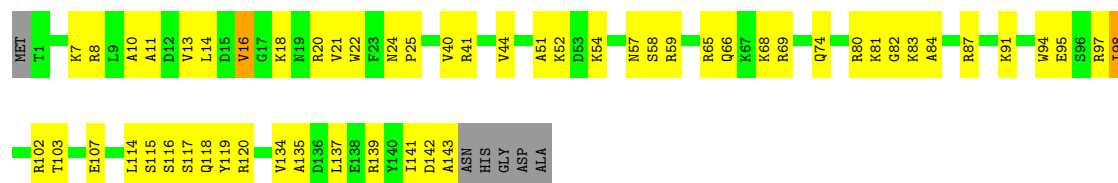
• Molecule 21: 50S RIBOSOMAL PROTEIN L18E

Chain O: 56% 42% ..



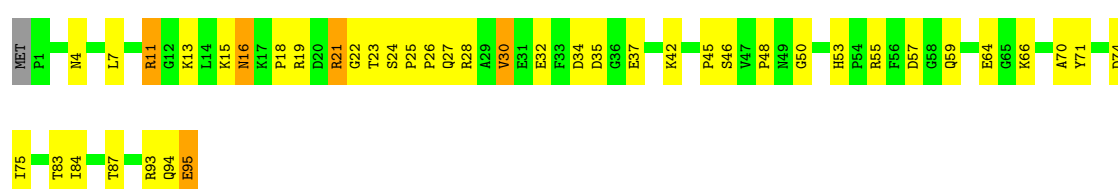
• Molecule 22: 50S RIBOSOMAL PROTEIN L19E

Chain P: 59% 36% ..



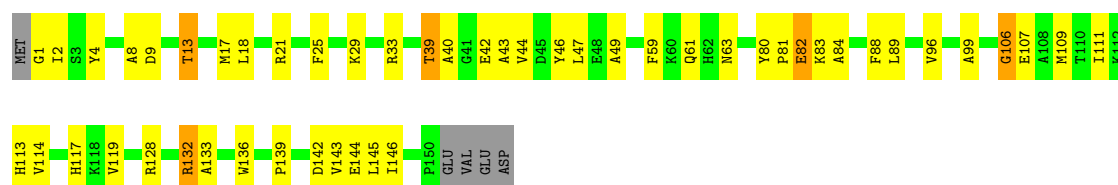
• Molecule 23: 50S RIBOSOMAL PROTEIN L21E

Chain Q: 55% 39% 5% .

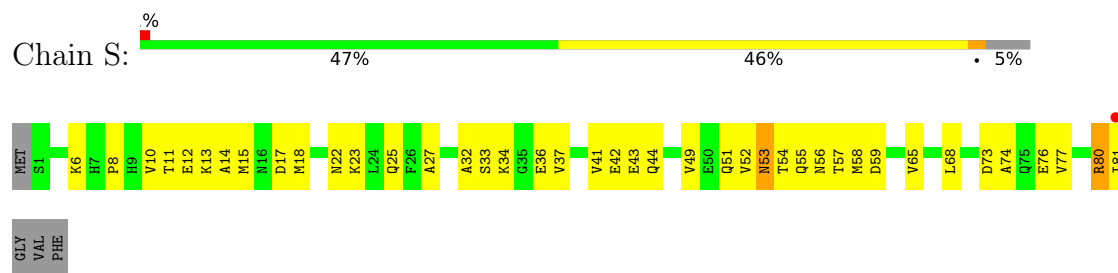


• Molecule 24: 50S RIBOSOMAL PROTEIN L22P

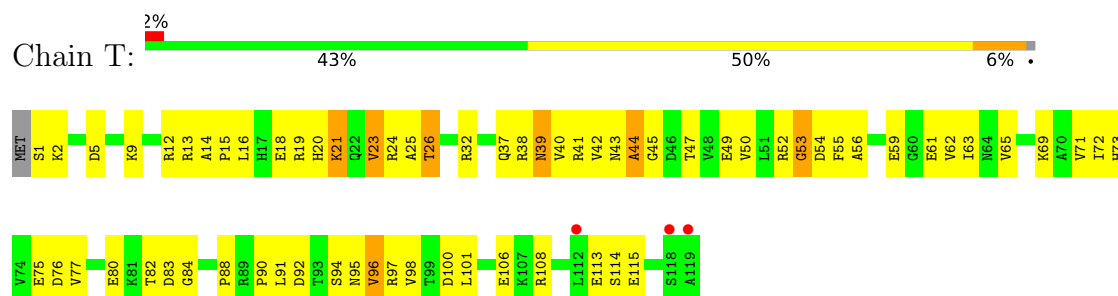
Chain R: 65% 29% ..



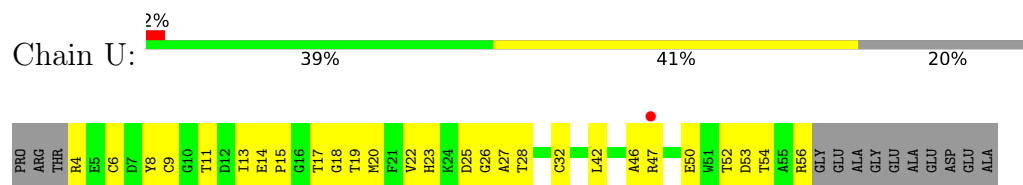
• Molecule 25: 50S RIBOSOMAL PROTEIN L23P



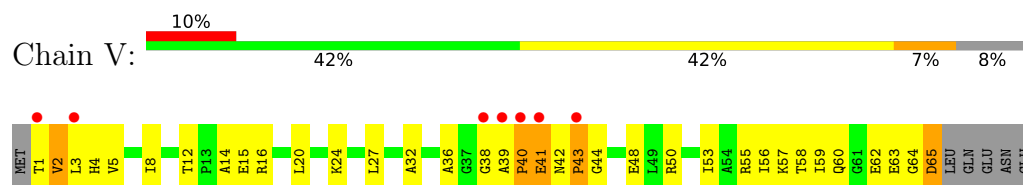
• Molecule 26: 50S RIBOSOMAL PROTEIN L24P



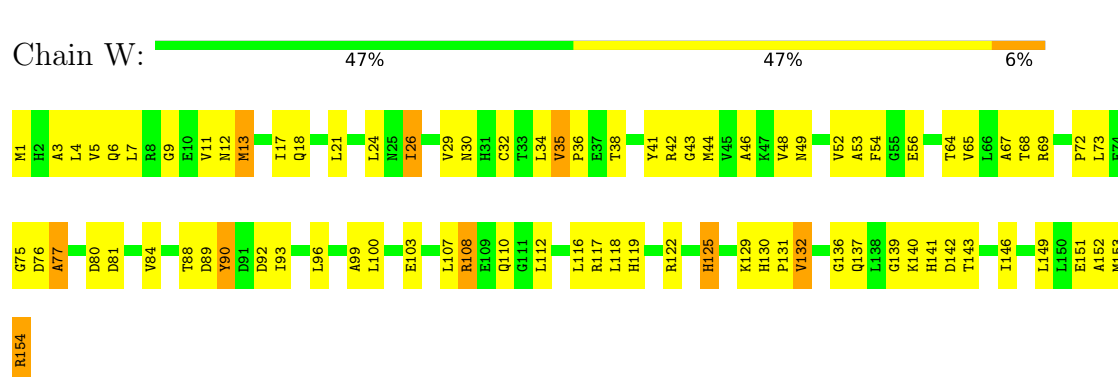
• Molecule 27: 50S RIBOSOMAL PROTEIN L24E



• Molecule 28: 50S RIBOSOMAL PROTEIN L29P

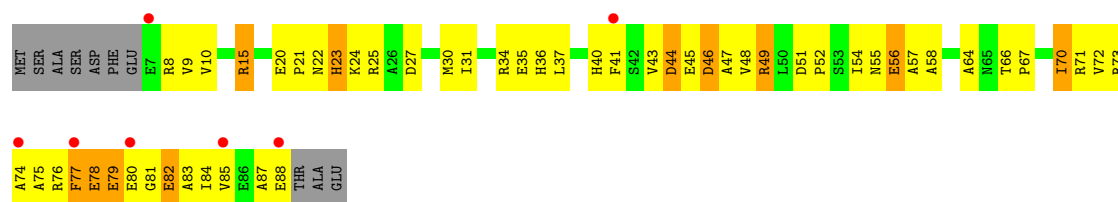


• Molecule 29: 50S RIBOSOMAL PROTEIN L30P

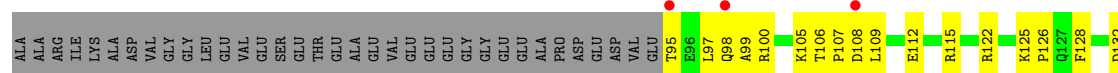
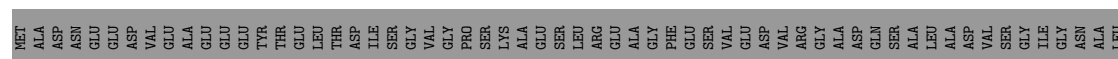
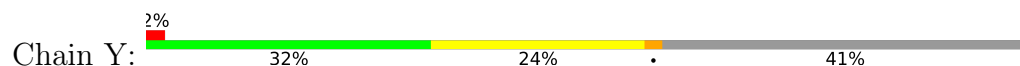


• Molecule 30: 50S RIBOSOMAL PROTEIN L31E





● Molecule 31: 50S RIBOSOMAL PROTEIN L32E



● Molecule 32: 50S RIBOSOMAL PROTEIN L37AE



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.69Å 299.78Å 573.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.98 – 2.90 49.95 – 2.89	Depositor EDS
% Data completeness (in resolution range)	83.8 (29.98-2.90) 83.4 (49.95-2.89)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.171 , 0.223 0.171 , 0.219	Depositor DCC
R_{free} test set	3279 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99111	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MHU, 004, OMG, PSU, MHT, K, NA, UR3, CL, 1MA, MG, OMU, MHW, DBB, CD, MHV

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	0.37	0/65957	0.69	13/102867 (0.0%)
2	1	0.38	0/438	0.61	0/578
3	2	0.34	0/401	0.56	0/529
4	3	0.37	0/771	0.57	0/1024
5	4	1.63	0/13	1.38	0/15
6	9	0.35	0/2904	0.69	1/4526 (0.0%)
7	A	0.33	0/1786	0.65	0/2408
8	B	0.33	0/2690	0.63	0/3652
9	C	0.36	0/1884	0.63	0/2551
10	D	0.32	0/1111	0.56	0/1498
11	E	0.33	0/1382	0.58	0/1880
12	F	0.33	0/901	0.57	0/1224
13	G	0.30	0/241	0.48	0/324
14	H	0.34	0/1302	0.64	0/1743
15	I	0.31	0/526	0.55	0/716
16	J	0.35	0/1136	0.59	0/1530
17	K	0.35	0/1001	0.67	0/1347
18	L	0.32	0/1130	0.63	0/1509
19	M	0.34	0/1582	0.60	0/2117
20	N	0.30	0/1474	0.64	0/1999
21	O	0.34	0/874	0.60	0/1181
22	P	0.33	0/1147	0.54	0/1528
23	Q	0.35	0/749	0.66	0/1005
24	R	0.34	0/1172	0.63	0/1578
25	S	0.34	0/648	0.59	0/875
26	T	0.32	0/958	0.61	0/1289
27	U	0.32	0/417	0.58	0/562
28	V	0.29	0/502	0.55	0/675
29	W	0.36	0/1219	0.62	0/1655
30	X	0.33	0/664	0.61	0/895
31	Y	0.35	0/1146	0.62	0/1536
32	Z	0.35	0/589	0.67	0/787

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98715	0.67	14/147603 (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	20
6	9	0	1
29	W	0	1
All	All	0	22

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	C1'-O4'-C4'	-6.45	104.74	109.90
1	0	1942	A	C5'-C4'-C3'	6.01	125.61	116.00
1	0	871	G	C5'-C4'-O4'	-5.83	102.10	109.10
1	0	2291	A	N9-C1'-C2'	5.68	121.39	114.00
1	0	2726	U	N1-C1'-C2'	5.63	121.33	114.00

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	482	G	Sidechain
1	0	518	G	Sidechain
1	0	792	G	Sidechain
1	0	817	G	Sidechain
1	0	867	A	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59020	0	29811	1125	0
2	1	431	0	426	27	0
3	2	396	0	413	30	0
4	3	755	0	728	38	0
5	4	63	0	50	0	0
6	9	2599	0	1325	72	0
7	A	1753	0	1766	116	0
8	B	2625	0	2533	203	0
9	C	1859	0	1816	140	0
10	D	1094	0	1085	111	0
11	E	1357	0	1266	79	0
12	F	890	0	843	56	0
13	G	240	0	231	19	0
14	H	1282	0	1292	88	0
15	I	519	0	500	62	0
16	J	1120	0	1098	75	0
17	K	992	0	1031	72	0
18	L	1118	0	1076	82	0
19	M	1558	0	1566	82	0
20	N	1445	0	1401	145	0
21	O	865	0	873	48	0
22	P	1136	0	1123	57	0
23	Q	735	0	729	45	0
24	R	1149	0	1122	59	0
25	S	641	0	605	39	0
26	T	950	0	923	71	0
27	U	410	0	364	35	0
28	V	499	0	511	43	0
29	W	1196	0	1137	116	0
30	X	654	0	653	59	0
31	Y	1130	0	1133	69	0
32	Z	578	0	539	24	0
33	0	109	0	0	0	0
33	3	1	0	0	0	0
33	4	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	74	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	2	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	2	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	4	10	0	14	1	0
39	0	5842	0	0	196	0
39	1	60	0	0	8	0
39	2	49	0	0	5	0
39	3	69	0	0	11	0
39	4	2	0	0	0	0
39	9	143	0	0	9	0
39	A	123	0	0	19	0
39	B	146	0	0	20	0
39	C	185	0	0	37	0
39	D	49	0	0	22	0
39	E	42	0	0	11	0
39	F	26	0	0	5	0
39	G	20	0	0	2	0
39	H	69	0	0	15	0
39	I	9	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	J	55	0	0	4	0
39	K	59	0	0	11	0
39	L	82	0	0	21	0
39	M	129	0	0	12	0
39	N	60	0	0	11	0
39	O	42	0	0	7	0
39	P	72	0	0	5	0
39	Q	48	0	0	7	0
39	R	85	0	0	6	0
39	S	30	0	0	5	0
39	T	39	0	0	8	0
39	U	29	0	0	3	0
39	V	13	0	0	3	0
39	W	69	0	0	12	0
39	X	26	0	0	6	0
39	Y	101	0	0	16	0
39	Z	37	0	0	2	0
All	All	99111	0	59983	2986	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 2986 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)
6:9:6:C:H5''	20:N:37:ARG:NH1	1.59	1.16
1:0:156:C:H5''	19:M:171:ARG:HD3	1.25	1.15
6:9:6:C:H5''	20:N:37:ARG:HH12	0.97	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.07
1:0:871:G:H5'	1:0:871:G:H8	1.10	1.06

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
3	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
4	3	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	14	42
5	4	2/8 (25%)	2 (100%)	0	0	100	100
7	A	235/240 (98%)	203 (86%)	28 (12%)	4 (2%)	9	31
8	B	335/338 (99%)	294 (88%)	36 (11%)	5 (2%)	10	34
9	C	244/246 (99%)	218 (89%)	21 (9%)	5 (2%)	7	27
10	D	134/177 (76%)	92 (69%)	39 (29%)	3 (2%)	6	24
11	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	25	58
12	F	117/120 (98%)	100 (86%)	12 (10%)	5 (4%)	2	10
13	G	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	11
14	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	8	28
15	I	68/162 (42%)	50 (74%)	16 (24%)	2 (3%)	4	18
16	J	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	7	26
17	K	130/132 (98%)	120 (92%)	10 (8%)	0	100	100
18	L	141/165 (86%)	113 (80%)	24 (17%)	4 (3%)	5	19
19	M	192/195 (98%)	175 (91%)	17 (9%)	0	100	100
20	N	184/187 (98%)	154 (84%)	21 (11%)	9 (5%)	2	8
21	O	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	17	48
22	P	141/149 (95%)	127 (90%)	14 (10%)	0	100	100
23	Q	93/96 (97%)	83 (89%)	9 (10%)	1 (1%)	14	42
24	R	148/155 (96%)	133 (90%)	14 (10%)	1 (1%)	22	54
25	S	79/85 (93%)	68 (86%)	11 (14%)	0	100	100
26	T	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	5	20
27	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
28	V	63/71 (89%)	53 (84%)	6 (10%)	4 (6%)	1	4
29	W	152/154 (99%)	138 (91%)	13 (9%)	1 (1%)	22	54
30	X	80/92 (87%)	66 (82%)	9 (11%)	5 (6%)	1	4
31	Y	140/241 (58%)	133 (95%)	7 (5%)	0	100	100
32	Z	71/83 (86%)	54 (76%)	14 (20%)	3 (4%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3707/4445 (83%)	3245 (88%)	397 (11%)	65 (2%)	8	29

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	A	34	ASP
7	A	37	VAL
8	B	184	ASP
9	C	8	LEU
10	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	
2	1	46/47 (98%)	46 (100%)	0	100	100
3	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
4	3	79/79 (100%)	79 (100%)	0	100	100
5	4	2/2 (100%)	2 (100%)	0	100	100
7	A	179/182 (98%)	168 (94%)	11 (6%)	18	48
8	B	282/283 (100%)	264 (94%)	18 (6%)	17	45
9	C	193/193 (100%)	181 (94%)	12 (6%)	18	47
10	D	117/148 (79%)	109 (93%)	8 (7%)	16	42
11	E	152/156 (97%)	146 (96%)	6 (4%)	32	66
12	F	93/94 (99%)	90 (97%)	3 (3%)	39	73
13	G	27/283 (10%)	27 (100%)	0	100	100
14	H	134/145 (92%)	128 (96%)	6 (4%)	27	61
15	I	58/130 (45%)	58 (100%)	0	100	100
16	J	118/121 (98%)	110 (93%)	8 (7%)	16	42
17	K	106/106 (100%)	105 (99%)	1 (1%)	78	93
18	L	113/127 (89%)	107 (95%)	6 (5%)	22	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	M	158/159 (99%)	151 (96%)	7 (4%)	28	61
20	N	149/150 (99%)	144 (97%)	5 (3%)	37	71
21	O	93/94 (99%)	90 (97%)	3 (3%)	39	73
22	P	113/117 (97%)	109 (96%)	4 (4%)	36	70
23	Q	79/80 (99%)	74 (94%)	5 (6%)	18	46
24	R	117/122 (96%)	113 (97%)	4 (3%)	37	71
25	S	71/74 (96%)	68 (96%)	3 (4%)	30	63
26	T	105/106 (99%)	98 (93%)	7 (7%)	16	43
27	U	44/52 (85%)	44 (100%)	0	100	100
28	V	51/57 (90%)	50 (98%)	1 (2%)	55	82
29	W	130/130 (100%)	122 (94%)	8 (6%)	18	47
30	X	66/74 (89%)	58 (88%)	8 (12%)	5	15
31	Y	120/196 (61%)	114 (95%)	6 (5%)	24	57
32	Z	60/68 (88%)	56 (93%)	4 (7%)	16	43
All	All	3097/3621 (86%)	2952 (95%)	145 (5%)	26	59

5 of 145 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
26	T	39	ASN
32	Z	44	GLU
29	W	13	MET
30	X	46	ASP
10	D	149	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
20	N	40	ASN
24	R	123	GLN
20	N	107	ASN
23	Q	40	HIS
26	T	43	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	23 (0%)
6	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	261 (9%)	24 (0%)

5 of 261 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1856	C
1	0	2467	A
1	0	2313	C
1	0	2526	C
1	0	871	G

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OMU	0	2587	35,1	14,22,23	1.06	1 (7%)	14,31,34	1.19	1 (7%)
5	004	4	7	5	9,10,11	2.92	3 (33%)	9,12,14	2.09	3 (33%)
5	DBB	4	3	5	4,5,6	1.05	0	1,5,7	0.24	0
1	1MA	0	628	35,1	15,25,26	0.76	0	15,37,40	1.41	1 (6%)
1	UR3	0	2619	1	14,22,23	0.82	0	15,32,35	0.59	0
5	MHW	4	1	5,33	9,9,10	2.56	4 (44%)	10,11,13	1.22	1 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MHU	4	5	5	14,15,16	2.86	8 (57%)	18,19,21	1.65	5 (27%)
5	MHV	4	6	38,5	7,9,10	2.05	2 (28%)	7,11,13	1.72	2 (28%)
1	OMG	0	2588	1	18,26,27	1.09	2 (11%)	20,38,41	2.59	5 (25%)
1	PSU	0	2621	1	17,21,22	1.64	3 (17%)	20,30,33	5.42	4 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	0	2587	35,1	-	0/7/27/28	0/2/2/2
5	004	4	7	5	-	2/4/6/8	0/1/1/1
5	DBB	4	3	5	-	0/3/4/6	-
1	1MA	0	628	35,1	-	0/3/25/26	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
5	MHW	4	1	5,33	-	0/2/2/4	0/1/1/1
5	MHU	4	5	5	-	0/9/12/14	0/1/1/1
5	MHV	4	6	38,5	-	0/1/12/14	0/1/1/1
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	4	7	004	CB-CA	7.09	1.60	1.52
1	0	2621	PSU	C5-C1'	-5.24	1.47	1.52
5	4	1	MHW	CA-N	4.54	1.42	1.35
5	4	5	MHU	CA-N	4.52	1.55	1.47
5	4	6	MHV	CB-CG	4.38	1.57	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.12	114.82	128.43
1	0	2621	PSU	C4-N3-C2	14.34	127.25	115.14
1	0	2588	OMG	C5-C6-N1	-8.58	111.69	123.43
1	0	2621	PSU	C5-C4-N3	-8.24	114.74	125.36
1	0	2588	OMG	C6-N1-C2	5.83	125.20	115.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	4	7	004	C-CA-CB-CG1
5	4	7	004	C-CA-CB-CG2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 233 ligands modelled in this entry, 232 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	$\# Z > 2$
38	MHT	4	101	5	9,11,11	1.66	3 (33%)	11,15,15	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	MHT	4	101	5	-	0/0/20/20	0/3/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	4	101	MHT	C8-C7	2.54	1.59	1.52
38	4	101	MHT	C5-C6	2.31	1.58	1.52
38	4	101	MHT	C8-C4	2.04	1.57	1.53

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	4	101	MHT	1	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	2749/2922 (94%)	-0.23	37 (1%) 77 77	18, 42, 85, 147	0
2	1	56/57 (98%)	-0.56	0 100 100	23, 28, 34, 41	0
3	2	46/50 (92%)	0.10	2 (4%) 35 31	24, 56, 82, 96	0
4	3	92/92 (100%)	0.02	1 (1%) 80 80	30, 48, 61, 79	0
5	4	2/8 (25%)	-0.11	0 100 100	49, 49, 49, 54	0
6	9	122/122 (100%)	-0.14	3 (2%) 57 55	36, 57, 84, 148	0
7	A	237/240 (98%)	-0.11	4 (1%) 70 69	21, 44, 80, 100	0
8	B	337/338 (99%)	-0.13	0 100 100	23, 50, 76, 86	0
9	C	246/246 (100%)	-0.32	0 100 100	19, 39, 62, 72	0
10	D	140/177 (79%)	1.73	56 (40%) 0 0	47, 94, 117, 125	0
11	E	172/178 (96%)	0.47	6 (3%) 44 38	41, 61, 83, 88	0
12	F	119/120 (99%)	0.35	3 (2%) 57 55	41, 63, 88, 104	0
13	G	29/348 (8%)	2.33	16 (55%) 0 0	71, 87, 95, 96	0
14	H	160/177 (90%)	0.10	2 (1%) 77 77	36, 52, 88, 105	0
15	I	70/162 (43%)	4.05	65 (92%) 0 0	108, 118, 136, 138	0
16	J	142/145 (97%)	-0.08	2 (1%) 75 75	34, 46, 66, 86	0
17	K	132/132 (100%)	-0.22	2 (1%) 73 73	26, 46, 65, 75	0
18	L	145/165 (87%)	0.38	8 (5%) 25 21	22, 60, 100, 114	0
19	M	194/195 (99%)	-0.48	0 100 100	25, 36, 52, 59	0
20	N	186/187 (99%)	0.05	5 (2%) 54 50	34, 58, 100, 110	0
21	O	115/116 (99%)	-0.13	0 100 100	33, 47, 66, 71	0
22	P	143/149 (95%)	-0.03	0 100 100	33, 49, 61, 73	0
23	Q	95/96 (98%)	-0.15	0 100 100	28, 39, 54, 66	0
24	R	150/155 (96%)	-0.20	0 100 100	28, 40, 58, 67	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	S	81/85 (95%)	0.01	1 (1%) 79 79	37, 52, 71, 79	0
26	T	119/120 (99%)	0.21	3 (2%) 57 55	35, 51, 80, 94	0
27	U	53/66 (80%)	0.08	1 (1%) 66 65	39, 51, 67, 78	0
28	V	65/71 (91%)	0.69	7 (10%) 5 4	46, 66, 105, 112	0
29	W	154/154 (100%)	-0.17	0 100 100	27, 42, 59, 71	0
30	X	82/92 (89%)	0.36	7 (8%) 10 8	38, 55, 76, 96	0
31	Y	142/241 (58%)	-0.10	4 (2%) 53 49	24, 40, 62, 81	0
32	Z	73/83 (87%)	-0.19	0 100 100	39, 53, 69, 87	0
All	All	6648/7489 (88%)	-0.03	235 (3%) 44 38	18, 46, 91, 148	0

The worst 5 of 235 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	I	88	GLN	8.5
15	I	132	VAL	8.5
15	I	128	THR	7.7
15	I	70	THR	7.4
15	I	66	GLY	7.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å ²)	Q<0.9
5	DBB	4	3	6/7	0.94	0.18	51,51,52,53	0
5	MHV	4	6	9/10	0.94	0.18	53,55,59,59	0
5	MHU	4	5	15/16	0.95	0.17	56,59,62,63	0
5	004	4	7	10/11	0.95	0.20	45,48,49,51	0
5	MHW	4	1	9/10	0.96	0.20	46,47,49,50	0
1	1MA	0	628	23/24	0.98	0.15	25,28,31,32	0
1	OMU	0	2587	21/22	0.98	0.15	29,32,37,38	0
1	OMG	0	2588	24/25	0.98	0.14	28,31,34,35	0
1	UR3	0	2619	21/22	0.98	0.13	30,35,39,42	0
1	PSU	0	2621	20/21	0.98	0.14	33,35,37,38	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. 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	B-factors(\AA^2)	Q<0.9
35	NA	0	3183	1/1	0.09	0.92	81,81,81,81	0
35	NA	0	3174	1/1	0.53	0.47	75,75,75,75	0
35	NA	R	202	1/1	0.60	0.59	75,75,75,75	0
35	NA	0	3134	1/1	0.61	0.61	72,72,72,72	0
35	NA	0	3175	1/1	0.71	0.45	54,54,54,54	0
35	NA	9	203	1/1	0.73	0.70	85,85,85,85	0
35	NA	0	3140	1/1	0.74	0.35	47,47,47,47	0
35	NA	0	3137	1/1	0.76	0.30	81,81,81,81	0
33	MG	0	3105	1/1	0.77	0.26	47,47,47,47	0
35	NA	0	3120	1/1	0.80	0.52	36,36,36,36	0
35	NA	0	3121	1/1	0.80	0.30	50,50,50,50	0
35	NA	0	3141	1/1	0.81	0.12	37,37,37,37	0
35	NA	C	301	1/1	0.82	0.25	32,32,32,32	0
35	NA	0	3117	1/1	0.83	0.43	56,56,56,56	0
35	NA	0	3170	1/1	0.83	0.35	72,72,72,72	0
35	NA	9	202	1/1	0.84	0.13	31,31,31,31	0
35	NA	0	3147	1/1	0.84	0.25	44,44,44,44	0
33	MG	0	3063	1/1	0.85	0.39	37,37,37,37	0
35	NA	0	3165	1/1	0.85	0.33	60,60,60,60	0
35	NA	0	3156	1/1	0.86	0.28	55,55,55,55	0
33	MG	0	3082	1/1	0.86	0.18	46,46,46,46	0
33	MG	0	3071	1/1	0.87	0.08	55,55,55,55	0
35	NA	0	3184	1/1	0.87	0.15	45,45,45,45	0
33	MG	0	3097	1/1	0.87	0.44	79,79,79,79	0
36	CL	0	3192	1/1	0.87	0.43	88,88,88,88	0
35	NA	0	3173	1/1	0.88	0.23	53,53,53,53	0
35	NA	0	3122	1/1	0.88	0.17	47,47,47,47	0
35	NA	0	3164	1/1	0.88	0.34	75,75,75,75	0
33	MG	0	3050	1/1	0.88	0.19	72,72,72,72	0
35	NA	0	3118	1/1	0.88	0.15	39,39,39,39	0
36	CL	0	3194	1/1	0.88	0.18	58,58,58,58	0
33	MG	0	3108	1/1	0.89	0.11	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	3161	1/1	0.89	0.48	54,54,54,54	0
33	MG	0	3093	1/1	0.89	0.16	45,45,45,45	0
35	NA	0	3138	1/1	0.89	0.31	41,41,41,41	0
33	MG	0	3092	1/1	0.90	0.16	42,42,42,42	0
33	MG	0	3047	1/1	0.90	0.20	62,62,62,62	0
35	NA	H	201	1/1	0.90	0.15	38,38,38,38	0
35	NA	0	3166	1/1	0.90	0.14	35,35,35,35	0
35	NA	0	3160	1/1	0.90	0.47	48,48,48,48	0
33	MG	0	3049	1/1	0.90	0.25	58,58,58,58	0
35	NA	0	3159	1/1	0.91	0.07	49,49,49,49	0
35	NA	0	3171	1/1	0.91	0.36	65,65,65,65	0
35	NA	0	3132	1/1	0.91	0.21	39,39,39,39	0
33	MG	T	201	1/1	0.91	0.11	45,45,45,45	0
33	MG	0	3034	1/1	0.91	0.09	29,29,29,29	0
35	NA	0	3154	1/1	0.91	0.36	40,40,40,40	0
33	MG	0	3051	1/1	0.91	0.12	58,58,58,58	0
36	CL	A	303	1/1	0.91	0.19	58,58,58,58	0
35	NA	0	3167	1/1	0.92	0.51	43,43,43,43	0
35	NA	0	3185	1/1	0.92	0.32	38,38,38,38	0
33	MG	0	3084	1/1	0.92	0.11	49,49,49,49	0
33	MG	0	3066	1/1	0.92	0.07	34,34,34,34	0
35	NA	0	3125	1/1	0.92	0.25	39,39,39,39	0
33	MG	0	3061	1/1	0.92	0.06	52,52,52,52	0
35	NA	R	201	1/1	0.92	0.10	33,33,33,33	0
33	MG	0	3077	1/1	0.92	0.17	58,58,58,58	0
35	NA	0	3179	1/1	0.92	0.23	64,64,64,64	0
35	NA	0	3181	1/1	0.92	0.31	46,46,46,46	0
33	MG	0	3046	1/1	0.92	0.11	52,52,52,52	0
35	NA	0	3145	1/1	0.93	0.06	55,55,55,55	0
33	MG	0	3101	1/1	0.93	0.08	73,73,73,73	0
35	NA	0	3148	1/1	0.93	0.13	29,29,29,29	0
33	MG	0	3069	1/1	0.93	0.08	56,56,56,56	0
33	MG	0	3087	1/1	0.93	0.29	75,75,75,75	0
35	NA	0	3157	1/1	0.93	0.56	71,71,71,71	0
33	MG	0	3089	1/1	0.93	0.13	47,47,47,47	0
34	K	0	3111	1/1	0.93	0.12	62,62,62,62	0
35	NA	0	3176	1/1	0.93	0.63	60,60,60,60	0
35	NA	0	3114	1/1	0.93	0.20	50,50,50,50	0
35	NA	0	3143	1/1	0.93	0.26	47,47,47,47	0
35	NA	0	3182	1/1	0.93	0.16	40,40,40,40	0
38	MHT	4	101	10/10	0.93	0.22	63,64,65,67	0
33	MG	9	201	1/1	0.94	0.09	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	K	201	1/1	0.94	0.07	46,46,46,46	0
35	NA	0	3144	1/1	0.94	0.13	44,44,44,44	0
33	MG	0	3060	1/1	0.94	0.08	27,27,27,27	0
35	NA	0	3168	1/1	0.94	0.20	40,40,40,40	0
33	MG	0	3073	1/1	0.94	0.07	28,28,28,28	0
35	NA	0	3130	1/1	0.94	0.42	61,61,61,61	0
33	MG	0	3103	1/1	0.94	0.08	60,60,60,60	0
35	NA	L	201	1/1	0.94	0.71	61,61,61,61	0
35	NA	Q	101	1/1	0.94	0.09	33,33,33,33	0
35	NA	0	3115	1/1	0.94	0.11	29,29,29,29	0
35	NA	0	3135	1/1	0.94	0.31	60,60,60,60	0
35	NA	0	3116	1/1	0.94	0.41	33,33,33,33	0
35	NA	0	3177	1/1	0.94	0.30	58,58,58,58	0
36	CL	0	3195	1/1	0.94	0.27	88,88,88,88	0
33	MG	0	3076	1/1	0.94	0.10	50,50,50,50	0
36	CL	O	202	1/1	0.94	0.18	74,74,74,74	0
33	MG	0	3086	1/1	0.94	0.05	41,41,41,41	0
33	MG	0	3083	1/1	0.95	0.07	25,25,25,25	0
35	NA	0	3139	1/1	0.95	0.17	62,62,62,62	0
35	NA	J	201	1/1	0.95	0.09	61,61,61,61	0
35	NA	0	3123	1/1	0.95	0.12	27,27,27,27	0
33	MG	0	3106	1/1	0.95	0.24	42,42,42,42	0
35	NA	0	3126	1/1	0.95	0.10	28,28,28,28	0
35	NA	0	3127	1/1	0.95	0.17	26,26,26,26	0
36	CL	0	3187	1/1	0.95	0.19	57,57,57,57	0
33	MG	0	3094	1/1	0.95	0.10	73,73,73,73	0
33	MG	0	3041	1/1	0.95	0.20	38,38,38,38	0
33	MG	0	3098	1/1	0.95	0.20	48,48,48,48	0
35	NA	0	3150	1/1	0.95	0.09	42,42,42,42	0
36	CL	J	203	1/1	0.95	0.14	63,63,63,63	0
36	CL	L	202	1/1	0.95	0.11	46,46,46,46	0
33	MG	0	3090	1/1	0.95	0.08	41,41,41,41	0
33	MG	0	3001	1/1	0.95	0.07	30,30,30,30	0
33	MG	0	3085	1/1	0.96	0.18	41,41,41,41	0
35	NA	0	3112	1/1	0.96	0.14	21,21,21,21	0
33	MG	0	3035	1/1	0.96	0.05	50,50,50,50	0
33	MG	0	3052	1/1	0.96	0.05	35,35,35,35	0
33	MG	0	3088	1/1	0.96	0.21	48,48,48,48	0
33	MG	0	3008	1/1	0.96	0.04	33,33,33,33	0
33	MG	0	3011	1/1	0.96	0.08	21,21,21,21	0
33	MG	0	3015	1/1	0.96	0.06	38,38,38,38	0
36	CL	0	3191	1/1	0.96	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	3	101	1/1	0.96	0.04	40,40,40,40	0
35	NA	0	3163	1/1	0.96	0.21	44,44,44,44	0
33	MG	0	3033	1/1	0.96	0.09	31,31,31,31	0
35	NA	0	3142	1/1	0.96	0.07	26,26,26,26	0
36	CL	J	202	1/1	0.96	0.18	55,55,55,55	0
33	MG	0	3002	1/1	0.96	0.04	26,26,26,26	0
36	CL	J	204	1/1	0.96	0.11	57,57,57,57	0
33	MG	0	3096	1/1	0.96	0.16	49,49,49,49	0
34	K	0	3110	1/1	0.96	0.20	86,86,86,86	0
35	NA	A	302	1/1	0.96	0.16	38,38,38,38	0
33	MG	0	3099	1/1	0.97	0.22	53,53,53,53	0
35	NA	0	3158	1/1	0.97	0.53	43,43,43,43	0
33	MG	0	3010	1/1	0.97	0.07	24,24,24,24	0
35	NA	0	3136	1/1	0.97	0.32	50,50,50,50	0
33	MG	0	3027	1/1	0.97	0.11	40,40,40,40	0
33	MG	0	3045	1/1	0.97	0.08	58,58,58,58	0
33	MG	0	3091	1/1	0.97	0.06	26,26,26,26	0
33	MG	0	3107	1/1	0.97	0.09	49,49,49,49	0
35	NA	0	3119	1/1	0.97	0.09	40,40,40,40	0
35	NA	M	201	1/1	0.97	0.13	30,30,30,30	0
33	MG	0	3065	1/1	0.97	0.10	38,38,38,38	0
33	MG	0	3109	1/1	0.97	0.11	20,20,20,20	0
35	NA	0	3169	1/1	0.97	0.14	35,35,35,35	0
33	MG	0	3056	1/1	0.97	0.09	42,42,42,42	0
36	CL	0	3188	1/1	0.97	0.14	57,57,57,57	0
33	MG	0	3067	1/1	0.97	0.11	41,41,41,41	0
35	NA	0	3146	1/1	0.97	0.12	26,26,26,26	0
36	CL	0	3193	1/1	0.97	0.13	56,56,56,56	0
33	MG	B	401	1/1	0.97	0.09	32,32,32,32	0
33	MG	0	3095	1/1	0.97	0.11	49,49,49,49	0
35	NA	0	3149	1/1	0.97	0.12	35,35,35,35	0
33	MG	0	3068	1/1	0.97	0.09	59,59,59,59	0
35	NA	0	3151	1/1	0.97	0.05	30,30,30,30	0
35	NA	0	3180	1/1	0.97	0.38	45,45,45,45	0
35	NA	0	3153	1/1	0.97	0.14	43,43,43,43	0
36	CL	N	201	1/1	0.97	0.13	57,57,57,57	0
33	MG	0	3058	1/1	0.97	0.06	27,27,27,27	0
36	CL	R	203	1/1	0.97	0.15	43,43,43,43	0
33	MG	0	3059	1/1	0.97	0.14	44,44,44,44	0
33	MG	0	3013	1/1	0.98	0.10	37,37,37,37	0
33	MG	0	3053	1/1	0.98	0.13	48,48,48,48	0
33	MG	4	102	1/1	0.98	0.08	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	3054	1/1	0.98	0.09	24,24,24,24	0
33	MG	A	301	1/1	0.98	0.08	44,44,44,44	0
33	MG	0	3055	1/1	0.98	0.13	40,40,40,40	0
33	MG	0	3014	1/1	0.98	0.07	31,31,31,31	0
33	MG	0	3057	1/1	0.98	0.08	32,32,32,32	0
33	MG	Y	301	1/1	0.98	0.12	34,34,34,34	0
33	MG	0	3006	1/1	0.98	0.05	46,46,46,46	0
33	MG	0	3038	1/1	0.98	0.08	28,28,28,28	0
33	MG	0	3039	1/1	0.98	0.10	33,33,33,33	0
35	NA	0	3113	1/1	0.98	0.26	44,44,44,44	0
33	MG	0	3040	1/1	0.98	0.14	70,70,70,70	0
33	MG	0	3062	1/1	0.98	0.07	51,51,51,51	0
33	MG	0	3016	1/1	0.98	0.11	23,23,23,23	0
35	NA	0	3152	1/1	0.98	0.11	34,34,34,34	0
33	MG	0	3064	1/1	0.98	0.18	96,96,96,96	0
33	MG	0	3043	1/1	0.98	0.06	35,35,35,35	0
35	NA	0	3155	1/1	0.98	0.20	39,39,39,39	0
33	MG	0	3044	1/1	0.98	0.06	37,37,37,37	0
33	MG	0	3017	1/1	0.98	0.05	26,26,26,26	0
35	NA	S	101	1/1	0.98	0.13	10,10,10,10	0
36	CL	0	3186	1/1	0.98	0.16	43,43,43,43	0
33	MG	0	3018	1/1	0.98	0.09	34,34,34,34	0
33	MG	0	3021	1/1	0.98	0.10	32,32,32,32	0
36	CL	0	3189	1/1	0.98	0.07	39,39,39,39	0
33	MG	0	3100	1/1	0.98	0.05	35,35,35,35	0
35	NA	0	3124	1/1	0.98	0.12	48,48,48,48	0
35	NA	0	3162	1/1	0.98	0.40	49,49,49,49	0
33	MG	0	3048	1/1	0.98	0.07	48,48,48,48	0
33	MG	0	3025	1/1	0.98	0.03	42,42,42,42	0
36	CL	3	103	1/1	0.98	0.08	53,53,53,53	0
33	MG	0	3104	1/1	0.98	0.06	40,40,40,40	0
36	CL	B	402	1/1	0.98	0.12	40,40,40,40	0
35	NA	0	3128	1/1	0.98	0.13	22,22,22,22	0
33	MG	0	3075	1/1	0.98	0.07	38,38,38,38	0
35	NA	0	3131	1/1	0.98	0.12	39,39,39,39	0
33	MG	0	3012	1/1	0.98	0.07	25,25,25,25	0
35	NA	0	3133	1/1	0.98	0.16	50,50,50,50	0
33	MG	0	3032	1/1	0.98	0.07	40,40,40,40	0
35	NA	0	3172	1/1	0.98	0.13	58,58,58,58	0
36	CL	Y	302	1/1	0.98	0.11	30,30,30,30	0
37	CD	3	102	1/1	0.98	0.05	55,55,55,55	0
37	CD	O	201	1/1	0.98	0.07	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	3081	1/1	0.98	0.16	41,41,41,41	0
33	MG	0	3079	1/1	0.99	0.03	42,42,42,42	0
33	MG	0	3080	1/1	0.99	0.09	65,65,65,65	0
33	MG	0	3004	1/1	0.99	0.07	27,27,27,27	0
33	MG	0	3042	1/1	0.99	0.10	31,31,31,31	0
33	MG	0	3026	1/1	0.99	0.07	19,19,19,19	0
33	MG	0	3009	1/1	0.99	0.07	22,22,22,22	0
33	MG	0	3028	1/1	0.99	0.09	39,39,39,39	0
36	CL	0	3190	1/1	0.99	0.12	46,46,46,46	0
33	MG	0	3029	1/1	0.99	0.08	33,33,33,33	0
33	MG	0	3030	1/1	0.99	0.08	31,31,31,31	0
35	NA	0	3178	1/1	0.99	0.10	29,29,29,29	0
33	MG	0	3031	1/1	0.99	0.08	28,28,28,28	0
35	NA	0	3129	1/1	0.99	0.10	25,25,25,25	0
33	MG	0	3005	1/1	0.99	0.10	27,27,27,27	0
33	MG	0	3019	1/1	0.99	0.05	23,23,23,23	0
33	MG	0	3020	1/1	0.99	0.08	22,22,22,22	0
33	MG	0	3003	1/1	0.99	0.12	31,31,31,31	0
33	MG	0	3070	1/1	0.99	0.06	25,25,25,25	0
33	MG	0	3036	1/1	0.99	0.05	32,32,32,32	0
33	MG	0	3072	1/1	0.99	0.08	47,47,47,47	0
36	CL	M	202	1/1	0.99	0.08	31,31,31,31	0
33	MG	0	3037	1/1	0.99	0.07	44,44,44,44	0
33	MG	0	3074	1/1	0.99	0.10	20,20,20,20	0
33	MG	0	3022	1/1	0.99	0.08	36,36,36,36	0
33	MG	0	3023	1/1	0.99	0.06	34,34,34,34	0
37	CD	1	101	1/1	0.99	0.08	56,56,56,56	0
33	MG	0	3024	1/1	0.99	0.06	12,12,12,12	0
33	MG	0	3078	1/1	0.99	0.04	22,22,22,22	0
33	MG	0	3102	1/1	0.99	0.08	23,23,23,23	0
37	CD	U	8701	1/1	1.00	0.08	60,60,60,60	0
37	CD	Z	101	1/1	1.00	0.11	59,59,59,59	0
33	MG	0	3007	1/1	1.00	0.07	12,12,12,12	0

6.5 Other polymers ⓘ

There are no such residues in this entry.