



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:18 am GMT

PDB ID : 1KD1  
Title : Co-crystal Structure of Spiramycin 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 : 2001-11-12  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

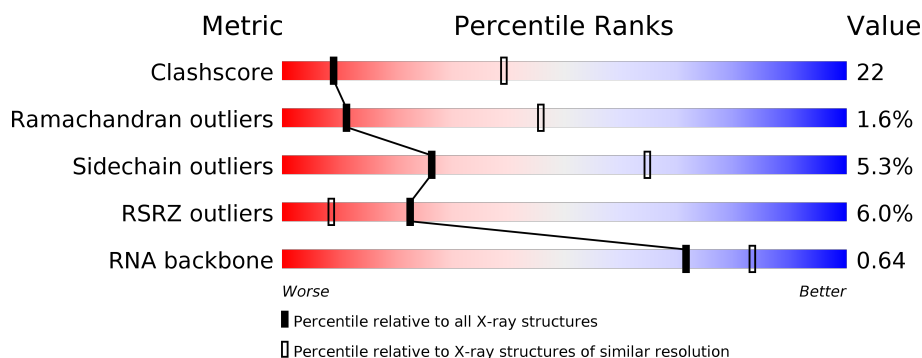
# 1 Overall quality at a glance

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	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div>47%</div> <div>39%</div> <div>7%</div> <div>6%</div> </div> </div>
2	B	122	<div> <div>5%</div> <div> <div>46%</div> <div>37%</div> <div>15%</div> </div> </div>
3	C	239	<div> <div>4%</div> <div> <div>54%</div> <div>39%</div> <div>6%</div> </div> </div>
4	D	337	<div> <div>%</div> <div> <div>51%</div> <div>43%</div> <div>6%</div> </div> </div>
5	E	246	<div> <div>53%</div> <div>41%</div> <div>6%</div> </div>
6	F	176	<div> <div>27%</div> <div> <div>28%</div> <div>43%</div> <div>6%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	SPR	A	9001	-	-	-	X
32	MG	A	8054	-	-	X	-
32	MG	A	8067	-	-	-	X
32	MG	Z	8109	-	-	-	X
33	NA	A	8303	-	-	-	X
33	NA	A	8308	-	-	-	X
33	NA	A	8310	-	-	-	X
33	NA	A	8321	-	-	-	X
33	NA	A	8323	-	-	-	X
33	NA	A	8331	-	-	-	X
33	NA	A	8332	-	-	-	X
33	NA	A	8335	-	-	-	X
33	NA	A	8356	-	-	-	X
33	NA	A	8362	-	-	-	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	8379	-	-	-	X
33	NA	A	8381	-	-	-	X
33	NA	A	8382	-	-	-	X
33	NA	B	8383	-	-	-	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	-
36	CD	4	8404	-	-	-	X
36	CD	V	8401	-	-	-	X

## 2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98587 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		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		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		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			

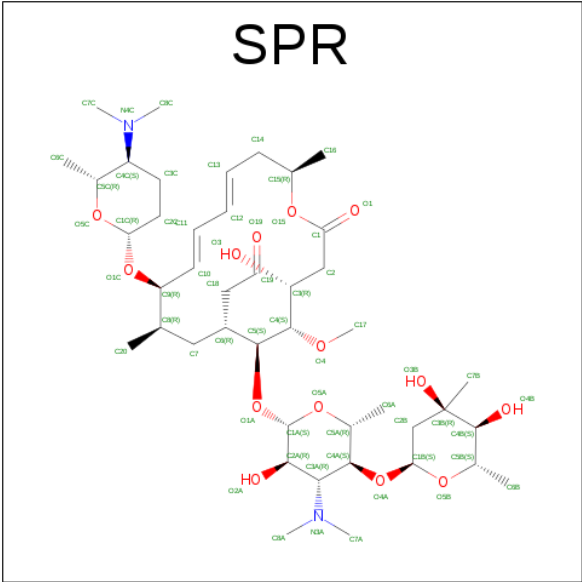
There is a discrepancy between the modelled and reference sequences:

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 SPIRAMYCIN I (three-letter code: SPR) (formula: C<sub>43</sub>H<sub>74</sub>N<sub>2</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			59	43	2	14		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	1	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	A	112	Total	Mg	0	0
			112	112		
32	4	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	J	1	Total Na 1 1	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	73	Total Na 73 73	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	3	Total Cl 3 3	0	0
34	C	1	Total Cl 1 1	0	0
34	Z	1	Total Cl 1 1	0	0
34	A	9	Total Cl 9 9	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	5910	Total 5910	O 5910	0	0
37	B	142	Total 142	O 142	0	0
37	C	126	Total 126	O 126	0	0
37	D	150	Total 150	O 150	0	0
37	E	169	Total 169	O 169	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	21	Total 21	O 21	0	0
37	J	78	Total 78	O 78	0	0
37	K	54	Total 54	O 54	0	0
37	L	65	Total 65	O 65	0	0
37	M	79	Total 79	O 79	0	0
37	N	132	Total 132	O 132	0	0
37	O	69	Total 69	O 69	0	0
37	P	45	Total 45	O 45	0	0
37	Q	65	Total 65	O 65	0	0
37	R	55	Total 55	O 55	0	0
37	S	83	Total 83	O 83	0	0
37	T	35	Total 35	O 35	0	0
37	U	39	Total 39	O 39	0	0
37	V	25	Total 25	O 25	0	0
37	W	15	Total 15	O 15	0	0
37	X	70	Total 70	O 70	0	0
37	Y	25	Total 25	O 25	0	0
37	Z	94	Total 94	O 94	0	0
37	1	41	Total 41	O 41	0	0

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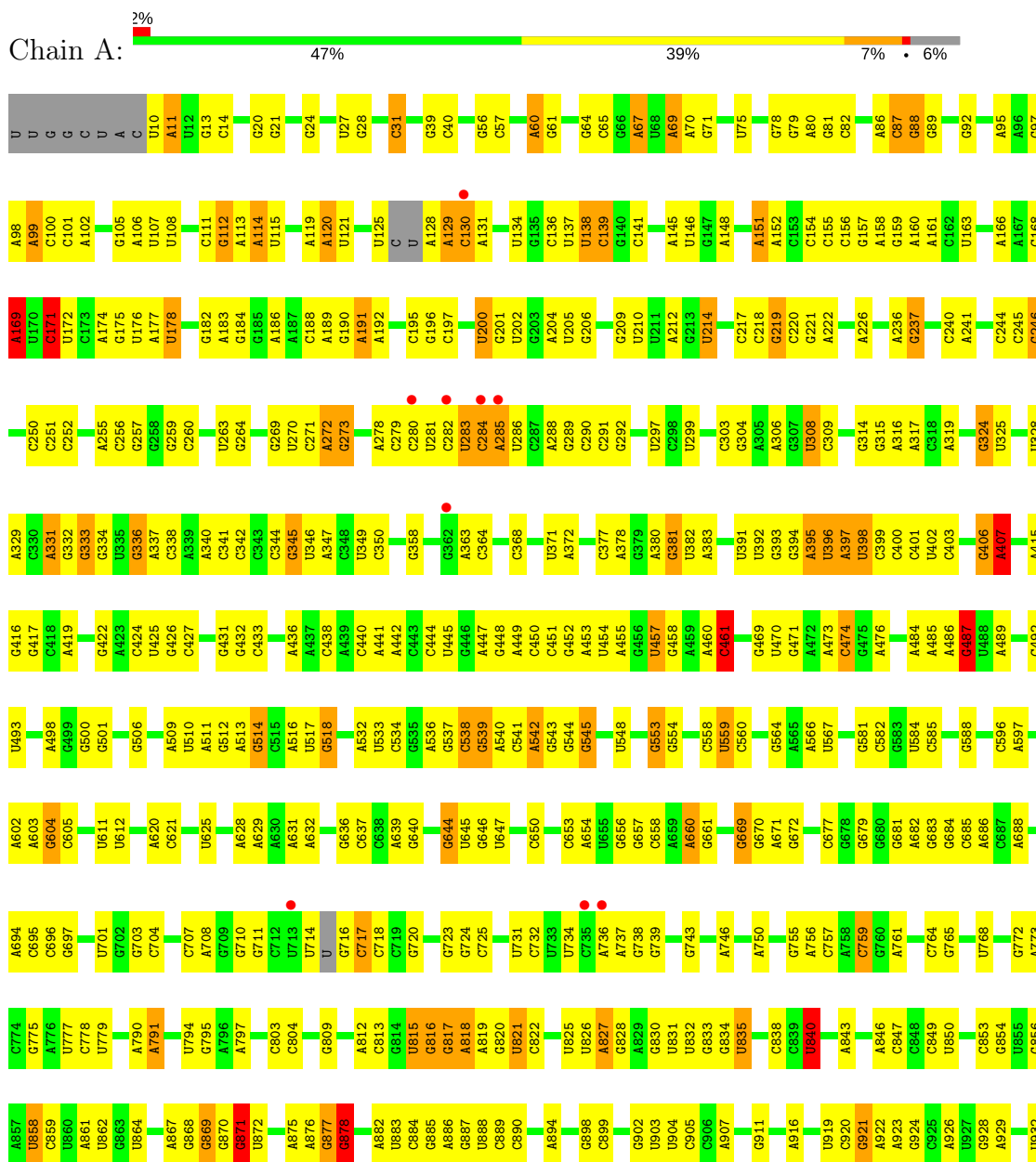
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	55	Total 55	O 55	0	0
37	3	42	Total 42	O 42	0	0
37	4	73	Total 73	O 73	0	0

### 3 Residue-property plots

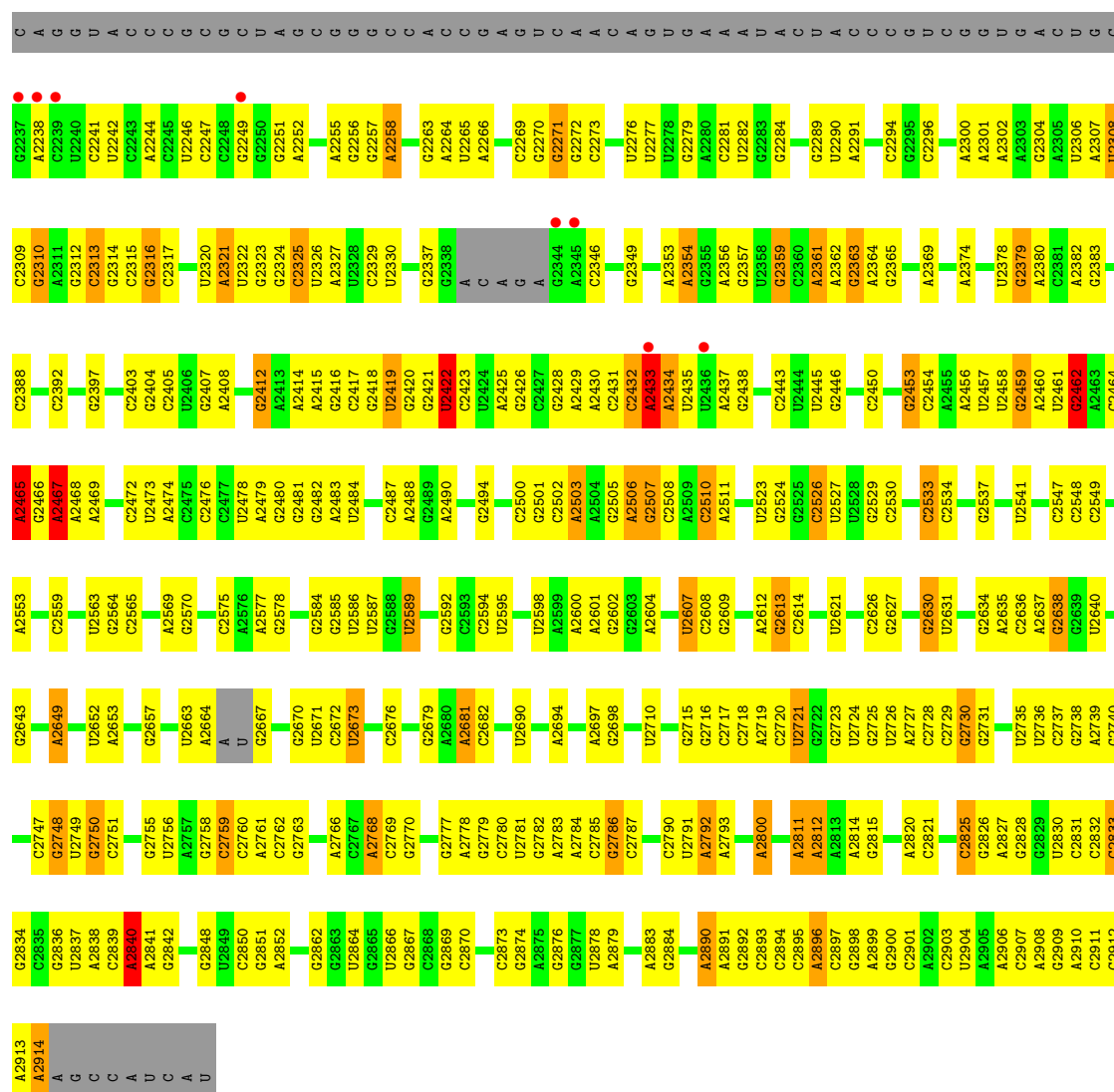
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 RRNA

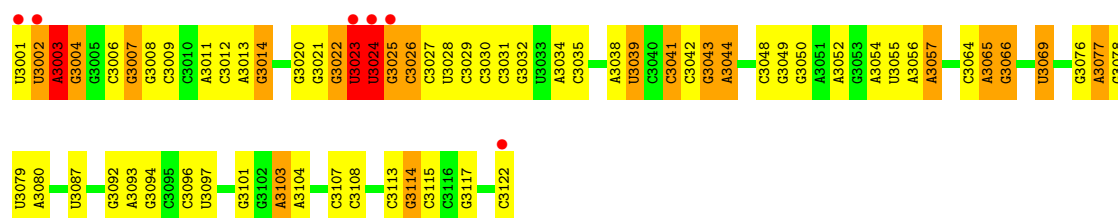


G2111	A2038	A	U1879	G1707	A1626	A1533	C1450	U1368	C1263	U1180	A1097	G940
A2112	A2039	C	C1880	A1710	G1627	A1534	C1451	A1369	U1264	A1181	A1098	G941
G2113	G1805	C	A1881	A1711	G1628	G1535	C1456	G1370	U1265	C1182	G1099	U942
C2114	G2044	C	C1882	A1712	G1629	C1536	A1458	U1457	C1267	C1183	C1103	
U2115	G2045	C1964	A1886	C1720	C1633	G1543	A1459	A1372	U1268	U1185	U1109	C946
U2116	G2046	C1965	U1887	C1721	G1634	U1544	C1462	A1375	G1269	C1186	U1109	U947
U2117	C2047	U1966	C1888	C1722	G1635	U1545	A1463	G1376	U1270	U1187	G1110	G948
A2118	G2050	U1967	A1889	G1723	G1636	G1546	U1464	C1377	U1278	A1188	U1114	G949
C2119	G2051	A1968	U1890	G1724	A1637	G1552	G1468	U1380	U1279	U1115	U1116	G950
U2120	G2052	A1969	U1891	C1725	A1641	G1553	U1470	U1381	U1288	U1117	G952	G951
G2121	G2053	U1970	U1892	C1726	A1642	U1554	C1469	C1384	C1289	A1191	U1117	G953
A2054	A2054	G1971	G1818	C1727	G1647	G1555	A1471	U1385	G1290	A1192	U1118	U954
A2055		U1972	G1819	G1730	G1648	U1556	C1472	U1386	U1291	A1193	A1118	A955
	U2059	A1973	G1820	C1731	A1649	U1557	A1472	C1385	U1292	G1197	U1120	
		G1974	G1821	C1732	G1650	U1558	C1473	U1386	U1293	U1198	U1121	G958
			G1822	A1733	A1651	U1559	C1474	G1390	U1294	A1199	A1123	G959
			G1823	G1734	A1652	U1560	C1475	G1391	U1295	U1200	G1039	G960
			G1824	C1735	U1654	U1561	C1476	A1392	G1296	C1201	C1126	A961
			G1825	C1736	G1655	G1562	C1477	A1393	G1297	U1205	C1127	
			G1826	A1737	A1656	G1563	U1478	C1394	C1301	U1206	U1128	C962
			G1827	C1738	A1657	C1564	C1479	U1408	G1312	U1207	C1129	C963
			A1829		A1658	U1565	C1483	G1398	C1303	C1208	U1130	
			U1833	U1741	A1659	A1573	C1484	A1399	A1308	G1209	G1131	G1045
			C1834	A1742	G1660	U1580	A1485	G1402	U1309	C1210	A1132	
			U1835	G1743		U1581	C1486	G1403	G1310	U1211	C1133	
			U1836	G1744	C1666	G1586	A1487	U1416	U1311	U1212	G1134	
			A1839	G1745	U1667	U1587	U1488	G1417	G1312	G1213	G1135	
			C1841	A1746	U1668	U1588	U1489	A1407	G1313	G1214	G1136	
			U1845	U1748	G1670	G1589	C1490	U1408	G1314	U1215	G1137	
			U1846			G1592	A1493	U1419	A1328	G1216	G1138	
			U1847	G1751	U1677	C1593	A1494	C1420	A1329	G1217	U1139	
			A1848	C1752	A1678	U1594	C1495	U1421	A1330	U1218	C1140	
			G1849	G1753	C1679	G1595	C1496	C1423	U1332	U1219	G1059	
			U1850	A1759	G1681	U1596	G1497	C1424	C1334	U1220	C	
			G1851	G1760	G1682	U1597	C1500	A1430	C1335	U1221	G1072	
			U1855	U1761	A1683	A1598	A1501	G1433	G1339	G1238	U	
			G1856	C1762	A1684	U1599	A1502	C1434	G1340	U1239	C	
			A1857	U1766	U1685	A1603	C1503	U1435	C1341	G1164	G1075	
			C1858	A1767	C1686	G1604	U1504	A1436	A1342	A1242	A1079	
			U1859	C1768	C1687	G1605	C1505	C1437	U1347	C1243	C1080	
			U1860	G1769	G1688	A1606	U1506	U1440	A1348	U1244	A1081	
			C1861	U1770	A1689	A1607	C1507	G1441	G1351	G1245	A1082	
			U1862	C1772	A1690	G1608	C1508	A1442	C1353	U1246	C1083	
			G1863	G1773	A1691	G1609	C1509	A1443	U1352	U1249	C1084	
			A1864	G1774	A1692	G1610	C1514	C1438	C1354	C1250	C1085	
			U1865	A1778	G1694	A1611	C1515	U1444	U1349	C1251	A1086	
			A1866	C1779	U1696	C1612	C1516	G1445	A1348	C1252	G1087	
			G1867	A1779	U1697	C1613	U1517	U1446	G1360	G1260	A1088	
			U1868	C1787	U1698	A1615	C1518	U1447	C1361	A1176	C1008	
			A1869	U1788	U1699	A1616	G1523		U1362	A1177		
			G1870	C1789	A1700	C1617	U1524		C1363			
			U1871	U1790	U1701	C1618	A1525					
			C1872	C1791	U1702	G1621	A1526					
			G1873	U1792	U1703	A1624	A1527					
			U1874	C1793	U1704	A1625	A1528					
			A1875	U1794	U1705	A1626	A1529					
			G1876	C1795	U1706	A1627						
			U1877	C1796	U1707	A1628						
			A1878	C1797	U1708	A1629						
			G1879	C1798	U1709	A1630						
			U1880	C1799	U1710	A1631						
			A1881	C1800	U1711	A1632						
			G1882	C1801	U1712	A1633						
			U1883	C1802	U1713	A1634						
			A1884	C1803	U1714	A1635						
			G1885	C1804	U1715	A1636						
			U1886	C1805	U1716	A1637						
			A1887	C1806	U1717	A1638						
			G1888	C1807	U1718	A1639						
			U1889	C1808	U1719	A1640						
			A1890	C1809	U1720	A1641						
			G1891	C1810	U1721	A1642						
			U1892	C1811	U1722	A1643						
			A1893	C1812	U1723	A1644						
			G1894	C1813	U1724	A1645						
			U1895	C1814	U1725	A1646						
			A1896	C1815	U1726	A1647						
			G1897	C1816	U1727	A1648						
			U1898	C1817	U1728	A1649						
			A1899	C1818	U1729	A1650						
			G1900	C1819	U1730	A1651						
			U1901	C1820	U1731	A1652						
			A1902	C1821	U1732	A1653						
			G1903	C1822	U1733	A1654						
			U1904	C1823	U1734	A1655						
			A1905	C1824	U1735	A1656						
			G1906	C1825	U1736	A1657						
			U1907	C1826	U1737	A1658						
			A1908	C1827	U1738	A1659						
			G1909	C1828	U1739	A1660						
			U1910	C1829	U1740	A1661						
			A1911	C1830	U1741	A1662						
			G1912	C1831	U1742	A1663						
			U1913	C1832	U1743	A1664						
			A1914	C1833	U1744	A1665						
			G1915	C1834	U1745	A1666						
			U1916	C1835	U1746	A1667						
			A1917	C1836	U1747	A1668						
			G1918	C1837	U1748	A1669						
			U1919	C1838	U1749	A1670						
			A1920	C1839	U1750	A1671						
			G1921	C1840	U1751	A1672						
			U1922	C1841	U1752	A1673						
			A1923	C1842	U1753	A1674						
			G1924	C1843	U1754	A1675						
			U1925	C1844	U1755	A1676						
			A1926	C1845	U1756	A1677						
			G1927	C1846	U1757	A1678						
			U1928	C1847	U1758	A1679						
			A1929	C1848	U1759	A1680						
			G1930	C1849	U1760	A1681						
			U1931	C1850	U1761	A1682						
			A1932	C1851	U1762	A1683						
			G1933	C1852	U1763	A1684						
			U1934	C1853	U1764	A1685						
			A1935	C1854	U1765	A1686						
			G1936	C1855	U1766	A1687						
			U1937	C1856	U1767	A1688						
			A1938	C1857	U1768	A1689						
			G1939	C1858	U1769	A1690						
			U1940	C1859	U1770	A1691						
			A1941	C1860	U1771	A1692						
			G1942	C1861	U1772	A1693						
			U1943	C1862	U1773	A1694						
			A1944	C1863	U1774	A1695						
			G1945	C1864	U1775	A1696						
			U1946	C1865	U1776	A1697						
			A1947	C1866	U1777	A1698						
			G1948	C1867	U1778	A1699						
			U1949	C1868	U1779	A1700						
			A1950	C1869	U1780	A1701						
			G1951	C1870	U1781	A1702						
			U1952	C1871	U1782	A1703						
			A1953	C1872	U1783	A1704						
			G1954	C1873	U							



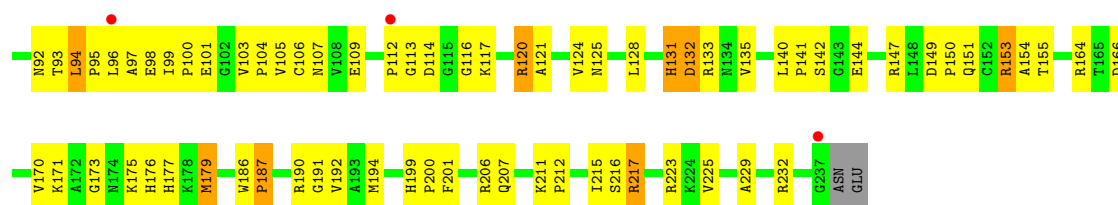


### • Molecule 2: 5S rRNA

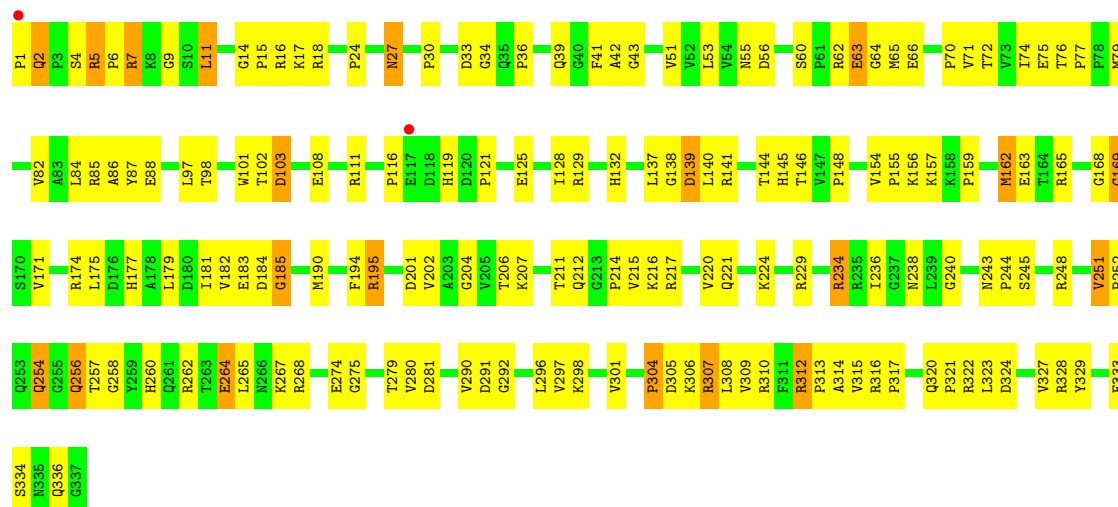


### • Molecule 3: RIBOSOMAL PROTEIN L2

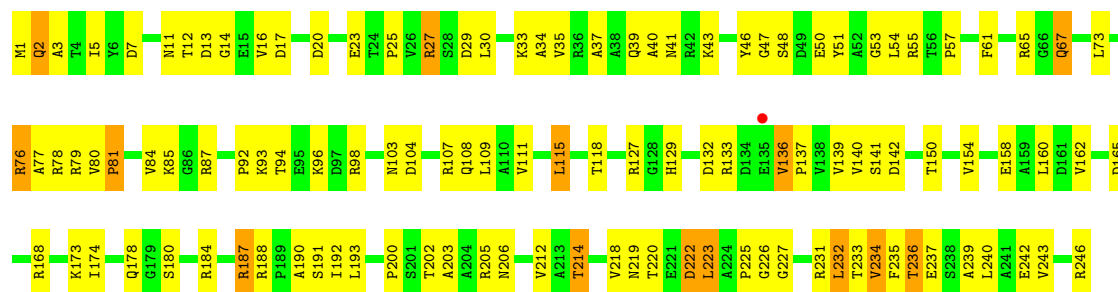




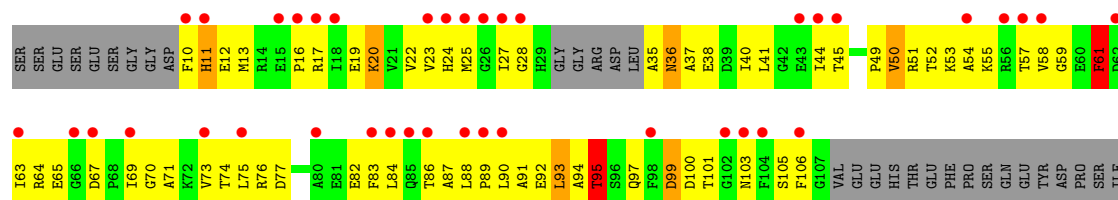
• Molecule 4: RIBOSOMAL PROTEIN L3

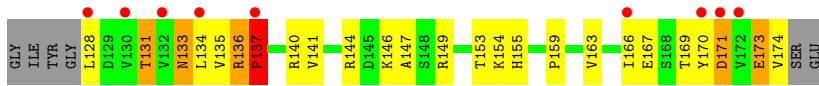


• Molecule 5: RIBOSOMAL PROTEIN L4



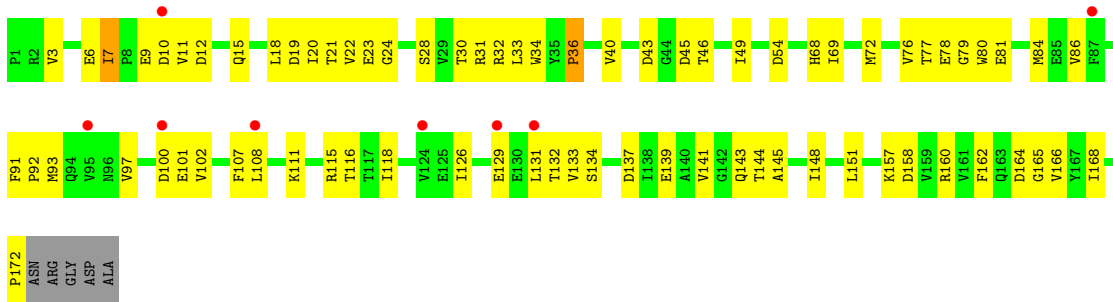
• Molecule 6: RIBOSOMAL PROTEIN L5





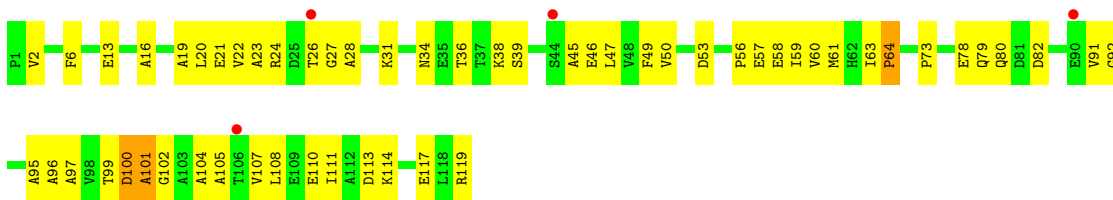
- Molecule 7: RIBOSOMAL PROTEIN L6

Chain G:  5% 55% 41% . .



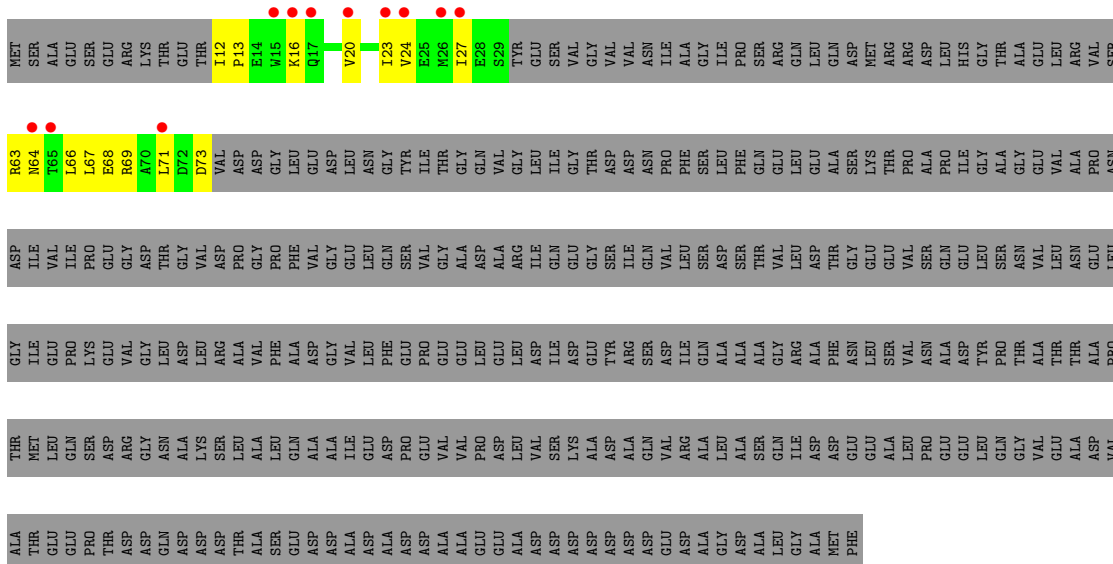
- Molecule 8: RIBOSOMAL PROTEIN L7AE

Chain H: 



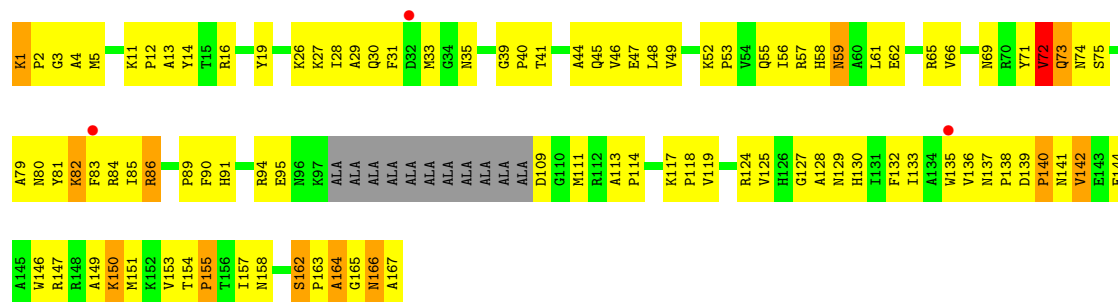
- Molecule 9: RIBOSOMAL PROTEIN L10

Chain I:  3% 92%

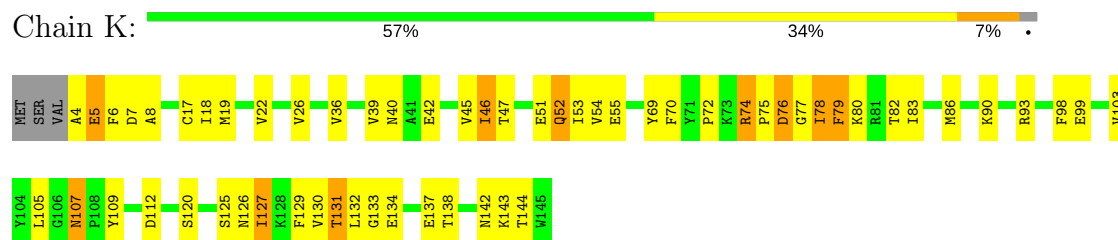


- Molecule 10: RIBOSOMAL PROTEIN L10E

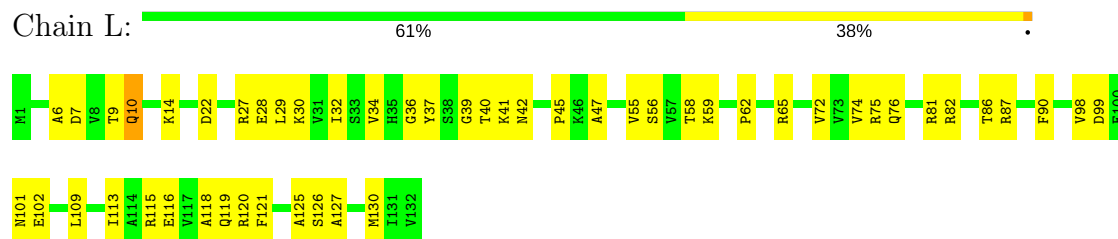
Chain J:  2% 35% 51% 7% 7%



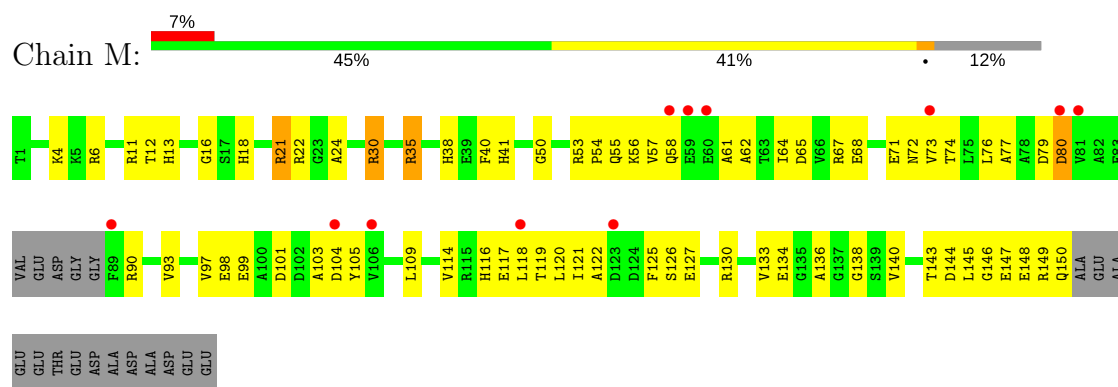
• Molecule 11: RIBOSOMAL PROTEIN L13



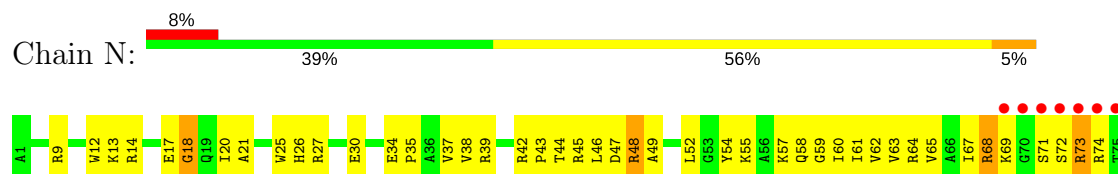
• Molecule 12: RIBOSOMAL PROTEIN L14



• Molecule 13: RIBOSOMAL PROTEIN L15

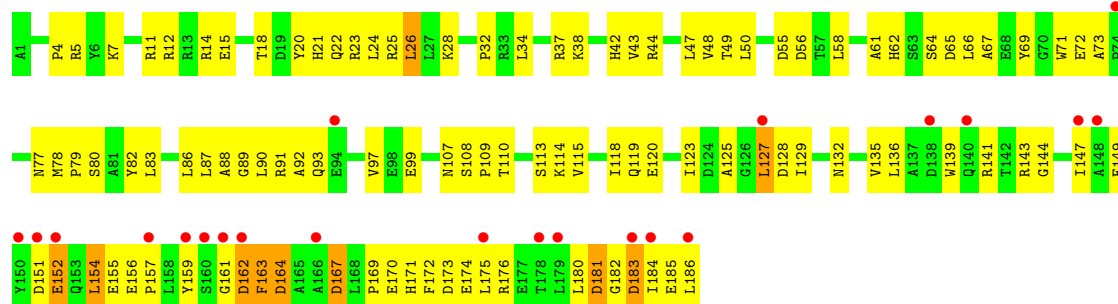


• Molecule 14: RIBOSOMAL PROTEIN L15E

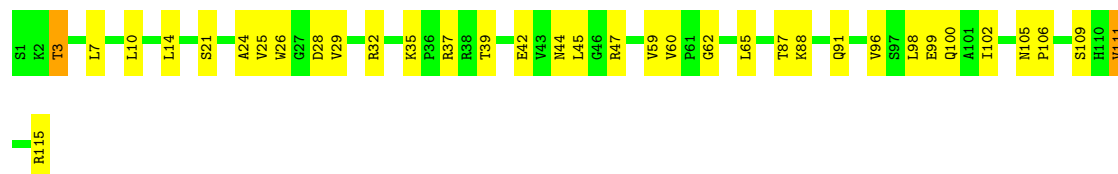




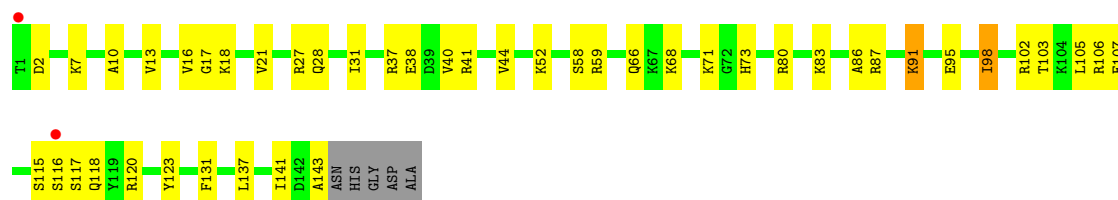
• Molecule 15: RIBOSOMAL PROTEIN L18



• Molecule 16: RIBOSOMAL PROTEIN L18E



• Molecule 17: RIBOSOMAL PROTEIN L19E

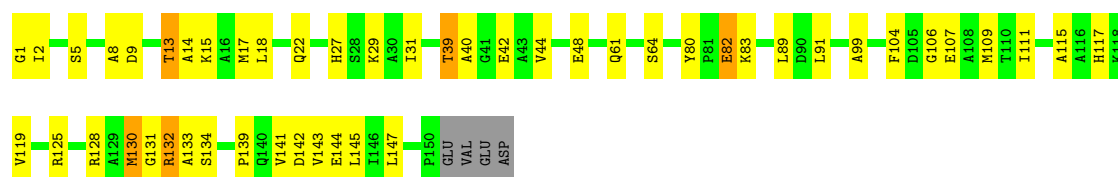


• Molecule 18: RIBOSOMAL PROTEIN L21E

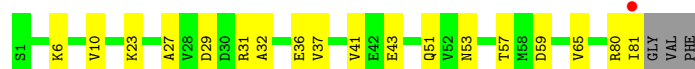
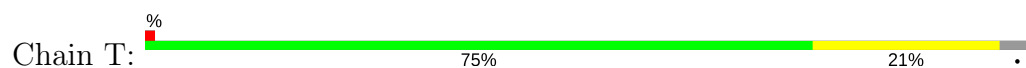


• Molecule 19: RIBOSOMAL PROTEIN L22

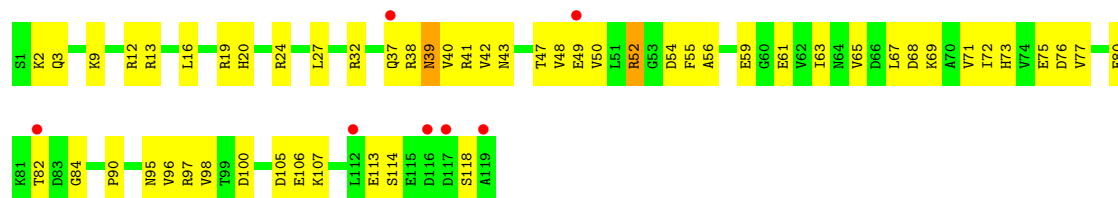




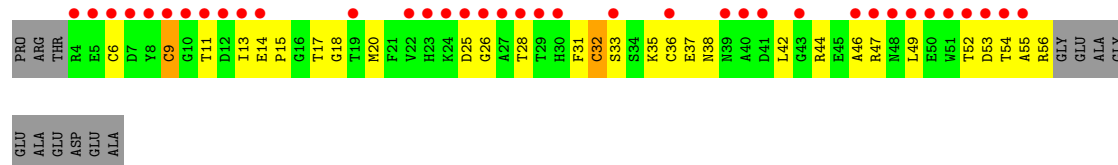
- Molecule 20: RIBOSOMAL PROTEIN L23



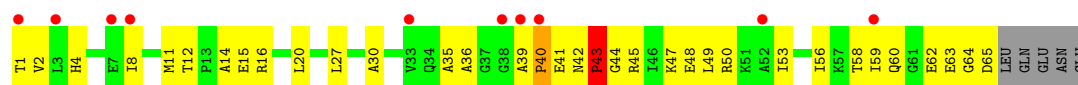
- Molecule 21: RIBOSOMAL PROTEIN L24



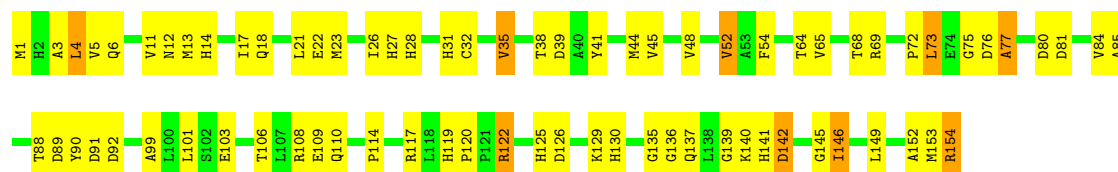
- Molecule 22: RIBOSOMAL PROTEIN L24E



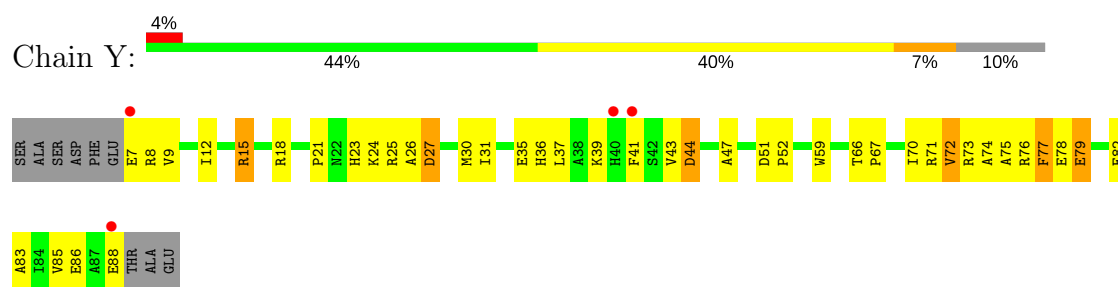
- Molecule 23: RIBOSOMAL PROTEIN L29



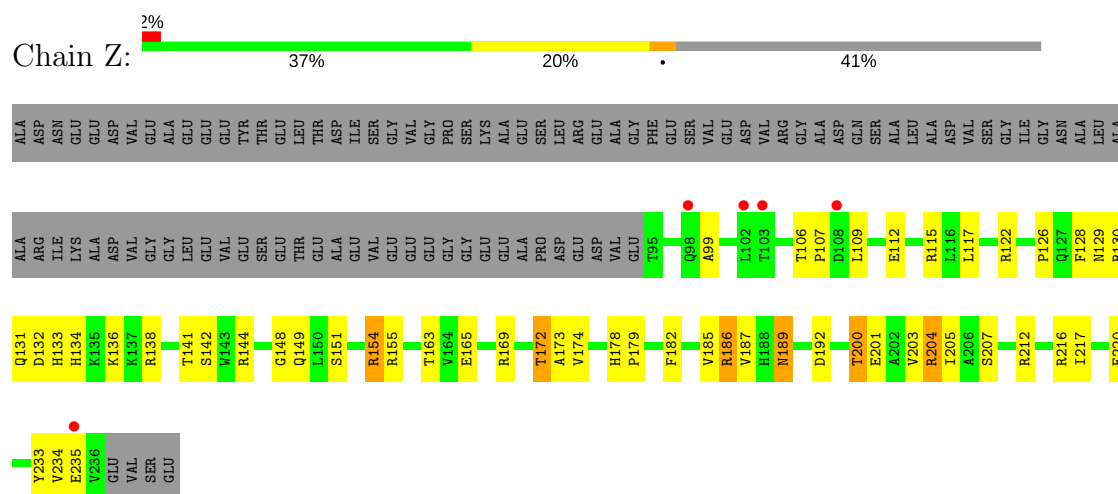
- Molecule 24: RIBOSOMAL PROTEIN L30



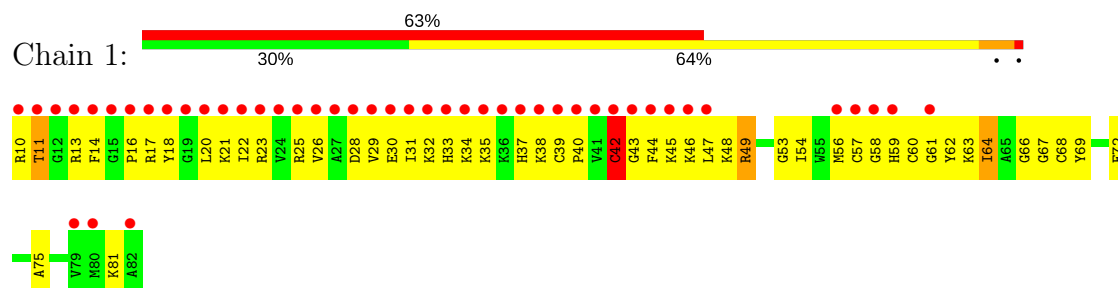
- Molecule 25: RIBOSOMAL PROTEIN L31E



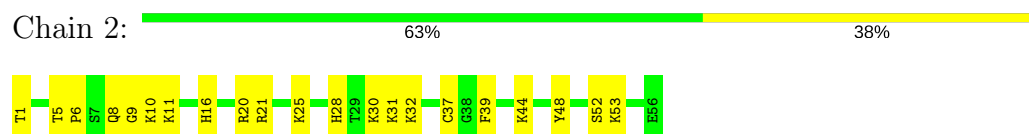
• Molecule 26: RIBOSOMAL PROTEIN L32E



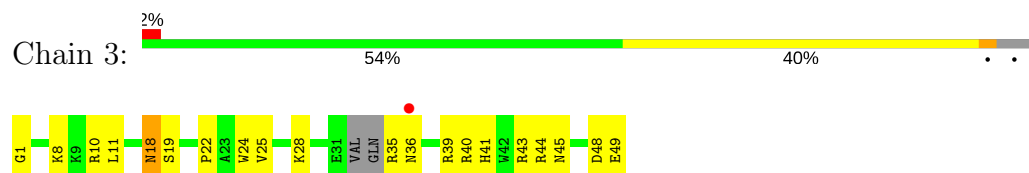
- Molecule 27: RIBOSOMAL PROTEIN L37Ae



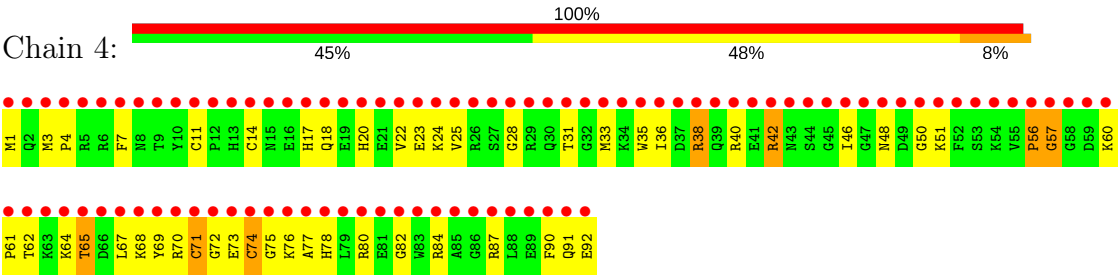
• Molecule 28: RIBOSOMAL PROTEIN L37E



- 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, $\alpha$ , $\beta$ , $\gamma$	212.90Å 300.47Å 575.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.00 50.07 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.7 (19.99-3.00) 91.1 (50.07-2.99)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	0.15	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.220 , 0.269 0.220 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	50.9	Xtriage
Anisotropy	0.399	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 65.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	98587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.62	12/66076 (0.0%)	0.79	45/103052 (0.0%)
2	B	0.90	12/2905 (0.4%)	0.98	17/4528 (0.4%)
3	C	0.53	0/1787	0.79	0/2409
4	D	0.52	0/2689	0.75	0/3652
5	E	0.54	0/1883	0.78	0/2551
6	F	0.43	0/1111	0.65	0/1498
7	G	0.47	0/1382	0.66	0/1880
8	H	0.44	0/896	0.64	0/1219
9	I	0.41	0/241	0.58	0/324
10	J	0.53	0/1246	0.83	1/1686 (0.1%)
11	K	0.52	0/1135	0.70	0/1530
12	L	0.51	0/1003	0.80	0/1351
13	M	0.49	0/1126	0.74	0/1504
14	N	0.67	0/1633	0.86	1/2180 (0.0%)
15	O	0.48	0/1473	0.76	0/1999
16	P	0.53	0/873	0.76	0/1181
17	Q	0.52	0/1143	0.67	0/1521
18	R	0.52	0/748	0.80	1/1005 (0.1%)
19	S	0.66	1/1172 (0.1%)	0.84	2/1578 (0.1%)
20	T	0.45	0/648	0.69	0/875
21	U	0.47	0/957	0.73	1/1289 (0.1%)
22	V	0.77	0/417	0.86	2/562 (0.4%)
23	W	0.42	0/502	0.63	0/675
24	X	0.54	0/1218	0.76	0/1655
25	Y	0.50	0/664	0.72	0/895
26	Z	0.53	0/1146	0.73	0/1536
27	1	0.85	0/575	0.87	1/763 (0.1%)
28	2	0.56	0/437	0.84	0/578
29	3	0.47	0/398	0.64	0/527
30	4	1.04	0/771	0.83	1/1024 (0.1%)
All	All	0.62	25/98255 (0.0%)	0.79	72/147027 (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	198
2	B	0	6
28	2	0	1
All	All	1	205

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2103	A	C5-C6	13.31	1.53	1.41
2	B	3025	G	O3'-P	11.56	1.75	1.61
2	B	3026	C	P-OP2	-10.89	1.30	1.49
2	B	3026	C	P-O5'	-9.81	1.50	1.59
2	B	3023	U	C2'-O2'	8.99	1.53	1.41

The worst 5 of 72 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP2-P-O3'	-18.78	63.89	105.20
1	A	1164	U	OP1-P-O3'	-18.34	64.85	105.20
1	A	2104	C	O5'-P-OP1	-14.12	92.99	105.70
2	B	3024	U	O5'-P-OP2	11.53	124.53	110.70
2	B	3026	C	O5'-P-OP2	-11.17	95.65	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 205 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	G	Sidechain
1	A	138	U	Sidechain
1	A	146	U	Sidechain
1	A	75	U	Sidechain
1	A	99	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	A	59017	0	29802	1290	0
2	B	2600	0	1326	80	0
3	C	1754	0	1763	132	0
4	D	2624	0	2533	190	0
5	E	1858	0	1816	149	0
6	F	1094	0	1085	135	0
7	G	1357	0	1266	85	0
8	H	885	0	854	63	0
9	I	240	0	231	21	0
10	J	1215	0	1215	175	0
11	K	1119	0	1098	70	0
12	L	993	0	1027	67	0
13	M	1114	0	1072	72	0
14	N	1605	0	1676	194	0
15	O	1444	0	1401	143	0
16	P	864	0	873	37	0
17	Q	1133	0	1127	53	0
18	R	734	0	727	30	0
19	S	1149	0	1122	60	0
20	T	641	0	605	23	0
21	U	949	0	923	59	0
22	V	410	0	368	45	0
23	W	499	0	511	33	0
24	X	1195	0	1137	99	0
25	Y	654	0	653	51	0
26	Z	1130	0	1133	71	0
27	1	563	0	601	80	0
28	2	430	0	426	27	0
29	3	393	0	406	27	0
30	4	755	0	732	58	0
31	A	59	0	73	9	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	112	0	0	5	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	73	0	0	1	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0
33	E	1	0	0	0	0
33	J	1	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	9	0	0	2	0
34	C	1	0	0	0	0
34	D	1	0	0	0	0
34	K	3	0	0	2	0
34	M	1	0	0	0	0
34	N	1	0	0	1	0
34	O	1	0	0	3	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	41	0	0	13	0
37	2	55	0	0	5	0
37	3	42	0	0	5	0
37	4	73	0	0	7	0
37	A	5910	0	0	300	0
37	B	142	0	0	16	0
37	C	126	0	0	23	0
37	D	150	0	0	28	0
37	E	169	0	0	40	0
37	F	51	0	0	22	0
37	G	42	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	H	26	0	0	9	0
37	I	21	0	0	5	0
37	J	78	0	0	26	0
37	K	54	0	0	8	0
37	L	65	0	0	12	0
37	M	79	0	0	18	0
37	N	132	0	0	36	0
37	O	69	0	0	23	0
37	P	45	0	0	9	0
37	Q	65	0	0	4	0
37	R	55	0	0	6	0
37	S	83	0	0	11	0
37	T	35	0	0	3	0
37	U	39	0	0	4	0
37	V	25	0	0	8	0
37	W	15	0	0	2	0
37	X	70	0	0	10	0
37	Y	25	0	0	11	0
37	Z	94	0	0	18	0
All	All	98587	0	59582	3325	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 22.

The worst 5 of 3325 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)
30:4:33:MET:SD	30:4:33:MET:CE	2.03	1.47
5:E:236:THR:HG22	5:E:239:ALA:H	1.09	1.15
1:A:2121:G:OP2	37:A:3494:HOH:O	1.64	1.15
1:A:2122:C:OP2	37:A:6549:HOH:O	1.64	1.15
1:A:1134:G:H4'	10:J:151:MET:HE1	1.28	1.12

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%)	205 (87%)	26 (11%)	4 (2%)	11	44
4	D	335/337 (99%)	307 (92%)	21 (6%)	7 (2%)	8	38
5	E	244/246 (99%)	225 (92%)	18 (7%)	1 (0%)	38	78
6	F	134/176 (76%)	95 (71%)	27 (20%)	12 (9%)	1	4
7	G	170/177 (96%)	158 (93%)	12 (7%)	0	100	100
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11	44
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	129 (85%)	17 (11%)	6 (4%)	3	20
11	K	140/145 (97%)	131 (94%)	5 (4%)	4 (3%)	5	28
12	L	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	12	48
13	M	141/164 (86%)	118 (84%)	20 (14%)	3 (2%)	8	38
14	N	192/194 (99%)	172 (90%)	18 (9%)	2 (1%)	18	59
15	O	184/186 (99%)	165 (90%)	13 (7%)	6 (3%)	4	25
16	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
17	Q	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	25	67
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	17	56
19	S	148/154 (96%)	138 (93%)	10 (7%)	0	100	100
20	T	79/84 (94%)	72 (91%)	7 (9%)	0	100	100
21	U	117/119 (98%)	108 (92%)	9 (8%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	26
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	25	67
25	Y	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	6	32
26	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	13	49

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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%)	41 (98%)	1 (2%)	0	100	100
30	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	8	36
All	All	3633/4235 (86%)	3299 (91%)	275 (8%)	59 (2%)	11	46

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	16	50
4	D	282/282 (100%)	264 (94%)	18 (6%)	20	57
5	E	193/193 (100%)	178 (92%)	15 (8%)	15	47
6	F	117/147 (80%)	106 (91%)	11 (9%)	10	37
7	G	152/155 (98%)	147 (97%)	5 (3%)	43	79
8	H	92/92 (100%)	91 (99%)	1 (1%)	78	93
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	11	40
11	K	118/121 (98%)	107 (91%)	11 (9%)	10	38
12	L	106/106 (100%)	103 (97%)	3 (3%)	49	82
13	M	112/126 (89%)	108 (96%)	4 (4%)	40	77
14	N	166/166 (100%)	157 (95%)	9 (5%)	26	64
15	O	149/149 (100%)	144 (97%)	5 (3%)	42	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	90 (97%)	3 (3%)	44	79
17	Q	113/116 (97%)	110 (97%)	3 (3%)	50	82
18	R	79/79 (100%)	75 (95%)	4 (5%)	28	66
19	S	117/121 (97%)	112 (96%)	5 (4%)	33	72
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	103 (98%)	2 (2%)	62	88
22	V	44/52 (85%)	42 (96%)	2 (4%)	32	71
23	W	51/56 (91%)	50 (98%)	1 (2%)	60	87
24	X	130/130 (100%)	122 (94%)	8 (6%)	21	58
25	Y	66/73 (90%)	61 (92%)	5 (8%)	15	48
26	Z	120/195 (62%)	112 (93%)	8 (7%)	19	54
27	1	56/56 (100%)	50 (89%)	6 (11%)	8	29
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	54	85
30	4	79/79 (100%)	73 (92%)	6 (8%)	15	48
All	All	3027/3441 (88%)	2867 (95%)	160 (5%)	26	65

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	155	PRO
13	M	35	ARG
27	1	11	THR
11	K	46	ILE
11	K	120	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 84 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	116	HIS
17	Q	73	HIS
28	2	16	HIS
14	N	58	GLN
14	N	176	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2745/2922 (93%)	248 (9%)	0
2	B	121/122 (99%)	15 (12%)	0
All	All	2866/3044 (94%)	263 (9%)	0

5 of 263 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

There are no RNA pucker outliers to report.

## 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	SPR	A	9001	1	61,62,62	2.99	28 (45%)	76,89,89	3.12	31 (40%)

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	SPR	A	9001	1	-	0/61/113/113	0/3/4/4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9001	SPR	C6-C5	-5.40	1.42	1.52
31	A	9001	SPR	O5A-C5A	-4.76	1.33	1.44
31	A	9001	SPR	O15-C1	-4.46	1.21	1.34
31	A	9001	SPR	O4A-C1B	-4.02	1.31	1.41
31	A	9001	SPR	O1C-C1C	-3.82	1.31	1.41

The worst 5 of 31 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9001	SPR	C8A-N3A-C7A	-9.17	82.41	110.41
31	A	9001	SPR	C5A-C4A-C3A	-7.41	93.97	110.55
31	A	9001	SPR	O19-C19-C18	-7.19	102.19	125.48
31	A	9001	SPR	O1C-C1C-O5C	-5.98	90.45	110.05
31	A	9001	SPR	C15-C14-C13	-5.86	102.86	113.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9001	SPR	9	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	2754/2922 (94%)	-0.07	48 (1%) 70 42	23, 51, 96, 143	0
2	B	122/122 (100%)	0.26	6 (4%) 30 12	37, 70, 100, 150	0
3	C	237/239 (99%)	0.12	10 (4%) 37 15	32, 63, 96, 110	0
4	D	337/337 (100%)	-0.14	2 (0%) 89 71	28, 57, 84, 95	0
5	E	246/246 (100%)	-0.20	1 (0%) 92 77	24, 50, 74, 85	0
6	F	140/176 (79%)	1.53	48 (34%) 0 0	60, 103, 122, 127	0
7	G	172/177 (97%)	0.47	8 (4%) 32 13	43, 68, 92, 98	0
8	H	119/119 (100%)	0.41	4 (3%) 46 20	59, 79, 102, 107	0
9	I	29/348 (8%)	1.84	11 (37%) 0 0	76, 94, 102, 104	0
10	J	156/167 (93%)	0.18	3 (1%) 67 37	35, 58, 85, 93	0
11	K	142/145 (97%)	-0.13	0 100 100	36, 50, 76, 84	0
12	L	132/132 (100%)	-0.01	0 100 100	35, 56, 78, 82	0
13	M	145/164 (88%)	0.50	11 (7%) 15 6	31, 74, 108, 117	0
14	N	194/194 (100%)	0.22	16 (8%) 12 5	37, 55, 91, 98	0
15	O	186/186 (100%)	0.69	22 (11%) 5 2	48, 74, 112, 122	0
16	P	115/115 (100%)	-0.05	0 100 100	39, 59, 75, 79	0
17	Q	143/148 (96%)	0.15	2 (1%) 75 49	38, 60, 76, 84	0
18	R	95/95 (100%)	-0.12	1 (1%) 80 55	38, 51, 64, 79	0
19	S	150/154 (97%)	-0.19	0 100 100	32, 45, 66, 75	0
20	T	81/84 (96%)	0.03	1 (1%) 79 53	47, 65, 84, 89	0
21	U	119/119 (100%)	0.38	7 (5%) 23 9	44, 62, 86, 97	0
22	V	53/66 (80%)	3.18	37 (69%) 0 0	85, 94, 102, 110	0
23	W	65/70 (92%)	1.12	10 (15%) 2 1	55, 81, 112, 118	0
24	X	154/154 (100%)	-0.20	0 100 100	32, 49, 66, 76	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.24	4 (4%) 30 12	42, 58, 84, 99	0
26	Z	142/240 (59%)	-0.10	5 (3%) 44 19	25, 46, 70, 85	0
27	1	73/73 (100%)	3.49	46 (63%) 0 0	79, 98, 103, 104	0
28	2	56/56 (100%)	-0.42	0 100 100	30, 39, 45, 49	0
29	3	46/48 (95%)	0.06	1 (2%) 62 33	40, 66, 90, 102	0
30	4	92/92 (100%)	6.46	92 (100%) 0 0	91, 103, 108, 111	0
All	All	6577/7279 (90%)	0.22	396 (6%) 23 9	23, 57, 102, 150	0

The worst 5 of 396 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	15.5
30	4	65	THR	13.0
30	4	82	GLY	12.9
30	4	84	ARG	12.4
30	4	83	TRP	11.9

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	A	8356	1/1	0.83	0.69	40.87	58,58,58,58	0
34	CL	A	8515	1/1	0.87	0.59	24.89	100,100,100,100	0
33	NA	A	8372	1/1	0.83	0.67	22.22	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8382	1/1	0.55	0.38	19.39	62,62,62,62	0
33	NA	B	8383	1/1	0.71	0.65	17.47	63,63,63,63	0
33	NA	A	8371	1/1	0.69	0.34	15.47	54,54,54,54	0
34	CL	D	8519	1/1	0.93	0.50	15.14	65,65,65,65	0
33	NA	A	8374	1/1	0.90	0.60	14.99	63,63,63,63	0
33	NA	A	8362	1/1	0.82	0.39	14.68	69,69,69,69	0
33	NA	A	8373	1/1	0.74	0.52	12.99	59,59,59,59	0
33	NA	A	8321	1/1	0.91	0.42	12.17	39,39,39,39	0
34	CL	A	8505	1/1	0.92	0.65	10.79	88,88,88,88	0
33	NA	A	8331	1/1	0.72	0.36	10.11	61,61,61,61	0
33	NA	A	8379	1/1	0.94	0.24	9.22	41,41,41,41	0
33	NA	A	8378	1/1	0.91	0.43	8.21	37,37,37,37	0
33	NA	A	8323	1/1	0.91	0.25	7.91	50,50,50,50	0
31	SPR	A	9001	59/59	0.83	0.36	7.31	78,88,95,95	0
33	NA	A	8376	1/1	0.96	0.28	7.04	78,78,78,78	0
33	NA	A	8308	1/1	0.88	0.22	6.51	69,69,69,69	0
33	NA	S	8386	1/1	0.83	0.27	6.29	53,53,53,53	0
33	NA	A	8335	1/1	0.98	0.23	5.87	52,52,52,52	0
33	NA	A	8365	1/1	0.74	0.40	5.32	49,49,49,49	0
33	NA	S	8337	1/1	0.70	0.32	3.42	49,49,49,49	0
33	NA	A	8310	1/1	0.91	0.23	3.29	29,29,29,29	0
32	MG	Z	8109	1/1	0.86	0.22	3.04	53,53,53,53	0
33	NA	A	8303	1/1	0.96	0.20	2.78	51,51,51,51	0
33	NA	A	8332	1/1	0.81	0.23	2.52	58,58,58,58	0
32	MG	A	8067	1/1	0.93	0.23	2.42	50,50,50,50	0
33	NA	A	8366	1/1	0.90	0.27	2.41	49,49,49,49	0
33	NA	A	8381	1/1	0.95	0.20	2.07	51,51,51,51	0
34	CL	A	8512	1/1	0.92	0.20	1.35	32,32,32,32	0
33	NA	A	8368	1/1	0.92	0.16	1.10	47,47,47,47	0
33	NA	A	8326	1/1	0.89	0.27	0.56	46,46,46,46	0
33	NA	A	8314	1/1	0.97	0.17	0.47	33,33,33,33	0
35	K	A	8602	1/1	0.83	0.29	0.38	68,68,68,68	0
32	MG	A	8064	1/1	0.95	0.16	0.18	24,24,24,24	0
32	MG	A	8101	1/1	0.94	0.16	0.11	55,55,55,55	0
33	NA	A	8361	1/1	0.97	0.14	0.09	53,53,53,53	0
34	CL	N	8518	1/1	0.82	0.22	-0.12	56,56,56,56	0
34	CL	P	8508	1/1	0.95	0.19	-0.23	93,93,93,93	0
32	MG	1	8105	1/1	0.86	0.29	-0.33	44,44,44,44	0
33	NA	A	8350	1/1	0.96	0.14	-0.39	34,34,34,34	0
33	NA	A	8305	1/1	0.89	0.15	-0.47	34,34,34,34	0
33	NA	A	8324	1/1	0.81	0.15	-0.48	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8044	1/1	0.98	0.14	-0.56	52,52,52,52	0
34	CL	O	8507	1/1	0.88	0.24	-0.60	62,62,62,62	0
36	CD	4	8404	1/1	0.59	0.79	-0.72	156,156,156,156	0
33	NA	J	8309	1/1	0.95	0.14	-0.79	21,21,21,21	0
36	CD	V	8401	1/1	0.79	0.48	-1.03	142,142,142,142	0
34	CL	K	8521	1/1	0.94	0.14	-1.04	46,46,46,46	0
33	NA	A	8333	1/1	0.88	0.13	-1.14	33,33,33,33	0
34	CL	4	8504	1/1	0.66	0.69	-1.16	95,95,95,95	0
33	NA	M	8380	1/1	0.98	0.15	-1.30	55,55,55,55	0
33	NA	A	8338	1/1	0.98	0.13	-1.32	67,67,67,67	0
32	MG	A	8086	1/1	0.98	0.07	-1.33	50,50,50,50	0
33	NA	A	8353	1/1	0.94	0.12	-1.53	38,38,38,38	0
32	MG	A	8112	1/1	0.98	0.15	-1.65	44,44,44,44	0
33	NA	A	8317	1/1	0.95	0.12	-1.88	27,27,27,27	0
32	MG	A	8074	1/1	0.95	0.08	-1.90	31,31,31,31	0
32	MG	U	8073	1/1	0.93	0.19	-2.03	42,42,42,42	0
32	MG	A	8018	1/1	0.95	0.11	-2.03	61,61,61,61	0
33	NA	A	8327	1/1	0.95	0.13	-2.09	32,32,32,32	0
36	CD	1	8403	1/1	0.85	0.28	-2.12	138,138,138,138	0
32	MG	A	8055	1/1	0.96	0.08	-2.36	71,71,71,71	0
32	MG	A	8107	1/1	0.99	0.04	-2.39	47,47,47,47	0
32	MG	C	8065	1/1	0.94	0.11	-2.49	57,57,57,57	0
36	CD	2	8402	1/1	0.98	0.06	-2.56	59,59,59,59	0
33	NA	A	8339	1/1	0.98	0.14	-2.57	16,16,16,16	0
33	NA	A	8320	1/1	0.93	0.12	-2.77	33,33,33,33	0
32	MG	A	8012	1/1	0.98	0.11	-2.79	52,52,52,52	0
32	MG	A	8058	1/1	0.98	0.09	-2.82	43,43,43,43	0
33	NA	K	8346	1/1	0.96	0.08	-2.84	27,27,27,27	0
33	NA	R	8348	1/1	0.93	0.11	-2.99	37,37,37,37	0
32	MG	A	8027	1/1	0.95	0.05	-3.10	63,63,63,63	0
32	MG	A	8060	1/1	0.96	0.12	-3.20	45,45,45,45	0
32	MG	A	8071	1/1	0.96	0.13	-3.26	91,91,91,91	0
32	MG	A	8057	1/1	0.95	0.11	-3.28	49,49,49,49	0
32	MG	A	8108	1/1	0.97	0.09	-3.29	88,88,88,88	0
32	MG	A	8001	1/1	0.79	0.12	-3.43	39,39,39,39	0
32	MG	A	8002	1/1	0.99	0.10	-3.52	31,31,31,31	0
32	MG	A	8015	1/1	0.93	0.10	-3.59	57,57,57,57	0
32	MG	A	8038	1/1	0.97	0.10	-3.61	35,35,35,35	0
32	MG	A	8056	1/1	0.98	0.09	-3.83	53,53,53,53	0
33	NA	A	8344	1/1	0.89	0.09	-3.95	30,30,30,30	0
33	NA	A	8343	1/1	0.89	0.09	-4.27	16,16,16,16	0
33	NA	C	8345	1/1	0.97	0.10	-4.43	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8062	1/1	0.90	0.11	-4.51	72,72,72,72	0
32	MG	A	8004	1/1	0.97	0.07	-4.53	48,48,48,48	0
32	MG	A	8096	1/1	0.92	0.09	-4.60	53,53,53,53	0
32	MG	A	8003	1/1	0.97	0.10	-4.67	24,24,24,24	0
32	MG	A	8053	1/1	0.94	0.11	-4.69	52,52,52,52	0
32	MG	A	8033	1/1	0.95	0.07	-4.82	30,30,30,30	0
32	MG	A	8006	1/1	0.94	0.08	-4.86	48,48,48,48	0
32	MG	A	8039	1/1	0.89	0.06	-5.21	50,50,50,50	0
32	MG	4	8078	1/1	0.90	0.26	-5.57	74,74,74,74	0
32	MG	A	8032	1/1	0.98	0.05	-5.63	34,34,34,34	0
32	MG	A	8017	1/1	0.98	0.03	-5.72	27,27,27,27	0
32	MG	A	8054	1/1	0.98	0.08	-6.47	48,48,48,48	0
32	MG	A	8019	1/1	0.99	0.07	-6.51	35,35,35,35	0
32	MG	A	8059	1/1	0.95	0.08	-6.53	31,31,31,31	0
32	MG	A	8008	1/1	0.97	0.07	-6.79	49,49,49,49	0
32	MG	A	8013	1/1	0.99	0.12	-7.34	46,46,46,46	0
32	MG	A	8010	1/1	0.96	0.05	-7.69	40,40,40,40	0
32	MG	A	8035	1/1	0.97	0.06	-7.73	54,54,54,54	0
32	MG	A	8014	1/1	0.97	0.06	-7.81	30,30,30,30	0
33	NA	N	8347	1/1	0.99	0.05	-7.92	21,21,21,21	0
32	MG	A	8091	1/1	0.96	0.07	-8.24	48,48,48,48	0
32	MG	A	8034	1/1	0.94	0.06	-8.99	39,39,39,39	0
32	MG	A	8020	1/1	0.98	0.05	-9.64	51,51,51,51	0
32	MG	A	8080	1/1	0.97	0.05	-10.62	50,50,50,50	0
33	NA	A	8325	1/1	0.97	0.09	-10.69	52,52,52,52	0
32	MG	A	8084	1/1	0.97	0.08	-10.93	48,48,48,48	0
32	MG	A	8077	1/1	0.97	0.07	-12.37	31,31,31,31	0
32	MG	A	8007	1/1	0.99	0.04	-12.43	23,23,23,23	0
32	MG	A	8052	1/1	0.99	0.05	-31.47	45,45,45,45	0
32	MG	A	8100	1/1	0.97	0.12	-	69,69,69,69	0
32	MG	A	8023	1/1	0.90	0.07	-	42,42,42,42	0
32	MG	A	8099	1/1	0.96	0.08	-	38,38,38,38	0
35	K	A	8603	1/1	0.84	0.36	-	88,88,88,88	0
33	NA	A	8354	1/1	0.90	0.16	-	40,40,40,40	0
33	NA	A	8336	1/1	0.89	0.19	-	49,49,49,49	0
34	CL	A	8517	1/1	0.87	0.31	-	55,55,55,55	0
32	MG	A	8119	1/1	0.88	0.36	-	71,71,71,71	0
32	MG	A	8037	1/1	0.99	0.10	-	48,48,48,48	0
34	CL	R	8511	1/1	0.81	0.44	-	63,63,63,63	0
32	MG	A	8005	1/1	0.98	0.10	-	44,44,44,44	0
32	MG	A	8009	1/1	0.98	0.06	-	20,20,20,20	0
33	NA	A	8315	1/1	0.97	0.14	-	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8330	1/1	0.93	0.19	-	43,43,43,43	0
33	NA	A	8370	1/1	0.86	0.35	-	49,49,49,49	0
33	NA	A	8318	1/1	0.95	0.17	-	34,34,34,34	0
33	NA	A	8355	1/1	0.85	0.36	-	55,55,55,55	0
33	NA	A	8334	1/1	0.97	0.06	-	36,36,36,36	0
32	MG	A	8022	1/1	0.96	0.09	-	41,41,41,41	0
32	MG	A	8081	1/1	0.93	0.18	-	58,58,58,58	0
33	NA	A	8306	1/1	0.92	0.51	-	56,56,56,56	0
34	CL	A	8522	1/1	0.89	0.43	-	75,75,75,75	0
34	CL	C	8509	1/1	0.94	0.28	-	86,86,86,86	0
33	NA	A	8385	1/1	0.88	0.39	-	41,41,41,41	0
33	NA	A	8377	1/1	0.85	0.25	-	60,60,60,60	0
33	NA	A	8307	1/1	0.94	0.10	-	39,39,39,39	0
32	MG	A	8049	1/1	0.50	0.60	-	89,89,89,89	0
34	CL	A	8513	1/1	0.94	0.12	-	56,56,56,56	0
32	MG	A	8087	1/1	0.96	0.06	-	48,48,48,48	0
32	MG	A	8011	1/1	0.98	0.10	-	52,52,52,52	0
32	MG	A	8040	1/1	0.88	0.19	-	78,78,78,78	0
32	MG	A	8110	1/1	0.89	0.13	-	47,47,47,47	0
32	MG	A	8090	1/1	0.74	0.29	-	36,36,36,36	0
32	MG	A	8066	1/1	0.95	0.13	-	83,83,83,83	0
32	MG	A	8051	1/1	0.94	0.09	-	56,56,56,56	0
32	MG	A	8068	1/1	0.94	0.13	-	58,58,58,58	0
32	MG	A	8043	1/1	0.95	0.08	-	39,39,39,39	0
36	CD	P	8405	1/1	0.74	0.44	-	169,169,169,169	0
32	MG	A	8113	1/1	0.90	0.11	-	45,45,45,45	0
33	NA	A	8316	1/1	0.94	0.34	-	51,51,51,51	0
33	NA	A	8357	1/1	0.89	0.17	-	67,67,67,67	0
33	NA	A	8364	1/1	0.79	0.32	-	40,40,40,40	0
33	NA	E	8304	1/1	0.88	0.12	-	35,35,35,35	0
33	NA	A	8342	1/1	0.94	0.24	-	47,47,47,47	0
33	NA	B	8351	1/1	0.79	0.23	-	69,69,69,69	0
33	NA	A	8329	1/1	0.40	0.52	-	70,70,70,70	0
32	MG	A	8116	1/1	0.88	0.17	-	67,67,67,67	0
33	NA	A	8367	1/1	0.92	0.20	-	52,52,52,52	0
33	NA	A	8375	1/1	0.91	0.34	-	53,53,53,53	0
33	NA	A	8313	1/1	0.90	0.23	-	63,63,63,63	0
32	MG	A	8115	1/1	0.89	0.10	-	59,59,59,59	0
32	MG	A	8063	1/1	0.97	0.06	-	78,78,78,78	0
34	CL	A	8503	1/1	0.83	0.33	-	50,50,50,50	0
33	NA	A	8311	1/1	0.96	0.09	-	42,42,42,42	0
32	MG	A	8030	1/1	0.99	0.09	-	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	L	8069	1/1	0.95	0.05	-	50,50,50,50	0
32	MG	A	8094	1/1	0.98	0.14	-	85,85,85,85	0
33	NA	A	8341	1/1	0.56	0.19	-	43,43,43,43	0
32	MG	A	8098	1/1	0.97	0.20	-	50,50,50,50	0
32	MG	A	8048	1/1	0.97	0.09	-	45,45,45,45	0
32	MG	A	8026	1/1	0.99	0.04	-	11,11,11,11	0
33	NA	A	8322	1/1	0.93	0.42	-	46,46,46,46	0
32	MG	A	8046	1/1	0.95	0.08	-	79,79,79,79	0
32	MG	A	8025	1/1	0.99	0.08	-	60,60,60,60	0
32	MG	A	8093	1/1	0.87	0.23	-	56,56,56,56	0
32	MG	A	8070	1/1	0.88	0.59	-	66,66,66,66	0
32	MG	A	8114	1/1	0.94	0.46	-	92,92,92,92	0
34	CL	A	8514	1/1	0.93	0.21	-	61,61,61,61	0
32	MG	A	8061	1/1	0.92	0.09	-	44,44,44,44	0
33	NA	A	8328	1/1	0.88	0.19	-	45,45,45,45	0
33	NA	A	8352	1/1	0.86	0.43	-	52,52,52,52	0
33	NA	A	8384	1/1	0.40	2.03	-	114,114,114,114	0
32	MG	A	8117	1/1	0.84	0.12	-	31,31,31,31	0
32	MG	A	8072	1/1	0.94	0.13	-	80,80,80,80	0
32	MG	A	8036	1/1	0.99	0.06	-	45,45,45,45	0
32	MG	A	8076	1/1	0.76	0.17	-	71,71,71,71	0
32	MG	A	8104	1/1	0.81	0.23	-	40,40,40,40	0
34	CL	A	8516	1/1	0.90	0.19	-	44,44,44,44	0
34	CL	M	8510	1/1	0.52	0.46	-	87,87,87,87	0
32	MG	A	8029	1/1	0.95	0.07	-	51,51,51,51	0
33	NA	A	8360	1/1	0.85	0.86	-	55,55,55,55	0
32	MG	A	8089	1/1	0.91	0.19	-	84,84,84,84	0
33	NA	A	8319	1/1	0.96	0.10	-	52,52,52,52	0
32	MG	A	8031	1/1	0.94	0.05	-	31,31,31,31	0
32	MG	B	8095	1/1	0.82	0.07	-	67,67,67,67	0
34	CL	S	8506	1/1	0.96	0.18	-	46,46,46,46	0
32	MG	A	8050	1/1	0.89	0.13	-	85,85,85,85	0
32	MG	A	8079	1/1	0.96	0.14	-	39,39,39,39	0
33	NA	A	8302	1/1	0.97	0.13	-	40,40,40,40	0
32	MG	A	8047	1/1	0.96	0.18	-	62,62,62,62	0
34	CL	K	8501	1/1	0.94	0.13	-	56,56,56,56	0
32	MG	A	8082	1/1	0.81	0.21	-	52,52,52,52	0
34	CL	Z	8520	1/1	0.90	0.18	-	35,35,35,35	0
32	MG	A	8103	1/1	0.90	0.29	-	55,55,55,55	0
32	MG	A	8021	1/1	0.98	0.07	-	27,27,27,27	0
32	MG	A	8075	1/1	0.93	0.08	-	57,57,57,57	0
32	MG	A	8111	1/1	0.98	0.07	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8028	1/1	0.98	0.07	-	44,44,44,44	0
33	NA	A	8301	1/1	0.89	0.20	-	43,43,43,43	0
32	MG	A	8097	1/1	0.98	0.22	-	44,44,44,44	0
33	NA	A	8369	1/1	0.72	0.38	-	52,52,52,52	0
32	MG	A	8042	1/1	0.96	0.09	-	44,44,44,44	0
32	MG	A	8106	1/1	0.96	0.08	-	47,47,47,47	0
33	NA	A	8363	1/1	0.84	0.41	-	66,66,66,66	0
32	MG	A	8045	1/1	0.92	0.08	-	54,54,54,54	0
32	MG	A	8102	1/1	0.89	1.19	-	87,87,87,87	0
32	MG	A	8085	1/1	0.91	0.14	-	72,72,72,72	0
32	MG	A	8016	1/1	0.96	0.09	-	41,41,41,41	0
35	K	A	8601	1/1	0.93	0.16	-	73,73,73,73	0
33	NA	T	8312	1/1	0.39	0.82	-	124,124,124,124	0
33	NA	A	8340	1/1	0.93	0.31	-	31,31,31,31	0
32	MG	A	8083	1/1	0.97	0.05	-	47,47,47,47	0
34	CL	K	8502	1/1	0.88	0.08	-	52,52,52,52	0
33	NA	A	8349	1/1	0.99	0.14	-	53,53,53,53	0
32	MG	A	8092	1/1	0.91	0.20	-	91,91,91,91	0
32	MG	A	8041	1/1	0.92	0.07	-	46,46,46,46	0
32	MG	A	8024	1/1	0.45	0.69	-	116,116,116,116	0
33	NA	A	8359	1/1	0.93	0.44	-	61,61,61,61	0
32	MG	A	8118	1/1	0.87	0.33	-	62,62,62,62	0
32	MG	A	8088	1/1	0.90	0.15	-	45,45,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.