



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 09:22 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

<https://www.wwpdb.org/validation/2017/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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

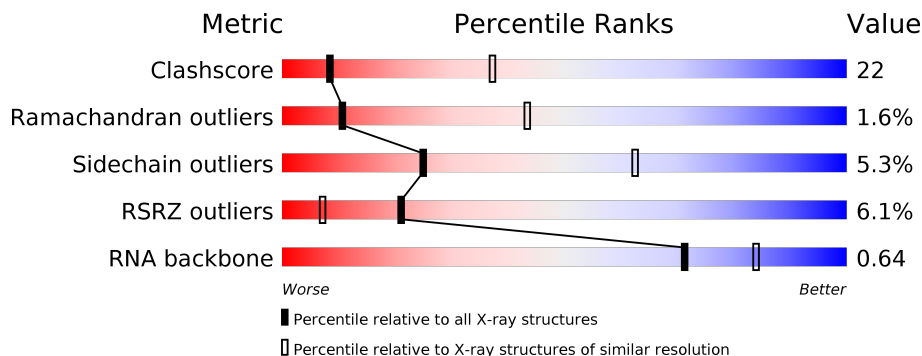
# 1 Overall quality at a glance

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	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)
RNA backbone	2636	1017 (3.30-2.70)

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>46%</div> <div>39%</div> <div>8%</div> <div>6%</div> </div> </div>
2	B	122	<div> <div>5%</div> <div> <div>46%</div> <div>37%</div> <div>12%</div> <div>5%</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>28%</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
32	MG	A	8024	-	-	-	X
32	MG	A	8049	-	-	-	X
32	MG	A	8054	-	-	X	-
33	NA	A	8329	-	-	-	X
33	NA	A	8365	-	-	-	X
33	NA	A	8373	-	-	-	X
33	NA	A	8384	-	-	-	X
33	NA	B	8383	-	-	-	X
33	NA	T	8312	-	-	-	X
34	CL	4	8504	-	-	-	X
34	CL	M	8510	-	-	-	X
34	CL	O	8507	-	-	X	-
36	CD	4	8404	-	-	-	X
36	CD	P	8405	-	-	-	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			

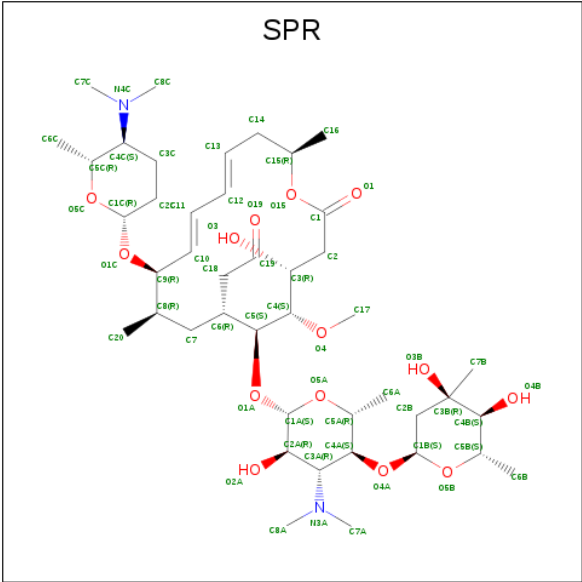
There is a discrepancy between the modelled and reference sequences:

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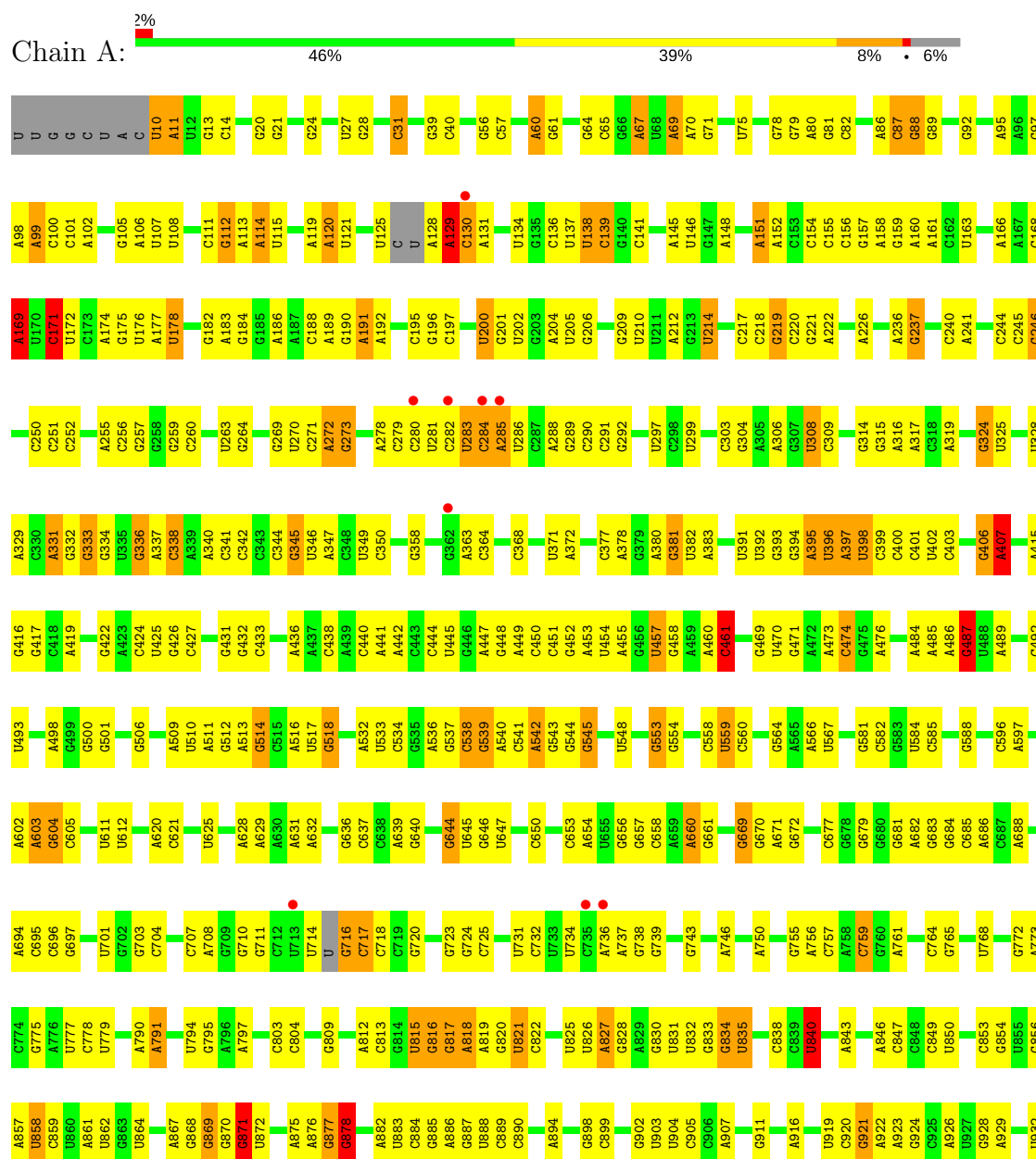
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	55	Total 55	O 55	0	0
37	3	42	Total 42	O 42	0	0
37	4	73	Total 73	O 73	0	0

### 3 Residue-property plots

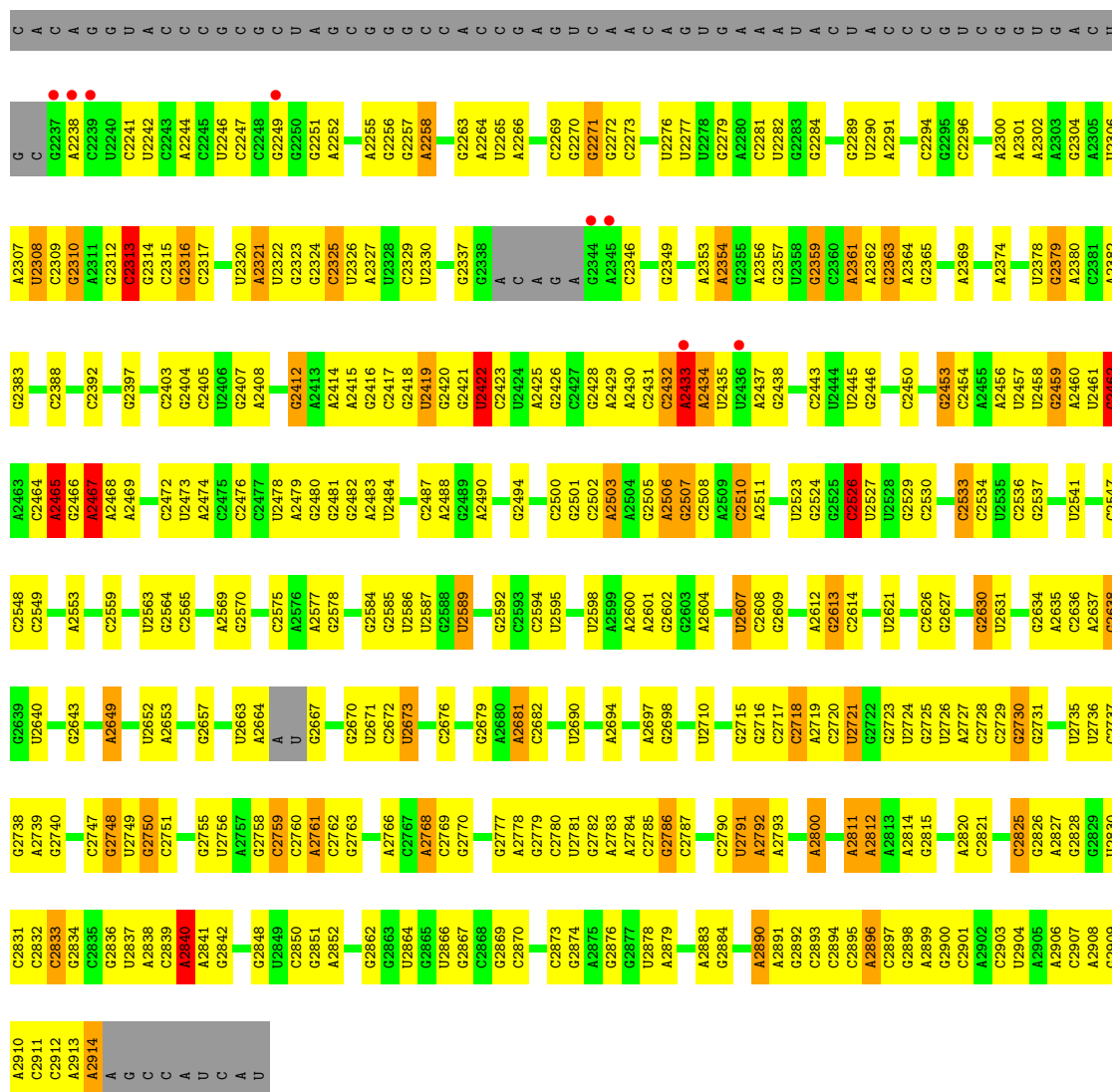
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

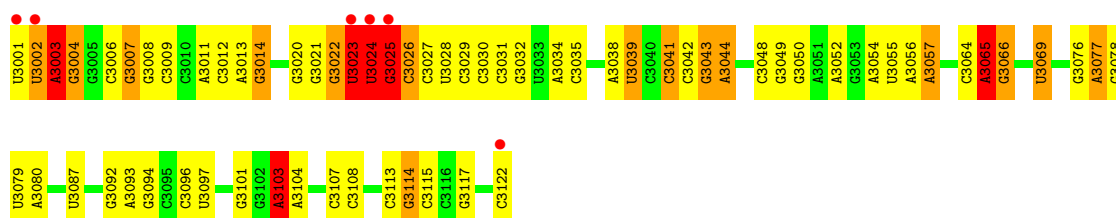


U2109	C2036	G	C1798	C1705	A1624	A1528	U1447	U1362	A1261	U1180	A1097	U1013	G940
G2110	C2037	G	C1878	G1706	U1625	G1529	C1450	G1363	C1262	A1181	A1098	A1013	G941
G2111	A2038	A	U1879	G1707	A1626	A1533	C1451	U1368	C1263	C1182	G1099	A1014	U942
C2112	A2039	C	G1805		G1627	U1534	U1450	A1369	U1264	C1183		C1015	
C2114	G2044	C	A1881	A1710	G1629	G1535	G1456	G1370	U1265	C1184		U1016	
U2115	G2045	C	G1806	A1711	A1630	C1536	G1457	U1371	U1266	U1185		C1019	C946
U2116	G2046	U	G1809	C1720	C1633	G1543	A1458	U1372	C1267	C1186	U1109	A1020	U947
U2117	C2047	C	C1810		U1634	U1544	A1459	A1375	C1268	U1187	G1110	A1021	G948
A2118	G2050	U	A1815	U1721	G1634	U1545	C1462	G1376	U1270	A1188	U1114	A1022	G949
C2119	G2051	C	G1816	C1722	U1635	G1546	U1463	U1377	U1271	U1115	U1115	A1023	G950
U2120	G2052	C	U1817	U1723	G1636	G1546	U1464		A1278	G1190	U1116	G1024	A951
G2121	G2053	G	C1818	C1724	A1637	G1552	U1464	U1380	U1279	A1191	U1117	C1025	G952
A2054	A2055	G	C1819	C1725	U1637	G1553			U1288	A1192	U1118	C1026	U954
A2055		U	A1820		A1641	U1554	G1468		U1289	G1119		G1027	A955
	U2059	U	G1821	G1730	A1642	G1555	C1469	U1383	G1290	U1197	U1120	U1028	G958
			U1822	C1731	U1647	U1556	A1470	C1384	U1291	U1198	A1123	U1029	C959
U2063	U2063	U	G1823	A1732	G1647	U1559	C1472	U1389	U1293	A1200		G1039	G960
U2064	U2064	U	C1824	C1733		U	U1473	G1390	U1298	C1201	C1126	A1040	A961
G2068	G2068	C	U1825	C1734	A1653	U1561	U1474	U1391	U1299	U1205	C1127	U1041	C962
U2069	U2069	C	G1826	G1735	U1654	C1562	U1475	G1392	G1300	U1206	U1128	U1042	C963
G2070	G2070	C	G1827	A1736	G1655	G1563		A1393	G1301	U1207	U1130	C1043	
C2071	C2071	U	U1828	C1737	A1656	G1563	C1477	G1311	C1302	C1208	G1131	C1044	U970
G2072	G2072	U	A1829	C1738	A1657	C1564	U1478	G1312	G1302	C1209	U1132	G1045	
G2073	G2073	U	U1833	U1741	A1658	U1573	C1483	A1414	G1303	C1209	A1132		
A2135	A2135	C	C1834	A1742	A1659	U1573	G1484	G1415	A1308	U1210	A1133	C1051	
G2136	G2136	U	U1835	G1743	G1660	A1580	A1485	G1416	G1134	U1052	U1134	G1052	
A	A	C	A1839	G1744	C1666	G1586	A1486	G1417	G1135	G1053	U1135	G1053	
C	C	C	U1840	G1745	U1667	G1587	A1487	U1418	U1136	G1055	U1136	G1055	
G	G	U	C1841	U1746	U1668	U1588	U1488	A1406	G1137	U1056	G1137	U1056	
C	C	U	U1842	C1747	U1669	G1589	G1489	A1407	G1138	A1057	U1138	U1057	
G	G	U	A1845	U1748	G1670	G1590	U1490	U1408	U1139	U1058	C1140	U1058	
G2080	G2080	C	U1846		U1677	G1592			U1217	U1218	C1140	U1059	
A2081	A2081	G	U1847	G1751	A1677	G1593	A1493	A1414	G1316	U1219		C1060	
A2082	A2082	U	A1848	G1752	A1678	C1594	A1494	G1415	G1325	U1220	G1151		
C2083	C2083	U	G1849	C1753	C1679	C1594	C1495	G1416	A1328	U1221		U1064	
A2084	A2084	U	U1850	A1759	C1680	G1595	G1496	G1417	A1329		C1156	G1065	
A2085	A2085	U	U1851	U1760	G1681	U1596	G1497	U1418	A1330		G1157	G1066	
		C	G1855	U1761	A1682	A1597		U1419	C1331	C1229	G1158	A1067	
A2089	A2089	U	G1856	U1766	G1683	A1598	U1500	C1420	A1332	A1232	G1159	C1068	
G2090	G2090	C	C1857	C1767	A1684	G1603	A1501	C1421	C1331	U1234	G1160	C1069	
G2091	G2091	A	U1857	A1767	A1685	G1604	U1502	C1422	C1332	A1161	G1161		
U2092	U2092	U	A1858	C1768	C1686	G1605	U1503	C1423	C1333	G1235	G1162		
G2093	G2093	U	U1859	U1769	G1687	G1606	U1504	C1424	C1334	U1236	G1163		
A2094	A2094	C	A1860	U1770	G1688	A1607	U1505		C1335	U1237	G1164		
G2095	G2095	U	U1861	U1771	A1689	A1607	U1506		G1339	C1238	G1165		
A2096	A2096	U	C1862	C1772	C1690	G1608	U1507		G1340	G1239	A1166		
G2097	G2097	C	G1863	G1773	A1691	G1609	C1507		A1341		G1167		
C2098	C2098	A	U1864	G1774	C1692	G1610	U1513		C1342	A1242	G1168		
G2099	G2099	G	A1865	C1775	A1693	G1611	A1514		U1347	C1243	U1169		
A2100	A2100	U	G1866	U1776	G1694	G1612	A1515		A1348	U1244	U1170		
A2101	A2101	C	U1867	A1778	U1696	G1613	A1516			C1245	A1171		
G2102	G2102	G	G1868	U1779	U1696	G1614	U1517		G1351	A1246	G1172		
A2103	A2103	C	U1871	C1787	C1699	A1615	U1523		G1441		A1173		
C2104	C2104	A	U1872	U1788	C1700	G1616	U1524		U1249	U1249	A1174		
C2105	C2105	C	C1872	G1789	U1702	C1617	U1525		C1352	C1250	G1175		
C2106	C2106	U	U1874	U1791	U1702	G1621	A1526		C1360	U1251	A1176		
A2108	A2108	A					A1527		C1361	G1260	A1177		

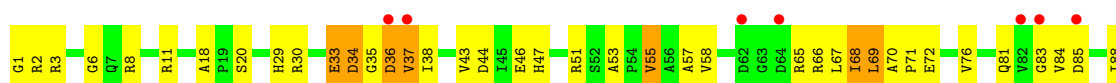


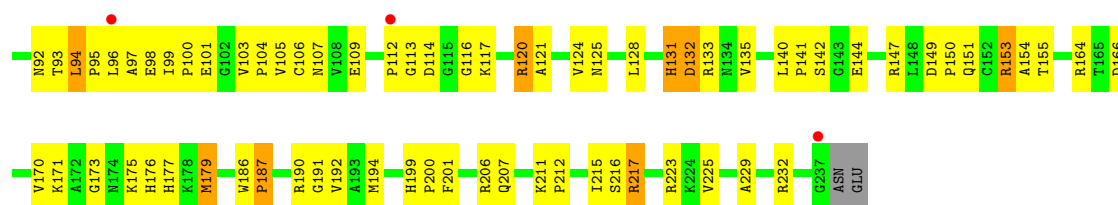


### • Molecule 2: 5S RRNA

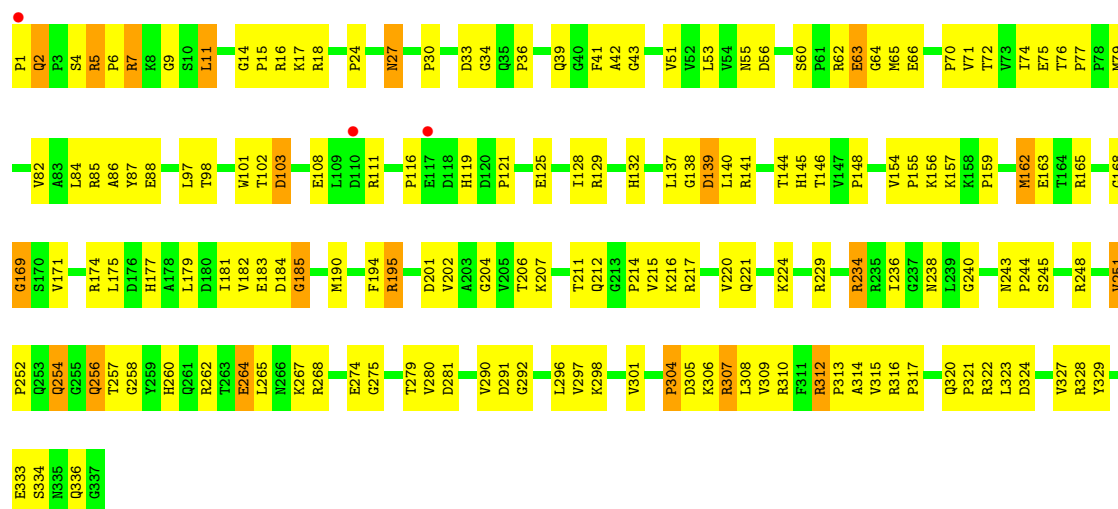


### • Molecule 3: RIBOSOMAL PROTEIN L2

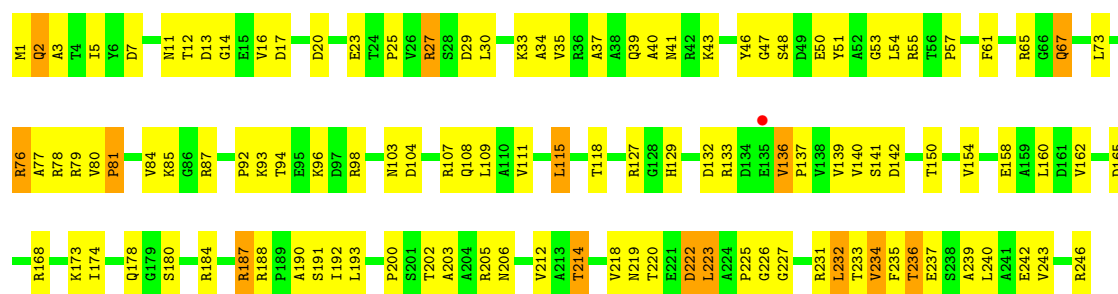




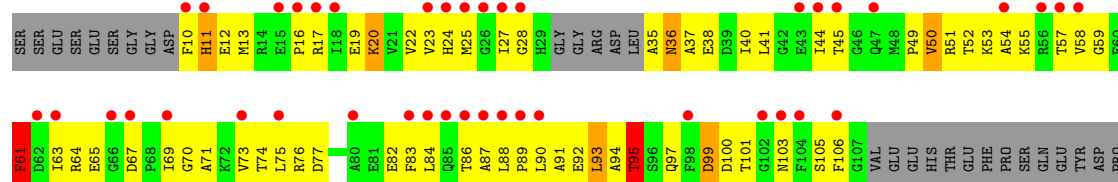
• Molecule 4: RIBOSOMAL PROTEIN L3



• Molecule 5: RIBOSOMAL PROTEIN L4

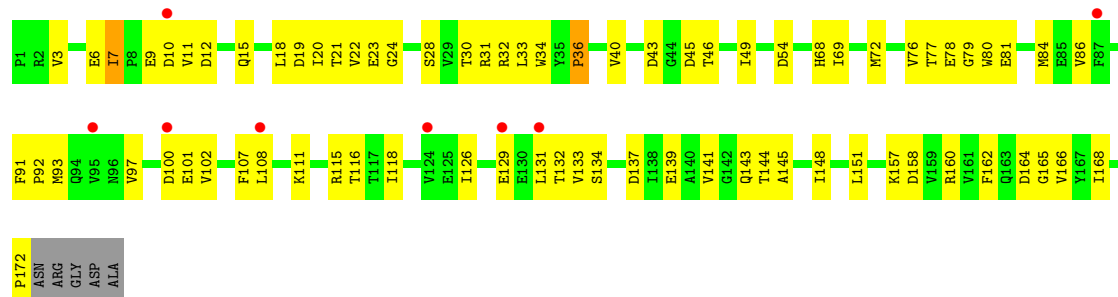


• Molecule 6: RIBOSOMAL PROTEIN L5

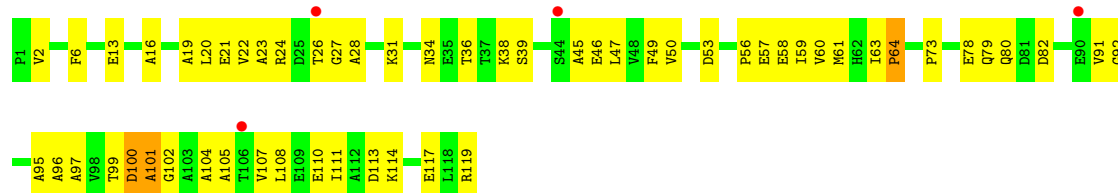


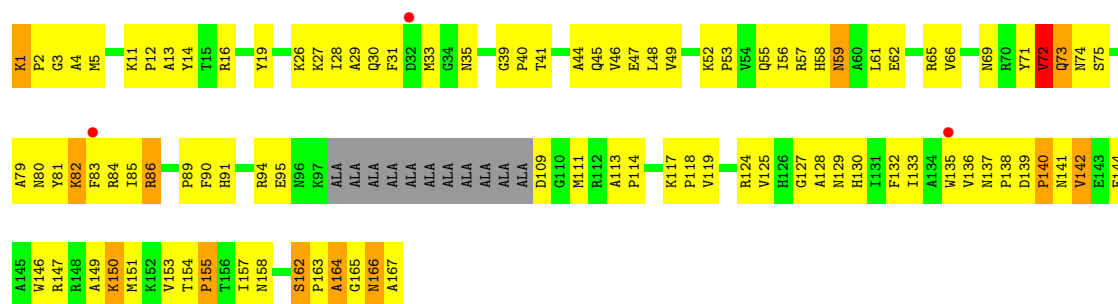


• Molecule 7: RIBOSOMAL PROTEIN L6

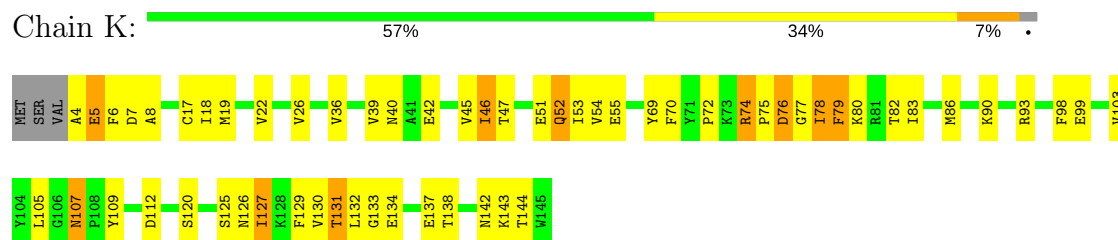


• Molecule 8: RIBOSOMAL PROTEIN L7AE

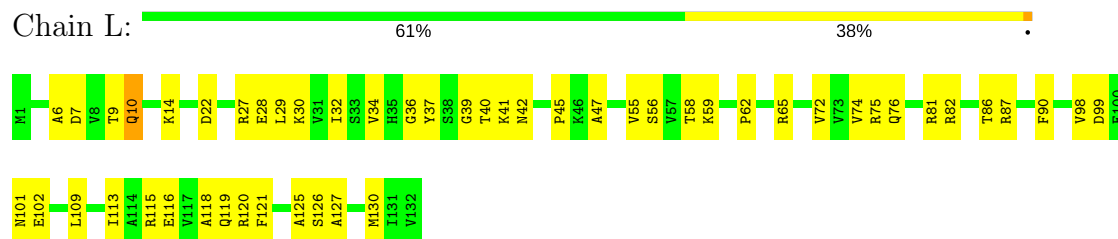




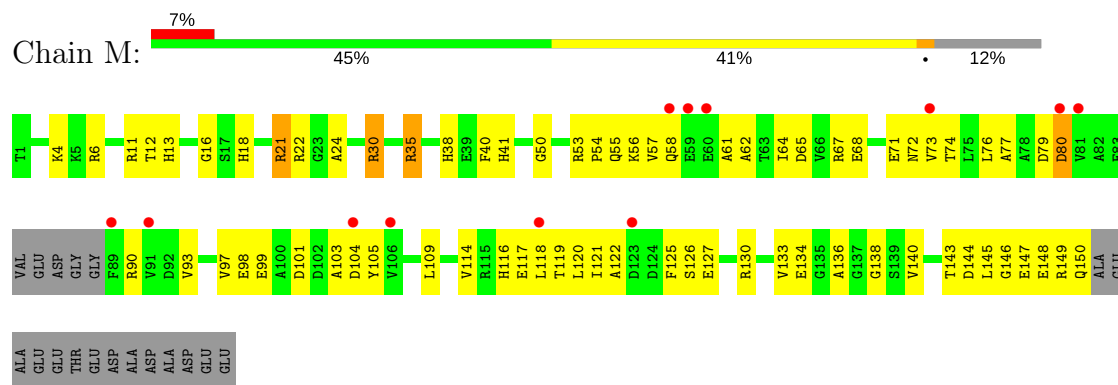
• Molecule 11: RIBOSOMAL PROTEIN L13



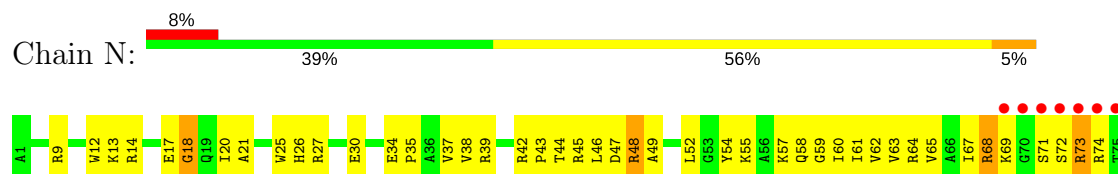
• Molecule 12: RIBOSOMAL PROTEIN L14



• Molecule 13: RIBOSOMAL PROTEIN L15

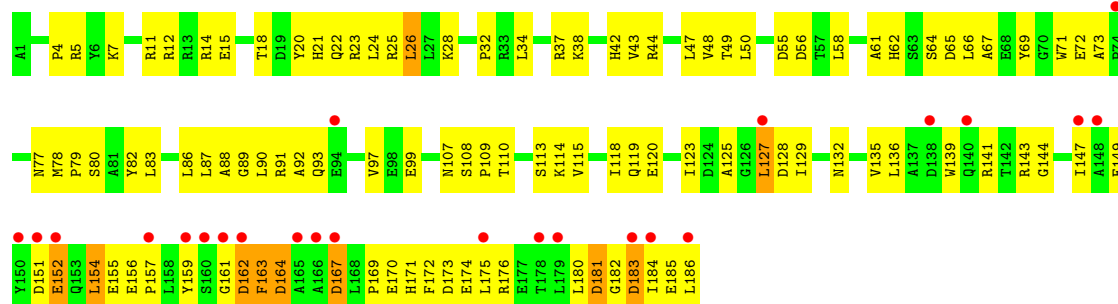


• Molecule 14: RIBOSOMAL PROTEIN L15E

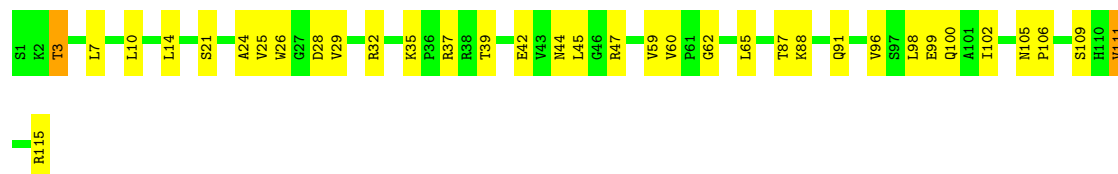




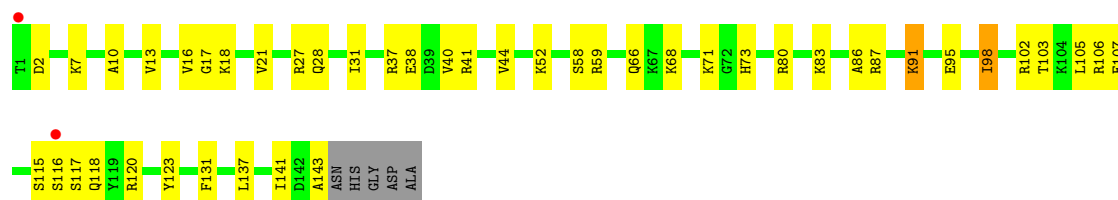
• Molecule 15: RIBOSOMAL PROTEIN L18



• Molecule 16: RIBOSOMAL PROTEIN L18E



• Molecule 17: RIBOSOMAL PROTEIN L19E

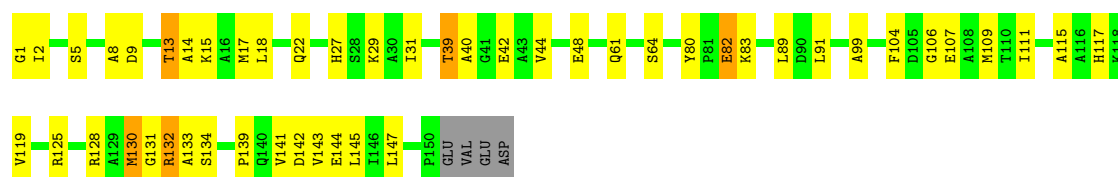


• Molecule 18: RIBOSOMAL PROTEIN L21E

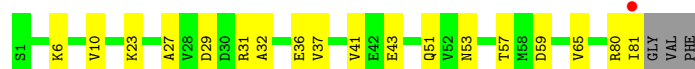
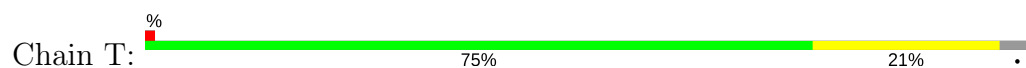


• Molecule 19: RIBOSOMAL PROTEIN L22

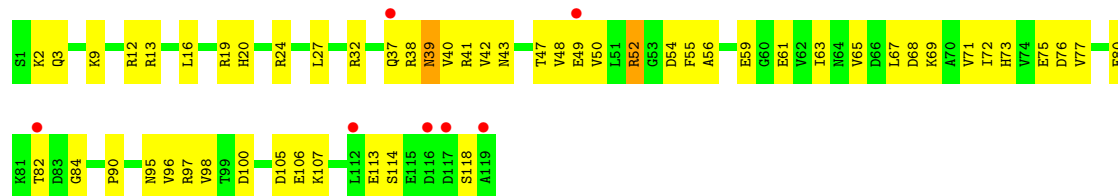




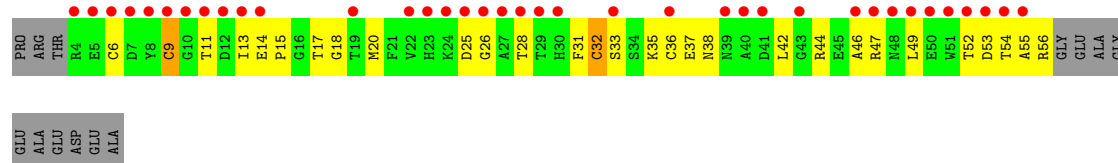
• Molecule 20: RIBOSOMAL PROTEIN L23



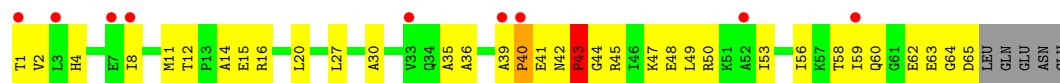
• Molecule 21: RIBOSOMAL PROTEIN L24



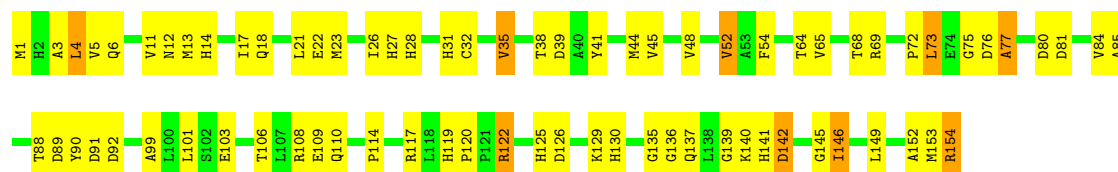
• Molecule 22: RIBOSOMAL PROTEIN L24E



• Molecule 23: RIBOSOMAL PROTEIN L29

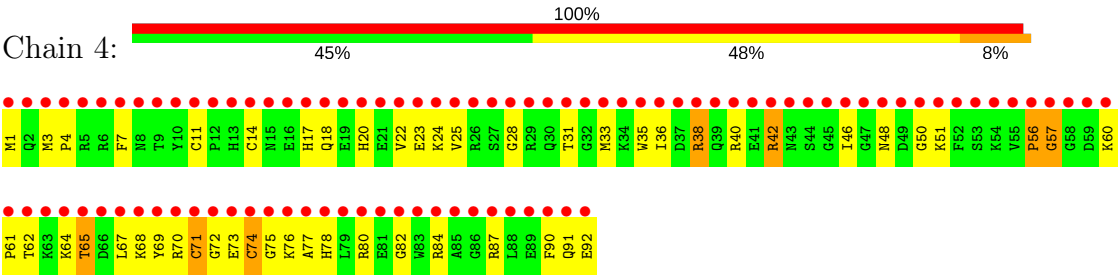


• Molecule 24: RIBOSOMAL PROTEIN L30



• Molecule 25: RIBOSOMAL PROTEIN L31E







## 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	Depositor
R, $R_{free}$	0.220 , 0.269 0.219 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
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%)	10	42
4	D	335/337 (99%)	307 (92%)	21 (6%)	7 (2%)	8	36
5	E	244/246 (99%)	225 (92%)	18 (7%)	1 (0%)	36	76
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%)	10	42
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	129 (85%)	17 (11%)	6 (4%)	3	19
11	K	140/145 (97%)	131 (94%)	5 (4%)	4 (3%)	5	26
12	L	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	11	45
13	M	141/164 (86%)	118 (84%)	20 (14%)	3 (2%)	8	36
14	N	192/194 (99%)	172 (90%)	18 (9%)	2 (1%)	17	56
15	O	184/186 (99%)	165 (90%)	13 (7%)	6 (3%)	4	23
16	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
17	Q	141/148 (95%)	138 (98%)	2 (1%)	1 (1%)	24	64
18	R	93/95 (98%)	87 (94%)	5 (5%)	1 (1%)	16	53
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%)	4	24
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	24	64
25	Y	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	6	31
26	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
27	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	12	47

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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%)	7	34
All	All	3633/4235 (86%)	3299 (91%)	275 (8%)	59 (2%)	11	43

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%)	15	48
4	D	282/282 (100%)	264 (94%)	18 (6%)	19	55
5	E	193/193 (100%)	178 (92%)	15 (8%)	14	45
6	F	117/147 (80%)	106 (91%)	11 (9%)	9	35
7	G	152/155 (98%)	147 (97%)	5 (3%)	41	77
8	H	92/92 (100%)	91 (99%)	1 (1%)	76	92
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	10	38
11	K	118/121 (98%)	107 (91%)	11 (9%)	10	36
12	L	106/106 (100%)	103 (97%)	3 (3%)	47	80
13	M	112/126 (89%)	108 (96%)	4 (4%)	38	75
14	N	166/166 (100%)	157 (95%)	9 (5%)	24	62
15	O	149/149 (100%)	144 (97%)	5 (3%)	40	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	90 (97%)	3 (3%)	42	78
17	Q	113/116 (97%)	110 (97%)	3 (3%)	48	81
18	R	79/79 (100%)	75 (95%)	4 (5%)	26	64
19	S	117/121 (97%)	112 (96%)	5 (4%)	32	70
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	103 (98%)	2 (2%)	60	87
22	V	44/52 (85%)	42 (96%)	2 (4%)	30	69
23	W	51/56 (91%)	50 (98%)	1 (2%)	58	86
24	X	130/130 (100%)	122 (94%)	8 (6%)	20	56
25	Y	66/73 (90%)	61 (92%)	5 (8%)	14	46
26	Z	120/195 (62%)	112 (93%)	8 (7%)	18	52
27	1	56/56 (100%)	50 (89%)	6 (11%)	7	28
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	52	83
30	4	79/79 (100%)	73 (92%)	6 (8%)	14	46
All	All	3027/3441 (88%)	2867 (95%)	160 (5%)	25	62

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	2747/2922 (94%)	248 (9%)	40 (1%)
2	B	121/122 (99%)	15 (12%)	5 (4%)
All	All	2868/3044 (94%)	263 (9%)	45 (1%)

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

5 of 45 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1377	C
1	A	1692	C
2	B	3023	U
1	A	1506	U
1	A	1856	C

## 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	3.01	28 (45%)	76,89,89	3.14	32 (42%)

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	-5.47	1.42	1.52
31	A	9001	SPR	O5A-C5A	-4.89	1.33	1.44
31	A	9001	SPR	O15-C1	-4.49	1.21	1.34
31	A	9001	SPR	O4A-C1B	-4.07	1.31	1.41
31	A	9001	SPR	O1C-C1C	-3.86	1.31	1.41

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9001	SPR	C8A-N3A-C7A	-9.28	82.41	110.40
31	A	9001	SPR	C5A-C4A-C3A	-7.54	93.97	110.51
31	A	9001	SPR	O19-C19-C18	-7.32	102.19	125.51
31	A	9001	SPR	O1C-C1C-O5C	-6.01	90.45	109.93
31	A	9001	SPR	C15-C14-C13	-5.92	102.86	113.93

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 [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, 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	47 (1%) 70 41	23, 51, 96, 143	0
2	B	122/122 (100%)	0.25	6 (4%) 29 11	37, 70, 100, 150	0
3	C	237/239 (99%)	0.12	10 (4%) 36 14	32, 63, 96, 110	0
4	D	337/337 (100%)	-0.13	3 (0%) 84 62	28, 57, 84, 95	0
5	E	246/246 (100%)	-0.18	1 (0%) 92 78	24, 50, 74, 85	0
6	F	140/176 (79%)	1.55	50 (35%) 0 0	60, 103, 122, 127	0
7	G	172/177 (97%)	0.48	8 (4%) 31 12	43, 68, 92, 98	0
8	H	119/119 (100%)	0.43	4 (3%) 45 19	59, 79, 102, 107	0
9	I	29/348 (8%)	1.89	12 (41%) 0 0	76, 94, 102, 104	0
10	J	156/167 (93%)	0.20	3 (1%) 66 37	35, 58, 85, 93	0
11	K	142/145 (97%)	-0.12	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%)	0.52	12 (8%) 11 3	31, 74, 108, 117	0
14	N	194/194 (100%)	0.22	16 (8%) 11 3	37, 55, 91, 98	0
15	O	186/186 (100%)	0.71	24 (12%) 3 1	48, 74, 112, 122	0
16	P	115/115 (100%)	-0.04	0 100 100	39, 59, 75, 79	0
17	Q	143/148 (96%)	0.17	2 (1%) 75 49	38, 60, 76, 84	0
18	R	95/95 (100%)	-0.11	1 (1%) 80 55	38, 51, 64, 79	0
19	S	150/154 (97%)	-0.17	0 100 100	32, 45, 66, 75	0
20	T	81/84 (96%)	0.05	1 (1%) 79 53	47, 65, 84, 89	0
21	U	119/119 (100%)	0.41	7 (5%) 22 8	44, 62, 86, 97	0
22	V	53/66 (80%)	3.20	37 (69%) 0 0	85, 94, 102, 110	0
23	W	65/70 (92%)	1.12	9 (13%) 3 1	55, 81, 112, 118	0
24	X	154/154 (100%)	-0.18	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%)	0.28	4 (4%) 29 11	42, 58, 84, 99	0
26	Z	142/240 (59%)	-0.09	5 (3%) 44 18	25, 46, 70, 85	0
27	1	73/73 (100%)	3.54	47 (64%) 0 0	79, 98, 103, 104	0
28	2	56/56 (100%)	-0.41	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%)	6.54	92 (100%) 0 0	91, 103, 108, 111	0
All	All	6577/7279 (90%)	0.24	402 (6%) 21 7	23, 57, 102, 150	0

The worst 5 of 402 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
30	4	37	ASP	15.8
30	4	65	THR	13.4
30	4	82	GLY	13.1
30	4	84	ARG	12.4
30	4	83	TRP	12.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	T	8312	1/1	0.38	0.82	124,124,124,124	0
33	NA	A	8384	1/1	0.40	2.02	114,114,114,114	0
33	NA	A	8329	1/1	0.40	0.52	70,70,70,70	0
32	MG	A	8024	1/1	0.45	0.69	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8049	1/1	0.50	0.60	89,89,89,89	0
34	CL	M	8510	1/1	0.52	0.46	87,87,87,87	0
33	NA	A	8382	1/1	0.54	0.38	62,62,62,62	0
33	NA	A	8341	1/1	0.56	0.19	43,43,43,43	0
36	CD	4	8404	1/1	0.58	0.79	156,156,156,156	0
34	CL	4	8504	1/1	0.67	0.71	95,95,95,95	0
33	NA	A	8371	1/1	0.69	0.33	54,54,54,54	0
33	NA	S	8337	1/1	0.70	0.33	49,49,49,49	0
33	NA	B	8383	1/1	0.71	0.62	63,63,63,63	0
33	NA	A	8331	1/1	0.72	0.35	61,61,61,61	0
32	MG	A	8090	1/1	0.73	0.29	36,36,36,36	0
33	NA	A	8369	1/1	0.73	0.38	52,52,52,52	0
36	CD	P	8405	1/1	0.73	0.45	169,169,169,169	0
33	NA	A	8365	1/1	0.74	0.41	49,49,49,49	0
33	NA	A	8373	1/1	0.74	0.52	59,59,59,59	0
32	MG	A	8076	1/1	0.76	0.16	71,71,71,71	0
33	NA	B	8351	1/1	0.78	0.23	69,69,69,69	0
36	CD	V	8401	1/1	0.78	0.48	142,142,142,142	0
32	MG	A	8001	1/1	0.79	0.12	39,39,39,39	0
33	NA	A	8364	1/1	0.80	0.32	40,40,40,40	0
33	NA	A	8324	1/1	0.80	0.15	51,51,51,51	0
32	MG	A	8082	1/1	0.81	0.21	52,52,52,52	0
34	CL	R	8511	1/1	0.81	0.45	63,63,63,63	0
32	MG	A	8104	1/1	0.81	0.23	40,40,40,40	0
33	NA	A	8332	1/1	0.81	0.22	58,58,58,58	0
33	NA	A	8362	1/1	0.82	0.38	69,69,69,69	0
34	CL	N	8518	1/1	0.82	0.22	56,56,56,56	0
32	MG	B	8095	1/1	0.82	0.07	67,67,67,67	0
34	CL	A	8503	1/1	0.83	0.33	50,50,50,50	0
33	NA	A	8372	1/1	0.83	0.66	55,55,55,55	0
33	NA	S	8386	1/1	0.83	0.27	53,53,53,53	0
33	NA	A	8356	1/1	0.83	0.68	58,58,58,58	0
35	K	A	8602	1/1	0.83	0.28	68,68,68,68	0
31	SPR	A	9001	59/59	0.83	0.36	78,88,95,95	0
33	NA	A	8363	1/1	0.84	0.41	66,66,66,66	0
32	MG	A	8117	1/1	0.84	0.12	31,31,31,31	0
33	NA	A	8360	1/1	0.85	0.86	55,55,55,55	0
36	CD	1	8403	1/1	0.85	0.27	138,138,138,138	0
35	K	A	8603	1/1	0.85	0.36	88,88,88,88	0
33	NA	A	8377	1/1	0.85	0.25	60,60,60,60	0
33	NA	A	8355	1/1	0.85	0.36	55,55,55,55	0
33	NA	A	8352	1/1	0.86	0.43	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	1	8105	1/1	0.86	0.28	44,44,44,44	0
33	NA	A	8370	1/1	0.86	0.34	49,49,49,49	0
32	MG	Z	8109	1/1	0.86	0.22	53,53,53,53	0
32	MG	A	8118	1/1	0.86	0.34	62,62,62,62	0
34	CL	A	8517	1/1	0.87	0.31	55,55,55,55	0
32	MG	A	8093	1/1	0.87	0.23	56,56,56,56	0
34	CL	A	8515	1/1	0.87	0.58	100,100,100,100	0
33	NA	E	8304	1/1	0.88	0.12	35,35,35,35	0
32	MG	A	8119	1/1	0.88	0.36	71,71,71,71	0
32	MG	A	8115	1/1	0.88	0.10	59,59,59,59	0
34	CL	O	8507	1/1	0.88	0.25	62,62,62,62	0
32	MG	A	8116	1/1	0.88	0.17	67,67,67,67	0
33	NA	A	8333	1/1	0.88	0.13	33,33,33,33	0
32	MG	A	8070	1/1	0.88	0.59	66,66,66,66	0
33	NA	A	8308	1/1	0.88	0.23	69,69,69,69	0
32	MG	A	8040	1/1	0.88	0.19	78,78,78,78	0
33	NA	A	8328	1/1	0.88	0.19	45,45,45,45	0
33	NA	A	8305	1/1	0.89	0.15	34,34,34,34	0
33	NA	A	8326	1/1	0.89	0.26	46,46,46,46	0
34	CL	K	8502	1/1	0.89	0.08	52,52,52,52	0
32	MG	A	8102	1/1	0.89	1.21	87,87,87,87	0
33	NA	A	8343	1/1	0.89	0.09	16,16,16,16	0
33	NA	A	8385	1/1	0.89	0.40	41,41,41,41	0
34	CL	A	8522	1/1	0.89	0.43	75,75,75,75	0
33	NA	A	8336	1/1	0.89	0.20	49,49,49,49	0
32	MG	A	8050	1/1	0.89	0.13	85,85,85,85	0
32	MG	A	8039	1/1	0.89	0.06	50,50,50,50	0
33	NA	A	8344	1/1	0.89	0.09	30,30,30,30	0
32	MG	A	8110	1/1	0.89	0.13	47,47,47,47	0
33	NA	A	8301	1/1	0.89	0.20	43,43,43,43	0
33	NA	A	8357	1/1	0.90	0.17	67,67,67,67	0
34	CL	Z	8520	1/1	0.90	0.18	35,35,35,35	0
32	MG	A	8103	1/1	0.90	0.30	55,55,55,55	0
32	MG	A	8088	1/1	0.90	0.15	45,45,45,45	0
32	MG	A	8023	1/1	0.90	0.07	42,42,42,42	0
33	NA	A	8313	1/1	0.90	0.22	63,63,63,63	0
32	MG	A	8062	1/1	0.90	0.11	72,72,72,72	0
33	NA	A	8374	1/1	0.90	0.60	63,63,63,63	0
32	MG	4	8078	1/1	0.90	0.25	74,74,74,74	0
33	NA	A	8366	1/1	0.90	0.26	49,49,49,49	0
32	MG	A	8113	1/1	0.90	0.10	45,45,45,45	0
34	CL	A	8516	1/1	0.90	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	A	8375	1/1	0.91	0.34	53,53,53,53	0
33	NA	A	8378	1/1	0.91	0.42	37,37,37,37	0
34	CL	A	8512	1/1	0.91	0.20	32,32,32,32	0
32	MG	A	8085	1/1	0.91	0.13	72,72,72,72	0
32	MG	A	8089	1/1	0.91	0.19	84,84,84,84	0
33	NA	A	8310	1/1	0.91	0.22	29,29,29,29	0
33	NA	A	8354	1/1	0.91	0.16	40,40,40,40	0
32	MG	A	8092	1/1	0.91	0.20	91,91,91,91	0
33	NA	A	8321	1/1	0.91	0.43	39,39,39,39	0
33	NA	A	8323	1/1	0.91	0.25	50,50,50,50	0
32	MG	A	8045	1/1	0.92	0.08	54,54,54,54	0
34	CL	D	8519	1/1	0.92	0.51	65,65,65,65	0
33	NA	R	8348	1/1	0.92	0.11	37,37,37,37	0
33	NA	A	8367	1/1	0.92	0.20	52,52,52,52	0
32	MG	A	8061	1/1	0.92	0.09	44,44,44,44	0
33	NA	A	8306	1/1	0.92	0.50	56,56,56,56	0
32	MG	A	8096	1/1	0.92	0.08	53,53,53,53	0
32	MG	A	8041	1/1	0.92	0.07	46,46,46,46	0
32	MG	A	8081	1/1	0.92	0.18	58,58,58,58	0
34	CL	A	8505	1/1	0.92	0.67	88,88,88,88	0
32	MG	A	8015	1/1	0.93	0.10	57,57,57,57	0
33	NA	A	8322	1/1	0.93	0.42	46,46,46,46	0
33	NA	A	8330	1/1	0.93	0.18	43,43,43,43	0
35	K	A	8601	1/1	0.93	0.16	73,73,73,73	0
33	NA	A	8320	1/1	0.93	0.12	33,33,33,33	0
33	NA	A	8340	1/1	0.93	0.30	31,31,31,31	0
32	MG	U	8073	1/1	0.93	0.20	42,42,42,42	0
32	MG	A	8067	1/1	0.93	0.24	50,50,50,50	0
32	MG	A	8114	1/1	0.93	0.47	92,92,92,92	0
34	CL	A	8514	1/1	0.93	0.21	61,61,61,61	0
33	NA	A	8368	1/1	0.93	0.15	47,47,47,47	0
33	NA	A	8359	1/1	0.93	0.42	61,61,61,61	0
33	NA	A	8307	1/1	0.94	0.11	39,39,39,39	0
34	CL	K	8521	1/1	0.94	0.14	46,46,46,46	0
34	CL	A	8513	1/1	0.94	0.12	56,56,56,56	0
34	CL	C	8509	1/1	0.94	0.29	86,86,86,86	0
32	MG	A	8075	1/1	0.94	0.08	57,57,57,57	0
33	NA	A	8318	1/1	0.94	0.17	34,34,34,34	0
32	MG	A	8068	1/1	0.94	0.13	58,58,58,58	0
33	NA	A	8353	1/1	0.94	0.12	38,38,38,38	0
32	MG	A	8006	1/1	0.94	0.08	48,48,48,48	0
32	MG	A	8053	1/1	0.94	0.11	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8051	1/1	0.94	0.09	56,56,56,56	0
33	NA	A	8316	1/1	0.94	0.34	51,51,51,51	0
33	NA	A	8342	1/1	0.94	0.24	47,47,47,47	0
32	MG	A	8072	1/1	0.94	0.13	80,80,80,80	0
32	MG	A	8034	1/1	0.94	0.06	39,39,39,39	0
32	MG	C	8065	1/1	0.94	0.11	57,57,57,57	0
32	MG	A	8029	1/1	0.94	0.07	51,51,51,51	0
33	NA	A	8379	1/1	0.94	0.24	41,41,41,41	0
32	MG	A	8101	1/1	0.94	0.16	55,55,55,55	0
32	MG	A	8031	1/1	0.94	0.05	31,31,31,31	0
34	CL	K	8501	1/1	0.94	0.13	56,56,56,56	0
33	NA	A	8327	1/1	0.95	0.13	32,32,32,32	0
32	MG	A	8033	1/1	0.95	0.07	30,30,30,30	0
32	MG	A	8046	1/1	0.95	0.08	79,79,79,79	0
32	MG	A	8066	1/1	0.95	0.13	83,83,83,83	0
32	MG	A	8027	1/1	0.95	0.05	63,63,63,63	0
32	MG	A	8074	1/1	0.95	0.08	31,31,31,31	0
32	MG	A	8059	1/1	0.95	0.08	31,31,31,31	0
32	MG	A	8043	1/1	0.95	0.08	39,39,39,39	0
33	NA	A	8381	1/1	0.95	0.20	51,51,51,51	0
32	MG	A	8064	1/1	0.95	0.16	24,24,24,24	0
32	MG	A	8079	1/1	0.95	0.15	39,39,39,39	0
32	MG	A	8047	1/1	0.95	0.18	62,62,62,62	0
33	NA	J	8309	1/1	0.95	0.14	21,21,21,21	0
33	NA	A	8317	1/1	0.95	0.12	27,27,27,27	0
32	MG	A	8057	1/1	0.95	0.11	49,49,49,49	0
32	MG	L	8069	1/1	0.95	0.06	50,50,50,50	0
32	MG	A	8018	1/1	0.95	0.11	61,61,61,61	0
34	CL	P	8508	1/1	0.95	0.18	93,93,93,93	0
32	MG	A	8055	1/1	0.96	0.08	71,71,71,71	0
32	MG	A	8099	1/1	0.96	0.08	38,38,38,38	0
32	MG	A	8106	1/1	0.96	0.08	47,47,47,47	0
33	NA	A	8350	1/1	0.96	0.15	34,34,34,34	0
33	NA	A	8311	1/1	0.96	0.09	42,42,42,42	0
33	NA	A	8319	1/1	0.96	0.11	52,52,52,52	0
32	MG	A	8016	1/1	0.96	0.09	41,41,41,41	0
33	NA	A	8303	1/1	0.96	0.20	51,51,51,51	0
34	CL	S	8506	1/1	0.96	0.18	46,46,46,46	0
32	MG	A	8022	1/1	0.96	0.09	41,41,41,41	0
32	MG	A	8087	1/1	0.96	0.06	48,48,48,48	0
33	NA	A	8376	1/1	0.96	0.28	78,78,78,78	0
32	MG	A	8071	1/1	0.96	0.14	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8042	1/1	0.96	0.09	44,44,44,44	0
33	NA	K	8346	1/1	0.96	0.08	27,27,27,27	0
32	MG	A	8014	1/1	0.96	0.06	30,30,30,30	0
32	MG	A	8091	1/1	0.96	0.07	48,48,48,48	0
32	MG	A	8060	1/1	0.96	0.12	45,45,45,45	0
32	MG	A	8084	1/1	0.97	0.08	48,48,48,48	0
32	MG	A	8108	1/1	0.97	0.09	88,88,88,88	0
32	MG	A	8004	1/1	0.97	0.07	48,48,48,48	0
32	MG	A	8010	1/1	0.97	0.05	40,40,40,40	0
32	MG	A	8100	1/1	0.97	0.12	69,69,69,69	0
33	NA	A	8334	1/1	0.97	0.06	36,36,36,36	0
33	NA	A	8314	1/1	0.97	0.18	33,33,33,33	0
32	MG	A	8063	1/1	0.97	0.06	78,78,78,78	0
32	MG	A	8003	1/1	0.97	0.10	24,24,24,24	0
32	MG	A	8080	1/1	0.97	0.05	50,50,50,50	0
33	NA	A	8302	1/1	0.97	0.13	40,40,40,40	0
32	MG	A	8083	1/1	0.97	0.05	47,47,47,47	0
32	MG	A	8008	1/1	0.97	0.07	49,49,49,49	0
32	MG	A	8048	1/1	0.97	0.09	45,45,45,45	0
33	NA	A	8325	1/1	0.97	0.09	52,52,52,52	0
33	NA	A	8361	1/1	0.97	0.14	53,53,53,53	0
33	NA	A	8315	1/1	0.97	0.15	30,30,30,30	0
32	MG	A	8038	1/1	0.97	0.10	35,35,35,35	0
32	MG	A	8035	1/1	0.97	0.06	54,54,54,54	0
33	NA	C	8345	1/1	0.97	0.10	42,42,42,42	0
32	MG	A	8086	1/1	0.98	0.07	50,50,50,50	0
32	MG	A	8005	1/1	0.98	0.10	44,44,44,44	0
32	MG	A	8032	1/1	0.98	0.05	34,34,34,34	0
32	MG	A	8056	1/1	0.98	0.10	53,53,53,53	0
32	MG	A	8028	1/1	0.98	0.07	44,44,44,44	0
32	MG	A	8097	1/1	0.98	0.22	44,44,44,44	0
32	MG	A	8017	1/1	0.98	0.03	27,27,27,27	0
32	MG	A	8044	1/1	0.98	0.14	52,52,52,52	0
32	MG	A	8019	1/1	0.98	0.07	35,35,35,35	0
32	MG	A	8111	1/1	0.98	0.07	69,69,69,69	0
32	MG	A	8020	1/1	0.98	0.05	51,51,51,51	0
32	MG	A	8077	1/1	0.98	0.07	31,31,31,31	0
32	MG	A	8009	1/1	0.98	0.06	20,20,20,20	0
32	MG	A	8011	1/1	0.98	0.10	52,52,52,52	0
33	NA	M	8380	1/1	0.98	0.15	55,55,55,55	0
33	NA	A	8335	1/1	0.98	0.23	52,52,52,52	0
32	MG	A	8054	1/1	0.98	0.08	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8012	1/1	0.98	0.11	52,52,52,52	0
32	MG	A	8094	1/1	0.98	0.14	85,85,85,85	0
32	MG	A	8098	1/1	0.98	0.20	50,50,50,50	0
33	NA	A	8339	1/1	0.98	0.14	16,16,16,16	0
36	CD	2	8402	1/1	0.98	0.06	59,59,59,59	0
32	MG	A	8058	1/1	0.98	0.10	43,43,43,43	0
32	MG	A	8112	1/1	0.98	0.15	44,44,44,44	0
33	NA	A	8338	1/1	0.98	0.13	67,67,67,67	0
32	MG	A	8021	1/1	0.98	0.07	27,27,27,27	0
32	MG	A	8107	1/1	0.99	0.04	47,47,47,47	0
32	MG	A	8052	1/1	0.99	0.05	45,45,45,45	0
32	MG	A	8025	1/1	0.99	0.09	60,60,60,60	0
32	MG	A	8026	1/1	0.99	0.05	11,11,11,11	0
33	NA	N	8347	1/1	0.99	0.05	21,21,21,21	0
33	NA	A	8349	1/1	0.99	0.14	53,53,53,53	0
32	MG	A	8002	1/1	0.99	0.10	31,31,31,31	0
32	MG	A	8007	1/1	0.99	0.04	23,23,23,23	0
32	MG	A	8037	1/1	0.99	0.10	48,48,48,48	0
32	MG	A	8013	1/1	0.99	0.12	46,46,46,46	0
32	MG	A	8036	1/1	0.99	0.06	45,45,45,45	0
32	MG	A	8030	1/1	0.99	0.09	26,26,26,26	0

## 6.5 Other polymers

There are no such residues in this entry.