



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:55 PM GMT

PDB ID : 1M1K  
Title : Co-crystal structure of azithromycin 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 : 2002-06-19  
Resolution : 3.20 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

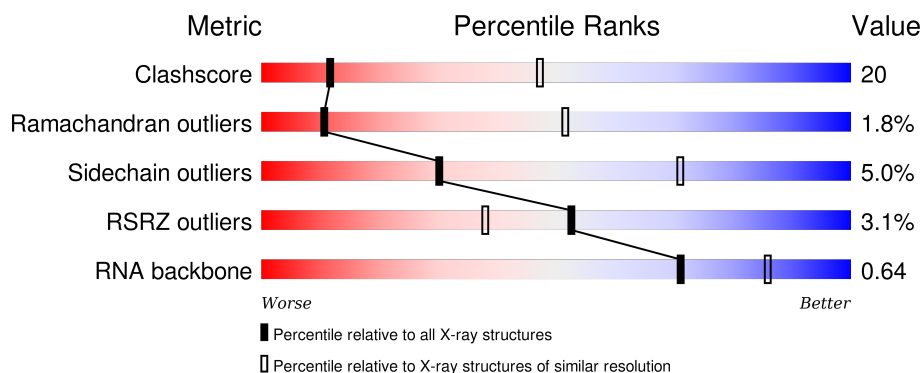
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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></div> <div>51% 36% 7% 6%</div> </div>
2	B	122	<div> <div>5%</div> <div>43% 42% 9% 6%</div> </div>
3	C	239	<div> <div>5%</div> <div>52% 42% 5%</div> </div>
4	D	337	<div> <div></div> <div>51% 43% 6%</div> </div>
5	E	246	<div> <div></div> <div>61% 34% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
6	F	176	
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	ZIT	A	8600	-	-	-	X
32	MG	A	8024	-	-	-	X
32	MG	A	8044	-	-	-	X
32	MG	A	8060	-	-	-	X
32	MG	A	8064	-	-	-	X
32	MG	A	8066	-	-	-	X
34	NA	A	8303	-	-	-	X
34	NA	A	8305	-	-	-	X
34	NA	A	8321	-	-	-	X
34	NA	A	8323	-	-	-	X
34	NA	A	8325	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8331	-	-	-	X
34	NA	A	8335	-	-	-	X
34	NA	A	8350	-	-	-	X
34	NA	A	8356	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8361	-	-	-	X
34	NA	A	8362	-	-	-	X
34	NA	A	8364	-	-	-	X
34	NA	A	8365	-	-	-	X
34	NA	A	8366	-	-	-	X
34	NA	A	8368	-	-	-	X
34	NA	A	8369	-	-	-	X
34	NA	A	8371	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8373	-	-	-	X
34	NA	A	8374	-	-	-	X
34	NA	A	8376	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8378	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	M	8380	-	-	-	X
34	NA	S	8386	-	-	-	X
35	CL	4	8504	-	-	-	X
35	CL	A	8505	-	-	-	X
35	CL	A	8513	-	-	X	-
35	CL	A	8515	-	-	-	X
35	CL	D	8519	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	K	8502	-	-	X	-
35	CL	N	8518	-	-	X	-
35	CL	O	8507	-	-	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	GB 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			

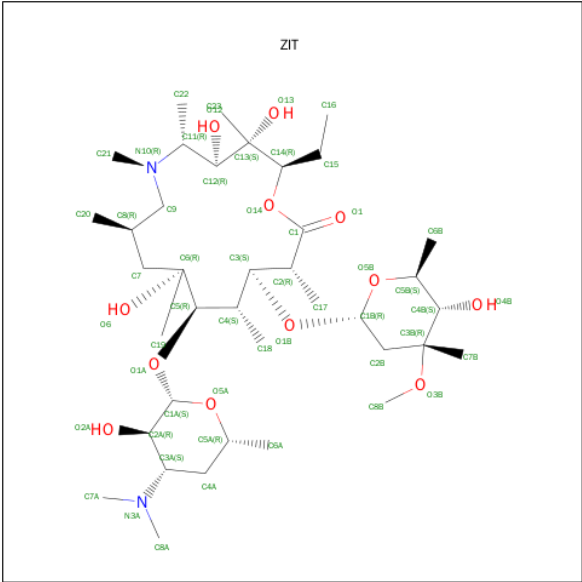
There is a discrepancy between the modelled and reference sequences:

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 AZITHROMYCIN (three-letter code: ZIT) (formula: C<sub>38</sub>H<sub>72</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			52	38	2	12		

- 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	D	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	109	Total	Mg	0	0
			109	109		
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 POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	4	Total Cl 4 4	0	0
35	C	1	Total Cl 1 1	0	0
35	A	9	Total Cl 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	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	5898	Total 5898	O 5898	0	0
37	B	140	Total 140	O 140	0	0
37	C	129	Total 129	O 129	0	0
37	D	152	Total 152	O 152	0	0
37	E	169	Total 169	O 169	0	0
37	F	52	Total 52	O 52	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	28	Total 28	O 28	0	0
37	I	21	Total 21	O 21	0	0
37	J	81	Total 81	O 81	0	0
37	K	56	Total 56	O 56	0	0
37	L	61	Total 61	O 61	0	0
37	M	81	Total 81	O 81	0	0
37	N	129	Total 129	O 129	0	0
37	O	68	Total 68	O 68	0	0
37	P	45	Total 45	O 45	0	0
37	Q	69	Total 69	O 69	0	0
37	R	56	Total 56	O 56	0	0
37	S	89	Total 89	O 89	0	0
37	T	36	Total 36	O 36	0	0
37	U	39	Total 39	O 39	0	0
37	V	27	Total 27	O 27	0	0
37	W	15	Total 15	O 15	0	0
37	X	73	Total 73	O 73	0	0
37	Y	30	Total 30	O 30	0	0
37	Z	93	Total 93	O 93	0	0
37	1	38	Total 38	O 38	0	0

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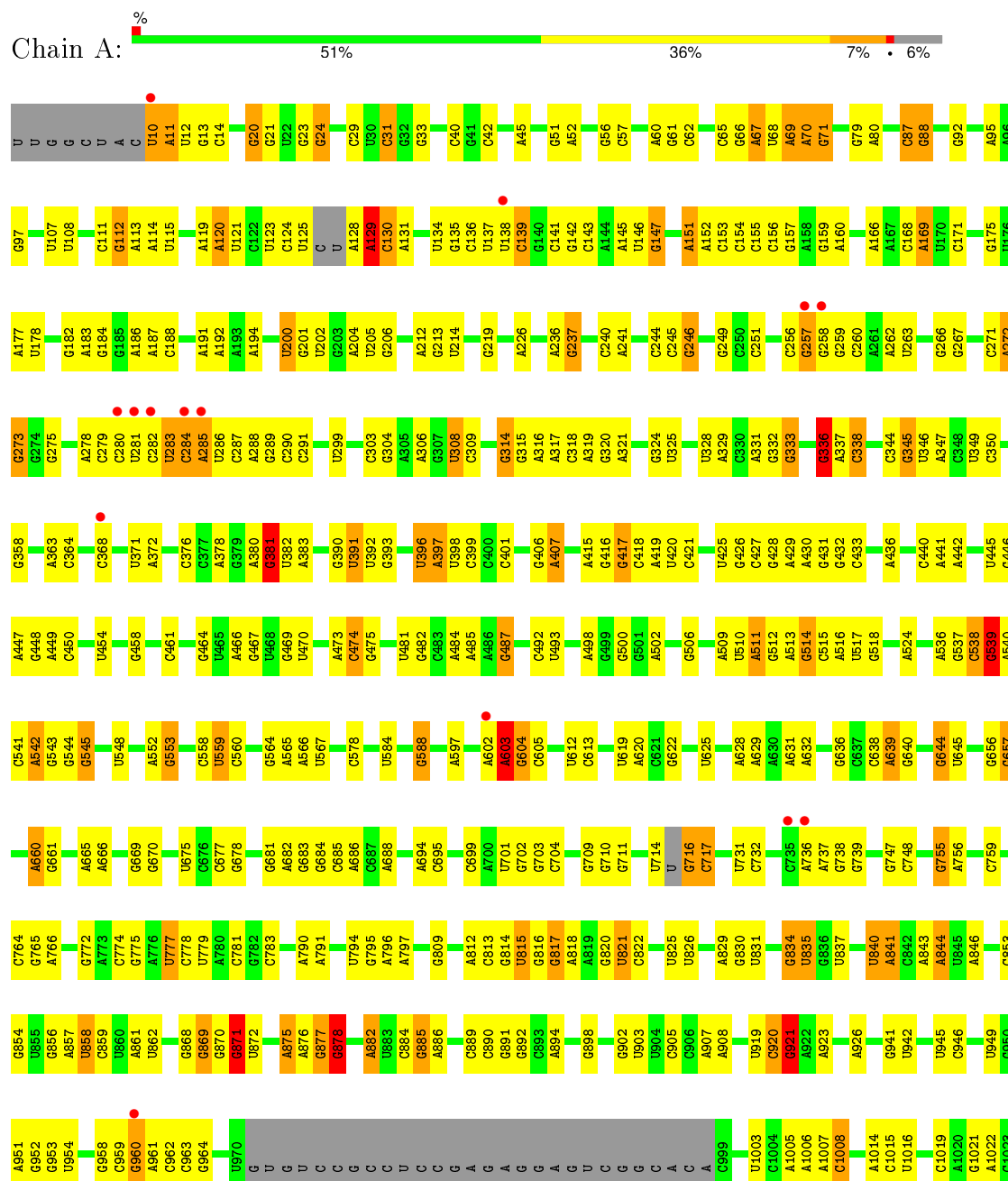
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	57	Total 57	O 57	0	0
37	3	39	Total 39	O 39	0	0
37	4	72	Total 72	O 72	0	0

### 3 Residue-property plots

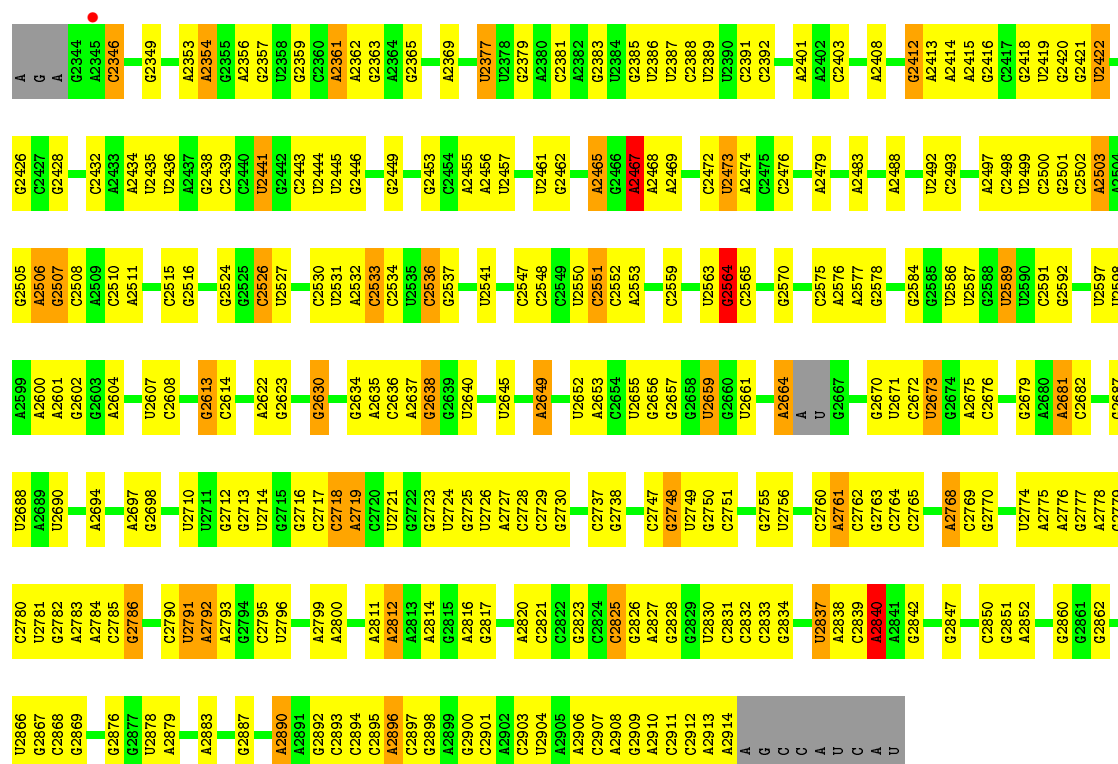
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

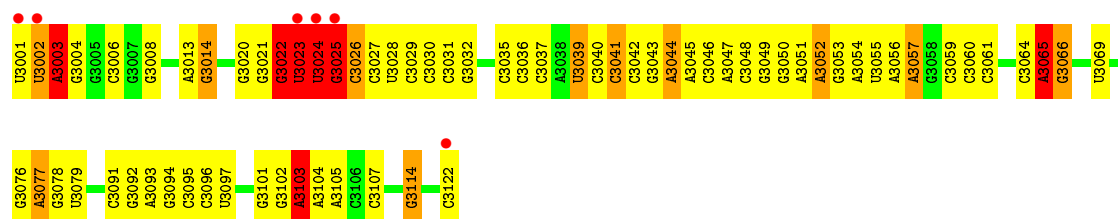
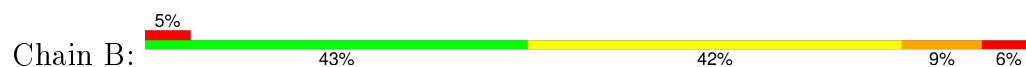




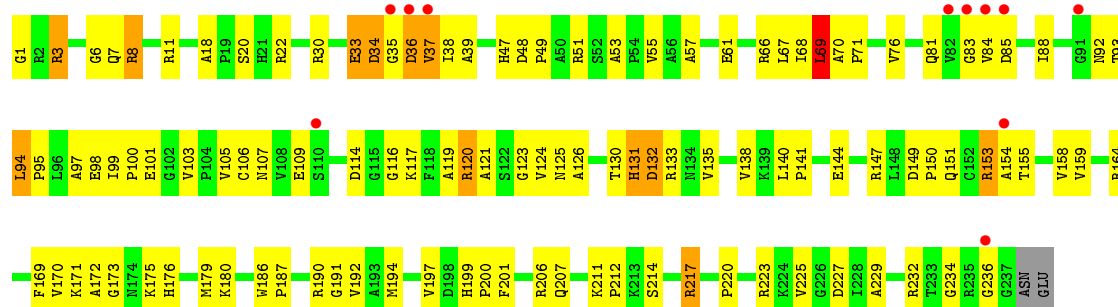
G2257	C2039	G1948	C1841	U1749	G1670	A1572	C1456	C1360	G1365	U1187	G1113	G1024
A2258	C2040	G1951	A1842	C1750	G1675	A1573	U1457	C1361	U1266	A1188	A1114	C1025
G2263	G2041	U	A1843	G1751	G1676	C1574	U1457	U1362	C1267	A1189	U1115	U1028
A2264	U2042	A	U1846	C1753	G1677	A1580	U1461	U1368	G1268	G1190	U1116	U1029
U2265	C2043	A	A1847	G1758	A1678	G1588	U1462	U1369	C1269	A1191	A1117	G1036
A2266	G2044	C	U1848	A1759	C1679	G1589	A1463	G1370	U1270	A1192	G1118	G1037
G2267	U2045	C	U1849	U1758	G1680	G1592	U1463	U1371	A1271	A1193	G1119	G1038
C2268	C2046	U	C1854	A1759	G1681	G1593	A1470	A1372	G1272	G1197	U1120	G1039
C2269	G2047	A	G1855	U1766	G1682	G1594	U1478	U1372	C1273	U1198	G1121	G1044
G2270	G2050	U	C1856	A1767	A1683	C1593	C1474	A1375	U1279	A1200	A1123	G1045
G2271	A2051	G	A1857	G1768	A1684	G1595	C1477	G1376	G1289	U1199	G1127	G1046
G2272	C2054	A	C1769	A1685	A1685	G1596	U1478	G1377	U1292	G1204	U1128	U1047
C2273	A2055	C	U1770	U1770	G1688	G1597	U1486	G1378	G1293	U1205	G1129	G1048
A2274	U2063	C	C1861	U1771	G1689	U1598	A1487	U1379	U1293	U1206	U1130	A1057
G2275	C2064	U	G1862	G1772	C1690	A1598	U1488	U1380	U1294	A1207	G1131	A1058
U2276	U2064	C	G1863	G1773	A1691	G1601	U1488	C1384	G1299	A1208	A1132	G1051
U2277	A1966	A	A1865	A1778	G1692	G1602	U1494	G1385	U1300	C1208	A1133	G1052
C2281	G2070	U	G1868	A1779	A1693	G1603	A1494	U1389	G1301	C1209	G1134	G1055
U2282	C2071	G	A1869	U1779	G1694	G1604	U1503	A1389	U1310	G1210	U1137	U1056
G2283	G2072	U	C1870	U1783	G1695	G1605	U1504	A1390	U1304	G1211	G1138	A1057
G2289	A2073	A	U1874	U1784	U1696	G1605	G1497	G1391	U1305	C1212	U1139	A1058
U2290	G1974	C	G1873	G1785	U1696	G1605	G1497	A1392	U1306	G1213	U1140	G1059
A2291	U1978	A	U1874	G1786	C1699	C1613	U1500	A1393	U1309	G1214	C1140	G1060
C2292	G2080	U	U1874	C1787	G1700	G1614	U1503	C1394	U1310	A1215	U1141	C1061
G2293	A2081	C	G1877	U1788	A1701	A1615	U1504	A1407	U1311	G1216	C1142	U1062
A2300	C2082	U	U1879	G1789	U1702	C1617	U1505	U1408	G1312	U1218	G1151	G1063
A2301	A2083	C	U1879	C1790	G1706	C1617	U1506	G1409	A1313	U1219	A1156	A1067
A2302	G2088	A	G1902	C1792	G1707	U1625	C1507	G1416	G1314	G1224	C1155	C1068
A2303	U1996	U	U1903	C1792	G1707	A1626	U1507	G1417	G1315	G1225	C1157	G1072
G2304	A1997	C	A1904	C1798	G1709	G1627	U1523	U1418	U1316	C1229	G1158	G1076
U2305	G2001	G	G1908	A1804	A1710	A1630	U1524	U1419	G1323	C1229	G1159	G1076
U2306	C2002	C	A1909	G1805	A1717	A1633	U1525	C1420	G1324	U1234	A1161	C1080
G2309	U2003	U	A1910	G1809	A1717	C1633	A1527	G1421	G1325	G1235	G1162	A1081
C2310	U2004	U	A1919	C1840	G1720	G1634	A1528	U1422	U1326	G1236	G1163	A1082
A2311	G2005	G	C1920	G1840	G1721	U1635	A1529	C1423	G1327	A1236	U1164	C1083
G2312	C2006	A	A1921	U1722	U1722	G1636	U1532	A1424	A1328	U1237	G1165	C1084
C2313	U2007	C	A1922	G1814	G1723	A1637	G1533	G1425	A1329	C1238	A1166	C1085
G2314	U2008	U	A1922	A1815	U1724	A1637	A1533	C1426	A1330	G1239	G1167	C1086
C2315	G2009	C	C1816	C1816	G1725	A1641	C1534	A1427	A1331	C1242	C1168	A1087
G2316	G1925	A	G1925	G1819	G1730	A1642	G1535	A1434	C1332	A1242	U1169	G1087
C2317	G1926	C	A1927	G1820	C1731	C1643	C1536	U1435	U1333	G1243	U1170	A1088
U2320	A1927	A	G1927	G1820	G1731	U1654	C1543	C1436	C1334	U1244	A1171	G1094
C2321	G2014	G	A1930	G1823	A1732	G1655	G1549	U1440	U1336	A1246	A1173	U1095
U2322	A2015	U	A1931	G1823	G1734	A1656	C1549	U1441	U1342	A1247	A1174	U1096
G2323	U2016	A	A1934	G1827	C1735	A1657	G1555	A1442	U1248	A1248	G1175	A1097
C2324	A1934	C	C1935	G1828	A1736	A1658	G1556	A1442	U1249	U1249	C1176	A1098
U2325	C1936	C	C1936	A1829	A1737	G1660	U1559	G1445	A1348	C1250	A1177	G1099
C2326	U2116	G	C1936	C1830	C1738	A1661	U1559	U1446	G1349	C1251	U1180	C1102
U2327	A2030	C	C1940	U1834	U1741	C1662	U1559	U1447	U1350	A1252	A1181	C1103
C2329	G2033	C	A1941	U1835	A1742	C1662	U1561	U1447	G1351	C1253	C1182	U1109
U2330	U2034	C	A1941	A1836	A1742	C1666	C1562	C1450	A1261	A1261	C1183	G1110
G2338	C2035	U	A1941	A1836	A1742	C1666	C1562	C1450	A1261	A1261	C1183	G1110
A2339	C2035	A	A1941	A1836	A1742	C1666	C1562	C1450	A1261	A1261	C1183	G1110
C	C2035	C	A1941	A1836	A1742	C1666	C1562	C1450	A1261	A1261	C1183	G1110
G2257	C2039	G1948	C1841	U1749	G1670	A1572	C1456	C1360	G1365	U1187	G1113	G1024
A2258	C2040	G1951	A1842	C1750	G1675	A1573	U1457	C1361	U1266	A1188	A1114	C1025
G2263	G2041	U	A1843	G1751	G1676	C1574	U1457	U1362	C1267	A1189	U1115	U1028
A2264	U2042	A	U1846	C1753	G1677	A1580	U1461	U1368	G1268	G1190	U1116	U1029
U2265	C2043	C	A1847	G1758	A1678	G1588	U1462	U1369	C1269	A1191	A1117	G1036
A2266	G2044	C	U1848	A1759	C1679	G1589	A1463	G1370	U1270	A1192	G1118	G1037
G2267	U2045	C	U1849	U1758	G1680	G1592	U1463	U1371	A1271	A1193	G1119	G1038
C2268	C2046	U	C1854	A1759	G1681	G1593	A1470	A1372	G1272	G1197	U1120	G1039
C2269	G2047	A	G1855	U1766	G1682	G1594	U1478	U1372	C1273	U1198	G1121	G1044
G2270	G2050	U	C1856	A1767	A1683	C1593	C1474	A1375	U1279	A1200	A1123	G1045
G2271	A2051	G	A1857	G1768	A1684	G1595	C1477	G1376	G1289	U1199	G1127	G1046
G2272	C2054	A	C1769	A1685	A1685	G1596	U1478	G1377	U1292	G1204	U1128	U1047
C2273	A2055	C	U1770	U1770	G1688	G1597	U1486	G1378	G1293	U1205	G1129	G1048
A2274	U2063	C	C1861	U1771	G1689	U1598	A1487	U1379	U1293	U1206	U1130	A1057
G2275	C2064	U	G1862	G1772	C1690	A1598	U1488	U1380	U1294	A1207	G1131	A1058
U2276	U2064	C	G1863	G1773	A1691	G1601	U1488	C1384	G1299	A1208	A1132	G1051
U2277	A1966	A	A1865	A1778	G1692	G1602	U1494	G1385	U1300	C1208	A1133	G1052
C2281	G2070	U	G1868	A1779	A1693	G1603	A1494	U1389	G1301	C1209	G1134	G1055
U2282	C2071	G	A1869	U1779	G1694	G1604	U1503	A1389	U1310	G1210	U1137	U1056
G2283	G2072	U	C1870	U1783	G1695	G1605	U1504	A1390	U1304	G1211	G1138	A1057
G2289	A2073	A	U1874	U1784	U1696	G1605	G1497	G1391	U1305	C1212	U1139	A1058
U2290	G1974	C	G1873	G1785	U1696	G1605	G1497	A1392	U1306	G1213	U1140	G1059
A2291	U1978	A	U1874	G1786	C1699	C1613	U1500	A1393	U1309	G1214	C1140	G1060
C2292	G2080	U	U1874	C1787	G1700	G1614	U1503	C1394	U1310	A1215	U1141	C1061
G2293	A2081	C	G1877	U1788	A1701	A1615	U1504	A1407	U1311	G1216	C1142	U1062
A2300	C2082	U	U1879	G1789	U1702	C1617	U1505	U1408	G1312	U1218	G1151	G1063
A2301	A2083	C	U1879	C1790	G1706	C1617	U1506	G1409	A1313	U1219	A1156	A1067
A2302	G2088	A	G1902	C1792	G1707	U1625	C1507	G1416	G1314	G1224	C1155	C1068
A2303	U1996	U	U1903	C1792	G1707	A1626	U1507	G1417	G1315	G1225	C1157	G1072
G2304	A1997	C	A1904	C1798	G1709	G1627	U1523	U1418	U1316	C1229	G1158	G1076
U2305	G2001	G	G1908	A1804	A1710	A1630	U1524	U1419	G1323	C1229	G1159	G1076
U2306	C2002	C	A1909	G1805	A1717	A1633	U1525	C1420	G1324	U1234	A1161	C1080
G2309	U2003	U	A1910	G1809	A1717	C1633	A1527	G1421	G1325	G1235	G1162	A1081
C2310	U2004	U	A1919	C1840	G1720	G1634	A1528	U1422	U1326	G1236	G1163	A1082
A2311	G2005	G	C1920	G1840	G1721	U1635	A1529	C1423	G1327	A1236	U1164	C1083
G2312	C2006	A	A1921	U1722	U1722	G1636	U1532	A1424	A1328	U1237	G1165	C1084
C2313	U2007	C	A1922	G1814	G1723	A1637	G1533	G1425	A1329	C1238	A1166	C1085
G2314	U2008	U	A1922	A1815	U1724	A1637	A1533	C1426	A1330	G1239	G1167	C1086
C2315	G2009	C	C1816	C1816	G1725	A1641	C1534	A1427	A1331	C1242	C1168	A1087
G2316	G1925	A	G1925	G1819	G1730	A1642	G1535	A1434	C1332	A1242	U1169	G1087
C2317	G1926	C	A1927	G1820	C1731	C1643	C1536	U1435	U1333	G1243	U1170	A1088
U2320	A1927	A	G1927	G1820	G1731	U1654	C1543	C1436	C1334	U1244	A1171	G1094
C2321	G2014	G	A1930	G1823	A1732	G1655	G1549	U1440	U1336	A1246	A1173	U1095
U2322	A2015	U	A1931	G1823	G1734	A1656	C1549	U1441	U1342	A1247	A1174	U1096
G2323	U2016	A	A1934	G1827	C1735	A1657	G1555	A1442	U1248	A1248	G1175	A1097
C2324	A1934	C	C1935	G1828	A1736	A1658	G1556	A1442	U1249	U1249	C1176	A1098
U2325	C19											



- Molecule 2: 5S rRNA

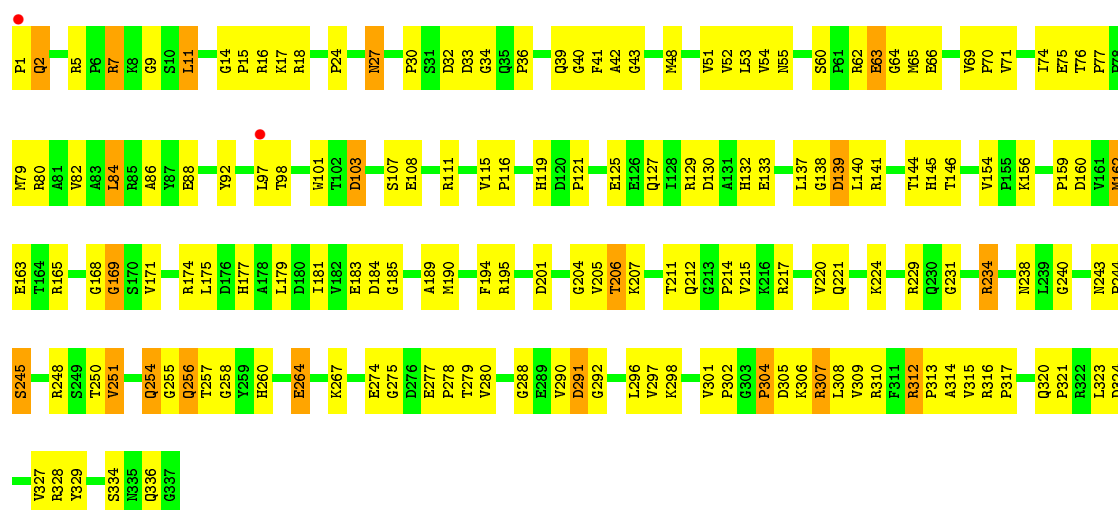


- Molecule 3: RIBOSOMAL PROTEIN L2



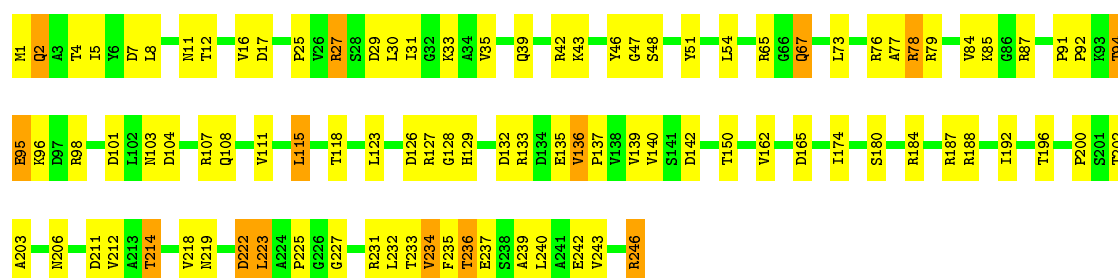
- Molecule 4: RIBOSOMAL PROTEIN L3





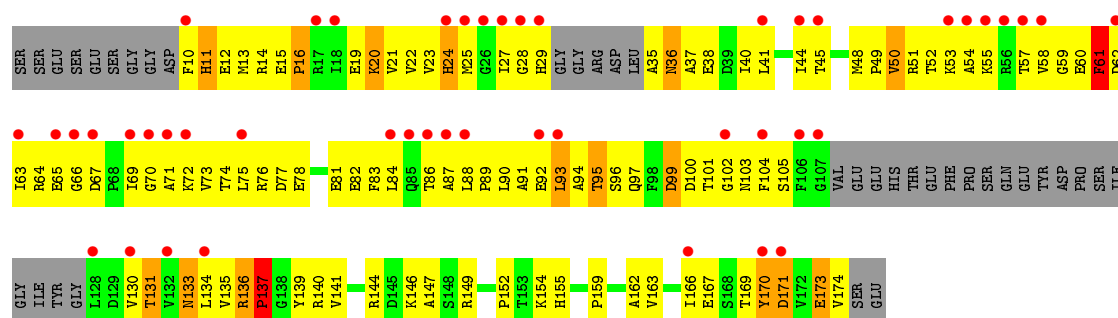
• Molecule 5: RIBOSOMAL PROTEIN L4

Chain E: 61% 34% 6%



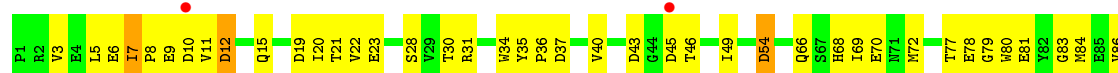
• Molecule 6: RIBOSOMAL PROTEIN L5

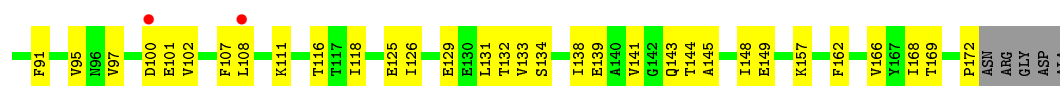
Chain F: 26% 20% 49% 9% 20%



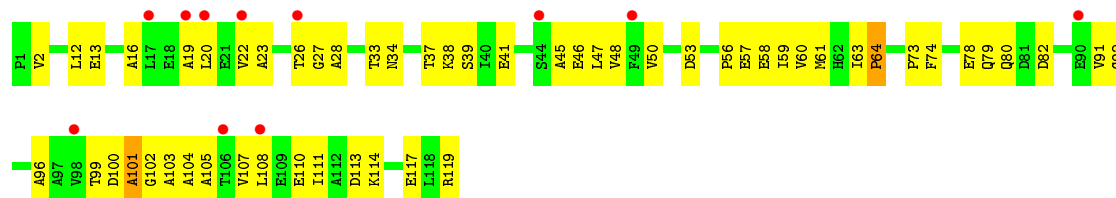
• Molecule 7: RIBOSOMAL PROTEIN L6

Chain G: 2% 56% 40%

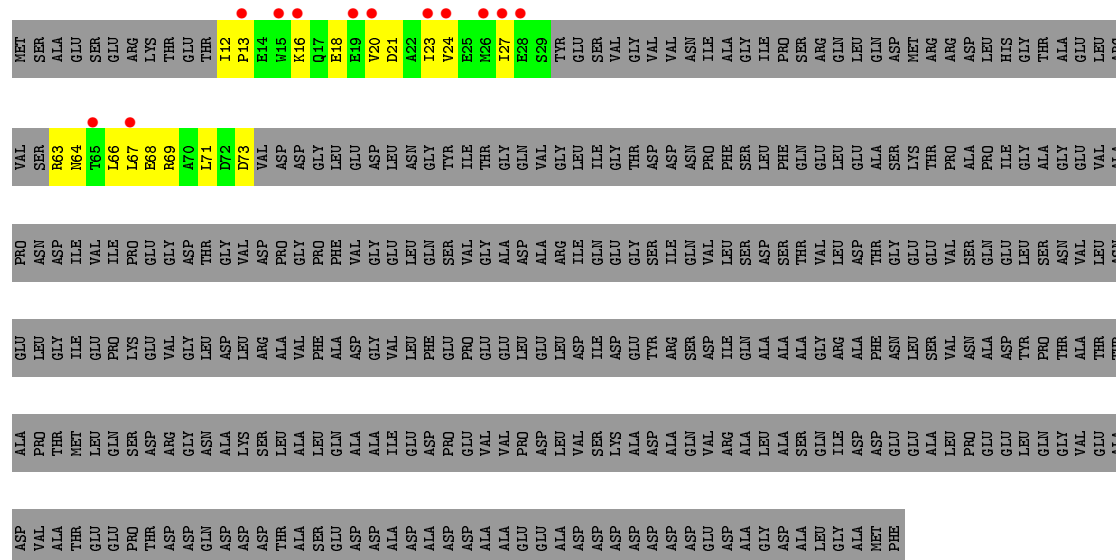




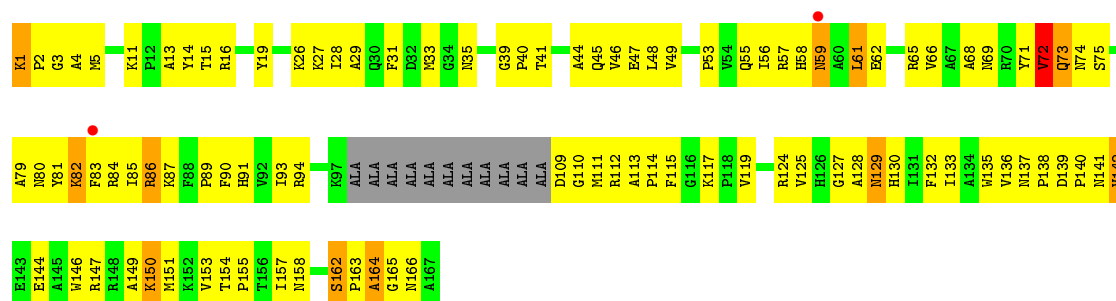
• Molecule 8: RIBOSOMAL PROTEIN L7AE

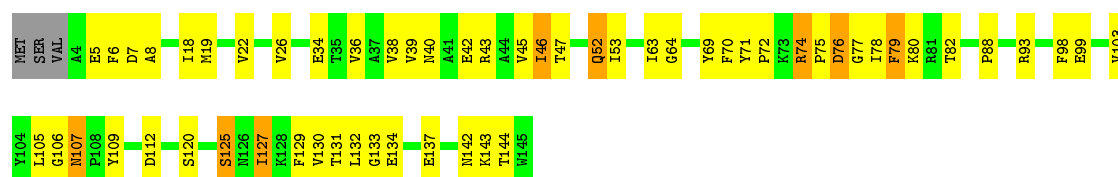


• Molecule 9: RIBOSOMAL PROTEIN L10



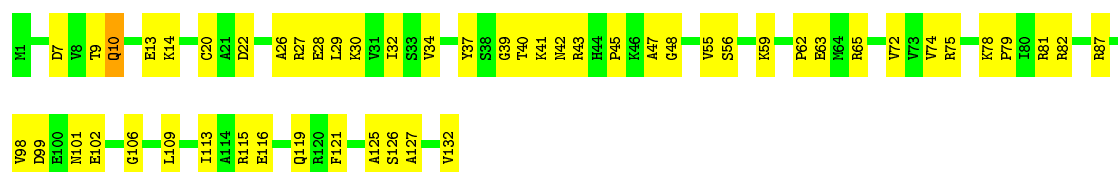
• Molecule 10: RIBOSOMAL PROTEIN L10E





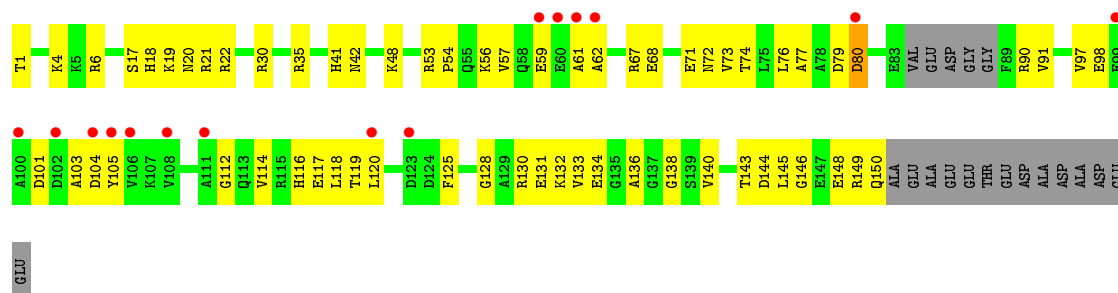
• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L: 61% 39%



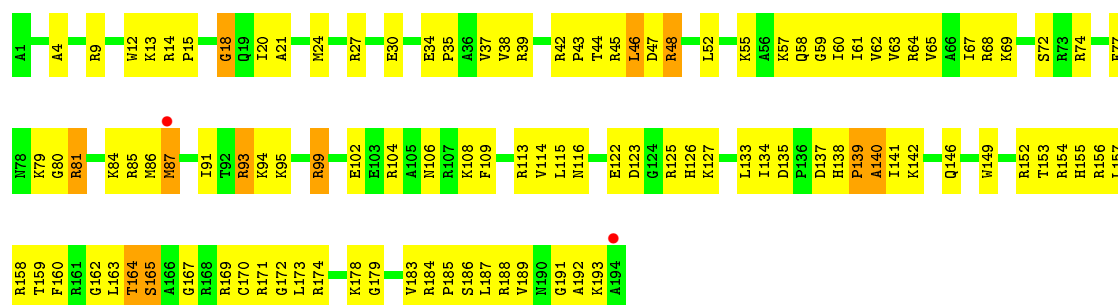
• Molecule 13: RIBOSOMAL PROTEIN L15

Chain M: 9% 50% 38% 12%



• Molecule 14: RIBOSOMAL PROTEIN L15E

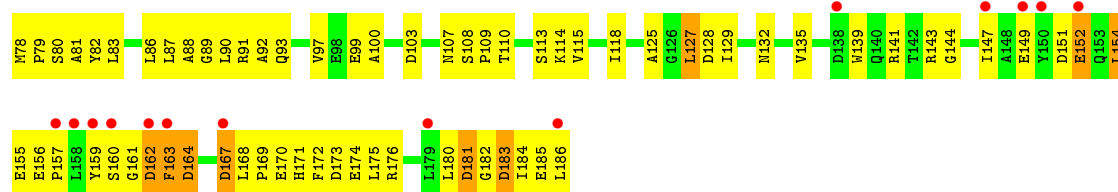
Chain N: 43% 51% 6%



• Molecule 15: RIBOSOMAL PROTEIN L18

Chain O: 8% 42% 52% 6%





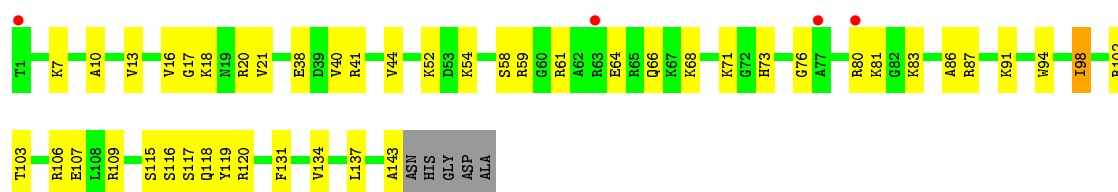
• Molecule 16: RIBOSOMAL PROTEIN L18E

Chain P: 60% 38%



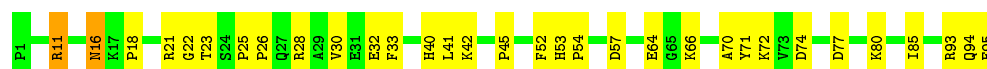
• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain Q: 3% 66% 30%



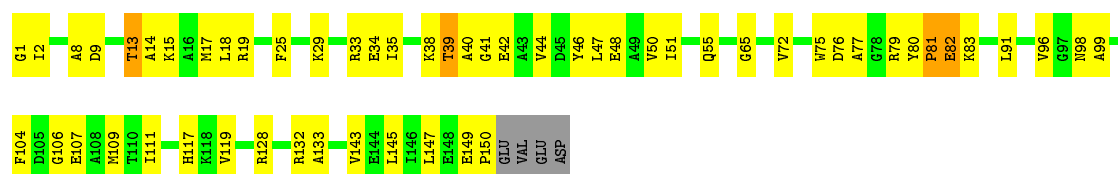
• Molecule 18: RIBOSOMAL PROTEIN L21E

Chain R: 66% 32%



• Molecule 19: RIBOSOMAL PROTEIN L22

Chain S: 61% 34%



• Molecule 20: RIBOSOMAL PROTEIN L23

Chain T: 73% 24%

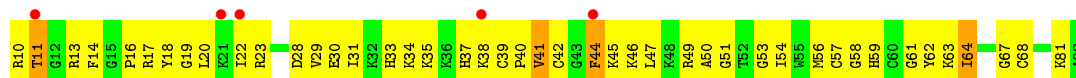


• Molecule 21: RIBOSOMAL PROTEIN L24





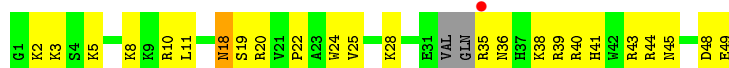
• Molecule 27: RIBOSOMAL PROTEIN L37Ae



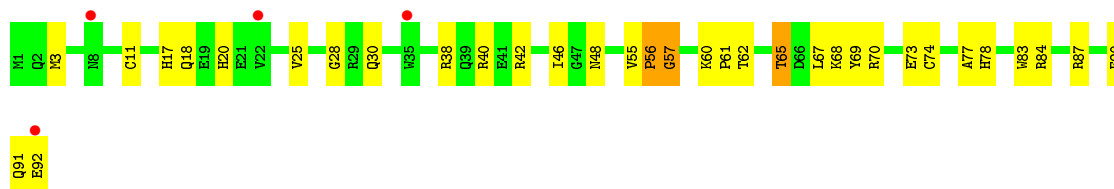
• Molecule 28: RIBOSOMAL PROTEIN L37E



• 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, $\alpha$ , $\beta$ , $\gamma$	213.75Å 301.57Å 574.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 49.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-3.20) 87.9 (49.69-3.00)	Depositor EDS
$R_{merge}$	0.19	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.27 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.214 , 0.250 0.198 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	60.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 74.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 366469 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	98587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.59	1/66076 (0.0%)	0.76	33/103052 (0.0%)
2	B	0.92	16/2905 (0.6%)	0.98	20/4528 (0.4%)
3	C	0.47	0/1787	0.75	0/2409
4	D	0.52	0/2689	0.74	0/3652
5	E	0.49	0/1883	0.73	0/2551
6	F	0.43	0/1111	0.68	0/1498
7	G	0.48	0/1382	0.67	0/1880
8	H	0.44	0/896	0.64	0/1219
9	I	0.51	0/241	0.63	0/324
10	J	0.50	0/1246	0.82	2/1686 (0.1%)
11	K	0.53	0/1135	0.69	0/1530
12	L	0.57	1/1003 (0.1%)	0.78	0/1351
13	M	0.47	0/1126	0.76	0/1504
14	N	0.56	0/1633	0.81	1/2180 (0.0%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.49	0/873	0.69	0/1181
17	Q	0.49	0/1143	0.66	0/1521
18	R	0.52	0/748	0.78	0/1005
19	S	0.52	0/1172	0.77	0/1578
20	T	0.48	0/648	0.69	0/875
21	U	0.46	0/957	0.73	0/1289
22	V	0.47	0/417	0.67	0/562
23	W	0.43	0/502	0.63	0/675
24	X	0.52	0/1218	0.72	0/1655
25	Y	0.49	0/664	0.71	0/895
26	Z	0.50	0/1146	0.73	0/1536
27	1	0.52	0/575	0.75	0/763
28	2	0.57	0/437	0.78	0/578
29	3	0.45	0/398	0.63	0/527
30	4	0.57	0/771	0.73	0/1024
All	All	0.57	18/98255 (0.0%)	0.76	56/147027 (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	141
2	B	0	5
All	All	1	146

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3025	G	O3'-P	10.69	1.74	1.61
2	B	3025	G	C4'-O4'	9.77	1.58	1.45
2	B	3023	U	C2'-O2'	9.46	1.53	1.41
2	B	3026	C	P-O5'	-8.76	1.50	1.59
2	B	3003	A	C5'-C4'	8.50	1.61	1.51

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.12	63.13	105.20
1	A	1164	U	OP2-P-O3'	-17.65	66.37	105.20
1	A	1165	G	O5'-P-OP1	-12.66	94.31	105.70
2	B	3024	U	O5'-P-OP2	11.59	124.60	110.70
2	B	3026	C	O5'-P-OP2	-11.13	95.68	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	G	Sidechain
1	A	146	U	Sidechain
1	A	20	G	Sidechain
1	A	24	G	Sidechain
1	A	33	G	Sidechain

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29803	1165	0
2	B	2600	0	1326	84	0
3	C	1754	0	1763	129	0
4	D	2624	0	2533	180	0
5	E	1858	0	1816	125	0
6	F	1094	0	1085	143	0
7	G	1357	0	1266	84	0
8	H	885	0	854	66	0
9	I	240	0	231	25	0
10	J	1215	0	1215	152	0
11	K	1119	0	1098	68	0
12	L	993	0	1027	56	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	159	0
15	O	1444	0	1401	142	0
16	P	864	0	873	46	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	28	0
19	S	1149	0	1122	64	0
20	T	641	0	605	22	0
21	U	949	0	923	55	0
22	V	410	0	364	36	0
23	W	499	0	511	33	0
24	X	1195	0	1137	99	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	59	0
27	1	563	0	597	51	0
28	2	430	0	426	28	0
29	3	393	0	406	30	0
30	4	755	0	728	41	0
31	A	52	0	72	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	1	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	3	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	4	0
35	L	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	2	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	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	38	0	0	8	0
37	2	57	0	0	4	0
37	3	39	0	0	4	0
37	4	72	0	0	12	0
37	A	5898	0	0	232	0
37	B	140	0	0	15	0
37	C	129	0	0	24	0
37	D	152	0	0	27	0
37	E	169	0	0	34	0
37	F	52	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	42	0	0	13	0
37	H	28	0	0	10	0
37	I	21	0	0	5	0
37	J	81	0	0	17	0
37	K	56	0	0	6	0
37	L	61	0	0	13	0
37	M	81	0	0	19	0
37	N	129	0	0	22	0
37	O	68	0	0	20	0
37	P	45	0	0	13	0
37	Q	69	0	0	6	0
37	R	56	0	0	3	0
37	S	89	0	0	8	0
37	T	36	0	0	4	0
37	U	39	0	0	5	0
37	V	27	0	0	5	0
37	W	15	0	0	3	0
37	X	73	0	0	7	0
37	Y	30	0	0	8	0
37	Z	93	0	0	14	0
All	All	98587	0	59571	3047	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

The worst 5 of 3047 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:H5'	1:A:1161:A:H5'	1.22	1.15
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.26	1.13
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.33	1.11
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.67	1.10
1:A:871:G:H8	1:A:871:G:H5'	1.14	1.07

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%)	204 (87%)	26 (11%)	5 (2%)	9	46
4	D	335/337 (99%)	303 (90%)	23 (7%)	9 (3%)	6	39
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	39	80
6	F	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	1	4
7	G	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11	52
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	5	32
11	K	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	9	46
12	L	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	13	55
13	M	141/164 (86%)	119 (84%)	20 (14%)	2 (1%)	14	57
14	N	192/194 (99%)	174 (91%)	15 (8%)	3 (2%)	12	54
15	O	184/186 (99%)	164 (89%)	13 (7%)	7 (4%)	4	28
16	P	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	21	67
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	26	72
18	R	93/95 (98%)	86 (92%)	6 (6%)	1 (1%)	17	62
19	S	148/154 (96%)	139 (94%)	8 (5%)	1 (1%)	26	72
20	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
21	U	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	21	67
22	V	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	9	48
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	33
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	26	72
25	Y	80/91 (88%)	71 (89%)	8 (10%)	1 (1%)	15	59
26	Z	140/240 (58%)	137 (98%)	3 (2%)	0	100	100
27	1	71/73 (97%)	61 (86%)	8 (11%)	2 (3%)	6	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	8	45
All	All	3633/4235 (86%)	3285 (90%)	281 (8%)	67 (2%)	11	51

5 of 67 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	17	57
4	D	282/282 (100%)	263 (93%)	19 (7%)	20	60
5	E	193/193 (100%)	175 (91%)	18 (9%)	11	41
6	F	117/147 (80%)	107 (92%)	10 (8%)	13	47
7	G	152/155 (98%)	148 (97%)	4 (3%)	54	85
8	H	92/92 (100%)	91 (99%)	1 (1%)	80	94
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	12	43
11	K	118/121 (98%)	108 (92%)	10 (8%)	13	47
12	L	106/106 (100%)	103 (97%)	3 (3%)	51	84
13	M	112/126 (89%)	108 (96%)	4 (4%)	42	79
14	N	166/166 (100%)	158 (95%)	8 (5%)	31	72
15	O	149/149 (100%)	143 (96%)	6 (4%)	38	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	90 (97%)	3 (3%)	46	81
17	Q	113/116 (97%)	110 (97%)	3 (3%)	52	85
18	R	79/79 (100%)	75 (95%)	4 (5%)	29	70
19	S	117/121 (97%)	114 (97%)	3 (3%)	54	85
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	101 (96%)	4 (4%)	40	78
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	50 (98%)	1 (2%)	63	88
24	X	130/130 (100%)	122 (94%)	8 (6%)	23	64
25	Y	66/73 (90%)	61 (92%)	5 (8%)	16	55
26	Z	120/195 (62%)	112 (93%)	8 (7%)	20	60
27	1	56/56 (100%)	53 (95%)	3 (5%)	27	68
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	57	86
30	4	79/79 (100%)	78 (99%)	1 (1%)	76	92
All	All	3027/3441 (88%)	2876 (95%)	151 (5%)	30	71

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	72	VAL
11	K	125	SER
26	Z	163	THR
10	J	82	LYS
11	K	46	ILE

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

Mol	Chain	Res	Type
13	M	58	GLN
16	P	100	GLN
29	3	16	ASN
13	M	116	HIS
14	N	176	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	245 (8%)	36 (1%)
2	B	121/122 (99%)	14 (11%)	6 (4%)
All	All	2868/3044 (94%)	259 (9%)	42 (1%)

5 of 259 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 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1450	C
1	A	1856	C
2	B	3025	G
1	A	1563	G
1	A	1692	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 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
31	ZIT	A	8600	-	54,54,54	1.68	10 (18%)	76,83,83	1.27	7 (9%)

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	ZIT	A	8600	-	-	0/72/107/107	0/3/3/3

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	8600	ZIT	C9-C8	2.05	1.61	1.53
31	A	8600	ZIT	O5A-C5A	2.30	1.49	1.44
31	A	8600	ZIT	C13-C14	2.43	1.59	1.54
31	A	8600	ZIT	C4-C5	2.78	1.61	1.54
31	A	8600	ZIT	C4A-C5A	2.80	1.57	1.51

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	8600	ZIT	C6-C5-C4	-4.10	108.35	114.11
31	A	8600	ZIT	C14-C13-C12	-2.06	104.66	108.11
31	A	8600	ZIT	C7A-N3A-C3A	2.01	118.91	113.09
31	A	8600	ZIT	O1B-C3-C4	2.29	111.08	108.19
31	A	8600	ZIT	C2A-C3A-N3A	2.34	117.17	110.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	8600	ZIT	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	42 (1%) 76 63	27, 56, 101, 149	0
2	B	122/122 (100%)	0.10	6 (4%) 33 20	43, 71, 98, 158	0
3	C	237/239 (99%)	0.08	11 (4%) 36 23	38, 62, 93, 114	0
4	D	337/337 (100%)	-0.10	2 (0%) 90 84	29, 64, 90, 99	0
5	E	246/246 (100%)	-0.12	0 100 100	30, 58, 81, 92	0
6	F	140/176 (79%)	1.40	46 (32%) 0 0	61, 108, 124, 131	0
7	G	172/177 (97%)	0.35	4 (2%) 64 49	50, 76, 97, 102	0
8	H	119/119 (100%)	0.49	11 (9%) 11 6	62, 82, 106, 110	0
9	I	29/348 (8%)	1.71	12 (41%) 0 0	80, 100, 109, 109	0
10	J	156/167 (93%)	0.06	2 (1%) 79 67	43, 65, 94, 101	0
11	K	142/145 (97%)	-0.10	0 100 100	45, 57, 80, 97	0
12	L	132/132 (100%)	-0.12	0 100 100	38, 58, 80, 87	0
13	M	145/164 (88%)	0.50	15 (10%) 9 5	33, 77, 113, 123	0
14	N	194/194 (100%)	-0.14	2 (1%) 84 75	42, 56, 73, 84	0
15	O	186/186 (100%)	0.40	15 (8%) 15 8	52, 74, 114, 124	0
16	P	115/115 (100%)	0.08	0 100 100	52, 66, 84, 88	0
17	Q	143/148 (96%)	0.25	4 (2%) 56 42	45, 65, 80, 89	0
18	R	95/95 (100%)	-0.08	0 100 100	38, 54, 70, 82	0
19	S	150/154 (97%)	-0.19	0 100 100	40, 54, 74, 82	0
20	T	81/84 (96%)	0.01	1 (1%) 81 69	55, 71, 90, 97	0
21	U	119/119 (100%)	0.46	6 (5%) 32 19	52, 69, 92, 103	0
22	V	53/66 (80%)	0.01	0 100 100	51, 64, 82, 89	0
23	W	65/70 (92%)	1.15	14 (21%) 1 1	62, 83, 118, 124	0
24	X	154/154 (100%)	-0.34	0 100 100	38, 56, 76, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	82/91 (90%)	0.15	1 (1%) 81 69	53, 67, 91, 107	0
26	Z	142/240 (59%)	-0.08	1 (0%) 89 83	33, 56, 77, 94	0
27	1	73/73 (100%)	0.06	5 (6%) 20 11	59, 71, 87, 94	0
28	2	56/56 (100%)	-0.29	0 100 100	35, 46, 51, 52	0
29	3	46/48 (95%)	0.14	1 (2%) 65 50	44, 72, 96, 106	0
30	4	92/92 (100%)	0.39	4 (4%) 39 25	44, 66, 79, 90	0
All	All	6577/7279 (90%)	0.05	205 (3%) 52 38	27, 62, 101, 158	0

The worst 5 of 205 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3001	U	8.4
23	W	1	THR	7.7
9	I	27	ILE	6.0
6	F	57	THR	6.0
15	O	186	LEU	5.7

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
35	CL	A	8515	1/1	0.66	0.88	82.65	110,110,110,110	0
34	NA	A	8374	1/1	0.31	1.55	69.20	89,89,89,89	0
34	NA	A	8356	1/1	0.90	0.70	61.24	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8362	1/1	0.94	0.67	42.13	62,62,62,62	0
34	NA	A	8378	1/1	0.91	1.10	32.36	48,48,48,48	0
34	NA	A	8321	1/1	0.91	0.47	32.11	42,42,42,42	0
32	MG	A	8064	1/1	0.92	0.44	20.95	36,36,36,36	0
34	NA	B	8383	1/1	0.81	0.54	20.65	40,40,40,40	0
34	NA	A	8326	1/1	0.64	1.01	20.05	92,92,92,92	0
34	NA	A	8303	1/1	0.66	0.40	19.95	54,54,54,54	0
34	NA	A	8323	1/1	0.81	0.44	19.57	57,57,57,57	0
34	NA	A	8371	1/1	0.74	0.34	19.33	48,48,48,48	0
32	MG	A	8066	1/1	0.72	0.70	19.25	48,48,48,48	0
34	NA	A	8377	1/1	0.75	0.33	18.16	68,68,68,68	0
34	NA	A	8359	1/1	0.94	0.53	14.81	75,75,75,75	0
34	NA	A	8361	1/1	0.95	0.51	14.28	46,46,46,46	0
34	NA	M	8380	1/1	0.90	0.65	13.08	75,75,75,75	0
32	MG	A	8024	1/1	0.79	0.48	11.78	79,79,79,79	0
35	CL	A	8505	1/1	0.83	0.43	11.03	92,92,92,92	0
34	NA	A	8372	1/1	0.87	0.48	10.82	87,87,87,87	0
34	NA	A	8373	1/1	0.81	0.53	10.39	67,67,67,67	0
34	NA	A	8325	1/1	0.87	0.27	9.41	62,62,62,62	0
34	NA	A	8376	1/1	0.94	0.28	9.01	49,49,49,49	0
34	NA	A	8366	1/1	0.82	0.40	8.81	79,79,79,79	0
34	NA	A	8368	1/1	0.81	0.26	8.18	65,65,65,65	0
34	NA	A	8335	1/1	0.96	0.27	7.88	61,61,61,61	0
34	NA	A	8369	1/1	0.93	0.33	7.68	55,55,55,55	0
34	NA	S	8386	1/1	0.51	0.45	6.62	97,97,97,97	0
34	NA	A	8382	1/1	0.90	0.29	6.23	74,74,74,74	0
35	CL	D	8519	1/1	0.92	0.44	5.70	65,65,65,65	0
34	NA	A	8350	1/1	0.98	0.21	5.64	43,43,43,43	0
34	NA	A	8364	1/1	0.64	0.23	5.38	52,52,52,52	0
34	NA	A	8305	1/1	0.77	0.25	5.20	46,46,46,46	0
32	MG	A	8044	1/1	0.98	0.21	4.30	58,58,58,58	0
31	ZIT	A	8600	52/52	0.84	0.29	4.13	81,91,95,96	0
34	NA	A	8365	1/1	0.86	0.58	4.12	76,76,76,76	0
35	CL	4	8504	1/1	0.86	0.54	2.83	93,93,93,93	0
32	MG	A	8060	1/1	0.95	0.20	2.09	51,51,51,51	0
34	NA	A	8331	1/1	0.93	0.19	2.08	55,55,55,55	0
35	CL	P	8508	1/1	0.82	0.36	1.76	97,97,97,97	0
34	NA	U	8343	1/1	0.89	0.25	1.47	38,38,38,38	0
34	NA	S	8337	1/1	0.81	0.21	1.35	58,58,58,58	0
35	CL	A	8510	1/1	0.77	0.34	1.06	97,97,97,97	0
34	NA	A	8379	1/1	0.95	0.18	1.01	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8112	1/1	0.88	0.22	0.90	50,50,50,50	0
32	MG	A	8013	1/1	0.96	0.20	0.85	56,56,56,56	0
32	MG	A	8067	1/1	0.88	0.21	0.45	51,51,51,51	0
34	NA	A	8314	1/1	0.93	0.18	-0.10	48,48,48,48	0
32	MG	A	8049	1/1	0.89	0.19	-0.10	74,74,74,74	0
34	NA	C	8345	1/1	0.93	0.21	-0.17	57,57,57,57	0
34	NA	A	8332	1/1	0.75	0.16	-0.20	50,50,50,50	0
32	MG	A	8053	1/1	0.78	0.15	-0.33	40,40,40,40	0
33	K	A	8201	1/1	0.96	0.16	-0.61	70,70,70,70	0
34	NA	A	8381	1/1	0.81	0.15	-0.66	61,61,61,61	0
32	MG	A	8058	1/1	0.98	0.18	-0.73	62,62,62,62	0
36	CD	1	8403	1/1	0.97	0.12	-0.75	77,77,77,77	0
32	MG	Z	8109	1/1	0.94	0.17	-0.78	61,61,61,61	0
32	MG	A	8059	1/1	0.94	0.15	-0.89	56,56,56,56	0
32	MG	A	8086	1/1	0.94	0.12	-0.98	56,56,56,56	0
35	CL	N	8518	1/1	0.94	0.20	-1.31	65,65,65,65	0
32	MG	A	8057	1/1	0.91	0.18	-1.33	54,54,54,54	0
36	CD	V	8401	1/1	1.00	0.11	-1.42	75,75,75,75	0
34	NA	A	8324	1/1	0.94	0.09	-1.43	48,48,48,48	0
36	CD	4	8404	1/1	0.96	0.11	-1.44	75,75,75,75	0
32	MG	A	8032	1/1	0.97	0.15	-1.44	63,63,63,63	0
35	CL	L	8512	1/1	0.90	0.13	-1.47	55,55,55,55	0
32	MG	A	8004	1/1	0.97	0.11	-1.48	60,60,60,60	0
34	NA	A	8333	1/1	0.89	0.12	-1.59	51,51,51,51	0
34	NA	A	8353	1/1	0.95	0.12	-1.60	46,46,46,46	0
36	CD	2	8402	1/1	0.99	0.08	-1.67	70,70,70,70	0
32	MG	A	8071	1/1	0.86	0.13	-1.67	85,85,85,85	0
34	NA	J	8309	1/1	0.96	0.15	-1.71	43,43,43,43	0
34	NA	K	8346	1/1	0.95	0.15	-2.00	33,33,33,33	0
33	K	A	8202	1/1	0.98	0.14	-2.04	61,61,61,61	0
32	MG	A	8008	1/1	0.95	0.13	-2.19	61,61,61,61	0
32	MG	A	8096	1/1	0.79	0.10	-2.27	64,64,64,64	0
32	MG	U	8073	1/1	0.79	0.08	-2.35	62,62,62,62	0
32	MG	A	8017	1/1	0.90	0.06	-2.57	42,42,42,42	0
32	MG	4	8078	1/1	0.91	0.06	-2.59	54,54,54,54	0
32	MG	D	8055	1/1	0.98	0.10	-2.68	51,51,51,51	0
34	NA	N	8347	1/1	0.98	0.12	-2.76	23,23,23,23	0
35	CL	K	8521	1/1	0.93	0.16	-2.91	64,64,64,64	0
34	NA	S	8338	1/1	0.98	0.09	-3.04	49,49,49,49	0
32	MG	A	8107	1/1	0.98	0.04	-3.08	60,60,60,60	0
32	MG	A	8012	1/1	0.95	0.10	-3.26	35,35,35,35	0
34	NA	A	8317	1/1	0.98	0.04	-3.27	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8080	1/1	0.97	0.13	-3.34	65,65,65,65	0
32	MG	A	8056	1/1	0.94	0.10	-3.39	61,61,61,61	0
32	MG	A	8033	1/1	0.95	0.11	-3.42	36,36,36,36	0
34	NA	R	8348	1/1	0.94	0.07	-3.49	39,39,39,39	0
32	MG	A	8027	1/1	0.96	0.05	-3.61	51,51,51,51	0
32	MG	A	8108	1/1	0.94	0.13	-3.65	85,85,85,85	0
32	MG	A	8074	1/1	0.95	0.04	-3.70	52,52,52,52	0
32	MG	A	8003	1/1	0.97	0.10	-3.95	26,26,26,26	0
32	MG	A	8018	1/1	0.98	0.11	-4.16	54,54,54,54	0
34	NA	A	8344	1/1	0.96	0.08	-4.26	39,39,39,39	0
32	MG	A	8001	1/1	0.87	0.10	-4.46	41,41,41,41	0
32	MG	A	8052	1/1	0.92	0.13	-4.65	58,58,58,58	0
32	MG	A	8019	1/1	0.99	0.06	-4.66	24,24,24,24	0
32	MG	A	8035	1/1	0.96	0.08	-4.83	60,60,60,60	0
32	MG	C	8065	1/1	0.99	0.05	-4.87	40,40,40,40	0
32	MG	A	8022	1/1	0.96	0.05	-4.93	55,55,55,55	0
32	MG	A	8007	1/1	0.98	0.09	-5.35	42,42,42,42	0
32	MG	A	8039	1/1	0.94	0.06	-5.39	67,67,67,67	0
32	MG	A	8038	1/1	0.96	0.08	-5.95	29,29,29,29	0
32	MG	A	8020	1/1	0.95	0.07	-6.61	36,36,36,36	0
34	NA	A	8320	1/1	0.97	0.12	-6.65	32,32,32,32	0
32	MG	A	8077	1/1	0.97	0.07	-6.82	37,37,37,37	0
32	MG	A	8054	1/1	0.95	0.06	-6.93	52,52,52,52	0
32	MG	A	8010	1/1	0.95	0.09	-7.46	43,43,43,43	0
32	MG	A	8002	1/1	0.96	0.07	-8.08	43,43,43,43	0
32	MG	A	8014	1/1	0.99	0.07	-8.88	24,24,24,24	0
34	NA	A	8327	1/1	0.95	0.09	-8.89	44,44,44,44	0
32	MG	A	8084	1/1	0.96	0.05	-9.79	41,41,41,41	0
32	MG	A	8110	1/1	0.95	0.08	-10.46	35,35,35,35	0
32	MG	A	8015	1/1	0.97	0.09	-11.06	57,57,57,57	0
32	MG	A	8006	1/1	0.96	0.04	-12.02	54,54,54,54	0
32	MG	A	8028	1/1	0.97	0.05	-12.79	57,57,57,57	0
34	NA	A	8339	1/1	0.98	0.06	-20.29	33,33,33,33	0
34	NA	A	8330	1/1	0.85	0.28	-	57,57,57,57	0
35	CL	K	8516	1/1	0.97	0.26	-	53,53,53,53	0
32	MG	A	8093	1/1	0.91	0.09	-	59,59,59,59	0
35	CL	A	8522	1/1	0.81	0.69	-	83,83,83,83	0
32	MG	A	8045	1/1	0.97	0.10	-	58,58,58,58	0
32	MG	A	8041	1/1	0.76	0.26	-	69,69,69,69	0
34	NA	A	8311	1/1	0.92	0.15	-	63,63,63,63	0
32	MG	A	8047	1/1	0.98	0.17	-	81,81,81,81	0
34	NA	A	8301	1/1	0.95	0.17	-	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
34	NA	A	8340	1/1	0.75	0.61	-	56,56,56,56	0
34	NA	B	8351	1/1	0.80	0.15	-	54,54,54,54	0
34	NA	A	8358	1/1	0.96	0.65	-	107,107,107,107	0
32	MG	1	8105	1/1	0.85	0.43	-	38,38,38,38	0
34	NA	A	8302	1/1	0.92	0.23	-	52,52,52,52	0
32	MG	A	8106	1/1	0.88	0.14	-	71,71,71,71	0
34	NA	A	8355	1/1	0.88	0.50	-	60,60,60,60	0
32	MG	A	8063	1/1	0.94	0.11	-	92,92,92,92	0
32	MG	A	8115	1/1	0.98	0.05	-	43,43,43,43	0
35	CL	A	8514	1/1	0.91	0.18	-	57,57,57,57	0
35	CL	A	8517	1/1	0.89	0.16	-	52,52,52,52	0
35	CL	C	8509	1/1	0.91	0.27	-	69,69,69,69	0
32	MG	A	8083	1/1	0.95	0.08	-	51,51,51,51	0
32	MG	A	8070	1/1	0.95	0.18	-	46,46,46,46	0
34	NA	A	8354	1/1	0.78	0.60	-	54,54,54,54	0
32	MG	A	8061	1/1	0.96	0.04	-	37,37,37,37	0
34	NA	A	8367	1/1	0.83	0.24	-	38,38,38,38	0
32	MG	A	8072	1/1	0.96	0.11	-	65,65,65,65	0
32	MG	A	8099	1/1	0.86	0.17	-	55,55,55,55	0
34	NA	E	8304	1/1	0.90	0.20	-	32,32,32,32	0
34	NA	A	8385	1/1	0.75	0.67	-	73,73,73,73	0
34	NA	A	8306	1/1	0.95	0.53	-	41,41,41,41	0
34	NA	A	8352	1/1	0.87	0.32	-	56,56,56,56	0
32	MG	A	8117	1/1	0.99	0.10	-	33,33,33,33	0
35	CL	S	8506	1/1	0.91	0.27	-	69,69,69,69	0
34	NA	A	8360	1/1	0.91	0.85	-	59,59,59,59	0
34	NA	A	8316	1/1	0.84	0.41	-	61,61,61,61	0
32	MG	A	8011	1/1	0.81	0.08	-	44,44,44,44	0
34	NA	A	8329	1/1	0.27	0.45	-	70,70,70,70	0
32	MG	A	8029	1/1	0.98	0.12	-	50,50,50,50	0
34	NA	A	8308	1/1	0.86	0.23	-	53,53,53,53	0
32	MG	A	8043	1/1	0.94	0.14	-	56,56,56,56	0
32	MG	A	8103	1/1	0.94	0.20	-	76,76,76,76	0
34	NA	A	8349	1/1	0.91	0.31	-	57,57,57,57	0
32	MG	A	8036	1/1	0.97	0.07	-	46,46,46,46	0
32	MG	A	8068	1/1	0.95	0.05	-	56,56,56,56	0
34	NA	A	8315	1/1	0.97	0.30	-	62,62,62,62	0
34	NA	A	8336	1/1	0.90	0.16	-	85,85,85,85	0
32	MG	A	8031	1/1	1.00	0.03	-	44,44,44,44	0
32	MG	A	8021	1/1	0.94	0.09	-	32,32,32,32	0
34	NA	A	8313	1/1	0.88	0.21	-	66,66,66,66	0
32	MG	B	8095	1/1	0.95	0.08	-	98,98,98,98	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	A	8342	1/1	0.86	0.37	-	51,51,51,51	0
32	MG	A	8101	1/1	0.91	0.14	-	60,60,60,60	0
35	CL	R	8511	1/1	0.60	0.59	-	102,102,102,102	0
35	CL	O	8507	1/1	0.71	0.52	-	84,84,84,84	0
32	MG	A	8076	1/1	0.95	0.09	-	75,75,75,75	0
32	MG	L	8069	1/1	0.91	0.16	-	79,79,79,79	0
32	MG	A	8085	1/1	0.97	0.15	-	68,68,68,68	0
32	MG	A	8051	1/1	0.96	0.13	-	66,66,66,66	0
32	MG	A	8009	1/1	0.95	0.05	-	46,46,46,46	0
32	MG	A	8016	1/1	0.96	0.13	-	50,50,50,50	0
32	MG	A	8111	1/1	0.90	0.08	-	62,62,62,62	0
35	CL	K	8501	1/1	0.96	0.33	-	81,81,81,81	0
34	NA	A	8341	1/1	0.58	0.30	-	63,63,63,63	0
35	CL	A	8503	1/1	0.80	0.51	-	74,74,74,74	0
35	CL	A	8513	1/1	0.83	0.15	-	67,67,67,67	0
32	MG	A	8100	1/1	0.90	0.15	-	88,88,88,88	0
32	MG	A	8090	1/1	0.93	0.16	-	47,47,47,47	0
32	MG	A	8030	1/1	0.99	0.10	-	40,40,40,40	0
32	MG	A	8104	1/1	0.97	0.07	-	50,50,50,50	0
34	NA	A	8375	1/1	0.68	0.28	-	86,86,86,86	0
32	MG	A	8088	1/1	0.84	0.13	-	64,64,64,64	0
32	MG	A	8079	1/1	0.97	0.08	-	42,42,42,42	0
32	MG	A	8114	1/1	0.88	0.27	-	47,47,47,47	0
32	MG	A	8098	1/1	0.99	0.25	-	52,52,52,52	0
35	CL	A	8520	1/1	0.84	0.19	-	65,65,65,65	0
34	NA	A	8307	1/1	0.87	0.42	-	48,48,48,48	0
34	NA	J	8322	1/1	0.71	0.43	-	62,62,62,62	0
32	MG	A	8025	1/1	0.98	0.05	-	54,54,54,54	0
36	CD	P	8405	1/1	0.91	0.09	-	152,152,152,152	0
34	NA	A	8319	1/1	0.99	0.14	-	57,57,57,57	0
35	CL	K	8502	1/1	0.95	0.15	-	87,87,87,87	0
34	NA	A	8363	1/1	0.56	0.91	-	79,79,79,79	0
32	MG	A	8081	1/1	0.96	0.12	-	67,67,67,67	0
34	NA	A	8318	1/1	0.90	0.69	-	45,45,45,45	0
32	MG	A	8040	1/1	0.90	0.09	-	63,63,63,63	0
32	MG	A	8113	1/1	0.90	0.15	-	53,53,53,53	0
34	NA	A	8328	1/1	0.70	0.29	-	61,61,61,61	0
32	MG	A	8026	1/1	0.97	0.09	-	49,49,49,49	0
32	MG	A	8062	1/1	0.97	0.09	-	61,61,61,61	0
32	MG	A	8087	1/1	0.84	0.10	-	75,75,75,75	0
32	MG	A	8089	1/1	0.90	0.11	-	70,70,70,70	0
32	MG	A	8042	1/1	0.93	0.23	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8097	1/1	0.92	0.30	-	45,45,45,45	0
32	MG	A	8116	1/1	0.83	0.10	-	54,54,54,54	0
32	MG	A	8034	1/1	0.97	0.03	-	32,32,32,32	0
34	NA	A	8357	1/1	0.79	0.07	-	64,64,64,64	0
32	MG	A	8046	1/1	0.96	0.10	-	72,72,72,72	0
32	MG	A	8082	1/1	0.89	0.22	-	83,83,83,83	0
32	MG	A	8091	1/1	0.94	0.06	-	58,58,58,58	0
34	NA	A	8334	1/1	0.94	0.20	-	45,45,45,45	0
32	MG	A	8037	1/1	0.95	0.12	-	61,61,61,61	0
32	MG	A	8005	1/1	0.96	0.13	-	60,60,60,60	0
34	NA	A	8370	1/1	0.95	0.20	-	42,42,42,42	0
34	NA	T	8312	1/1	0.79	0.25	-	51,51,51,51	0
32	MG	A	8023	1/1	0.98	0.03	-	33,33,33,33	0
32	MG	A	8102	1/1	0.95	0.28	-	75,75,75,75	0
32	MG	A	8050	1/1	0.88	0.26	-	67,67,67,67	0
32	MG	A	8048	1/1	0.96	0.08	-	41,41,41,41	0
32	MG	A	8075	1/1	0.94	0.11	-	56,56,56,56	0
34	NA	A	8384	1/1	0.40	1.14	-	90,90,90,90	0
34	NA	A	8310	1/1	0.81	0.20	-	29,29,29,29	0
32	MG	A	8094	1/1	0.96	0.09	-	66,66,66,66	0
32	MG	A	8092	1/1	0.84	0.32	-	95,95,95,95	0

## 6.5 Other polymers

There are no such residues in this entry.