



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 03:20 pm GMT

PDB ID : 3CXC  
Title : The structure of an enhanced oxazolidinone inhibitor bound to the 50S ribosomal subunit of *H. marismortui*  
Authors : Ippolito, J.A.; Wang, D.; Kanyo, Z.F.; Duffy, E.M.  
Deposited on : 2008-04-24  
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 : trunk30967  
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) : trunk30967

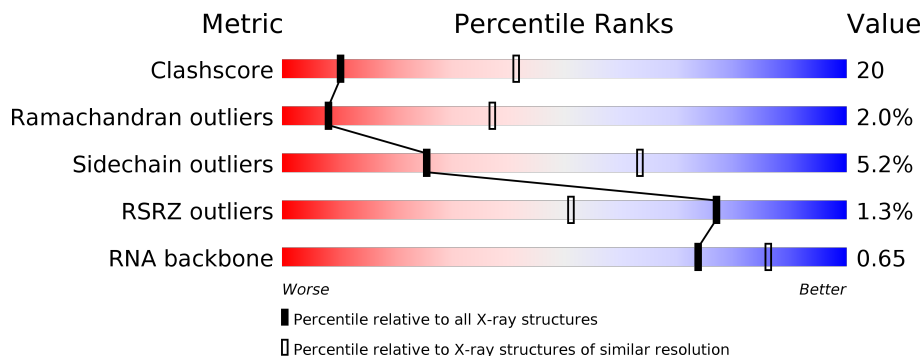
# 1 Overall quality at a glance

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	0	2922	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>40%</div> <div>6%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>38%</div> <div>49%</div> <div>11%</div> </div> <div>.</div> </div>
3	4	3	<div> <div> <div></div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
4	A	239	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>5%</div> </div> <div>.</div> </div>
5	B	337	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>42%</div> <div>6%</div> </div> </div>
6	C	246	<div> <div> <div></div> <div>55%</div> <div>39%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	D	176	
8	E	177	
9	F	119	
10	G	348	
11	H	167	
12	I	145	
13	J	132	
14	K	164	
15	L	194	
16	M	186	
17	N	115	
18	O	148	
19	P	95	
20	Q	154	
21	R	84	
22	S	119	
23	T	66	
24	U	70	
25	V	154	
26	W	91	
27	X	240	
28	Y	73	
29	Z	56	
30	1	48	
31	2	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
33	MG	0	8024	-	-	-	X
33	MG	0	8114	-	-	-	X
35	NA	0	8329	-	-	-	X
35	NA	0	8363	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8384	-	-	-	X
35	NA	H	8322	-	-	-	X
35	NA	Q	8386	-	-	-	X
35	NA	R	8312	-	-	-	X
37	CD	2	8404	-	-	X	-

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98635 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(\*CP\*CP\*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PRO	CONFLICT	UNP P20279

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	J	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	145	Total	C	N	O	S	0	0	0
			1118	670	222	226				

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.



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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

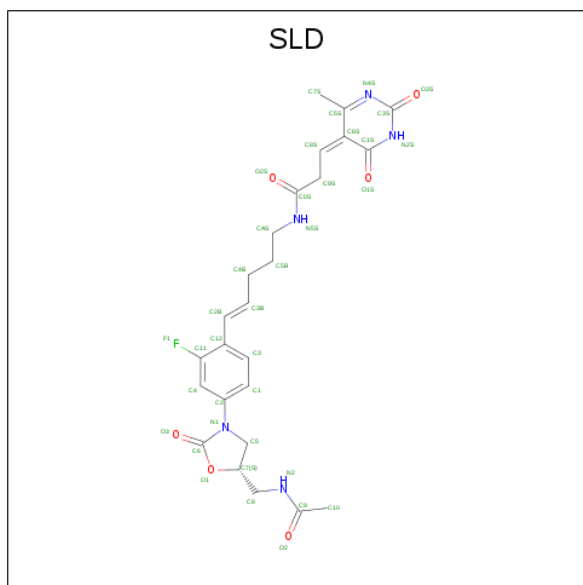
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is (3Z)-N-[(4E)-5-(4-{(5S)-5-[(acetylamino)methyl]-2-oxo-1,3-oxazolidin-3-yl}-2-fluorophenyl)pent-4-en-1-yl]-3-(4-methyl-2,6-dioxo-1,6-dihydropyrimidin-5(2H)-ylidene)propanamide (three-letter code: SLD) (formula: C<sub>25</sub>H<sub>28</sub>FN<sub>5</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	F	N	O	0	0
			37	25	1	5	6		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	J	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	2	Total 2	Mg 2	0	0
33	S	1	Total 1	Mg 1	0	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	73	Total 73	Na 73	0	0
35	P	1	Total 1	Na 1	0	0
35	Q	2	Total 2	Na 2	0	0
35	K	1	Total 1	Na 1	0	0
35	H	2	Total 2	Na 2	0	0
35	I	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	A	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	8	Total 8	Cl 8	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cl 1	0	0
36	J	1	Total 1	Cl 1	0	0
36	Q	1	Total 1	Cl 1	0	0
36	K	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	I	3	Total 3	Cl 3	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	X	1	Total 1	Cl 1	0	0
36	2	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	Z	1	Total 1	Cd 1	0	0
37	Y	1	Total 1	Cd 1	0	0
37	T	1	Total 1	Cd 1	0	0
37	2	1	Total 1	Cd 1	0	0
37	N	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5806	Total 5806	O 5806	0	0
38	9	147	Total 147	O 147	0	0
38	4	1	Total 1	O 1	0	0
38	A	136	Total 136	O 136	0	0
38	B	160	Total 160	O 160	0	0
38	C	180	Total 180	O 180	0	0
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	26	Total 26	O 26	0	0
38	G	21	Total 21	O 21	0	0
38	H	82	Total 82	O 82	0	0
38	I	61	Total 61	O 61	0	0
38	J	63	Total 63	O 63	0	0
38	K	85	Total 85	O 85	0	0
38	L	130	Total 130	O 130	0	0
38	M	69	Total 69	O 69	0	0
38	N	45	Total 45	O 45	0	0
38	O	70	Total 70	O 70	0	0
38	P	56	Total 56	O 56	0	0
38	Q	92	Total 92	O 92	0	0
38	R	40	Total 40	O 40	0	0
38	S	37	Total 37	O 37	0	0

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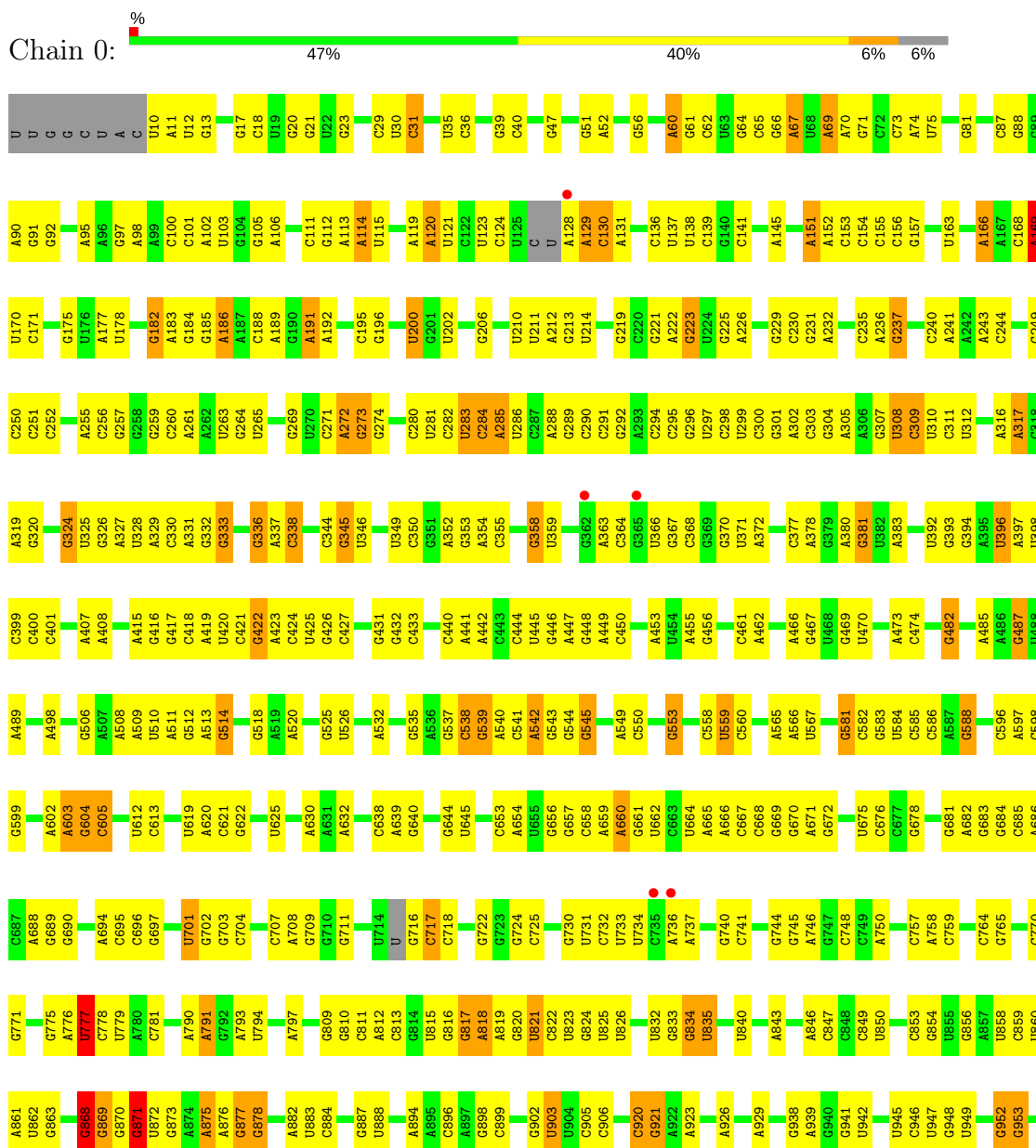
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	27	Total 27	O 27	0	0
38	U	13	Total 13	O 13	0	0
38	V	74	Total 74	O 74	0	0
38	W	29	Total 29	O 29	0	0
38	X	105	Total 105	O 105	0	0
38	Y	41	Total 41	O 41	0	0
38	Z	57	Total 57	O 57	0	0
38	1	45	Total 45	O 45	0	0
38	2	76	Total 76	O 76	0	0

### 3 Residue-property plots

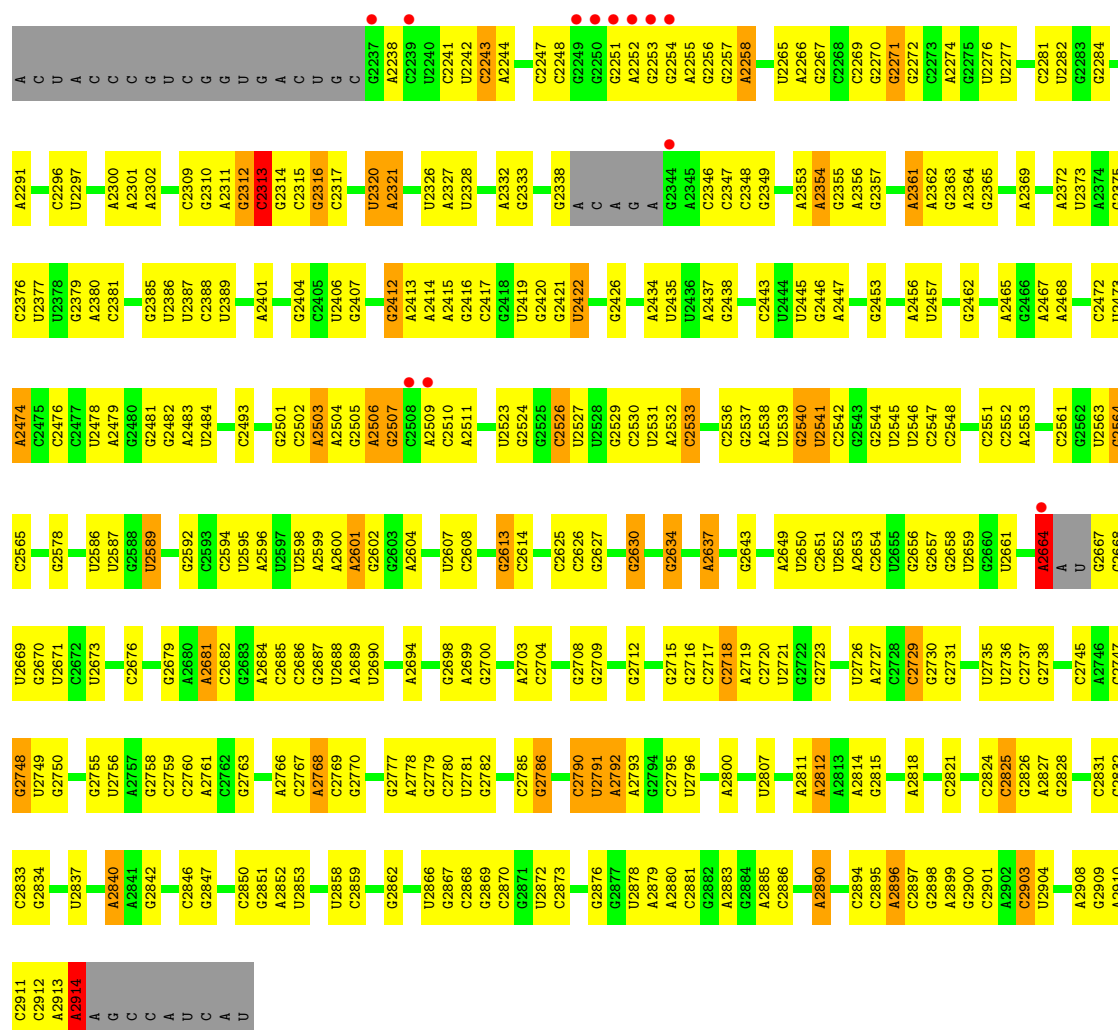
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

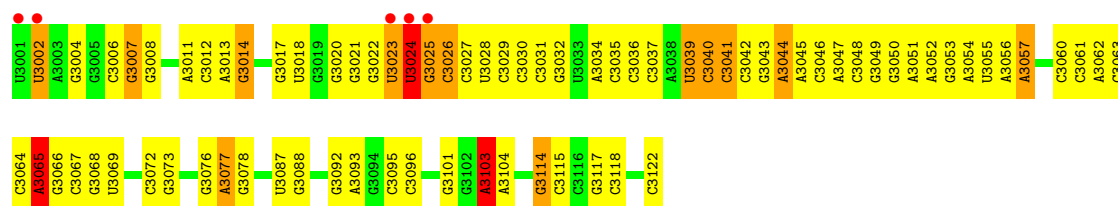


A	G2082	C1988	A1910	U1748	A1656	C1574	G1498	U1419	A1313	G1223	A1154	U1029	G958
U	A2083	U1992	G1917	G1751	A1657	C1575	U1499	C1420	U1314	G1224	G1155	U1030	C959
G	C1993	U1993	U1918	G1752	A1658	A1580	U1500	U1421	U1320	C1225	C1156	G1031	G960
U	A2090	A1994	A1919	A1755	C1666	C1584	U1503	U1422	A1321	G1226	G1158	G1044	A961
G	G2090	U1995	C1920	G1756	U1668	C1585	U1504	A1424	G1322	G1229	G1159	G1045	C962
A	G2091	U1996	A1921	U1757	A1669	G1586	U1505	G1425	G1323	C1230	G1160	C963	G964
G	G2094	G2000	A1922	U1758	G1670	U1587	U1506	C1426	G1324	C1231	G1161	G1052	G968
G	A2095	G2001	G1925	A1759	C1675	G1592	U1511	A1427	G1325	U1234	G1162	G1055	G969
A	A2096	C2002	G1926	G1760	U1676	C1593	U1512	G1430	A1328	G1235	U1170	G1059	U970
A	U2003	U2004	A1927	U1761	G1677	C1594	C1513	C1431	A1329	U1236	G1163	G1064	G
C	A2101	U2004	C1928	G1762	U1677	C1595	C1514	U1432	A1330	U1237	G1165	G1065	U
A	G2102	G2005	G1929	C1763	A1676	G1596	A1515	G1433	A1331	G1238	A1166	G1069	C
C	C2105	U2008	A1930	U1766	C1679	U1597	C1516	A1434	G1332	G1239	U1171	A1070	C
U	C2106	U2008	A1931	A1767	A1682	U1598	U1517	U1435	U1333	A1242	A1171	U1064	U
A	U2107	A2011	G1932	G1768	A1683	U1599	U1518	C1436	C1334	U1243	A1172	G1065	C
A	C	U2012	A1934	C1769	A1684	G1600	G1520	U1440	C1335	U1244	A1173	G1069	C
C	G2110	G2013	C1935	U1770	A1685	A1603	C1521	G1441	C1342	A1245	A1174	C1071	C
A	G2111	G2014	C1936	G1771	C1686	G1604	U1522	G1442	C1343	A1246	G1175	A1072	U
G	A2112	A2015	U1937	C1772	C1687	G1605	U1523	G1443	G1344	U1247	U1180	G1072	C
G	G2113	U2016	G1938	G1773	C1687	G1605	U1524	G1444	A1345	U1248	A1181	C1078	C
U	U2114	U2016	U1939	G1774	C1692	G1609	G1525	G1445	U1346	U1249	C1182	A1078	G
A	U2115	G2023	A1852	G1774	C1692	C1609	A1526	G1445	U1346	U1250	C1183	A1079	A
C	U2116	U2023	A1853	G1774	C1692	C1609	A1527	G1445	U1346	U1251	C1184	G1080	G
C	C2119	U2028	C1854	A1778	G1697	G1610	A1528	C1450	A1352	A1252	C1185	A1081	A
C	U2120	C2029	G1855	A1779	U1698	G1611	A1529	C1451	C1353	C1253	U1186	G1086	G
G	G2121	A2030	C1856	G1780	U1698	A1612	G1529	G1452	C1353	U1256	C1187	A1087	A
C	C2121	U2030	A1857	G1781	U1701	G1613	G1535	U1453	C1360	U1266	U1187	G1087	G
C	G2033	G2033	G1861	G1782	U1702	G1614	U1536	U1454	C1361	U1267	A1188	A1088	A
G	U2034	U2034	C1862	A1783	U1703	A1615	C1537	C1455	U1362	G1268	A1189	G1088	G
U	C2035	C2035	G1863	U1784	U1704	A1616	C1537	C1456	U1363	G1269	G1190	U1109	U
A	G2036	C2036	C1864	C1787	A1711	C1617	U1538	U1457	C1366	U1270	A1191	G1110	C
G	U2036	U2036	A1864	C1787	A1712	G1618	U1539	G1457	C1366	C1273	A1192	G1110	G
C	A2039	C2040	C1872	U1788	C1714	A1624	C1545	G1460	A1372	U1276	A1114	A1114	C
C	G2041	U2042	G1877	G1789	G1715	U1625	G1546	U1461	U1276	C1277	U1115	U1115	A
G	U2042	U2043	G1878	U1791	A1716	A1626	A1547	A1463	A1375	G1277	U1116	U1116	C
C	G2044	G2044	U1879	C1792	A1717	G1627	U1548	U1464	G1376	U1278	A1117	A1117	C
C	G2050	G2050	C1793	C1793	U1717	G1627	U1549	C1474	C1377	U1279	A1118	A1118	A
A	G2053	A2054	C1882	U1722	U1722	C1633	G1552	A1470	A1381	G1283	A1200	G1119	C999
A	A2055	A2055	U1798	G1723	G1723	G1634	C1552	A1471	A1381	G1283	A1201	U1120	C1000
C	U2055	U2055	G1799	U1724	U1724	U1635	C1553	A1472	G1382	G1284	C1201	U1120	C1001
C	G2060	A2060	G1800	C1725	C1725	G1636	G1557	U1473	U1383	G1289	G1202	U1120	G1002
C	A2061	C2061	A1801	G1725	A1637	A1637	C1558	C1474	C1384	C1289	A1123	U1120	G1003
A	A2062	A2062	G1802	U1730	U1638	U1638	A1559	C1477	G1385	G1290	C1129	A1006	U1006
A	U2063	U2063	C1803	C1730	U1639	U1639	U1559	C1477	G1385	G1290	U1130	A1007	C1007
C	C2065	C2065	A1804	U1731	U1639	U1639	U1559	C1477	G1385	G1290	U1131	A1008	C1008
A	G2070	G2070	G1805	A1732	C1640	C1640	U1561	U1478	A1393	U1298	G1131	U1009	U1009
C	C2071	C2071	G1806	U1733	A1641	A1641	C1562	U1483	A1394	G1299	A1132	U1009	U1009
A	A2072	A2072	U1807	C1734	G1734	C1643	C1563	G1484	G1398	G1300	G1133	A1014	C1014
C	U2073	U2073	U1808	A1735	U1735	C1644	C1564	G1485	A1399	U1304	G1134	C1015	C1015
C	G2074	G2074	U1809	C1736	U1736	C1644	C1564	G1486	A1407	C1305	G1137	U1016	U1016
A	A2074	A2074	G1810	U1741	U1741	G1649	C1565	A1487	U1407	U1306	G1138	C1019	C1019
A	C2071	C2071	C1810	A1742	A1742	C1650	C1566	A1488	U1408	A1307	G1139	C1020	C1020
A	G2072	G2072	U1813	G1743	G1743	C1651	A1567	U1489	U1409	A1308	C1140	G1021	G1021
A	U2073	U2073	U1814	G1744	G1744	C1652	U1568	A1494	G1409	U1309	G1216	A1022	A1022
A	G2074	G2074	C1818	U1745	U1745	C1653	U1569	C1495	G1416	U1310	G1217	U1218	U1218
U	U2074	U2074	A1746	G1746	G1746	C1654	A1572	G1496	G1417	G1311	U1218	G1150	G1150
U	U2074	U2074	G1820	A1747	A1747	G1655	A1573	G1497	U1418	G1312	U1219	G1151	U1028





### • Molecule 2: 5S RIBOSOMAL RNA

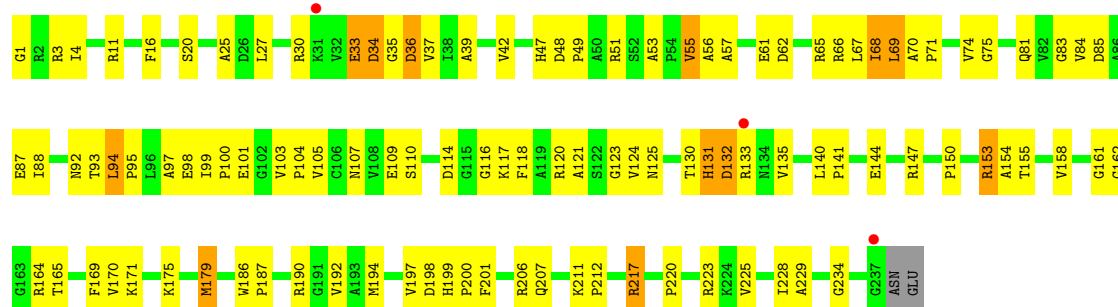


### • Molecule 3: 5'-R(\*CP\*CP\*A)-3'

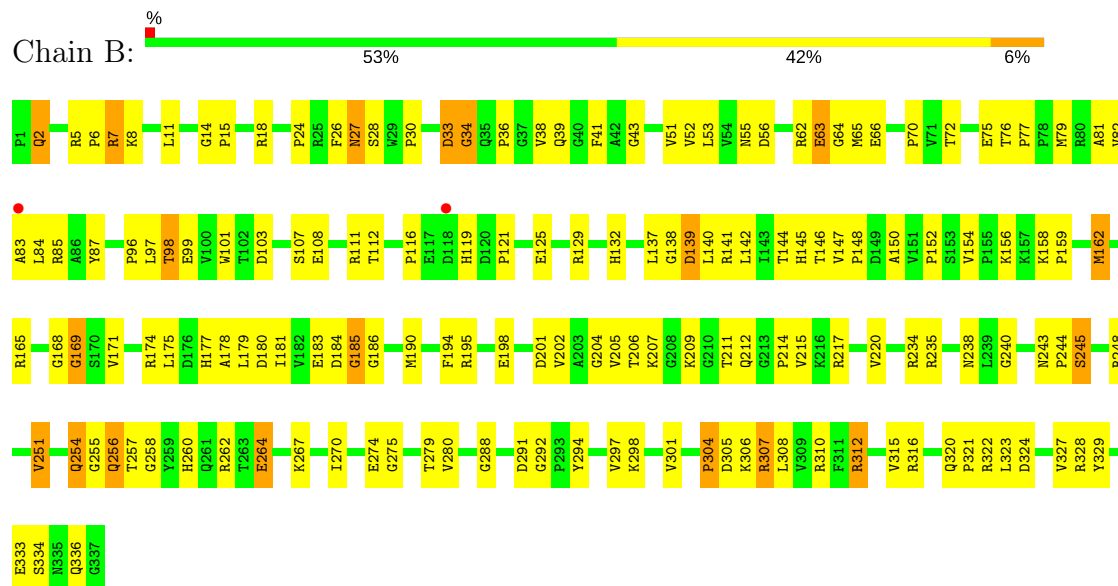


### • Molecule 4: RIBOSOMAL PROTEIN L2

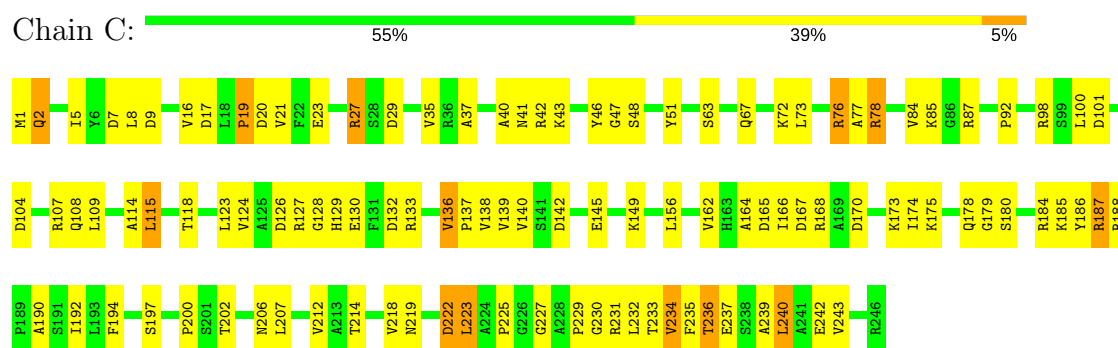




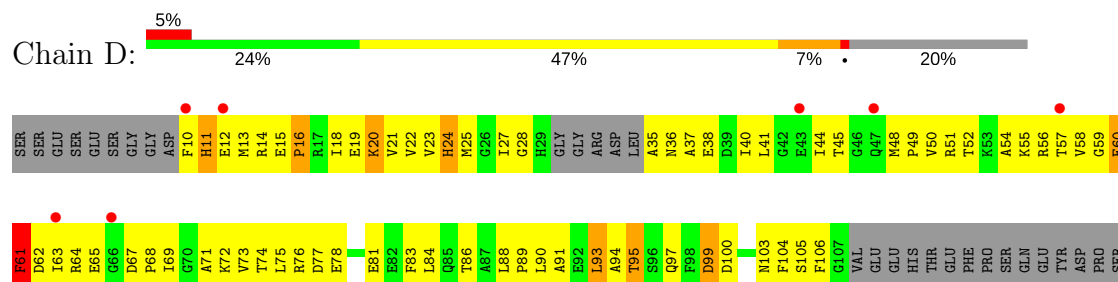
• Molecule 5: RIBOSOMAL PROTEIN L3



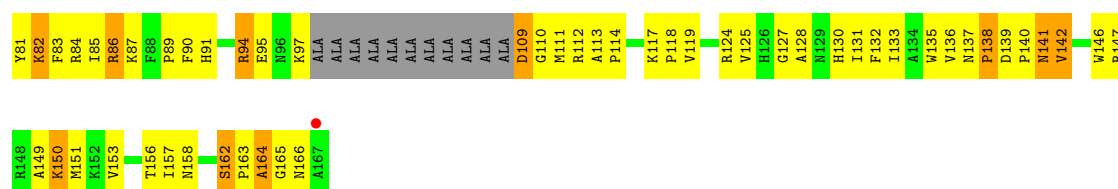
• Molecule 6: RIBOSOMAL PROTEIN L4



• Molecule 7: RIBOSOMAL PROTEIN L5

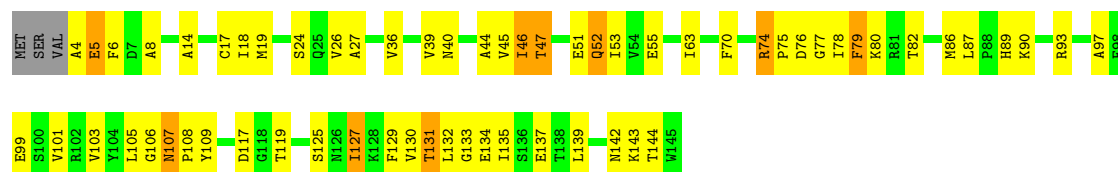






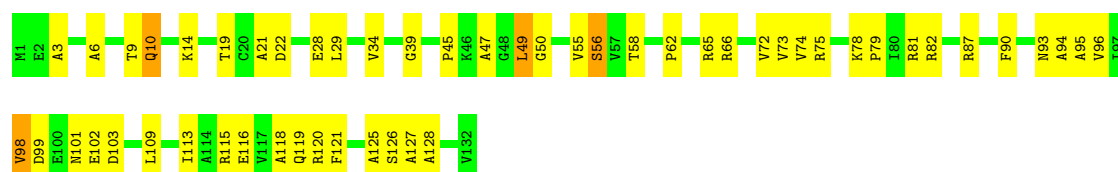
• Molecule 12: RIBOSOMAL PROTEIN L13

Chain I: 55% 37% 6%



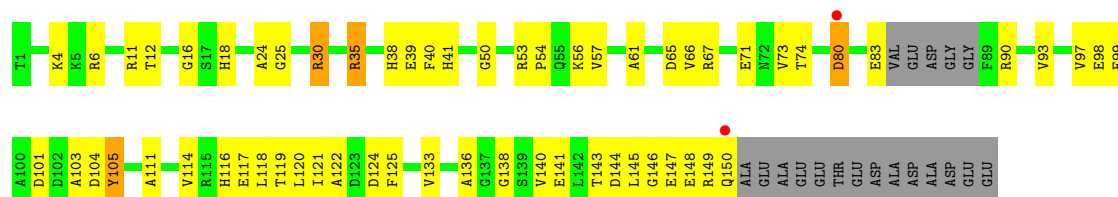
• Molecule 13: RIBOSOMAL PROTEIN L14

Chain J: 60% 37%



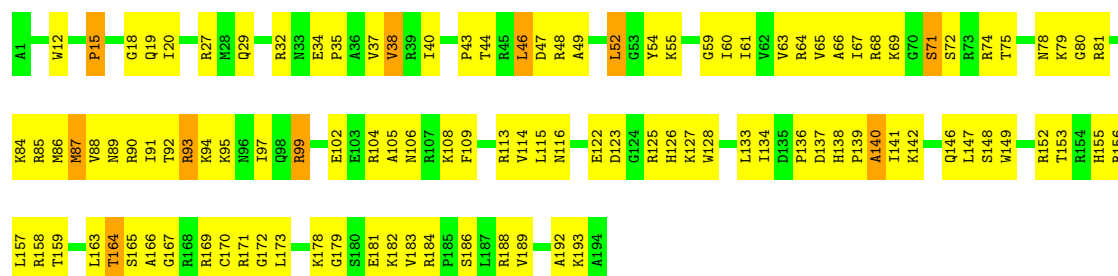
• Molecule 14: RIBOSOMAL PROTEIN L15

Chain K: % 51% 35% 12%

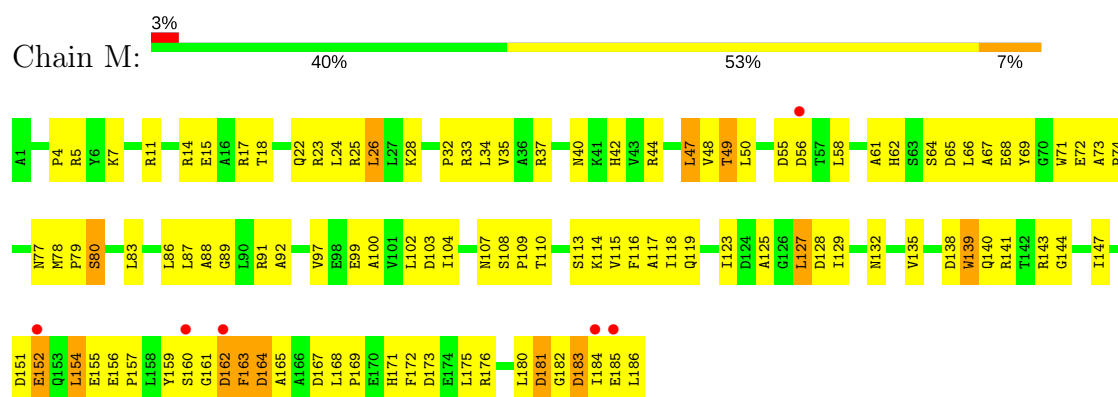


• Molecule 15: RIBOSOMAL PROTEIN L15E

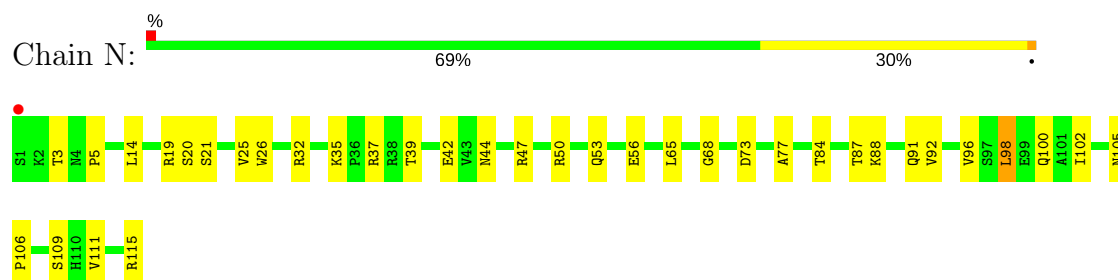
Chain L: 43% 52% 5%



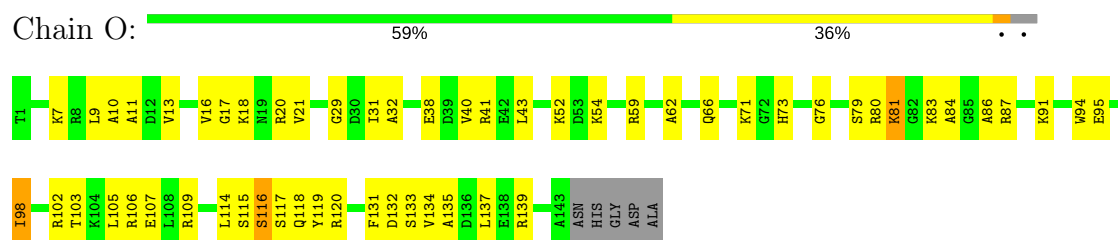
• Molecule 16: RIBOSOMAL PROTEIN L18



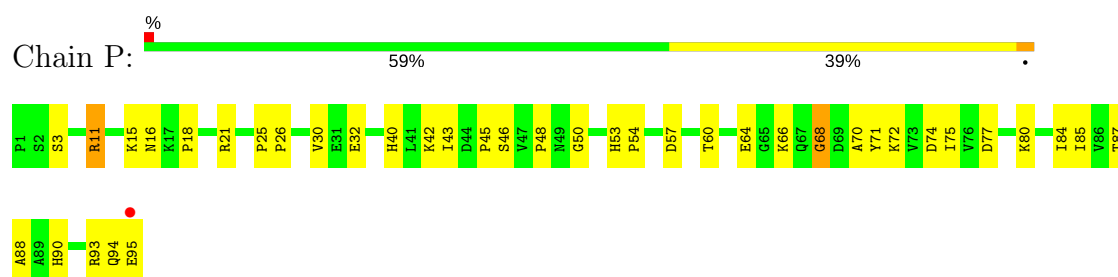
• Molecule 17: RIBOSOMAL PROTEIN L18E



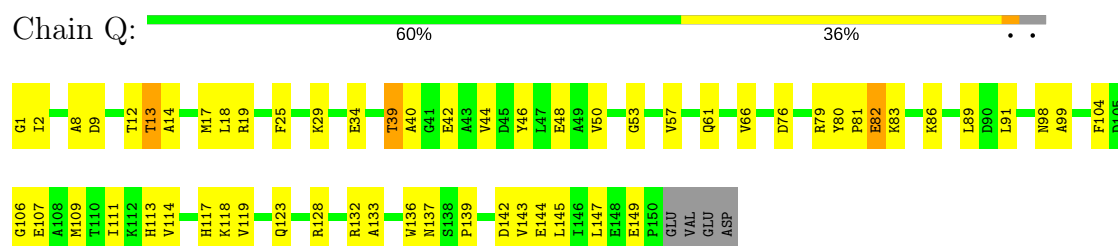
• Molecule 18: RIBOSOMAL PROTEIN L19E



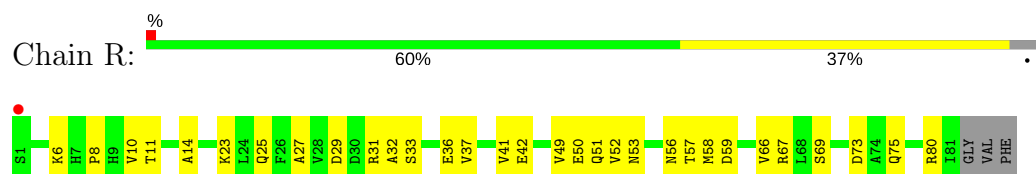
• Molecule 19: RIBOSOMAL PROTEIN L21E



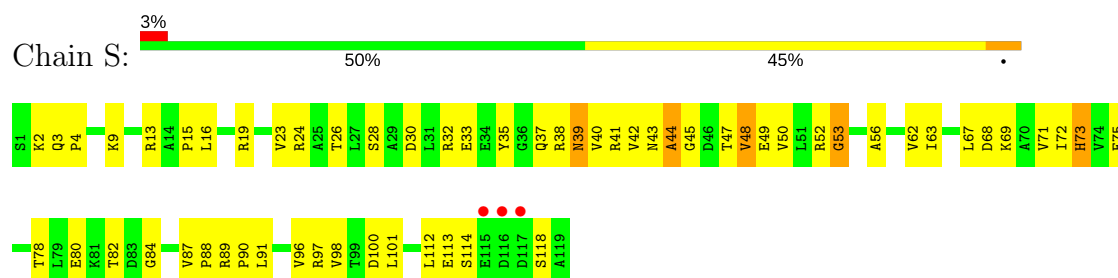
• Molecule 20: RIBOSOMAL PROTEIN L22



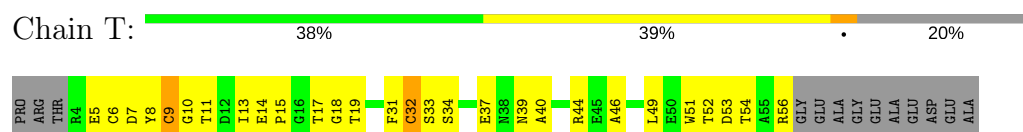
- Molecule 21: RIBOSOMAL PROTEIN L23



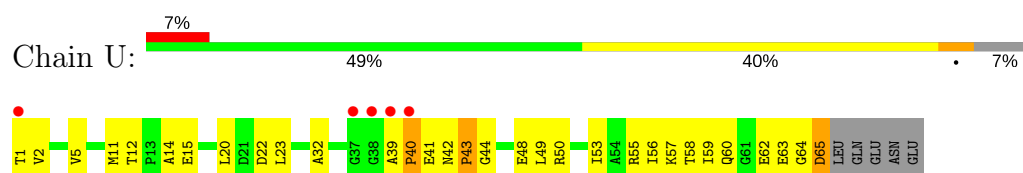
- Molecule 22: RIBOSOMAL PROTEIN L24



- Molecule 23: RIBOSOMAL PROTEIN L24E



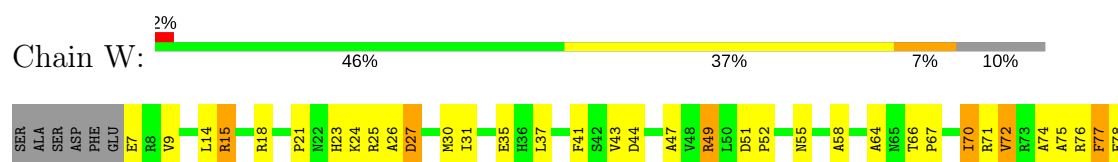
- Molecule 24: RIBOSOMAL PROTEIN L29



- Molecule 25: RIBOSOMAL PROTEIN L30



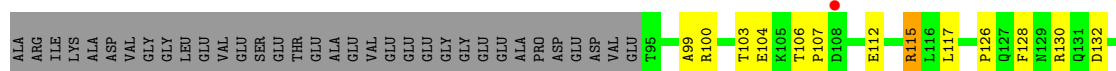
- Molecule 26: RIBOSOMAL PROTEIN L31E





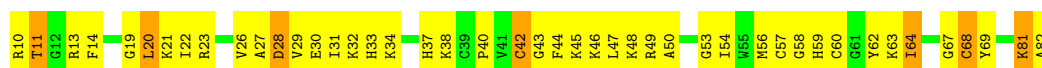
• Molecule 27: RIBOSOMAL PROTEIN L32E

Chain X: 39% 18% 41%



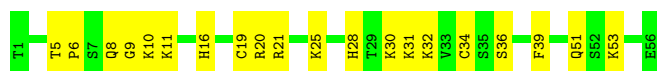
• Molecule 28: RIBOSOMAL PROTEIN L37AE

Chain Y: 38% 52% 10%



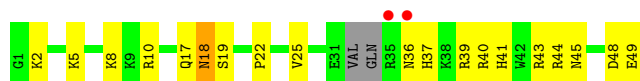
• Molecule 29: RIBOSOMAL PROTEIN L37E

Chain Z: 64% 36%



• Molecule 30: RIBOSOMAL PROTEIN L39E

Chain 1: 4% 56% 38%



• Molecule 31: RIBOSOMAL PROTEIN L44E

Chain 2: 2% 60% 35%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	213.66Å 300.71Å 575.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-3.00) 90.8 (20.00-2.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.77 (at 2.98Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.186 , 0.229 0.186 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	66.9	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 63.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	98635	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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, K, CD, SLD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	0	0.52	4/66076 (0.0%)	0.71	23/103052 (0.0%)
2	9	0.46	0/2905	0.76	3/4528 (0.1%)
3	4	0.89	0/65	1.01	0/99
4	A	0.39	0/1787	0.70	0/2409
5	B	0.40	0/2690	0.68	0/3652
6	C	0.45	0/1884	0.71	0/2551
7	D	0.37	0/1111	0.62	0/1498
8	E	0.38	0/1382	0.61	0/1880
9	F	0.38	0/897	0.60	0/1219
10	G	0.38	0/241	0.58	0/324
11	H	0.44	0/1247	0.79	3/1686 (0.2%)
12	I	0.43	0/1136	0.65	0/1530
13	J	0.41	0/1004	0.72	0/1351
14	K	0.41	0/1130	0.71	0/1509
15	L	0.49	0/1634	0.75	1/2180 (0.0%)
16	M	0.39	0/1474	0.68	0/1999
17	N	0.41	0/874	0.67	0/1181
18	O	0.41	0/1143	0.60	0/1521
19	P	0.44	0/749	0.74	1/1005 (0.1%)
20	Q	0.44	0/1172	0.69	0/1578
21	R	0.38	0/648	0.62	0/875
22	S	0.40	0/958	0.69	0/1289
23	T	0.61	2/417 (0.5%)	0.68	0/562
24	U	0.36	0/502	0.60	0/675
25	V	0.43	0/1219	0.67	0/1655
26	W	0.41	0/664	0.65	0/895
27	X	0.43	0/1146	0.68	0/1536
28	Y	0.54	1/576 (0.2%)	0.80	0/763
29	Z	0.54	0/438	0.78	2/578 (0.3%)
30	1	0.43	0/399	0.58	0/527
31	2	0.73	2/771 (0.3%)	0.72	0/1024
All	All	0.49	9/98339 (0.0%)	0.70	33/147131 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	70
2	9	0	2
25	V	0	1
All	All	0	73

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	14	CYS	CB-SG	-12.55	1.60	1.82
1	0	2102	G	C6-O6	-6.72	1.18	1.24
28	Y	60	CYS	CB-SG	-6.10	1.71	1.82
1	0	2474	A	N1-C2	5.85	1.39	1.34
23	T	9	CYS	CB-SG	-5.75	1.72	1.81

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	8.48	128.16	109.50
1	0	1979	G	C2'-C3'-O3'	6.90	124.75	113.70
11	H	74	ASN	N-CA-C	-6.85	92.50	111.00
2	9	3103	A	C5'-C4'-O4'	6.75	117.20	109.10
1	0	1563	G	C2'-C3'-O3'	6.72	124.45	113.70

There are no chirality outliers.

5 of 73 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	202	U	Sidechain
1	0	223	G	Sidechain
1	0	261	A	Sidechain
1	0	324	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	0	59017	0	29800	1222	0
2	9	2600	0	1326	88	0
3	4	59	0	35	2	0
4	A	1754	0	1763	127	0
5	B	2625	0	2533	170	0
6	C	1859	0	1816	112	0
7	D	1094	0	1085	125	0
8	E	1357	0	1266	65	0
9	F	886	0	854	67	0
10	G	240	0	231	22	0
11	H	1216	0	1215	155	0
12	I	1120	0	1098	69	0
13	J	994	0	1027	57	0
14	K	1118	0	1076	64	0
15	L	1606	0	1676	142	0
16	M	1445	0	1401	139	0
17	N	865	0	873	35	0
18	O	1133	0	1127	57	0
19	P	735	0	729	29	0
20	Q	1149	0	1122	61	0
21	R	641	0	605	24	0
22	S	950	0	923	53	0
23	T	410	0	364	33	0
24	U	499	0	511	32	0
25	V	1196	0	1137	97	0
26	W	654	0	653	46	0
27	X	1130	0	1133	51	0
28	Y	564	0	598	54	0
29	Z	431	0	426	24	0
30	1	394	0	406	32	0
31	2	755	0	729	51	0
32	0	37	0	28	4	0
33	0	107	0	0	0	0
33	2	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	2	0	0	0	0
35	0	73	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
36	0	8	0	0	1	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	P	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	2	1	0	0	2	0
37	N	1	0	0	0	0
37	T	1	0	0	0	0
37	Y	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5806	0	0	72	0
38	1	45	0	0	1	0
38	2	76	0	0	4	0
38	4	1	0	0	0	0
38	9	147	0	0	5	0
38	A	136	0	0	11	0
38	B	160	0	0	17	0
38	C	180	0	0	10	0
38	D	49	0	0	8	0
38	E	47	0	0	1	0
38	F	26	0	0	6	0
38	G	21	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	82	0	0	9	0
38	I	61	0	0	3	0
38	J	63	0	0	4	0
38	K	85	0	0	9	0
38	L	130	0	0	5	0
38	M	69	0	0	8	0
38	N	45	0	0	5	0
38	O	70	0	0	0	0
38	P	56	0	0	1	0
38	Q	92	0	0	4	0
38	R	40	0	0	1	0
38	S	37	0	0	3	0
38	T	27	0	0	2	0
38	U	13	0	0	1	0
38	V	74	0	0	6	0
38	W	29	0	0	3	0
38	X	105	0	0	4	0
38	Y	41	0	0	5	0
38	Z	57	0	0	1	0
All	All	98635	0	59566	2990	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 2990 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)
24:U:12:THR:HG22	24:U:15:GLU:HG3	1.24	1.14
13:J:10:GLN:NE2	13:J:10:GLN:H	1.47	1.13
1:O:871:G:H8	1:O:871:G:H5'	1.13	1.10
11:H:86:ARG:NH1	11:H:133:ILE:HG13	1.66	1.08
15:L:87:MET:HB3	31:2:46:ILE:HD13	1.31	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	
4	A	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	10	42
5	B	335/337 (99%)	300 (90%)	28 (8%)	7 (2%)	8	36
6	C	244/246 (99%)	213 (87%)	28 (12%)	3 (1%)	14	51
7	D	134/176 (76%)	96 (72%)	26 (19%)	12 (9%)	1	4
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	27	67
9	F	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	6	30
10	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	3	18
11	H	152/167 (91%)	132 (87%)	16 (10%)	4 (3%)	6	30
12	I	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	8	36
13	J	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	11	45
14	K	141/164 (86%)	116 (82%)	23 (16%)	2 (1%)	12	47
15	L	192/194 (99%)	167 (87%)	20 (10%)	5 (3%)	6	30
16	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	3	20
17	N	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	19	59
18	O	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	24	64
19	P	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	7	34
20	Q	148/154 (96%)	134 (90%)	14 (10%)	0	100	100
21	R	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
22	S	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	10	42
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	8	37
24	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	24
25	V	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	24	64
26	W	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	6	31
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100	100
28	Y	71/73 (97%)	58 (82%)	10 (14%)	3 (4%)	3	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Z	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
30	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
31	2	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	7	34
All	All	3633/4235 (86%)	3224 (89%)	338 (9%)	71 (2%)	8	37

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	139	ASP
7	D	93	LEU
7	D	95	THR
7	D	137	PRO
7	D	173	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	179/181 (99%)	168 (94%)	11 (6%)	20	57
5	B	282/282 (100%)	264 (94%)	18 (6%)	19	55
6	C	193/193 (100%)	178 (92%)	15 (8%)	14	45
7	D	117/147 (80%)	108 (92%)	9 (8%)	14	46
8	E	152/155 (98%)	146 (96%)	6 (4%)	35	73
9	F	92/92 (100%)	91 (99%)	1 (1%)	76	92
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	111 (91%)	11 (9%)	10	38
12	I	118/121 (98%)	110 (93%)	8 (7%)	17	52
13	J	106/106 (100%)	102 (96%)	4 (4%)	36	73
14	K	113/126 (90%)	108 (96%)	5 (4%)	31	69
15	L	166/166 (100%)	157 (95%)	9 (5%)	24	62
16	M	149/149 (100%)	141 (95%)	8 (5%)	24	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	93/93 (100%)	90 (97%)	3 (3%)	42	78
18	O	113/116 (97%)	109 (96%)	4 (4%)	39	75
19	P	79/79 (100%)	75 (95%)	4 (5%)	26	64
20	Q	117/121 (97%)	114 (97%)	3 (3%)	49	81
21	R	71/73 (97%)	69 (97%)	2 (3%)	47	80
22	S	105/105 (100%)	100 (95%)	5 (5%)	28	66
23	T	44/52 (85%)	44 (100%)	0	100	100
24	U	51/56 (91%)	49 (96%)	2 (4%)	35	73
25	V	130/130 (100%)	122 (94%)	8 (6%)	20	56
26	W	66/73 (90%)	62 (94%)	4 (6%)	20	57
27	X	120/195 (62%)	113 (94%)	7 (6%)	22	59
28	Y	56/56 (100%)	52 (93%)	4 (7%)	16	50
29	Z	46/46 (100%)	45 (98%)	1 (2%)	55	84
30	1	42/44 (96%)	41 (98%)	1 (2%)	52	83
31	2	79/79 (100%)	75 (95%)	4 (5%)	26	64
All	All	3028/3441 (88%)	2871 (95%)	157 (5%)	25	63

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	I	46	ILE
14	K	117	GLU
27	X	204	ARG
12	I	52	GLN
13	J	10	GLN

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

Mol	Chain	Res	Type
14	K	41	HIS
17	N	53	GLN
30	1	16	ASN
15	L	26	HIS
16	M	107	ASN



### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	241 (8%)	25 (0%)
2	9	121/122 (99%)	18 (14%)	3 (2%)
3	4	2/3 (66%)	1 (50%)	0
All	All	2868/3047 (94%)	260 (9%)	28 (0%)

5 of 260 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1450	C
1	0	1856	C
2	9	3024	U
1	0	1563	G
1	0	1667	A

## 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	$\# Z  > 2$
32	SLD	0	9500	-	37,39,39	4.57	16 (43%)	47,53,53	2.64	17 (36%)

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
32	SLD	0	9500	-	-	0/23/51/51	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	SLD	C9S-C8S	-9.92	1.35	1.50
32	0	9500	SLD	C9S-C0S	-5.74	1.43	1.51
32	0	9500	SLD	O1-C7	-3.60	1.41	1.46
32	0	9500	SLD	C3-C12	2.80	1.46	1.41
32	0	9500	SLD	F1-C11	3.50	1.44	1.35

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	SLD	O3-C6-N1	-8.71	122.04	128.97
32	0	9500	SLD	C5-N1-C6	-5.57	108.17	111.26
32	0	9500	SLD	C7-O1-C6	-2.93	107.83	110.22
32	0	9500	SLD	O1-C6-N1	-2.85	108.18	109.97
32	0	9500	SLD	CAS-N5S-C0S	-2.41	118.28	122.85

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9500	SLD	4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	0	2754/2922 (94%)	-0.44	32 (1%) 79 53	35, 63, 107, 150	0
2	9	122/122 (100%)	-0.02	5 (4%) 37 15	52, 80, 106, 150	0
3	4	3/3 (100%)	-0.43	0 100 100	49, 49, 51, 51	0
4	A	237/239 (99%)	-0.48	3 (1%) 77 51	44, 69, 101, 121	0
5	B	337/337 (100%)	-0.38	2 (0%) 89 71	42, 72, 98, 108	0
6	C	246/246 (100%)	-0.54	0 100 100	36, 63, 87, 99	0
7	D	140/176 (79%)	0.32	9 (6%) 19 6	70, 115, 131, 137	0
8	E	172/177 (97%)	-0.28	3 (1%) 70 41	61, 84, 102, 107	0
9	F	119/119 (100%)	-0.07	2 (1%) 70 41	70, 88, 112, 118	0
10	G	29/348 (8%)	0.09	1 (3%) 45 19	85, 105, 113, 117	0
11	H	156/167 (93%)	-0.30	2 (1%) 77 51	51, 72, 100, 108	0
12	I	142/145 (97%)	-0.51	0 100 100	50, 66, 85, 102	0
13	J	132/132 (100%)	-0.38	0 100 100	53, 71, 89, 96	0
14	K	145/164 (88%)	-0.29	2 (1%) 75 49	39, 83, 117, 129	0
15	L	194/194 (100%)	-0.63	0 100 100	47, 62, 79, 90	0
16	M	186/186 (100%)	-0.04	6 (3%) 47 20	58, 81, 120, 133	0
17	N	115/115 (100%)	-0.35	1 (0%) 84 62	56, 72, 90, 94	0
18	O	143/148 (96%)	-0.49	0 100 100	50, 72, 87, 94	0
19	P	95/95 (100%)	-0.48	1 (1%) 80 55	51, 62, 75, 88	0
20	Q	150/154 (97%)	-0.53	0 100 100	46, 61, 81, 88	0
21	R	81/84 (96%)	-0.35	1 (1%) 79 53	59, 76, 95, 103	0
22	S	119/119 (100%)	-0.34	3 (2%) 57 29	55, 74, 97, 113	0
23	T	53/66 (80%)	-0.31	0 100 100	57, 73, 92, 99	0
24	U	65/70 (92%)	0.11	5 (7%) 13 4	68, 91, 123, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	V	154/154 (100%)	-0.54	0 100 100	51, 64, 82, 94	0
26	W	82/91 (90%)	-0.25	2 (2%) 59 30	58, 75, 99, 117	0
27	X	142/240 (59%)	-0.60	1 (0%) 87 68	43, 61, 82, 101	0
28	Y	73/73 (100%)	-0.28	0 100 100	62, 76, 95, 104	0
29	Z	56/56 (100%)	-0.71	0 100 100	42, 52, 58, 68	0
30	1	46/48 (95%)	-0.15	2 (4%) 35 13	49, 77, 105, 117	0
31	2	92/92 (100%)	-0.19	2 (2%) 62 33	53, 73, 87, 98	0
All	All	6580/7282 (90%)	-0.38	85 (1%) 77 51	35, 69, 108, 150	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	6.1
1	0	2250	G	5.8
22	S	116	ASP	4.8
2	9	3025	G	4.7
24	U	1	THR	4.5

## 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
35	NA	9	8351	1/1	0.33	0.25	94,94,94,94	0
35	NA	Q	8386	1/1	0.43	0.64	107,107,107,107	0
35	NA	0	8384	1/1	0.48	0.62	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8363	1/1	0.49	0.62	83,83,83,83	0
35	NA	R	8312	1/1	0.53	0.92	84,84,84,84	0
35	NA	0	8329	1/1	0.56	1.24	98,98,98,98	0
35	NA	0	8371	1/1	0.65	0.72	69,69,69,69	0
33	MG	0	8049	1/1	0.66	0.33	90,90,90,90	0
35	NA	H	8322	1/1	0.70	0.41	78,78,78,78	0
35	NA	0	8324	1/1	0.71	0.39	58,58,58,58	0
35	NA	0	8361	1/1	0.73	0.36	77,77,77,77	0
34	K	0	8201	1/1	0.75	0.12	141,141,141,141	0
33	MG	0	8024	1/1	0.76	0.62	98,98,98,98	0
35	NA	0	8368	1/1	0.77	0.36	69,69,69,69	0
35	NA	0	8340	1/1	0.77	0.37	69,69,69,69	0
35	NA	0	8385	1/1	0.78	0.36	73,73,73,73	0
35	NA	0	8341	1/1	0.78	0.34	60,60,60,60	0
35	NA	9	8383	1/1	0.78	0.38	67,67,67,67	0
33	MG	0	8114	1/1	0.79	0.69	95,95,95,95	0
35	NA	0	8352	1/1	0.80	0.33	61,61,61,61	0
35	NA	0	8382	1/1	0.80	0.17	89,89,89,89	0
37	CD	N	8405	1/1	0.80	0.23	150,150,150,150	0
35	NA	0	8332	1/1	0.80	0.37	50,50,50,50	0
35	NA	0	8362	1/1	0.81	0.25	79,79,79,79	0
35	NA	0	8323	1/1	0.81	0.44	66,66,66,66	0
35	NA	0	8326	1/1	0.81	0.30	73,73,73,73	0
34	K	0	8202	1/1	0.81	0.77	92,92,92,92	0
35	NA	0	8307	1/1	0.82	0.32	71,71,71,71	0
36	CL	0	8505	1/1	0.82	0.44	99,99,99,99	0
33	MG	A	8105	1/1	0.82	0.30	52,52,52,52	0
35	NA	0	8366	1/1	0.82	0.36	82,82,82,82	0
33	MG	0	8113	1/1	0.83	0.10	60,60,60,60	0
35	NA	0	8365	1/1	0.83	0.43	47,47,47,47	0
36	CL	K	8510	1/1	0.83	0.25	104,104,104,104	0
35	NA	0	8378	1/1	0.84	0.75	65,65,65,65	0
33	MG	0	8102	1/1	0.84	0.38	91,91,91,91	0
35	NA	0	8316	1/1	0.84	0.21	52,52,52,52	0
35	NA	0	8369	1/1	0.84	0.35	96,96,96,96	0
35	NA	0	8360	1/1	0.84	0.41	69,69,69,69	0
36	CL	0	8515	1/1	0.85	0.30	100,100,100,100	0
33	MG	0	8071	1/1	0.85	0.07	104,104,104,104	0
33	MG	0	8013	1/1	0.85	0.17	60,60,60,60	0
33	MG	0	8092	1/1	0.86	0.37	111,111,111,111	0
35	NA	0	8350	1/1	0.86	0.28	57,57,57,57	0
33	MG	0	8066	1/1	0.86	0.17	105,105,105,105	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8313	1/1	0.86	0.21	89,89,89,89	0
33	MG	0	8046	1/1	0.87	0.15	86,86,86,86	0
35	NA	0	8381	1/1	0.87	0.31	69,69,69,69	0
35	NA	0	8325	1/1	0.87	0.28	64,64,64,64	0
36	CL	P	8511	1/1	0.87	0.37	84,84,84,84	0
35	NA	0	8364	1/1	0.88	0.24	66,66,66,66	0
33	MG	0	8085	1/1	0.88	0.22	92,92,92,92	0
36	CL	B	8519	1/1	0.88	0.38	95,95,95,95	0
35	NA	0	8374	1/1	0.88	0.14	77,77,77,77	0
35	NA	0	8328	1/1	0.88	0.22	55,55,55,55	0
33	MG	0	8011	1/1	0.88	0.19	50,50,50,50	0
33	MG	0	8022	1/1	0.88	0.58	83,83,83,83	0
33	MG	0	8045	1/1	0.89	0.25	91,91,91,91	0
36	CL	N	8508	1/1	0.89	0.22	116,116,116,116	0
35	NA	0	8333	1/1	0.89	0.26	40,40,40,40	0
33	MG	S	8073	1/1	0.89	0.14	71,71,71,71	0
33	MG	0	8003	1/1	0.89	0.15	51,51,51,51	0
33	MG	0	8076	1/1	0.89	0.16	102,102,102,102	0
35	NA	0	8370	1/1	0.90	0.40	76,76,76,76	0
36	CL	I	8502	1/1	0.90	0.11	93,93,93,93	0
36	CL	A	8509	1/1	0.90	0.72	89,89,89,89	0
35	NA	0	8311	1/1	0.90	0.26	73,73,73,73	0
35	NA	P	8348	1/1	0.90	0.09	68,68,68,68	0
33	MG	0	8028	1/1	0.90	0.17	57,57,57,57	0
36	CL	2	8504	1/1	0.90	0.49	100,100,100,100	0
35	NA	0	8375	1/1	0.91	0.69	81,81,81,81	0
35	NA	Q	8337	1/1	0.91	0.26	64,64,64,64	0
35	NA	0	8357	1/1	0.91	0.26	61,61,61,61	0
33	MG	0	8097	1/1	0.91	0.30	53,53,53,53	0
36	CL	I	8501	1/1	0.91	0.18	99,99,99,99	0
33	MG	0	8104	1/1	0.92	0.14	66,66,66,66	0
33	MG	0	8111	1/1	0.92	0.12	75,75,75,75	0
35	NA	0	8310	1/1	0.92	0.20	46,46,46,46	0
33	MG	0	8107	1/1	0.92	0.09	55,55,55,55	0
33	MG	0	8100	1/1	0.92	0.19	97,97,97,97	0
36	CL	Q	8506	1/1	0.92	0.23	80,80,80,80	0
33	MG	0	8081	1/1	0.92	0.08	67,67,67,67	0
36	CL	0	8513	1/1	0.92	0.24	74,74,74,74	0
33	MG	0	8103	1/1	0.92	0.42	97,97,97,97	0
35	NA	0	8377	1/1	0.92	0.58	75,75,75,75	0
33	MG	0	8054	1/1	0.93	0.19	45,45,45,45	0
35	NA	0	8336	1/1	0.93	0.13	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8330	1/1	0.93	0.11	61,61,61,61	0
35	NA	C	8304	1/1	0.93	0.38	51,51,51,51	0
36	CL	0	8503	1/1	0.93	0.30	82,82,82,82	0
33	MG	0	8115	1/1	0.93	0.12	73,73,73,73	0
35	NA	0	8308	1/1	0.93	0.25	77,77,77,77	0
35	NA	0	8372	1/1	0.93	0.74	72,72,72,72	0
33	MG	0	8112	1/1	0.93	0.15	64,64,64,64	0
33	MG	9	8095	1/1	0.93	0.36	106,106,106,106	0
35	NA	0	8353	1/1	0.93	0.14	43,43,43,43	0
32	SLD	0	9500	37/37	0.93	0.21	46,50,53,59	0
33	MG	0	8082	1/1	0.93	0.16	79,79,79,79	0
35	NA	0	8354	1/1	0.93	0.41	58,58,58,58	0
33	MG	0	8108	1/1	0.93	0.27	102,102,102,102	0
33	MG	0	8099	1/1	0.93	0.23	80,80,80,80	0
33	MG	0	8116	1/1	0.94	0.17	84,84,84,84	0
35	NA	0	8321	1/1	0.94	0.42	67,67,67,67	0
33	MG	J	8069	1/1	0.94	0.05	87,87,87,87	0
36	CL	0	8514	1/1	0.94	0.13	75,75,75,75	0
33	MG	0	8035	1/1	0.94	0.06	69,69,69,69	0
33	MG	0	8062	1/1	0.94	0.09	90,90,90,90	0
35	NA	0	8317	1/1	0.94	0.11	57,57,57,57	0
35	NA	0	8373	1/1	0.94	0.24	57,57,57,57	0
33	MG	0	8067	1/1	0.94	0.12	81,81,81,81	0
36	CL	M	8507	1/1	0.94	0.24	86,86,86,86	0
33	MG	0	8020	1/1	0.94	0.19	53,53,53,53	0
35	NA	0	8356	1/1	0.94	0.96	73,73,73,73	0
35	NA	0	8359	1/1	0.94	0.15	81,81,81,81	0
35	NA	0	8338	1/1	0.94	0.08	66,66,66,66	0
33	MG	0	8064	1/1	0.94	0.37	39,39,39,39	0
33	MG	0	8029	1/1	0.95	0.07	60,60,60,60	0
35	NA	0	8335	1/1	0.95	0.17	83,83,83,83	0
35	NA	0	8334	1/1	0.95	0.20	48,48,48,48	0
33	MG	0	8053	1/1	0.95	0.29	63,63,63,63	0
33	MG	0	8072	1/1	0.95	0.33	78,78,78,78	0
36	CL	I	8521	1/1	0.95	0.25	69,69,69,69	0
33	MG	0	8034	1/1	0.95	0.10	46,46,46,46	0
36	CL	0	8517	1/1	0.95	0.33	82,82,82,82	0
33	MG	0	8051	1/1	0.95	0.19	97,97,97,97	0
35	NA	0	8303	1/1	0.95	0.49	55,55,55,55	0
33	MG	0	8018	1/1	0.95	0.09	57,57,57,57	0
33	MG	0	8101	1/1	0.95	0.14	94,94,94,94	0
33	MG	0	8087	1/1	0.95	0.07	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8339	1/1	0.95	0.13	33,33,33,33	0
33	MG	B	8055	1/1	0.95	0.06	71,71,71,71	0
33	MG	0	8090	1/1	0.95	0.33	81,81,81,81	0
35	NA	0	8376	1/1	0.95	0.46	79,79,79,79	0
33	MG	0	8016	1/1	0.96	0.07	71,71,71,71	0
33	MG	0	8026	1/1	0.96	0.08	39,39,39,39	0
33	MG	0	8001	1/1	0.96	0.17	46,46,46,46	0
35	NA	0	8367	1/1	0.96	0.25	85,85,85,85	0
33	MG	0	8042	1/1	0.96	0.15	61,61,61,61	0
33	MG	0	8008	1/1	0.96	0.16	52,52,52,52	0
35	NA	L	8347	1/1	0.96	0.13	55,55,55,55	0
33	MG	0	8075	1/1	0.96	0.09	77,77,77,77	0
33	MG	0	8031	1/1	0.96	0.12	54,54,54,54	0
33	MG	0	8060	1/1	0.96	0.15	63,63,63,63	0
36	CL	J	8512	1/1	0.96	0.21	67,67,67,67	0
33	MG	0	8044	1/1	0.96	0.27	59,59,59,59	0
36	CL	L	8518	1/1	0.96	0.10	69,69,69,69	0
35	NA	A	8345	1/1	0.96	0.10	48,48,48,48	0
33	MG	0	8096	1/1	0.96	0.09	70,70,70,70	0
33	MG	9	8052	1/1	0.96	0.10	60,60,60,60	0
33	MG	0	8110	1/1	0.96	0.12	56,56,56,56	0
33	MG	X	8109	1/1	0.96	0.17	66,66,66,66	0
35	NA	0	8301	1/1	0.96	0.12	59,59,59,59	0
35	NA	0	8306	1/1	0.96	0.38	59,59,59,59	0
33	MG	0	8009	1/1	0.96	0.18	44,44,44,44	0
33	MG	0	8057	1/1	0.96	0.08	53,53,53,53	0
35	NA	0	8302	1/1	0.96	0.16	55,55,55,55	0
35	NA	0	8343	1/1	0.96	0.14	48,48,48,48	0
35	NA	0	8358	1/1	0.96	0.28	109,109,109,109	0
33	MG	0	8040	1/1	0.96	0.08	88,88,88,88	0
33	MG	0	8088	1/1	0.96	0.22	40,40,40,40	0
36	CL	0	8516	1/1	0.96	0.26	64,64,64,64	0
33	MG	0	8079	1/1	0.96	0.12	53,53,53,53	0
33	MG	0	8043	1/1	0.97	0.07	64,64,64,64	0
33	MG	0	8019	1/1	0.97	0.15	43,43,43,43	0
35	NA	0	8305	1/1	0.97	0.08	42,42,42,42	0
33	MG	0	8086	1/1	0.97	0.06	62,62,62,62	0
33	MG	2	8078	1/1	0.97	0.04	65,65,65,65	0
36	CL	0	8522	1/1	0.97	0.63	92,92,92,92	0
35	NA	0	8355	1/1	0.97	0.40	77,77,77,77	0
33	MG	0	8050	1/1	0.97	0.14	68,68,68,68	0
35	NA	0	8318	1/1	0.97	0.23	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	X	8520	1/1	0.97	0.28	57,57,57,57	0
33	MG	0	8070	1/1	0.97	0.07	63,63,63,63	0
33	MG	0	8002	1/1	0.97	0.09	51,51,51,51	0
33	MG	0	8025	1/1	0.97	0.06	59,59,59,59	0
35	NA	K	8380	1/1	0.97	0.36	85,85,85,85	0
35	NA	0	8327	1/1	0.97	0.10	46,46,46,46	0
33	MG	0	8089	1/1	0.97	0.07	82,82,82,82	0
35	NA	0	8314	1/1	0.97	0.23	53,53,53,53	0
33	MG	0	8004	1/1	0.97	0.19	50,50,50,50	0
33	MG	4	8063	1/1	0.97	0.11	62,62,62,62	0
33	MG	0	8106	1/1	0.97	0.26	78,78,78,78	0
35	NA	0	8344	1/1	0.97	0.12	48,48,48,48	0
35	NA	0	8379	1/1	0.97	0.24	48,48,48,48	0
33	MG	0	8036	1/1	0.97	0.06	52,52,52,52	0
33	MG	0	8117	1/1	0.98	0.07	45,45,45,45	0
33	MG	0	8007	1/1	0.98	0.12	47,47,47,47	0
33	MG	0	8027	1/1	0.98	0.08	65,65,65,65	0
33	MG	0	8037	1/1	0.98	0.07	54,54,54,54	0
33	MG	0	8083	1/1	0.98	0.07	65,65,65,65	0
33	MG	0	8048	1/1	0.98	0.06	66,66,66,66	0
33	MG	0	8077	1/1	0.98	0.13	54,54,54,54	0
35	NA	0	8349	1/1	0.98	0.44	69,69,69,69	0
35	NA	0	8331	1/1	0.98	0.12	60,60,60,60	0
33	MG	0	8041	1/1	0.98	0.24	68,68,68,68	0
33	MG	0	8059	1/1	0.98	0.06	60,60,60,60	0
33	MG	0	8039	1/1	0.98	0.10	53,53,53,53	0
33	MG	0	8006	1/1	0.98	0.28	60,60,60,60	0
33	MG	0	8084	1/1	0.98	0.05	70,70,70,70	0
33	MG	0	8032	1/1	0.98	0.08	52,52,52,52	0
33	MG	0	8014	1/1	0.98	0.18	46,46,46,46	0
33	MG	0	8098	1/1	0.98	0.06	50,50,50,50	0
35	NA	0	8315	1/1	0.98	0.19	70,70,70,70	0
33	MG	0	8047	1/1	0.98	0.10	90,90,90,90	0
33	MG	0	8058	1/1	0.98	0.11	61,61,61,61	0
37	CD	Y	8403	1/1	0.98	0.07	84,84,84,84	0
35	NA	0	8319	1/1	0.98	0.18	41,41,41,41	0
35	NA	H	8309	1/1	0.98	0.25	49,49,49,49	0
33	MG	0	8033	1/1	0.98	0.11	48,48,48,48	0
35	NA	0	8320	1/1	0.98	0.20	40,40,40,40	0
33	MG	0	8074	1/1	0.98	0.07	51,51,51,51	0
33	MG	0	8093	1/1	0.98	0.10	63,63,63,63	0
35	NA	0	8342	1/1	0.98	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	I	8346	1/1	0.99	0.08	45,45,45,45	0
37	CD	Z	8402	1/1	0.99	0.07	89,89,89,89	0
37	CD	T	8401	1/1	0.99	0.07	83,83,83,83	0
33	MG	0	8038	1/1	0.99	0.19	56,56,56,56	0
33	MG	0	8094	1/1	0.99	0.07	97,97,97,97	0
33	MG	0	8056	1/1	0.99	0.09	60,60,60,60	0
33	MG	0	8061	1/1	0.99	0.05	45,45,45,45	0
33	MG	0	8023	1/1	0.99	0.06	46,46,46,46	0
33	MG	0	8030	1/1	0.99	0.16	48,48,48,48	0
33	MG	A	8065	1/1	0.99	0.15	55,55,55,55	0
33	MG	0	8068	1/1	0.99	0.06	64,64,64,64	0
37	CD	2	8404	1/1	0.99	0.09	90,90,90,90	0
33	MG	0	8012	1/1	0.99	0.06	42,42,42,42	0
33	MG	0	8080	1/1	0.99	0.08	52,52,52,52	0
33	MG	0	8017	1/1	0.99	0.15	43,43,43,43	0
33	MG	0	8010	1/1	0.99	0.10	47,47,47,47	0
33	MG	0	8015	1/1	0.99	0.11	60,60,60,60	0
33	MG	0	8005	1/1	0.99	0.10	58,58,58,58	0
33	MG	0	8021	1/1	0.99	0.18	54,54,54,54	0
33	MG	0	8091	1/1	0.99	0.06	65,65,65,65	0

## 6.5 Other polymers

There are no such residues in this entry.