



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:30 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk28620

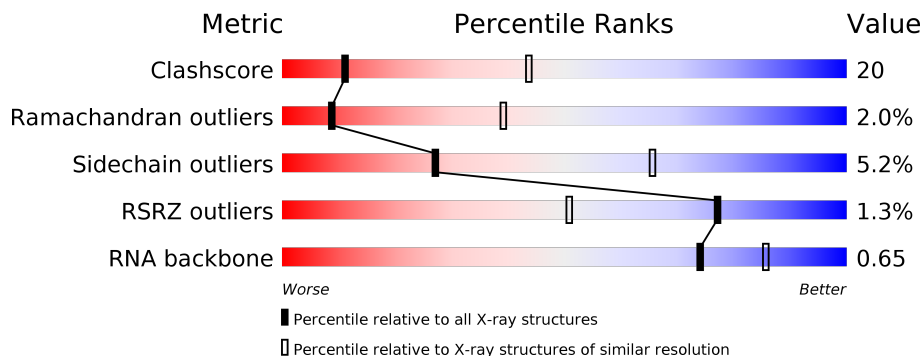
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)
RNA backbone	2435	1007 (3.34-2.66)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>41%</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>12%</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>
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	8006	-	-	-	X
33	MG	0	8020	-	-	-	X
33	MG	0	8038	-	-	-	X
33	MG	0	8044	-	-	-	X
33	MG	0	8049	-	-	-	X
33	MG	0	8053	-	-	-	X
33	MG	0	8054	-	-	-	X
33	MG	0	8064	-	-	-	X
33	MG	0	8108	-	-	-	X
34	K	0	8202	-	-	-	X
35	NA	0	8303	-	-	-	X
35	NA	0	8308	-	-	-	X
35	NA	0	8310	-	-	-	X
35	NA	0	8320	-	-	-	X
35	NA	0	8321	-	-	-	X
35	NA	0	8323	-	-	-	X
35	NA	0	8324	-	-	-	X
35	NA	0	8325	-	-	-	X
35	NA	0	8326	-	-	-	X
35	NA	0	8332	-	-	-	X
35	NA	0	8333	-	-	-	X
35	NA	0	8335	-	-	-	X
35	NA	0	8350	-	-	-	X
35	NA	0	8356	-	-	-	X
35	NA	0	8361	-	-	-	X
35	NA	0	8362	-	-	-	X
35	NA	0	8364	-	-	-	X
35	NA	0	8365	-	-	-	X
35	NA	0	8366	-	-	-	X
35	NA	0	8367	-	-	-	X
35	NA	0	8368	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8372	-	-	-	X
35	NA	0	8373	-	-	-	X
35	NA	0	8376	-	-	-	X
35	NA	0	8377	-	-	-	X
35	NA	0	8378	-	-	-	X
35	NA	0	8379	-	-	-	X
35	NA	9	8383	-	-	-	X
35	NA	K	8380	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	NA	Q	8386	-	-	-	X
36	CL	0	8505	-	-	-	X
36	CL	2	8504	-	-	-	X
36	CL	B	8519	-	-	-	X
36	CL	I	8521	-	-	-	X
36	CL	J	8512	-	-	-	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			

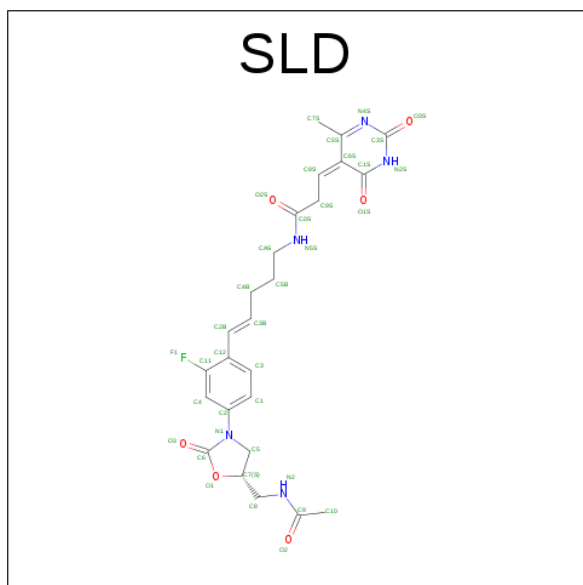
There is a discrepancy between the modelled and reference sequences:

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		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	2	1	Total 1	Mg 1	0	0
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 Cl 8 8	0	0
36	P	1	Total Cl 1 1	0	0
36	J	1	Total Cl 1 1	0	0
36	Q	1	Total Cl 1 1	0	0
36	K	1	Total Cl 1 1	0	0
36	B	1	Total Cl 1 1	0	0
36	I	3	Total Cl 3 3	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	X	1	Total Cl 1 1	0	0
36	2	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	M	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	Z	1	Total Cd 1 1	0	0
37	Y	1	Total Cd 1 1	0	0
37	T	1	Total Cd 1 1	0	0
37	2	1	Total Cd 1 1	0	0
37	N	1	Total Cd 1 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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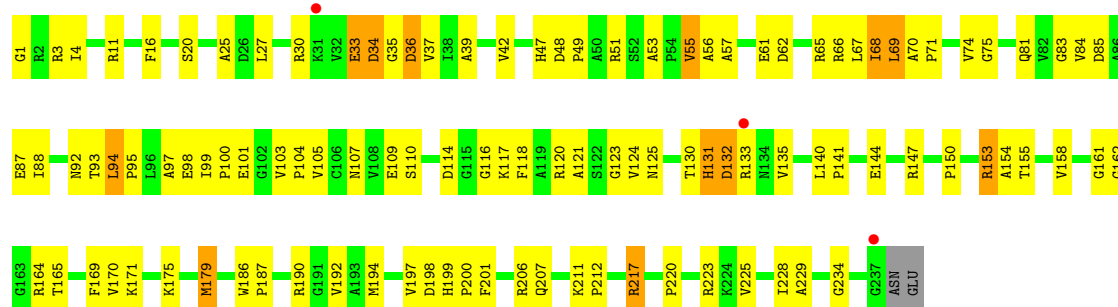
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	27	Total 27	O 27	0	0
38	U	13	Total 13	O 13	0	0
38	V	74	Total 74	O 74	0	0
38	W	29	Total 29	O 29	0	0
38	X	105	Total 105	O 105	0	0
38	Y	41	Total 41	O 41	0	0
38	Z	57	Total 57	O 57	0	0
38	1	45	Total 45	O 45	0	0
38	2	76	Total 76	O 76	0	0



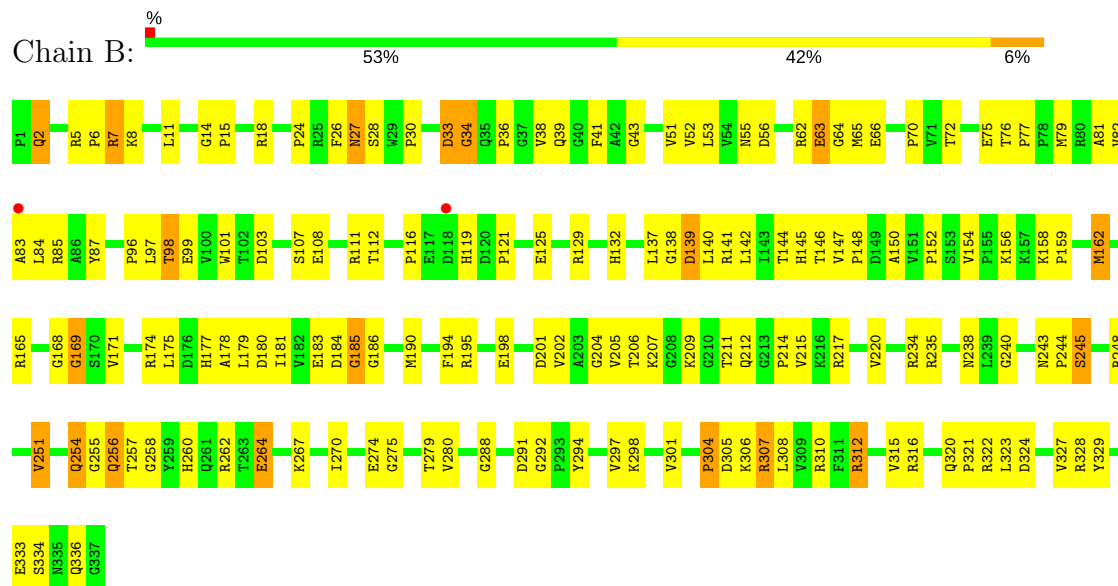


A	G2082	C1988	A1910	U1748	A1656	C1574	G1498	U1419	A1313	G1223	A1154	U1029	G958
U	A2083	U1992	G1917	G1751	A1657	C1575	U1499	C1420	U1314	G1224	G1155	U1030	C959
G	A1993	C1993	U1918	G1752	A1658	A1580	U1500	U1421	U1320	C1225	C1156	G1031	G960
U	A2090	A1994	C1920	A1755	C1666	C1584	U1503	U1422	A1321	G1226	G1158	G1044	A961
G	G2090	U1995	C1921	G1756	U1668	C1585	U1504	C1424	G1322	G1229	G1159	G1045	C962
A	G2091	U1996	A1922	U1757	A1669	G1586	U1505	G1425	G1323	C1230	G1160	G1059	C963
G	G2094	G2000	A1925	U1758	G1670	U1587	U1506	C1426	G1324	G1231	G1161	G1060	G964
A	A2095	G2001	G1926	A1759	C1675	C1592	U1511	A1427	G1325	U1234	G1162	G1062	G968
G	A2096	C2002	U1927	G1760	G1676	C1593	G1512	G1430	A1328	G1235	G1163	G1065	G969
A	U2003	U2003	U1928	U1761	U1677	C1594	C1513	G1431	A1329	U1236	U1170	U1064	U970
C	A2101	G2004	C1928	G1762	A1677	G1594	C1514	U1432	A1330	G1238	G1172	G1065	G
A	G2102	G2005	G1929	C1763	A1678	G1595	A1515	G1433	A1331	G1239	G1173	G1069	U
C	C2105	U2008	A1930	U1766	C1679	U1596	C1516	A1434	G1332	A1242	U1174	A1070	C
U	C2106	U2009	A1931	A1767	A1682	U1597	U1517	U1435	U1333	A1243	G1175	G1071	U
A	U2107	A2011	G1932	C1768	A1683	U1598	U1518	C1436	C1334	U1244	A1176	G1072	C
C	G2110	U2012	U1934	G1769	A1684	G1600	G1520	U1440	C1335	C1245	A1177	C1069	C
A	G2111	G2013	C1936	U1770	A1685	A1603	C1521	G1441	C1342	A1246	G1178	A1078	C
G	A2112	U2014	U1937	C1772	C1687	G1604	U1522	G1442	C1343	A1247	U1180	G1079	G
G	G2113	U2015	G1938	G1773	C1688	G1605	U1523	G1443	C1344	U1248	A1181	G1087	C
U	U2114	U2016	U1939	G1774	C1692	G1606	U1524	G1444	A1345	U1249	C1182	G1088	U
A	U2115	G2023	A1852	G1775	C1693	G1607	U1525	G1445	U1346	C1250	C1183	A1078	G
C	U2116	U2024	C1853	G1776	C1694	G1608	A1526	G1446	A1347	C1251	G1184	C1080	A
C	C2119	U2025	C1854	A1778	G1697	G1609	A1527	C1447	A1348	A1252	C1185	C1081	G
C	U2120	C2029	G1855	U1779	U1698	G1610	A1528	C1448	C1349	C1253	U1186	A1086	A
G	G2121	A2030	C1856	G1780	C1699	A1612	G1529	G1449	C1350	U1254	C1187	G1087	G
C	G2122	U2031	A1857	G1781	U1701	G1613	U1530	U1450	C1351	U1255	U1188	A1088	A
G	G2123	G2033	G1858	G1782	U1702	G1614	G1531	U1451	C1352	U1256	C1189	G1089	G
C	U2124	U2034	C1859	U1783	A1710	A1615	C1532	U1452	U1353	C1257	G1190	U1109	U
U	G2125	C2035	G1860	U1784	U1711	A1616	C1533	U1453	C1354	U1258	A1191	G1110	C
A	G2126	U2036	C1861	C1787	A1712	G1617	U1534	U1454	C1355	C1259	A1192	G1111	G
G	G2127	G2037	C1862	U1788	G1713	G1618	U1535	G1455	C1356	C1273	A1193	A1114	C
C	U2128	A2039	C1863	G1789	C1714	A1624	C1545	U1456	A1372	U1276	G1196	U1115	A
G	A2135	C2040	G1790	G1715	C1716	U1625	G1546	U1457	C1373	G1277	G1197	U1116	C
G	G2136	G2041	U1791	A1716	A1696	A1696	A1547	A1463	C1374	U1278	U1198	A1117	A
C	A	U2042	C1792	A1717	G1627	G1627	U1548	U1464	C1375	U1279	U1199	A1118	C
C	C	G2044	C1793	U1718	C1633	C1633	C1549	C1474	C1376	U1280	A1200	G1119	C
A	G	U2045	C1794	U1719	G1634	G1634	U1550	U1475	C1377	G1281	C1201	U1120	A
C	C	G2046	U1722	U1720	U1635	U1635	C1551	U1476	C1378	G1282	C1202	G1121	C
A	U	A2054	G1723	G1721	U1636	U1636	C1552	C1477	C1379	G1283	A1203	U1122	C
C	C	A2055	U1724	U1722	U1637	U1637	C1553	U1478	C1380	G1284	C1204	A1123	C
C	U	C2056	C1725	C1725	A1637	A1637	C1554	C1479	C1381	C1285	U1205	C1129	C
G	G	G2057	G1730	G1726	U1638	U1638	U1555	U1480	C1382	G1286	U1206	U1130	A
A	A	A2060	U1731	U1727	U1639	U1639	U1556	U1481	C1383	G1287	A1207	G1131	C
C	C	C2061	A1732	A1728	C1640	C1640	U1557	U1482	C1384	U1288	C1208	A1132	C
A	A	A2062	U1733	U1729	A1641	A1641	C1558	U1483	C1385	G1289	C1209	U1133	A
C	C	U2063	G1734	G1734	C1642	C1642	C1559	U1484	C1386	G1290	G1210	G1134	C
A	A	G2064	C1735	C1735	C1643	C1643	C1560	U1485	C1387	G1291	G1211	G1135	C
C	C	C2065	A1736	A1736	C1644	C1644	C1561	U1486	C1388	U1304	C1212	G1137	C
U	U	G2070	U1737	U1737	U1645	U1645	C1562	U1487	A1407	C1305	C1213	G1138	C
A	A	A2071	U1738	U1738	G1646	G1646	C1563	U1488	U1408	U1306	G1214	U1139	C
C	C	G2072	G1742	G1742	C1647	C1647	C1564	U1489	C1389	C1307	C1215	C1140	C
A	A	U2073	G1743	G1743	C1648	C1648	C1565	U1490	G1390	G1216	G1217	G1150	C
G	G	A2074	G1744	G1744	C1649	C1649	C1566	U1491	C1391	U1310	U1218	G1151	C
A	A	U2075	U1745	U1745	U1650	U1650	C1567	U1492	C1392	G1312	G1219	G1152	C
C	C	C2076	C1746	C1746	C1651	C1651	U1568	U1493	C1393	U1311	U1219	G1153	C
U	U	A2077	G1747	G1747	C1652	C1652	U1569	U1494	C1394	U1312	U1220	G1154	C
A	A	U2078	U1748	U1748	C1653	C1653	U1570	U1495	C1395	U1313	U1221	G1155	C
C	C	G2079	G1749	G1749	C1654	C1654	U1571	U1496	C1396	U1314	U1222	G1156	C
A	A	U2080	U1749	U1749	C1655	C1655	U1572	U1497	C1397	U1315	U1223	G1157	C
C	C	A2081	G1750	G1750	C1656	C1656	U1573	U1498	C1398	U1316	U1224	G1158	C
U	U	U2082	U1751	U1751	C1657	C1657	U1574	U1499	C1399	U1317	U1225	G1159	C
A	A	C2083	U1752	U1752	C1658	C1658	U1575	U1500	C1400	U1318	U1226	G1160	C
C	C	G2084	G1753	G1753	C1659	C1659	U1576	U1501	C1401	U1319	U1227	G1161	C
A	A	U2085	U1754	U1754	C1660	C1660	U1577	U1502	C1402	U1320	U1228	G1162	C
C	C	A2086	U1755	U1755	C1661	C1661	U1578	U1503	C1403	U1321	U1229	G1163	C
U	U	U2087	U1756	U1756	C1662	C1662	U1579	U1504	C1404	U1322	U1230	G1164	C
A	A	C2088	U1757	U1757	C1663	C1663	U1580	U1505	C1405	U1323	U1231	G1165	C
C	C	G2089	U1758	U1758	C1664	C1664	U1581	U1506	C1406	U1324	U1232	G1166	C
A	A	U2090	U1759	U1759	C1665	C1665	U1582	U1507	C1407	U1325	U1233	G1167	C
C	C	A2091	U1760	U1760	C1666	C1666	U1583	U1508	C1408	U1326	U1234	G1168	C
U	U	U2092	U1761	U1761	C1667	C1667	U1584	U1509	C1409	U1327	U1235	G1169	C
A	A	C2093	U1762	U1762	C1668	C1668	U1585	U1510	C1410	U1328	U1236	G1170	C
C	C	G2094	U1763	U1763	C1669	C1669	U1586	U1511	C1411	U1329	U1237	G1171	C
A	A	U2095	U1764	U1764	C1670	C1670	U1587	U1512	C1412	U1330	U1238	G1172	C
C	C	A2096	U1765	U1765	C1671	C1671	U1588	U1513	C1413	U1331	U1239	G1173	C
U	U	U2097	U1766	U1766	C1672	C1672	U1589	U1514	C1414	U1332	U1240	G1174	C
A	A	C2098	U1767	U1767	C1673	C1673	U1590	U1515	C1415	U1333	U1241	G1175	C
C	C	G2099	U1768	U1768	C1674	C1674	U1591	U1516	C1416	U1334	U1242	G1176	C
A	A	U2100	U1769	U1769	C1675	C1675	U1592	U1517	C1417	U1335	U1243	G1177	C
C	C	A2101	U1770	U1770	C1676	C1676	U1593	U1518	C1418	U1336	U1244	G1178	C
U	U	U2102	U1771	U1771	C1677	C1677	U1594	U1519	C1419	U1337	U1245	G1179	C
A	A	C2103	U1772	U1772	C1678	C1678	U1595	U1520	C1420	U1338	U1246	G1180	C
C	C	G2104	U1773	U1773	C1679	C1679	U1596	U1521	C1421	U1339	U1247	G1181	C
A	A	U2105	U1774	U1774	C1680	C1680	U1597	U1522	C1422	U1340	U1248	G1182	C
C	C	A2106	U1775	U1775	C1681	C1681	U1598	U1523	C1423	U1341	U1249	G1183	C
U	U	U2107	U1776	U1776	C1682	C1682	U1599	U1524	C1424	U1342	U1250	G1184	C
A	A	C2108	U1777	U1777	C1683	C1683	U1600	U1525	C1425	U1343	U1251	G1185	C
C	C	G2109	U1778	U1778	C1684	C1684	U1601	U1526	C1426	U1344	U1252	G1186	C
A	A	U2110	U1779	U1779	C1685	C1685	U1602	U1527	C1427	U1345	U1253	G1187	C
C	C	A2111	U1780	U1780	C1686	C1686	U1603	U1528	C1428	U1346	U1254	G1188	C
U	U	U2112	U1781	U1781	C1687	C1687	U1604	U1529	C1429	U1347	U1255	G1189	C
A	A	C2113	U1782	U1782	C1688	C1688	U1605	U1530	C1430	U1348	U1256	G1190	C
C	C	G2114	U1783	U1783	C1689	C1689	U1606	U1531	C1431	U1349	U1257	G1191	C
A	A	U2115	U1784	U1784	C1690	C1690	U1607	U1532	C1432	U1350	U1258	G1192	C
C	C	A2116	U1785	U1785	C1691	C1691	U1608	U1533	C1433	U1351	U1259	G1193	C
U	U	U2117	U1786	U1786	C1692	C1692	U1609	U1534	C1434	U1352	U1260	G1194	C
A	A	C2118	U1787	U1787	C1693	C1693	U1610	U1535	C1435	U1353	U1261	G1195	C
C	C	G2119	U1788	U1788	C1694	C1694	U1611	U1536	C1436	U1354	U1262	G1196	C
A	A	U2120	U1789	U1789									

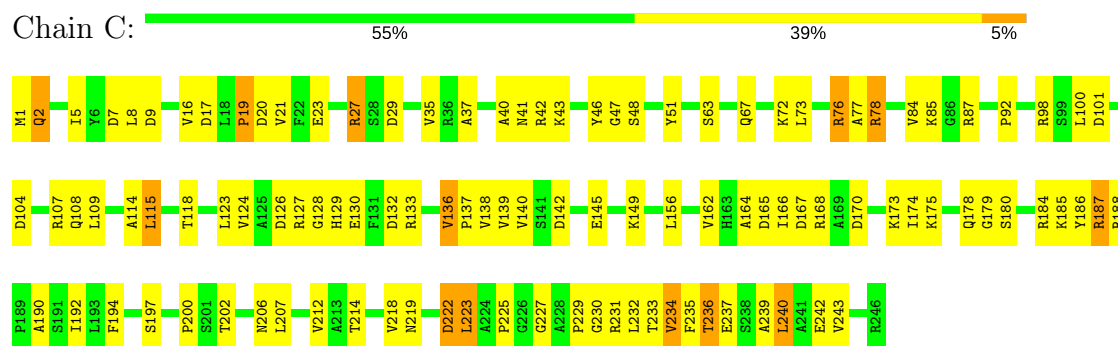




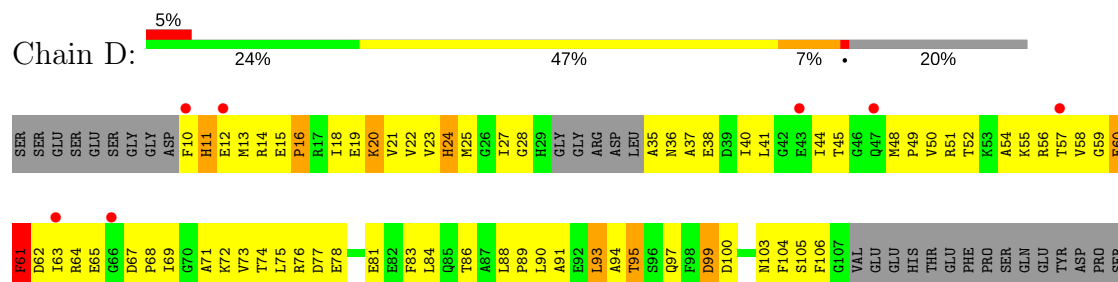
• Molecule 5: RIBOSOMAL PROTEIN L3



• Molecule 6: RIBOSOMAL PROTEIN L4

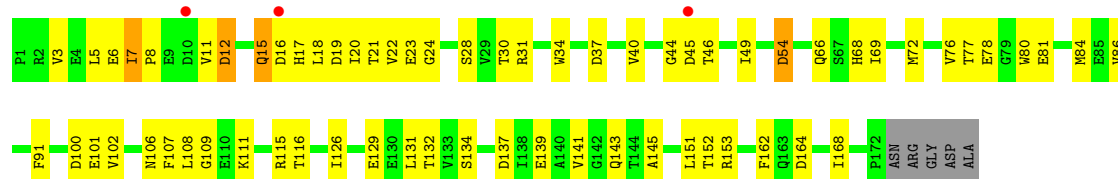


• Molecule 7: RIBOSOMAL PROTEIN L5

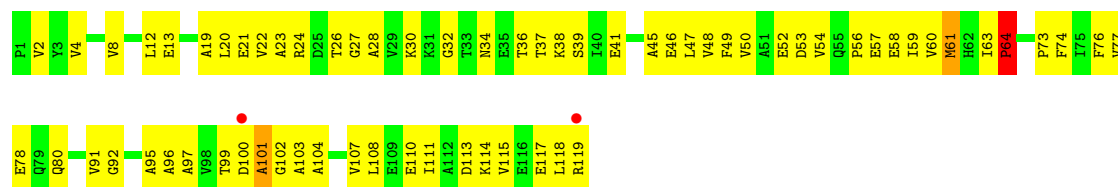
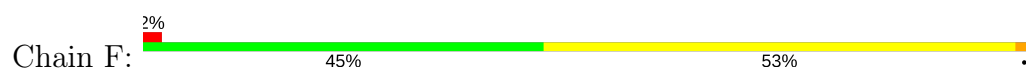




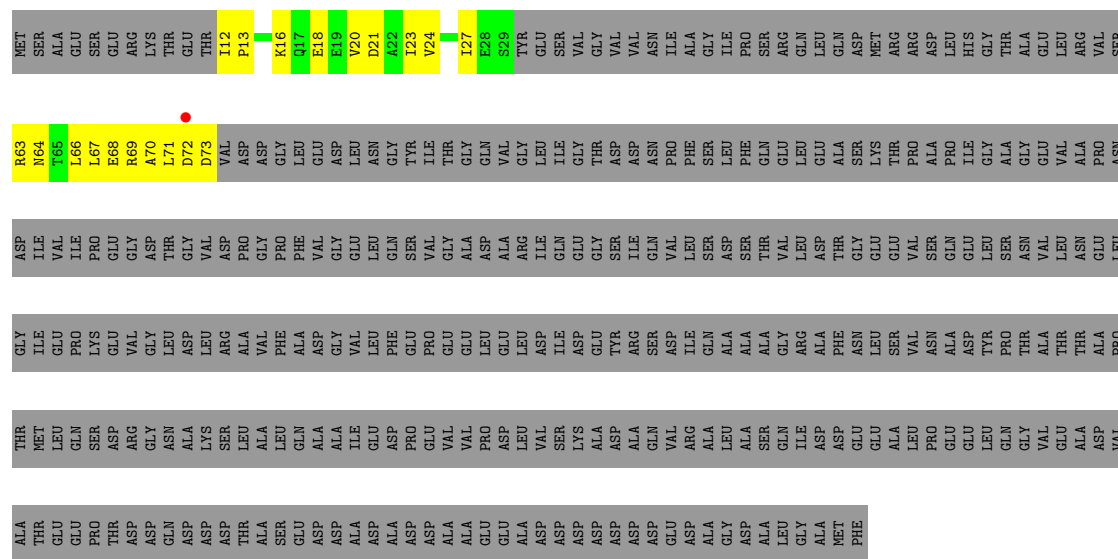
• Molecule 8: RIBOSOMAL PROTEIN L6



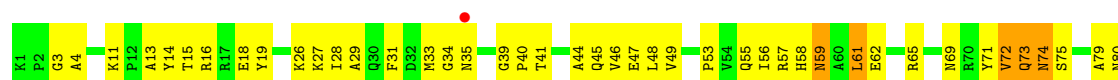
• Molecule 9: RIBOSOMAL PROTEIN L7AE

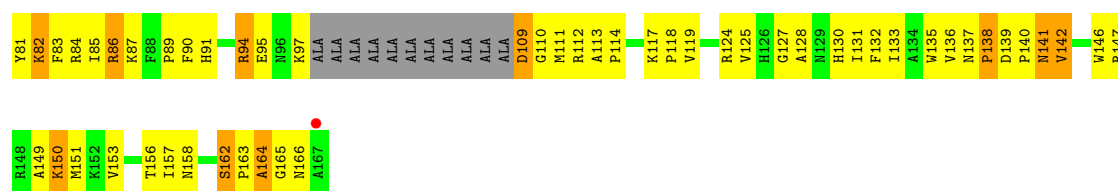


• Molecule 10: RIBOSOMAL PROTEIN L10



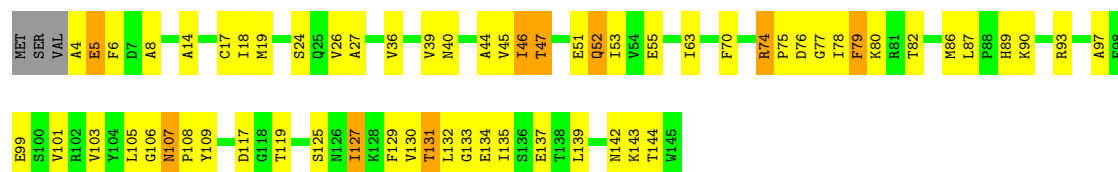
• Molecule 11: RIBOSOMAL PROTEIN L10E





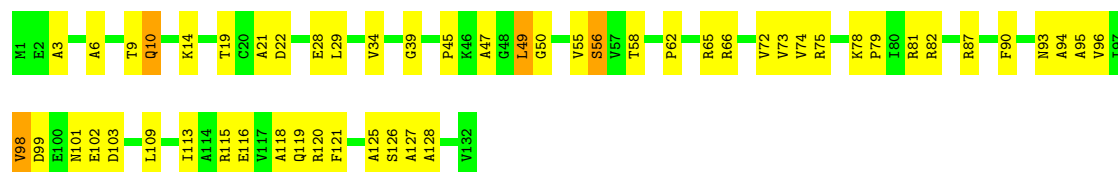
• Molecule 12: RIBOSOMAL PROTEIN L13

Chain I: 55% 37% 6%



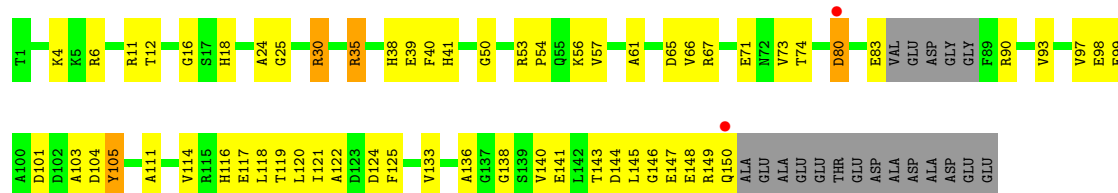
• Molecule 13: RIBOSOMAL PROTEIN L14

Chain J: 60% 37%



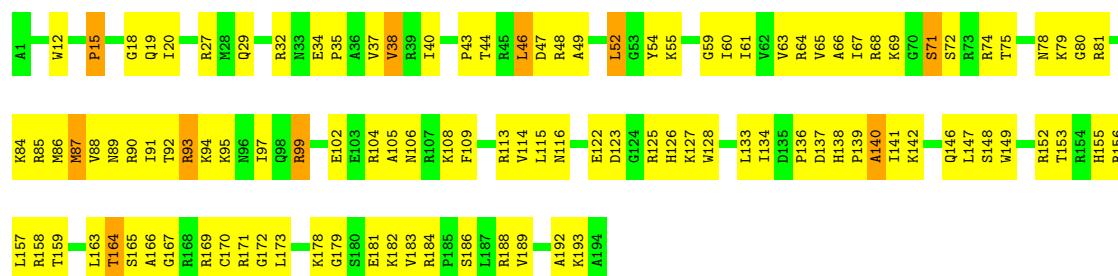
• Molecule 14: RIBOSOMAL PROTEIN L15

Chain K: 51% 35% 12%

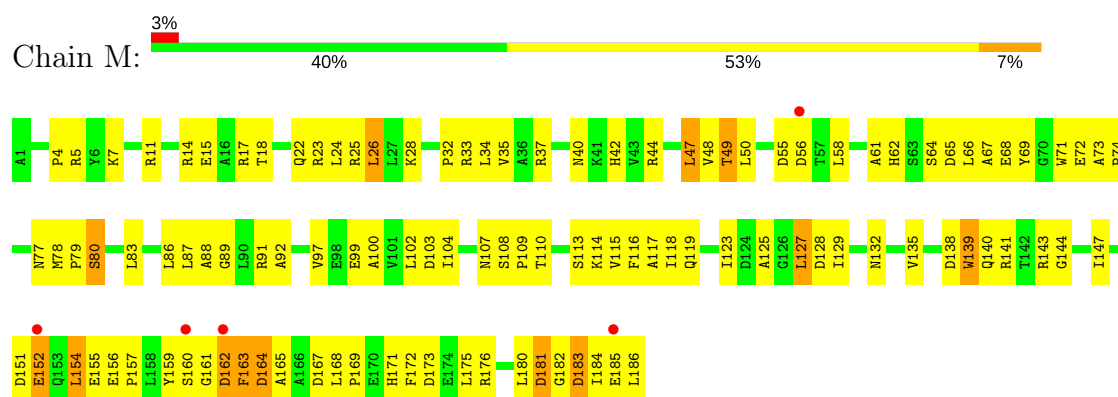


• Molecule 15: RIBOSOMAL PROTEIN L15E

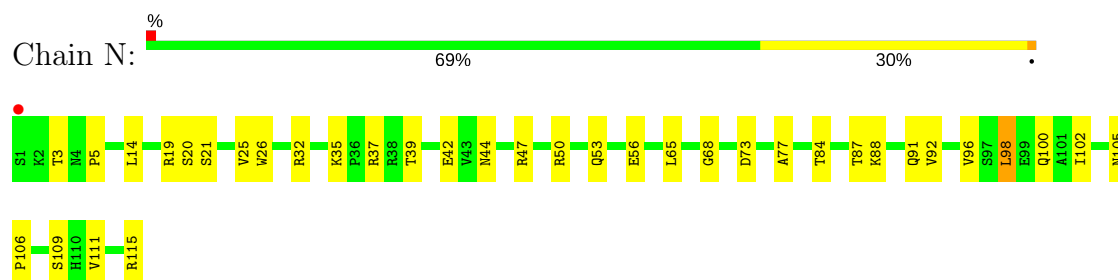
Chain L: 43% 52% 5%



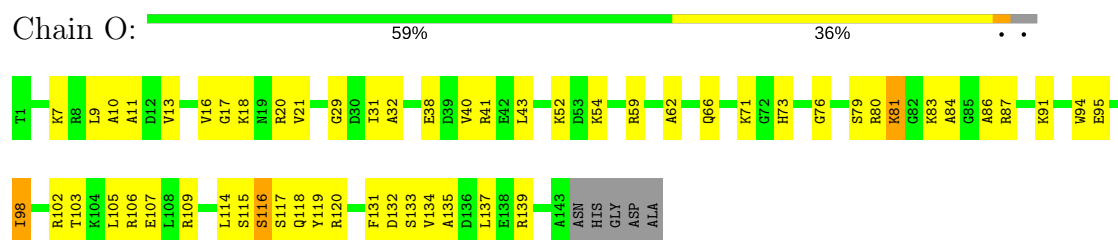
• Molecule 16: RIBOSOMAL PROTEIN L18



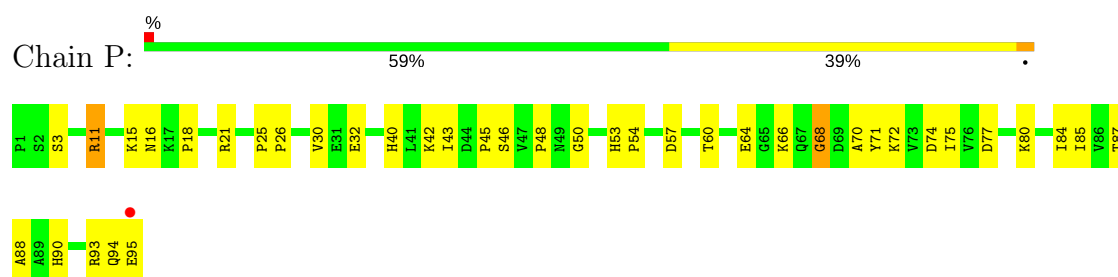
• Molecule 17: RIBOSOMAL PROTEIN L18E



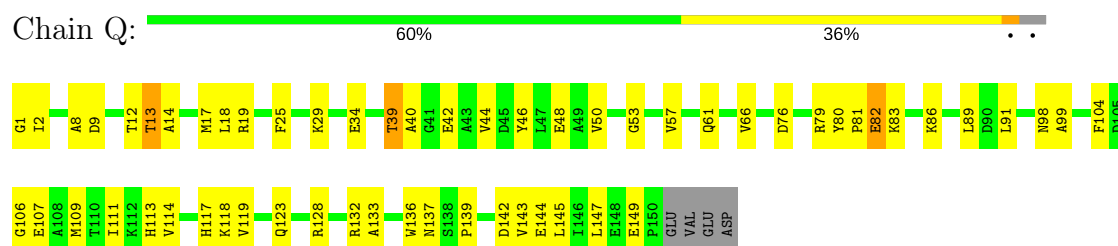
• Molecule 18: RIBOSOMAL PROTEIN L19E



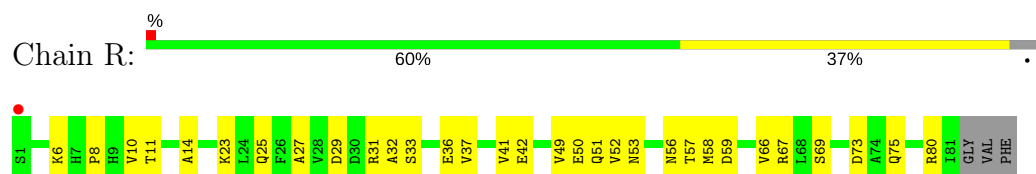
• Molecule 19: RIBOSOMAL PROTEIN L21E



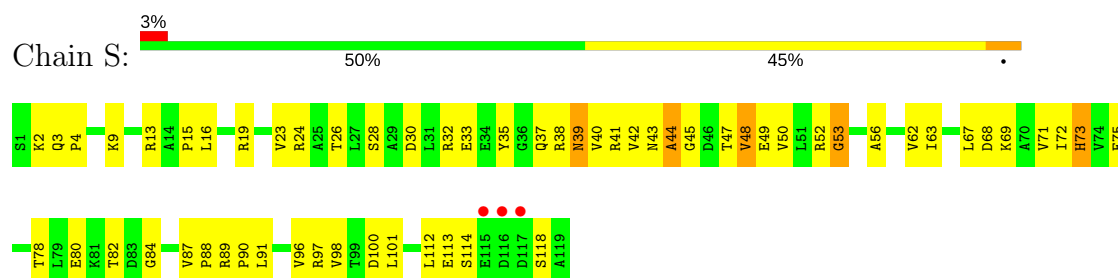
• Molecule 20: RIBOSOMAL PROTEIN L22



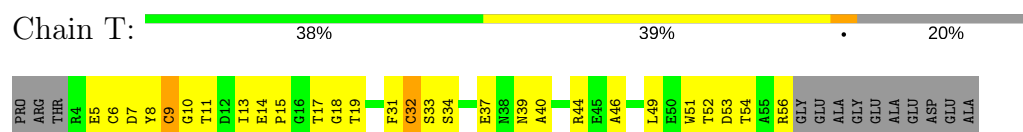
- Molecule 21: RIBOSOMAL PROTEIN L23



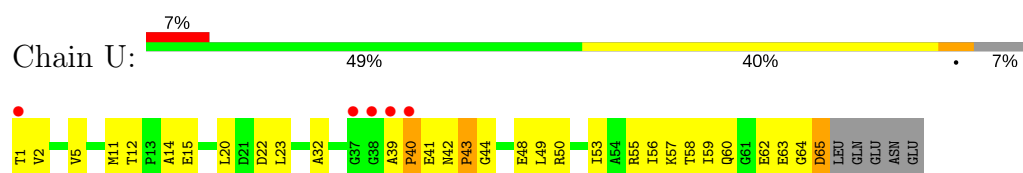
- Molecule 22: RIBOSOMAL PROTEIN L24



- Molecule 23: RIBOSOMAL PROTEIN L24E



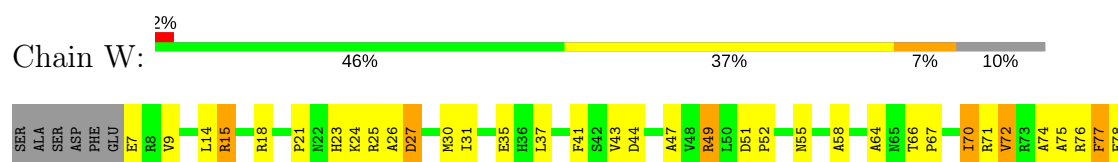
- Molecule 24: RIBOSOMAL PROTEIN L29



- Molecule 25: RIBOSOMAL PROTEIN L30



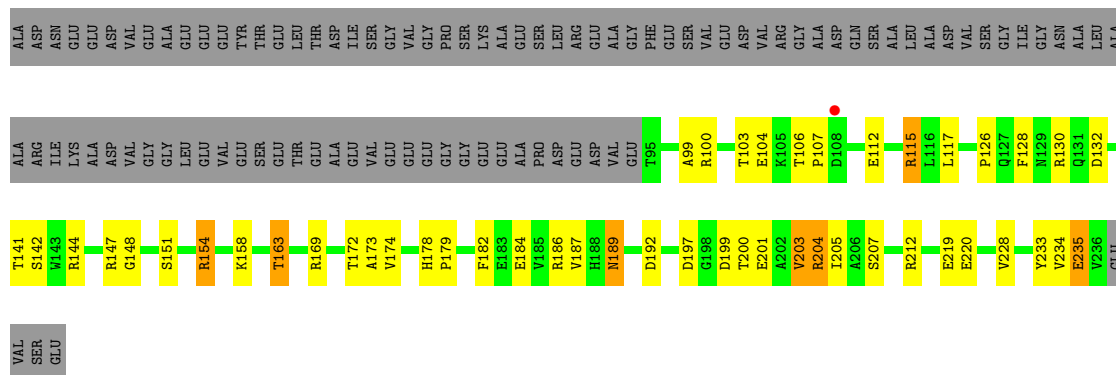
- Molecule 26: RIBOSOMAL PROTEIN L31E





• 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%



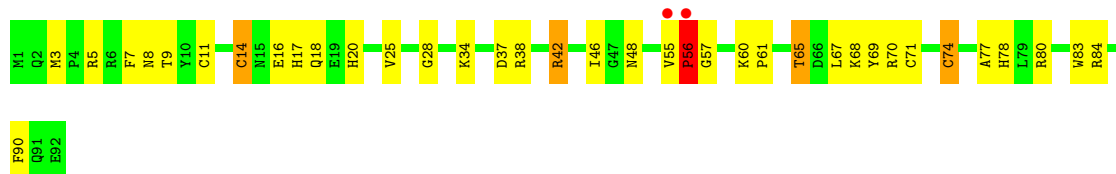
• Molecule 30: RIBOSOMAL PROTEIN L39E

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>	2.45 (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.	DCC
Wilson B-factor (Å <sup>2</sup> )	68.8	Xtriage
Anisotropy	0.431	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>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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%)	11	44
5	B	335/337 (99%)	300 (90%)	28 (8%)	7 (2%)	8	38
6	C	244/246 (99%)	213 (87%)	28 (12%)	3 (1%)	15	53
7	D	134/176 (76%)	96 (72%)	26 (19%)	12 (9%)	1	4
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	28	70
9	F	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	6	31
10	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	3	20
11	H	152/167 (91%)	132 (87%)	16 (10%)	4 (3%)	6	31
12	I	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	8	38
13	J	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	12	48
14	K	141/164 (86%)	116 (82%)	23 (16%)	2 (1%)	13	49
15	L	192/194 (99%)	167 (87%)	20 (10%)	5 (3%)	6	31
16	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	4	21
17	N	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	20	62
18	O	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	25	67
19	P	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	8	36
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%)	11	44
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	9	39
24	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	5	26
25	V	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	25	67
26	W	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	6	32
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100	100
28	Y	71/73 (97%)	58 (82%)	10 (14%)	3 (4%)	3	18

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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%)	8	36
All	All	3633/4235 (86%)	3224 (89%)	338 (9%)	71 (2%)	9	39

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%)	22	59
5	B	282/282 (100%)	264 (94%)	18 (6%)	20	57
6	C	193/193 (100%)	178 (92%)	15 (8%)	15	47
7	D	117/147 (80%)	108 (92%)	9 (8%)	15	48
8	E	152/155 (98%)	146 (96%)	6 (4%)	37	75
9	F	92/92 (100%)	91 (99%)	1 (1%)	78	93
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	111 (91%)	11 (9%)	11	40
12	I	118/121 (98%)	110 (93%)	8 (7%)	18	54
13	J	106/106 (100%)	102 (96%)	4 (4%)	38	75
14	K	113/126 (90%)	108 (96%)	5 (4%)	33	72
15	L	166/166 (100%)	157 (95%)	9 (5%)	26	64
16	M	149/149 (100%)	141 (95%)	8 (5%)	26	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	93/93 (100%)	90 (97%)	3 (3%)	44	79
18	O	113/116 (97%)	109 (96%)	4 (4%)	41	78
19	P	79/79 (100%)	75 (95%)	4 (5%)	28	66
20	Q	117/121 (97%)	114 (97%)	3 (3%)	51	83
21	R	71/73 (97%)	69 (97%)	2 (3%)	49	82
22	S	105/105 (100%)	100 (95%)	5 (5%)	30	69
23	T	44/52 (85%)	44 (100%)	0	100	100
24	U	51/56 (91%)	49 (96%)	2 (4%)	37	75
25	V	130/130 (100%)	122 (94%)	8 (6%)	21	58
26	W	66/73 (90%)	62 (94%)	4 (6%)	22	59
27	X	120/195 (62%)	113 (94%)	7 (6%)	23	61
28	Y	56/56 (100%)	52 (93%)	4 (7%)	17	52
29	Z	46/46 (100%)	45 (98%)	1 (2%)	57	86
30	1	42/44 (96%)	41 (98%)	1 (2%)	54	85
31	2	79/79 (100%)	75 (95%)	4 (5%)	28	66
All	All	3028/3441 (88%)	2871 (95%)	157 (5%)	27	65

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%)	0
2	9	121/122 (99%)	18 (14%)	0
3	4	2/3 (66%)	1 (50%)	0
All	All	2868/3047 (94%)	260 (9%)	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

There are no RNA pucker outliers to report.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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	4.52	16 (43%)	47,53,53	2.63	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	-9.72	1.35	1.50
32	0	9500	SLD	C9S-C0S	-5.74	1.43	1.51
32	0	9500	SLD	O1-C7	-3.58	1.41	1.46
32	0	9500	SLD	C3-C12	2.76	1.46	1.41
32	0	9500	SLD	F1-C11	3.49	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	-8.78	122.04	129.01
32	0	9500	SLD	C5-N1-C6	-5.50	108.17	111.24
32	0	9500	SLD	C7-O1-C6	-2.93	107.83	110.22
32	0	9500	SLD	O1-C6-N1	-2.82	108.18	109.97
32	0	9500	SLD	CAS-N5S-C0S	-2.38	118.28	122.84

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 ⓘ

### 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	0	2754/2922 (94%)	-0.44	32 (1%) 79 53	35, 63, 107, 150	0
2	9	122/122 (100%)	-0.02	5 (4%) 38 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%) 20 7	70, 115, 131, 137	0
8	E	172/177 (97%)	-0.28	3 (1%) 70 42	61, 84, 102, 107	0
9	F	119/119 (100%)	-0.07	2 (1%) 70 42	70, 88, 112, 118	0
10	G	29/348 (8%)	0.09	1 (3%) 46 20	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	5 (2%) 55 26	58, 81, 120, 133	0
17	N	115/115 (100%)	-0.35	1 (0%) 84 61	56, 72, 90, 94	0
18	O	143/148 (96%)	-0.48	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%) 58 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%) 14 5	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 <span>100</span> <span>100</span>	51, 64, 82, 94	0
26	W	82/91 (90%)	-0.25	2 (2%) <span>59</span> <span>30</span>	58, 75, 99, 117	0
27	X	142/240 (59%)	-0.60	1 (0%) <span>87</span> <span>67</span>	43, 61, 82, 101	0
28	Y	73/73 (100%)	-0.27	0 <span>100</span> <span>100</span>	62, 76, 95, 104	0
29	Z	56/56 (100%)	-0.71	0 <span>100</span> <span>100</span>	42, 52, 58, 68	0
30	1	46/48 (95%)	-0.14	2 (4%) <span>36</span> <span>15</span>	49, 77, 105, 117	0
31	2	92/92 (100%)	-0.19	2 (2%) <span>62</span> <span>33</span>	53, 73, 87, 98	0
All	All	6580/7282 (90%)	-0.38	84 (1%) <span>77</span> <span>51</span>	35, 69, 108, 150	0

The worst 5 of 84 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. 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	NA	0	8356	1/1	0.94	0.96	<span>55.52</span>	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8371	1/1	0.66	0.72	38.24	69,69,69,69	0
35	NA	0	8377	1/1	0.93	0.58	31.35	75,75,75,75	0
35	NA	0	8323	1/1	0.81	0.44	30.91	66,66,66,66	0
34	K	0	8202	1/1	0.81	0.77	26.95	92,92,92,92	0
35	NA	0	8378	1/1	0.84	0.77	26.66	65,65,65,65	0
35	NA	0	8376	1/1	0.95	0.46	23.49	79,79,79,79	0
35	NA	0	8372	1/1	0.93	0.74	23.45	72,72,72,72	0
36	CL	0	8505	1/1	0.83	0.43	20.77	99,99,99,99	0
35	NA	0	8303	1/1	0.94	0.50	18.70	55,55,55,55	0
33	MG	0	8064	1/1	0.94	0.36	17.82	39,39,39,39	0
35	NA	0	8321	1/1	0.94	0.41	15.67	67,67,67,67	0
35	NA	0	8368	1/1	0.77	0.36	14.46	69,69,69,69	0
35	NA	0	8361	1/1	0.72	0.37	13.98	77,77,77,77	0
36	CL	B	8519	1/1	0.88	0.38	13.66	95,95,95,95	0
35	NA	Q	8386	1/1	0.42	0.64	11.18	107,107,107,107	0
35	NA	0	8379	1/1	0.97	0.24	10.88	48,48,48,48	0
35	NA	0	8350	1/1	0.85	0.28	10.75	57,57,57,57	0
36	CL	2	8504	1/1	0.90	0.49	10.69	100,100,100,100	0
33	MG	0	8044	1/1	0.96	0.27	10.09	59,59,59,59	0
35	NA	0	8366	1/1	0.82	0.36	9.71	82,82,82,82	0
33	MG	0	8108	1/1	0.93	0.27	9.57	102,102,102,102	0
35	NA	0	8332	1/1	0.81	0.37	9.01	50,50,50,50	0
35	NA	0	8325	1/1	0.86	0.28	8.96	64,64,64,64	0
35	NA	0	8362	1/1	0.81	0.24	8.55	79,79,79,79	0
35	NA	K	8380	1/1	0.97	0.36	8.20	85,85,85,85	0
33	MG	0	8053	1/1	0.95	0.30	7.74	63,63,63,63	0
35	NA	0	8364	1/1	0.89	0.24	7.43	66,66,66,66	0
35	NA	0	8333	1/1	0.89	0.26	5.99	40,40,40,40	0
33	MG	0	8006	1/1	0.98	0.28	5.96	60,60,60,60	0
35	NA	0	8308	1/1	0.93	0.25	5.75	77,77,77,77	0
35	NA	0	8324	1/1	0.71	0.39	5.62	58,58,58,58	0
35	NA	9	8383	1/1	0.78	0.40	4.75	67,67,67,67	0
35	NA	0	8373	1/1	0.94	0.24	4.74	57,57,57,57	0
35	NA	0	8326	1/1	0.81	0.30	4.56	73,73,73,73	0
35	NA	0	8367	1/1	0.96	0.25	4.36	85,85,85,85	0
33	MG	0	8020	1/1	0.94	0.19	4.07	53,53,53,53	0
35	NA	0	8365	1/1	0.83	0.42	3.68	47,47,47,47	0
36	CL	I	8521	1/1	0.95	0.25	3.38	69,69,69,69	0
33	MG	0	8038	1/1	0.99	0.19	2.85	56,56,56,56	0
35	NA	0	8320	1/1	0.98	0.21	2.81	40,40,40,40	0
35	NA	0	8335	1/1	0.95	0.17	2.60	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8049	1/1	0.66	0.32	2.52	90,90,90,90	0
33	MG	0	8054	1/1	0.93	0.19	2.50	45,45,45,45	0
35	NA	0	8310	1/1	0.92	0.20	2.39	46,46,46,46	0
36	CL	J	8512	1/1	0.96	0.21	2.01	67,67,67,67	0
35	NA	H	8309	1/1	0.98	0.26	1.91	49,49,49,49	0
32	SLD	0	9500	37/37	0.92	0.21	1.91	46,50,53,59	0
36	CL	N	8508	1/1	0.89	0.22	1.89	116,116,116,116	0
35	NA	Q	8337	1/1	0.91	0.26	1.52	64,64,64,64	0
33	MG	0	8060	1/1	0.96	0.15	1.41	63,63,63,63	0
35	NA	0	8359	1/1	0.94	0.15	1.32	81,81,81,81	0
33	MG	0	8014	1/1	0.98	0.18	1.22	46,46,46,46	0
33	MG	0	8001	1/1	0.96	0.17	1.13	46,46,46,46	0
33	MG	0	8004	1/1	0.97	0.19	1.09	50,50,50,50	0
33	MG	0	8008	1/1	0.96	0.16	1.03	52,52,52,52	0
33	MG	0	8013	1/1	0.85	0.17	0.84	60,60,60,60	0
33	MG	X	8109	1/1	0.96	0.18	0.77	66,66,66,66	0
35	NA	0	8374	1/1	0.88	0.14	0.46	77,77,77,77	0
33	MG	0	8017	1/1	0.99	0.15	0.35	43,43,43,43	0
35	NA	0	8353	1/1	0.93	0.14	0.34	43,43,43,43	0
33	MG	0	8112	1/1	0.93	0.15	0.27	64,64,64,64	0
35	NA	0	8339	1/1	0.94	0.14	0.05	33,33,33,33	0
33	MG	A	8065	1/1	0.99	0.15	0.05	55,55,55,55	0
33	MG	0	8003	1/1	0.89	0.15	-0.04	51,51,51,51	0
33	MG	0	8077	1/1	0.98	0.13	-0.19	54,54,54,54	0
33	MG	0	8019	1/1	0.97	0.15	-0.43	43,43,43,43	0
35	NA	0	8343	1/1	0.96	0.14	-0.51	48,48,48,48	0
34	K	0	8201	1/1	0.75	0.13	-0.62	141,141,141,141	0
35	NA	0	8344	1/1	0.97	0.11	-0.64	48,48,48,48	0
35	NA	0	8331	1/1	0.98	0.12	-0.65	60,60,60,60	0
33	MG	0	8058	1/1	0.98	0.11	-0.71	61,61,61,61	0
33	MG	0	8007	1/1	0.98	0.12	-0.73	47,47,47,47	0
33	MG	0	8067	1/1	0.94	0.12	-0.73	81,81,81,81	0
35	NA	L	8347	1/1	0.96	0.13	-0.86	55,55,55,55	0
33	MG	S	8073	1/1	0.89	0.14	-0.94	71,71,71,71	0
33	MG	0	8015	1/1	0.99	0.11	-0.99	60,60,60,60	0
37	CD	Y	8403	1/1	0.98	0.07	-1.30	84,84,84,84	0
33	MG	0	8057	1/1	0.96	0.09	-1.32	53,53,53,53	0
35	NA	0	8338	1/1	0.95	0.09	-1.35	66,66,66,66	0
35	NA	0	8317	1/1	0.94	0.11	-1.38	57,57,57,57	0
33	MG	0	8086	1/1	0.97	0.06	-1.41	62,62,62,62	0
37	CD	2	8404	1/1	0.99	0.09	-1.43	90,90,90,90	0
37	CD	Z	8402	1/1	0.99	0.07	-1.50	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	I	8346	1/1	0.99	0.08	-1.52	45,45,45,45	0
33	MG	9	8052	1/1	0.96	0.10	-1.64	60,60,60,60	0
33	MG	0	8039	1/1	0.98	0.10	-1.70	53,53,53,53	0
33	MG	4	8063	1/1	0.97	0.11	-1.73	62,62,62,62	0
33	MG	0	8062	1/1	0.94	0.09	-1.77	90,90,90,90	0
33	MG	0	8074	1/1	0.98	0.07	-1.81	51,51,51,51	0
33	MG	0	8107	1/1	0.93	0.09	-1.91	55,55,55,55	0
35	NA	0	8327	1/1	0.98	0.10	-1.96	46,46,46,46	0
33	MG	0	8027	1/1	0.98	0.07	-2.00	65,65,65,65	0
33	MG	0	8010	1/1	0.99	0.10	-2.00	47,47,47,47	0
35	NA	A	8345	1/1	0.96	0.10	-2.02	48,48,48,48	0
36	CL	L	8518	1/1	0.96	0.10	-2.09	69,69,69,69	0
35	NA	P	8348	1/1	0.89	0.09	-2.14	68,68,68,68	0
33	MG	0	8002	1/1	0.97	0.09	-2.15	51,51,51,51	0
37	CD	T	8401	1/1	0.99	0.07	-2.21	83,83,83,83	0
33	MG	0	8056	1/1	0.99	0.09	-2.47	60,60,60,60	0
33	MG	0	8080	1/1	0.99	0.08	-2.66	52,52,52,52	0
33	MG	B	8055	1/1	0.95	0.06	-2.68	71,71,71,71	0
33	MG	0	8018	1/1	0.95	0.09	-2.77	57,57,57,57	0
33	MG	2	8078	1/1	0.98	0.04	-2.99	65,65,65,65	0
33	MG	0	8096	1/1	0.96	0.09	-3.15	70,70,70,70	0
33	MG	0	8016	1/1	0.96	0.07	-3.25	71,71,71,71	0
33	MG	0	8091	1/1	0.99	0.06	-3.47	65,65,65,65	0
33	MG	0	8012	1/1	0.99	0.06	-3.51	42,42,42,42	0
33	MG	0	8032	1/1	0.98	0.08	-3.70	52,52,52,52	0
35	NA	0	8305	1/1	0.97	0.08	-3.81	42,42,42,42	0
33	MG	J	8069	1/1	0.94	0.05	-3.89	87,87,87,87	0
33	MG	0	8033	1/1	0.98	0.11	-4.56	48,48,48,48	0
33	MG	0	8059	1/1	0.98	0.06	-5.88	60,60,60,60	0
33	MG	0	8084	1/1	0.99	0.05	-6.30	70,70,70,70	0
33	MG	0	8035	1/1	0.94	0.06	-6.42	69,69,69,69	0
35	NA	R	8312	1/1	0.53	0.93	-	84,84,84,84	0
33	MG	0	8099	1/1	0.93	0.23	-	80,80,80,80	0
33	MG	0	8005	1/1	0.99	0.10	-	58,58,58,58	0
33	MG	0	8093	1/1	0.98	0.10	-	63,63,63,63	0
35	NA	0	8330	1/1	0.93	0.11	-	61,61,61,61	0
33	MG	0	8104	1/1	0.92	0.13	-	66,66,66,66	0
33	MG	0	8076	1/1	0.89	0.16	-	102,102,102,102	0
35	NA	0	8316	1/1	0.84	0.21	-	52,52,52,52	0
33	MG	0	8111	1/1	0.92	0.12	-	75,75,75,75	0
35	NA	0	8340	1/1	0.78	0.36	-	69,69,69,69	0
36	CL	I	8501	1/1	0.91	0.18	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8363	1/1	0.50	0.60	-	83,83,83,83	0
33	MG	0	8045	1/1	0.89	0.25	-	91,91,91,91	0
35	NA	0	8336	1/1	0.93	0.13	-	63,63,63,63	0
33	MG	0	8022	1/1	0.88	0.57	-	83,83,83,83	0
36	CL	0	8514	1/1	0.94	0.14	-	75,75,75,75	0
33	MG	0	8041	1/1	0.98	0.24	-	68,68,68,68	0
36	CL	I	8502	1/1	0.90	0.11	-	93,93,93,93	0
33	MG	0	8026	1/1	0.96	0.08	-	39,39,39,39	0
35	NA	0	8313	1/1	0.85	0.22	-	89,89,89,89	0
36	CL	K	8510	1/1	0.83	0.26	-	104,104,104,104	0
33	MG	0	8030	1/1	0.99	0.16	-	48,48,48,48	0
35	NA	C	8304	1/1	0.93	0.38	-	51,51,51,51	0
33	MG	0	8066	1/1	0.86	0.18	-	105,105,105,105	0
33	MG	0	8029	1/1	0.95	0.07	-	60,60,60,60	0
33	MG	0	8075	1/1	0.96	0.09	-	77,77,77,77	0
36	CL	0	8515	1/1	0.86	0.29	-	100,100,100,100	0
36	CL	P	8511	1/1	0.87	0.37	-	84,84,84,84	0
33	MG	0	8114	1/1	0.78	0.70	-	95,95,95,95	0
33	MG	0	8089	1/1	0.97	0.07	-	82,82,82,82	0
33	MG	0	8115	1/1	0.93	0.12	-	73,73,73,73	0
33	MG	0	8050	1/1	0.97	0.14	-	68,68,68,68	0
36	CL	X	8520	1/1	0.97	0.28	-	57,57,57,57	0
33	MG	0	8101	1/1	0.95	0.14	-	94,94,94,94	0
33	MG	0	8098	1/1	0.98	0.06	-	50,50,50,50	0
36	CL	0	8517	1/1	0.95	0.33	-	82,82,82,82	0
35	NA	0	8375	1/1	0.91	0.69	-	81,81,81,81	0
35	NA	0	8385	1/1	0.78	0.36	-	73,73,73,73	0
33	MG	0	8048	1/1	0.98	0.06	-	66,66,66,66	0
36	CL	A	8509	1/1	0.90	0.74	-	89,89,89,89	0
33	MG	0	8094	1/1	0.99	0.07	-	97,97,97,97	0
33	MG	0	8025	1/1	0.97	0.06	-	59,59,59,59	0
33	MG	0	8116	1/1	0.94	0.16	-	84,84,84,84	0
33	MG	0	8037	1/1	0.98	0.07	-	54,54,54,54	0
35	NA	0	8329	1/1	0.56	1.25	-	98,98,98,98	0
35	NA	0	8311	1/1	0.90	0.26	-	73,73,73,73	0
35	NA	9	8351	1/1	0.33	0.26	-	94,94,94,94	0
33	MG	0	8082	1/1	0.92	0.16	-	79,79,79,79	0
33	MG	0	8042	1/1	0.96	0.14	-	61,61,61,61	0
35	NA	0	8319	1/1	0.98	0.18	-	41,41,41,41	0
36	CL	0	8522	1/1	0.97	0.64	-	92,92,92,92	0
35	NA	0	8384	1/1	0.47	0.63	-	85,85,85,85	0
33	MG	A	8105	1/1	0.82	0.30	-	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
33	MG	0	8031	1/1	0.96	0.12	-	54,54,54,54	0
35	NA	0	8352	1/1	0.81	0.32	-	61,61,61,61	0
33	MG	0	8061	1/1	0.99	0.05	-	45,45,45,45	0
33	MG	0	8011	1/1	0.88	0.19	-	50,50,50,50	0
35	NA	0	8370	1/1	0.90	0.40	-	76,76,76,76	0
33	MG	0	8036	1/1	0.97	0.05	-	52,52,52,52	0
35	NA	0	8328	1/1	0.88	0.23	-	55,55,55,55	0
33	MG	0	8110	1/1	0.96	0.12	-	56,56,56,56	0
36	CL	Q	8506	1/1	0.92	0.23	-	80,80,80,80	0
35	NA	0	8382	1/1	0.79	0.18	-	89,89,89,89	0
33	MG	0	8043	1/1	0.97	0.07	-	64,64,64,64	0
36	CL	0	8513	1/1	0.92	0.24	-	74,74,74,74	0
37	CD	N	8405	1/1	0.81	0.23	-	150,150,150,150	0
33	MG	0	8040	1/1	0.96	0.08	-	88,88,88,88	0
35	NA	0	8369	1/1	0.84	0.35	-	96,96,96,96	0
33	MG	0	8023	1/1	0.99	0.06	-	46,46,46,46	0
33	MG	0	8088	1/1	0.96	0.22	-	40,40,40,40	0
35	NA	0	8355	1/1	0.96	0.40	-	77,77,77,77	0
33	MG	0	8117	1/1	0.98	0.07	-	45,45,45,45	0
35	NA	0	8318	1/1	0.97	0.23	-	48,48,48,48	0
33	MG	0	8009	1/1	0.96	0.18	-	44,44,44,44	0
33	MG	0	8070	1/1	0.97	0.06	-	63,63,63,63	0
33	MG	0	8079	1/1	0.96	0.12	-	53,53,53,53	0
35	NA	0	8307	1/1	0.83	0.32	-	71,71,71,71	0
33	MG	0	8087	1/1	0.95	0.07	-	82,82,82,82	0
36	CL	0	8503	1/1	0.94	0.29	-	82,82,82,82	0
33	MG	0	8047	1/1	0.98	0.10	-	90,90,90,90	0
35	NA	0	8349	1/1	0.98	0.44	-	69,69,69,69	0
33	MG	0	8034	1/1	0.95	0.10	-	46,46,46,46	0
33	MG	0	8085	1/1	0.88	0.22	-	92,92,92,92	0
33	MG	0	8092	1/1	0.87	0.36	-	111,111,111,111	0
33	MG	0	8100	1/1	0.92	0.19	-	97,97,97,97	0
35	NA	0	8360	1/1	0.84	0.41	-	69,69,69,69	0
33	MG	0	8046	1/1	0.86	0.15	-	86,86,86,86	0
33	MG	0	8068	1/1	0.99	0.07	-	64,64,64,64	0
35	NA	0	8334	1/1	0.96	0.20	-	48,48,48,48	0
35	NA	0	8357	1/1	0.92	0.26	-	61,61,61,61	0
33	MG	0	8102	1/1	0.84	0.40	-	91,91,91,91	0
33	MG	0	8113	1/1	0.84	0.10	-	60,60,60,60	0
33	MG	0	8097	1/1	0.91	0.30	-	53,53,53,53	0
33	MG	9	8095	1/1	0.93	0.36	-	106,106,106,106	0
35	NA	0	8341	1/1	0.79	0.33	-	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8083	1/1	0.98	0.07	-	65,65,65,65	0
33	MG	0	8021	1/1	0.99	0.18	-	54,54,54,54	0
35	NA	0	8306	1/1	0.96	0.38	-	59,59,59,59	0
33	MG	0	8071	1/1	0.84	0.07	-	104,104,104,104	0
36	CL	M	8507	1/1	0.94	0.24	-	86,86,86,86	0
33	MG	0	8051	1/1	0.95	0.19	-	97,97,97,97	0
33	MG	0	8103	1/1	0.92	0.42	-	97,97,97,97	0
35	NA	0	8301	1/1	0.96	0.12	-	59,59,59,59	0
36	CL	0	8516	1/1	0.96	0.26	-	64,64,64,64	0
33	MG	0	8081	1/1	0.92	0.08	-	67,67,67,67	0
33	MG	0	8024	1/1	0.75	0.62	-	98,98,98,98	0
35	NA	0	8314	1/1	0.97	0.23	-	53,53,53,53	0
35	NA	0	8315	1/1	0.98	0.20	-	70,70,70,70	0
35	NA	0	8302	1/1	0.96	0.16	-	55,55,55,55	0
35	NA	0	8354	1/1	0.92	0.41	-	58,58,58,58	0
35	NA	0	8358	1/1	0.96	0.28	-	109,109,109,109	0
33	MG	0	8028	1/1	0.90	0.17	-	57,57,57,57	0
33	MG	0	8106	1/1	0.97	0.26	-	78,78,78,78	0
35	NA	0	8381	1/1	0.87	0.30	-	69,69,69,69	0
35	NA	H	8322	1/1	0.70	0.42	-	78,78,78,78	0
33	MG	0	8090	1/1	0.95	0.33	-	81,81,81,81	0
33	MG	0	8072	1/1	0.95	0.34	-	78,78,78,78	0
35	NA	0	8342	1/1	0.98	0.14	-	42,42,42,42	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.