



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 12:36 AM 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 validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

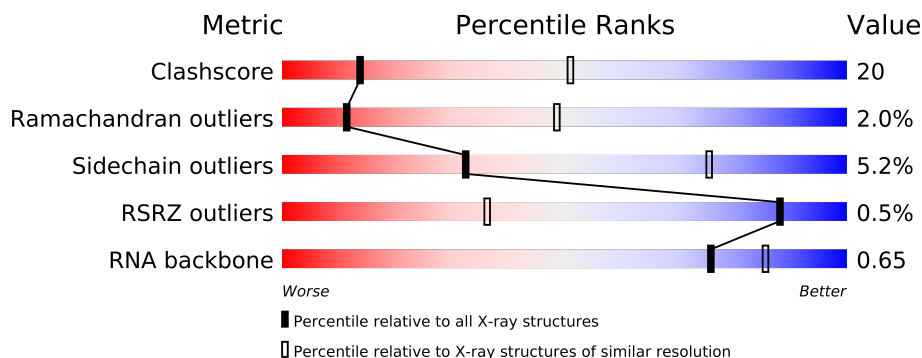
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	4	3	
4	A	239	
5	B	337	
6	C	246	
7	D	176	
8	E	177	
9	F	119	
10	G	348	
11	H	167	
12	I	145	
13	J	132	
14	K	164	

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Mol	Chain	Length	Quality of chain
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 that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
32	SLD	0	9500	-	X
33	MG	0	8006	-	X
33	MG	0	8009	-	X
33	MG	0	8020	-	X
33	MG	0	8021	-	X
33	MG	0	8022	-	X
33	MG	0	8024	-	X
33	MG	0	8030	-	X
33	MG	0	8038	-	X
33	MG	0	8041	-	X
33	MG	0	8042	-	X
33	MG	0	8044	-	X
33	MG	0	8045	-	X
33	MG	0	8046	-	X
33	MG	0	8049	-	X
33	MG	0	8051	-	X
33	MG	0	8053	-	X
33	MG	0	8054	-	X
33	MG	0	8064	-	X
33	MG	0	8072	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8085	-	X
33	MG	0	8088	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8097	-	X
33	MG	0	8099	-	X
33	MG	0	8100	-	X
33	MG	0	8102	-	X
33	MG	0	8103	-	X
33	MG	0	8106	-	X
33	MG	0	8108	-	X
33	MG	0	8113	-	X
33	MG	0	8114	-	X
33	MG	0	8115	-	X
33	MG	9	8095	-	X
33	MG	A	8105	-	X
34	K	0	8202	-	X
35	NA	0	8302	-	X
35	NA	0	8303	-	X
35	NA	0	8306	-	X
35	NA	0	8307	-	X
35	NA	0	8308	-	X
35	NA	0	8311	-	X
35	NA	0	8313	-	X
35	NA	0	8314	-	X
35	NA	0	8315	-	X
35	NA	0	8316	-	X
35	NA	0	8318	-	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	8328	-	X
35	NA	0	8329	-	X
35	NA	0	8332	-	X
35	NA	0	8333	-	X
35	NA	0	8334	-	X
35	NA	0	8335	-	X
35	NA	0	8340	-	X
35	NA	0	8341	-	X
35	NA	0	8349	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	8350	-	X
35	NA	0	8352	-	X
35	NA	0	8354	-	X
35	NA	0	8355	-	X
35	NA	0	8356	-	X
35	NA	0	8357	-	X
35	NA	0	8358	-	X
35	NA	0	8360	-	X
35	NA	0	8361	-	X
35	NA	0	8362	-	X
35	NA	0	8363	-	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	8369	-	X
35	NA	0	8370	-	X
35	NA	0	8371	-	X
35	NA	0	8372	-	X
35	NA	0	8373	-	X
35	NA	0	8375	-	X
35	NA	0	8376	-	X
35	NA	0	8377	-	X
35	NA	0	8378	-	X
35	NA	0	8379	-	X
35	NA	0	8381	-	X
35	NA	0	8382	-	X
35	NA	0	8384	-	X
35	NA	0	8385	-	X
35	NA	9	8383	-	X
35	NA	C	8304	-	X
35	NA	H	8322	-	X
35	NA	K	8380	-	X
35	NA	Q	8386	-	X
35	NA	R	8312	-	X
36	CL	0	8503	-	X
36	CL	0	8505	-	X
36	CL	0	8513	-	X
36	CL	0	8515	-	X
36	CL	0	8516	-	X
36	CL	0	8517	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	CL	0	8522	-	X
36	CL	2	8504	-	X
36	CL	A	8509	-	X
36	CL	B	8519	-	X
36	CL	I	8521	-	X
36	CL	P	8511	-	X
36	CL	Q	8506	-	X
36	CL	X	8520	-	X
37	CD	N	8405	-	X

2 Entry composition

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

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			

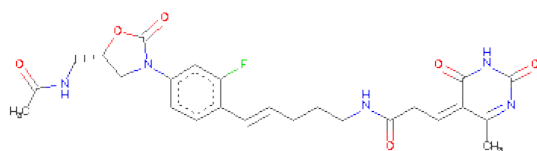
There is a discrepancy between the modelled and reference sequences:

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: C₂₅H₂₈FN₅O₆).



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

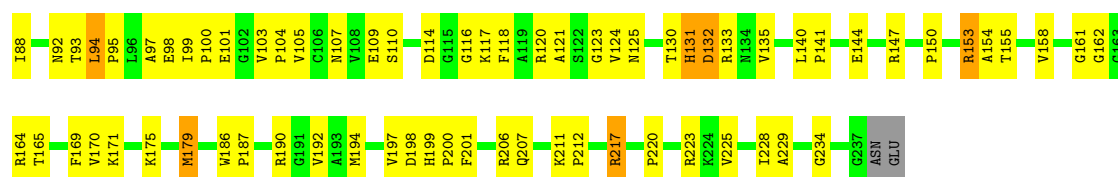
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	27	Total 27	O 27	0	0
38	U	13	Total 13	O 13	0	0
38	V	74	Total 74	O 74	0	0
38	W	29	Total 29	O 29	0	0
38	X	105	Total 105	O 105	0	0
38	Y	41	Total 41	O 41	0	0
38	Z	57	Total 57	O 57	0	0
38	1	45	Total 45	O 45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

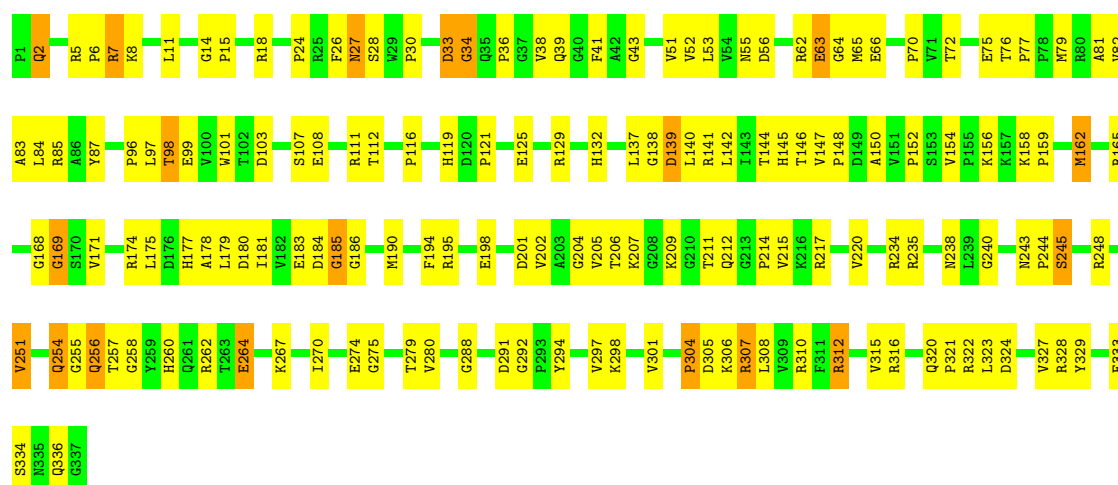
U	G2082	G2083	U1992	A1910	U1748	A1656	C1574	G1498	U1419	A1313	G1223	A1154	U1029	G958
A	A2083	A2089	C1993	G1917	G1751	A1657	C1575	U1499	C1420	U1314	G1224	G1155	U1030	C959
G	A2089	G2090	C1995	U1918	G1752	A1658	A1580	U1500	U1422	U1320	G1225	C1156	G1031	G960
U	G2090	G2091	U1996	A1919	A1755	C1666	G1584	U1503	A1424	A1321	G1226	G1157	G1044	A961
A	G2091	G2094	G2000	A1920	G1756	U1668	C1585	U1504	G1425	G1322	G1229	G1159	G1045	C962
G	G2094	A2095	G2001	A1921	U1757	A1669	G1586	U1505	C1426	G1323	C1229	G1160	C963	C963
A	A2095	A2096	G2002	A1922	U1758	A1670	U1587	U1506	A1427	G1324	U1234	G1161	G1052	G964
G	A2096	G2002	U2003	G1925	G1759	C1675	G1589	U1511	G1430	A1328	G1235	G1162	G1055	G968
A	G2002	U2003	U2004	G1926	G1760	G1676	G1592	G1512	G1431	A1329	G1236	U1170	G1055	G969
C	A2101	U2004	G2005	A1927	U1761	U1677	C1594	C1513	U1432	A1330	U1237	G	U	U970
A	G2102	C2102	G2005	C1928	C1762	A1676	G1585	A1514	G1433	A1331	U1238	G1165	G1059	G
C	C2102	C2105	U2008	A1829	C1763	C1679	U1596	A1515	A1434	C1332	G1239	A1166	G1060	U
U	C2105	C2106	U2008	A1830	U1766	A1682	U1597	C1516	U1435	U1333	U1242	U1171	U1064	C
A	C2106	U2107	A2011	A1831	G1767	A1683	A1598	U1517	U1436	C1334	G1065	G1172	G1065	C
A	U2107	C2110	U2011	A1845	A1767	G1683	U1599	U1519	U1440	U1244	C1069	A1173	C1069	C
C	G2110	G2111	G2013	U1846	G1768	A1684	A1600	G1520	G1441	C1335	C1245	A1174	C1070	C
C	G2111	G2014	G2014	A1847	C1769	A1685	A1603	C1521	G1442	C1342	A1246	G1175	A1071	C
A	G2112	A2015	A2015	G1848	U1770	A1686	G1604	A1522	U1443	C1343	A1247	U1180	G1072	U
G	A2015	G2113	U2016	G1849	C1772	C1687	G1605	U1523	G1444	G1344	U1248	A1181	C1072	C
G	G2113	C2113	U2016	G1850	G1773	C1687	G1605	U1524	G1445	A1345	U1249	C1182	A1078	C
U	C2113	C2114	G2023	G1851	G1774	C1692	G1609	U1525	G1445	U1346	C1250	C1183	A1078	G
A	U2115	U2116	G2023	A1852	G1774	C1692	G1610	A1526	G1445	U1346	C1251	C1184	A1078	A
C	U2116	U2116	G2023	A1853	G1774	C1692	G1611	A1527	G1445	U1346	C1252	C1185	A1078	A
C	U2116	U2116	G2023	A1854	G1774	C1692	G1612	A1528	G1445	U1346	C1253	U1185	A1081	G
C	U2116	U2116	G2023	A1855	G1774	C1692	G1613	A1529	G1445	U1346	C1254	U1186	A1081	A
C	U2116	U2116	G2023	A1856	G1774	C1692	G1614	U1530	G1445	U1346	C1255	U1187	A1081	G
C	U2116	U2116	G2023	A1857	G1774	C1692	G1615	U1531	G1445	U1346	C1256	U1188	A1081	A
C	U2116	U2116	G2023	A1858	G1774	C1692	G1616	U1532	G1445	U1346	C1257	U1189	A1081	G
C	U2116	U2116	G2023	A1859	G1774	C1692	G1617	U1533	G1445	U1346	C1258	U1190	A1081	U
C	U2116	U2116	G2023	A1860	G1774	C1692	G1618	U1534	G1445	U1346	C1259	U1191	A1081	U
C	U2116	U2116	G2023	A1861	G1774	C1692	G1619	U1535	G1445	U1346	C1260	U1192	A1081	C
C	U2116	U2116	G2023	A1862	G1774	C1692	G1620	U1536	G1445	U1346	C1261	U1193	A1081	G
C	U2116	U2116	G2023	A1863	G1774	C1692	G1621	U1537	G1445	U1346	C1262	U1194	A1081	G
C	U2116	U2116	G2023	A1864	G1774	C1692	G1622	U1538	G1445	U1346	C1263	U1195	A1081	G
C	U2116	U2116	G2023	A1865	G1774	C1692	G1623	U1539	G1445	U1346	C1264	U1196	A1081	G
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C	U2116	U2116	G2023	A1867	G1774	C1692	G1625	U1541	G1445	U1346	C1266	U1198	A1081	C
C	U2116	U2116	G2023	A1868	G1774	C1692	G1626	U1542	G1445	U1346	C1267	U1199	A1081	A
C	U2116	U2116	G2023	A1869	G1774	C1692	G1627	U1543	G1445	U1346	C1268	U1200	A1081	C
C	U2116	U2116	G2023	A1870	G1774	C1692	G1628	U1544	G1445	U1346	C1269	A1201	A1081	C
C	U2116	U2116	G2023	A1871	G1774	C1692	G1629	U1545	G1445	U1346	C1270	A1202	A1081	C
C	U2116	U2116	G2023	A1872	G1774	C1692	G1630	U1546	G1445	U1346	C1271	A1203	A1081	C
C	U2116	U2116	G2023	A1873	G1774	C1692	G1631	U1547	G1445	U1346	C1272	A1204	A1081	C
C	U2116	U2116	G2023	A1874	G1774	C1692	G1632	U1548	G1445	U1346	C1273	A1205	A1081	C
C	U2116	U2116	G2023	A1875	G1774	C1692	G1633	U1549	G1445	U1346	C1274	A1206	A1081	C
C	U2116	U2116	G2023	A1876	G1774	C1692	G1634	U1550	G1445	U1346	C1275	A1207	A1081	C
C	U2116	U2116	G2023	A1877	G1774	C1692	G1635	U1551	G1445	U1346	C1276	A1208	A1081	C
C	U2116	U2116	G2023	A1878	G1774	C1692	G1636	U1552	G1445	U1346	C1277	A1209	A1081	C
C	U2116	U2116	G2023	A1879	G1774	C1692	G1637	U1553	G1445	U1346	C1278	A1210	A1081	C
C	U2116	U2116	G2023	A1880	G1774	C1692	G1638	U1554	G1445	U1346	C1279	A1211	A1081	C
C	U2116	U2116	G2023	A1881	G1774	C1692	G1639	U1555	G1445	U1346	C1280	A1212	A1081	C
C	U2116	U2116	G2023	A1882	G1774	C1692	G1640	U1556	G1445	U1346	C1281	A1213	A1081	C
C	U2116	U2116	G2023	A1883	G1774	C1692	G1641	U1557	G1445	U1346	C1282	A1214	A1081	C
C	U2116	U2116	G2023	A1884	G1774	C1692	G1642	U1558	G1445	U1346	C1283	A1215	A1081	C
C	U2116	U2116	G2023	A1885	G1774	C1692	G1643	U1559	G1445	U1346	C1284	A1216	A1081	C
C	U2116	U2116	G2023	A1886	G1774	C1692	G1644	U1560	G1445	U1346	C1285	A1217	A1081	C
C	U2116	U2116	G2023	A1887	G1774	C1692	G1645	U1561	G1445	U1346	C1286	A1218	A1081	C
C	U2116	U2116	G2023	A1888	G1774	C1692	G1646	U1562	G1445	U1346	C1287	A1219	A1081	C
C	U2116	U2116	G2023	A1889	G1774	C1692	G1647	U1563	G1445	U1346	C1288	A1220	A1081	C
C	U2116	U2116	G2023	A1890	G1774	C1692	G1648	U1564	G1445	U1346	C1289	A1221	A1081	C
C	U2116	U2116	G2023	A1891	G1774	C1692	G1649	U1565	G1445	U1346	C1290	A1222	A1081	C
C	U2116	U2116	G2023	A1892	G1774	C1692	G1650	U1566	G1445	U1346	C1291	A1223	A1081	C
C	U2116	U2116	G2023	A1893	G1774	C1692	G1651	U1567	G1445	U1346	C1292	A1224	A1081	C
C	U2116	U2116	G2023	A1894	G1774	C1692	G1652	U1568	G1445	U1346	C1293	A1225	A1081	C
C	U2116	U2116	G2023	A1895	G1774	C1692	G1653	U1569	G1445	U1346	C1294	A1226	A1081	C
C	U2116	U2116	G2023	A1896	G1774	C1692	G1654	U1570	G1445	U1346	C1295	A1227	A1081	C
C	U2116	U2116	G2023	A1897	G1774	C1692	G1655	U1571	G1445	U1346	C1296	A1228	A1081	C
C	U2116	U2116	G2023	A1898	G1774	C1692	G1656	U1572	G1445	U1346	C1297	A1229	A1081	C
C	U2116	U2116	G2023	A1899	G1774	C1692	G1657	U1573	G1445	U1346	C1298	A1230	A1081	C
C	U2116	U2116	G2023	A1900	G1774	C1692	G1658	U1574	G1445	U1346	C1299	A1231	A1081	C
C	U2116	U2116	G2023	A1901	G1774	C1692	G1659	U1575	G1445	U1346	C1300	A1232	A1081	C
C	U2116	U2116	G2023	A1902	G1774	C1692	G1660	U1576	G1445	U1346	C1301	A1233	A1081	C
C	U2116	U2116	G2023	A1903	G1774	C1692	G1661	U1577	G1445	U1346	C1302	A1234	A1081	C
C	U2116	U2116	G2023	A1904	G1774	C1692	G1662	U1578	G1445	U1346	C1303	A1235	A1081	C
C	U2116	U2116	G2023	A1905	G1774	C1692	G1663	U1579	G1445	U1346	C1304	A1236	A1081	C
C	U2116	U2116	G2023	A1906	G1774	C1692	G1664	U1580	G1445	U1346	C1305	A1237	A1081	C
C	U2116	U2116	G2023	A1907	G1774	C1692	G1665	U1581	G1445	U1346	C1306	A1238	A1081	C
C	U2116	U2116	G2023	A1908	G1774	C1692	G1666	U1582	G1445	U1346	C1307	A1239	A1081	C
C	U2116	U2116	G2023	A1909	G1774	C1692	G1667	U1583	G1445	U1346	C1308	A1240	A1081	C
C	U2116	U2116	G2023	A1910	G1774	C1692	G1668	U1584	G1445	U1346	C1309	A1241	A1081	C
C	U2116	U2116	G2023	A1911	G1774	C1692	G1669	U1585	G1445	U1346	C1310	A1242	A1081	C
C	U2116	U2116	G2023	A1912	G1774	C1692	G1670	U1586	G1445	U1346	C1311	A1243	A1081	C
C	U2116	U2116	G2023	A1913	G1774	C1692	G1671	U1587	G1445	U1346	C1312	A1244	A1081	C
C	U2116	U2116	G2023	A1914	G1774	C1692	G1672	U1588	G1445	U1346	C1313	A1245	A1081	C
C	U2116	U2116	G2023	A1915	G1774	C1692	G1673	U1589	G1445	U1346	C1314	A1246	A1081	C
C	U2116	U2116	G2023	A1916	G1774	C1692	G1674	U1590	G1445	U1346	C1315	A1247	A1081	C
C	U2116	U2116	G2023	A1917	G1774	C1692	G1675	U1591	G1445	U1346	C1316	A1248	A1081	C
C	U2116	U2116	G2023	A1918	G1774	C1692	G1676	U1592	G1445	U1346	C1317	A1249	A1081	C
C	U2116	U2116	G2023	A1919	G1774	C1692	G1677	U1593	G1445	U1346	C1318	A1250	A1081	C
C	U2116	U2116	G2023	A1920	G1774	C1692	G1678	U1594	G1445	U1346	C1319	A1251	A1081	C
C	U2116	U2116	G2023	A1921	G1774	C1692	G1679	U1595	G					





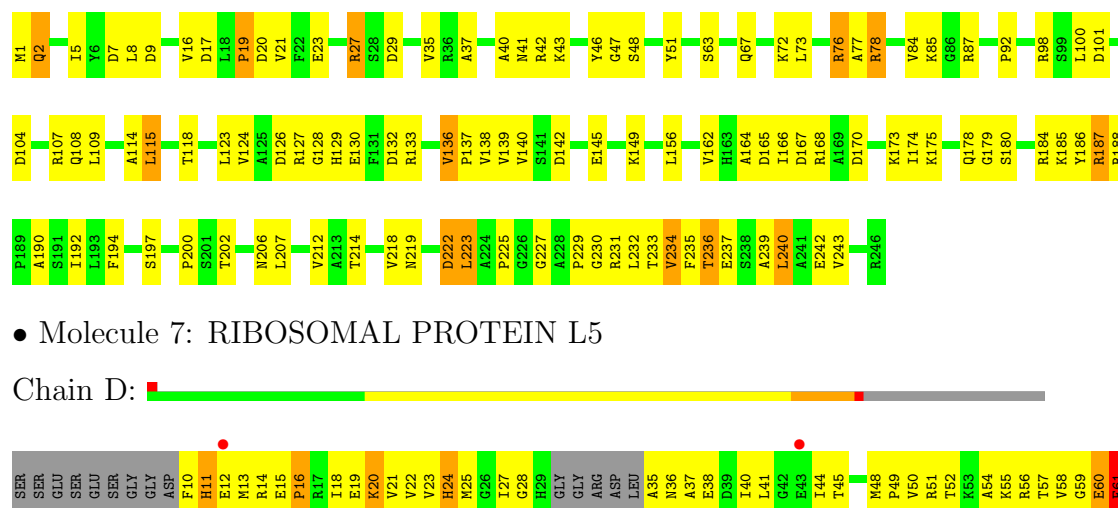
• Molecule 5: RIBOSOMAL PROTEIN L3

Chain B:

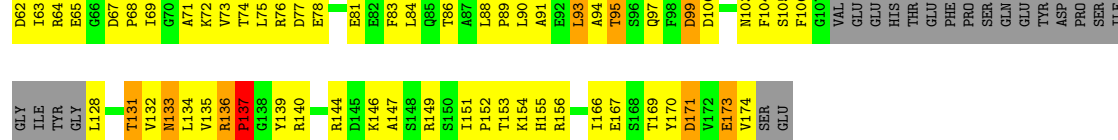


• Molecule 6: RIBOSOMAL PROTEIN L4

Chain C:

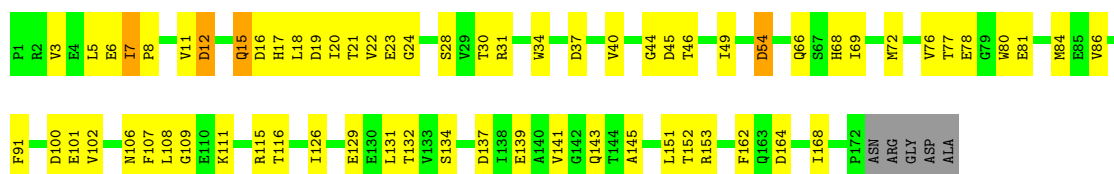


• Molecule 7: RIBOSOMAL PROTEIN L5



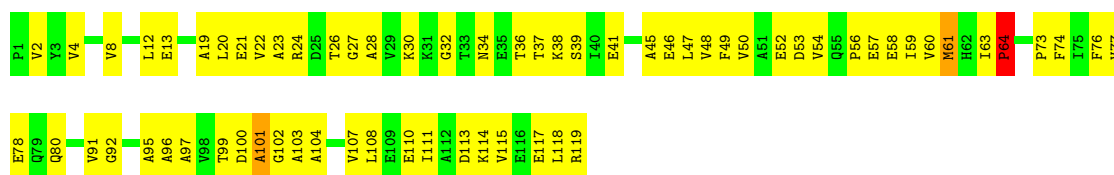
• Molecule 8: RIBOSOMAL PROTEIN L6

Chain E:



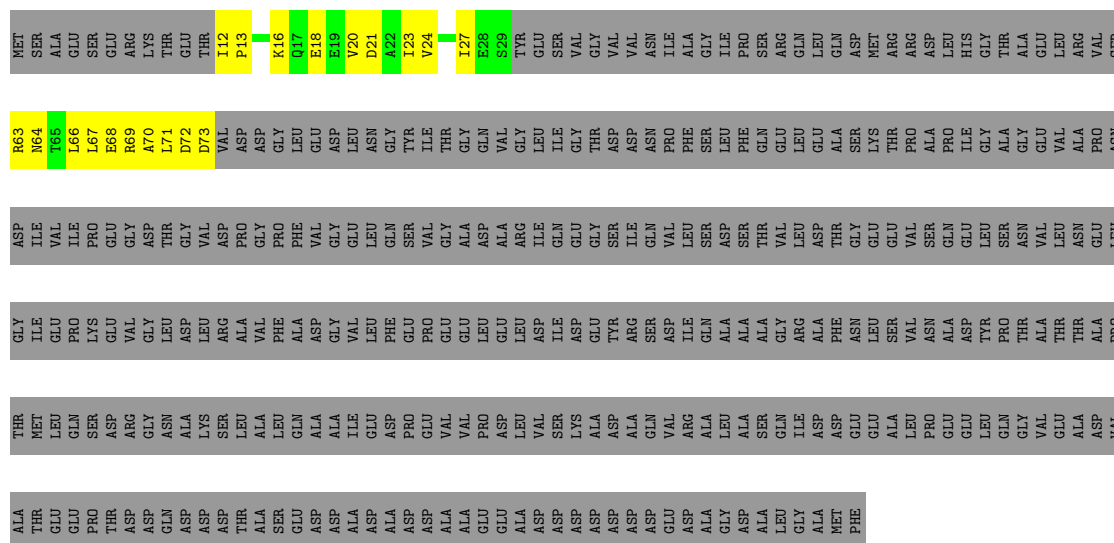
• Molecule 9: RIBOSOMAL PROTEIN L7AE

Chain F:



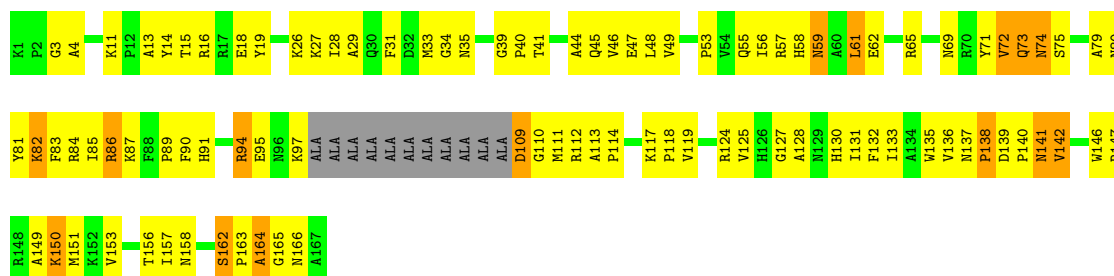
• Molecule 10: RIBOSOMAL PROTEIN L10

Chain G:



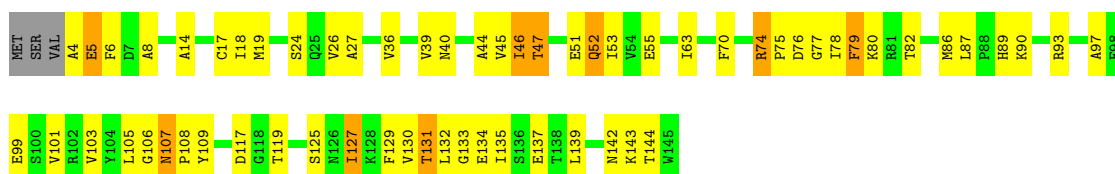
• Molecule 11: RIBOSOMAL PROTEIN L10E

Chain H:



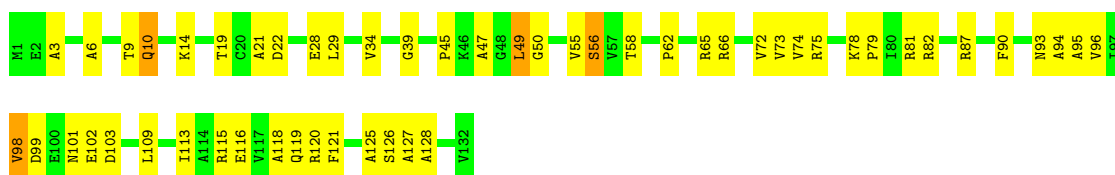
• Molecule 12: RIBOSOMAL PROTEIN L13

Chain I:



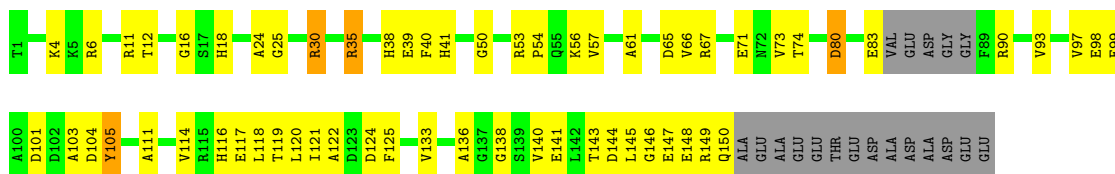
• Molecule 13: RIBOSOMAL PROTEIN L14

Chain J:



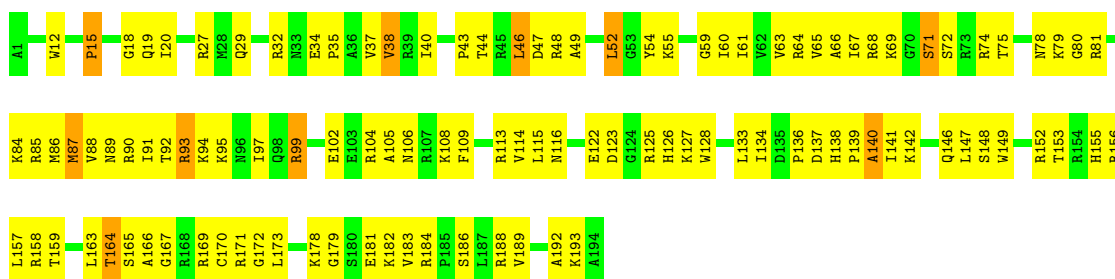
• Molecule 14: RIBOSOMAL PROTEIN L15

Chain K:



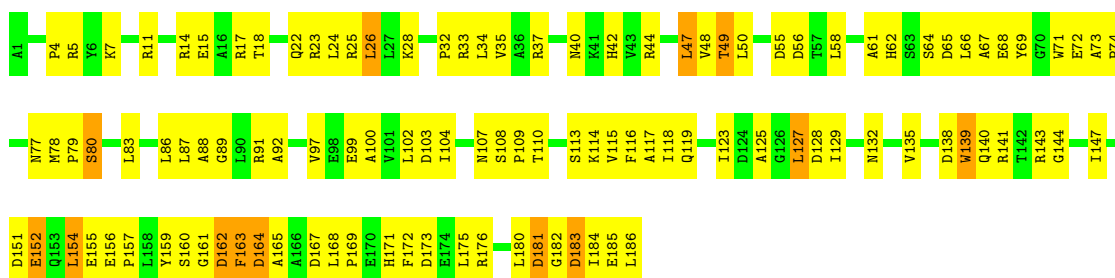
• Molecule 15: RIBOSOMAL PROTEIN L15E

Chain L:



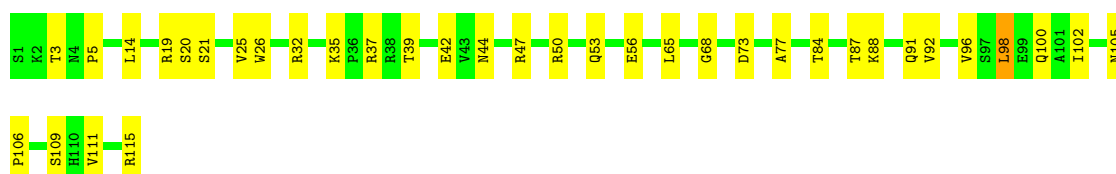
• Molecule 16: RIBOSOMAL PROTEIN L18

Chain M:



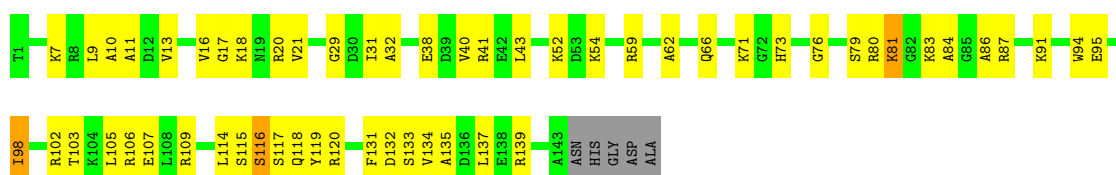
• Molecule 17: RIBOSOMAL PROTEIN L18E

Chain N:



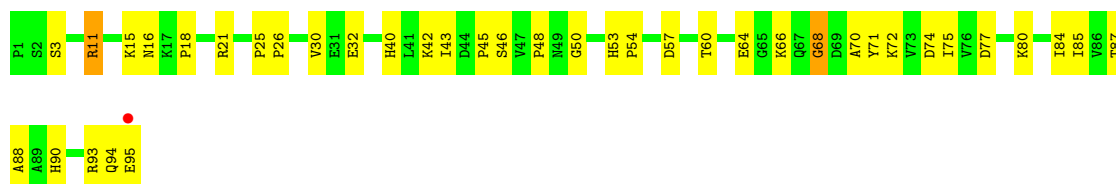
• Molecule 18: RIBOSOMAL PROTEIN L19E

Chain O:



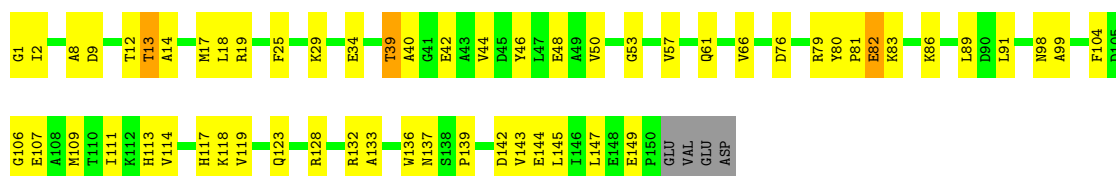
• Molecule 19: RIBOSOMAL PROTEIN L21E

Chain P:



• Molecule 20: RIBOSOMAL PROTEIN L22

Chain Q:



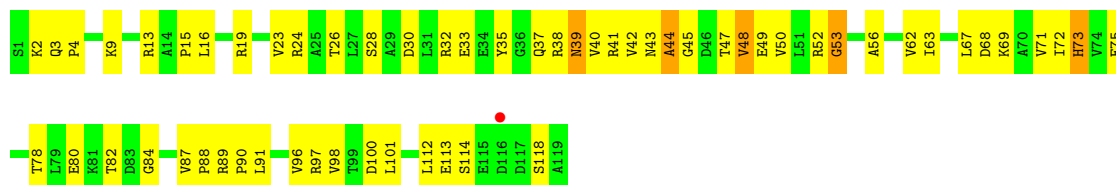
• Molecule 21: RIBOSOMAL PROTEIN L23

Chain R:



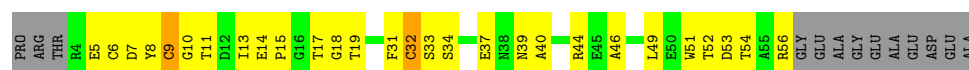
• Molecule 22: RIBOSOMAL PROTEIN L24

Chain S:



• Molecule 23: RIBOSOMAL PROTEIN L24E

Chain T: 



- Molecule 24: RIBOSOMAL PROTEIN L29

Chain U: 



- Molecule 25: RIBOSOMAL PROTEIN L30

Chain V: 



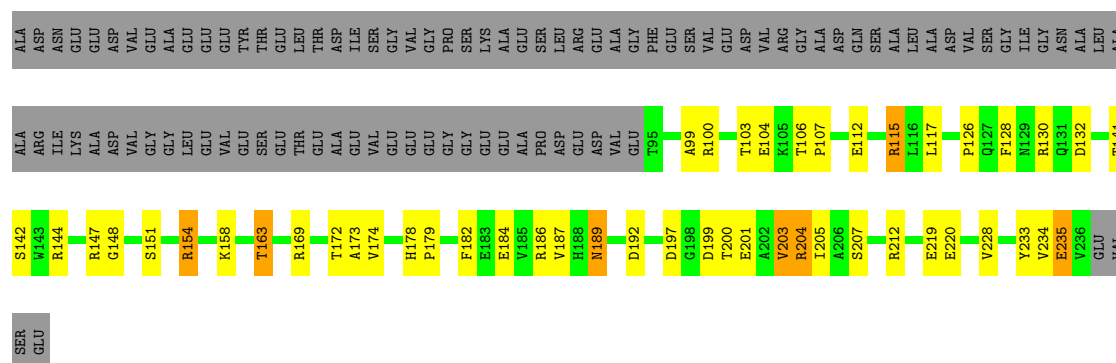
- Molecule 26: RIBOSOMAL PROTEIN L31E

Chain W: 



- Molecule 27: RIBOSOMAL PROTEIN L32E

Chain X: 



- Molecule 28: RIBOSOMAL PROTEIN L37AE

Chain Y: 



- Molecule 29: RIBOSOMAL PROTEIN L37E

Chain Z:



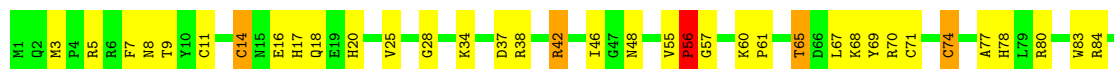
- Molecule 30: RIBOSOMAL PROTEIN L39E

Chain 1:



- Molecule 31: RIBOSOMAL PROTEIN L44E

Chain 2:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	68.8	Xtriage
Anisotropy	0.431	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 45.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 360129 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98635	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	S	1	0	0	0	0
33	X	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	26	0	0	6	0
38	G	21	0	0	2	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

The worst 5 of 2990 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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%)	14	54
5	B	335/337 (99%)	300 (90%)	28 (8%)	7 (2%)	11	47
6	C	244/246 (99%)	213 (87%)	28 (12%)	3 (1%)	19	64
7	D	134/176 (76%)	96 (72%)	26 (19%)	12 (9%)	1	5
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	33	81
9	F	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	8	39
10	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	5	25
11	H	152/167 (91%)	132 (87%)	16 (10%)	4 (3%)	8	39
12	I	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	11	47
13	J	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	15	58
14	K	141/164 (86%)	116 (82%)	23 (16%)	2 (1%)	16	60
15	L	192/194 (99%)	167 (87%)	20 (10%)	5 (3%)	8	39
16	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	5	27
17	N	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	25	73
18	O	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	30	78
19	P	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	10	45
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%)	14	54
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	11	48
24	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	6	33
25	V	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	30	78
26	W	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	9	40
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100	100
28	Y	71/73 (97%)	58 (82%)	10 (14%)	3 (4%)	4	24
29	Z	54/56 (96%)	50 (93%)	4 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
31	2	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	10	45
All	All	3633/4235 (86%)	3224 (89%)	338 (9%)	71 (2%)	11	48

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%)	26	68
5	B	282/282 (100%)	264 (94%)	18 (6%)	25	66
6	C	193/193 (100%)	178 (92%)	15 (8%)	18	55
7	D	117/147 (80%)	108 (92%)	9 (8%)	18	56
8	E	152/155 (98%)	146 (96%)	6 (4%)	43	85
9	F	92/92 (100%)	91 (99%)	1 (1%)	84	97
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	111 (91%)	11 (9%)	14	47
12	I	118/121 (98%)	110 (93%)	8 (7%)	22	63
13	J	106/106 (100%)	102 (96%)	4 (4%)	44	85
14	K	113/126 (90%)	108 (96%)	5 (4%)	39	82
15	L	166/166 (100%)	157 (95%)	9 (5%)	31	74
16	M	149/149 (100%)	141 (95%)	8 (5%)	31	74
17	N	93/93 (100%)	90 (97%)	3 (3%)	51	89
18	O	113/116 (97%)	109 (96%)	4 (4%)	48	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	P	79/79 (100%)	75 (95%)	4 (5%)	33	76
20	Q	117/121 (97%)	114 (97%)	3 (3%)	59	91
21	R	71/73 (97%)	69 (97%)	2 (3%)	56	91
22	S	105/105 (100%)	100 (95%)	5 (5%)	35	79
23	T	44/52 (85%)	44 (100%)	0	100	100
24	U	51/56 (91%)	49 (96%)	2 (4%)	43	85
25	V	130/130 (100%)	122 (94%)	8 (6%)	26	67
26	W	66/73 (90%)	62 (94%)	4 (6%)	26	68
27	X	120/195 (62%)	113 (94%)	7 (6%)	28	71
28	Y	56/56 (100%)	52 (93%)	4 (7%)	21	61
29	Z	46/46 (100%)	45 (98%)	1 (2%)	64	93
30	1	42/44 (96%)	41 (98%)	1 (2%)	61	92
31	2	79/79 (100%)	75 (95%)	4 (5%)	33	76
All	All	3028/3441 (88%)	2871 (95%)	157 (5%)	32	75

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	-	39,39,39	6.56	18 (46%)	53,53,53	2.48	17 (32%)

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 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	SLD	C8S-C6S	33.10	1.58	1.33
32	0	9500	SLD	C5S-N4S	10.68	1.45	1.33
32	0	9500	SLD	C9S-C8S	-9.35	1.35	1.50
32	0	9500	SLD	C6-N1	8.01	1.45	1.36
32	0	9500	SLD	C6S-C1S	7.57	1.58	1.44

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	-8.38	122.04	128.86
32	0	9500	SLD	O1-C6-O3	6.47	129.77	122.32
32	0	9500	SLD	C5-N1-C6	-5.44	108.17	111.26
32	0	9500	SLD	C3S-N4S-C5S	4.99	123.64	118.93
32	0	9500	SLD	C2-N1-C6	4.57	131.36	125.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	0	2754/2922 (94%)	-0.50	20 (0%) 84 28	35, 63, 107, 150	0
2	9	122/122 (100%)	-0.10	4 (3%) 44 8	52, 80, 106, 150	0
3	4	3/3 (100%)	-0.57	0 100 100	49, 49, 51, 51	0
4	A	237/239 (99%)	-0.32	0 100 100	44, 69, 101, 121	0
5	B	337/337 (100%)	-0.27	0 100 100	42, 72, 98, 108	0
6	C	246/246 (100%)	-0.36	0 100 100	36, 63, 87, 99	0
7	D	140/176 (79%)	0.15	2 (1%) 72 18	70, 115, 131, 137	0
8	E	172/177 (97%)	-0.20	0 100 100	61, 84, 102, 107	0
9	F	119/119 (100%)	-0.11	0 100 100	70, 88, 112, 118	0
10	G	29/348 (8%)	-0.02	0 100 100	85, 105, 113, 117	0
11	H	156/167 (93%)	-0.23	0 100 100	51, 72, 100, 108	0
12	I	142/145 (97%)	-0.35	0 100 100	50, 66, 85, 102	0
13	J	132/132 (100%)	-0.27	0 100 100	53, 71, 89, 96	0
14	K	145/164 (88%)	-0.23	0 100 100	39, 83, 117, 129	0
15	L	194/194 (100%)	-0.42	0 100 100	47, 62, 79, 90	0
16	M	186/186 (100%)	-0.06	0 100 100	58, 81, 120, 133	0
17	N	115/115 (100%)	-0.26	0 100 100	56, 72, 90, 94	0
18	O	143/148 (96%)	-0.33	0 100 100	50, 72, 87, 94	0
19	P	95/95 (100%)	-0.32	1 (1%) 77 21	51, 62, 75, 88	0
20	Q	150/154 (97%)	-0.37	0 100 100	46, 61, 81, 88	0
21	R	81/84 (96%)	-0.24	0 100 100	59, 76, 95, 103	0
22	S	119/119 (100%)	-0.26	1 (0%) 83 26	55, 74, 97, 113	0
23	T	53/66 (80%)	-0.22	0 100 100	57, 73, 92, 99	0
24	U	65/70 (92%)	-0.00	2 (3%) 47 9	68, 91, 123, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	154/154 (100%)	-0.38	0 100 100	51, 64, 82, 94	0
26	W	82/91 (90%)	-0.19	0 100 100	58, 75, 99, 117	0
27	X	142/240 (59%)	-0.42	0 100 100	43, 61, 82, 101	0
28	Y	73/73 (100%)	-0.22	0 100 100	62, 76, 95, 104	0
29	Z	56/56 (100%)	-0.50	0 100 100	42, 52, 58, 68	0
30	1	46/48 (95%)	-0.15	1 (2%) 59 12	49, 77, 105, 117	0
31	2	92/92 (100%)	-0.18	0 100 100	53, 73, 87, 98	0
All	All	6580/7282 (90%)	-0.36	31 (0%) 88 36	35, 69, 108, 150	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	6.3
1	0	2250	G	4.9
2	9	3002	U	4.2
2	9	3025	G	3.9
2	9	3023	U	3.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8352	1/1	0.32	136.61	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8356	1/1	0.96	54.03	73,73,73,73	0
35	NA	0	8329	1/1	1.26	51.08	98,98,98,98	0
35	NA	0	8385	1/1	0.33	44.57	73,73,73,73	0
35	NA	0	8384	1/1	0.58	41.86	85,85,85,85	0
36	CL	A	8509	1/1	0.99	40.70	89,89,89,89	0
35	NA	0	8371	1/1	0.66	38.95	69,69,69,69	0
33	MG	0	8024	1/1	0.70	38.50	98,98,98,98	0
35	NA	0	8311	1/1	0.27	31.02	73,73,73,73	0
34	K	0	8202	1/1	0.82	28.69	92,92,92,92	0
33	MG	0	8072	1/1	0.30	26.68	78,78,78,78	0
35	NA	0	8363	1/1	0.56	25.16	83,83,83,83	0
35	NA	0	8377	1/1	0.47	24.88	75,75,75,75	0
35	NA	0	8349	1/1	0.45	24.25	69,69,69,69	0
33	MG	0	8103	1/1	0.49	23.71	97,97,97,97	0
35	NA	0	8376	1/1	0.43	23.70	79,79,79,79	0
33	MG	0	8092	1/1	0.27	23.64	111,111,111,111	0
36	CL	0	8522	1/1	0.63	23.50	92,92,92,92	0
35	NA	0	8323	1/1	0.40	23.40	66,66,66,66	0
33	MG	0	8041	1/1	0.27	23.40	68,68,68,68	0
35	NA	0	8378	1/1	0.74	23.31	65,65,65,65	0
35	NA	0	8379	1/1	0.28	23.15	48,48,48,48	0
35	NA	0	8372	1/1	0.71	19.99	72,72,72,72	0
36	CL	X	8520	1/1	0.28	19.78	57,57,57,57	0
35	NA	0	8368	1/1	0.39	18.55	69,69,69,69	0
35	NA	0	8321	1/1	0.42	18.47	67,67,67,67	0
35	NA	0	8360	1/1	0.44	18.39	69,69,69,69	0
35	NA	0	8370	1/1	0.35	18.07	76,76,76,76	0
35	NA	0	8361	1/1	0.41	16.94	77,77,77,77	0
35	NA	0	8354	1/1	0.44	16.57	58,58,58,58	0
33	MG	0	8064	1/1	0.32	16.39	39,39,39,39	0
35	NA	0	8381	1/1	0.29	16.37	69,69,69,69	0
36	CL	Q	8506	1/1	0.26	15.97	80,80,80,80	0
35	NA	0	8306	1/1	0.33	15.83	59,59,59,59	0
33	MG	0	8022	1/1	0.52	14.02	83,83,83,83	0
36	CL	B	8519	1/1	0.41	13.83	95,95,95,95	0
35	NA	0	8303	1/1	0.37	13.01	55,55,55,55	0
35	NA	0	8340	1/1	0.35	11.98	69,69,69,69	0
36	CL	2	8504	1/1	0.45	11.94	100,100,100,100	0
33	MG	0	8097	1/1	0.30	11.84	53,53,53,53	0
33	MG	0	8114	1/1	0.81	11.72	95,95,95,95	0
33	MG	0	8044	1/1	0.28	10.87	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8316	1/1	0.17	10.81	52,52,52,52	0
33	MG	0	8106	1/1	0.24	10.80	78,78,78,78	0
35	NA	0	8332	1/1	0.40	10.68	50,50,50,50	0
36	CL	0	8505	1/1	0.31	10.62	99,99,99,99	0
35	NA	Q	8386	1/1	0.60	10.30	107,107,107,107	0
35	NA	0	8341	1/1	0.37	10.27	60,60,60,60	0
33	MG	0	8113	1/1	0.14	9.50	60,60,60,60	0
35	NA	0	8366	1/1	0.37	9.22	82,82,82,82	0
36	CL	0	8503	1/1	0.30	9.22	82,82,82,82	0
35	NA	0	8325	1/1	0.26	9.17	64,64,64,64	0
33	MG	0	8085	1/1	0.25	8.93	92,92,92,92	0
35	NA	0	8362	1/1	0.23	8.88	79,79,79,79	0
33	MG	0	8051	1/1	0.22	8.39	97,97,97,97	0
35	NA	0	8302	1/1	0.17	8.30	55,55,55,55	0
35	NA	0	8350	1/1	0.24	8.25	57,57,57,57	0
35	NA	K	8380	1/1	0.36	7.99	85,85,85,85	0
35	NA	0	8308	1/1	0.29	7.79	77,77,77,77	0
35	NA	0	8375	1/1	0.63	7.73	81,81,81,81	0
35	NA	0	8307	1/1	0.35	7.51	71,71,71,71	0
35	NA	0	8315	1/1	0.17	7.32	70,70,70,70	0
35	NA	0	8364	1/1	0.23	7.25	66,66,66,66	0
33	MG	A	8105	1/1	0.32	6.86	52,52,52,52	0
33	MG	0	8108	1/1	0.24	6.80	102,102,102,102	0
36	CL	0	8513	1/1	0.24	6.77	74,74,74,74	0
35	NA	0	8333	1/1	0.27	6.73	40,40,40,40	0
35	NA	0	8369	1/1	0.36	6.52	96,96,96,96	0
35	NA	R	8312	1/1	0.90	6.20	84,84,84,84	0
33	MG	0	8053	1/1	0.27	6.14	63,63,63,63	0
33	MG	0	8102	1/1	0.34	6.14	91,91,91,91	0
35	NA	0	8324	1/1	0.40	6.07	58,58,58,58	0
35	NA	0	8313	1/1	0.24	6.06	89,89,89,89	0
35	NA	0	8382	1/1	0.21	5.64	89,89,89,89	0
33	MG	0	8100	1/1	0.21	5.47	97,97,97,97	0
33	MG	0	8021	1/1	0.17	5.36	54,54,54,54	0
35	NA	0	8357	1/1	0.23	5.35	61,61,61,61	0
33	MG	0	8006	1/1	0.25	5.24	60,60,60,60	0
36	CL	P	8511	1/1	0.34	4.90	84,84,84,84	0
35	NA	0	8358	1/1	0.27	4.82	109,109,109,109	0
33	MG	0	8045	1/1	0.24	4.74	91,91,91,91	0
36	CL	0	8515	1/1	0.26	4.62	100,100,100,100	0
35	NA	0	8365	1/1	0.48	4.59	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8326	1/1	0.29	4.56	73,73,73,73	0
35	NA	0	8367	1/1	0.21	4.38	85,85,85,85	0
35	NA	0	8314	1/1	0.25	4.26	53,53,53,53	0
35	NA	0	8355	1/1	0.42	4.25	77,77,77,77	0
35	NA	9	8383	1/1	0.37	4.07	67,67,67,67	0
33	MG	0	8030	1/1	0.17	3.77	48,48,48,48	0
33	MG	0	8088	1/1	0.23	3.75	40,40,40,40	0
35	NA	0	8335	1/1	0.17	3.68	83,83,83,83	0
36	CL	0	8516	1/1	0.27	3.66	64,64,64,64	0
36	CL	0	8517	1/1	0.27	3.62	82,82,82,82	0
33	MG	9	8095	1/1	0.32	3.59	106,106,106,106	0
35	NA	0	8373	1/1	0.20	3.54	57,57,57,57	0
35	NA	C	8304	1/1	0.34	3.31	51,51,51,51	0
35	NA	0	8318	1/1	0.20	3.27	48,48,48,48	0
35	NA	0	8334	1/1	0.23	3.24	48,48,48,48	0
33	MG	0	8020	1/1	0.18	3.13	53,53,53,53	0
35	NA	0	8328	1/1	0.18	3.06	55,55,55,55	0
36	CL	I	8521	1/1	0.23	2.86	69,69,69,69	0
33	MG	0	8054	1/1	0.18	2.83	45,45,45,45	0
33	MG	0	8046	1/1	0.17	2.75	86,86,86,86	0
33	MG	0	8090	1/1	0.29	2.65	81,81,81,81	0
33	MG	0	8099	1/1	0.24	2.62	80,80,80,80	0
35	NA	H	8322	1/1	0.42	2.48	78,78,78,78	0
33	MG	0	8038	1/1	0.17	2.44	56,56,56,56	0
33	MG	0	8115	1/1	0.16	2.33	73,73,73,73	0
37	CD	N	8405	1/1	0.24	2.31	150,150,150,150	0
33	MG	0	8042	1/1	0.14	2.26	61,61,61,61	0
32	SLD	0	9500	37/37	0.21	2.11	46,50,53,59	0
33	MG	0	8049	1/1	0.30	2.10	90,90,90,90	0
33	MG	0	8009	1/1	0.17	2.02	44,44,44,44	0
36	CL	M	8507	1/1	0.25	1.83	86,86,86,86	0
36	CL	J	8512	1/1	0.21	1.79	67,67,67,67	0
33	MG	0	8011	1/1	0.19	1.72	50,50,50,50	0
35	NA	0	8320	1/1	0.17	1.70	40,40,40,40	0
35	NA	H	8309	1/1	0.24	1.66	49,49,49,49	0
33	MG	0	8060	1/1	0.14	1.51	63,63,63,63	0
33	MG	0	8082	1/1	0.14	1.47	79,79,79,79	0
33	MG	X	8109	1/1	0.20	1.36	66,66,66,66	0
35	NA	0	8374	1/1	0.16	1.33	77,77,77,77	0
33	MG	0	8014	1/1	0.18	1.31	46,46,46,46	0
36	CL	K	8510	1/1	0.24	1.28	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8310	1/1	0.17	1.22	46,46,46,46	0
33	MG	0	8013	1/1	0.17	1.17	60,60,60,60	0
35	NA	Q	8337	1/1	0.23	1.11	64,64,64,64	0
33	MG	0	8004	1/1	0.18	1.01	50,50,50,50	0
33	MG	0	8001	1/1	0.16	1.00	46,46,46,46	0
35	NA	0	8339	1/1	0.15	0.96	33,33,33,33	0
36	CL	I	8501	1/1	0.18	0.81	99,99,99,99	0
35	NA	0	8359	1/1	0.14	0.80	81,81,81,81	0
33	MG	0	8101	1/1	0.13	0.75	94,94,94,94	0
36	CL	0	8514	1/1	0.14	0.72	75,75,75,75	0
36	CL	N	8508	1/1	0.19	0.72	116,116,116,116	0
33	MG	0	8008	1/1	0.15	0.72	52,52,52,52	0
33	MG	0	8112	1/1	0.15	0.69	64,64,64,64	0
33	MG	0	8116	1/1	0.16	0.64	84,84,84,84	0
35	NA	0	8319	1/1	0.17	0.46	41,41,41,41	0
35	NA	0	8331	1/1	0.14	0.44	60,60,60,60	0
35	NA	9	8351	1/1	0.34	0.36	94,94,94,94	0
33	MG	0	8079	1/1	0.12	0.34	53,53,53,53	0
33	MG	0	8017	1/1	0.15	0.30	43,43,43,43	0
33	MG	0	8104	1/1	0.15	0.09	66,66,66,66	0
33	MG	0	8076	1/1	0.15	0.09	102,102,102,102	0
33	MG	0	8003	1/1	0.14	0.06	51,51,51,51	0
35	NA	0	8330	1/1	0.12	-0.02	61,61,61,61	0
35	NA	0	8353	1/1	0.12	-0.02	43,43,43,43	0
33	MG	0	8028	1/1	0.16	-0.04	57,57,57,57	0
34	K	0	8201	1/1	0.13	-0.29	141,141,141,141	0
33	MG	0	8077	1/1	0.12	-0.46	54,54,54,54	0
35	NA	0	8342	1/1	0.13	-0.46	42,42,42,42	0
33	MG	0	8007	1/1	0.12	-0.55	47,47,47,47	0
33	MG	A	8065	1/1	0.13	-0.55	55,55,55,55	0
35	NA	0	8301	1/1	0.11	-0.60	59,59,59,59	0
33	MG	0	8034	1/1	0.11	-0.65	46,46,46,46	0
35	NA	L	8347	1/1	0.14	-0.66	55,55,55,55	0
33	MG	0	8110	1/1	0.13	-0.70	56,56,56,56	0
33	MG	0	8015	1/1	0.11	-0.90	60,60,60,60	0
33	MG	0	8066	1/1	0.15	-0.91	105,105,105,105	0
35	NA	0	8343	1/1	0.12	-0.92	48,48,48,48	0
33	MG	0	8111	1/1	0.11	-1.02	75,75,75,75	0
33	MG	0	8005	1/1	0.11	-1.10	58,58,58,58	0
37	CD	Y	8403	1/1	0.08	-1.13	84,84,84,84	0
33	MG	0	8058	1/1	0.09	-1.18	61,61,61,61	0
33	MG	S	8073	1/1	0.11	-1.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8093	1/1	0.11	-1.24	63,63,63,63	0
36	CL	I	8502	1/1	0.12	-1.29	93,93,93,93	0
37	CD	2	8404	1/1	0.09	-1.33	90,90,90,90	0
35	NA	I	8346	1/1	0.09	-1.38	45,45,45,45	0
33	MG	0	8086	1/1	0.06	-1.40	62,62,62,62	0
35	NA	0	8317	1/1	0.10	-1.41	57,57,57,57	0
33	MG	4	8063	1/1	0.11	-1.44	62,62,62,62	0
33	MG	0	8062	1/1	0.09	-1.48	90,90,90,90	0
33	MG	0	8057	1/1	0.08	-1.51	53,53,53,53	0
33	MG	0	8107	1/1	0.09	-1.52	55,55,55,55	0
35	NA	0	8327	1/1	0.11	-1.56	46,46,46,46	0
37	CD	Z	8402	1/1	0.06	-1.59	89,89,89,89	0
33	MG	0	8010	1/1	0.11	-1.63	47,47,47,47	0
33	MG	0	8074	1/1	0.06	-1.67	51,51,51,51	0
33	MG	0	8096	1/1	0.11	-1.67	70,70,70,70	0
33	MG	0	8098	1/1	0.10	-1.73	50,50,50,50	0
35	NA	0	8338	1/1	0.06	-1.74	66,66,66,66	0
33	MG	0	8039	1/1	0.10	-1.75	53,53,53,53	0
33	MG	0	8068	1/1	0.07	-1.84	64,64,64,64	0
33	MG	0	8117	1/1	0.08	-1.84	45,45,45,45	0
36	CL	L	8518	1/1	0.10	-1.86	69,69,69,69	0
33	MG	0	8070	1/1	0.09	-1.89	63,63,63,63	0
33	MG	0	8002	1/1	0.09	-1.99	51,51,51,51	0
33	MG	0	8019	1/1	0.12	-2.05	43,43,43,43	0
35	NA	A	8345	1/1	0.10	-2.08	48,48,48,48	0
33	MG	0	8018	1/1	0.09	-2.10	57,57,57,57	0
33	MG	9	8052	1/1	0.09	-2.12	60,60,60,60	0
35	NA	P	8348	1/1	0.09	-2.13	68,68,68,68	0
35	NA	0	8344	1/1	0.08	-2.21	48,48,48,48	0
33	MG	0	8056	1/1	0.10	-2.22	60,60,60,60	0
33	MG	0	8027	1/1	0.06	-2.26	65,65,65,65	0
33	MG	0	8031	1/1	0.11	-2.31	54,54,54,54	0
33	MG	0	8029	1/1	0.06	-2.40	60,60,60,60	0
33	MG	0	8040	1/1	0.09	-2.40	88,88,88,88	0
33	MG	0	8080	1/1	0.08	-2.53	52,52,52,52	0
33	MG	0	8067	1/1	0.10	-2.54	81,81,81,81	0
33	MG	B	8055	1/1	0.06	-2.58	71,71,71,71	0
33	MG	0	8081	1/1	0.08	-2.64	67,67,67,67	0
37	CD	T	8401	1/1	0.06	-2.67	83,83,83,83	0
33	MG	0	8087	1/1	0.08	-2.70	82,82,82,82	0
33	MG	0	8016	1/1	0.08	-2.78	71,71,71,71	0
33	MG	0	8050	1/1	0.16	-2.84	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	2	8078	1/1	0.04	-2.92	65,65,65,65	0
33	MG	0	8083	1/1	0.08	-2.93	65,65,65,65	0
33	MG	0	8012	1/1	0.06	-3.06	42,42,42,42	0
33	MG	0	8033	1/1	0.11	-3.07	48,48,48,48	0
35	NA	0	8336	1/1	0.08	-3.24	63,63,63,63	0
33	MG	0	8075	1/1	0.08	-3.39	77,77,77,77	0
33	MG	0	8091	1/1	0.05	-3.43	65,65,65,65	0
33	MG	J	8069	1/1	0.05	-3.58	87,87,87,87	0
33	MG	0	8048	1/1	0.05	-3.60	66,66,66,66	0
33	MG	0	8094	1/1	0.06	-3.80	97,97,97,97	0
35	NA	0	8305	1/1	0.08	-4.03	42,42,42,42	0
33	MG	0	8043	1/1	0.07	-4.14	64,64,64,64	0
33	MG	0	8037	1/1	0.06	-4.20	54,54,54,54	0
33	MG	0	8089	1/1	0.09	-4.32	82,82,82,82	0
33	MG	0	8059	1/1	0.07	-4.45	60,60,60,60	0
33	MG	0	8071	1/1	0.07	-4.59	104,104,104,104	0
33	MG	0	8036	1/1	0.05	-4.76	52,52,52,52	0
33	MG	0	8032	1/1	0.06	-4.96	52,52,52,52	0
33	MG	0	8061	1/1	0.05	-5.49	45,45,45,45	0
33	MG	0	8026	1/1	0.10	-5.99	39,39,39,39	0
33	MG	0	8035	1/1	0.06	-6.17	69,69,69,69	0
33	MG	0	8084	1/1	0.05	-6.98	70,70,70,70	0
33	MG	0	8047	1/1	0.10	-7.84	90,90,90,90	0
33	MG	0	8025	1/1	0.06	-8.09	59,59,59,59	0
33	MG	0	8023	1/1	0.05	-51.62	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.