



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:29 am GMT

PDB ID : 3CC2
Title : The Refined Crystal Structure of the Haloarcula Marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution with rrnA Sequence for the 23S rRNA and Genome-derived Sequences for r-Proteins
Authors : Gurel, G.; Blaha, G.
Deposited on : 2008-02-23
Resolution : 2.40 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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) : recalc28949

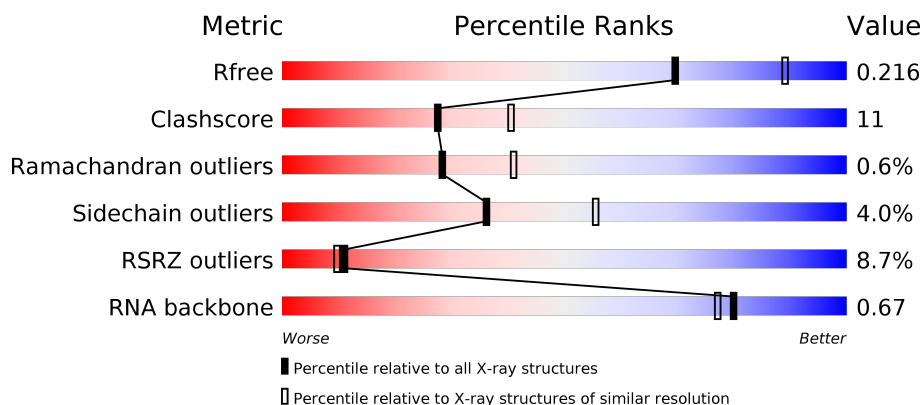
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
R_{free}	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>9%</div> <div>70%</div> <div>26%</div> <div>..</div> </div>
2	B	338	<div> <div>12%</div> <div>71%</div> <div>25%</div> <div>.</div> </div>
3	C	246	<div> <div>6%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
4	D	177	<div> <div>49%</div> <div>47%</div> <div>29%</div> <div>21%</div> </div>

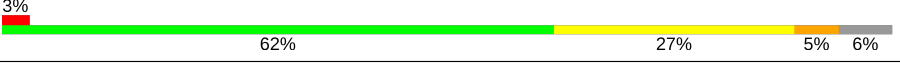

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

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
32	MG	0	8060	-	-	-	X
32	MG	0	8064	-	-	-	X
32	MG	0	8066	-	-	-	X
34	NA	0	8302	-	-	-	X
34	NA	0	8303	-	-	-	X
34	NA	0	8305	-	-	-	X
34	NA	0	8320	-	-	-	X
34	NA	0	8323	-	-	-	X
34	NA	0	8325	-	-	-	X
34	NA	0	8326	-	-	-	X
34	NA	0	8327	-	-	-	X
34	NA	0	8331	-	-	-	X
34	NA	0	8335	-	-	-	X
34	NA	0	8340	-	-	-	X
34	NA	0	8350	-	-	-	X
34	NA	0	8356	-	-	-	X
34	NA	0	8359	-	-	-	X
34	NA	0	8362	-	-	-	X
34	NA	0	8364	-	-	-	X
34	NA	0	8366	-	-	-	X
34	NA	0	8368	-	-	-	X
34	NA	0	8371	-	-	-	X
34	NA	0	8372	-	-	-	X
34	NA	0	8374	-	-	-	X
34	NA	0	8376	-	-	-	X
34	NA	0	8378	-	-	-	X
34	NA	0	8379	-	-	-	X
34	NA	R	8386	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 99049 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 protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	0	0
			1753	1072	352	324	5			

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 9 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	70	Total	C	N	O	S	0	0	0
			519	323	81	114	1			

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

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

- Molecule 12 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
12	L	145	Total	C	N	O	0	0	0
			1118	670	222	226			

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	143	Total	C	N	O		0	0	0
			1136	683	229	224				

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	109	Total	Mg	0	0
			109	109		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	1	Total	Mg	0	0
			1	1		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	73	Total Na 73 73	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	A	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	9	3	Total Na 3 3	0	0
34	L	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cd 1	0	0
36	Z	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	3	1	Total 1	Cd 1	0	0
36	U	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	5949	Total 5949	O 5949	0	0
37	A	117	Total 117	O 117	0	0
37	B	146	Total 146	O 146	0	0
37	C	170	Total 170	O 170	0	0
37	D	47	Total 47	O 47	0	0
37	E	42	Total 42	O 42	0	0
37	F	24	Total 24	O 24	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	19	Total 19	O 19	0	0
37	H	72	Total 72	O 72	0	0
37	I	9	Total 9	O 9	0	0
37	J	51	Total 51	O 51	0	0
37	K	56	Total 56	O 56	0	0
37	L	72	Total 72	O 72	0	0
37	M	119	Total 119	O 119	0	0
37	N	65	Total 65	O 65	0	0
37	O	39	Total 39	O 39	0	0
37	P	63	Total 63	O 63	0	0
37	Q	52	Total 52	O 52	0	0
37	R	80	Total 80	O 80	0	0
37	S	33	Total 33	O 33	0	0
37	T	38	Total 38	O 38	0	0
37	U	27	Total 27	O 27	0	0
37	V	14	Total 14	O 14	0	0
37	W	66	Total 66	O 66	0	0
37	X	29	Total 29	O 29	0	0
37	Y	94	Total 94	O 94	0	0
37	Z	26	Total 26	O 26	0	0
37	1	53	Total 53	O 53	0	0

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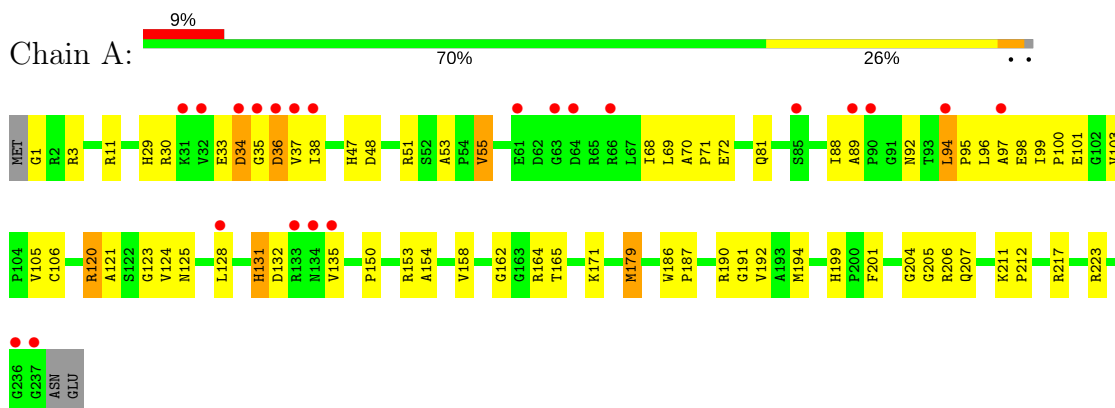
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	40	Total 40	O 40	0	0
37	3	72	Total 72	O 72	0	0
37	9	139	Total 139	O 139	0	0

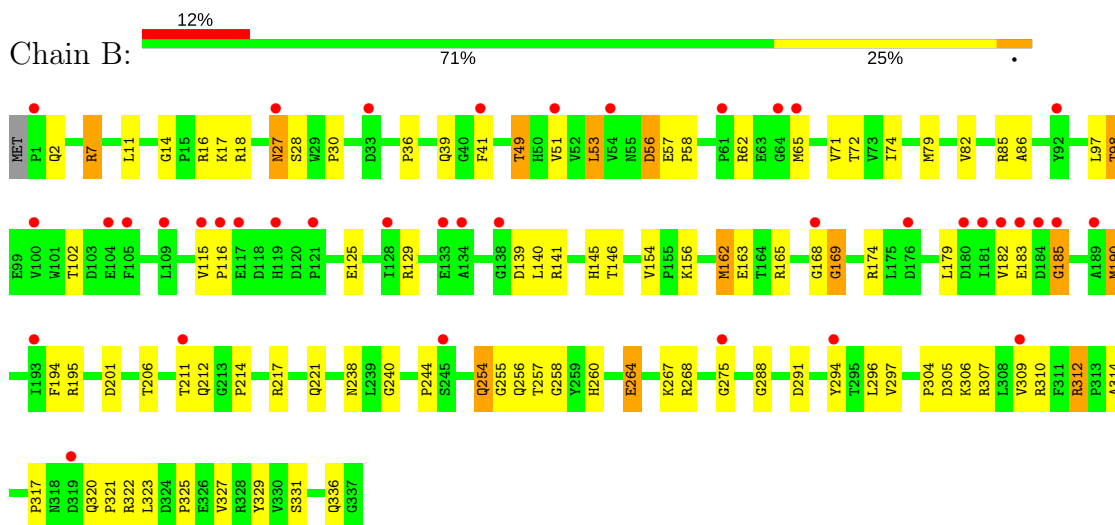
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

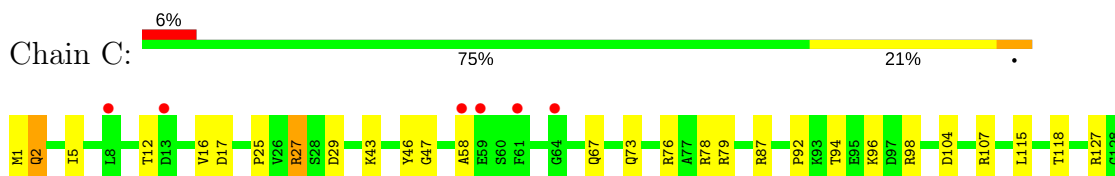
• Molecule 1: 50S ribosomal protein L2P

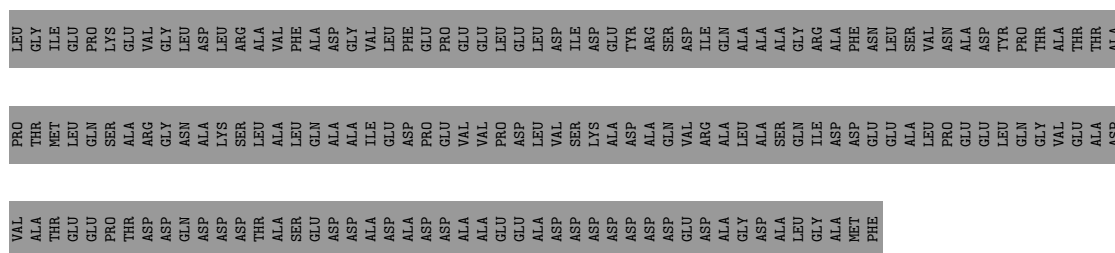


• Molecule 2: 50S ribosomal protein L3P

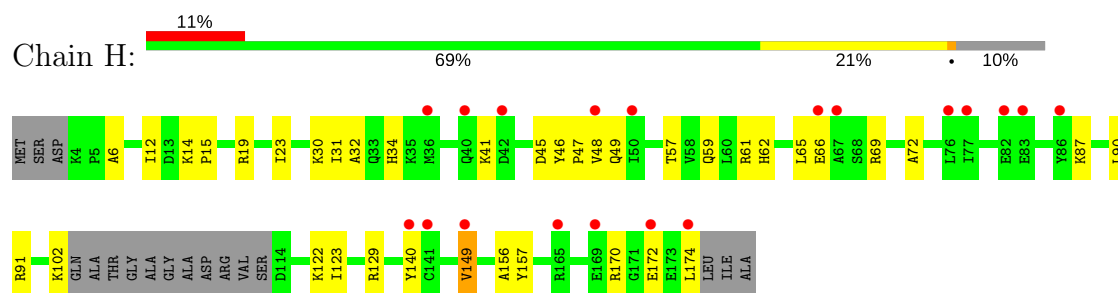


• Molecule 3: 50S ribosomal protein L4P

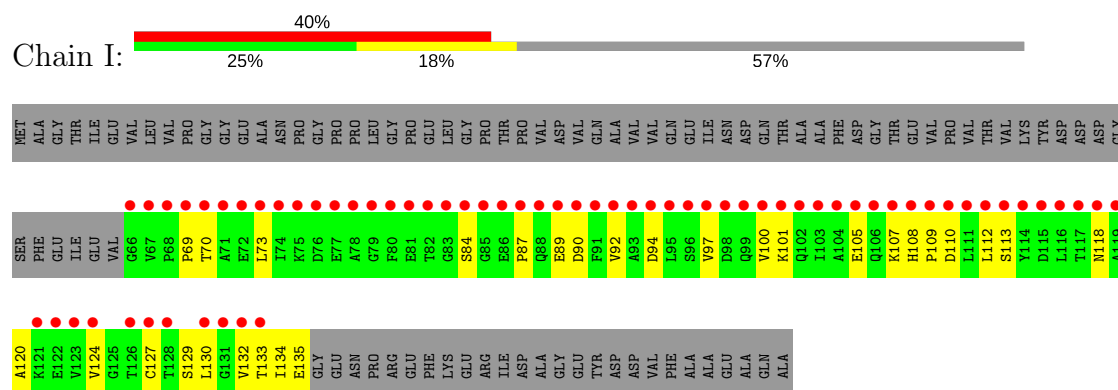




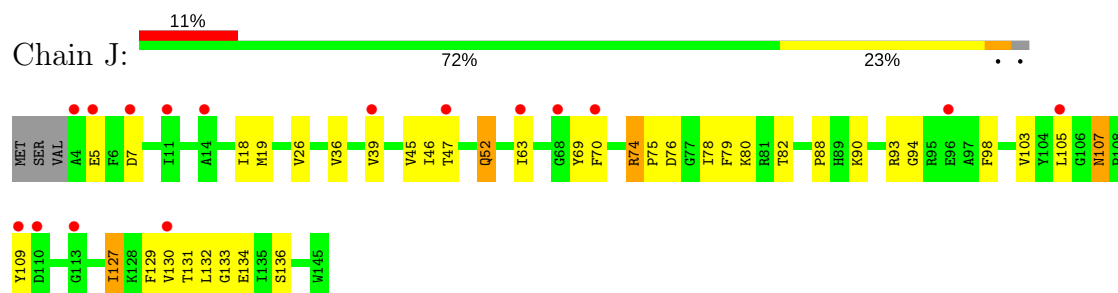
- Molecule 8: 50S ribosomal protein L10e



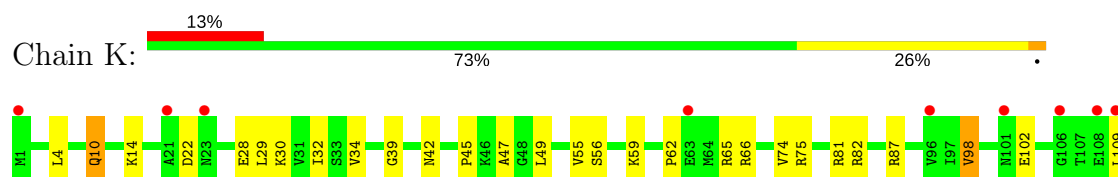
- Molecule 9: 50S ribosomal protein L11P



- Molecule 10: 50S ribosomal protein L13P

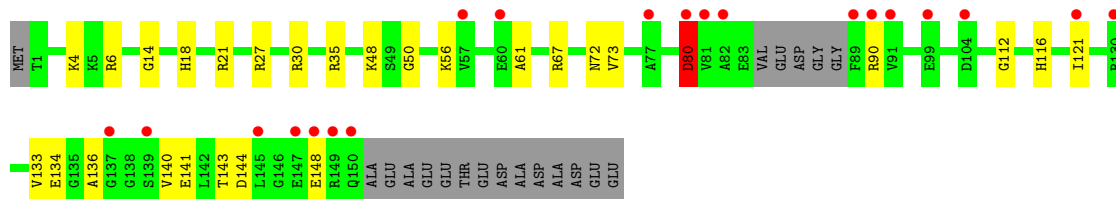


- Molecule 11: 50S ribosomal protein L14P

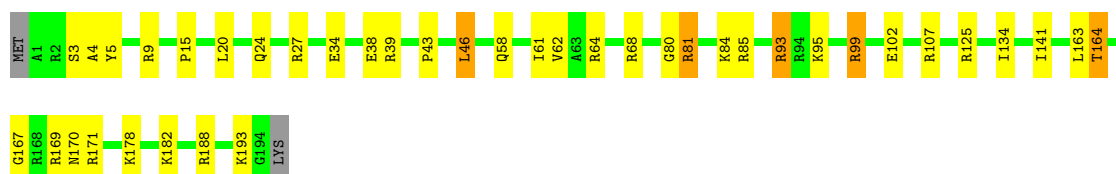
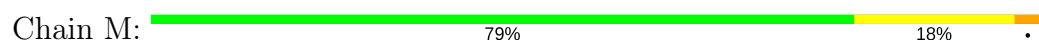




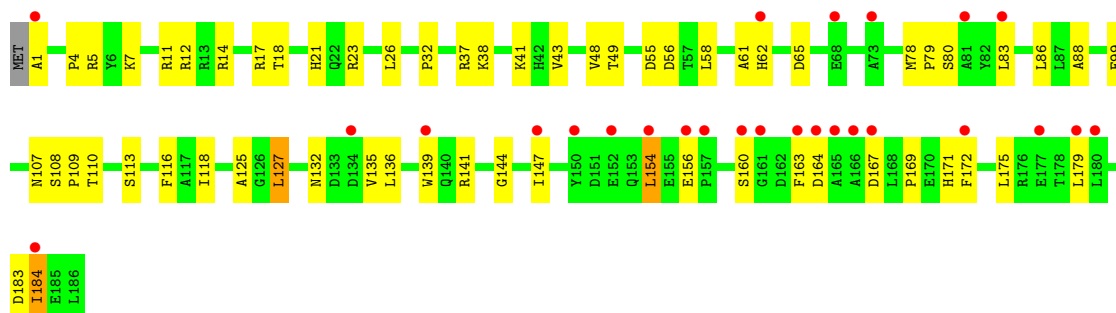
- Molecule 12: 50S ribosomal protein L15P



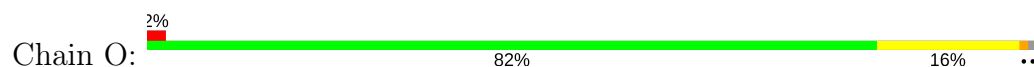
- Molecule 13: 50S ribosomal protein L15e



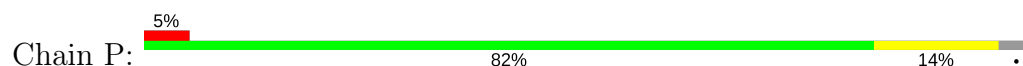
- Molecule 14: 50S ribosomal protein L18P



- Molecule 15: 50S ribosomal protein L18e

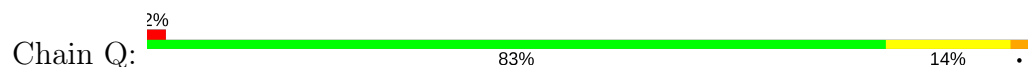


- Molecule 16: 50S ribosomal protein L19e





- Molecule 17: 50S ribosomal protein L21e

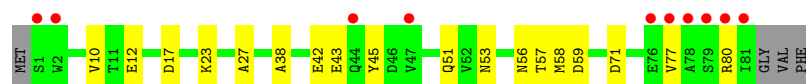


- Molecule 18: 50S ribosomal protein L22P

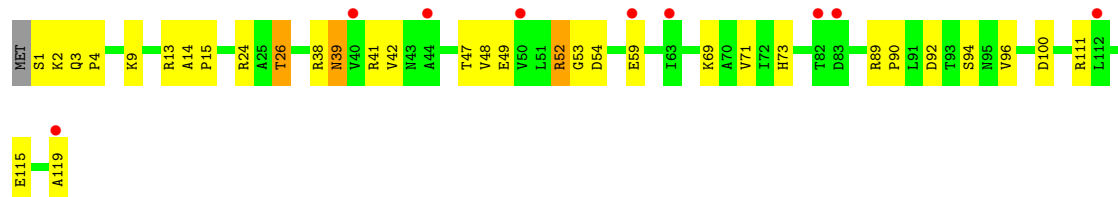


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- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P

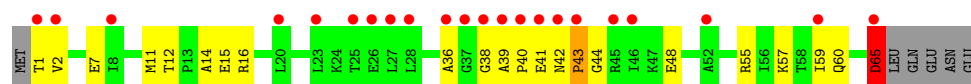


- Molecule 21: 50S ribosomal protein L24e

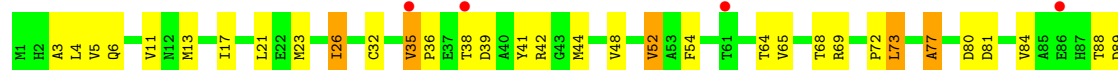


- Molecule 22: 50S ribosomal protein L29P

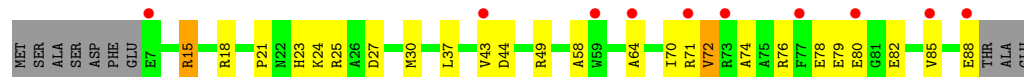




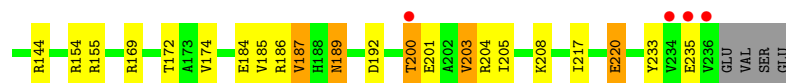
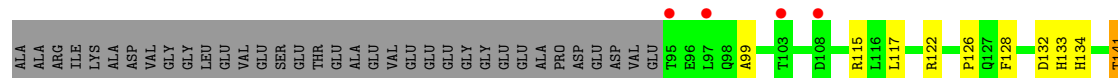
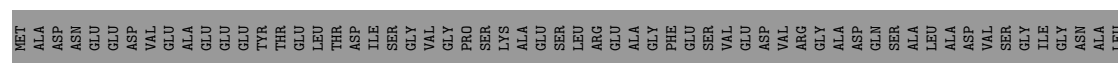
• Molecule 23: 50S ribosomal protein L30P



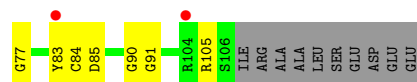
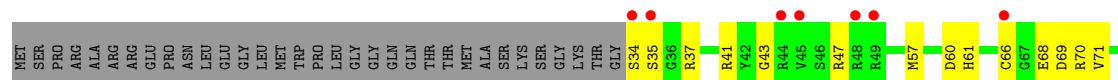
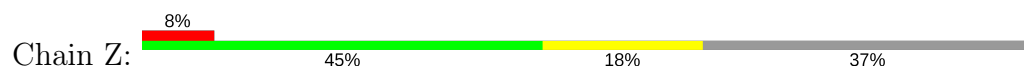
• Molecule 24: 50S ribosomal protein L31e



• Molecule 25: 50S ribosomal protein L32e



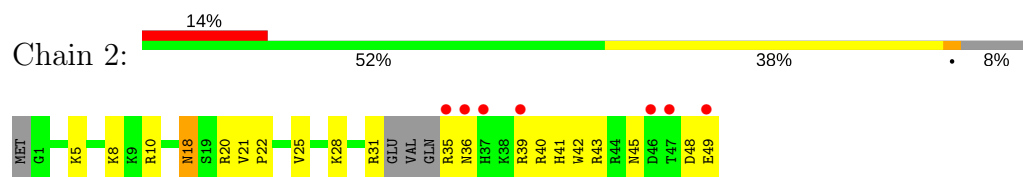
• Molecule 26: 50S ribosomal protein L37Ae



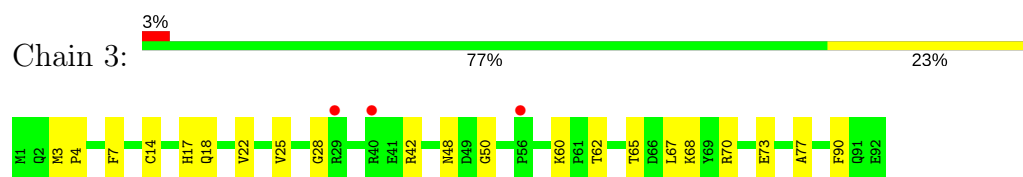
• Molecule 27: 50S ribosomal protein L37e



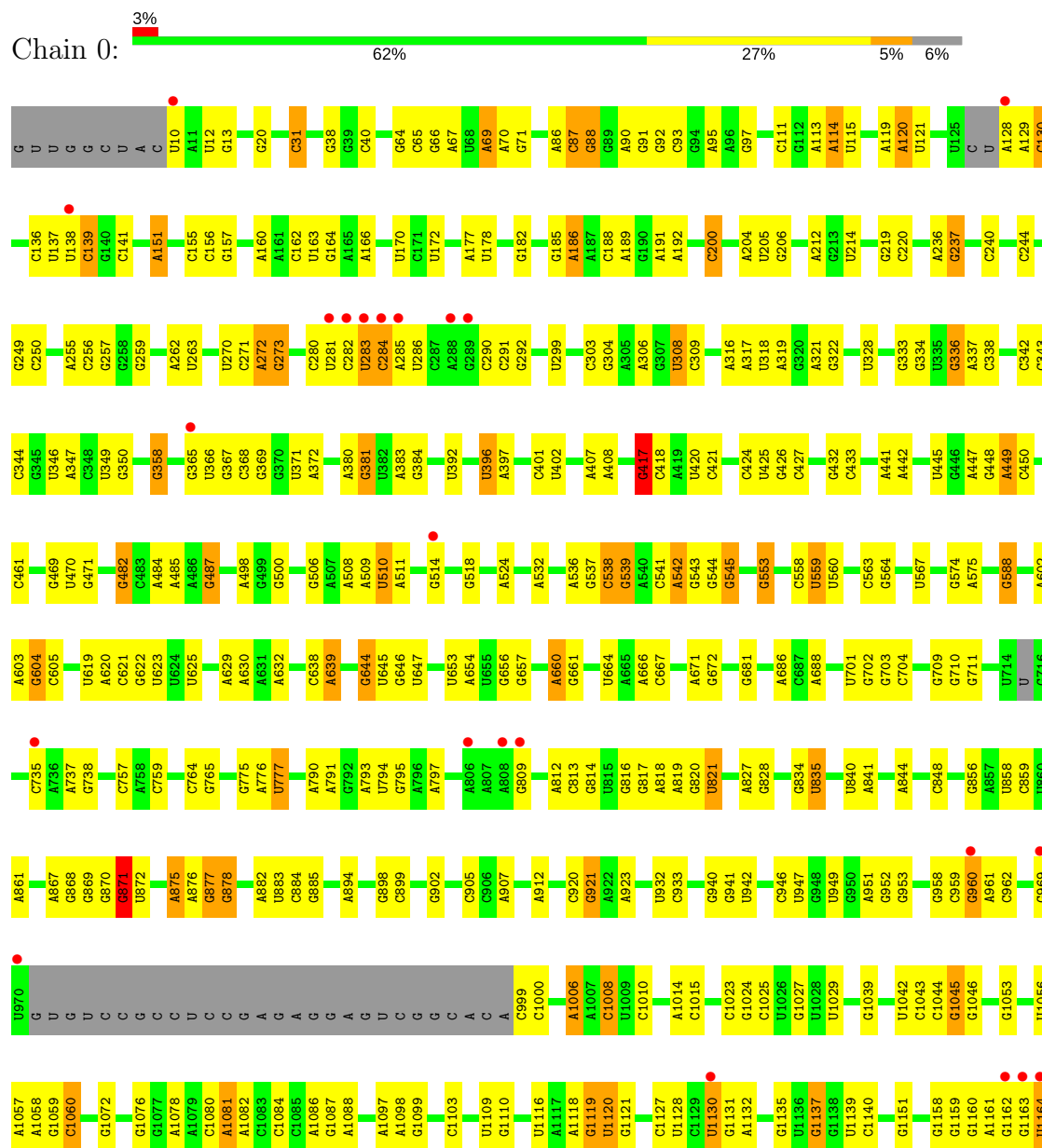
• Molecule 28: 50S ribosomal protein L39e



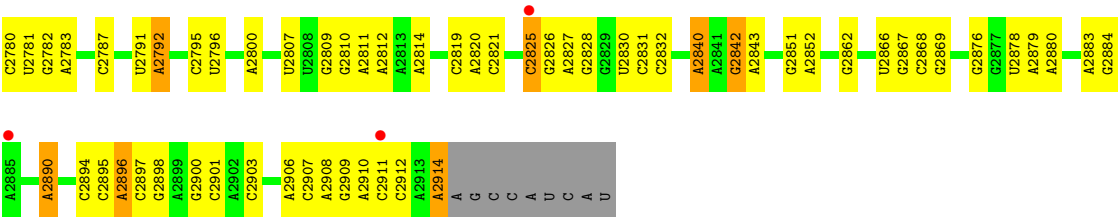
• Molecule 29: 50S ribosomal protein L44E



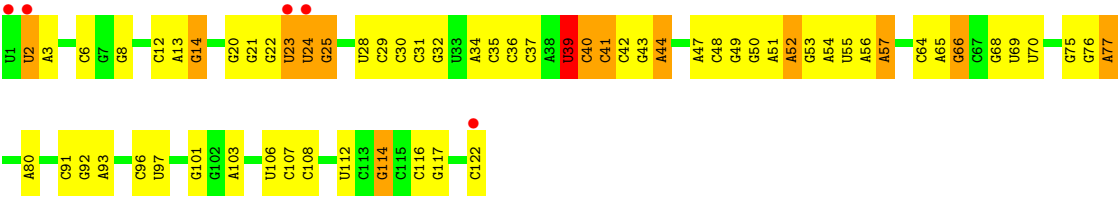
• Molecule 30: 23S RIBOSOMAL RNA



C2667	G2537	G2453	G2338	A	G1971	G1848	A1716	A1597	C1462	A1341	G1235	G1165
G2668	A2538	A2456	A	C	U1972	C1856	A1717	A1598	U1463	C1342	A1236	A1166
U2669	U2541	U2457	A	C	A1973	C1863	U1722	A1603	A1470	C1343	U1237	G1167
U2671	C2542	G2457	G	C	G1976	G1867	U1723	G1604	U1350	U1350	C1238	C1168
C2672	G2543	U2457	A	C	U1977	G1868	U1724	G1605	C1474	U1351	G1239	U1170
U2673	G2544	G2457	A	C	A1978	G1867	C1725	G1611	U1352	A1352	G1240	U1171
C2676	C2462	A2463	G	A	G1979	G1868	G1730	G1612	C1477	C1353	G1241	A1172
C2676	A2463	A2464	G	G	U1980	G1868	A1731	A1613	A1482	C1360	C1242	A1173
A2681	A2465	A2465	U	A	U1985	G1877	C1732	G1614	A1483	U1244	C1245	A1174
C2682	G2466	G2466	A	C	U1985	G1877	A1733	A1615	G1484	C1246	A1246	G1175
U2690	A2467	A2468	C	C	U1992	G1878	C1734	A1624	A1485	U1367	U1249	G1176
A2691	A2468	A2469	C	C	C1993	C1860	C1735	U1625	A1493	A1369	C1250	G1177
G2694	C2472	C2472	C	C	U1994	A1881	A1736	U1626	U1370	G1370	C1251	G1178
U2694	G2476	G2477	C	C	G1995	C1882	C1737	U1627	A1497	A1372	U1180	A1181
C2698	U2478	U2478	G	G	U1996	G1883	U1741	G1627	G1497	U1372	A1252	A1182
U2710	A2479	A2479	C	C	U1997	G1884	A1742	A1632	U1500	C1377	C1183	C1183
G2711	G2483	G2483	U	A	G2001	A1909	G1782	C1633	U1503	C1384	G1257	U1185
G2712	U2487	U2487	G	G	C2002	A1919	U1766	G1634	U1504	U1384	G1258	C1186
G2716	G2488	G2488	C	C	U2003	G1920	U1771	U1635	U1505	A1393	U1266	U1187
C2717	U2489	U2489	C	C	G2005	A1921	C1772	U1636	U1506	C1394	C1267	A1188
A2719	G2490	G2490	G	G	U2008	A1922	G1773	A1641	U1521	A1406	C1268	A1189
G2720	U2491	U2491	C	C	G2009	G1925	A1778	A1642	U1524	A1407	G1269	G1190
U2721	U2492	U2492	C	C	A2010	G1926	A1779	U1654	A1526	U1408	A1278	A1191
G2722	U2493	U2493	C	C	U2011	C1928	U1783	G1655	A1527	G1409	U1279	A1192
G2723	U2494	U2494	C	C	G2012	G1929	U1784	A1656	A1528	A1413	C1289	A1193
U2724	U2495	U2495	C	C	U2013	C1930	U1785	A1657	G1529	A1414	G1290	G1195
G2725	U2496	U2496	G	G	A2015	A1941	C1787	C1666	G1535	G1417	A1294	G1196
U2726	U2497	U2497	A	A	U2016	C1942	U1788	A1667	C1536	U1418	G1295	G1197
C2729	U2498	U2498	A	A	G2019	C1943	G1789	U1668	C1545	U1419	A1299	A1199
G2730	U2499	U2499	C	C	A2031	G1946	C1798	C1675	G1546	C1423	G1300	C1201
G2738	U2500	U2500	A	A	U2032	G1947	G1799	G1676	U1556	A1424	U1304	G1202
C2747	U2501	U2501	C	C	G2033	G1948	A1815	U1677	G1557	U1427	C1305	U1205
G2748	U2502	U2502	U	U	U2034	G1949	C1816	A1678	G1557	C1428	U1306	U1206
U2749	U2503	U2503	C	C	G2044	G1950	G1819	C1680	A1559	U1429	A1313	A1207
G2750	U2504	U2504	A	A	U2045	G1951	G1820	G1681	U1561	G1430	G1315	C1208
C2751	U2505	U2505	A	A	G2050	G1952	U1825	A1682	C1562	U1435	U1210	G1209
G2754	U2506	U2506	C	C	A2054	G1953	C1826	A1683	C1562	G1433	G1316	C1211
U2755	U2507	U2507	U	U	C2061	G1954	U1826	A1684	U1565	U1434	C1316	C1212
G2756	U2508	U2508	A	A	A2062	G1955	A1829	A1685	G1571	C1436	G1325	C1213
C2762	U2509	U2509	C	C	U2063	G1956	A1830	C1692	U1571	U1436	U1325	G1214
A2768	U2510	U2510	C	C	U2064	G1957	C1834	G1697	G1588	C1439	A1328	A1215
C2769	U2511	U2511	C	C	G2070	G1958	U1835	U1698	G1589	U1440	G1329	G1216
G2770	U2512	U2512	U	U	C2071	G1959	A1840	C1699	U1596	A1441	U1330	U1217
C2777	U2513	U2513	C	C	G2072	G1960	A1841	U1701	G1593	A1442	U1333	U1219
A2778	U2514	U2514	G	G	C2073	G1961	A1842	U1702	C1593	C1450	C1334	C1229
G2779	U2515	U2515	U	U	A2074	G1962	A1843	C1714	G1594	G1453	G1339	A1230
	U2516	U2516	C	C	U2081	G1963	A1844	C1715	U1596	U1453	G1340	U1234



● Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.65Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.95 – 2.40 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (49.95-2.40) 90.6 (85.47-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.199 , 0.231 0.183 , 0.216	Depositor DCC
R_{free} test set	6200 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	99049	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, OMG, CL, NA, K, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	0/1786	0.66	0/2408
2	B	0.32	0/2690	0.64	0/3652
3	C	0.36	0/1885	0.64	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.31	0/1382	0.56	0/1880
6	F	0.32	0/901	0.54	0/1224
7	G	0.42	0/241	0.74	0/324
8	H	0.39	0/1302	0.68	0/1743
9	I	0.34	0/526	0.53	0/716
10	J	0.33	0/1136	0.58	0/1530
11	K	0.32	0/1004	0.65	0/1351
12	L	0.34	0/1130	0.65	0/1509
13	M	0.33	0/1582	0.62	0/2116
14	N	0.28	0/1474	0.61	0/1999
15	O	0.32	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.33	0/749	0.67	0/1005
18	R	1.31	7/1172 (0.6%)	1.13	5/1578 (0.3%)
19	S	0.33	0/648	0.59	1/875 (0.1%)
20	T	0.31	0/958	0.62	1/1289 (0.1%)
21	U	0.36	0/417	0.60	0/562
22	V	0.36	0/502	0.68	1/675 (0.1%)
23	W	0.33	0/1219	0.65	1/1655 (0.1%)
24	X	0.36	0/664	0.59	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.34	0/584	0.66	0/781
27	1	0.42	0/438	0.65	0/578
28	2	0.33	0/401	0.56	0/529
29	3	0.36	0/771	0.59	0/1024
30	0	0.33	0/65958	0.69	21/102869 (0.0%)
31	9	0.29	0/2904	0.69	1/4526 (0.0%)
All	All	0.36	7/98702 (0.0%)	0.68	32/147588 (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
18	R	1	0
30	0	0	39
31	9	0	1
All	All	1	40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CA-C	-29.63	0.93	1.52
18	R	150	PRO	CB-CG	16.19	2.31	1.50
18	R	150	PRO	N-CA	14.71	1.72	1.47
18	R	150	PRO	CA-CB	12.12	1.77	1.53
18	R	150	PRO	CG-CD	11.79	1.89	1.50

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	N-CA-C	-24.01	49.68	112.10
18	R	150	PRO	CB-CA-C	-19.94	62.16	112.00
18	R	150	PRO	CA-C-O	-16.63	80.28	120.20
30	0	1942	A	C5'-C4'-C3'	8.15	129.05	116.00
18	R	150	PRO	CA-N-CD	7.93	122.80	111.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 40 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	270	U	Sidechain
30	0	396	U	Sidechain
30	0	417	G	Sidechain
30	0	449	A	Sidechain
30	0	469	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	74	0
2	B	2625	0	2533	80	0
3	C	1860	0	1813	65	0
4	D	1094	0	1085	45	0
5	E	1357	0	1266	42	0
6	F	890	0	843	26	0
7	G	240	0	231	11	0
8	H	1282	0	1292	34	0
9	I	519	0	500	23	0
10	J	1120	0	1098	39	0
11	K	994	0	1027	40	0
12	L	1118	0	1076	26	0
13	M	1558	0	1572	44	0
14	N	1445	0	1401	55	0
15	O	865	0	873	19	0
16	P	1136	0	1123	20	0
17	Q	735	0	728	11	0
18	R	1149	0	1122	31	0
19	S	641	0	605	13	0
20	T	950	0	923	24	0
21	U	410	0	364	16	0
22	V	499	0	511	19	0
23	W	1196	0	1137	66	0
24	X	654	0	653	21	0
25	Y	1130	0	1133	30	0
26	Z	573	0	532	14	0
27	1	431	0	426	17	0
28	2	396	0	413	24	0
29	3	755	0	728	16	0
30	0	59021	0	29809	870	0
31	9	2599	0	1325	72	0
32	0	109	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	73	0	0	0	0
34	9	3	0	0	0	0
34	A	1	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	L	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	0	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	5949	0	0	149	0
37	1	53	0	0	2	0
37	2	40	0	0	4	0
37	3	72	0	0	6	0
37	9	139	0	0	7	0
37	A	117	0	0	14	0
37	B	146	0	0	13	0
37	C	170	0	0	18	0
37	D	47	0	0	5	0
37	E	42	0	0	4	0
37	F	24	0	0	2	0
37	G	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	H	72	0	0	5	0
37	I	9	0	0	3	0
37	J	51	0	0	2	0
37	K	56	0	0	5	0
37	L	72	0	0	9	0
37	M	119	0	0	9	0
37	N	65	0	0	10	0
37	O	39	0	0	3	0
37	P	63	0	0	1	0
37	Q	52	0	0	3	0
37	R	80	0	0	2	0
37	S	33	0	0	2	0
37	T	38	0	0	2	0
37	U	27	0	0	1	0
37	V	14	0	0	1	0
37	W	66	0	0	5	0
37	X	29	0	0	5	0
37	Y	94	0	0	10	0
37	Z	26	0	0	2	0
All	All	99049	0	59908	1694	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 11.

The worst 5 of 1694 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.89	1.50
14:N:37:ARG:NH1	31:9:6:C:H5''	1.61	1.14
30:0:871:G:C8	30:0:871:G:H5'	1.86	1.10
30:0:960:G:H4'	37:0:6980:HOH:O	1.49	1.09
18:R:150:PRO:CG	18:R:150:PRO:CB	2.30	1.08

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	
1	A	235/240 (98%)	220 (94%)	13 (6%)	2 (1%)	20	29
2	B	335/338 (99%)	315 (94%)	17 (5%)	3 (1%)	20	29
3	C	244/246 (99%)	231 (95%)	13 (5%)	0	100	100
4	D	134/177 (76%)	115 (86%)	15 (11%)	4 (3%)	5	4
5	E	170/178 (96%)	165 (97%)	5 (3%)	0	100	100
6	F	117/120 (98%)	106 (91%)	9 (8%)	2 (2%)	11	13
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	148 (95%)	8 (5%)	0	100	100
9	I	68/162 (42%)	57 (84%)	11 (16%)	0	100	100
10	J	140/145 (97%)	132 (94%)	7 (5%)	1 (1%)	25	37
11	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	22	33
12	L	141/165 (86%)	126 (89%)	14 (10%)	1 (1%)	25	37
13	M	192/196 (98%)	187 (97%)	5 (3%)	0	100	100
14	N	184/187 (98%)	170 (92%)	11 (6%)	3 (2%)	11	15
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	140 (99%)	1 (1%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	144 (97%)	4 (3%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	48 (94%)	2 (4%)	1 (2%)	9	10
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	11	15
23	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	25	37
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	14	19
25	Y	140/241 (58%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	63 (89%)	6 (8%)	2 (3%)	6	5
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
All	All	3705/4472 (83%)	3505 (95%)	177 (5%)	23 (1%)	28	41

5 of 23 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
6	F	101	ALA
10	J	5	GLU
12	L	80	ASP
14	N	154	LEU

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	
1	A	179/182 (98%)	171 (96%)	8 (4%)	32	50
2	B	282/283 (100%)	268 (95%)	14 (5%)	28	45
3	C	193/193 (100%)	179 (93%)	14 (7%)	16	26
4	D	117/148 (79%)	112 (96%)	5 (4%)	33	52
5	E	152/156 (97%)	148 (97%)	4 (3%)	51	72
6	F	93/94 (99%)	92 (99%)	1 (1%)	78	90
7	G	27/282 (10%)	26 (96%)	1 (4%)	39	59
8	H	134/145 (92%)	129 (96%)	5 (4%)	39	59
9	I	58/130 (45%)	57 (98%)	1 (2%)	66	82
10	J	118/121 (98%)	110 (93%)	8 (7%)	18	29
11	K	106/106 (100%)	103 (97%)	3 (3%)	49	70
12	L	113/127 (89%)	110 (97%)	3 (3%)	50	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	152 (96%)	6 (4%)	38	58
14	N	149/150 (99%)	146 (98%)	3 (2%)	60	79
15	O	93/94 (99%)	90 (97%)	3 (3%)	44	65
16	P	113/117 (97%)	111 (98%)	2 (2%)	64	81
17	Q	79/80 (99%)	75 (95%)	4 (5%)	28	44
18	R	117/122 (96%)	115 (98%)	2 (2%)	66	82
19	S	71/74 (96%)	69 (97%)	2 (3%)	49	70
20	T	105/106 (99%)	98 (93%)	7 (7%)	19	30
21	U	44/53 (83%)	44 (100%)	0	100	100
22	V	51/57 (90%)	49 (96%)	2 (4%)	37	56
23	W	130/130 (100%)	123 (95%)	7 (5%)	26	41
24	X	66/74 (89%)	60 (91%)	6 (9%)	11	16
25	Y	120/196 (61%)	112 (93%)	8 (7%)	19	30
26	Z	60/94 (64%)	58 (97%)	2 (3%)	43	64
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	54	74
29	3	79/79 (100%)	78 (99%)	1 (1%)	73	87
All	All	3095/3646 (85%)	2972 (96%)	123 (4%)	36	55

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	46	ILE
13	M	68	ARG
25	Y	172	THR
10	J	74	ARG
11	K	49	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	88	GLN
28	2	18	ASN
13	M	137	ASN

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Mol	Chain	Res	Type
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	224 (8%)	0
31	9	121/122 (99%)	16 (13%)	0
All	All	2866/3045 (94%)	240 (8%)	0

5 of 240 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

There are no RNA pucker outliers to report.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

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
30	OMU	0	2587	30	14,22,23	0.98	1 (7%)	18,31,34	3.64	2 (11%)
30	OMG	0	2588	30	18,26,27	1.04	2 (11%)	22,38,41	2.48	4 (18%)
30	UR3	0	2619	30	14,22,23	0.72	0	16,32,35	0.74	0
30	PSU	0	2621	30	16,21,22	1.58	3 (18%)	20,30,33	6.13	4 (20%)
30	1MA	0	628	30,34	16,25,26	1.01	1 (6%)	13,37,40	1.20	1 (7%)

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
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,34	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.79	1.48	1.52
30	0	2588	OMG	C8-N7	-2.03	1.30	1.34
30	0	2621	PSU	C2-N1	2.52	1.43	1.38
30	0	2587	OMU	C4-N3	2.67	1.37	1.33
30	0	2621	PSU	C4-N3	2.73	1.38	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.33	114.50	128.40
30	0	2621	PSU	C5-C4-N3	-12.89	114.85	125.43
30	0	2588	OMG	C5-C6-N1	-8.36	111.57	123.48
30	0	628	1MA	C2-N3-C4	-3.75	110.65	116.41
30	0	2587	OMU	C5-C4-N3	-3.54	114.66	123.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 231 ligands modelled in this entry, 231 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	A	237/240 (98%)	0.81	22 (9%) 9 8	19, 38, 77, 98	0
2	B	337/338 (99%)	1.01	39 (11%) 5 5	21, 46, 74, 84	0
3	C	246/246 (100%)	0.68	14 (5%) 24 23	15, 36, 60, 71	0
4	D	140/177 (79%)	2.73	86 (61%) 0 0	47, 90, 115, 123	0
5	E	172/178 (96%)	1.15	28 (16%) 2 2	39, 61, 81, 85	0
6	F	119/120 (99%)	1.03	25 (21%) 1 1	34, 61, 90, 104	0
7	G	29/348 (8%)	2.34	13 (44%) 0 0	69, 86, 95, 98	0
8	H	160/177 (90%)	1.03	19 (11%) 5 4	30, 48, 83, 90	0
9	I	70/162 (43%)	5.01	65 (92%) 0 0	122, 136, 154, 155	0
10	J	142/145 (97%)	1.05	16 (11%) 6 5	29, 43, 66, 89	0
11	K	132/132 (100%)	1.07	17 (12%) 4 3	27, 42, 65, 77	0
12	L	145/165 (87%)	0.99	20 (13%) 3 3	18, 55, 101, 117	0
13	M	194/196 (98%)	0.21	0 100 100	20, 31, 47, 55	0
14	N	186/187 (99%)	1.01	26 (13%) 3 3	32, 53, 102, 112	0
15	O	115/116 (99%)	0.25	2 (1%) 70 68	29, 45, 62, 70	0
16	P	143/149 (95%)	0.78	7 (4%) 30 29	31, 45, 57, 68	0
17	Q	95/96 (98%)	0.53	2 (2%) 64 61	26, 35, 54, 66	0
18	R	150/155 (96%)	0.69	3 (2%) 65 63	22, 37, 58, 71	0
19	S	81/85 (95%)	0.89	10 (12%) 5 4	31, 48, 72, 82	0
20	T	119/120 (99%)	0.74	9 (7%) 15 13	29, 46, 78, 98	0
21	U	53/67 (79%)	0.96	5 (9%) 9 8	34, 48, 66, 76	0
22	V	65/71 (91%)	2.07	22 (33%) 0 0	40, 62, 106, 113	0
23	W	154/154 (100%)	0.77	11 (7%) 17 15	28, 42, 59, 71	0
24	X	82/92 (89%)	1.15	10 (12%) 5 4	36, 50, 78, 94	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.46	8 (5%) 25 24	22, 36, 60, 80	0
26	Z	73/116 (62%)	0.92	9 (12%) 5 4	34, 48, 68, 87	0
27	1	56/57 (98%)	0.74	0 100 100	19, 24, 31, 40	0
28	2	46/50 (92%)	1.02	7 (15%) 2 2	26, 50, 75, 89	0
29	3	92/92 (100%)	0.51	3 (3%) 47 45	22, 45, 62, 76	0
30	0	2749/2923 (94%)	0.24	78 (2%) 53 51	16, 36, 81, 155	0
31	9	122/122 (100%)	0.13	5 (4%) 38 36	31, 54, 77, 138	0
All	All	6646/7517 (88%)	0.67	581 (8%) 11 10	15, 42, 89, 155	0

The worst 5 of 581 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	15.0
9	I	91	PHE	12.4
14	N	166	ALA	11.4
4	D	63	ILE	10.1
9	I	88	GLN	9.8

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	OMU	0	2587	21/22	0.90	0.17	-	22,25,27,28	0
30	UR3	0	2619	21/22	0.91	0.20	-	24,27,31,36	0
30	1MA	0	628	23/24	0.93	0.20	-	20,22,23,25	0
30	PSU	0	2621	20/21	0.92	0.22	-	20,23,27,27	0
30	OMG	0	2588	24/25	0.91	0.18	-	22,25,27,28	0

6.3 Carbohydrates [i](#)

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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
34	NA	0	8374	1/1	0.94	0.61	38.29	47,47,47,47	0
34	NA	0	8372	1/1	0.95	0.59	29.03	60,60,60,60	0
34	NA	R	8386	1/1	0.59	0.68	23.84	80,80,80,80	0
34	NA	0	8368	1/1	0.47	0.41	17.56	48,48,48,48	0
34	NA	0	8371	1/1	0.55	0.36	16.25	48,48,48,48	0
34	NA	0	8376	1/1	0.84	0.43	15.96	42,42,42,42	0
34	NA	0	8379	1/1	0.80	0.57	14.90	46,46,46,46	0
32	MG	0	8060	1/1	0.96	0.28	11.87	33,33,33,33	0
32	MG	0	8066	1/1	0.95	0.59	11.38	88,88,88,88	0
34	NA	0	8331	1/1	0.90	0.32	10.97	35,35,35,35	0
34	NA	0	8340	1/1	0.59	0.47	10.91	49,49,49,49	0
34	NA	0	8350	1/1	0.95	0.42	10.69	41,41,41,41	0
34	NA	0	8335	1/1	0.53	0.38	9.27	31,31,31,31	0
34	NA	0	8320	1/1	0.84	0.35	7.90	37,37,37,37	0
34	NA	0	8362	1/1	0.84	0.39	7.40	46,46,46,46	0
34	NA	0	8326	1/1	0.42	0.25	6.50	37,37,37,37	0
34	NA	0	8323	1/1	0.72	0.28	6.30	31,31,31,31	0
34	NA	0	8302	1/1	0.91	0.23	5.73	44,44,44,44	0
34	NA	0	8364	1/1	0.95	0.31	5.25	40,40,40,40	0
34	NA	0	8359	1/1	0.85	0.27	5.17	39,39,39,39	0
34	NA	0	8366	1/1	0.82	0.22	4.04	63,63,63,63	0
34	NA	0	8305	1/1	0.86	0.28	3.98	33,33,33,33	0
34	NA	0	8325	1/1	0.92	0.25	3.30	50,50,50,50	0
34	NA	0	8378	1/1	0.73	0.38	3.10	40,40,40,40	0
32	MG	0	8064	1/1	0.85	0.22	2.76	26,26,26,26	0
34	NA	0	8327	1/1	0.71	0.25	2.62	36,36,36,36	0
34	NA	0	8356	1/1	0.86	0.22	2.35	35,35,35,35	0
34	NA	0	8303	1/1	0.93	0.24	2.34	32,32,32,32	0
34	NA	0	8321	1/1	0.87	0.28	1.86	42,42,42,42	0
34	NA	0	8373	1/1	0.67	0.18	1.75	44,44,44,44	0
34	NA	0	8324	1/1	0.77	0.21	1.59	48,48,48,48	0
32	MG	0	8080	1/1	0.76	0.24	1.54	40,40,40,40	0
35	CL	M	8518	1/1	0.95	0.20	0.99	32,32,32,32	0
32	MG	0	8015	1/1	0.93	0.25	0.97	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8369	1/1	0.96	0.23	0.95	42,42,42,42	0
32	MG	0	8057	1/1	0.83	0.19	0.88	34,34,34,34	0
34	NA	0	8365	1/1	0.81	0.23	0.58	31,31,31,31	0
34	NA	0	8361	1/1	0.68	0.24	0.47	41,41,41,41	0
34	NA	0	8339	1/1	0.80	0.21	0.40	19,19,19,19	0
34	NA	9	8383	1/1	0.75	0.17	0.03	46,46,46,46	0
34	NA	M	8347	1/1	0.85	0.17	-0.02	19,19,19,19	0
34	NA	0	8333	1/1	0.63	0.17	-0.04	23,23,23,23	0
32	MG	0	8109	1/1	0.84	0.19	-0.26	25,25,25,25	0
32	MG	0	8012	1/1	0.90	0.16	-0.33	30,30,30,30	0
35	CL	J	8521	1/1	0.61	0.23	-0.34	47,47,47,47	0
34	NA	0	8353	1/1	0.95	0.18	-0.68	17,17,17,17	0
34	NA	C	8304	1/1	0.85	0.17	-0.71	29,29,29,29	0
35	CL	0	8515	1/1	0.92	0.16	-0.73	53,53,53,53	0
32	MG	0	8086	1/1	0.86	0.14	-0.77	37,37,37,37	0
34	NA	0	8314	1/1	0.93	0.20	-0.77	38,38,38,38	0
34	NA	0	8382	1/1	0.58	0.17	-0.79	67,67,67,67	0
32	MG	0	8038	1/1	0.81	0.16	-0.84	21,21,21,21	0
34	NA	Q	8348	1/1	0.83	0.16	-0.85	30,30,30,30	0
34	NA	0	8309	1/1	0.69	0.15	-1.15	25,25,25,25	0
34	NA	L	8380	1/1	0.92	0.20	-1.34	44,44,44,44	0
34	NA	J	8346	1/1	0.74	0.18	-1.36	37,37,37,37	0
35	CL	0	8512	1/1	0.92	0.16	-1.38	35,35,35,35	0
35	CL	B	8519	1/1	0.76	0.19	-1.38	34,34,34,34	0
32	MG	0	8054	1/1	0.89	0.18	-1.42	16,16,16,16	0
32	MG	0	8008	1/1	0.90	0.14	-1.61	26,26,26,26	0
34	NA	0	8317	1/1	0.84	0.15	-1.70	28,28,28,28	0
34	NA	A	8345	1/1	0.80	0.13	-1.89	43,43,43,43	0
32	MG	0	8044	1/1	0.85	0.14	-2.00	33,33,33,33	0
32	MG	0	8013	1/1	0.93	0.17	-2.04	22,22,22,22	0
32	MG	0	8020	1/1	0.91	0.14	-2.04	22,22,22,22	0
32	MG	0	8007	1/1	0.90	0.16	-2.09	21,21,21,21	0
32	MG	0	8074	1/1	0.97	0.07	-2.16	35,35,35,35	0
32	MG	0	8010	1/1	0.75	0.18	-2.17	24,24,24,24	0
32	MG	Y	8108	1/1	0.67	0.14	-2.23	25,25,25,25	0
34	NA	0	8332	1/1	0.93	0.12	-2.25	31,31,31,31	0
36	CD	Z	8403	1/1	0.95	0.11	-2.27	43,43,43,43	0
34	NA	0	8344	1/1	0.83	0.12	-2.30	24,24,24,24	0
35	CL	0	8505	1/1	0.91	0.12	-2.38	41,41,41,41	0
32	MG	3	8078	1/1	0.86	0.12	-2.53	37,37,37,37	0
32	MG	0	8056	1/1	0.72	0.13	-2.55	34,34,34,34	0
35	CL	0	8516	1/1	0.90	0.14	-2.67	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CD	U	8401	1/1	0.90	0.09	-2.75	48,48,48,48	0
32	MG	0	8053	1/1	0.92	0.15	-2.76	33,33,33,33	0
35	CL	O	8508	1/1	0.93	0.08	-2.84	51,51,51,51	0
34	NA	0	8343	1/1	0.86	0.11	-2.92	28,28,28,28	0
32	MG	0	8107	1/1	0.86	0.13	-2.93	68,68,68,68	0
32	MG	0	8003	1/1	0.88	0.16	-2.97	21,21,21,21	0
36	CD	3	8404	1/1	0.94	0.07	-3.05	45,45,45,45	0
32	MG	0	8033	1/1	0.58	0.14	-3.11	19,19,19,19	0
32	MG	0	8077	1/1	0.72	0.17	-3.13	22,22,22,22	0
32	MG	T	8073	1/1	0.75	0.13	-3.16	40,40,40,40	0
36	CD	1	8402	1/1	0.96	0.09	-3.17	45,45,45,45	0
33	K	0	8201	1/1	0.82	0.17	-3.32	60,60,60,60	0
32	MG	0	8058	1/1	0.82	0.09	-3.34	29,29,29,29	0
32	MG	0	8111	1/1	0.87	0.08	-3.37	23,23,23,23	0
34	NA	0	8334	1/1	0.97	0.09	-3.65	36,36,36,36	0
32	MG	0	8067	1/1	0.90	0.11	-3.73	28,28,28,28	0
32	MG	B	8055	1/1	0.37	0.12	-3.97	42,42,42,42	0
32	MG	0	8084	1/1	0.83	0.16	-3.97	38,38,38,38	0
34	NA	0	8338	1/1	0.83	0.10	-4.17	41,41,41,41	0
32	MG	0	8004	1/1	0.91	0.13	-4.20	19,19,19,19	0
34	NA	0	8310	1/1	0.97	0.12	-4.28	30,30,30,30	0
32	MG	0	8021	1/1	0.95	0.10	-4.42	25,25,25,25	0
32	MG	0	8017	1/1	0.90	0.12	-4.64	11,11,11,11	0
32	MG	0	8096	1/1	0.76	0.10	-5.31	34,34,34,34	0
32	MG	0	8027	1/1	0.83	0.09	-5.52	36,36,36,36	0
35	CL	3	8504	1/1	0.95	0.09	-5.81	43,43,43,43	0
32	MG	0	8113	1/1	0.97	0.07	-6.02	31,31,31,31	0
32	MG	0	8106	1/1	0.91	0.04	-6.07	31,31,31,31	0
32	MG	0	8006	1/1	0.86	0.08	-6.49	29,29,29,29	0
32	MG	0	8032	1/1	0.93	0.08	-6.65	26,26,26,26	0
32	MG	0	8028	1/1	0.94	0.07	-6.69	27,27,27,27	0
32	MG	0	8052	1/1	0.39	0.14	-7.54	48,48,48,48	0
32	MG	0	8019	1/1	0.81	0.07	-7.59	23,23,23,23	0
32	MG	0	8091	1/1	0.86	0.08	-8.36	41,41,41,41	0
32	MG	0	8035	1/1	0.81	0.10	-9.60	34,34,34,34	0
33	K	0	8202	1/1	0.95	0.11	-10.18	37,37,37,37	0
32	MG	A	8065	1/1	0.94	0.05	-10.92	23,23,23,23	0
32	MG	0	8001	1/1	0.96	0.10	-12.13	24,24,24,24	0
32	MG	0	8039	1/1	0.94	0.06	-13.27	33,33,33,33	0
32	MG	0	8018	1/1	0.67	0.09	-15.81	30,30,30,30	0
32	MG	0	8002	1/1	0.86	0.12	-16.00	25,25,25,25	0
32	MG	0	8048	1/1	0.94	0.28	-	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8005	1/1	0.94	0.13	-	25,25,25,25	0
32	MG	0	8079	1/1	0.85	0.15	-	20,20,20,20	0
34	NA	R	8337	1/1	0.89	0.15	-	33,33,33,33	0
32	MG	0	8009	1/1	0.82	0.21	-	25,25,25,25	0
32	MG	0	8114	1/1	0.90	0.13	-	38,38,38,38	0
32	MG	0	8031	1/1	0.95	0.14	-	24,24,24,24	0
32	MG	0	8089	1/1	0.79	0.16	-	43,43,43,43	0
34	NA	0	8375	1/1	0.86	0.33	-	38,38,38,38	0
32	MG	0	8112	1/1	0.53	0.28	-	39,39,39,39	0
32	MG	0	8029	1/1	0.85	0.10	-	34,34,34,34	0
32	MG	0	8034	1/1	0.88	0.12	-	30,30,30,30	0
32	MG	0	8047	1/1	0.78	0.26	-	59,59,59,59	0
32	MG	0	8071	1/1	0.73	0.12	-	61,61,61,61	0
34	NA	H	8322	1/1	0.78	0.33	-	54,54,54,54	0
34	NA	0	8363	1/1	0.84	0.52	-	50,50,50,50	0
32	MG	0	8093	1/1	0.84	0.21	-	37,37,37,37	0
32	MG	0	8042	1/1	0.93	0.17	-	31,31,31,31	0
34	NA	0	8306	1/1	0.96	0.18	-	29,29,29,29	0
35	CL	0	8522	1/1	0.83	0.21	-	44,44,44,44	0
34	NA	0	8384	1/1	0.60	0.15	-	53,53,53,53	0
34	NA	0	8313	1/1	0.90	0.10	-	55,55,55,55	0
32	MG	0	8099	1/1	0.84	0.33	-	40,40,40,40	0
34	NA	0	8316	1/1	0.72	0.28	-	38,38,38,38	0
35	CL	A	8509	1/1	0.94	0.18	-	49,49,49,49	0
32	MG	0	8036	1/1	0.86	0.11	-	31,31,31,31	0
32	MG	0	8097	1/1	0.74	0.11	-	30,30,30,30	0
35	CL	N	8507	1/1	0.96	0.10	-	44,44,44,44	0
32	MG	0	8083	1/1	0.74	0.15	-	33,33,33,33	0
32	MG	9	8095	1/1	0.86	0.23	-	64,64,64,64	0
34	NA	0	8311	1/1	0.83	0.28	-	52,52,52,52	0
32	MG	K	8069	1/1	0.81	0.19	-	47,47,47,47	0
32	MG	0	8025	1/1	0.78	0.13	-	32,32,32,32	0
32	MG	0	8043	1/1	0.90	0.07	-	32,32,32,32	0
32	MG	0	8024	1/1	0.92	0.25	-	22,22,22,22	0
34	NA	0	8328	1/1	0.95	0.13	-	31,31,31,31	0
32	MG	0	8110	1/1	0.89	0.11	-	29,29,29,29	0
32	MG	0	8040	1/1	0.91	0.18	-	38,38,38,38	0
32	MG	0	8046	1/1	0.61	0.14	-	39,39,39,39	0
36	CD	O	8405	1/1	0.95	0.07	-	71,71,71,71	0
34	NA	9	8351	1/1	0.91	0.07	-	45,45,45,45	0
32	MG	0	8081	1/1	0.94	0.09	-	39,39,39,39	0
32	MG	0	8022	1/1	0.94	0.17	-	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8041	1/1	0.94	0.15	-	34,34,34,34	0
32	MG	0	8062	1/1	0.63	0.21	-	42,42,42,42	0
35	CL	0	8514	1/1	0.85	0.23	-	39,39,39,39	0
32	MG	0	8045	1/1	0.63	0.18	-	55,55,55,55	0
32	MG	0	8011	1/1	0.88	0.20	-	21,21,21,21	0
32	MG	0	8051	1/1	0.90	0.15	-	54,54,54,54	0
34	NA	0	8329	1/1	0.73	0.17	-	55,55,55,55	0
34	NA	0	8315	1/1	0.96	0.23	-	30,30,30,30	0
32	MG	0	8049	1/1	0.77	0.22	-	54,54,54,54	0
34	NA	0	8377	1/1	0.76	0.33	-	50,50,50,50	0
35	CL	J	8502	1/1	0.88	0.18	-	55,55,55,55	0
32	MG	0	8030	1/1	0.42	0.15	-	21,21,21,21	0
34	NA	0	8381	1/1	0.80	0.20	-	43,43,43,43	0
32	MG	0	8085	1/1	0.90	0.13	-	37,37,37,37	0
32	MG	0	8087	1/1	0.92	0.16	-	57,57,57,57	0
32	MG	0	8103	1/1	0.76	0.18	-	55,55,55,55	0
35	CL	J	8501	1/1	0.79	0.10	-	46,46,46,46	0
35	CL	0	8503	1/1	0.94	0.19	-	38,38,38,38	0
32	MG	0	8088	1/1	0.85	0.17	-	24,24,24,24	0
32	MG	0	8102	1/1	0.87	0.16	-	48,48,48,48	0
32	MG	0	8050	1/1	0.66	0.14	-	66,66,66,66	0
34	NA	9	8352	1/1	0.92	0.20	-	41,41,41,41	0
34	NA	0	8385	1/1	0.85	0.37	-	44,44,44,44	0
35	CL	0	8517	1/1	0.87	0.12	-	47,47,47,47	0
32	MG	0	8014	1/1	0.23	0.17	-	25,25,25,25	0
32	MG	0	8092	1/1	0.68	0.15	-	66,66,66,66	0
32	MG	0	8105	1/1	0.90	0.10	-	45,45,45,45	0
32	MG	0	8115	1/1	0.93	0.08	-	41,41,41,41	0
32	MG	0	8059	1/1	0.89	0.14	-	22,22,22,22	0
32	MG	0	8070	1/1	0.76	0.20	-	44,44,44,44	0
32	MG	0	8075	1/1	0.90	0.11	-	27,27,27,27	0
34	NA	0	8342	1/1	0.84	0.24	-	35,35,35,35	0
32	MG	0	8094	1/1	0.68	0.17	-	59,59,59,59	0
34	NA	0	8355	1/1	0.82	0.44	-	53,53,53,53	0
34	NA	0	8360	1/1	0.65	0.37	-	41,41,41,41	0
34	NA	0	8336	1/1	0.82	0.10	-	37,37,37,37	0
32	MG	0	8116	1/1	0.91	0.08	-	35,35,35,35	0
34	NA	0	8367	1/1	0.88	0.34	-	46,46,46,46	0
34	NA	0	8358	1/1	0.88	0.30	-	73,73,73,73	0
32	MG	0	8026	1/1	0.95	0.15	-	23,23,23,23	0
34	NA	0	8330	1/1	0.92	0.10	-	37,37,37,37	0
32	MG	0	8104	1/1	0.88	0.30	-	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8100	1/1	0.78	0.22	-	63,63,63,63	0
32	MG	0	8098	1/1	0.85	0.23	-	25,25,25,25	0
34	NA	0	8357	1/1	0.94	0.07	-	39,39,39,39	0
34	NA	0	8341	1/1	0.84	0.19	-	41,41,41,41	0
35	CL	0	8511	1/1	0.92	0.12	-	37,37,37,37	0
32	MG	0	8072	1/1	0.88	0.13	-	47,47,47,47	0
32	MG	0	8076	1/1	0.45	0.14	-	44,44,44,44	0
34	NA	0	8307	1/1	0.81	0.34	-	42,42,42,42	0
32	MG	0	8037	1/1	0.94	0.06	-	35,35,35,35	0
34	NA	0	8354	1/1	0.85	0.20	-	23,23,23,23	0
34	NA	0	8319	1/1	0.80	0.19	-	31,31,31,31	0
32	MG	0	8101	1/1	0.72	0.24	-	44,44,44,44	0
35	CL	0	8513	1/1	0.86	0.16	-	44,44,44,44	0
34	NA	S	8312	1/1	0.95	0.11	-	28,28,28,28	0
34	NA	0	8308	1/1	0.89	0.12	-	45,45,45,45	0
32	MG	0	8082	1/1	0.87	0.12	-	62,62,62,62	0
35	CL	Y	8520	1/1	0.89	0.12	-	35,35,35,35	0
32	MG	0	8023	1/1	0.87	0.25	-	28,28,28,28	0
32	MG	0	8061	1/1	0.84	0.17	-	30,30,30,30	0
35	CL	R	8506	1/1	0.77	0.22	-	40,40,40,40	0
32	MG	0	8068	1/1	0.47	0.17	-	46,46,46,46	0
32	MG	0	8090	1/1	0.36	0.38	-	56,56,56,56	0
35	CL	L	8510	1/1	0.90	0.14	-	40,40,40,40	0
34	NA	0	8318	1/1	0.69	0.32	-	47,47,47,47	0
32	MG	0	8016	1/1	0.95	0.14	-	30,30,30,30	0
32	MG	0	8063	1/1	0.68	0.13	-	60,60,60,60	0
34	NA	0	8301	1/1	0.97	0.20	-	34,34,34,34	0
34	NA	0	8370	1/1	0.83	0.68	-	70,70,70,70	0
34	NA	0	8349	1/1	0.90	0.18	-	32,32,32,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.