



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 05:22 AM GMT

PDB ID : 1VQ5
Title : The structure of the transition state analogue "RAA" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.60 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>

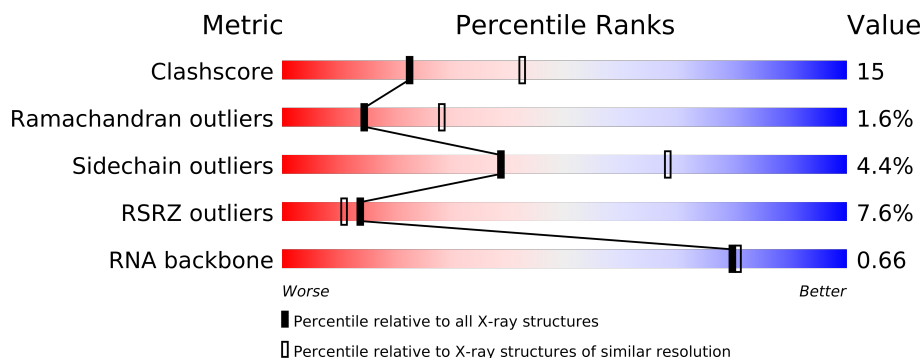
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.60 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	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (2.60-2.60)
RNA backbone	1838	1002 (3.12-2.08)

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	8	
4	A	240	
5	B	338	
6	C	246	
7	D	177	
8	E	178	
9	F	120	
10	G	348	
11	H	171	
12	J	145	
13	K	132	
14	L	165	

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Mol	Chain	Length	Quality of chain
15	M	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	
30	2	50	
31	3	92	
32	I	162	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8011	-	X
33	MG	0	8016	-	X
33	MG	0	8023	-	X
33	MG	0	8041	-	X
33	MG	0	8049	-	X
33	MG	0	8053	-	X
33	MG	0	8060	-	X
33	MG	0	8080	-	X
33	MG	0	8087	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8100	-	X
33	MG	0	8101	-	X
33	MG	0	8113	-	X
33	MG	Y	8109	-	X
35	NA	0	9103	-	X
35	NA	0	9105	-	X
35	NA	0	9106	-	X
35	NA	0	9107	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	9110	-	X
35	NA	0	9113	-	X
35	NA	0	9118	-	X
35	NA	0	9120	-	X
35	NA	0	9121	-	X
35	NA	0	9123	-	X
35	NA	0	9125	-	X
35	NA	0	9129	-	X
35	NA	0	9131	-	X
35	NA	0	9135	-	X
35	NA	0	9142	-	X
35	NA	0	9150	-	X
35	NA	0	9152	-	X
35	NA	0	9153	-	X
35	NA	0	9155	-	X
35	NA	0	9156	-	X
35	NA	0	9160	-	X
35	NA	0	9162	-	X
35	NA	0	9164	-	X
35	NA	0	9165	-	X
35	NA	0	9169	-	X
35	NA	0	9170	-	X
35	NA	0	9173	-	X
35	NA	0	9174	-	X
35	NA	0	9175	-	X
35	NA	0	9176	-	X
35	NA	0	9177	-	X
35	NA	0	9178	-	X
35	NA	0	9179	-	X
35	NA	0	9181	-	X
35	NA	0	9182	-	X
35	NA	0	9184	-	X
35	NA	0	9185	-	X
35	NA	B	9158	-	X
35	NA	L	9180	-	X
35	NA	R	9186	-	X
35	NA	S	9112	-	X
36	CL	0	9315	-	X
36	CL	0	9316	-	X
36	CL	A	9309	-	X
36	CL	N	9307	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99060 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
			59021	26350	10878	19048	2745			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	modified residue	GB 3377779
0	2587	OMU	U	modified residue	GB 3377779
0	2588	OMG	G	modified residue	GB 3377779
0	2619	UR3	U	modified residue	GB 3377779
0	2621	PSU	U	modified residue	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'-D*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			126	61	23	37	5			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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 50S ribosomal protein L5P.

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 50S ribosomal protein L6P.

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 50S ribosomal protein L7AE.

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

- Molecule 10 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	160	Total	C	N	O	S	0	0	0
			1266	785	237	238	6			

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	132	Total	C	N	O	S	0	0	0
			992	609	187	192	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	HIS	CONFLICT	UNP P22450

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called 50S Ribosomal Protein L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	194	Total	C	N	O	S	0	0	0
			1560	943	332	284	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	CONFLICT	GB 55231501
M	194	ALA	GLY	CONFLICT	GB 55231501

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	73	Total	C	N	O	S	0	0	0
			578	346	116	111	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	10	ARG	SER	CONFLICT	GB 55231162

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	106	Total	Mg	0	0
			106	106		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	2	Total	Mg	0	0
			2	2		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	2	Total	Mg	0	0
			2	2		
33	3	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	3	Total K 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	71	Total Na 71 71	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	2	Total Na 2 2	0	0
35	B	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	A	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	2	Total Na 2 2	0	0
35	L	1	Total Na 1 1	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total 1	Cl 1	0	0
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	O	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0
37	3	1	Total 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5820	Total 5820	O 5820	0	0
38	9	133	Total 133	O 133	0	0
38	4	8	Total 8	O 8	0	0
38	A	117	Total 117	O 117	0	0
38	B	150	Total 150	O 150	0	0
38	C	165	Total 165	O 165	0	0

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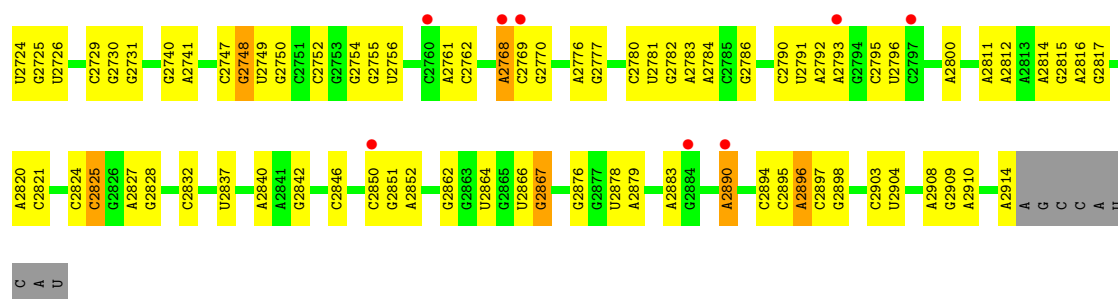
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	21	Total 21	O 21	0	0
38	G	16	Total 16	O 16	0	0
38	H	66	Total 66	O 66	0	0
38	J	52	Total 52	O 52	0	0
38	K	54	Total 54	O 54	0	0
38	L	83	Total 83	O 83	0	0
38	M	118	Total 118	O 118	0	0
38	N	66	Total 66	O 66	0	0
38	O	39	Total 39	O 39	0	0
38	P	65	Total 65	O 65	0	0
38	Q	52	Total 52	O 52	0	0
38	R	85	Total 85	O 85	0	0
38	S	31	Total 31	O 31	0	0
38	T	39	Total 39	O 39	0	0
38	U	25	Total 25	O 25	0	0
38	V	13	Total 13	O 13	0	0
38	W	68	Total 68	O 68	0	0
38	X	27	Total 27	O 27	0	0
38	Y	92	Total 92	O 92	0	0

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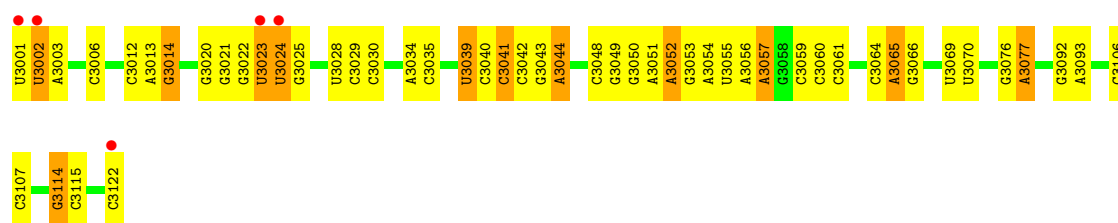
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Z	30	Total 30	O 30	0	0
38	1	59	Total 59	O 59	0	0
38	2	42	Total 42	O 42	0	0
38	3	74	Total 74	O 74	0	0
38	I	10	Total 10	O 10	0	0

G2634	G2524	G2418	G2324	A2067	G1950	G1806	A1701	G1595	C1450	A1328	C1209	U1130
G2637	G2525	G2419	G2325	G2068	G1951	A1811	U1702	U1596	C1451	A1331	G1210	G1131
G2643	G2526	G2420	C2329	G2072	A	G1819	A1710	A1598	G1452	C1332	C1213	A1132
G2644	G2527	G2421	U2330	G2073	A	G1820	A1711	A1599	G1453	U1333	G1214	G1135
U2645	C2533	G2422	C2331	A2074	C	G1829	A1712	A1603	G1458	C1334	A1215	U1136
U2649	U2534	G2423	G2338	U2076	U	A1839	G1713	G1604	A1458	C1335	G1216	G1137
U2652	C2535	G2426	A	G2079	A	C1830	G1714	G1605	C1462	U1336	G1224	A1150
U2653	U2536	G2427	C	G2080	G	U1834	G1715	G1614	A1463	G1340	C1225	G1151
G2654	G2537	G2428	A	A2081	A	U1835	A1716	C1614	A1341	A1341	C1229	G1158
U2655	A	G2438	G	G2083	C	U1835	A1717	A1624	C1474	C1342	C1229	G1159
U2656	C2542	G2439	A2237	G	C	A1839	G1718	U1625	C1477	C1343	U1234	G1160
U2659	C2548	U2443	G2239	A2096	U1964	A1840	U1722	A1626	U1478	G1351	A1235	A1161
A2664	U	U2444	U2240	A2101	G	U1845	G1723	U1626	C1477	A1352	G1236	G1162
U2667	A	G2445	U2241	A2102	U1971	U1846	U1724	A1631	G1483	C1353	U1237	G1163
G2668	C2551	U2446	C2243	A2103	A1973	A1847	G1725	C1633	G1484	C1360	U1238	U1164
G2669	A2552	G2447	G2248	C2104	G1976	G1848	G1730	G1634	A1485	G1363	G1239	G1165
G2670	U2563	G2448	G2249	C2105	U1977	G1849	C1731	G1635	A1494	G1372	A1242	A1166
U2671	G2564	G2449	G2250	C2106	A1978	G1855	A1732	G1636	G1495	A1372	C1243	G1167
C2676	U2565	G2452	A2252	G2110	G1979	C1856	C1734	A1637	G1496	G1375	U1244	C1168
G2679	G2566	G2453	G2253	U2115	U1986	G1863	U1741	U1641	U1500	A1376	C1245	A1171
A2680	A2567	A2454	G2254	U2116	A1997	G1867	A1742	A1642	U1503	G1377	A1246	G1172
G2682	G2570	G2455	A2255	G2134	U2004	G1868	G1743	C1644	U1504	C1377	U1249	A1173
G2683	C2575	G2456	G2256	A2135	U2008	G1877	G1744	A1656	U1505	U1380	C1250	A1174
A2684	A2577	G2457	G2257	G2136	U2016	U1878	G1756	A1657	U1506	G1385	C1251	G1175
G2685	G2578	G2458	G2258	A	U2016	U1879	U1761	A1658	C1514	G1391	C1252	G1176
G2690	U2586	G2459	U2265	C	U2016	C1881	G1756	A1659	U1524	A1392	U1270	G1177
A2691	G2587	A2460	A2266	G	A2011	U1904	G1756	G1663	A1526	G1398	C1273	G1178
G2692	U2588	G2461	A2267	C	U2012	U1905	U1766	A1664	A1527	A1399	G1273	G1179
U2693	U2589	G2462	C2268	G	G2013	U1905	U1766	G1665	A1528	A1406	A1278	G1180
A2694	G2591	G2463	G2269	U	G2014	U1905	U1766	G1666	A1529	A1407	U1279	G1181
G2698	G2592	G2464	G2270	C	U2015	U1905	U1766	G1667	G1529	U1408	C1289	A1188
A2699	U2597	G2465	G2271	A	U2016	U1905	U1766	G1668	G1535	G1409	G1290	A1189
G2708	U2598	G2466	G2272	C	U2016	U1905	U1766	G1669	C1536	G1417	A1294	G1190
G2709	A2601	G2467	U2265	A	U2016	U1905	U1766	G1670	U1544	U1418	A1294	A1191
U2710	G2602	G2468	A2266	G	U2016	U1905	U1766	G1671	C1545	U1419	A1294	A1192
G2711	G2603	G2469	A2267	U	U2016	U1905	U1766	G1672	U1545	C1420	G1299	A1193
G2712	A2604	G2470	C2268	C	U2016	U1905	U1766	G1673	U1546	G1423	G1300	A1194
G2713	U2607	G2471	G2269	A	U2016	U1905	U1766	G1674	U1547	A1424	U1304	G1195
U2714	C2608	G2472	U2265	C	U2016	U1905	U1766	G1675	U1548	A1427	C1305	U1198
G2715	G2609	G2473	A2266	G	U2016	U1905	U1766	G1676	C1549	U1435	U1306	A1199
G2716	U2610	G2474	A2267	U	U2016	U1905	U1766	G1677	U1550	A1434	A1307	C1201
G2717	G2611	G2475	C2268	C	U2016	U1905	U1766	G1678	U1551	A1435	A1308	A1202
G2718	C2614	G2476	G2269	A	U2016	U1905	U1766	G1679	U1552	U1436	U1309	G1203
A2719	U2619	G2477	U2265	G	U2016	U1905	U1766	G1680	U1553	G1437	U1310	G1204
G2720	U2620	G2478	A2266	C	U2016	U1905	U1766	G1681	U1554	U1438	G1311	U1205
G2721	G2722	G2479	A2267	U	U2016	U1905	U1766	G1682	U1555	U1439	U1312	U1206
G2723	G2723	G2480	U2265	G	U2016	U1905	U1766	G1683	U1556	U1440	U1313	A1207
		G2481	C2268	A	U2016	U1905	U1766	G1684	U1557	U1441	U1314	C1208
		G2482	G2269	C	U2016	U1905	U1766	G1685	U1558	U1442	U1315	
		G2483	U2265	G	U2016	U1905	U1766	G1686	U1559	U1443	U1316	
		G2484	A2266	U	U2016	U1905	U1766	G1687	U1560	U1444	U1317	
		G2485	A2267	C	U2016	U1905	U1766	G1688	U1561	U1445	U1318	
		G2486	C2268	A	U2016	U1905	U1766	G1689	U1562	U1446	U1319	
		G2487	U2265	G	U2016	U1905	U1766	G1690	U1563	U1447	U1320	
		G2488	A2266	C	U2016	U1905	U1766	G1691	U1564	U1448	U1321	
		G2489	A2267	U	U2016	U1905	U1766	G1692	U1565	U1449	U1322	
		G2490	C2268	A	U2016	U1905	U1766	G1693	U1566	U1450	U1323	
		G2491	U2265	G	U2016	U1905	U1766	G1694	U1567	U1451	U1324	
		G2492	A2266	C	U2016	U1905	U1766	G1695	U1568	U1452	U1325	
		G2493	A2267	U	U2016	U1905	U1766	G1696	U1569	U1453	U1326	
		G2494	C2268	A	U2016	U1905	U1766	G1697	U1570	U1454	U1327	
		G2495	U2265	G	U2016	U1905	U1766	G1698	U1571	U1455	U1328	
		G2496	A2266	C	U2016	U1905	U1766	G1699	U1572	U1456	U1329	
		G2497	A2267	U	U2016	U1905	U1766	G1700	U1573	U1457	U1330	
		G2498	C2268	A	U2016	U1905	U1766	G1701	U1574	U1458	U1331	
		G2499	U2265	G	U2016	U1905	U1766	G1702	U1575	U1459	U1332	
		G2500	A2266	C	U2016	U1905	U1766	G1703	U1576	U1460	U1333	
		G2501	A2267	U	U2016	U1905	U1766	G1704	U1577	U1461	U1334	
		G2502	C2268	A	U2016	U1905	U1766	G1705	U1578	U1462	U1335	
		G2503	U2265	G	U2016	U1905	U1766	G1706	U1579	U1463	U1336	
		G2504	A2266	C	U2016	U1905	U1766	G1707	U1580	U1464	U1337	
		G2505	A2267	U	U2016	U1905	U1766	G1708	U1581	U1465	U1338	
		G2506	C2268	A	U2016	U1905	U1766	G1709	U1582	U1466	U1339	
		G2507	U2265	G	U2016	U1905	U1766	G1710	U1583	U1467	U1340	
		G2508	A2266	C	U2016	U1905	U1766	G1711	U1584	U1468	U1341	
		G2509	A2267	U	U2016	U1905	U1766	G1712	U1585	U1469	U1342	
		G2510	C2268	A	U2016	U1905	U1766	G1713	U1586	U1470	U1343	
		G2511	U2265	G	U2016	U1905	U1766	G1714	U1587	U1471	U1344	
		G2512	A2266	C	U2016	U1905	U1766	G1715	U1588	U1472	U1345	
		G2513	A2267	U	U2016	U1905	U1766	G1716	U1589	U1473	U1346	
		G2514	C2268	A	U2016	U1905	U1766	G1717	U1590	U1474	U1347	
		G2515	U2265	G	U2016	U1905	U1766	G1718	U1591	U1475	U1348	
		G2516	A2266	C	U2016	U1905	U1766	G1719	U1592	U1476	U1349	
		G2517	A2267	U	U2016	U1905	U1766	G1720	U1593	U1477	U1350	
		G2518	C2268	A	U2016	U1905	U1766	G1721	U1594	U1478	U1351	
		G2519	U2265	G	U2016	U1905	U1766	G1722	U1595	U1479	U1352	
		G2520	A2266	C	U2016	U1905	U1766	G1723	U1596	U1480	U1353	
		G2521	A2267	U	U2016	U1905	U1766	G1724	U1597	U1481	U1354	
		G2522	C2268	A	U2016	U1905	U1766	G1725	U1598	U1482	U1355	
		G2523	U2265	G	U2016	U1905	U1766	G1726	U1599	U1483	U1356	
		G2524	A2266	C	U2016	U1905	U1766	G1727	U1600	U1484	U1357	
		G2525	A2267	U	U2016	U1905	U1766	G1728	U1601	U1485	U1358	
		G2526	C2268	A	U2016	U1905	U1766	G1729	U1602	U1486	U1359	
		G2527	U2265	G	U2016	U1905	U1766	G1730	U1603	U1487	U1360	
		G2528	A2266	C	U2016	U1905	U1766	G1731	U1604	U1488	U1361	
		G2529	A2267	U	U2016	U1905	U1766	G1732	U1605	U1489	U1362	
		G2530	C2268	A	U2016	U1905	U1766	G1733	U1606	U1490	U1363	
		G2531	U2265	G	U2016	U1905	U1766	G1734	U1607	U1491	U1364	
		G2532	A2266	C	U2016	U1905	U1766	G1735	U1608	U1492	U1365	
		G2533	A2267	U	U2016	U1905	U1766	G1736	U1609	U1493	U1366	
		G2534	C2268	A	U2016	U1905	U1766	G1737	U1610	U1494	U1367	
		G2535	U2265	G	U2016	U1905	U1766	G1738	U1611	U1495	U1368	
		G2536	A2266	C	U2016	U1905	U1766	G1739	U1612	U1496	U1369	
		G2537	A2267	U	U2016	U1905	U1766	G1740	U1613	U1497	U1370	
		G2538	C2268	A	U2016	U1905	U1766	G1741	U1614	U1498	U1371	
		G2539	U2265	G	U2016	U1905	U1766	G1742	U1615	U1499	U1372	
		G2540	A2266	C	U2016	U1905	U1766	G1743	U1616	U1500	U1373	
		G2541	A2267	U	U201							



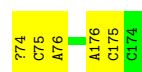
• Molecule 2: 5S ribosomal RNA

Chain 9:



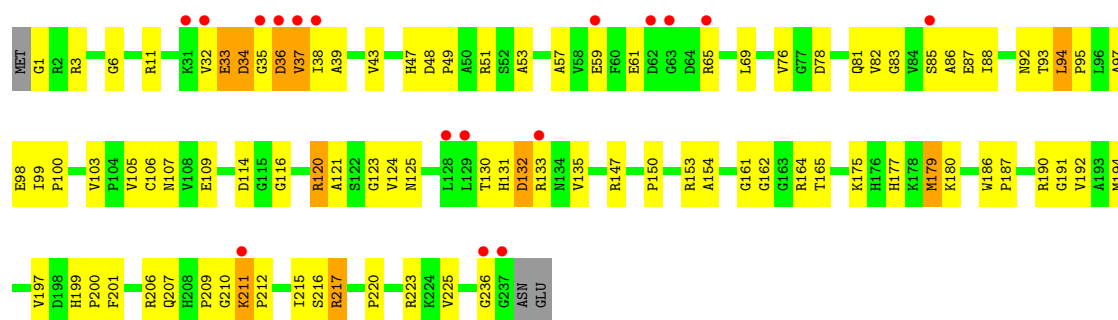
• Molecule 3: 5'-D*(DC)P*(DC)P*(5AA)P*(2OP)P*(PO2)P*AP*C*C-3'

Chain 4:



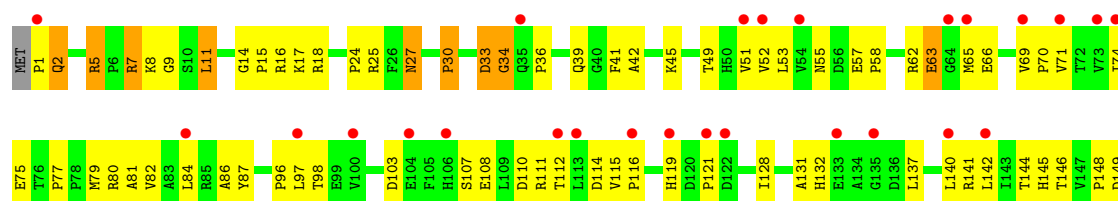
• Molecule 4: 50S ribosomal protein L2P

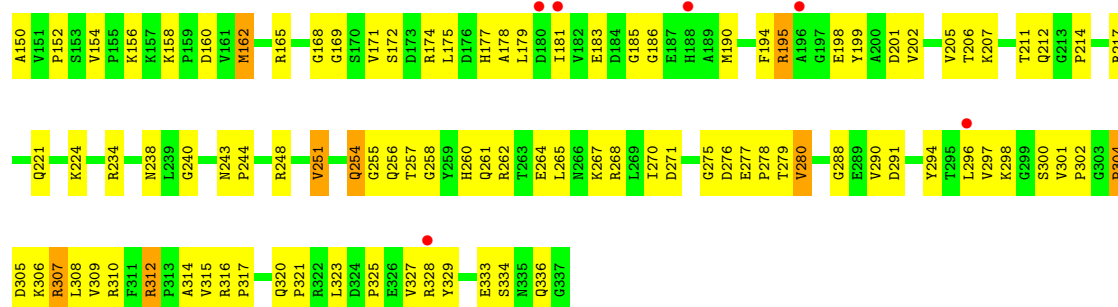
Chain A:



• Molecule 5: 50S ribosomal protein L3P

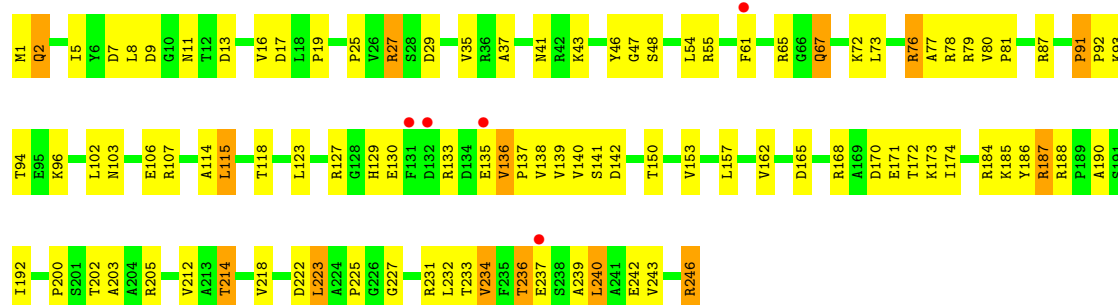
Chain B:





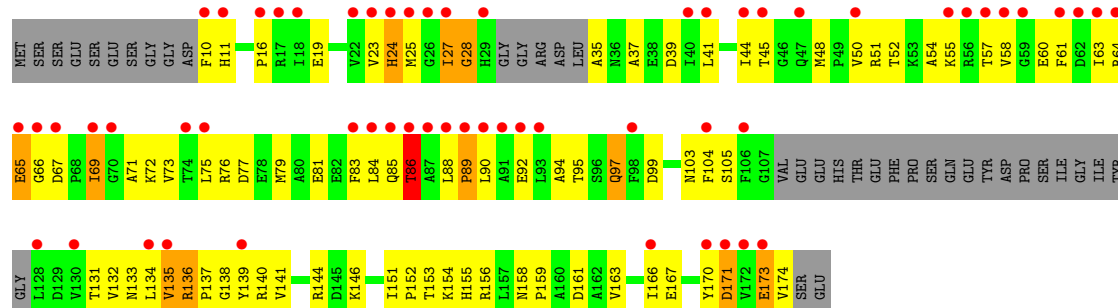
• Molecule 6: 50S ribosomal protein L4E

Chain C:



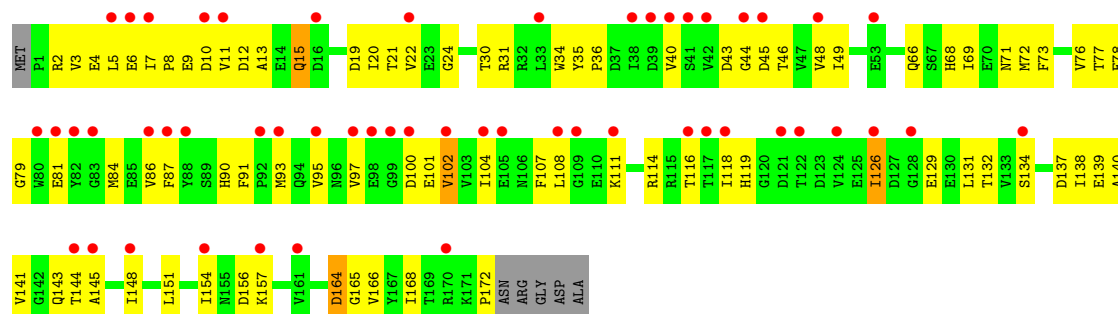
• Molecule 7: 50S ribosomal protein L5P

Chain D:



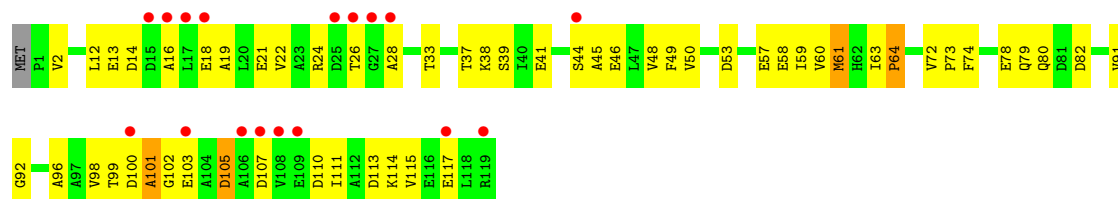
• Molecule 8: 50S ribosomal protein L6P

Chain E:



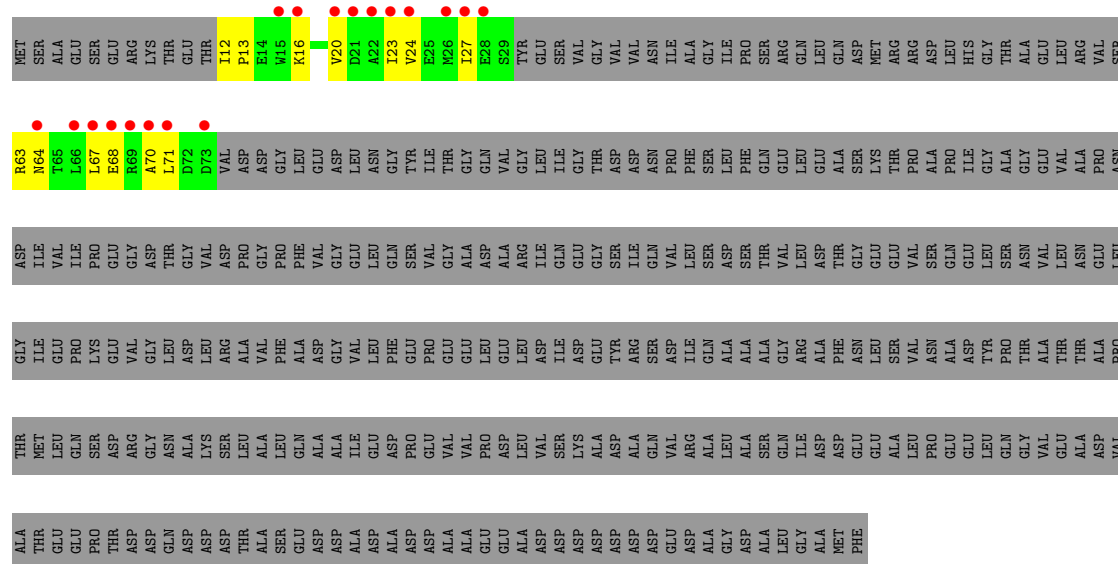
• Molecule 9: 50S ribosomal protein L7AE

Chain F: 



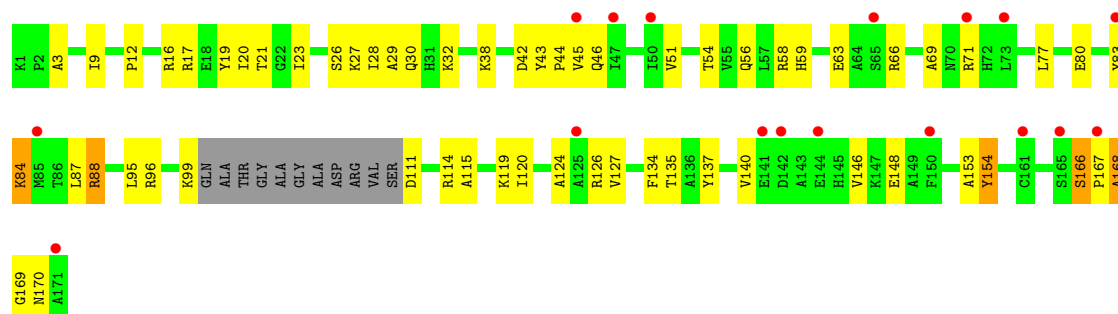
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G: 



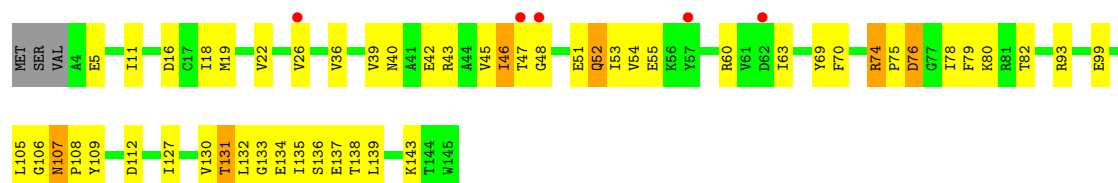
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H: 



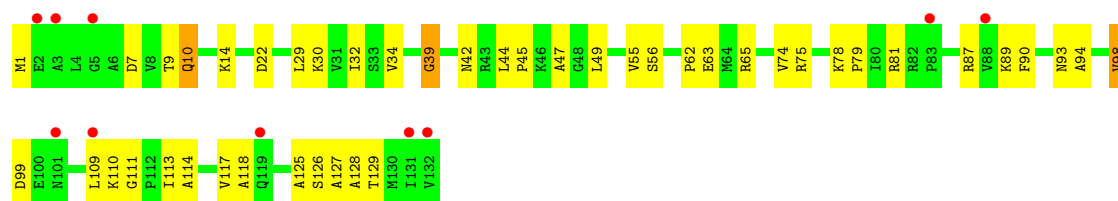
• Molecule 12: 50S ribosomal protein L13P

Chain J: 



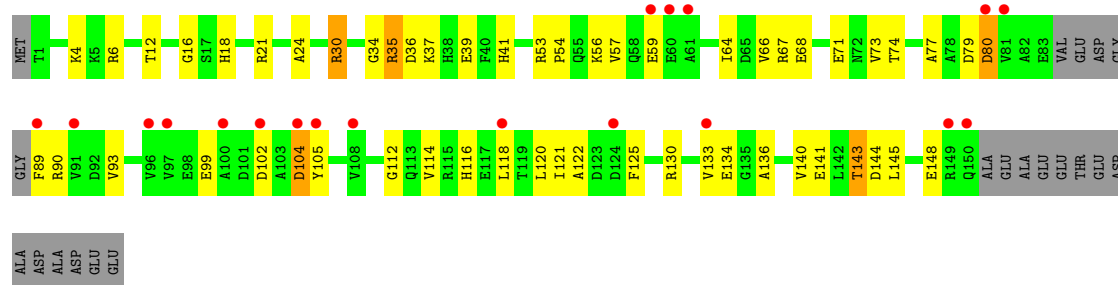
- Molecule 13: 50S ribosomal protein L14P

Chain K:



- Molecule 14: 50S ribosomal protein L15P

Chain L:



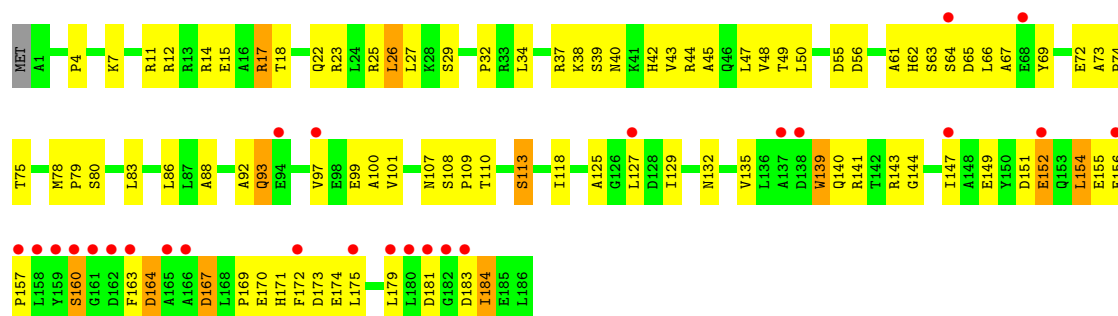
- Molecule 15: 50S Ribosomal Protein L15E

Chain M:



- Molecule 16: 50S ribosomal protein L18P

Chain N:



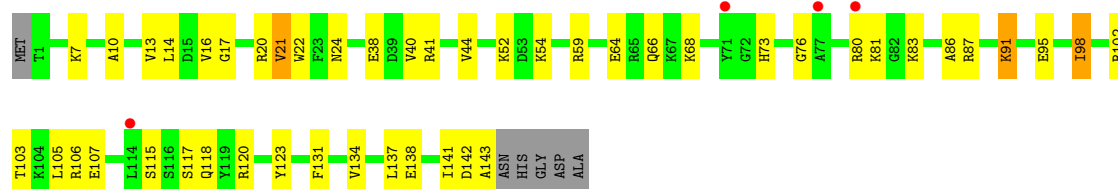
- Molecule 17: 50S ribosomal protein L18e

Chain O:



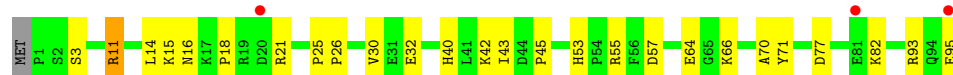
- Molecule 18: 50S ribosomal protein L19E

Chain P:



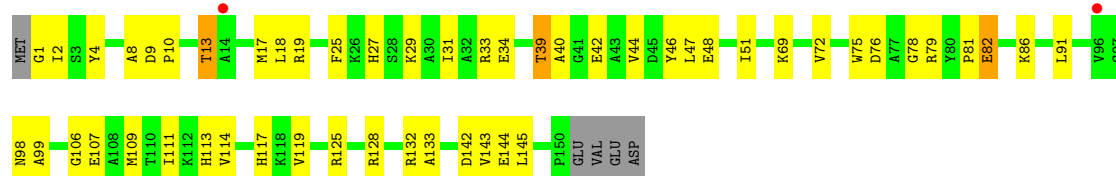
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



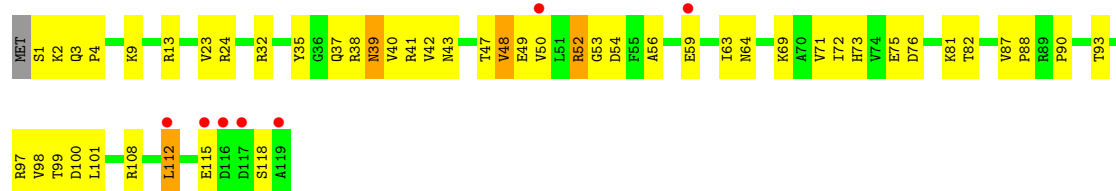
- Molecule 21: 50S ribosomal protein L23P

Chain S:



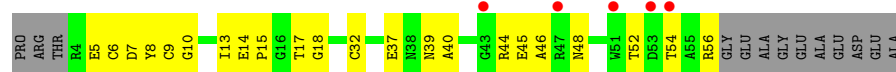
- Molecule 22: 50S ribosomal protein L24P

Chain T:

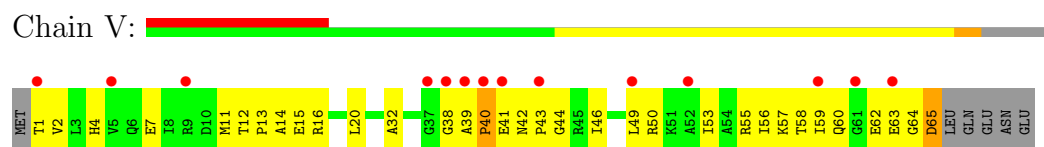


- Molecule 23: 50S ribosomal protein L24E

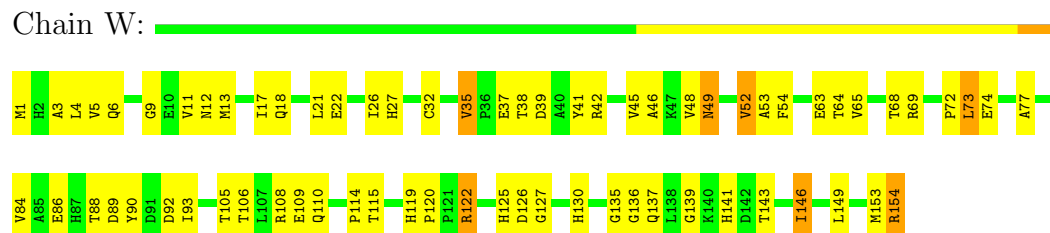
Chain U:



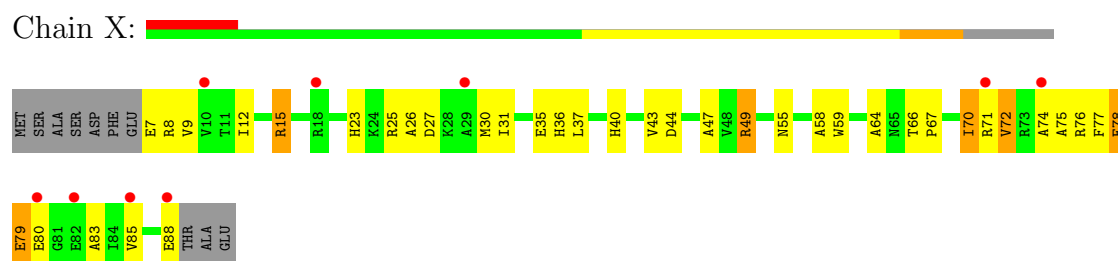
- Molecule 24: 50S ribosomal protein L29P



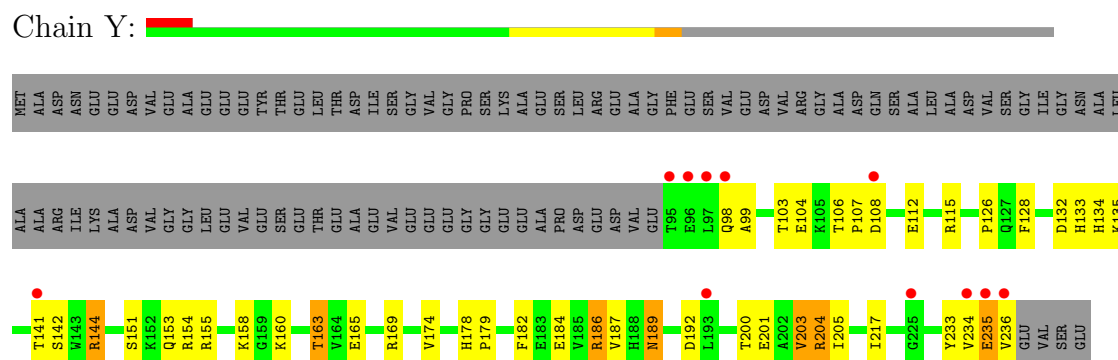
- Molecule 25: 50S ribosomal protein L30P



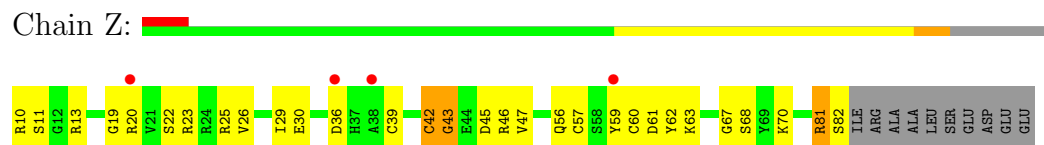
- Molecule 26: 50S ribosomal protein L31e



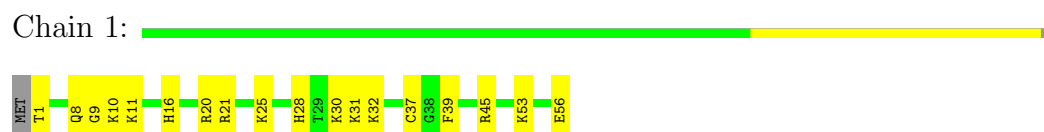
- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae

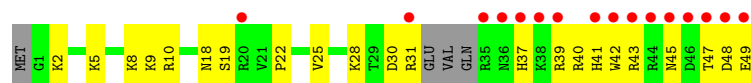


- Molecule 29: 50S ribosomal protein L37e



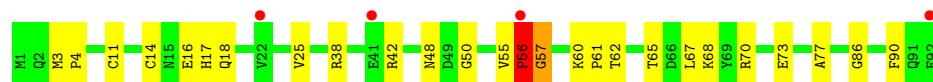
- Molecule 30: 50S ribosomal protein L39e

Chain 2: 



- Molecule 31: 50S ribosomal protein L44E

Chain 3: 



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P

Chain I: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.79Å 300.61Å 573.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-2.60) 90.1 (49.67-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.197 , 0.237 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 602690 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	99060	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.51% 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, OMG, CL, NA, K, PO2, CD, 5AA, DCZ, OMU, UR3, 2OP, 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	0	0.38	0/65959	0.69	20/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.53	0/83	0.82	0/119
4	A	0.33	0/1786	0.64	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.39	0/1884	0.66	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.29	0/241	0.45	0/324
11	H	0.34	0/1287	0.63	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.64	0/1509
15	M	0.35	0/1584	0.61	0/2119
16	N	0.28	0/1474	0.62	0/1999
17	O	0.34	0/874	0.59	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.37	0/749	0.68	0/1005
20	R	0.35	0/1172	0.64	0/1578
21	S	0.33	0/648	0.58	0/875
22	T	0.32	0/958	0.65	1/1289 (0.1%)
23	U	0.34	0/417	0.56	0/562
24	V	0.28	0/502	0.51	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.34	0/664	0.59	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.37	0/589	0.65	0/787
29	1	0.41	0/438	0.64	0/578
30	2	0.32	0/401	0.55	0/529
31	3	0.38	0/771	0.59	0/1024
32	I	0.29	0/526	0.53	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.37	0/98775	0.67	22/147696 (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	1	52
25	W	0	1
All	All	1	53

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.50	130.40	109.50
1	0	1942	A	C5'-C4'-C3'	7.87	128.58	116.00
2	9	3039	U	N1-C1'-C2'	6.80	122.84	114.00
1	0	871	G	C5'-C4'-O4'	-6.76	100.98	109.10
1	0	1819	G	C5'-C4'-C3'	6.21	125.94	116.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 53 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	189	A	Sidechain
1	0	26	U	Sidechain
1	0	333	G	Sidechain
1	0	48	A	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	59021	0	29813	777	1
2	9	2600	0	1326	52	1
3	4	126	0	75	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	158	1
6	C	1859	0	1816	111	0
7	D	1094	0	1085	93	0
8	E	1357	0	1266	78	0
9	F	890	0	843	51	0
10	G	240	0	231	11	0
11	H	1266	0	1268	60	0
12	J	1120	0	1098	62	0
13	K	992	0	1031	51	1
14	L	1118	0	1076	53	0
15	M	1560	0	1568	62	0
16	N	1445	0	1401	109	0
17	O	865	0	873	29	0
18	P	1136	0	1123	51	0
19	Q	735	0	729	23	0
20	R	1149	0	1122	55	0
21	S	641	0	605	19	0
22	T	950	0	923	50	0
23	U	410	0	364	21	0
24	V	499	0	511	34	0
25	W	1196	0	1137	95	0
26	X	654	0	653	44	0
27	Y	1130	0	1133	53	0
28	Z	578	0	539	24	0
29	1	431	0	426	27	0
30	2	396	0	413	29	0
31	3	755	0	728	19	0
32	I	519	0	500	58	0
33	0	106	0	0	0	0
33	2	1	0	0	0	0
33	3	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	2	0	0	0	0
33	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	71	0	0	0	0
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	1	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	0	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5820	0	0	111	0
38	1	59	0	0	2	0
38	2	42	0	0	2	0
38	3	74	0	0	3	0
38	4	8	0	0	0	0
38	9	133	0	0	3	0
38	A	117	0	0	9	0
38	B	150	0	0	16	0
38	C	165	0	0	15	0
38	D	49	0	0	11	0
38	E	47	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	F	21	0	0	3	0
38	G	16	0	0	0	0
38	H	66	0	0	6	0
38	I	10	0	0	2	0
38	J	52	0	0	1	0
38	K	54	0	0	3	0
38	L	83	0	0	10	0
38	M	118	0	0	3	0
38	N	66	0	0	8	0
38	O	39	0	0	4	0
38	P	65	0	0	3	0
38	Q	52	0	0	5	0
38	R	85	0	0	4	0
38	S	31	0	0	3	0
38	T	39	0	0	1	0
38	U	25	0	0	0	0
38	V	13	0	0	2	0
38	W	68	0	0	6	0
38	X	27	0	0	2	0
38	Y	92	0	0	5	0
38	Z	30	0	0	2	0
All	All	99060	0	59975	2235	3

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 15.

The worst 5 of 2235 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.12
15:M:164:THR:HG22	15:M:167:GLY:H	1.13	1.09
1:0:156:C:H5''	15:M:171:ARG:HD3	1.35	1.08
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.30	1.08
11:H:166:SER:HB2	11:H:167:PRO:HD3	1.35	1.07

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:9:3020:G:OP1	5:B:195:ARG:NH2[7_545]	1.98	0.22
1:0:1171:A:N3	1:0:1964:U:O5'[3_655]	2.13	0.07
13:K:63:GLU:CB	13:K:63:GLU:CB[3_655]	2.13	0.07

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	235/240 (98%)	206 (88%)	24 (10%)	5 (2%)	11	19
5	B	335/338 (99%)	294 (88%)	35 (10%)	6 (2%)	13	25
6	C	244/246 (99%)	217 (89%)	26 (11%)	1 (0%)	43	72
7	D	134/177 (76%)	97 (72%)	25 (19%)	12 (9%)	1	1
8	E	170/178 (96%)	156 (92%)	13 (8%)	1 (1%)	33	63
9	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	6	8
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	142 (91%)	11 (7%)	3 (2%)	12	23
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	16	32
13	K	130/132 (98%)	119 (92%)	8 (6%)	3 (2%)	10	17
14	L	141/165 (86%)	120 (85%)	19 (14%)	2 (1%)	16	32
15	M	192/194 (99%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	167 (91%)	11 (6%)	6 (3%)	6	9
17	O	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	25	49
18	P	141/149 (95%)	135 (96%)	6 (4%)	0	100	100
19	Q	93/96 (97%)	87 (94%)	6 (6%)	0	100	100
20	R	148/155 (96%)	138 (93%)	8 (5%)	2 (1%)	16	32
21	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
22	T	117/120 (98%)	107 (92%)	10 (8%)	0	100	100
23	U	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	11	21
24	V	63/71 (89%)	55 (87%)	6 (10%)	2 (3%)	6	9
25	W	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	30	58
26	X	80/92 (87%)	70 (88%)	8 (10%)	2 (2%)	9	14
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	3	3
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	88 (98%)	0	2 (2%)	10	18
32	I	68/162 (42%)	51 (75%)	17 (25%)	0	100	100
All	All	3705/4430 (84%)	3350 (90%)	295 (8%)	60 (2%)	14	28

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	ASP
4	A	132	ASP
9	F	101	ALA
11	H	168	ALA
12	J	5	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	179/182 (98%)	169 (94%)	10 (6%)	30	55
5	B	282/283 (100%)	265 (94%)	17 (6%)	27	51
6	C	193/193 (100%)	176 (91%)	17 (9%)	14	27
7	D	117/148 (79%)	112 (96%)	5 (4%)	40	69
8	E	152/156 (97%)	148 (97%)	4 (3%)	59	85
9	F	93/94 (99%)	92 (99%)	1 (1%)	84	96
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	126 (96%)	6 (4%)	38	67
12	J	118/121 (98%)	109 (92%)	9 (8%)	19	36
13	K	106/106 (100%)	101 (95%)	5 (5%)	36	65
14	L	113/127 (89%)	107 (95%)	6 (5%)	32	58
15	M	158/158 (100%)	151 (96%)	7 (4%)	39	68
16	N	149/150 (99%)	144 (97%)	5 (3%)	49	78
17	O	93/94 (99%)	90 (97%)	3 (3%)	51	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	P	113/117 (97%)	109 (96%)	4 (4%)	48	77
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	74
20	R	117/122 (96%)	114 (97%)	3 (3%)	59	85
21	S	71/74 (96%)	69 (97%)	2 (3%)	56	84
22	T	105/106 (99%)	101 (96%)	4 (4%)	44	74
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	68	90
25	W	130/130 (100%)	124 (95%)	6 (5%)	37	66
26	X	66/74 (89%)	61 (92%)	5 (8%)	19	36
27	Y	120/196 (61%)	111 (92%)	9 (8%)	19	36
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	87
31	3	79/79 (100%)	76 (96%)	3 (4%)	44	74
32	I	58/130 (45%)	57 (98%)	1 (2%)	73	92
All	All	3093/3611 (86%)	2956 (96%)	137 (4%)	39	68

5 of 137 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	46	ILE
14	L	35	ARG
27	Y	174	VAL
12	J	74	ARG
13	K	7	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	170	ASN
19	Q	16	ASN
30	2	41	HIS
16	N	40	ASN
18	P	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	32 (1%)
2	9	121/122 (99%)	15 (12%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	250 (8%)	33 (1%)

5 of 250 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1692	C
1	0	2726	U
1	0	1450	C
1	0	1563	G

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

6 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	$\# Z > 2$
1	OMU	0	2587	1,35	20,22,23	0.71	1 (5%)	24,31,34	0.72	0
1	OMG	0	2588	1,3	24,26,27	0.93	2 (8%)	32,38,41	5.31	3 (9%)
1	UR3	0	2619	1	20,22,23	0.79	0	23,32,35	0.81	0
1	PSU	0	2621	1	19,21,22	1.23	2 (10%)	23,30,33	1.06	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	1MA	0	628	1	23,25,26	0.86	0	32,37,40	1.00	1 (3%)
3	5AA	4	76	1,3	24,26,27	0.76	1 (4%)	35,38,41	0.90	1 (2%)

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
1	OMU	0	2587	1,35	-	0/8/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1	-	1/8/25/26	0/1/3/3
3	5AA	4	76	1,3	-	0/12/29/30	0/1/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.15	1.43	1.37
1	0	2588	OMG	P-OP1	2.83	1.49	1.46
1	0	2621	PSU	C6-N1	2.79	1.34	1.32
1	0	2587	OMU	P-OP1	2.25	1.49	1.46
3	4	76	5AA	P-OP1	2.03	1.49	1.46

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-29.46	130.17	134.14
3	4	76	5AA	C2-N1-C6	3.37	118.83	111.53
1	0	2588	OMG	C6-N1-C2	3.19	125.09	119.51
1	0	628	1MA	C2-N3-C4	-3.12	110.89	116.23
1	0	2621	PSU	C5-C4-N3	-2.34	114.59	118.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 234 ligands modelled in this entry, 234 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.

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%)	0.36	96 (3%) 42 38	24, 51, 98, 161	0
2	9	122/122 (100%)	0.51	5 (4%) 35 32	46, 68, 96, 153	0
3	4	8/8 (100%)	0.45	0 100 100	42, 45, 47, 54	0
4	A	237/240 (98%)	0.43	17 (7%) 15 12	31, 55, 94, 120	0
5	B	337/338 (99%)	0.99	32 (9%) 8 6	33, 65, 94, 103	0
6	C	246/246 (100%)	0.01	5 (2%) 62 60	26, 51, 75, 86	0
7	D	140/177 (79%)	2.06	58 (41%) 1 0	64, 110, 134, 141	0
8	E	172/178 (96%)	1.65	53 (30%) 1 1	50, 81, 105, 115	0
9	F	119/120 (99%)	0.75	17 (14%) 3 2	57, 81, 107, 122	0
10	G	29/348 (8%)	2.79	18 (62%) 0 0	74, 95, 105, 107	0
11	H	160/171 (93%)	0.92	17 (10%) 7 5	42, 63, 94, 101	0
12	J	142/145 (97%)	0.71	5 (3%) 42 38	42, 59, 82, 97	0
13	K	132/132 (100%)	0.76	10 (7%) 14 11	37, 62, 86, 90	0
14	L	145/165 (87%)	0.74	19 (13%) 4 3	28, 74, 118, 131	0
15	M	194/194 (100%)	0.04	0 100 100	33, 48, 64, 72	0
16	N	186/187 (99%)	0.82	26 (13%) 3 2	43, 69, 118, 124	0
17	O	115/116 (99%)	0.24	2 (1%) 67 66	43, 61, 79, 89	0
18	P	143/149 (95%)	0.57	4 (2%) 50 48	46, 62, 75, 81	0
19	Q	95/96 (98%)	0.37	3 (3%) 45 42	40, 50, 66, 77	0
20	R	150/155 (96%)	0.22	2 (1%) 74 75	36, 51, 72, 82	0
21	S	81/85 (95%)	0.37	6 (7%) 14 12	48, 65, 85, 94	0
22	T	119/120 (99%)	0.44	7 (5%) 22 18	44, 61, 90, 111	0
23	U	53/66 (80%)	0.92	5 (9%) 9 6	48, 63, 80, 88	0
24	V	65/71 (91%)	1.21	14 (21%) 1 1	59, 83, 117, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.41	0 100 100	41, 57, 78, 88	0
26	X	82/92 (89%)	0.81	9 (10%) 6 4	49, 66, 89, 106	0
27	Y	142/241 (58%)	0.52	11 (7%) 13 10	32, 51, 74, 95	0
28	Z	73/83 (87%)	0.29	4 (5%) 24 20	45, 64, 78, 96	0
29	1	56/57 (98%)	-0.15	0 100 100	31, 38, 46, 61	0
30	2	46/50 (92%)	1.68	16 (34%) 1 1	40, 70, 123, 128	0
31	3	92/92 (100%)	0.37	4 (4%) 34 30	37, 60, 74, 89	0
32	I	70/162 (43%)	3.64	54 (77%) 0 0	108, 129, 152, 155	0
All	All	6659/7482 (89%)	0.57	519 (7%) 14 10	24, 58, 109, 161	0

The worst 5 of 519 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	93	GLN	11.8
32	I	133	THR	8.9
32	I	71	GLY	7.6
32	I	137	VAL	7.4
10	G	27	ILE	7.2

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

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
3	5AA	4	76	24/25	0.22	2.19	40,44,46,47	0
1	UR3	0	2619	21/22	0.20	1.42	33,38,39,42	0
1	1MA	0	628	23/24	0.20	0.20	28,34,37,38	0
1	OMG	0	2588	24/25	0.19	-1.15	30,33,38,40	0
1	PSU	0	2621	20/21	0.16	-1.32	31,34,40,41	0
1	OMU	0	2587	21/22	0.17	-1.40	31,35,40,41	0

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	9184	1/1	0.85	90.28	83,83,83,83	0
35	NA	B	9158	1/1	0.74	62.46	70,70,70,70	0
35	NA	0	9178	1/1	0.50	49.80	57,57,57,57	0
35	NA	0	9160	1/1	0.39	45.88	46,46,46,46	0
35	NA	0	9121	1/1	0.78	34.92	55,55,55,55	0
35	NA	0	9162	1/1	0.56	34.84	64,64,64,64	0
33	MG	0	8101	1/1	0.38	31.82	72,72,72,72	0
35	NA	0	9113	1/1	0.34	29.12	67,67,67,67	0
33	MG	0	8092	1/1	0.41	22.74	90,90,90,90	0
33	MG	0	8087	1/1	0.25	20.36	59,59,59,59	0
35	NA	0	9152	1/1	0.40	19.87	61,61,61,61	0
35	NA	0	9175	1/1	0.37	18.97	52,52,52,52	0
35	NA	0	9120	1/1	0.36	16.62	52,52,52,52	0
33	MG	0	8100	1/1	0.42	14.30	70,70,70,70	0
35	NA	0	9106	1/1	0.35	14.23	38,38,38,38	0
33	MG	0	8016	1/1	0.28	14.10	50,50,50,50	0
35	NA	0	9174	1/1	0.30	13.93	62,62,62,62	0
35	NA	L	9180	1/1	0.48	13.30	51,51,51,51	0
35	NA	0	9135	1/1	0.35	13.23	52,52,52,52	0
35	NA	0	9182	1/1	0.55	12.89	81,81,81,81	0
35	NA	0	9123	1/1	0.36	12.70	44,44,44,44	0
33	MG	0	8049	1/1	0.38	11.99	81,81,81,81	0
35	NA	0	9169	1/1	0.36	11.80	60,60,60,60	0
35	NA	0	9176	1/1	0.33	11.07	49,49,49,49	0
35	NA	0	9177	1/1	0.39	10.50	68,68,68,68	0
35	NA	0	9170	1/1	0.32	10.19	49,49,49,49	0
36	CL	0	9315	1/1	0.24	10.00	80,80,80,80	0
35	NA	0	9156	1/1	0.28	9.63	49,49,49,49	0
35	NA	0	9118	1/1	0.26	8.31	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9165	1/1	0.27	7.17	47,47,47,47	0
35	NA	0	9107	1/1	0.23	6.95	46,46,46,46	0
35	NA	0	9179	1/1	0.31	6.69	70,70,70,70	0
35	NA	0	9129	1/1	0.23	6.61	57,57,57,57	0
35	NA	0	9185	1/1	0.28	6.08	51,51,51,51	0
35	NA	0	9155	1/1	0.48	5.93	79,79,79,79	0
35	NA	0	9142	1/1	0.24	5.78	47,47,47,47	0
35	NA	0	9164	1/1	0.23	5.74	53,53,53,53	0
33	MG	Y	8109	1/1	0.30	4.61	44,44,44,44	0
35	NA	0	9103	1/1	0.23	4.50	43,43,43,43	0
33	MG	0	8060	1/1	0.20	4.47	46,46,46,46	0
33	MG	0	8041	1/1	0.22	4.28	79,79,79,79	0
35	NA	R	9186	1/1	0.35	4.11	78,78,78,78	0
35	NA	0	9110	1/1	0.33	3.97	43,43,43,43	0
33	MG	0	8080	1/1	0.19	3.76	41,41,41,41	0
33	MG	0	8113	1/1	0.19	3.67	52,52,52,52	0
35	NA	0	9125	1/1	0.20	3.33	59,59,59,59	0
33	MG	0	8011	1/1	0.19	3.24	20,20,20,20	0
36	CL	A	9309	1/1	0.28	3.22	61,61,61,61	0
35	NA	0	9105	1/1	0.24	3.19	44,44,44,44	0
33	MG	0	8023	1/1	0.22	2.96	52,52,52,52	0
35	NA	0	9153	1/1	0.24	2.89	21,21,21,21	0
35	NA	0	9181	1/1	0.26	2.85	56,56,56,56	0
35	NA	0	9173	1/1	0.20	2.79	62,62,62,62	0
36	CL	0	9316	1/1	0.31	2.51	66,66,66,66	0
33	MG	0	8053	1/1	0.19	2.41	57,57,57,57	0
35	NA	0	9150	1/1	0.21	2.26	42,42,42,42	0
35	NA	S	9112	1/1	0.27	2.14	73,73,73,73	0
35	NA	0	9131	1/1	0.18	2.12	41,41,41,41	0
36	CL	N	9307	1/1	0.32	2.08	72,72,72,72	0
33	MG	0	8090	1/1	0.27	2.02	65,65,65,65	0
33	MG	0	8063	1/1	0.19	1.92	71,71,71,71	0
35	NA	0	9172	1/1	0.23	1.88	62,62,62,62	0
33	MG	0	8005	1/1	0.20	1.85	36,36,36,36	0
35	NA	0	9163	1/1	0.20	1.80	65,65,65,65	0
35	NA	0	9161	1/1	0.20	1.66	56,56,56,56	0
36	CL	0	9312	1/1	0.27	1.55	59,59,59,59	0
33	MG	0	8103	1/1	0.27	1.38	65,65,65,65	0
36	CL	O	9308	1/1	0.25	1.37	79,79,79,79	0
35	NA	0	9159	1/1	0.21	1.31	50,50,50,50	0
33	MG	0	8072	1/1	0.21	1.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8028	1/1	0.17	1.12	41,41,41,41	0
33	MG	0	8099	1/1	0.18	1.09	53,53,53,53	0
35	NA	0	9124	1/1	0.20	1.03	66,66,66,66	0
35	NA	0	9114	1/1	0.20	0.99	64,64,64,64	0
33	MG	0	8075	1/1	0.16	0.98	57,57,57,57	0
35	NA	0	9171	1/1	0.20	0.91	52,52,52,52	0
35	NA	0	9111	1/1	0.22	0.81	61,61,61,61	0
34	K	0	9003	1/1	0.19	0.76	64,64,64,64	0
36	CL	B	9319	1/1	0.23	0.51	55,55,55,55	0
33	MG	0	8116	1/1	0.19	0.44	62,62,62,62	0
33	MG	0	8093	1/1	0.19	0.27	66,66,66,66	0
36	CL	L	9310	1/1	0.19	0.23	63,63,63,63	0
35	NA	0	9101	1/1	0.21	0.11	40,40,40,40	0
35	NA	0	9143	1/1	0.18	0.10	33,33,33,33	0
33	MG	0	8032	1/1	0.18	0.08	41,41,41,41	0
35	NA	0	9126	1/1	0.17	0.01	41,41,41,41	0
35	NA	H	9122	1/1	0.18	-0.06	72,72,72,72	0
35	NA	0	9102	1/1	0.21	-0.13	45,45,45,45	0
33	MG	0	8071	1/1	0.17	-0.20	66,66,66,66	0
35	NA	A	9145	1/1	0.19	-0.20	48,48,48,48	0
36	CL	J	9301	1/1	0.21	-0.22	78,78,78,78	0
35	NA	0	9127	1/1	0.15	-0.26	42,42,42,42	0
35	NA	0	9117	1/1	0.26	-0.52	61,61,61,61	0
33	MG	0	8045	1/1	0.19	-0.56	73,73,73,73	0
35	NA	R	9137	1/1	0.18	-0.63	44,44,44,44	0
35	NA	0	9133	1/1	0.13	-0.68	34,34,34,34	0
35	NA	0	9157	1/1	0.11	-0.73	73,73,73,73	0
35	NA	0	9166	1/1	0.13	-0.73	69,69,69,69	0
36	CL	0	9311	1/1	0.15	-0.76	53,53,53,53	0
33	MG	0	8013	1/1	0.18	-0.79	33,33,33,33	0
33	MG	0	8017	1/1	0.14	-0.80	29,29,29,29	0
35	NA	0	9140	1/1	0.20	-0.84	47,47,47,47	0
36	CL	J	9321	1/1	0.17	-0.91	55,55,55,55	0
35	NA	0	9134	1/1	0.12	-0.92	41,41,41,41	0
36	CL	J	9302	1/1	0.19	-0.94	79,79,79,79	0
33	MG	0	8058	1/1	0.16	-0.94	56,56,56,56	0
33	MG	0	8021	1/1	0.15	-1.04	32,32,32,32	0
33	MG	0	8047	1/1	0.16	-1.06	86,86,86,86	0
33	MG	0	8086	1/1	0.11	-1.12	50,50,50,50	0
37	CD	Z	9203	1/1	0.08	-1.14	67,67,67,67	0
35	NA	Q	9148	1/1	0.16	-1.18	38,38,38,38	0
35	NA	0	9116	1/1	0.14	-1.18	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8104	1/1	0.16	-1.29	55,55,55,55	0
33	MG	0	8038	1/1	0.16	-1.34	32,32,32,32	0
33	MG	0	8030	1/1	0.15	-1.35	35,35,35,35	0
33	MG	0	8018	1/1	0.14	-1.40	42,42,42,42	0
36	CL	M	9318	1/1	0.14	-1.43	47,47,47,47	0
33	MG	0	8081	1/1	0.14	-1.43	52,52,52,52	0
35	NA	R	9138	1/1	0.15	-1.63	63,63,63,63	0
33	MG	0	8096	1/1	0.13	-1.66	53,53,53,53	0
33	MG	0	8057	1/1	0.14	-1.66	42,42,42,42	0
33	MG	0	8119	1/1	0.19	-1.67	62,62,62,62	0
33	MG	0	8050	1/1	0.13	-1.68	69,69,69,69	0
33	MG	A	8065	1/1	0.14	-1.69	45,45,45,45	0
37	CD	3	9204	1/1	0.05	-1.73	64,64,64,64	0
35	NA	C	9104	1/1	0.11	-1.76	40,40,40,40	0
33	MG	B	8055	1/1	0.17	-1.76	62,62,62,62	0
33	MG	0	8064	1/1	0.14	-1.77	30,30,30,30	0
33	MG	0	8106	1/1	0.07	-1.77	54,54,54,54	0
35	NA	0	9130	1/1	0.09	-1.80	45,45,45,45	0
34	K	0	9001	1/1	0.15	-1.87	71,71,71,71	0
35	NA	9	9151	1/1	0.10	-1.88	64,64,64,64	0
33	MG	T	8073	1/1	0.12	-1.91	59,59,59,59	0
33	MG	0	8002	1/1	0.14	-1.92	39,39,39,39	0
35	NA	0	9149	1/1	0.16	-1.93	38,38,38,38	0
33	MG	0	8019	1/1	0.13	-1.95	35,35,35,35	0
36	CL	0	9314	1/1	0.11	-1.98	49,49,49,49	0
33	MG	0	8031	1/1	0.13	-2.07	30,30,30,30	0
36	CL	R	9306	1/1	0.09	-2.10	57,57,57,57	0
35	NA	0	9144	1/1	0.13	-2.12	33,33,33,33	0
36	CL	0	9313	1/1	0.14	-2.18	60,60,60,60	0
35	NA	0	9119	1/1	0.09	-2.19	44,44,44,44	0
33	MG	0	8035	1/1	0.10	-2.20	49,49,49,49	0
36	CL	0	9305	1/1	0.11	-2.22	55,55,55,55	0
35	NA	0	9141	1/1	0.09	-2.24	45,45,45,45	0
33	MG	0	8117	1/1	0.14	-2.25	37,37,37,37	0
33	MG	0	8034	1/1	0.13	-2.36	38,38,38,38	0
33	MG	3	8078	1/1	0.10	-2.37	43,43,43,43	0
33	MG	0	8012	1/1	0.13	-2.42	32,32,32,32	0
35	NA	0	9128	1/1	0.09	-2.48	43,43,43,43	0
35	NA	0	9115	1/1	0.14	-2.49	37,37,37,37	0
36	CL	0	9317	1/1	0.09	-2.50	61,61,61,61	0
33	MG	A	8066	1/1	0.06	-2.50	66,66,66,66	0
35	NA	H	9109	1/1	0.12	-2.58	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8024	1/1	0.13	-2.76	39,39,39,39	0
33	MG	0	8070	1/1	0.10	-2.82	57,57,57,57	0
33	MG	0	8107	1/1	0.11	-2.85	53,53,53,53	0
37	CD	O	9205	1/1	0.04	-2.87	143,143,143,143	0
37	CD	1	9202	1/1	0.07	-2.90	62,62,62,62	0
33	MG	0	8074	1/1	0.07	-2.95	37,37,37,37	0
33	MG	0	8067	1/1	0.14	-2.97	49,49,49,49	0
36	CL	0	9322	1/1	0.18	-3.05	77,77,77,77	0
33	MG	0	8015	1/1	0.11	-3.06	33,33,33,33	0
33	MG	0	8037	1/1	0.11	-3.11	45,45,45,45	0
33	MG	0	8033	1/1	0.10	-3.17	38,38,38,38	0
36	CL	3	9304	1/1	0.12	-3.17	61,61,61,61	0
33	MG	0	8040	1/1	0.13	-3.24	56,56,56,56	0
35	NA	J	9146	1/1	0.06	-3.26	42,42,42,42	0
34	K	0	9002	1/1	0.11	-3.27	48,48,48,48	0
37	CD	U	9201	1/1	0.10	-3.30	74,74,74,74	0
33	MG	0	8020	1/1	0.13	-3.36	31,31,31,31	0
33	MG	0	8001	1/1	0.12	-3.38	35,35,35,35	0
33	MG	0	8108	1/1	0.09	-3.42	58,58,58,58	0
33	MG	0	8044	1/1	0.12	-3.44	55,55,55,55	0
33	MG	B	8056	1/1	0.11	-3.47	47,47,47,47	0
33	MG	4	8118	1/1	0.13	-3.60	41,41,41,41	0
33	MG	0	8085	1/1	0.16	-3.60	72,72,72,72	0
35	NA	M	9147	1/1	0.10	-3.61	25,25,25,25	0
33	MG	0	8102	1/1	0.08	-3.62	58,58,58,58	0
33	MG	0	8094	1/1	0.11	-3.64	73,73,73,73	0
35	NA	9	9183	1/1	0.12	-3.81	60,60,60,60	0
33	MG	0	8003	1/1	0.15	-3.86	31,31,31,31	0
33	MG	0	8027	1/1	0.07	-3.86	37,37,37,37	0
33	MG	0	8061	1/1	0.08	-3.97	37,37,37,37	0
33	MG	9	8095	1/1	0.10	-3.97	77,77,77,77	0
35	NA	0	9139	1/1	0.15	-3.98	31,31,31,31	0
33	MG	0	8062	1/1	0.07	-4.05	51,51,51,51	0
33	MG	0	8112	1/1	0.05	-4.05	39,39,39,39	0
33	MG	0	8097	1/1	0.08	-4.26	40,40,40,40	0
33	MG	0	8098	1/1	0.09	-4.29	47,47,47,47	0
36	CL	0	9303	1/1	0.11	-4.30	53,53,53,53	0
33	MG	2	8076	1/1	0.13	-4.33	55,55,55,55	0
33	MG	0	8008	1/1	0.08	-4.39	37,37,37,37	0
33	MG	0	8039	1/1	0.06	-4.57	52,52,52,52	0
33	MG	0	8089	1/1	0.10	-4.58	56,56,56,56	0
33	MG	0	8042	1/1	0.06	-4.74	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8110	1/1	0.12	-4.97	32,32,32,32	0
33	MG	K	8069	1/1	0.07	-4.99	52,52,52,52	0
35	NA	0	9168	1/1	0.09	-5.01	49,49,49,49	0
35	NA	0	9108	1/1	0.09	-5.05	49,49,49,49	0
33	MG	0	8115	1/1	0.08	-5.14	57,57,57,57	0
33	MG	9	8052	1/1	0.12	-5.21	54,54,54,54	0
33	MG	0	8088	1/1	0.12	-5.24	38,38,38,38	0
33	MG	0	8084	1/1	0.13	-5.30	38,38,38,38	0
33	MG	0	8043	1/1	0.10	-5.49	47,47,47,47	0
33	MG	0	8007	1/1	0.11	-5.55	27,27,27,27	0
33	MG	0	8010	1/1	0.10	-5.75	28,28,28,28	0
33	MG	0	8054	1/1	0.09	-5.84	29,29,29,29	0
35	NA	0	9154	1/1	0.10	-5.91	33,33,33,33	0
33	MG	0	8059	1/1	0.14	-5.95	51,51,51,51	0
33	MG	0	8079	1/1	0.10	-6.02	29,29,29,29	0
33	MG	0	8014	1/1	0.06	-6.05	43,43,43,43	0
33	MG	0	8009	1/1	0.13	-6.12	30,30,30,30	0
33	MG	0	8051	1/1	0.08	-6.14	72,72,72,72	0
35	NA	0	9132	1/1	0.04	-6.29	34,34,34,34	0
33	MG	0	8091	1/1	0.07	-6.73	79,79,79,79	0
33	MG	0	8077	1/1	0.09	-6.83	28,28,28,28	0
33	MG	0	8068	1/1	0.07	-7.04	60,60,60,60	0
33	MG	0	8026	1/1	0.09	-7.07	24,24,24,24	0
33	MG	0	8006	1/1	0.09	-7.26	37,37,37,37	0
35	NA	0	9167	1/1	0.06	-7.55	52,52,52,52	0
33	MG	0	8048	1/1	0.05	-7.64	56,56,56,56	0
33	MG	0	8083	1/1	0.08	-7.73	42,42,42,42	0
33	MG	0	8029	1/1	0.06	-7.76	36,36,36,36	0
36	CL	Y	9320	1/1	0.10	-7.83	52,52,52,52	0
33	MG	0	8022	1/1	0.09	-8.37	35,35,35,35	0
33	MG	0	8114	1/1	0.07	-8.55	56,56,56,56	0
33	MG	0	8025	1/1	0.13	-8.69	46,46,46,46	0
33	MG	0	8046	1/1	0.09	-9.90	59,59,59,59	0
33	MG	0	8004	1/1	0.09	-10.96	34,34,34,34	0
33	MG	0	8111	1/1	0.09	-12.95	52,52,52,52	0
35	NA	0	9136	1/1	0.08	-13.69	55,55,55,55	0
33	MG	0	8082	1/1	0.15	-14.00	76,76,76,76	0
33	MG	0	8036	1/1	0.12	-19.08	35,35,35,35	0

6.5 Other polymers ⓘ

There are no such residues in this entry.