



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:40 PM GMT

PDB ID : 1VQ7
Title : The structure of the transition state analogue "DCA" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.50 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>

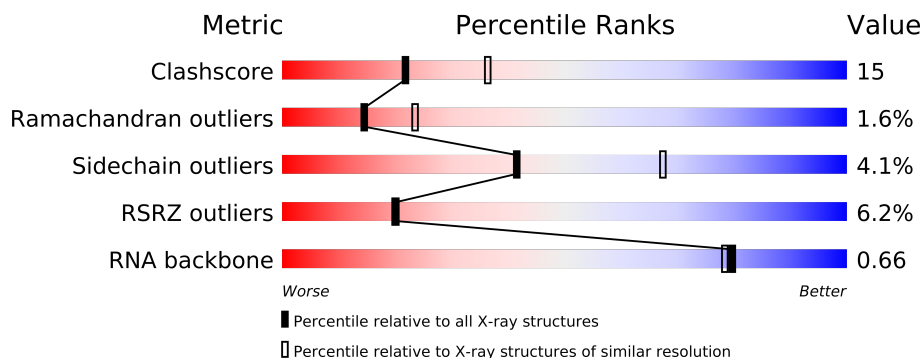
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.50 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	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)
RNA backbone	1838	1107 (3.10-1.90)

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	

Continued on next page...

Continued from previous page...

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	8013	-	X
33	MG	0	8016	-	X
33	MG	0	8023	-	X
33	MG	0	8029	-	X
33	MG	0	8041	-	X
33	MG	0	8045	-	X
33	MG	0	8047	-	X
33	MG	0	8049	-	X
33	MG	0	8060	-	X
33	MG	0	8085	-	X
33	MG	0	8087	-	X
33	MG	0	8090	-	X
33	MG	0	8092	-	X
33	MG	0	8094	-	X
33	MG	0	8101	-	X
33	MG	0	8103	-	X
34	K	0	9003	-	X
35	NA	0	9102	-	X
35	NA	0	9106	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	9107	-	X
35	NA	0	9111	-	X
35	NA	0	9118	-	X
35	NA	0	9121	-	X
35	NA	0	9125	-	X
35	NA	0	9135	-	X
35	NA	0	9140	-	X
35	NA	0	9142	-	X
35	NA	0	9150	-	X
35	NA	0	9152	-	X
35	NA	0	9156	-	X
35	NA	0	9160	-	X
35	NA	0	9161	-	X
35	NA	0	9162	-	X
35	NA	0	9163	-	X
35	NA	0	9170	-	X
35	NA	0	9171	-	X
35	NA	0	9172	-	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	9182	-	X
35	NA	0	9185	-	X
35	NA	0	9186	-	X
35	NA	B	9158	-	X
35	NA	L	9180	-	X
35	NA	S	9112	-	X
36	CL	0	9315	-	X
36	CL	0	9322	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99063 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'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			130	63	23	39	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	108	Total	Mg	0	0
			108	108		
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	1	Total	Mg	0	0
			1	1		
33	4	1	Total	Mg	0	0
			1	1		
33	T	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	0	0
			3	3		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	72	Total 72	Na 72	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	H	2	Total 2	Na 2	0	0
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	A	1	Total 1	Na 1	0	0
35	T	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	L	1	Total 1	Na 1	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	11	Total 11	Cl 11	0	0
36	J	3	Total 3	Cl 3	0	0
36	B	1	Total 1	Cl 1	0	0
36	A	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	O	1	Total 1	Cl 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	R	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	5809	Total 5809	O 5809	0	0
38	9	137	Total 137	O 137	0	0
38	4	8	Total 8	O 8	0	0
38	A	119	Total 119	O 119	0	0
38	B	153	Total 153	O 153	0	0
38	C	168	Total 168	O 168	0	0
38	D	47	Total 47	O 47	0	0
38	E	43	Total 43	O 43	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	F	23	Total 23	O 23	0	0
38	G	18	Total 18	O 18	0	0
38	H	65	Total 65	O 65	0	0
38	J	51	Total 51	O 51	0	0
38	K	58	Total 58	O 58	0	0
38	L	82	Total 82	O 82	0	0
38	M	116	Total 116	O 116	0	0
38	N	63	Total 63	O 63	0	0
38	O	42	Total 42	O 42	0	0
38	P	64	Total 64	O 64	0	0
38	Q	51	Total 51	O 51	0	0
38	R	84	Total 84	O 84	0	0
38	S	30	Total 30	O 30	0	0
38	T	42	Total 42	O 42	0	0
38	U	29	Total 29	O 29	0	0
38	V	14	Total 14	O 14	0	0
38	W	68	Total 68	O 68	0	0
38	X	27	Total 27	O 27	0	0
38	Y	96	Total 96	O 96	0	0
38	Z	32	Total 32	O 32	0	0
38	1	53	Total 53	O 53	0	0

Continued on next page...

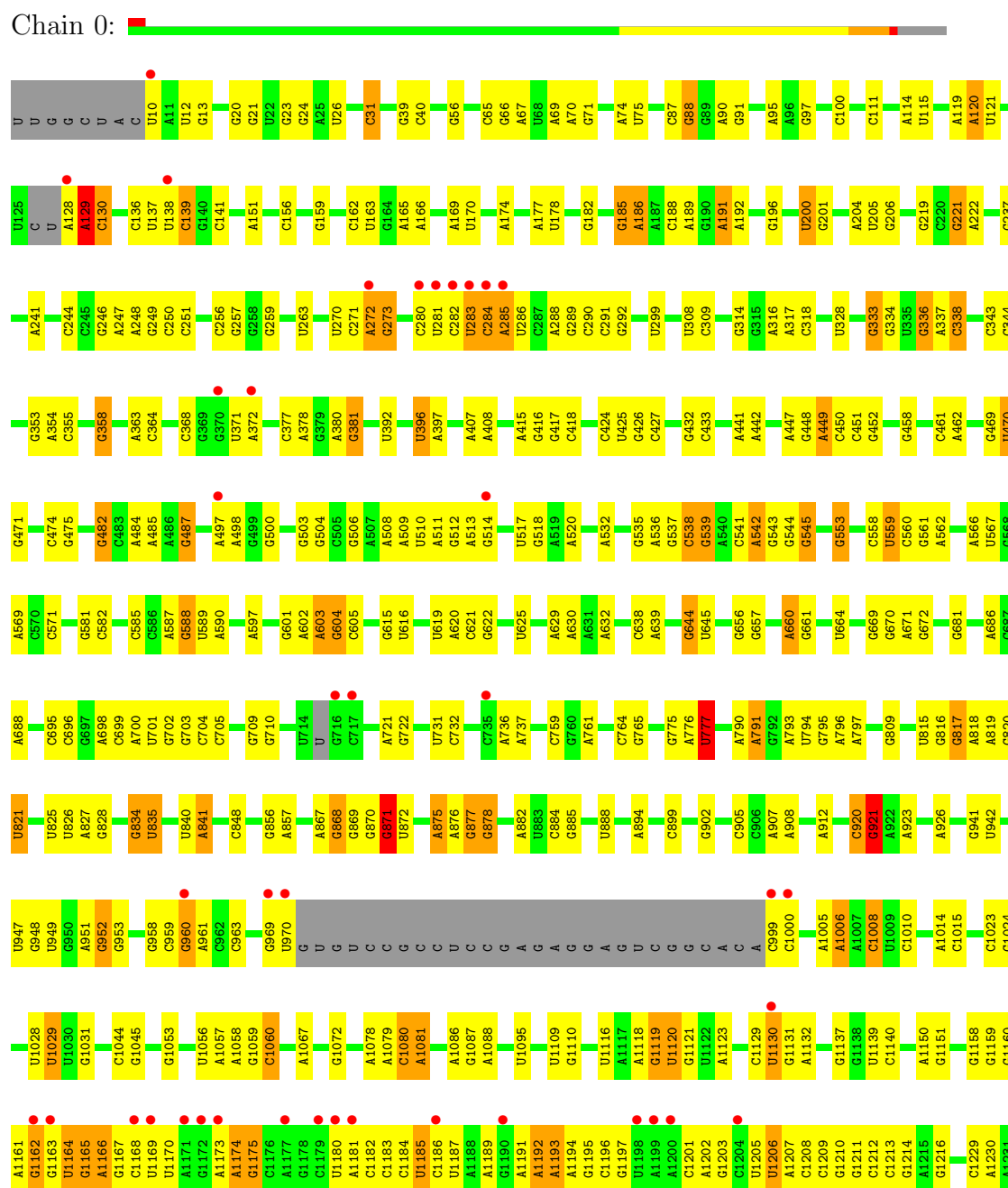
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	2	40	Total 40	O 40	0	0
38	3	74	Total 74	O 74	0	0
38	I	9	Total 9	O 9	0	0

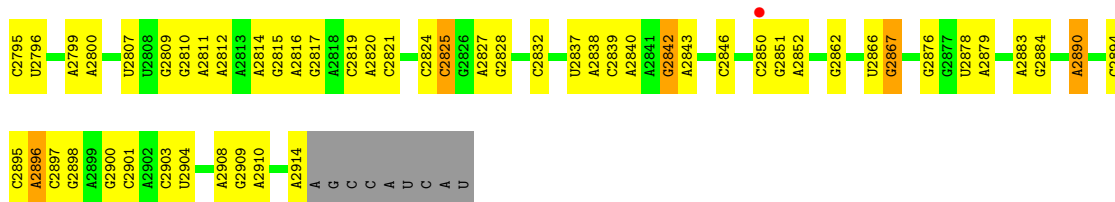
3 Residue-property plots

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

- Molecule 1: 23S ribosomal rna



G2708	U2587	U2473	G2379	A2274	C2035	G1923	G1798	A1711	C1592	C1462	C1342	A1232
G2709	G2568	A2474	A2382	G2275	C2036	G1929	G1799	A1712	C1593	A1463	C1343	A1233
U2710	U2589	C2475	C2281	C2281	A2039	G1942	G1805	G1713	C1594	A1470	G1351	U1234
G2716	C2591	C2477	G2385	U2282	U2043	C1943	G1806	C1714	G1595	A1471	C1353	U1236
C2717	G2592	U2478	U2387	A2291	G2044	A1942	A1811	C1715	A1597	A1472	G1354	U1237
C2718	A2601	G2480	C2388	C2389	G2044	G1948	A1811	A1716	A1598	C1472	A1355	C1238
A2719	G2602	A2483	A2401	A2300	G2053	G1949	A1815	A1717	A1603	U1473	A1355	G1239
C2720	U2607	A2488	A2402	A2302	A2054	G1950	G1819	U1722	G1604	C1474	C1360	A1242
G2722	C2608	G2489	C2403	A2302	A2055	G1951	G1820	U1724	G1605	U1478	G1363	C1243
G2723	G2613	A2408	A2408	C2309	C2061	A	U1825	C1725	C1613	A1482	U1370	U1244
U2724	C2614	G2412	A2412	G2310	A2062	A	U1826	G1730	G1614	C1483	G1372	C1245
G2726	U2615	A2413	A2413	A2311	U2063	C	C1826	C1731	A1624	C1484	U1371	A1246
A2727	G2616	A2414	A2414	C2312	U2064	A	A1829	A1732	A1625	A1485	C1372	C1250
C2728	U2499	A2415	A2415	C2313	A2067	U	C1830	A1733	A1626	A1495	A1375	C1251
C2729	C2500	G2422	A2422	C2315	G2068	G	C1834	C1734	U1634	G1496	G1376	C1268
G2730	G2501	G2423	G2423	G2317	G2072	A	U1835	G1739	G1634	U1500	U1380	U1270
G2731	C2502	U2424	U2424	C2320	A2074	C	A1840	U1741	U1635	A1504	G1386	C1273
U2735	A2503	G2425	G2425	A2321	G2075	U1964	A1845	G1742	G1636	U1503	U1387	U1279
U2736	G2504	A2426	A2426	G2325	G2076	G1970	U1846	G1744	A1642	U1505	A1406	A1294
G2740	A2505	G2427	G2427	U2326	C2077	G1971	A1847	G1745	A1642	U1506	A1407	G1299
A2741	G2507	U2428	U2428	A2327	U2078	U1972	G1848	C1746	U1654	A1526	A1413	G1300
C2742	C2508	G2435	G2435	C2327	G2079	G1973	G1849	A1747	U1655	A1527	A1414	U1304
G2747	A2509	U2436	U2436	U2328	G2080	A1973	G1855	G1751	A1656	A1528	G1415	C1305
C2748	C2510	G2437	G2437	C2329	A2081	G1976	G1856	G1752	A1657	U1530	G1416	U1306
U2749	U2512	C2438	C2438	U2330	G2089	U1977	U1857	C1762	A1658	U1531	G1417	A1307
G2750	A2521	U2439	U2439	G2333	G2090	A1978	U1874	U1766	U1676	U1532	U1418	A1308
C2751	G2524	G2445	G2445	C2334	G2091	U1979	G1877	C1767	U1677	G1535	U1419	U1309
U2752	U2525	A2446	A2446	G2335	G2092	U1980	G1883	C1768	A1677	C1536	C1420	U1310
G2753	C2526	G2447	G2447	G2336	G2093	U1985	G1867	C1769	U1668	C1537	G1423	G1312
G2754	C2526	U2448	U2448	G2337	G2094	U1985	G1868	G1773	C1675	G1543	A1424	G1323
U2755	U2527	A2449	A2449	G2338	A2095	C1993	U1874	G1774	U1676	C1545	A1427	G1329
A2664	A	C2443	C2443	A2338	A2096	C1996	G1877	G1775	U1677	U1559	U1434	A1328
U2756	U	G2444	G2444	G2339	C2101	U1996	G1878	A1776	U1677	U1561	U1435	A1329
C2762	C2533	A2445	A2445	C2340	G2102	U2004	G1879	A1777	A1682	U1562	A1436	A1330
G2765	C2534	G2446	G2446	G2341	C2105	G2005	C1880	G1778	G1683	C1562	C1436	A1331
A2766	U2535	G2451	G2451	A2342	C2106	U2008	A1881	G1779	U1684	U1544	U1440	U1333
C2767	C2536	G2452	G2452	A2343	G2110	U2008	C1882	A1776	A1685	C1564	C1441	C1334
A2768	U2541	G2453	G2453	A2344	G2128	A2011	G1884	G1777	C1686	A1580	A1442	C1335
C2769	C2542	A2454	A2454	A2345	G2135	U2012	G1891	A1778	U1687	U1587	C1450	U1336
G2770	C2548	U2457	U2457	A2354	G2136	G2013	G1891	A1779	C1687	U1588	G1451	G1340
A2775	C2552	G2462	G2462	A2355	A	G2014	A1904	G1785	C1692	U1589	C1452	A1341
U2776	A2553	A2463	A2463	A2356	C	G2016	U1905	C1786	C1692	U1589	G1452	G1340
G2778	U2563	G2464	G2464	A2364	C	U2016	G1909	C1787	G1697	U1589	G1452	G1340
A2786	G2564	A2465	A2465	A2364	C	U2016	A1909	U1788	U1698	A1580	C1452	G1340
C2786	C2565	A2466	A2466	A2369	U	U2028	C2079	G1789	U1701	U1587	G1452	G1340
U2790	G2578	A2467	A2467	A2372	C	A2030	A1919	C1790	A1701	U1587	G1452	G1340
U2791	A2698	A2468	A2468	U2373	G	A2030	C1920	U1791	U1702	U1587	G1452	G1340
A2792	G2700	A2469	A2469	G2373	A	G2033	A1921	A1797	C1705	U1587	G1452	G1340
		C2472	C2472	C2373	G	U2034	A1922					



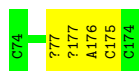
• Molecule 2: 5S ribosomal RNA

Chain 9:



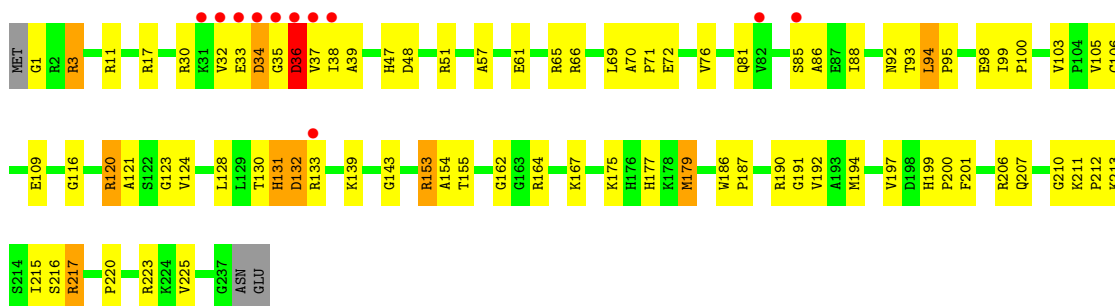
• Molecule 3: 5'-R(*CP*CP*(5AA)P*(2OP)P*(PAE)P*AP*C*C)-3'

Chain 4:



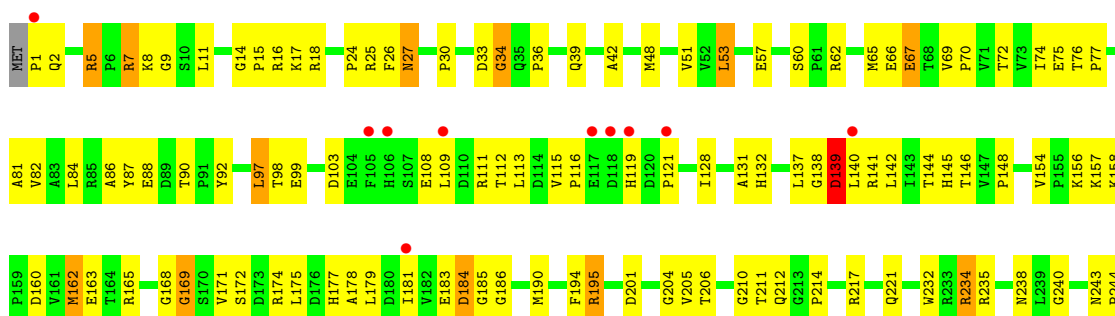
• Molecule 4: 50S ribosomal protein L2P

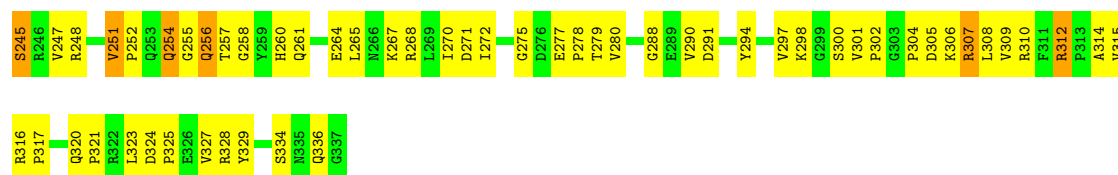
Chain A:



• Molecule 5: 50S ribosomal protein L3P

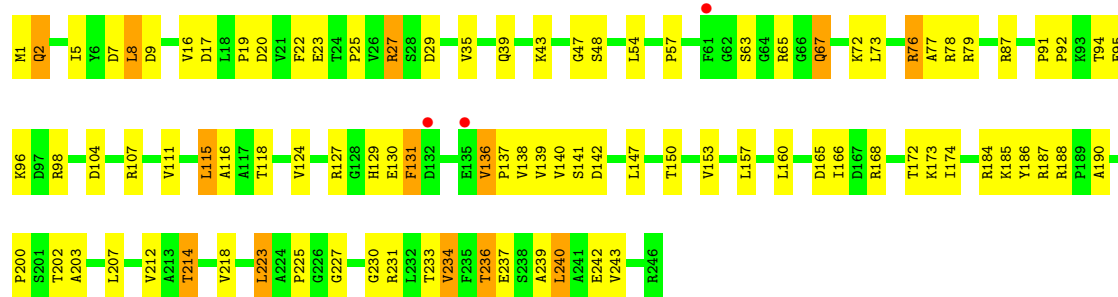
Chain B:





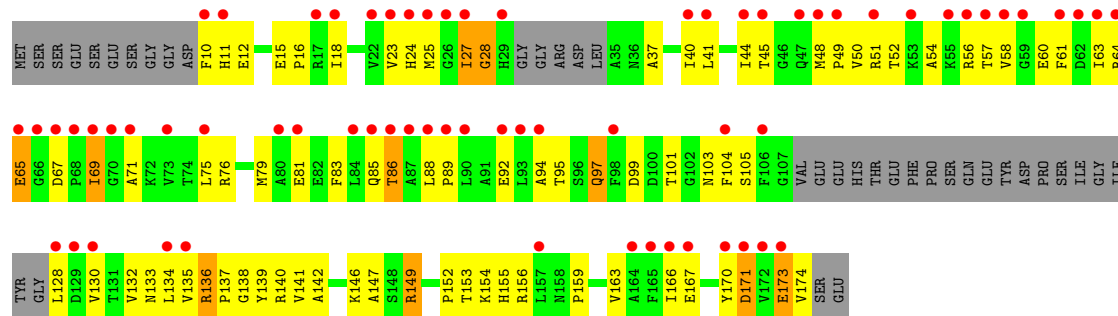
• Molecule 6: 50S ribosomal protein L4E

Chain C:



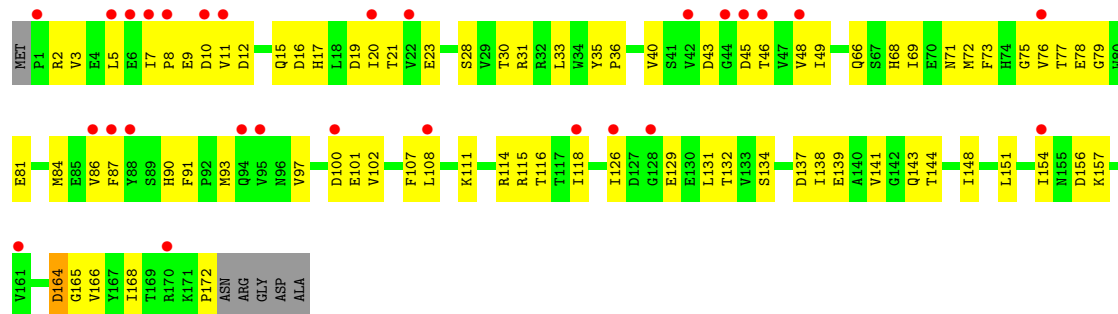
• Molecule 7: 50S ribosomal protein L5P

Chain D:



• Molecule 8: 50S ribosomal protein L6P

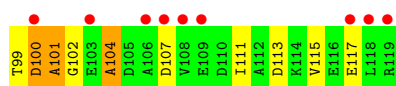
Chain E:



• Molecule 9: 50S ribosomal protein L7AE

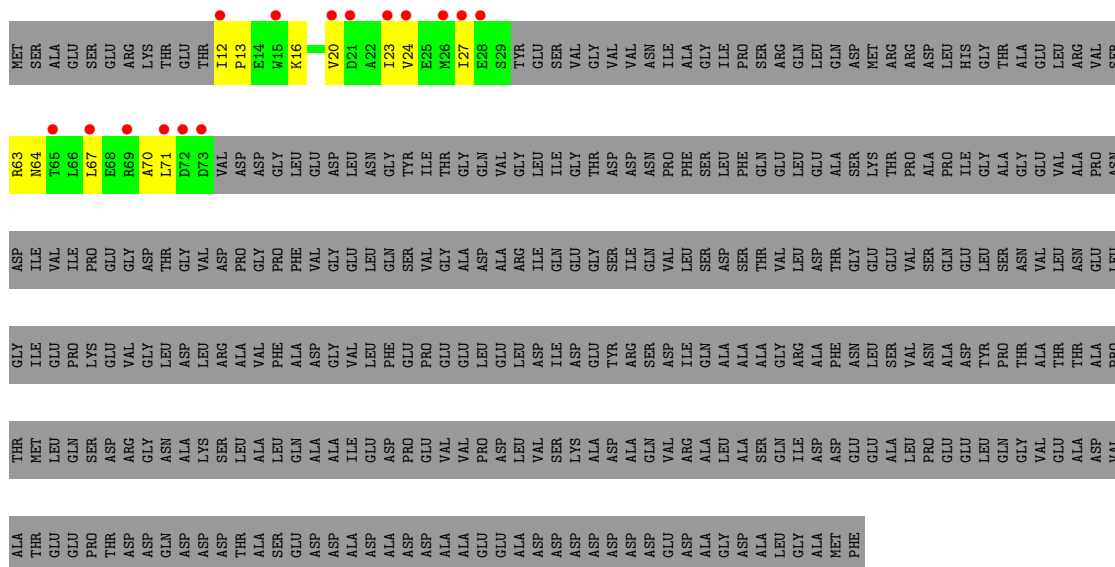
Chain F:





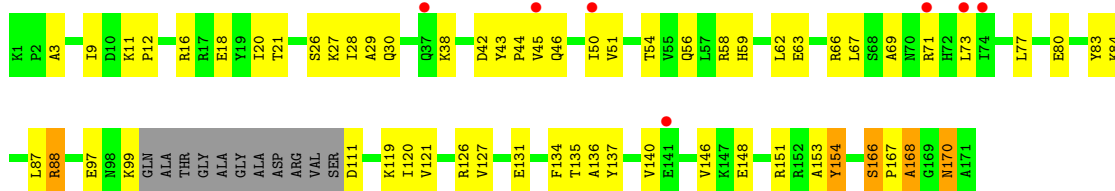
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

Chain G:



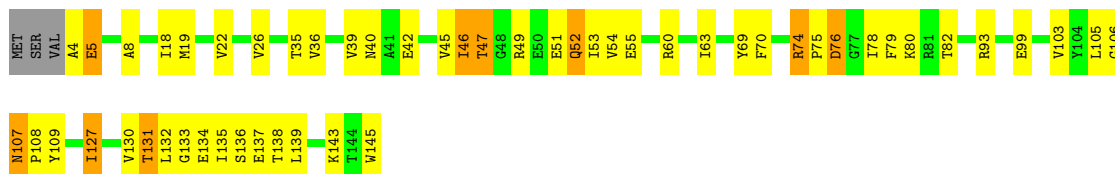
• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

Chain H:



• Molecule 12: 50S ribosomal protein L13P

Chain J:



• Molecule 13: 50S ribosomal protein L14P

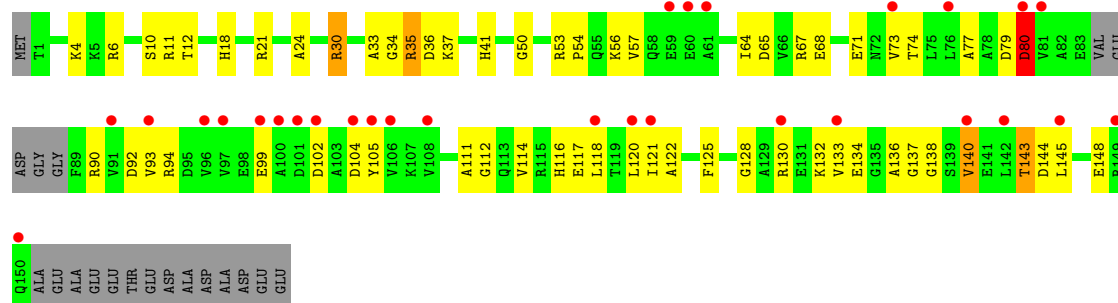
Chain K:





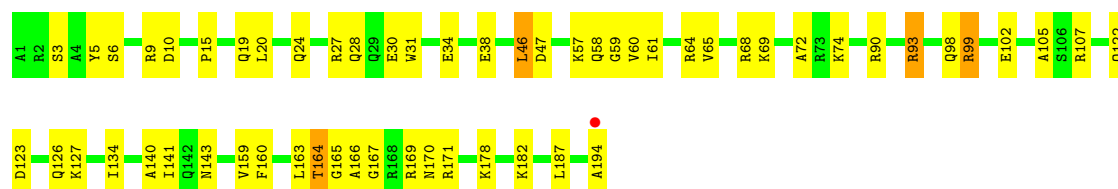
• Molecule 14: 50S ribosomal protein L15P

Chain L:



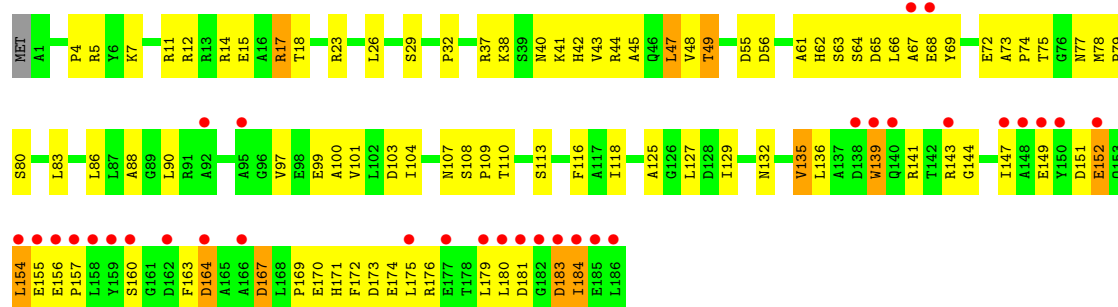
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



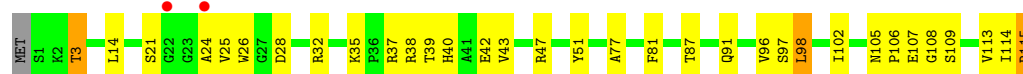
• Molecule 16: 50S ribosomal protein L18P

Chain N:



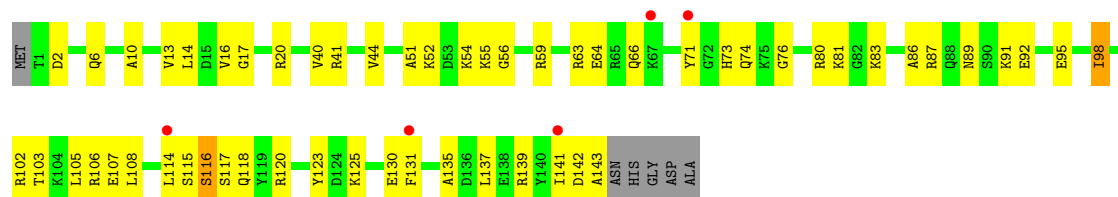
• Molecule 17: 50S ribosomal protein L18e

Chain O:



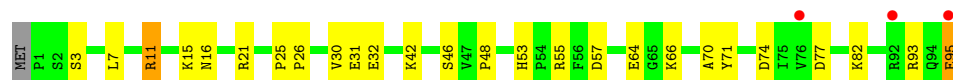
• Molecule 18: 50S ribosomal protein L19E

Chain P:



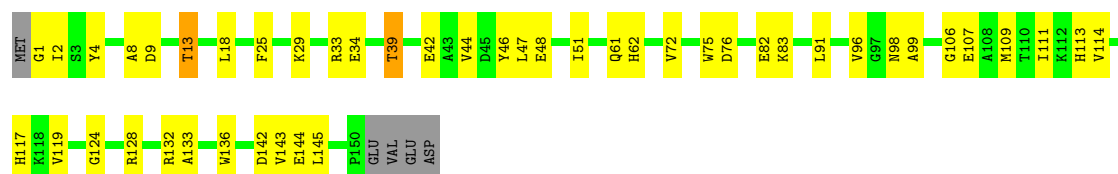
- Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



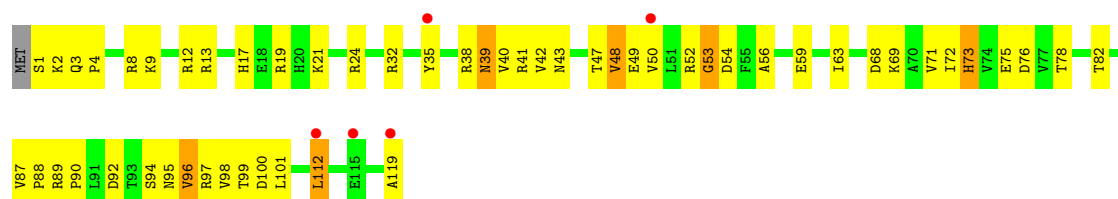
- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



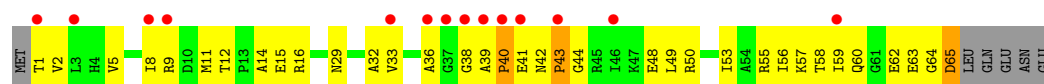
- Molecule 23: 50S ribosomal protein L24E

Chain U:



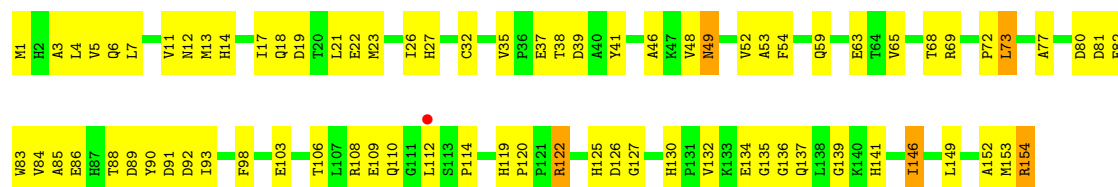
- Molecule 24: 50S ribosomal protein L29P

Chain V:



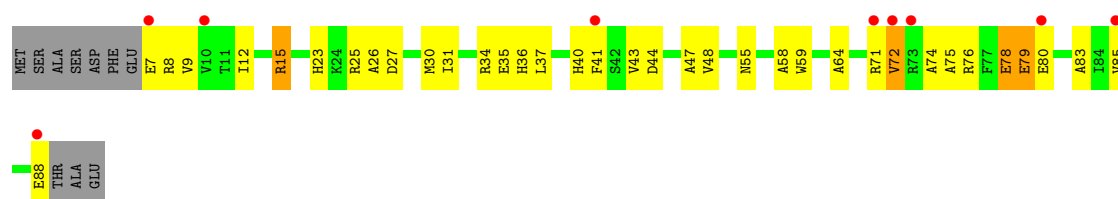
- Molecule 25: 50S ribosomal protein L30P

Chain W:



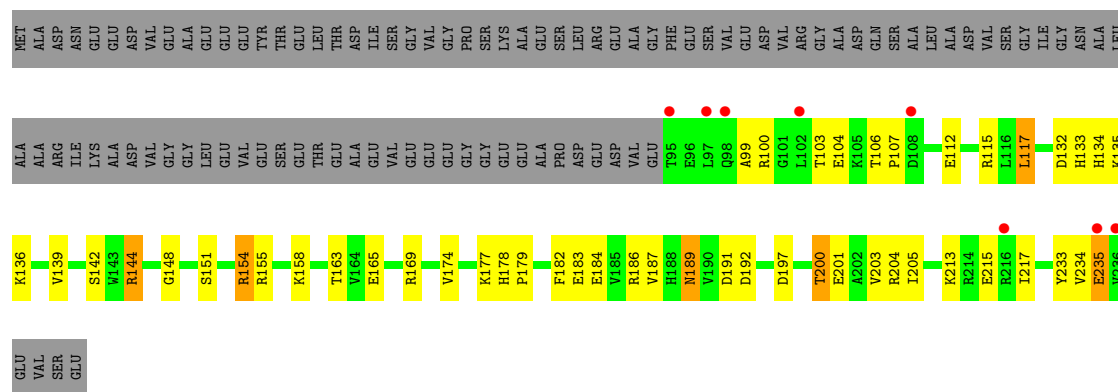
- Molecule 26: 50S ribosomal protein L31e

Chain X:



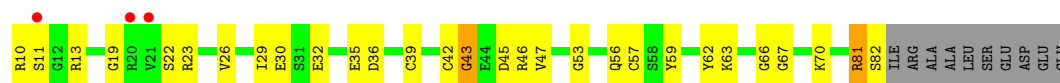
- Molecule 27: 50S ribosomal protein L32E

Chain Y:



- Molecule 28: 50S ribosomal protein L37Ae

Chain Z:



- Molecule 29: 50S ribosomal protein L37e

Chain 1:



- Molecule 30: 50S ribosomal protein L39e

Chain 2: 



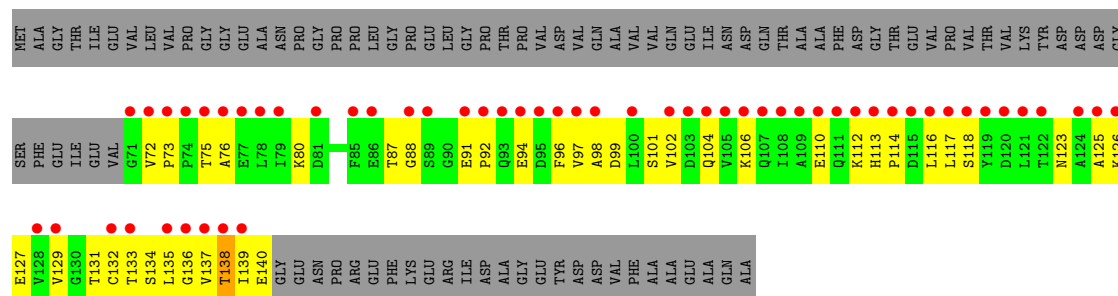
- Molecule 31: 50S ribosomal protein L44E

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	211.15Å 300.13Å 573.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.61 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (50.00-2.50) 89.0 (49.61-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.206 , 0.244 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 600554 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99063	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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, CD, 5AA, PAE, 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	0.37	0/65959	0.69	23/102870 (0.0%)
2	9	0.33	0/2905	0.70	1/4528 (0.0%)
3	4	0.43	0/102	0.65	0/149
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.63	0/3652
6	C	0.38	0/1884	0.66	0/2551
7	D	0.30	0/1111	0.54	0/1498
8	E	0.31	0/1382	0.57	0/1880
9	F	0.31	0/901	0.55	0/1224
10	G	0.27	0/241	0.45	0/324
11	H	0.33	0/1287	0.65	0/1725
12	J	0.35	0/1136	0.60	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.33	0/1130	0.65	0/1509
15	M	0.35	0/1584	0.62	0/2119
16	N	0.29	0/1474	0.63	0/1999
17	O	0.34	0/874	0.60	0/1181
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.35	0/749	0.67	0/1005
20	R	0.36	0/1172	0.63	0/1578
21	S	0.33	0/648	0.60	0/875
22	T	0.31	0/958	0.63	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.29	0/502	0.53	0/675
25	W	0.33	0/1219	0.63	0/1655
26	X	0.33	0/664	0.58	0/895
27	Y	0.36	0/1146	0.65	0/1536
28	Z	0.36	0/589	0.65	0/787
29	1	0.41	0/438	0.66	0/578
30	2	0.32	0/401	0.52	0/529
31	3	0.39	0/771	0.61	0/1024
32	I	0.31	0/526	0.54	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98794	0.67	24/147726 (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	54
2	9	0	3
All	All	1	57

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.68	130.79	109.50
1	0	1942	A	C5'-C4'-C3'	8.39	129.43	116.00
1	0	1979	G	C2'-C3'-O3'	7.72	126.49	109.50
1	0	871	G	C5'-C4'-O4'	-7.18	100.48	109.10
2	9	3039	U	N1-C1'-C2'	7.03	123.14	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 57 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	174	A	Sidechain
1	0	191	A	Sidechain
1	0	221	G	Sidechain
1	0	246	G	Sidechain
1	0	26	U	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	813	0
2	9	2600	0	1326	57	0
3	4	130	0	77	5	0
4	A	1753	0	1766	106	0
5	B	2625	0	2533	167	0
6	C	1859	0	1816	100	0
7	D	1094	0	1085	85	0
8	E	1357	0	1266	84	0
9	F	890	0	843	43	0
10	G	240	0	231	14	0
11	H	1266	0	1268	64	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	57	0
14	L	1118	0	1076	53	0
15	M	1560	0	1568	58	0
16	N	1445	0	1401	104	0
17	O	865	0	873	32	0
18	P	1136	0	1123	51	0
19	Q	735	0	729	21	0
20	R	1149	0	1122	60	0
21	S	641	0	605	21	0
22	T	950	0	923	56	0
23	U	410	0	364	29	0
24	V	499	0	511	35	0
25	W	1196	0	1137	95	0
26	X	654	0	653	34	0
27	Y	1130	0	1133	56	0
28	Z	578	0	539	25	0
29	1	431	0	426	21	0
30	2	396	0	413	28	0
31	3	755	0	728	27	0
32	I	519	0	500	47	0
33	0	108	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	1	0	0	0	0
33	B	2	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	Y	1	0	0	0	0
34	0	3	0	0	0	0
35	0	72	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	1	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	11	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
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	5809	0	0	103	0
38	1	53	0	0	2	0
38	2	40	0	0	3	0
38	3	74	0	0	4	0
38	4	8	0	0	1	0
38	9	137	0	0	5	0
38	A	119	0	0	13	0
38	B	153	0	0	15	0
38	C	168	0	0	12	0
38	D	47	0	0	10	0
38	E	43	0	0	7	0
38	F	23	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	G	18	0	0	2	0
38	H	65	0	0	4	0
38	I	9	0	0	2	0
38	J	51	0	0	4	0
38	K	58	0	0	6	0
38	L	82	0	0	12	0
38	M	116	0	0	5	0
38	N	63	0	0	10	0
38	O	42	0	0	3	0
38	P	64	0	0	3	0
38	Q	51	0	0	3	0
38	R	84	0	0	3	0
38	S	30	0	0	1	0
38	T	42	0	0	2	0
38	U	29	0	0	2	0
38	V	14	0	0	1	0
38	W	68	0	0	2	0
38	X	27	0	0	2	0
38	Y	96	0	0	5	0
38	Z	32	0	0	2	0
All	All	99063	0	59977	2271	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 2271 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:H:46:GLN:HB3	11:H:167:PRO:HD2	1.28	1.16
5:B:62:ARG:HA	5:B:65:MET:HE3	1.29	1.14
1:0:156:C:H5''	15:M:171:ARG:HD3	1.29	1.14
1:0:1160:G:H5'	1:0:1161:A:H5'	1.20	1.11
1:0:1242:A:H5'	12:J:82:THR:HG23	1.34	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/240 (98%)	210 (89%)	21 (9%)	4 (2%)	14	22
5	B	335/338 (99%)	298 (89%)	31 (9%)	6 (2%)	13	20
6	C	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	43	66
7	D	134/177 (76%)	101 (75%)	23 (17%)	10 (8%)	2	1
8	E	170/178 (96%)	158 (93%)	12 (7%)	0	100	100
9	F	117/120 (98%)	108 (92%)	3 (3%)	6 (5%)	3	3
10	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
11	H	156/171 (91%)	145 (93%)	8 (5%)	3 (2%)	12	19
12	J	140/145 (97%)	131 (94%)	7 (5%)	2 (1%)	16	27
13	K	130/132 (98%)	116 (89%)	11 (8%)	3 (2%)	10	14
14	L	141/165 (86%)	121 (86%)	16 (11%)	4 (3%)	8	10
15	M	192/194 (99%)	183 (95%)	9 (5%)	0	100	100
16	N	184/187 (98%)	165 (90%)	12 (6%)	7 (4%)	5	6
17	O	113/116 (97%)	107 (95%)	5 (4%)	1 (1%)	25	42
18	P	141/149 (95%)	138 (98%)	2 (1%)	1 (1%)	30	50
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
21	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	25	42
23	U	51/66 (77%)	46 (90%)	5 (10%)	0	100	100
24	V	63/71 (89%)	57 (90%)	4 (6%)	2 (3%)	6	8
25	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	30	50
26	X	80/92 (87%)	70 (88%)	9 (11%)	1 (1%)	18	29
27	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	9 (13%)	2 (3%)	8	10
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	9	13
31	3	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	10	15
32	I	68/162 (42%)	50 (74%)	17 (25%)	1 (2%)	15	25
All	All	3705/4430 (84%)	3373 (91%)	273 (7%)	59 (2%)	14	23

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	36	ASP
4	A	37	VAL
5	B	34	GLY
5	B	139	ASP
5	B	184	ASP

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%)	170 (95%)	9 (5%)	34	58
5	B	282/283 (100%)	266 (94%)	16 (6%)	29	50
6	C	193/193 (100%)	178 (92%)	15 (8%)	18	32
7	D	117/148 (79%)	111 (95%)	6 (5%)	33	57
8	E	152/156 (97%)	151 (99%)	1 (1%)	91	98
9	F	93/94 (99%)	93 (100%)	0	100	100
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	124 (94%)	8 (6%)	26	46
12	J	118/121 (98%)	109 (92%)	9 (8%)	19	33
13	K	106/106 (100%)	102 (96%)	4 (4%)	44	71
14	L	113/127 (89%)	107 (95%)	6 (5%)	32	54
15	M	158/158 (100%)	153 (97%)	5 (3%)	51	77
16	N	149/150 (99%)	142 (95%)	7 (5%)	36	61
17	O	93/94 (99%)	89 (96%)	4 (4%)	40	65
18	P	113/117 (97%)	110 (97%)	3 (3%)	57	83
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	71
20	R	117/122 (96%)	115 (98%)	2 (2%)	73	92
21	S	71/74 (96%)	70 (99%)	1 (1%)	78	94
22	T	105/106 (99%)	99 (94%)	6 (6%)	29	50
23	U	44/52 (85%)	44 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	V	51/57 (90%)	49 (96%)	2 (4%)	43	70
25	W	130/130 (100%)	126 (97%)	4 (3%)	52	79
26	X	66/74 (89%)	62 (94%)	4 (6%)	26	46
27	Y	120/196 (61%)	112 (93%)	8 (7%)	23	40
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	86
31	3	79/79 (100%)	77 (98%)	2 (2%)	60	85
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3611 (86%)	2967 (96%)	126 (4%)	41	67

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	J	47	THR
14	L	80	ASP
27	Y	144	ARG
12	J	74	ARG
12	J	131	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	143	ASN
20	R	61	GLN
30	2	18	ASN
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%)	16 (13%)	1 (0%)
3	4	1/8 (12%)	0	0
All	All	2867/3052 (93%)	251 (8%)	33 (1%)

5 of 251 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 33 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1667	A
1	0	2726	U
1	0	1377	C
1	0	1450	C

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	20,22,23	0.69	1 (5%)	24,31,34	0.74	0
1	OMG	0	2588	1,3	24,26,27	0.79	0	32,38,41	5.35	3 (9%)
1	UR3	0	2619	1	20,22,23	0.76	0	23,32,35	0.79	0
1	PSU	0	2621	1	19,21,22	1.16	3 (15%)	23,30,33	1.07	1 (4%)
1	1MA	0	628	1	23,25,26	0.81	0	32,37,40	1.01	1 (3%)
3	5AA	4	76	1,3	24,26,27	1.02	2 (8%)	35,38,41	0.91	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	-	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)
3	4	76	5AA	C3'-N3'	-3.17	1.42	1.47
1	0	2621	PSU	C2-N1	3.15	1.43	1.37
3	4	76	5AA	P-OP1	2.14	1.49	1.46
1	0	2621	PSU	C6-N1	2.12	1.34	1.32
1	0	2587	OMU	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	-29.70	130.14	134.14
3	4	76	5AA	C2-N1-C6	3.36	118.82	111.53
1	0	2588	OMG	C6-N1-C2	3.23	125.15	119.51
1	0	628	1MA	C2-N3-C4	-3.16	110.83	116.23
1	0	2621	PSU	C5-C4-N3	-2.32	114.63	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%)	-0.14	61 (2%) 59 61	24, 49, 93, 155	0
2	9	122/122 (100%)	0.07	5 (4%) 35 36	45, 66, 91, 152	0
3	4	8/8 (100%)	-0.28	0 100 100	41, 45, 49, 60	0
4	A	237/240 (98%)	0.28	11 (4%) 31 32	30, 51, 89, 114	0
5	B	337/338 (99%)	0.26	10 (2%) 48 50	31, 61, 90, 100	0
6	C	246/246 (100%)	-0.05	3 (1%) 75 77	28, 48, 71, 82	0
7	D	140/177 (79%)	2.28	67 (47%) 1 0	59, 106, 130, 136	0
8	E	172/178 (96%)	1.08	28 (16%) 2 2	52, 76, 101, 111	0
9	F	119/120 (99%)	0.89	21 (17%) 2 2	52, 74, 100, 116	0
10	G	29/348 (8%)	2.32	15 (51%) 0 0	74, 92, 104, 108	0
11	H	160/171 (93%)	0.33	7 (4%) 33 34	42, 60, 91, 100	0
12	J	142/145 (97%)	0.14	0 100 100	40, 56, 77, 99	0
13	K	132/132 (100%)	0.12	1 (0%) 83 84	35, 58, 80, 85	0
14	L	145/165 (87%)	0.78	29 (20%) 2 1	28, 69, 114, 127	0
15	M	194/194 (100%)	-0.07	1 (0%) 88 90	32, 43, 59, 66	0
16	N	186/187 (99%)	0.76	33 (17%) 2 2	40, 64, 113, 119	0
17	O	115/116 (99%)	0.20	2 (1%) 67 69	39, 58, 75, 90	0
18	P	143/149 (95%)	0.34	5 (3%) 42 43	43, 58, 70, 78	0
19	Q	95/96 (98%)	0.12	3 (3%) 45 47	38, 47, 60, 72	0
20	R	150/155 (96%)	-0.07	0 100 100	33, 48, 65, 76	0
21	S	81/85 (95%)	0.17	2 (2%) 54 57	45, 59, 78, 88	0
22	T	119/120 (99%)	0.43	5 (4%) 35 36	40, 58, 85, 96	0
23	U	53/66 (80%)	0.29	2 (3%) 38 40	46, 62, 76, 86	0
24	V	65/71 (91%)	1.43	14 (21%) 1 1	56, 76, 112, 120	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	0.05	1 (0%) 86 88	39, 55, 74, 86	0
26	X	82/92 (89%)	0.61	9 (10%) 6 6	46, 63, 85, 101	0
27	Y	142/241 (58%)	0.25	8 (5%) 24 24	30, 49, 70, 92	0
28	Z	73/83 (87%)	0.19	3 (4%) 35 36	46, 60, 76, 94	0
29	1	56/57 (98%)	-0.41	0 100 100	27, 34, 39, 52	0
30	2	46/50 (92%)	1.53	15 (32%) 1 1	36, 65, 120, 122	0
31	3	92/92 (100%)	0.27	4 (4%) 34 35	35, 55, 71, 87	0
32	I	70/162 (43%)	4.04	56 (80%) 0 0	108, 126, 148, 149	0
All	All	6659/7482 (89%)	0.22	421 (6%) 20 19	24, 55, 103, 155	0

The worst 5 of 421 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	133	THR	13.5
32	I	96	PHE	13.0
24	V	1	THR	11.6
32	I	102	VAL	10.9
32	I	93	GLN	10.3

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
1	UR3	0	2619	21/22	0.14	2.43	33,38,40,43	0
1	1MA	0	628	23/24	0.15	0.38	31,35,37,38	0
1	OMU	0	2587	21/22	0.12	-0.40	31,34,37,38	0
1	OMG	0	2588	24/25	0.12	-0.42	30,34,37,38	0
3	5AA	4	76	24/25	0.12	-0.79	39,44,45,46	0
1	PSU	0	2621	20/21	0.11	-1.77	28,31,39,40	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	B	9158	1/1	0.96	104.90	69,69,69,69	0
35	NA	0	9118	1/1	0.16	53.89	54,54,54,54	0
33	MG	0	8092	1/1	0.39	32.09	95,95,95,95	0
35	NA	0	9160	1/1	0.32	26.46	41,41,41,41	0
35	NA	0	9161	1/1	0.25	21.85	49,49,49,49	0
35	NA	0	9171	1/1	0.23	20.16	60,60,60,60	0
36	CL	0	9322	1/1	0.40	19.64	76,76,76,76	0
35	NA	0	9121	1/1	0.41	18.61	50,50,50,50	0
35	NA	0	9174	1/1	0.24	16.27	59,59,59,59	0
33	MG	0	8087	1/1	0.19	16.07	57,57,57,57	0
33	MG	0	8049	1/1	0.30	14.43	90,90,90,90	0
35	NA	L	9180	1/1	0.44	14.17	50,50,50,50	0
35	NA	0	9185	1/1	0.32	14.06	60,60,60,60	0
35	NA	0	9175	1/1	0.26	13.87	42,42,42,42	0
35	NA	0	9142	1/1	0.18	13.71	52,52,52,52	0
34	K	0	9003	1/1	0.29	13.64	82,82,82,82	0
35	NA	0	9178	1/1	0.30	12.84	53,53,53,53	0
33	MG	0	8085	1/1	0.22	12.81	93,93,93,93	0
35	NA	0	9170	1/1	0.34	11.92	61,61,61,61	0
35	NA	0	9162	1/1	0.28	10.77	58,58,58,58	0
35	NA	S	9112	1/1	0.55	10.76	76,76,76,76	0
35	NA	0	9152	1/1	0.20	9.98	60,60,60,60	0
35	NA	0	9179	1/1	0.20	9.23	57,57,57,57	0
35	NA	0	9125	1/1	0.21	9.18	64,64,64,64	0
36	CL	0	9315	1/1	0.20	8.77	69,69,69,69	0
35	NA	0	9182	1/1	0.25	8.77	74,74,74,74	0
35	NA	0	9163	1/1	0.27	8.26	71,71,71,71	0
35	NA	0	9156	1/1	0.24	7.79	50,50,50,50	0
35	NA	0	9140	1/1	0.23	7.54	49,49,49,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9150	1/1	0.18	7.50	44,44,44,44	0
35	NA	0	9111	1/1	0.23	7.39	65,65,65,65	0
33	MG	0	8041	1/1	0.23	7.30	59,59,59,59	0
35	NA	0	9176	1/1	0.21	7.24	43,43,43,43	0
33	MG	0	8023	1/1	0.17	6.78	53,53,53,53	0
33	MG	0	8016	1/1	0.18	5.97	35,35,35,35	0
35	NA	0	9186	1/1	0.29	5.95	75,75,75,75	0
35	NA	0	9172	1/1	0.24	5.49	59,59,59,59	0
33	MG	0	8060	1/1	0.17	5.01	39,39,39,39	0
35	NA	0	9106	1/1	0.17	4.63	34,34,34,34	0
33	MG	0	8045	1/1	0.21	4.58	65,65,65,65	0
33	MG	0	8094	1/1	0.15	4.49	62,62,62,62	0
33	MG	0	8103	1/1	0.15	4.30	66,66,66,66	0
33	MG	0	8013	1/1	0.21	3.90	33,33,33,33	0
33	MG	0	8090	1/1	0.32	3.31	80,80,80,80	0
35	NA	0	9102	1/1	0.14	3.10	42,42,42,42	0
33	MG	0	8029	1/1	0.17	3.08	32,32,32,32	0
33	MG	0	8047	1/1	0.17	2.97	102,102,102,102	0
33	MG	0	8101	1/1	0.14	2.54	69,69,69,69	0
35	NA	0	9107	1/1	0.13	2.54	43,43,43,43	0
35	NA	0	9177	1/1	0.16	2.41	55,55,55,55	0
35	NA	0	9173	1/1	0.15	2.39	42,42,42,42	0
35	NA	0	9135	1/1	0.16	2.14	43,43,43,43	0
35	NA	0	9155	1/1	0.28	1.99	60,60,60,60	0
35	NA	0	9113	1/1	0.14	1.76	59,59,59,59	0
33	MG	0	8099	1/1	0.14	1.75	59,59,59,59	0
33	MG	0	8082	1/1	0.14	1.74	66,66,66,66	0
35	NA	0	9114	1/1	0.15	1.71	66,66,66,66	0
35	NA	0	9101	1/1	0.15	1.66	46,46,46,46	0
33	MG	B	8055	1/1	0.21	1.62	60,60,60,60	0
33	MG	0	8058	1/1	0.15	1.60	45,45,45,45	0
35	NA	0	9159	1/1	0.15	1.57	50,50,50,50	0
35	NA	0	9129	1/1	0.12	1.50	53,53,53,53	0
35	NA	0	9184	1/1	0.14	1.33	75,75,75,75	0
35	NA	0	9134	1/1	0.15	1.30	34,34,34,34	0
35	NA	0	9165	1/1	0.22	1.11	39,39,39,39	0
33	MG	0	8038	1/1	0.15	1.10	28,28,28,28	0
35	NA	H	9122	1/1	0.21	1.09	77,77,77,77	0
35	NA	0	9127	1/1	0.14	0.86	39,39,39,39	0
33	MG	0	8012	1/1	0.14	0.85	35,35,35,35	0
33	MG	0	8072	1/1	0.15	0.46	51,51,51,51	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	9133	1/1	0.13	0.42	27,27,27,27	0
33	MG	0	8053	1/1	0.13	0.27	51,51,51,51	0
33	MG	0	8066	1/1	0.14	0.27	114,114,114,114	0
33	MG	0	8036	1/1	0.12	0.09	39,39,39,39	0
33	MG	0	8025	1/1	0.12	0.05	48,48,48,48	0
35	NA	0	9166	1/1	0.12	0.04	77,77,77,77	0
35	NA	0	9169	1/1	0.14	0.04	46,46,46,46	0
33	MG	0	8026	1/1	0.12	-0.01	24,24,24,24	0
35	NA	0	9126	1/1	0.13	-0.04	40,40,40,40	0
33	MG	0	8062	1/1	0.11	-0.18	53,53,53,53	0
35	NA	A	9145	1/1	0.16	-0.24	39,39,39,39	0
33	MG	0	8028	1/1	0.14	-0.28	43,43,43,43	0
35	NA	0	9116	1/1	0.12	-0.32	36,36,36,36	0
35	NA	0	9120	1/1	0.12	-0.32	56,56,56,56	0
33	MG	0	8032	1/1	0.14	-0.41	39,39,39,39	0
33	MG	0	8020	1/1	0.14	-0.42	32,32,32,32	0
33	MG	0	8114	1/1	0.11	-0.47	64,64,64,64	0
35	NA	0	9115	1/1	0.12	-0.50	37,37,37,37	0
35	NA	0	9117	1/1	0.21	-0.67	72,72,72,72	0
33	MG	0	8070	1/1	0.11	-0.68	53,53,53,53	0
33	MG	B	8056	1/1	0.15	-0.71	49,49,49,49	0
35	NA	0	9141	1/1	0.09	-0.75	46,46,46,46	0
35	NA	0	9168	1/1	0.10	-0.77	52,52,52,52	0
33	MG	0	8018	1/1	0.11	-0.78	40,40,40,40	0
33	MG	0	8104	1/1	0.12	-0.87	53,53,53,53	0
35	NA	0	9124	1/1	0.09	-0.88	59,59,59,59	0
33	MG	0	8027	1/1	0.10	-0.92	44,44,44,44	0
35	NA	0	9138	1/1	0.10	-1.01	51,51,51,51	0
37	CD	3	9204	1/1	0.10	-1.02	62,62,62,62	0
35	NA	H	9109	1/1	0.10	-1.03	31,31,31,31	0
33	MG	0	8048	1/1	0.12	-1.04	60,60,60,60	0
33	MG	0	8079	1/1	0.11	-1.05	28,28,28,28	0
33	MG	0	8034	1/1	0.12	-1.06	39,39,39,39	0
35	NA	9	9183	1/1	0.12	-1.09	55,55,55,55	0
33	MG	0	8086	1/1	0.06	-1.09	50,50,50,50	0
33	MG	0	8081	1/1	0.12	-1.15	43,43,43,43	0
35	NA	0	9119	1/1	0.11	-1.17	42,42,42,42	0
36	CL	0	9303	1/1	0.12	-1.22	54,54,54,54	0
33	MG	0	8097	1/1	0.11	-1.24	45,45,45,45	0
35	NA	J	9146	1/1	0.11	-1.25	37,37,37,37	0
35	NA	Q	9148	1/1	0.13	-1.25	36,36,36,36	0
36	CL	J	9301	1/1	0.09	-1.27	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	O	9308	1/1	0.10	-1.27	68,68,68,68	0
36	CL	0	9311	1/1	0.10	-1.30	51,51,51,51	0
36	CL	J	9321	1/1	0.10	-1.31	54,54,54,54	0
35	NA	0	9167	1/1	0.09	-1.36	40,40,40,40	0
35	NA	9	9151	1/1	0.14	-1.52	76,76,76,76	0
37	CD	Z	9203	1/1	0.08	-1.54	61,61,61,61	0
36	CL	A	9309	1/1	0.14	-1.61	58,58,58,58	0
33	MG	0	8106	1/1	0.07	-1.62	51,51,51,51	0
36	CL	B	9319	1/1	0.11	-1.66	47,47,47,47	0
33	MG	A	8065	1/1	0.11	-1.67	42,42,42,42	0
33	MG	0	8015	1/1	0.10	-1.67	30,30,30,30	0
35	NA	0	9110	1/1	0.10	-1.69	37,37,37,37	0
33	MG	0	8064	1/1	0.09	-1.71	25,25,25,25	0
35	NA	M	9147	1/1	0.09	-1.79	18,18,18,18	0
33	MG	0	8030	1/1	0.11	-1.79	35,35,35,35	0
35	NA	0	9181	1/1	0.09	-1.80	51,51,51,51	0
36	CL	0	9314	1/1	0.08	-1.81	50,50,50,50	0
36	CL	0	9316	1/1	0.09	-1.86	56,56,56,56	0
36	CL	0	9313	1/1	0.11	-1.86	62,62,62,62	0
35	NA	0	9157	1/1	0.07	-1.87	60,60,60,60	0
36	CL	L	9310	1/1	0.08	-1.88	58,58,58,58	0
33	MG	0	8107	1/1	0.07	-1.88	45,45,45,45	0
35	NA	C	9104	1/1	0.07	-1.89	32,32,32,32	0
33	MG	0	8011	1/1	0.11	-1.91	23,23,23,23	0
37	CD	U	9201	1/1	0.06	-1.94	73,73,73,73	0
35	NA	0	9103	1/1	0.10	-1.96	44,44,44,44	0
33	MG	0	8093	1/1	0.10	-2.00	56,56,56,56	0
33	MG	0	8037	1/1	0.10	-2.03	46,46,46,46	0
33	MG	0	8076	1/1	0.11	-2.06	57,57,57,57	0
35	NA	0	9131	1/1	0.10	-2.11	35,35,35,35	0
33	MG	0	8009	1/1	0.10	-2.14	31,31,31,31	0
33	MG	0	8057	1/1	0.11	-2.18	39,39,39,39	0
33	MG	0	8102	1/1	0.09	-2.20	51,51,51,51	0
33	MG	0	8003	1/1	0.12	-2.25	26,26,26,26	0
36	CL	N	9307	1/1	0.12	-2.29	61,61,61,61	0
33	MG	0	8014	1/1	0.10	-2.31	42,42,42,42	0
33	MG	0	8098	1/1	0.10	-2.32	45,45,45,45	0
35	NA	0	9153	1/1	0.09	-2.32	17,17,17,17	0
33	MG	0	8100	1/1	0.10	-2.35	68,68,68,68	0
33	MG	9	8095	1/1	0.10	-2.35	72,72,72,72	0
35	NA	R	9137	1/1	0.07	-2.36	42,42,42,42	0
33	MG	0	8019	1/1	0.08	-2.38	33,33,33,33	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	0	8017	1/1	0.07	-2.51	31,31,31,31	0
33	MG	0	8074	1/1	0.07	-2.53	34,34,34,34	0
33	MG	0	8077	1/1	0.11	-2.53	29,29,29,29	0
36	CL	M	9318	1/1	0.09	-2.56	36,36,36,36	0
36	CL	J	9302	1/1	0.09	-2.61	70,70,70,70	0
35	NA	0	9108	1/1	0.10	-2.70	48,48,48,48	0
37	CD	O	9205	1/1	0.07	-2.71	137,137,137,137	0
36	CL	3	9304	1/1	0.07	-2.73	47,47,47,47	0
33	MG	0	8005	1/1	0.10	-2.73	24,24,24,24	0
33	MG	0	8084	1/1	0.10	-2.81	40,40,40,40	0
33	MG	0	8067	1/1	0.11	-2.83	52,52,52,52	0
33	MG	0	8118	1/1	0.09	-2.89	63,63,63,63	0
36	CL	R	9306	1/1	0.08	-2.89	53,53,53,53	0
36	CL	0	9305	1/1	0.07	-2.90	52,52,52,52	0
35	NA	0	9128	1/1	0.07	-2.92	40,40,40,40	0
33	MG	0	8039	1/1	0.08	-2.95	49,49,49,49	0
33	MG	0	8007	1/1	0.09	-2.95	23,23,23,23	0
33	MG	0	8035	1/1	0.07	-2.97	50,50,50,50	0
35	NA	0	9105	1/1	0.10	-3.04	35,35,35,35	0
33	MG	0	8096	1/1	0.07	-3.24	38,38,38,38	0
33	MG	0	8001	1/1	0.07	-3.25	36,36,36,36	0
33	MG	T	8073	1/1	0.04	-3.30	49,49,49,49	0
36	CL	0	9312	1/1	0.06	-3.31	52,52,52,52	0
35	NA	0	9130	1/1	0.05	-3.33	36,36,36,36	0
33	MG	0	8031	1/1	0.07	-3.41	30,30,30,30	0
37	CD	1	9202	1/1	0.02	-3.44	54,54,54,54	0
33	MG	0	8050	1/1	0.07	-3.49	63,63,63,63	0
33	MG	0	8068	1/1	0.05	-3.53	58,58,58,58	0
35	NA	0	9154	1/1	0.08	-3.62	26,26,26,26	0
34	K	0	9001	1/1	0.10	-3.63	66,66,66,66	0
35	NA	0	9123	1/1	0.11	-3.66	52,52,52,52	0
33	MG	3	8078	1/1	0.06	-3.70	46,46,46,46	0
33	MG	0	8111	1/1	0.06	-3.73	57,57,57,57	0
35	NA	0	9132	1/1	0.06	-3.92	29,29,29,29	0
33	MG	0	8021	1/1	0.11	-3.96	25,25,25,25	0
33	MG	0	8054	1/1	0.10	-4.03	24,24,24,24	0
33	MG	Y	8109	1/1	0.07	-4.07	40,40,40,40	0
33	MG	4	8119	1/1	0.08	-4.20	41,41,41,41	0
33	MG	0	8061	1/1	0.10	-4.26	34,34,34,34	0
33	MG	0	8108	1/1	0.06	-4.44	56,56,56,56	0
36	CL	0	9320	1/1	0.09	-4.49	48,48,48,48	0
35	NA	0	9164	1/1	0.10	-4.51	52,52,52,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	T	9143	1/1	0.06	-4.56	31,31,31,31	0
35	NA	0	9144	1/1	0.04	-4.57	35,35,35,35	0
33	MG	0	8044	1/1	0.07	-4.61	47,47,47,47	0
33	MG	0	8116	1/1	0.06	-4.68	50,50,50,50	0
35	NA	0	9149	1/1	0.07	-4.74	36,36,36,36	0
33	MG	0	8080	1/1	0.07	-4.83	37,37,37,37	0
33	MG	0	8112	1/1	0.05	-5.00	37,37,37,37	0
36	CL	0	9317	1/1	0.04	-5.19	61,61,61,61	0
33	MG	0	8024	1/1	0.08	-5.31	49,49,49,49	0
33	MG	0	8063	1/1	0.07	-5.39	53,53,53,53	0
33	MG	0	8008	1/1	0.07	-5.49	35,35,35,35	0
33	MG	0	8004	1/1	0.06	-5.74	33,33,33,33	0
33	MG	0	8033	1/1	0.07	-5.78	39,39,39,39	0
33	MG	0	8022	1/1	0.05	-5.88	35,35,35,35	0
34	K	0	9002	1/1	0.06	-6.01	43,43,43,43	0
33	MG	0	8091	1/1	0.06	-6.49	74,74,74,74	0
33	MG	9	8052	1/1	0.05	-6.91	50,50,50,50	0
33	MG	0	8088	1/1	0.05	-7.01	39,39,39,39	0
35	NA	0	9139	1/1	0.06	-7.08	22,22,22,22	0
33	MG	0	8002	1/1	0.03	-7.28	28,28,28,28	0
33	MG	0	8083	1/1	0.06	-7.56	35,35,35,35	0
33	MG	0	8051	1/1	0.08	-7.60	56,56,56,56	0
35	NA	0	9136	1/1	0.07	-7.80	53,53,53,53	0
33	MG	0	8071	1/1	0.07	-8.02	53,53,53,53	0
33	MG	0	8059	1/1	0.09	-8.18	51,51,51,51	0
33	MG	0	8117	1/1	0.07	-8.55	32,32,32,32	0
33	MG	0	8043	1/1	0.07	-8.89	42,42,42,42	0
33	MG	K	8069	1/1	0.08	-10.24	41,41,41,41	0
33	MG	0	8010	1/1	0.06	-10.46	30,30,30,30	0
33	MG	0	8046	1/1	0.04	-10.69	52,52,52,52	0
33	MG	0	8042	1/1	0.06	-11.09	45,45,45,45	0
33	MG	0	8006	1/1	0.07	-11.47	32,32,32,32	0
33	MG	0	8089	1/1	0.06	-12.17	60,60,60,60	0
33	MG	0	8075	1/1	0.04	-12.50	39,39,39,39	0
33	MG	0	8040	1/1	0.08	-13.63	45,45,45,45	0
33	MG	0	8110	1/1	0.04	-14.51	34,34,34,34	0
33	MG	0	8115	1/1	0.08	-20.50	52,52,52,52	0
33	MG	0	8113	1/1	0.09	-57.00	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.