



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 17, 2020 – 06:47 PM EDT

PDB ID : 1VQM
Title : The structure of the transition state analogue "DAN" bound to the large ribosomal subunit of haloarcula marismortui
Authors : Schmeing, T.M.; Steitz, T.A.
Deposited on : 2004-12-16
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.4
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.4

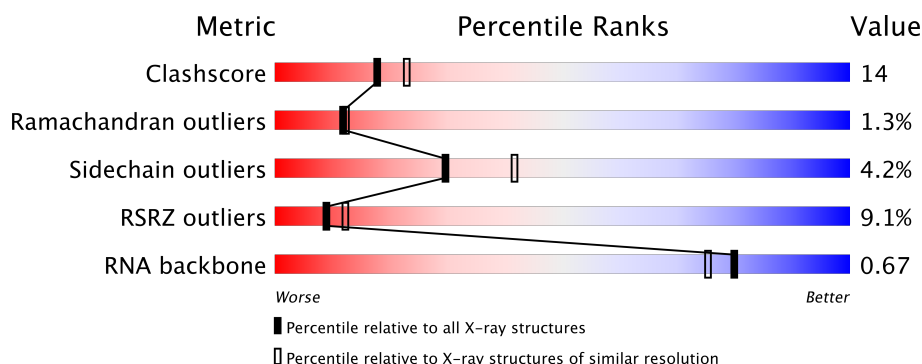
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)
RNA backbone	3102	1090 (2.70-1.90)

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

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>25%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>10%</div> <div>.</div> </div> </div>
3	4	7	<div> <div></div> <div> <div></div> <div>57%</div> <div>29%</div> <div>14%</div> </div> </div>
4	A	240	<div> <div>8%</div> <div> <div></div> <div>59%</div> <div>36%</div> <div>.</div> <div>.</div> </div> </div>
5	B	338	<div> <div>4%</div> <div> <div></div> <div>56%</div> <div>41%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
15	M	195	
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	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	3	92	
32	I	162	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	MG	0	8014	-	-	-	X
33	MG	0	8022	-	-	-	X
33	MG	0	8040	-	-	-	X
33	MG	0	8047	-	-	-	X
33	MG	0	8052	-	-	-	X
33	MG	0	8065	-	-	-	X
33	MG	0	8094	-	-	-	X
35	NA	0	9140	-	-	-	X
35	NA	0	9179	-	-	-	X
35	NA	0	9185	-	-	-	X
37	SR	0	9500	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99045 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S ribosomal rna.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			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*(PPU)P*(PO2)P*(DA)P*C*C')-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	7	Total	C	N	O	P	0	0	0
			135	68	24	38	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	87	Total	Mg	0	0
			87	87		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	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	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	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	62	Total Na 62 62	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	3	1	Total Na 1 1	0	0
35	R	3	Total Na 3 3	0	0
35	9	3	Total Na 3 3	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
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0
36	Y	1	Total Cl 1 1	0	0
36	L	1	Total Cl 1 1	0	0
36	3	1	Total Cl 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	M	1	Total	Cl	0	0
			1	1		

- Molecule 37 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	98	Total	Sr	0	0
			98	98		
37	1	2	Total	Sr	0	0
			2	2		
37	H	1	Total	Sr	0	0
			1	1		
37	B	2	Total	Sr	0	0
			2	2		
37	3	1	Total	Sr	0	0
			1	1		
37	A	3	Total	Sr	0	0
			3	3		
37	R	1	Total	Sr	0	0
			1	1		
37	9	3	Total	Sr	0	0
			3	3		
37	L	1	Total	Sr	0	0
			1	1		
37	S	1	Total	Sr	0	0
			1	1		
37	F	1	Total	Sr	0	0
			1	1		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5739	Total 5739	O 5739	0	0
39	9	132	Total 132	O 132	0	0
39	4	8	Total 8	O 8	0	0
39	A	123	Total 123	O 123	0	0
39	B	139	Total 139	O 139	0	0
39	C	177	Total 177	O 177	0	0
39	D	50	Total 50	O 50	0	0
39	E	43	Total 43	O 43	0	0
39	F	28	Total 28	O 28	0	0
39	G	16	Total 16	O 16	0	0
39	H	71	Total 71	O 71	0	0
39	J	53	Total 53	O 53	0	0
39	K	57	Total 57	O 57	0	0
39	L	82	Total 82	O 82	0	0
39	M	125	Total 125	O 125	0	0
39	N	59	Total 59	O 59	0	0
39	O	35	Total 35	O 35	0	0
39	P	59	Total 59	O 59	0	0
39	Q	48	Total 48	O 48	0	0
39	R	86	Total 86	O 86	0	0
39	S	31	Total 31	O 31	0	0

Continued on next page...

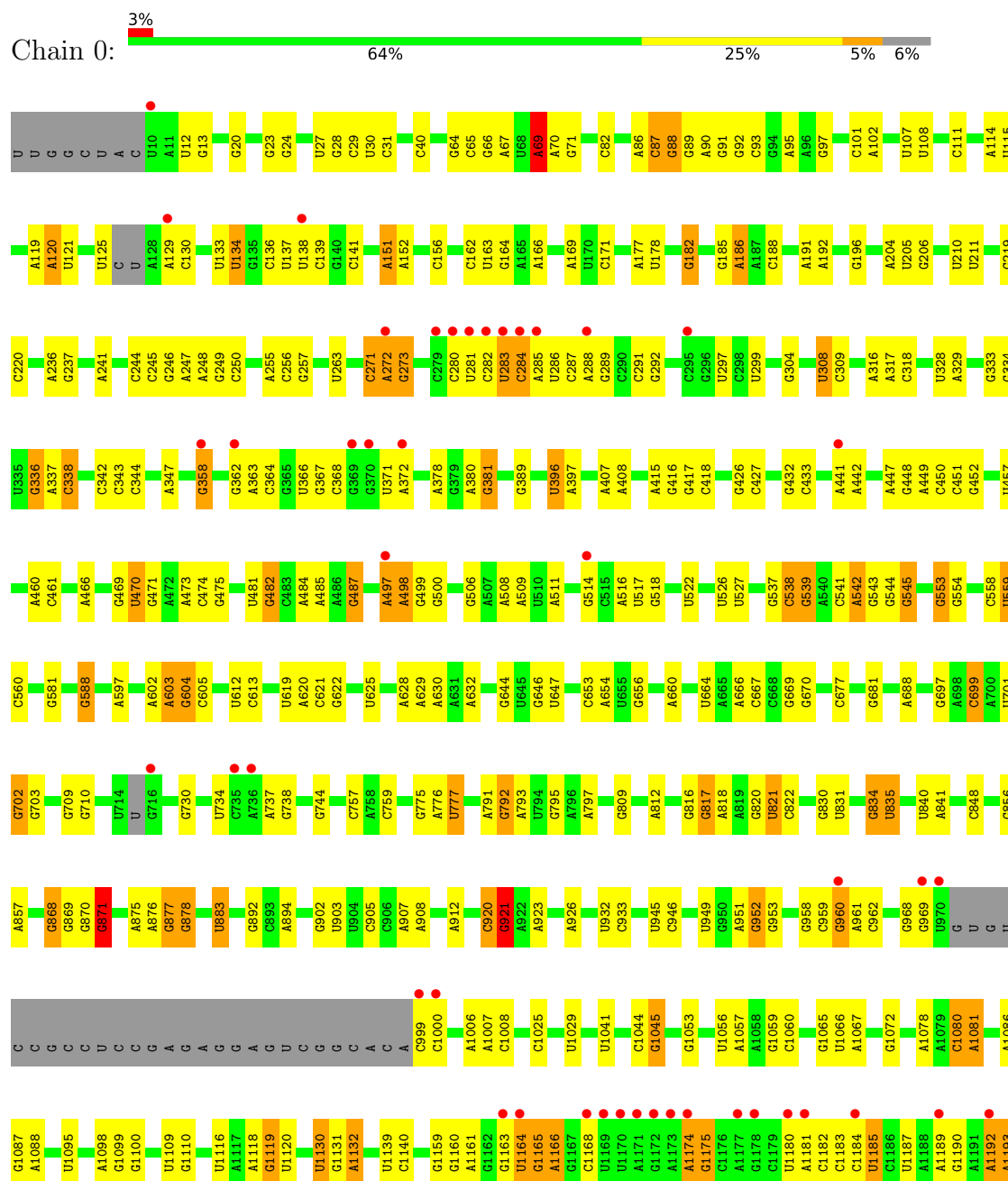
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	T	36	Total 36	O 36	0	0
39	U	26	Total 26	O 26	0	0
39	V	11	Total 11	O 11	0	0
39	W	68	Total 68	O 68	0	0
39	X	23	Total 23	O 23	0	0
39	Y	93	Total 93	O 93	0	0
39	Z	28	Total 28	O 28	0	0
39	1	51	Total 51	O 51	0	0
39	2	41	Total 41	O 41	0	0
39	3	67	Total 67	O 67	0	0
39	I	9	Total 9	O 9	0	0

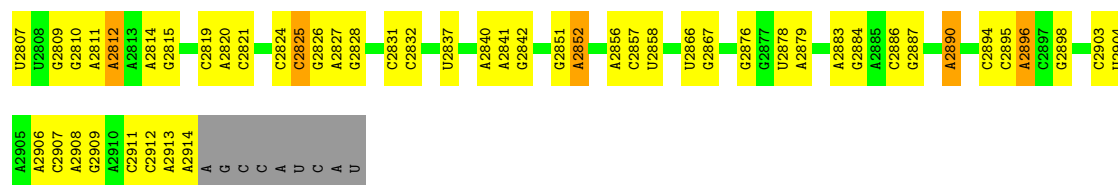
3 Residue-property plots

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

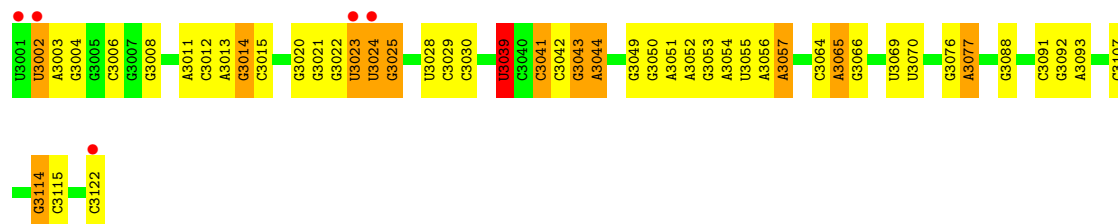
- Molecule 1: 23S ribosomal rna



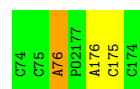
C9682	U2566	G2480	A2354	C	A	A2089	C	U1838	A1716	G1592	G1415	A1294	C1196
U2690	U2587	G2481	G2355	C	C	G2090	C	A1839	A1717	G1593	G1418	A1298	G1197
A2694	G2588	G2482	A2356	A	A	G2091	C	A1840	U1722	C1594	U1418	U1298	U1198
G2698	U2589	G2483	G2357	G	G	A2096	C	A1845	G1723	G1595	U1419	G1299	A1199
A2699	G2590	G2484	A2361	U	U	A2101	C	A1846	U1724	U1596	U1422	U1304	A1200
G2700	G2591	G2485	A2362	A	A	A2102	C	A1847	C1725	A1597	C1423	C1305	C1201
G2712	G2592	G2486	G2363	C	C	A2103	C	A1848	G1730	A1598	U1426	G1311	A1202
G2716	U2597	G2487	A2364	C	C	G2102	C	G1849	A1731	C1602	U1435	U1314	C1203
C2717	U2598	G2488	G2365	C	C	A2103	C	G1853	A1732	A1603	U1436	G1315	U1204
A2718	A2600	G2489	A2366	C	C	G2110	C	C1856	U1733	G1604	U1437	U1316	U1205
G2719	A2601	G2490	A2367	C	C	A2112	C	G1863	A1736	G1605	U1438	G1317	U1206
A2720	G2602	G2491	G2368	U	U	G2113	C	G1868	U1741	A1615	G1441	G1318	A1207
U2721	U2607	G2492	A2369	A	A	G2114	C	G1869	U1742	A1616	A1442	G1319	C1208
U2722	C2608	G2493	A2370	C	C	U2115	C	G1870	G1745	C1617	U1443	U1320	G1210
G2723	G2613	G2494	A2371	G	G	U2116	C	G1871	U1754	A1624	U1444	G1321	G1211
U2724	U2619	G2495	A2372	C	C	G2134	C	G1872	G1755	U1625	U1445	A1328	C1212
G2725	U2620	G2496	A2373	C	C	A2136	C	G1873	C1752	A1626	U1446	U1329	G1216
U2726	U2621	G2497	A2374	C	C	G2137	C	G1874	A1756	G1627	U1447	A1331	G1217
A2727	C2626	G2498	A2375	C	C	A	C	G1875	A1757	U1628	U1448	U1332	U1218
C2747	G2627	G2499	A2376	C	C	C	C	G1876	G1756	A1630	U1449	C1333	U1219
U2748	U2627	G2500	A2377	C	C	U	U	G1877	U1757	A1631	U1450	C1334	U1220
G2749	U2628	G2501	A2378	C	C	G	G	G1878	U1758	U1632	U1451	U1335	G1226
G2750	G2632	G2502	A2379	C	C	C	C	G1879	C1759	U1633	U1452	U1336	C1229
U2760	U2633	G2503	A2380	C	C	U	U	G1880	U1760	G1634	U1453	G1340	A1230
A2761	G2634	G2504	A2381	C	C	C	C	G1881	U1761	U1635	U1454	A1341	A1231
C2762	U2637	G2505	A2382	C	C	G	G	A1919	U1762	A1636	U1455	G1342	A1232
G2765	G2642	G2506	A2383	C	C	A	A	G1920	U1763	U1637	U1456	C1343	A1233
C2766	U2643	G2507	A2384	C	C	C	C	A1921	G1777	A1641	U1457	G1351	U1234
U2767	G2644	G2508	A2385	C	C	U	U	A1922	U1778	A1642	U1458	U1235	G1236
A2768	U2645	G2509	A2386	C	C	U	U	G1923	A1779	U1654	U1459	A1237	U1237
C2769	U2646	G2510	A2387	C	C	C	C	G1924	U1780	G1655	U1460	G1238	G1239
G2770	U2647	G2511	A2388	C	C	A	A	A1940	C1786	A1656	U1503	C1360	A1242
G2779	A2649	G2512	A2389	C	C	A	A	C1941	U1787	A1657	U1504	C1361	G1245
C2780	U2650	G2513	A2390	C	C	C	C	A1942	C1788	A1658	U1505	G1362	C1243
U2781	U2651	G2514	A2391	C	C	U	U	C1943	U1789	U1666	U1506	G1363	U1244
G2782	U2652	G2515	A2392	C	C	A	A	G1944	G1795	U1667	U1524	C1366	A1246
A2783	A2653	G2516	A2393	C	C	U	U	C1945	A1796	U1668	G1525	A1369	U1249
C2784	U2654	G2517	A2394	C	C	A	A	G1946	C1797	A1681	U1526	A1372	U1250
G2785	U2655	G2518	A2395	C	C	C	C	G1947	G1798	G1682	U1527	C1251	C1251
U2786	A2656	G2519	A2396	C	C	U	U	G1948	G1799	A1683	A1528	G1252	C1253
C2787	U2657	G2520	A2397	C	C	U	U	G1949	U1809	A1684	G1552	C1377	C1253
C2790	G2657	G2521	A2398	C	C	C	C	G1950	C1818	C1686	U1553	G1378	U1261
U2791	U2658	G2522	A2399	C	C	U	U	G1951	G1819	C1687	U1554	C1384	A1266
A2792	G2659	G2523	A2400	C	C	A	A	U	G1820	U1689	G1555	U1398	U1267
U2793	U2660	G2524	A2401	C	C	C	C	A	C1829	C1692	U1559	C1267	C1268
G2794	U2661	G2525	A2402	C	C	U	U	C	A1830	U1701	U	C1400	G1269
C2795	U2662	G2526	A2403	C	C	C	C	U	U1702	U1702	A1561	A1406	U1279
U2796	U2663	G2527	A2404	C	C	A	A	A	C1834	C1714	A1573	A1407	U1408
A2800	G2664	G2528	A2405	C	C	U	U	U	U1835	C1574	C1575	U1409	C1289



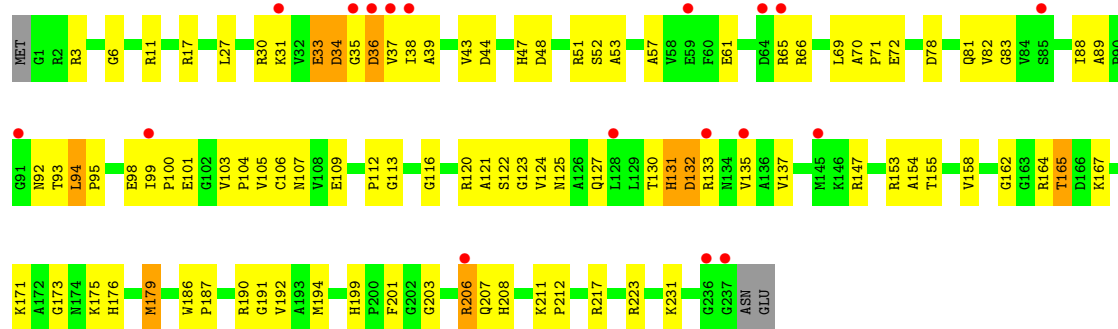
• Molecule 2: 5S ribosomal RNA



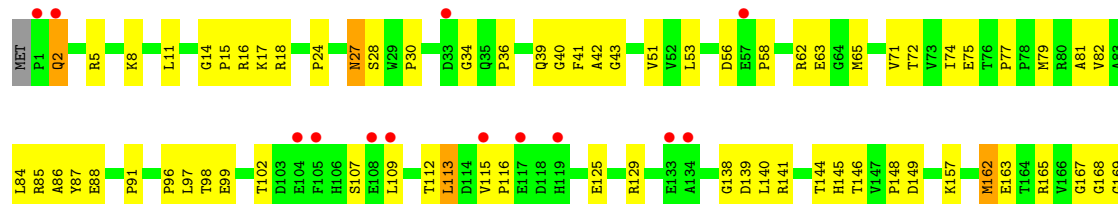
• Molecule 3: 5'-R(*CP*CP*(PPU)P*(PO2)P*(DA)P*C*C)-3'

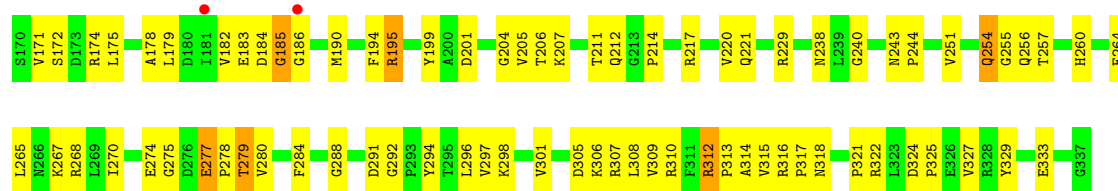


• Molecule 4: 50S ribosomal protein L2P

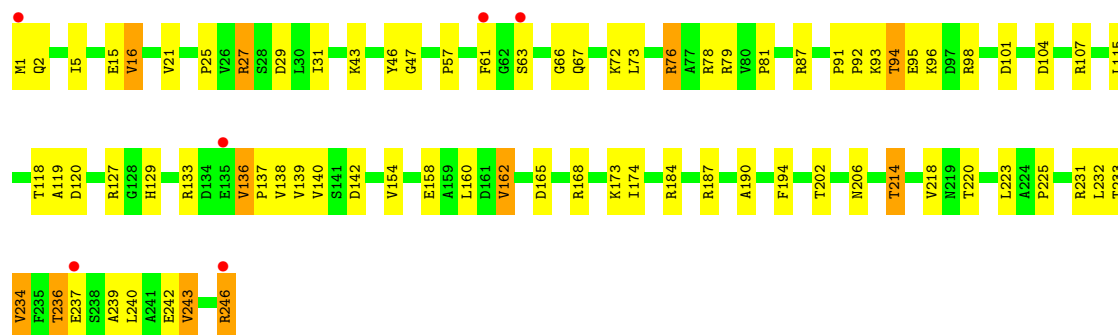


• Molecule 5: 50S ribosomal protein L3P

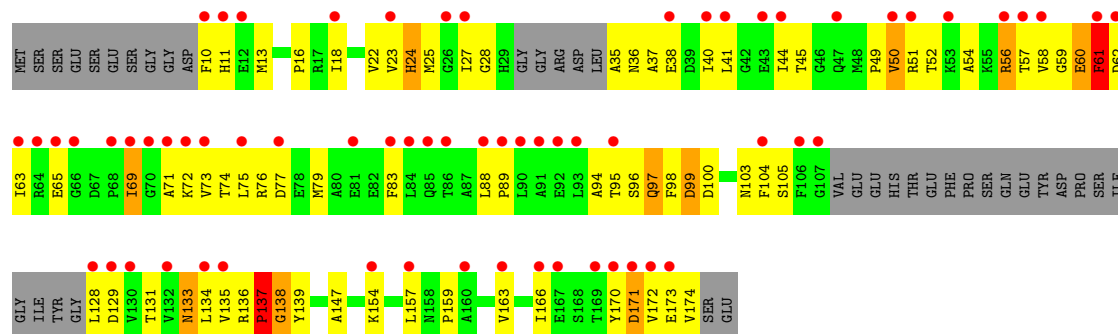




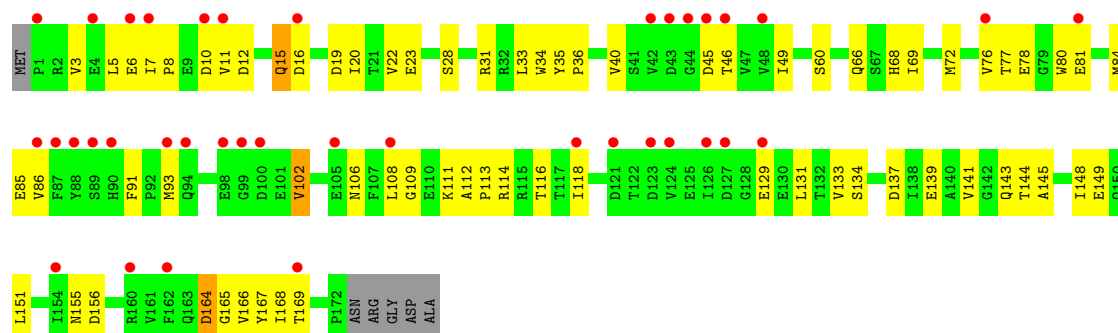
• Molecule 6: 50S ribosomal protein L4E



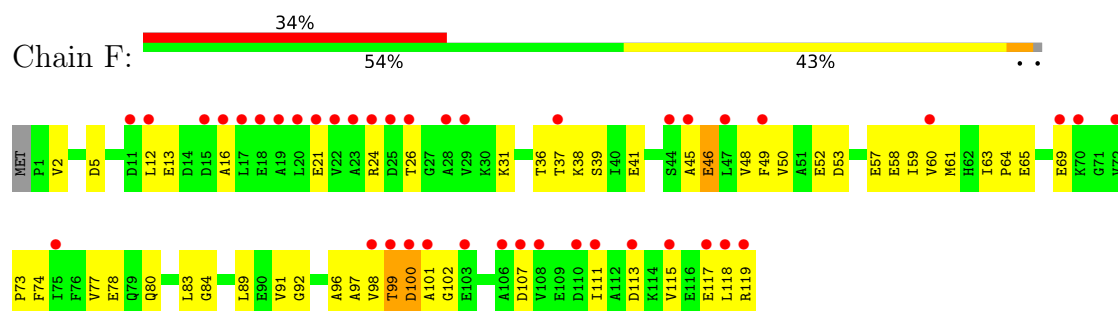
• Molecule 7: 50S ribosomal protein L5P



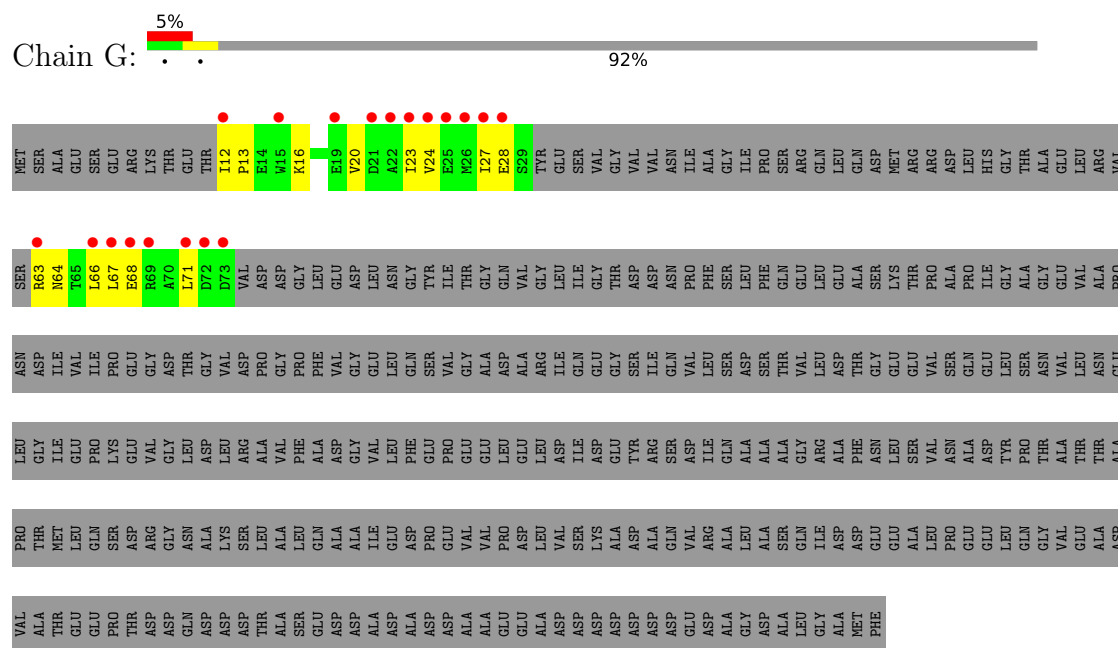
• Molecule 8: 50S ribosomal protein L6P



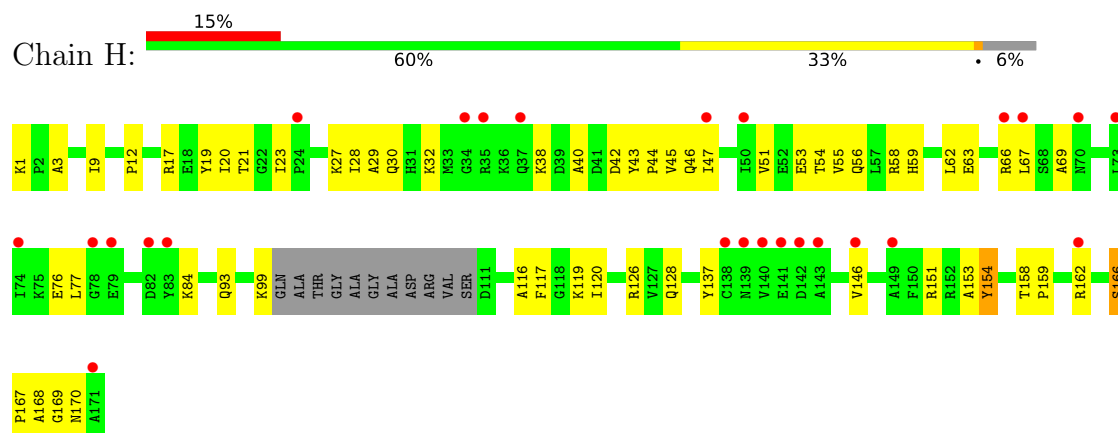
- Molecule 9: 50S ribosomal protein L7AE



- Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG

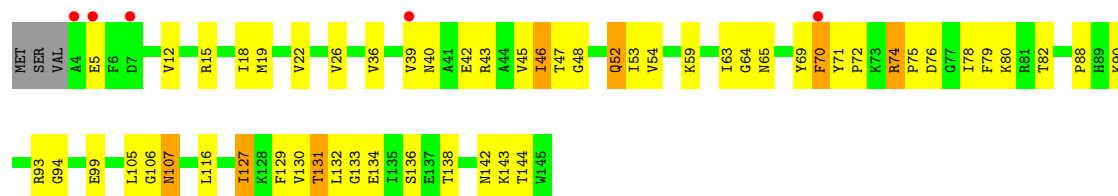


- Molecule 11: 50S RIBOSOMAL PROTEIN L10E

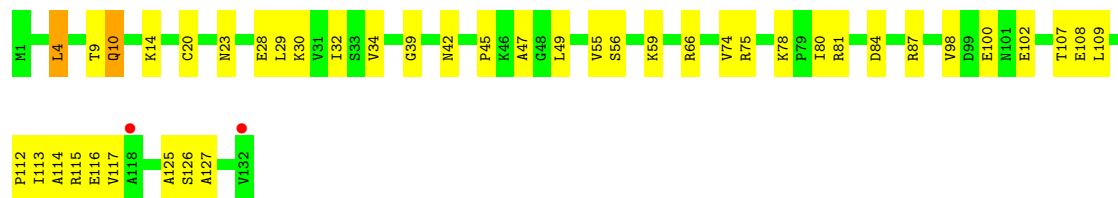


- Molecule 12: 50S ribosomal protein L13P

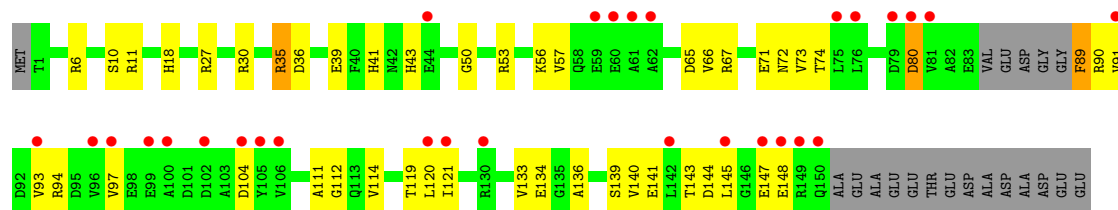




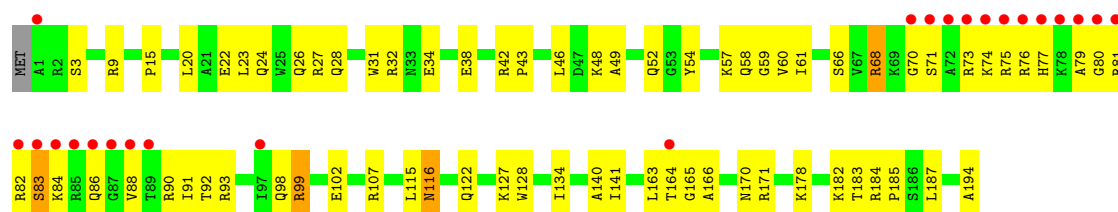
• Molecule 13: 50S ribosomal protein L14P



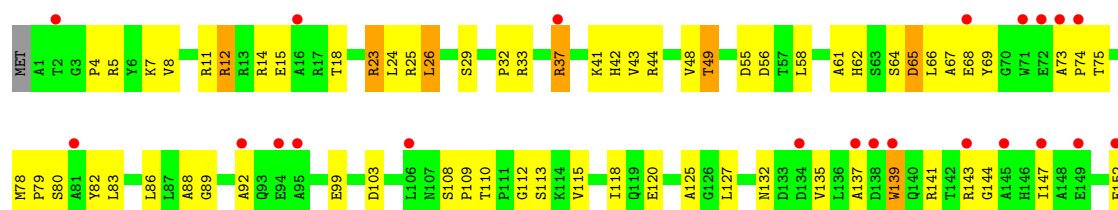
• Molecule 14: 50S ribosomal protein L15P

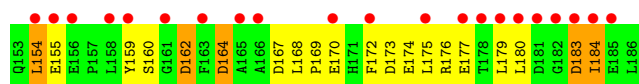


• Molecule 15: 50S Ribosomal Protein L15E



• Molecule 16: 50S ribosomal protein L18P





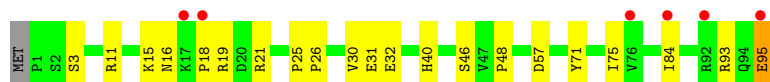
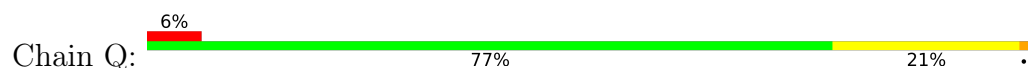
- Molecule 17: 50S ribosomal protein L18e



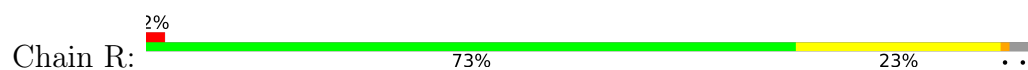
- Molecule 18: 50S ribosomal protein L19E



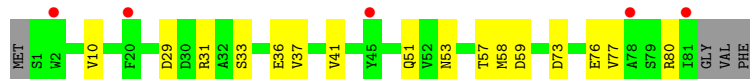
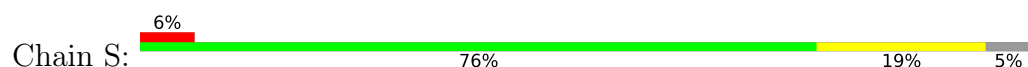
- Molecule 19: 50S ribosomal protein L21e



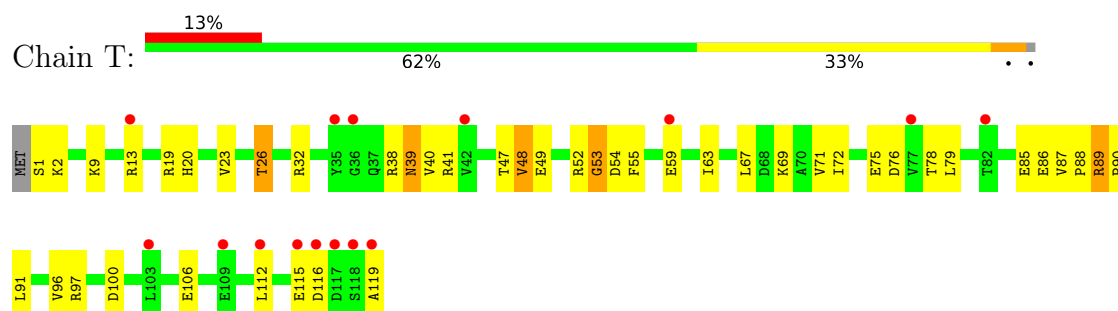
- Molecule 20: 50S ribosomal protein L22P



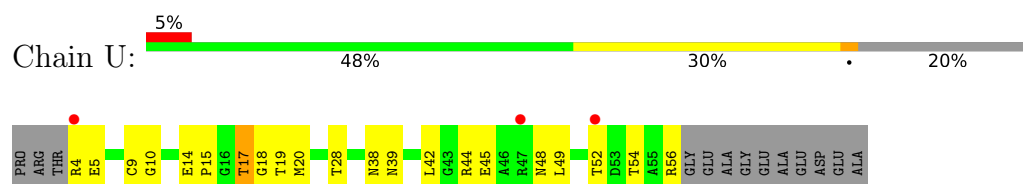
- Molecule 21: 50S ribosomal protein L23P



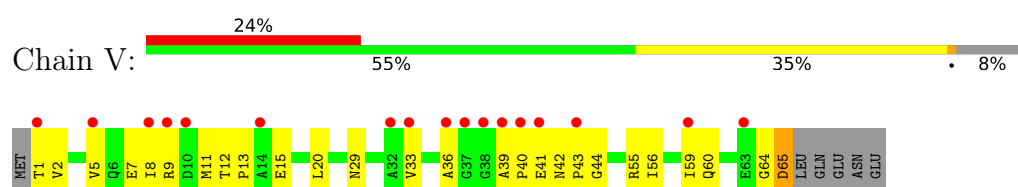
- Molecule 22: 50S ribosomal protein L24P



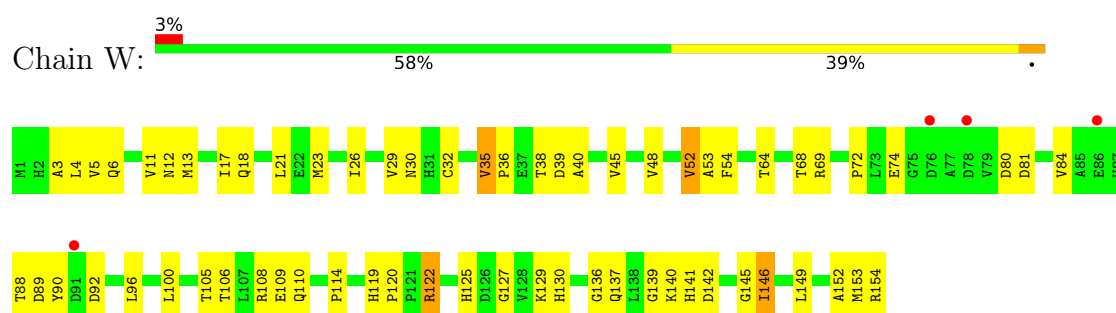
- Molecule 23: 50S ribosomal protein L24E



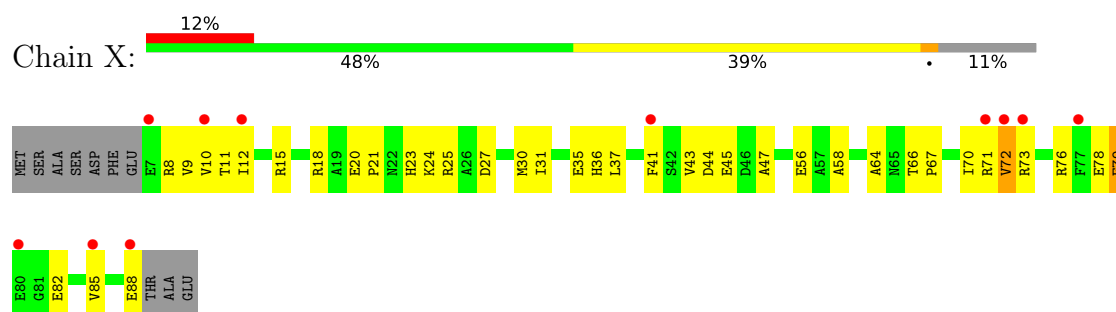
- Molecule 24: 50S ribosomal protein L29P



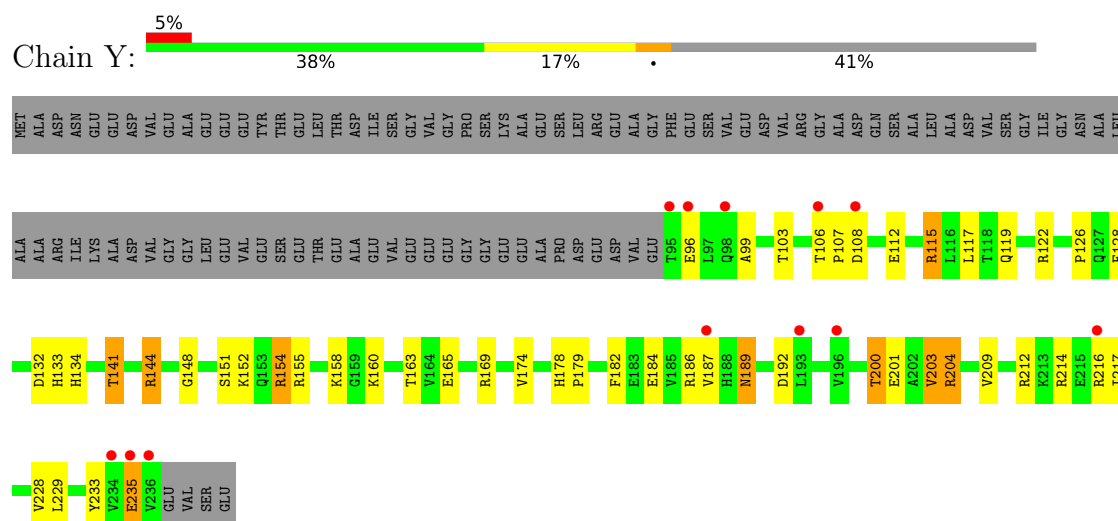
- Molecule 25: 50S ribosomal protein L30P



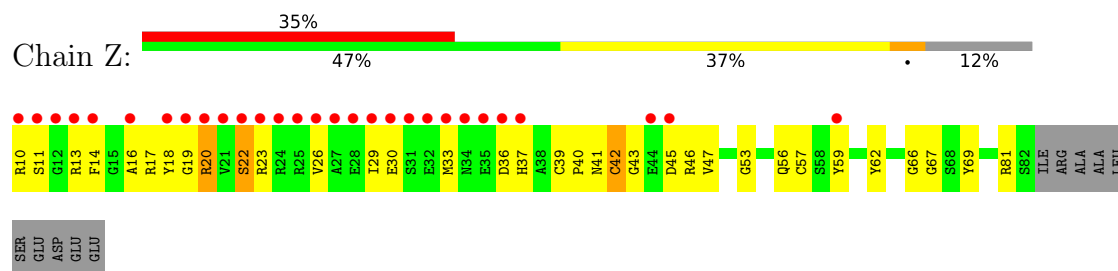
- Molecule 26: 50S ribosomal protein L31e



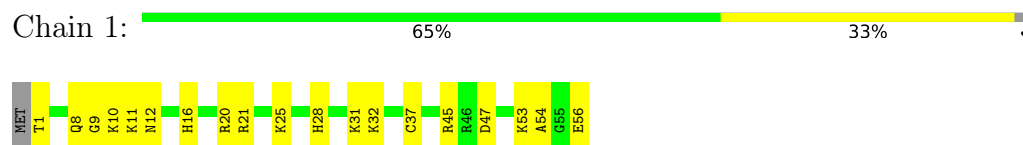
- Molecule 27: 50S ribosomal protein L32E



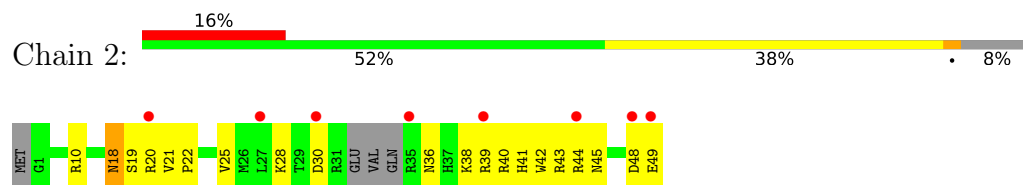
• Molecule 28: 50S ribosomal protein L37Ae



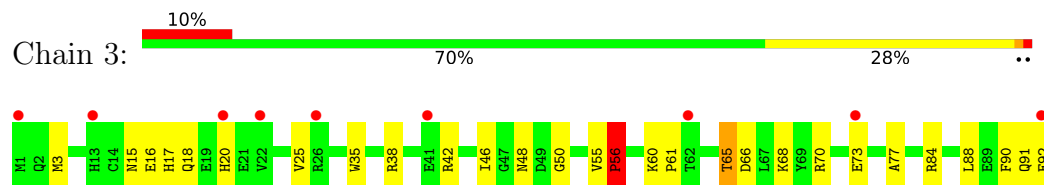
• Molecule 29: 50S ribosomal protein L37e



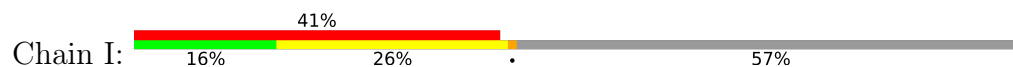
• Molecule 30: 50S ribosomal protein L39e



• Molecule 31: 50S ribosomal protein L44E



• Molecule 32: 50S RIBOSOMAL PROTEIN L11P



MET	SER		
ALA	PHE	A125	
GLY	GLU	K126	
THR	ILE	E127	
ILE	GLU	V128	
GLU	VAL	V129	
VAL	G71	G130	
LEU	T131	C132	
VAL	V72	T133	
VAL	P73	S134	
PRO	P74	L135	
GLY	T75	G136	
GLY	A76	V137	
GLU	E77	T138	
ALA	L78	I139	
ASN	I79	E140	
PRO	K80	GLY	
GLY	D81	GLU	
PRO	E82	ASN	
PRO	A83	PRO	
LEU	G84	ARG	
GLY	F85	GLU	
PRO	E86	PHE	
GLU	T87	LYS	
LEU	G88	GLU	
GLY	S89	ARG	
PRO	G90	ILE	
THR	E91	ASP	
PRO	P92	ALA	
VAL	Q93	GLY	
ASP	E94	GLU	
VAL	D95	TYR	
GLN	F96	ASP	
ALA	V97	ASP	
VAL	A98	VAL	
VAL	D99	PHE	
GLN	L100	ALA	
GLU	S101	ALA	
ILE	V102	GLU	
ASN	D103	GLN	
ASP	Q104	ALA	
GLN	V105	GLN	
THR	K106	ALA	
ALA	Q107	GLY	
ALA	I108	ALA	
PHE	A109		
ASP	E110		
GLY	Q111		
THR	K112		
GLU	H113		
VAL	P114		
PRO	D115		
VAL	L116		
THR	L117		
VAL	S118		
LYS	Y119		
TYR	D120		
ASP	L121		
ASP	T122		
ASP	N123		
GLY	A124		

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	211.44Å 298.56Å 574.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 49.61 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (50.00-2.30) 89.8 (49.61-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.247 0.206 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 61.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99045	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, PPU, CL, SR, NA, K, PO2, CD, OMU, UR3, 1MA, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.38	0/65959	0.70	24/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.48	0/102	0.75	0/149
4	A	0.33	0/1786	0.65	0/2408
5	B	0.32	0/2690	0.64	0/3652
6	C	0.37	0/1884	0.65	0/2551
7	D	0.29	0/1111	0.53	0/1498
8	E	0.31	0/1382	0.56	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.27	0/241	0.46	0/324
11	H	0.33	0/1287	0.64	0/1725
12	J	0.34	0/1136	0.60	0/1530
13	K	0.35	0/1001	0.66	0/1347
14	L	0.32	0/1130	0.63	0/1509
15	M	0.35	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.60	0/1999
17	O	0.32	0/874	0.58	1/1181 (0.1%)
18	P	0.34	0/1147	0.55	0/1528
19	Q	0.35	0/749	0.68	0/1005
20	R	0.35	0/1172	0.66	1/1578 (0.1%)
21	S	0.32	0/648	0.58	0/875
22	T	0.30	0/958	0.62	0/1289
23	U	0.34	0/417	0.56	0/562
24	V	0.26	0/502	0.50	0/675
25	W	0.33	0/1219	0.59	0/1655
26	X	0.32	0/664	0.59	0/895
27	Y	0.35	0/1146	0.65	0/1536
28	Z	0.33	0/589	0.59	0/787
29	1	0.44	0/438	0.66	0/578
30	2	0.34	0/401	0.58	0/529
31	3	0.35	0/771	0.58	0/1024
32	I	0.28	0/526	0.50	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.36	0/98794	0.67	27/147726 (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	0	44
2	9	0	1
All	All	0	45

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1819	G	C5'-C4'-C3'	7.74	128.38	116.00
1	0	871	G	C5'-C4'-O4'	-7.70	99.86	109.10
1	0	1942	A	C5'-C4'-C3'	7.40	127.83	116.00
2	9	3039	U	N1-C1'-C2'	6.97	123.06	114.00
1	0	1979	G	C2'-C3'-O3'	6.95	124.81	113.70

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	396	U	Sidechain
1	0	460	A	Sidechain
1	0	469	G	Sidechain
1	0	470	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	714	0
2	9	2600	0	1326	52	0
3	4	135	0	83	3	0
4	A	1753	0	1766	108	0
5	B	2625	0	2532	133	0
6	C	1859	0	1816	89	0
7	D	1094	0	1085	77	0
8	E	1357	0	1266	55	0
9	F	890	0	843	47	0
10	G	240	0	231	14	0
11	H	1266	0	1268	57	0
12	J	1120	0	1098	78	0
13	K	992	0	1031	46	0
14	L	1118	0	1076	50	0
15	M	1560	0	1568	72	0
16	N	1445	0	1401	86	0
17	O	865	0	873	37	0
18	P	1136	0	1123	38	0
19	Q	735	0	729	17	0
20	R	1149	0	1122	36	0
21	S	641	0	605	16	0
22	T	950	0	924	49	0
23	U	410	0	364	21	0
24	V	499	0	511	31	0
25	W	1196	0	1137	91	0
26	X	654	0	653	38	0
27	Y	1130	0	1133	61	0
28	Z	578	0	539	39	0
29	1	431	0	426	26	0
30	2	396	0	413	28	0
31	3	755	0	728	28	0
32	I	519	0	500	50	0
33	0	87	0	0	0	0
33	2	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	62	0	0	0	0
35	3	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	3	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	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	0	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	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	98	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	3	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	L	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5739	0	0	94	0
39	1	51	0	0	1	0
39	2	41	0	0	1	0
39	3	67	0	0	3	0
39	4	8	0	0	0	0
39	9	132	0	0	8	0
39	A	123	0	0	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	B	139	0	0	19	0
39	C	177	0	0	16	0
39	D	50	0	0	5	0
39	E	43	0	0	2	0
39	F	28	0	0	2	0
39	G	16	0	0	2	0
39	H	71	0	0	8	0
39	I	9	0	0	1	0
39	J	53	0	0	3	0
39	K	57	0	0	4	0
39	L	82	0	0	11	0
39	M	125	0	0	7	0
39	N	59	0	0	7	0
39	O	35	0	0	3	0
39	P	59	0	0	0	0
39	Q	48	0	0	5	0
39	R	86	0	0	2	0
39	S	31	0	0	1	0
39	T	36	0	0	1	0
39	U	26	0	0	1	0
39	V	11	0	0	1	0
39	W	68	0	0	3	0
39	X	23	0	0	3	0
39	Y	93	0	0	9	0
39	Z	28	0	0	3	0
All	All	99045	0	59983	2061	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

The worst 5 of 2061 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.23	1.17
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.31	1.10
2:9:3076:G:H3'	2:9:3077:A:H5''	1.35	1.08
6:C:236:THR:HG22	6:C:239:ALA:H	1.14	1.06
1:0:133:U:H2'	1:0:134:U:H5''	1.37	1.02

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%)	213 (91%)	17 (7%)	5 (2%)	7	5
5	B	335/338 (99%)	312 (93%)	18 (5%)	5 (2%)	10	10
6	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
7	D	134/177 (76%)	104 (78%)	18 (13%)	12 (9%)	1	0
8	E	170/178 (96%)	164 (96%)	6 (4%)	0	100	100
9	F	117/120 (98%)	104 (89%)	11 (9%)	2 (2%)	9	8
10	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	H	156/171 (91%)	141 (90%)	13 (8%)	2 (1%)	12	12
12	J	140/145 (97%)	132 (94%)	5 (4%)	3 (2%)	7	5
13	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	19	23
14	L	141/165 (86%)	120 (85%)	20 (14%)	1 (1%)	22	26
15	M	192/195 (98%)	180 (94%)	11 (6%)	1 (0%)	29	35
16	N	184/187 (98%)	162 (88%)	15 (8%)	7 (4%)	3	1
17	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
18	P	141/149 (95%)	137 (97%)	4 (3%)	0	100	100
19	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	17	20
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	55 (87%)	7 (11%)	1 (2%)	9	9
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	58 (82%)	10 (14%)	3 (4%)	3	1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	14	15
32	I	68/162 (42%)	52 (76%)	14 (21%)	2 (3%)	4	3
All	All	3705/4431 (84%)	3409 (92%)	249 (7%)	47 (1%)	12	12

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	37	VAL
7	D	137	PRO
9	F	101	ALA
11	H	166	SER
12	J	143	LYS

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%)	21	29
5	B	282/283 (100%)	268 (95%)	14 (5%)	24	34
6	C	193/193 (100%)	174 (90%)	19 (10%)	8	9
7	D	117/148 (79%)	110 (94%)	7 (6%)	19	26
8	E	152/156 (97%)	145 (95%)	7 (5%)	27	38
9	F	93/94 (99%)	90 (97%)	3 (3%)	39	54
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	130 (98%)	2 (2%)	65	79
12	J	118/121 (98%)	110 (93%)	8 (7%)	16	21
13	K	106/106 (100%)	102 (96%)	4 (4%)	33	47
14	L	113/127 (89%)	109 (96%)	4 (4%)	36	50
15	M	158/159 (99%)	153 (97%)	5 (3%)	39	54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	142 (95%)	7 (5%)	26	37
17	O	93/94 (99%)	91 (98%)	2 (2%)	52	69
18	P	113/117 (97%)	110 (97%)	3 (3%)	44	61
19	Q	79/80 (99%)	75 (95%)	4 (5%)	24	33
20	R	117/122 (96%)	117 (100%)	0	100	100
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	33	47
23	U	44/52 (85%)	43 (98%)	1 (2%)	50	67
24	V	51/57 (90%)	50 (98%)	1 (2%)	55	72
25	W	130/130 (100%)	126 (97%)	4 (3%)	40	55
26	X	66/74 (89%)	62 (94%)	4 (6%)	18	25
27	Y	120/196 (61%)	109 (91%)	11 (9%)	9	11
28	Z	60/68 (88%)	59 (98%)	1 (2%)	60	76
29	1	46/47 (98%)	45 (98%)	1 (2%)	52	69
30	2	42/46 (91%)	41 (98%)	1 (2%)	49	66
31	3	79/79 (100%)	77 (98%)	2 (2%)	47	65
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2964 (96%)	129 (4%)	30	42

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	F	46	GLU
13	K	84	ASP
27	Y	189	ASN
11	H	84	LYS
12	J	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
16	N	93	GLN
18	P	88	GLN
30	2	16	ASN
16	N	107	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	O	100	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	235 (8%)	36 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)
3	4	1/7 (14%)	0	0
All	All	2867/3051 (93%)	249 (8%)	37 (1%)

5 of 249 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 37 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1506	U
1	0	1730	G
1	0	2791	U
1	0	1684	A
1	0	1685	A

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	PSU	0	2621	1	17,21,22	1.68	3 (17%)	20,30,33	5.43	4 (20%)
3	PPU	4	76	1,3	32,40,41	1.19	1 (3%)	33,57,60	0.84	2 (6%)
1	UR3	0	2619	1	14,22,23	0.87	1 (7%)	15,32,35	0.59	0
1	OMG	0	2588	1,3	18,26,27	1.06	2 (11%)	20,38,41	2.61	5 (25%)
1	1MA	0	628	1	15,25,26	0.72	0	15,37,40	1.36	1 (6%)
1	OMU	0	2587	1	14,22,23	0.99	1 (7%)	14,31,34	1.17	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
3	PPU	4	76	1,3	-	0/21/43/44	0/4/4/4
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMG	0	2588	1,3	-	2/5/27/28	0/3/3/3
1	1MA	0	628	1	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	4	76	PPU	OC-CM	-5.45	1.26	1.42
1	0	2621	PSU	C5-C1'	-4.96	1.48	1.52
1	0	2588	OMG	C6-N1	3.28	1.38	1.33
1	0	2621	PSU	C4-N3	3.02	1.38	1.33
1	0	2621	PSU	C2-N1	2.79	1.43	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.24	114.72	128.43
1	0	2621	PSU	C4-N3-C2	14.32	127.23	115.14
1	0	2588	OMG	C5-C6-N1	-8.61	111.65	123.43
1	0	2621	PSU	C5-C4-N3	-8.22	114.76	125.36
1	0	2588	OMG	C6-N1-C2	5.84	125.22	115.93

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	2588	OMG	C3'-C2'-O2'-CM2
1	0	2588	OMG	C1'-C2'-O2'-CM2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	4	76	PPU	1	0
1	0	2587	OMU	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 312 ligands modelled in this entry, 312 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2749/2922 (94%)	-0.12	75 (2%) 54 62	26, 50, 94, 154	0
2	9	122/122 (100%)	0.14	5 (4%) 37 44	45, 70, 97, 154	0
3	4	5/7 (71%)	-0.62	0 100 100	46, 48, 54, 54	0
4	A	237/240 (98%)	0.54	18 (7%) 13 18	31, 55, 88, 108	0
5	B	337/338 (99%)	0.41	15 (4%) 33 40	32, 57, 83, 94	0
6	C	246/246 (100%)	0.19	6 (2%) 59 66	29, 51, 76, 90	0
7	D	140/177 (79%)	2.40	65 (46%) 0 0	64, 100, 128, 135	0
8	E	172/178 (96%)	1.14	38 (22%) 0 1	47, 71, 89, 96	0
9	F	119/120 (99%)	1.46	41 (34%) 0 0	51, 77, 106, 112	0
10	G	29/348 (8%)	2.78	19 (65%) 0 0	75, 97, 105, 106	0
11	H	160/171 (93%)	0.89	25 (15%) 2 2	49, 66, 97, 105	0
12	J	142/145 (97%)	0.28	5 (3%) 44 51	40, 55, 76, 95	0
13	K	132/132 (100%)	0.08	2 (1%) 73 79	36, 52, 74, 83	0
14	L	145/165 (87%)	1.00	29 (20%) 1 1	29, 70, 114, 125	0
15	M	194/195 (99%)	0.99	23 (11%) 4 6	36, 49, 90, 98	0
16	N	186/187 (99%)	1.27	43 (23%) 0 1	48, 70, 117, 121	0
17	O	115/116 (99%)	0.39	4 (3%) 44 51	42, 60, 75, 81	0
18	P	143/149 (95%)	0.30	4 (2%) 53 60	41, 56, 69, 81	0
19	Q	95/96 (98%)	0.38	6 (6%) 20 25	42, 54, 70, 78	0
20	R	150/155 (96%)	0.12	3 (2%) 65 71	33, 49, 69, 77	0
21	S	81/85 (95%)	0.43	5 (6%) 20 26	42, 60, 81, 98	0
22	T	119/120 (99%)	0.89	15 (12%) 3 5	46, 59, 89, 113	0
23	U	53/66 (80%)	0.38	3 (5%) 23 30	46, 57, 77, 84	0
24	V	65/71 (91%)	1.83	17 (26%) 0 0	55, 80, 116, 121	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%)	0.34	4 (2%) 56 63	42, 56, 79, 88	0
26	X	82/92 (89%)	0.91	11 (13%) 3 4	46, 60, 88, 105	0
27	Y	142/241 (58%)	0.40	12 (8%) 10 14	32, 49, 70, 90	0
28	Z	73/83 (87%)	2.19	29 (39%) 0 0	51, 83, 99, 106	0
29	1	56/57 (98%)	-0.28	0 100 100	30, 36, 45, 54	0
30	2	46/50 (92%)	1.06	8 (17%) 1 1	39, 63, 88, 100	0
31	3	92/92 (100%)	0.62	9 (9%) 7 10	39, 61, 76, 90	0
32	I	70/162 (43%)	6.05	66 (94%) 0 0	114, 127, 144, 146	0
All	All	6651/7482 (88%)	0.43	605 (9%) 9 12	26, 56, 102, 154	0

The worst 5 of 605 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	71	GLY	20.6
24	V	1	THR	16.1
7	D	63	ILE	14.8
15	M	70	GLY	13.7
32	I	133	THR	13.6

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OMG	0	2588	24/25	0.97	0.12	34,37,42,43	0
3	PPU	4	76	37/38	0.98	0.12	38,43,49,54	0
1	UR3	0	2619	21/22	0.98	0.14	39,40,43,47	0
1	PSU	0	2621	20/21	0.98	0.13	35,39,43,44	0
1	1MA	0	628	23/24	0.98	0.15	35,37,40,44	0
1	OMU	0	2587	21/22	0.98	0.12	35,40,43,43	0

6.3 Carbohydrates ⓘ

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
37	SR	0	9537	1/1	0.14	0.21	159,159,159,159	0
33	MG	0	8047	1/1	0.18	1.13	111,111,111,111	0
35	NA	0	9129	1/1	0.29	0.32	82,82,82,82	0
37	SR	0	9547	1/1	0.38	0.28	184,184,184,184	0
33	MG	0	8102	1/1	0.43	0.16	76,76,76,76	0
33	MG	0	8108	1/1	0.47	0.13	107,107,107,107	0
38	CD	Z	9203	1/1	0.48	0.19	93,93,93,93	0
33	MG	0	8094	1/1	0.51	0.68	93,93,93,93	0
35	NA	0	9184	1/1	0.56	0.21	83,83,83,83	0
35	NA	0	9111	1/1	0.67	0.27	70,70,70,70	0
35	NA	0	9185	1/1	0.67	0.47	62,62,62,62	0
35	NA	0	9179	1/1	0.69	1.23	96,96,96,96	0
35	NA	9	9151	1/1	0.71	0.23	83,83,83,83	0
33	MG	0	8050	1/1	0.72	0.18	86,86,86,86	0
35	NA	S	9112	1/1	0.72	0.31	85,85,85,85	0
33	MG	0	8059	1/1	0.72	0.40	71,71,71,71	0
33	MG	0	8065	1/1	0.74	0.47	90,90,90,90	0
35	NA	0	9178	1/1	0.75	0.26	57,57,57,57	0
33	MG	0	8042	1/1	0.76	0.09	58,58,58,58	0
33	MG	0	8052	1/1	0.76	0.41	87,87,87,87	0
33	MG	0	8022	1/1	0.76	1.07	123,123,123,123	0
36	CL	0	9316	1/1	0.77	0.24	86,86,86,86	0
33	MG	0	8091	1/1	0.77	0.08	58,58,58,58	0
33	MG	0	8014	1/1	0.77	0.86	94,94,94,94	0
37	SR	0	9484	1/1	0.77	0.08	139,139,139,139	0
37	SR	9	9588	1/1	0.78	0.14	141,141,141,141	0
33	MG	0	8032	1/1	0.78	0.10	47,47,47,47	0
33	MG	0	8040	1/1	0.78	0.44	100,100,100,100	0
33	MG	0	8072	1/1	0.79	0.33	78,78,78,78	0
37	SR	0	9500	1/1	0.79	1.25	200,200,200,200	0
35	NA	0	9140	1/1	0.79	0.55	67,67,67,67	0
35	NA	0	9171	1/1	0.81	0.25	66,66,66,66	0
35	NA	H	9122	1/1	0.81	0.19	78,78,78,78	0
33	MG	0	8089	1/1	0.81	0.23	64,64,64,64	0
35	NA	0	9168	1/1	0.82	0.15	68,68,68,68	0
33	MG	0	8107	1/1	0.82	0.16	67,67,67,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	9182	1/1	0.82	0.14	81,81,81,81	0
33	MG	0	8084	1/1	0.83	0.33	84,84,84,84	0
35	NA	0	9102	1/1	0.83	0.24	64,64,64,64	0
35	NA	0	9174	1/1	0.83	0.51	71,71,71,71	0
35	NA	0	9163	1/1	0.83	0.19	65,65,65,65	0
35	NA	0	9170	1/1	0.84	0.38	87,87,87,87	0
33	MG	0	8041	1/1	0.84	0.12	56,56,56,56	0
35	NA	0	9158	1/1	0.84	0.23	62,62,62,62	0
33	MG	0	8099	1/1	0.84	0.19	74,74,74,74	0
33	MG	0	8116	1/1	0.84	0.08	59,59,59,59	0
33	MG	0	8092	1/1	0.84	0.49	79,79,79,79	0
35	NA	0	9164	1/1	0.84	0.34	62,62,62,62	0
35	NA	0	9125	1/1	0.85	0.56	87,87,87,87	0
33	MG	0	8054	1/1	0.85	0.14	60,60,60,60	0
33	MG	0	8101	1/1	0.85	0.15	68,68,68,68	0
33	MG	0	8114	1/1	0.86	0.39	79,79,79,79	0
33	MG	0	8093	1/1	0.86	0.18	52,52,52,52	0
35	NA	0	9157	1/1	0.86	0.17	52,52,52,52	0
35	NA	9	9152	1/1	0.87	0.48	76,76,76,76	0
33	MG	0	8113	1/1	0.87	0.13	49,49,49,49	0
35	NA	0	9161	1/1	0.88	0.20	61,61,61,61	0
37	SR	0	9504	1/1	0.88	0.12	107,107,107,107	0
37	SR	0	9626	1/1	0.88	0.38	147,147,147,147	0
34	K	0	9001	1/1	0.88	0.71	92,92,92,92	0
35	NA	9	9183	1/1	0.88	0.13	80,80,80,80	0
35	NA	0	9118	1/1	0.88	0.30	71,71,71,71	0
35	NA	0	9172	1/1	0.88	0.36	78,78,78,78	0
35	NA	0	9107	1/1	0.89	0.25	59,59,59,59	0
33	MG	0	8063	1/1	0.89	0.12	67,67,67,67	0
35	NA	3	9169	1/1	0.89	0.40	98,98,98,98	0
33	MG	0	8117	1/1	0.89	0.15	48,48,48,48	0
38	CD	O	9205	1/1	0.89	0.04	138,138,138,138	0
37	SR	B	9521	1/1	0.89	0.40	184,184,184,184	0
35	NA	R	9137	1/1	0.89	0.11	43,43,43,43	0
33	MG	0	8090	1/1	0.89	0.18	67,67,67,67	0
35	NA	0	9173	1/1	0.89	0.37	69,69,69,69	0
34	K	0	9002	1/1	0.89	0.12	90,90,90,90	0
33	MG	0	8046	1/1	0.90	0.10	47,47,47,47	0
35	NA	0	9126	1/1	0.90	0.11	64,64,64,64	0
35	NA	0	9110	1/1	0.90	0.15	49,49,49,49	0
33	MG	0	8045	1/1	0.90	0.32	82,82,82,82	0
35	NA	0	9156	1/1	0.90	0.34	59,59,59,59	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8024	1/1	0.90	0.42	76,76,76,76	0
35	NA	0	9130	1/1	0.90	0.14	53,53,53,53	0
35	NA	0	9167	1/1	0.91	0.16	57,57,57,57	0
35	NA	0	9149	1/1	0.91	0.21	52,52,52,52	0
37	SR	0	9459	1/1	0.91	0.07	107,107,107,107	0
35	NA	0	9175	1/1	0.91	0.19	55,55,55,55	0
33	MG	B	8055	1/1	0.91	0.27	94,94,94,94	0
33	MG	0	8079	1/1	0.91	0.14	33,33,33,33	0
33	MG	9	8095	1/1	0.91	0.26	61,61,61,61	0
36	CL	B	9319	1/1	0.91	0.23	62,62,62,62	0
35	NA	0	9131	1/1	0.91	0.21	52,52,52,52	0
35	NA	0	9113	1/1	0.91	0.11	74,74,74,74	0
33	MG	0	8051	1/1	0.91	0.29	33,33,33,33	0
37	SR	0	9467	1/1	0.92	0.10	91,91,91,91	0
35	NA	0	9154	1/1	0.92	0.26	57,57,57,57	0
37	SR	0	9517	1/1	0.92	0.04	117,117,117,117	0
37	SR	0	9529	1/1	0.92	0.09	120,120,120,120	0
33	MG	0	8082	1/1	0.92	0.41	89,89,89,89	0
33	MG	0	8115	1/1	0.92	0.17	61,61,61,61	0
33	MG	0	8021	1/1	0.92	0.18	58,58,58,58	0
33	MG	0	8080	1/1	0.92	0.20	58,58,58,58	0
33	MG	0	8085	1/1	0.93	0.32	68,68,68,68	0
35	NA	C	9104	1/1	0.93	0.11	33,33,33,33	0
35	NA	0	9155	1/1	0.93	0.29	62,62,62,62	0
35	NA	0	9177	1/1	0.93	0.35	78,78,78,78	0
35	NA	0	9132	1/1	0.93	0.15	57,57,57,57	0
33	MG	0	8103	1/1	0.93	0.20	74,74,74,74	0
33	MG	0	8075	1/1	0.93	0.05	41,41,41,41	0
33	MG	T	8073	1/1	0.93	0.12	52,52,52,52	0
33	MG	0	8039	1/1	0.93	0.09	66,66,66,66	0
35	NA	J	9146	1/1	0.93	0.12	58,58,58,58	0
33	MG	0	8043	1/1	0.93	0.06	57,57,57,57	0
37	SR	0	9539	1/1	0.93	0.50	162,162,162,162	0
37	SR	0	9532	1/1	0.93	0.05	127,127,127,127	0
37	SR	0	9475	1/1	0.94	0.12	84,84,84,84	0
36	CL	0	9322	1/1	0.94	0.20	58,58,58,58	0
33	MG	Y	8109	1/1	0.94	0.12	47,47,47,47	0
37	SR	0	9581	1/1	0.94	0.10	136,136,136,136	0
35	NA	0	9159	1/1	0.94	0.21	54,54,54,54	0
33	MG	0	8096	1/1	0.94	0.12	51,51,51,51	0
35	NA	0	9141	1/1	0.94	0.08	64,64,64,64	0
33	MG	2	8076	1/1	0.94	0.20	64,64,64,64	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
33	MG	0	8097	1/1	0.94	0.23	63,63,63,63	0
35	NA	0	9124	1/1	0.94	0.12	54,54,54,54	0
35	NA	0	9181	1/1	0.94	0.20	55,55,55,55	0
37	SR	0	9590	1/1	0.94	0.10	98,98,98,98	0
35	NA	0	9127	1/1	0.94	0.19	71,71,71,71	0
33	MG	0	8060	1/1	0.94	0.17	97,97,97,97	0
33	MG	0	8106	1/1	0.94	0.08	50,50,50,50	0
33	MG	0	8083	1/1	0.94	0.08	59,59,59,59	0
36	CL	N	9307	1/1	0.95	0.14	65,65,65,65	0
33	MG	0	8002	1/1	0.95	0.10	37,37,37,37	0
33	MG	0	8027	1/1	0.95	0.25	40,40,40,40	0
36	CL	J	9302	1/1	0.95	0.08	63,63,63,63	0
37	SR	0	9560	1/1	0.95	0.08	98,98,98,98	0
35	NA	0	9128	1/1	0.95	0.09	48,48,48,48	0
35	NA	Q	9148	1/1	0.95	0.12	48,48,48,48	0
33	MG	0	8058	1/1	0.95	0.56	92,92,92,92	0
33	MG	0	8015	1/1	0.95	0.10	33,33,33,33	0
35	NA	0	9116	1/1	0.95	0.45	55,55,55,55	0
37	SR	0	9468	1/1	0.95	0.03	120,120,120,120	0
36	CL	J	9321	1/1	0.95	0.13	68,68,68,68	0
36	CL	0	9315	1/1	0.95	0.10	59,59,59,59	0
35	NA	0	9134	1/1	0.95	0.06	52,52,52,52	0
35	NA	0	9162	1/1	0.95	0.18	50,50,50,50	0
33	MG	0	8088	1/1	0.95	0.08	39,39,39,39	0
37	SR	0	9505	1/1	0.95	0.08	91,91,91,91	0
35	NA	0	9160	1/1	0.95	0.16	45,45,45,45	0
33	MG	0	8104	1/1	0.95	0.10	59,59,59,59	0
37	SR	0	9465	1/1	0.96	0.09	101,101,101,101	0
36	CL	0	9317	1/1	0.96	0.07	57,57,57,57	0
33	MG	0	8098	1/1	0.96	0.07	47,47,47,47	0
35	NA	0	9166	1/1	0.96	0.08	68,68,68,68	0
33	MG	0	8013	1/1	0.96	0.37	24,24,24,24	0
33	MG	0	8028	1/1	0.96	0.12	37,37,37,37	0
33	MG	0	8074	1/1	0.96	0.19	32,32,32,32	0
33	MG	0	8019	1/1	0.96	0.05	51,51,51,51	0
37	SR	0	9489	1/1	0.96	0.08	92,92,92,92	0
33	MG	0	8067	1/1	0.96	0.10	44,44,44,44	0
37	SR	0	9515	1/1	0.96	0.16	94,94,94,94	0
33	MG	A	8066	1/1	0.96	0.13	53,53,53,53	0
33	MG	0	8057	1/1	0.96	0.34	68,68,68,68	0
33	MG	0	8012	1/1	0.96	0.22	46,46,46,46	0
35	NA	0	9165	1/1	0.96	0.23	46,46,46,46	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	A	9309	1/1	0.96	0.11	60,60,60,60	0
36	CL	J	9301	1/1	0.96	0.10	59,59,59,59	0
35	NA	0	9120	1/1	0.96	0.26	61,61,61,61	0
37	SR	F	9595	1/1	0.96	0.15	104,104,104,104	0
35	NA	R	9186	1/1	0.96	0.19	71,71,71,71	0
35	NA	0	9150	1/1	0.96	0.16	52,52,52,52	0
37	SR	9	9503	1/1	0.96	0.04	116,116,116,116	0
35	NA	R	9138	1/1	0.96	0.11	76,76,76,76	0
37	SR	0	9522	1/1	0.96	0.07	118,118,118,118	0
33	MG	0	8061	1/1	0.96	0.12	81,81,81,81	0
33	MG	0	8068	1/1	0.96	0.13	55,55,55,55	0
35	NA	0	9139	1/1	0.96	0.08	50,50,50,50	0
35	NA	M	9147	1/1	0.96	0.18	45,45,45,45	0
36	CL	0	9311	1/1	0.96	0.10	64,64,64,64	0
37	SR	0	9585	1/1	0.96	0.10	94,94,94,94	0
37	SR	0	9452	1/1	0.96	0.11	107,107,107,107	0
35	NA	0	9106	1/1	0.97	0.37	44,44,44,44	0
37	SR	0	9566	1/1	0.97	0.07	80,80,80,80	0
35	NA	0	9136	1/1	0.97	0.14	38,38,38,38	0
37	SR	0	9455	1/1	0.97	0.07	77,77,77,77	0
37	SR	0	9508	1/1	0.97	0.07	91,91,91,91	0
37	SR	0	9417	1/1	0.97	0.13	61,61,61,61	0
36	CL	Y	9320	1/1	0.97	0.10	49,49,49,49	0
33	MG	0	8017	1/1	0.97	0.12	30,30,30,30	0
37	SR	0	9482	1/1	0.97	0.26	122,122,122,122	0
37	SR	0	9534	1/1	0.97	0.17	108,108,108,108	0
37	SR	0	9473	1/1	0.97	0.02	79,79,79,79	0
36	CL	L	9310	1/1	0.97	0.09	58,58,58,58	0
36	CL	0	9314	1/1	0.97	0.09	55,55,55,55	0
37	SR	0	9442	1/1	0.97	0.11	65,65,65,65	0
37	SR	0	9429	1/1	0.97	0.11	71,71,71,71	0
37	SR	0	9464	1/1	0.97	0.05	83,83,83,83	0
35	NA	0	9115	1/1	0.97	0.17	47,47,47,47	0
37	SR	A	9437	1/1	0.97	0.12	73,73,73,73	0
35	NA	0	9135	1/1	0.97	0.18	54,54,54,54	0
35	NA	0	9114	1/1	0.97	0.13	46,46,46,46	0
37	SR	0	9530	1/1	0.97	0.14	73,73,73,73	0
37	SR	H	9486	1/1	0.97	0.22	114,114,114,114	0
33	MG	0	8030	1/1	0.97	0.05	37,37,37,37	0
37	SR	0	9477	1/1	0.97	0.07	83,83,83,83	0
37	SR	0	9629	1/1	0.97	0.08	77,77,77,77	0
33	MG	0	8031	1/1	0.97	0.09	55,55,55,55	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9469	1/1	0.97	0.03	91,91,91,91	0
37	SR	0	9509	1/1	0.97	0.12	91,91,91,91	0
35	NA	0	9108	1/1	0.98	0.15	35,35,35,35	0
33	MG	0	8008	1/1	0.98	0.19	22,22,22,22	0
37	SR	0	9433	1/1	0.98	0.13	75,75,75,75	0
37	SR	0	9435	1/1	0.98	0.08	75,75,75,75	0
37	SR	0	9488	1/1	0.98	0.12	84,84,84,84	0
33	MG	0	8037	1/1	0.98	0.07	42,42,42,42	0
37	SR	0	9427	1/1	0.98	0.13	58,58,58,58	0
33	MG	0	8029	1/1	0.98	0.31	37,37,37,37	0
37	SR	0	9466	1/1	0.98	0.04	101,101,101,101	0
36	CL	O	9308	1/1	0.98	0.08	66,66,66,66	0
33	MG	0	8025	1/1	0.98	0.40	33,33,33,33	0
33	MG	0	8003	1/1	0.98	0.16	38,38,38,38	0
33	MG	K	8069	1/1	0.98	0.19	26,26,26,26	0
37	SR	0	9446	1/1	0.98	0.11	93,93,93,93	0
36	CL	0	9305	1/1	0.98	0.07	58,58,58,58	0
37	SR	0	9490	1/1	0.98	0.09	108,108,108,108	0
37	SR	S	9470	1/1	0.98	0.12	99,99,99,99	0
37	SR	0	9450	1/1	0.98	0.07	76,76,76,76	0
37	SR	0	9405	1/1	0.98	0.15	59,59,59,59	0
33	MG	0	8020	1/1	0.98	0.19	38,38,38,38	0
35	NA	0	9105	1/1	0.98	0.10	45,45,45,45	0
33	MG	0	8118	1/1	0.98	0.15	30,30,30,30	0
37	SR	0	9495	1/1	0.98	0.10	102,102,102,102	0
37	SR	0	9420	1/1	0.98	0.14	73,73,73,73	0
37	SR	0	9483	1/1	0.98	0.07	80,80,80,80	0
37	SR	B	9458	1/1	0.98	0.08	83,83,83,83	0
35	NA	0	9117	1/1	0.98	0.12	44,44,44,44	0
33	MG	0	8056	1/1	0.98	0.18	47,47,47,47	0
35	NA	0	9143	1/1	0.98	0.08	46,46,46,46	0
33	MG	0	8026	1/1	0.98	0.18	35,35,35,35	0
35	NA	0	9123	1/1	0.98	0.09	42,42,42,42	0
37	SR	0	9447	1/1	0.98	0.11	69,69,69,69	0
37	SR	0	9570	1/1	0.98	0.04	105,105,105,105	0
37	SR	0	9414	1/1	0.98	0.11	58,58,58,58	0
37	SR	0	9431	1/1	0.98	0.15	66,66,66,66	0
37	SR	0	9568	1/1	0.98	0.07	77,77,77,77	0
33	MG	0	8044	1/1	0.98	0.06	44,44,44,44	0
33	MG	0	8036	1/1	0.98	0.10	60,60,60,60	0
33	MG	0	8070	1/1	0.98	0.16	28,28,28,28	0
37	SR	0	9426	1/1	0.98	0.08	72,72,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	0	9449	1/1	0.98	0.07	66,66,66,66	0
36	CL	3	9304	1/1	0.99	0.10	65,65,65,65	0
37	SR	0	9441	1/1	0.99	0.07	68,68,68,68	0
36	CL	0	9303	1/1	0.99	0.10	50,50,50,50	0
37	SR	0	9474	1/1	0.99	0.11	61,61,61,61	0
37	SR	0	9423	1/1	0.99	0.09	58,58,58,58	0
37	SR	0	9422	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9545	1/1	0.99	0.05	79,79,79,79	0
37	SR	A	9497	1/1	0.99	0.10	91,91,91,91	0
37	SR	0	9415	1/1	0.99	0.11	58,58,58,58	0
37	SR	0	9506	1/1	0.99	0.04	71,71,71,71	0
33	MG	0	8004	1/1	0.99	0.11	36,36,36,36	0
38	CD	3	9204	1/1	0.99	0.05	63,63,63,63	0
37	SR	0	9448	1/1	0.99	0.06	63,63,63,63	0
35	NA	0	9101	1/1	0.99	0.17	50,50,50,50	0
37	SR	1	9460	1/1	0.99	0.11	53,53,53,53	0
36	CL	M	9318	1/1	0.99	0.18	43,43,43,43	0
37	SR	0	9407	1/1	0.99	0.15	46,46,46,46	0
37	SR	0	9601	1/1	0.99	0.04	95,95,95,95	0
37	SR	0	9413	1/1	0.99	0.12	50,50,50,50	0
33	MG	0	8038	1/1	0.99	0.26	27,27,27,27	0
36	CL	0	9312	1/1	0.99	0.09	60,60,60,60	0
37	SR	0	9440	1/1	0.99	0.04	73,73,73,73	0
33	MG	0	8112	1/1	0.99	0.07	43,43,43,43	0
37	SR	0	9432	1/1	0.99	0.13	67,67,67,67	0
36	CL	R	9306	1/1	0.99	0.07	48,48,48,48	0
33	MG	0	8001	1/1	0.99	0.24	19,19,19,19	0
38	CD	U	9201	1/1	0.99	0.09	60,60,60,60	0
37	SR	0	9438	1/1	0.99	0.10	68,68,68,68	0
37	SR	0	9462	1/1	0.99	0.12	73,73,73,73	0
37	SR	0	9445	1/1	0.99	0.10	59,59,59,59	0
37	SR	0	9411	1/1	0.99	0.18	46,46,46,46	0
33	MG	0	8005	1/1	0.99	0.10	34,34,34,34	0
37	SR	0	9416	1/1	0.99	0.10	47,47,47,47	0
37	SR	3	9439	1/1	0.99	0.03	74,74,74,74	0
37	SR	0	9456	1/1	0.99	0.09	64,64,64,64	0
33	MG	0	8110	1/1	0.99	0.10	46,46,46,46	0
37	SR	0	9425	1/1	0.99	0.12	59,59,59,59	0
37	SR	0	9434	1/1	0.99	0.13	68,68,68,68	0
33	MG	0	8009	1/1	0.99	0.13	26,26,26,26	0
37	SR	0	9501	1/1	0.99	0.11	76,76,76,76	0
37	SR	0	9457	1/1	0.99	0.10	54,54,54,54	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
37	SR	1	9419	1/1	0.99	0.11	42,42,42,42	0
37	SR	0	9498	1/1	0.99	0.05	66,66,66,66	0
37	SR	A	9436	1/1	0.99	0.07	57,57,57,57	0
37	SR	R	9418	1/1	0.99	0.14	59,59,59,59	0
37	SR	0	9412	1/1	0.99	0.12	46,46,46,46	0
36	CL	0	9313	1/1	0.99	0.07	57,57,57,57	0
37	SR	0	9454	1/1	0.99	0.07	83,83,83,83	0
37	SR	0	9443	1/1	0.99	0.09	59,59,59,59	0
37	SR	0	9480	1/1	0.99	0.05	95,95,95,95	0
37	SR	0	9461	1/1	0.99	0.04	80,80,80,80	0
37	SR	0	9453	1/1	0.99	0.07	71,71,71,71	0
37	SR	0	9410	1/1	0.99	0.12	41,41,41,41	0
37	SR	0	9478	1/1	1.00	0.06	76,76,76,76	0
37	SR	0	9430	1/1	1.00	0.10	50,50,50,50	0
37	SR	0	9428	1/1	1.00	0.07	55,55,55,55	0
37	SR	0	9408	1/1	1.00	0.16	41,41,41,41	0
37	SR	0	9406	1/1	1.00	0.17	36,36,36,36	0
37	SR	L	9409	1/1	1.00	0.13	44,44,44,44	0
37	SR	0	9451	1/1	1.00	0.11	60,60,60,60	0
37	SR	9	9481	1/1	1.00	0.06	88,88,88,88	0
37	SR	0	9424	1/1	1.00	0.14	47,47,47,47	0
38	CD	1	9202	1/1	1.00	0.04	55,55,55,55	0
37	SR	0	9421	1/1	1.00	0.11	74,74,74,74	0
37	SR	0	9444	1/1	1.00	0.09	56,56,56,56	0

6.5 Other polymers ⓘ

There are no such residues in this entry.