



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2018 – 02:44 pm GMT

PDB ID : 1VQP  
Title : The structure of the transition state analogue "RAP" bound to the large ribosomal subunit of haloarcula marismortui  
Authors : Schmeing, T.M.; Steitz, T.A.  
Deposited on : 2004-12-16  
Resolution : 2.25 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk31020  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk31020

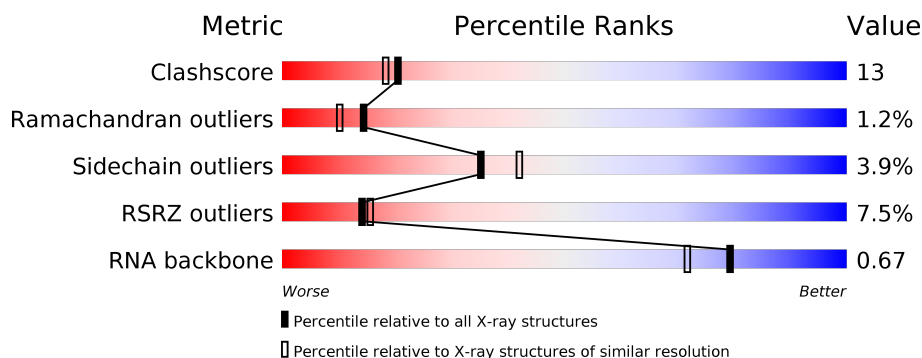
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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.



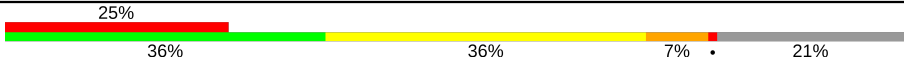
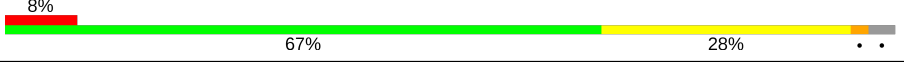

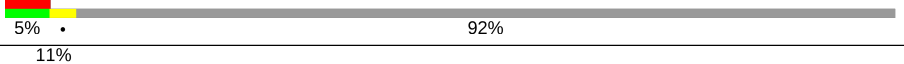

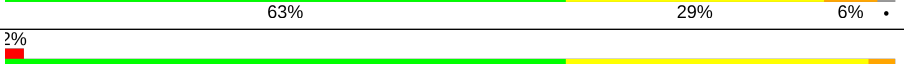
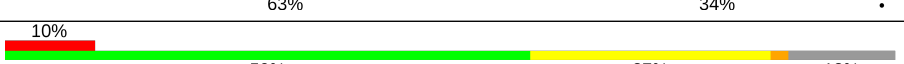
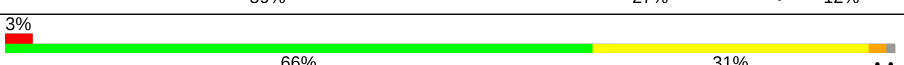
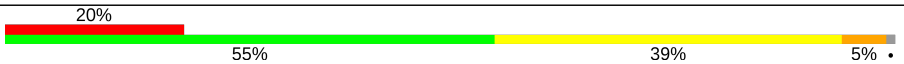


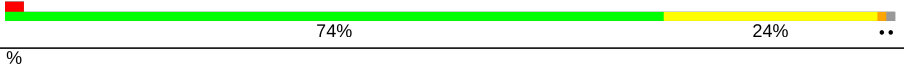

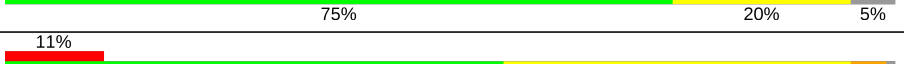
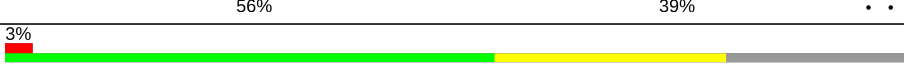



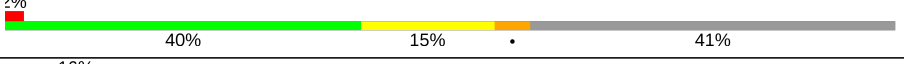
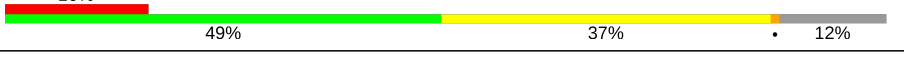





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	1286 (2.26-2.26)
Ramachandran outliers	120053	1253 (2.26-2.26)
Sidechain outliers	120020	1254 (2.26-2.26)
RSRZ outliers	108989	1158 (2.26-2.26)
RNA backbone	2636	1032 (2.72-1.80)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2922	<div> <div>4%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>6%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>7%</div> <div></div> </div> </div>
3	4	8	<div> <div></div> <div> <div></div> <div>38%</div> <div>63%</div> </div> </div>
4	A	240	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>32%</div> <div>5%</div> </div> </div>
5	B	338	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>33%</div> </div> </div>
6	C	246	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>29%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
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	
31	3	92	

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Mol	Chain	Length	Quality of chain
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	8022	-	-	-	X
33	MG	0	8024	-	-	-	X
33	MG	0	8059	-	-	-	X
35	NA	0	9118	-	-	-	X
35	NA	0	9125	-	-	-	X
35	NA	0	9169	-	-	-	X
35	NA	S	9112	-	-	-	X
37	SR	0	9500	-	-	-	X
37	SR	0	9547	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99070 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\*(DC)P\*(DC)P\*(PPU)\*(LOF)P\*(PO2)P\*AP\*C\*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	8	Total	C	N	O	P	0	0	0
			132	67	23	37	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7AE.

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

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

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

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L10E.

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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



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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	88	Total	Mg	0	0
			88	88		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	T	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	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	64	Total	Na	0	0
			64	64		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	D	1	Total 1	Na 1	0	0
35	H	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	3	Total 3	Na 3	0	0
35	9	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	10	Total 10	Cl 10	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
36	R	1	Total 1	Cl 1	0	0
36	Y	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	3	1	Total 1	Cl 1	0	0

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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	5757	Total O 5757 5757	0	0
39	9	139	Total O 139 139	0	0
39	4	6	Total O 6 6	0	0
39	A	124	Total O 124 124	0	0
39	B	140	Total O 140 140	0	0
39	C	172	Total O 172 172	0	0
39	D	50	Total O 50 50	0	0
39	E	40	Total O 40 40	0	0
39	F	25	Total O 25 25	0	0
39	G	16	Total O 16 16	0	0
39	H	69	Total O 69 69	0	0
39	J	52	Total O 52 52	0	0
39	K	59	Total O 59 59	0	0
39	L	83	Total O 83 83	0	0
39	M	131	Total O 131 131	0	0
39	N	58	Total O 58 58	0	0
39	O	39	Total O 39 39	0	0
39	P	57	Total O 57 57	0	0
39	Q	51	Total O 51 51	0	0
39	R	87	Total O 87 87	0	0
39	S	32	Total O 32 32	0	0

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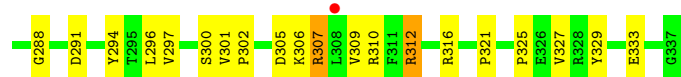
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39	T	36	Total 36	O 36	0	0
39	U	30	Total 30	O 30	0	0
39	V	11	Total 11	O 11	0	0
39	W	72	Total 72	O 72	0	0
39	X	24	Total 24	O 24	0	0
39	Y	88	Total 88	O 88	0	0
39	Z	31	Total 31	O 31	0	0
39	1	49	Total 49	O 49	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0
39	I	9	Total 9	O 9	0	0



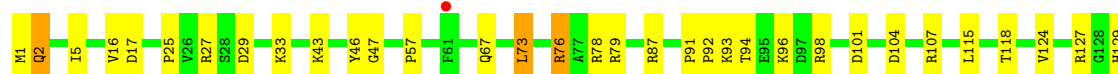
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A2811	G2466	U2564	U2671	A2467	U	A	A2083	U	U1838	G1723	C1594	U1422	C1253	C1182
A2812	A2468	C2565	C2676	A2469	C	C	G2090	G	A1839	U1724	U1595	C1423	C1257	C1183
A2813	C2469		G2237	G2238	A	A	G2091	C	A1840	C1725	A1597	C1426	G1258	C1184
A2814	C2472	A2568	A2238	C2239	C	C	A2096	C	A1845	G1730	A1598		C1268	U1186
A2815	A2569	A2578	U2478	U2240	G	G	A2101	U1964	U1846	C1731	A1603	U1432	G1269	U1187
C2819	G2578	U2586	C2477	C2243	U	U	G2102	U1965	A1847	A1732	G1604	A1441		A1188
A2820	U2478	U2587	A2354	C2243	C	C	A2103	U1966	A1847	A1733	A1605	A1442	U1279	A1189
C2821	A2354	G2588	A2354	C2243	A	A	C2104	U1967			A1607			
C2824	A2361	U2588	A2361	G2250	C	C		G1971	C1863	A1736				
C2825	A2362	U2589	A2362	G2251	C	C	G2110	U1972	C1866		C1613	A1458	U1287	A1192
G2826	G2363	U2590	G2363	A2252	G	G	G2111	U1973		G1739		U1288	U1287	A1193
A2827	G2364	A2482	G2364	G2253	C	C	A2112	A1973	G1863	U1740	C1614	C1289		A1194
G2828	G2365	G2484	G2365	G2253	C	C	G2113	G1979	G1867	U1741	A1615	A1463		G1195
	A2369	U2484	A2369	A2258	U	U		G1979	G1867	G1744	U1625	A1470		C1196
	A2485	U2485	A2369	U2265	C	C	G2128	A1980	G1868	G1745	A1626			U1197
	A2490	A2600	A2372	A2266	A	A		A1981			A1627			A1199
	G2491	G2602	U2373	A2266	C	C		C1982						A1200
	C2493	U2607	A2374	G2270	C	C	U2133	U1983	G1873	U1748	A1630	U1473		C1201
	C2502	C2608	G2375	G2271	G	G	A2135	U1992	U1874			C1474		A1202
	A2503		G2379	G2272	C	C	G2136	U1996	G1877	G1751		A1476		C1203
	A2504		A2398	G2283	C	C			G1878	G1752	G1633	C1477		C1204
	G2505		G2399	A2291	A	A		U2003	U1879					U1205
	A2506		G2399	A2291	C	C		U2004	A1755		A1641	A1482		A1206
	G2507		A2408	G2299	C	C		G2005	C1860		A1642	C1483		A1207
	C2508		A2408	G2299	C	C		C2006	A1881			U1503		C1208
	U2509		A2412	A2300	A	A		A2007	G1884		A1656	U1504		G1209
	C2510		G2413	A2300	C	C		U2008	G1902			U1505		G1210
	U2511		A2414	A2302	U	U			U1766		A1659	U1506		G1211
	U2512		A2415	A2302	G	G			A1767		G1660			C1212
	A2521		G2416	C2309	C	C			C1768					G1214
	G2524		G2417	C2313	C	C			C1769		C1666	A1522		A1215
	G2525		U2419	G2314	A	A			G1778		A1523	U1524		G1217
	C2526		G2420	G2315	G	G			A1921		U1667	U1525		U1218
	U2531		G2421	G2316	U	U			C1920		A1668	A1526		U1219
	A2532		U2422	G2317	C	C			A1919			A1527		
	C2533		G2426	U2320	A	A			C1920		C1679	A1528		
	U2534		C2427	A2321	A	A			A1922		G1681	G1529		
	C2535		U2435	U2322	C	C			G1926		G1682	G1552		G1226
	G2536		U2443	G2323	G	G			A1927		G1683			A1230
	U2537		G2444	G2323	A	A			U1783		A1684			A1231
	A2538		U2444	U2326	U	U			G1789		C1686	G1555		A1232
	U2541		U2445	U2326	C	C			G1794		C1687			A1233
	C2542		G2446	U2329	A	A			G1795			U1559		U1234
	U2547		U2446	U2330	G	G			A1796		C1692	U		A1235
	C2549		G2453	U2333	C	C			A1797			C1561		U1236
	A2564		U2457	G2334	U	U			G1946		C1692	C1562		C1237
	U2567		U2457	G2335	C	C			G1947		G1700	G1563		C1238
	A		G2462	G2335	C	C			G1948		A1701	C1564		G1239
	U			G2338	A	A			G1949		U1702			
	G2667			A	C	C			G1950		G1706	A1573		A1242
				C	C	C			G1951			C1574		C1243
				A	A	A			U			A1406		U1244
					C	C			A			A1407		C1245
					U	U			G1818		C1714	G1588		A1246
					C	C			G1819		C1715	G1589		C1250
					A	A			G1820		A1716	U1418		
					C	C			U					
					A	A			A1829		A1717			



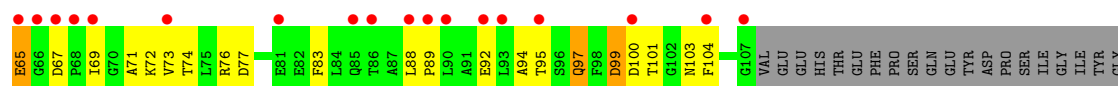
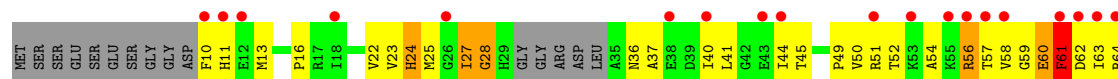




• Molecule 6: 50S ribosomal protein L4E



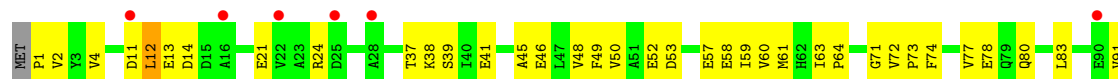
• Molecule 7: 50S ribosomal protein L5P

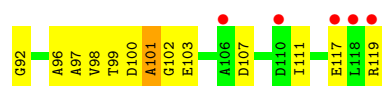


• Molecule 8: 50S ribosomal protein L6P

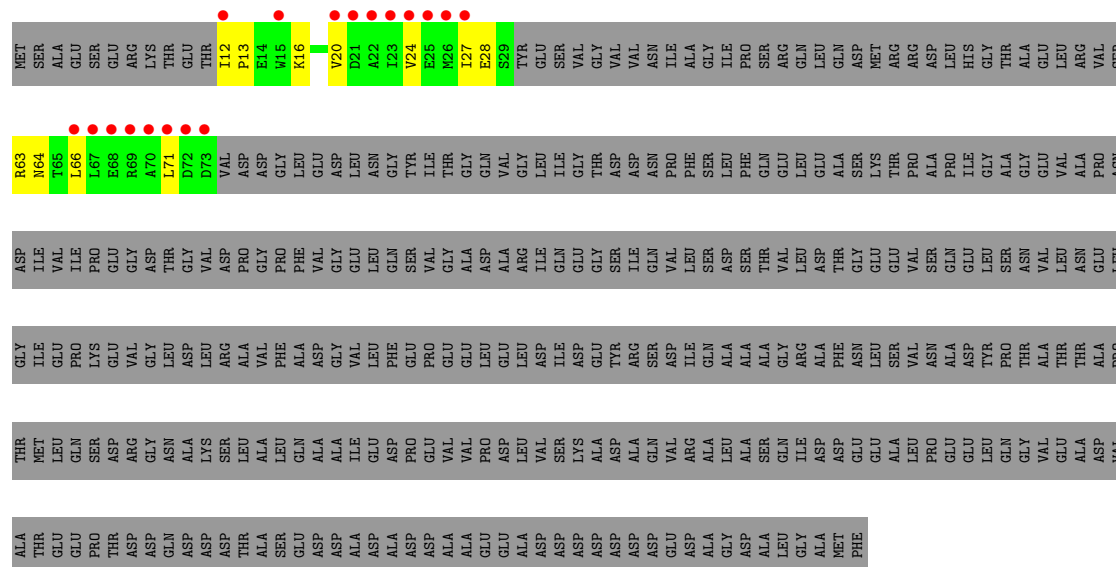


• Molecule 9: 50S ribosomal protein L7AE

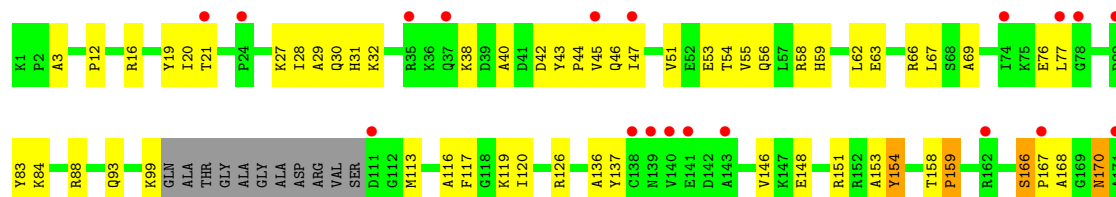




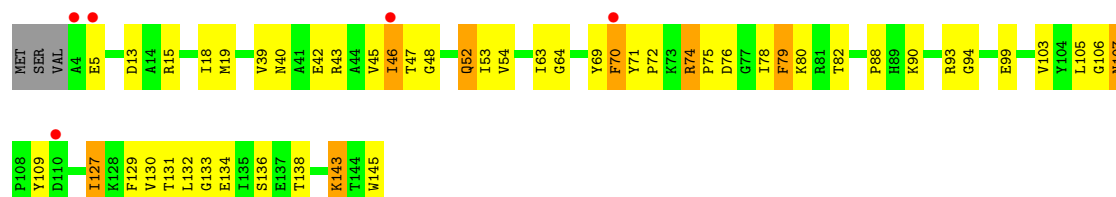
• Molecule 10: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



• Molecule 11: 50S RIBOSOMAL PROTEIN L10E

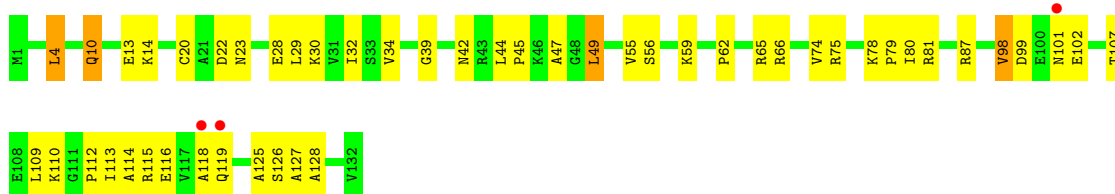


• Molecule 12: 50S ribosomal protein L13P

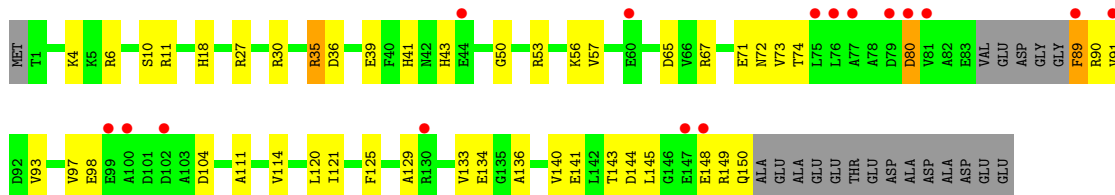


• Molecule 13: 50S ribosomal protein L14P

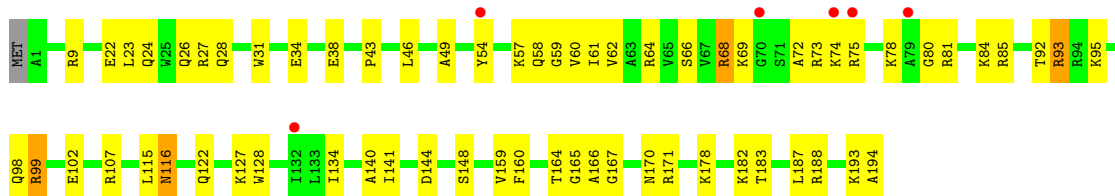




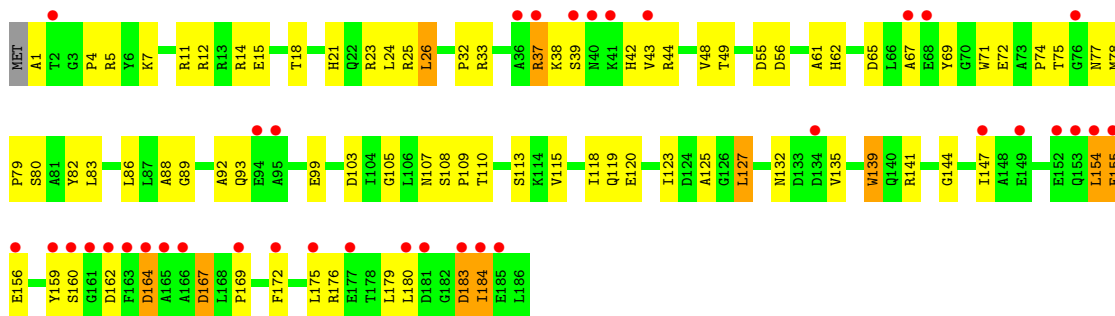
• Molecule 14: 50S ribosomal protein L15P



• Molecule 15: 50S Ribosomal Protein L15E



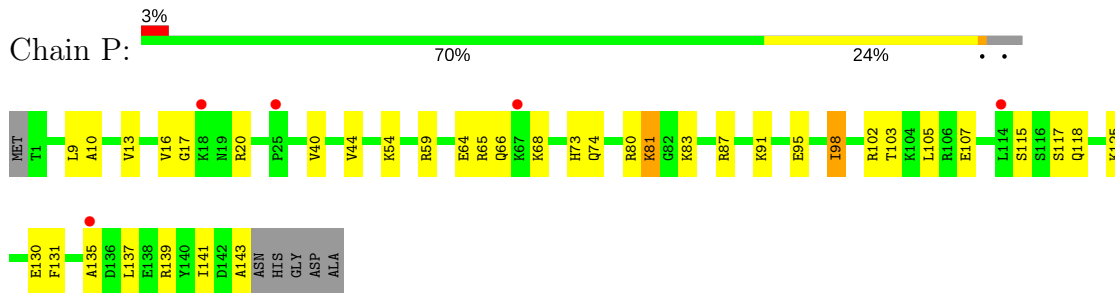
• Molecule 16: 50S ribosomal protein L18P



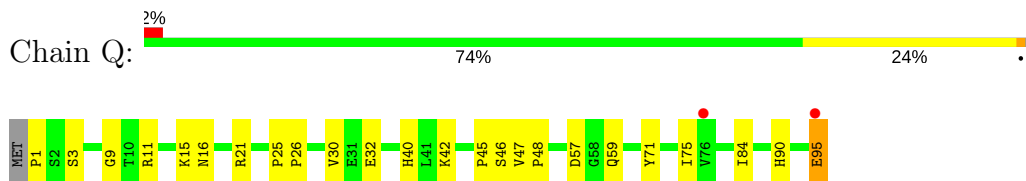
• Molecule 17: 50S ribosomal protein L18e



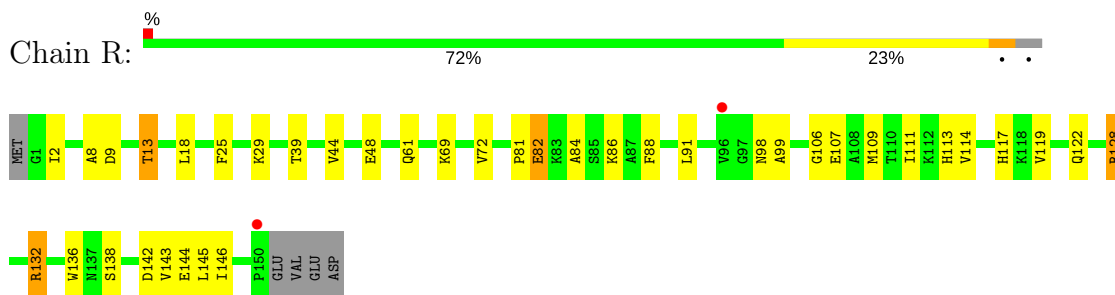
- Molecule 18: 50S ribosomal protein L19E



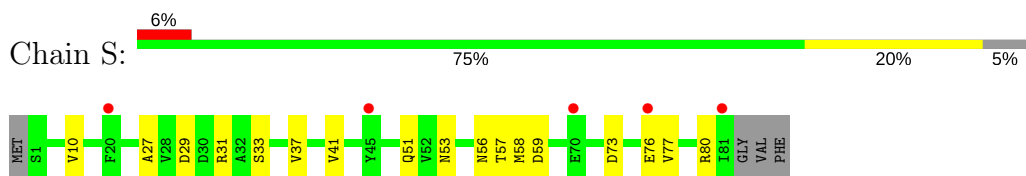
- Molecule 19: 50S ribosomal protein L21e



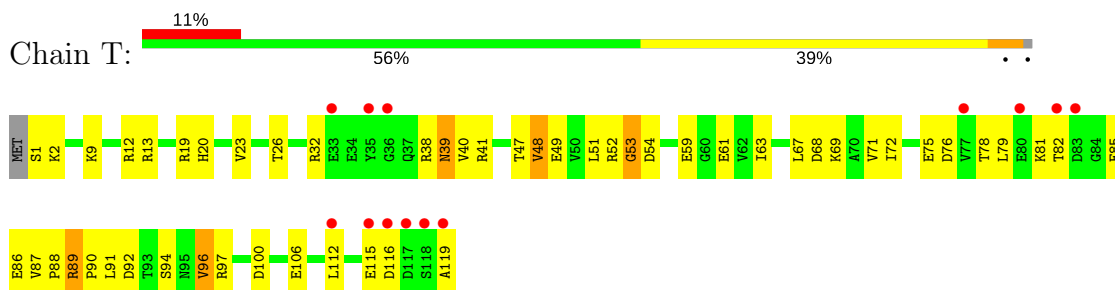
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P



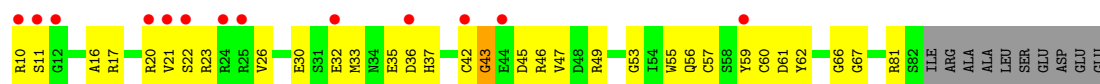
- Molecule 22: 50S ribosomal protein L24P



- Molecule 23: 50S ribosomal protein L24E







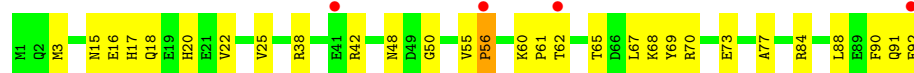
- Molecule 29: 50S ribosomal protein L37e



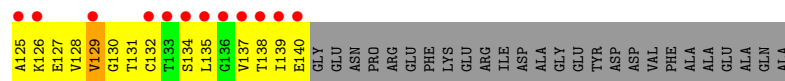
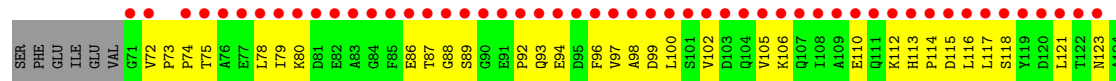
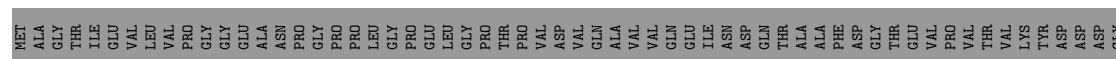
- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



- Molecule 32: 50S RIBOSOMAL PROTEIN L11P



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.61Å 298.19Å 574.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.25 37.18 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-2.25) 90.5 (37.18-2.25)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.74 (at 2.24Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.218 , 0.247 0.209 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99070	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.45% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, HFA, DCZ, 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	0.36	0/65959	0.70	24/102870 (0.0%)
2	9	0.32	0/2905	0.70	1/4528 (0.0%)
3	4	0.51	0/83	0.79	0/119
4	A	0.32	0/1786	0.67	0/2408
5	B	0.32	0/2690	0.65	0/3652
6	C	0.37	0/1884	0.65	1/2551 (0.0%)
7	D	0.28	0/1111	0.53	0/1498
8	E	0.30	0/1382	0.56	0/1880
9	F	0.30	0/901	0.53	0/1224
10	G	0.26	0/241	0.46	0/324
11	H	0.32	0/1287	0.65	0/1725
12	J	0.34	0/1136	0.60	0/1530
13	K	0.34	0/1001	0.67	0/1347
14	L	0.32	0/1130	0.65	0/1509
15	M	0.33	0/1584	0.60	0/2119
16	N	0.28	0/1474	0.61	0/1999
17	O	0.31	0/874	0.58	1/1181 (0.1%)
18	P	0.33	0/1147	0.54	0/1528
19	Q	0.34	0/749	0.69	0/1005
20	R	0.35	0/1172	0.66	1/1578 (0.1%)
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.29	0/958	0.62	0/1289
23	U	0.32	0/417	0.57	0/562
24	V	0.26	0/502	0.51	0/675
25	W	0.34	0/1219	0.60	0/1655
26	X	0.32	0/664	0.57	0/895
27	Y	0.35	0/1146	0.64	0/1536
28	Z	0.31	0/589	0.60	0/787
29	1	0.43	0/438	0.65	0/578
30	2	0.34	0/401	0.57	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	0.35	0/98775	0.68	29/147696 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	45
2	9	0	2
All	All	0	47

There are no bond length outliers.

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-8.48	98.93	109.10
1	0	1942	A	C5'-C4'-C3'	7.65	128.23	116.00
1	0	1819	G	C5'-C4'-C3'	7.08	127.34	116.00
1	0	777	U	O4'-C1'-N1	7.08	113.87	108.20
2	9	3039	U	N1-C1'-C2'	6.91	122.98	114.00

There are no chirality outliers.

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	24	G	Sidechain
1	0	333	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29813	686	0
2	9	2600	0	1326	56	0
3	4	132	0	79	4	0
4	A	1753	0	1766	110	0
5	B	2625	0	2531	132	0
6	C	1859	0	1816	92	0
7	D	1094	0	1085	87	0
8	E	1357	0	1266	57	0
9	F	890	0	843	45	0
10	G	240	0	231	10	0
11	H	1266	0	1268	61	0
12	J	1120	0	1098	73	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	48	0
15	M	1560	0	1568	61	0
16	N	1445	0	1401	85	0
17	O	865	0	873	33	0
18	P	1136	0	1123	34	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	39	0
21	S	641	0	605	15	0
22	T	950	0	923	56	0
23	U	410	0	364	17	0
24	V	499	0	511	34	0
25	W	1196	0	1137	85	0
26	X	654	0	653	39	0
27	Y	1130	0	1133	50	0
28	Z	578	0	539	23	0
29	1	431	0	426	22	0
30	2	396	0	413	32	0
31	3	755	0	728	25	0
32	I	519	0	500	56	0
33	0	88	0	0	0	0
33	9	1	0	0	0	0
33	A	2	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	3	0	0	0	0
35	0	64	0	0	0	0
35	9	1	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	5757	0	0	88	0
39	1	49	0	0	1	0
39	2	38	0	0	2	0
39	3	66	0	0	2	0
39	4	6	0	0	0	0
39	9	139	0	0	7	0
39	A	124	0	0	16	0
39	B	140	0	0	18	0
39	C	172	0	0	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	D	50	0	0	12	0
39	E	40	0	0	3	0
39	F	25	0	0	2	0
39	G	16	0	0	1	0
39	H	69	0	0	6	0
39	I	9	0	0	0	0
39	J	52	0	0	3	0
39	K	59	0	0	3	0
39	L	83	0	0	9	0
39	M	131	0	0	5	0
39	N	58	0	0	4	0
39	O	39	0	0	5	0
39	P	57	0	0	1	0
39	Q	51	0	0	5	0
39	R	87	0	0	3	0
39	S	32	0	0	0	0
39	T	36	0	0	6	0
39	U	30	0	0	3	0
39	V	11	0	0	1	0
39	W	72	0	0	3	0
39	X	24	0	0	4	0
39	Y	88	0	0	7	0
39	Z	31	0	0	2	0
All	All	99070	0	59977	2013	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 13.

The worst 5 of 2013 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)
13:K:29:LEU:HB3	13:K:55:VAL:HG11	1.29	1.14
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.27	1.09
5:B:212:GLN:HB2	5:B:257:THR:HG21	1.28	1.07
25:W:21:LEU:HD21	25:W:48:VAL:HG11	1.31	1.06
6:C:236:THR:HG22	6:C:239:ALA:H	1.19	1.06

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%)	212 (90%)	19 (8%)	4 (2%)	10	5
5	B	335/338 (99%)	316 (94%)	16 (5%)	3 (1%)	19	16
6	C	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
7	D	134/177 (76%)	108 (81%)	14 (10%)	12 (9%)	1	0
8	E	170/178 (96%)	166 (98%)	4 (2%)	0	100	100
9	F	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	10	5
10	G	25/348 (7%)	25 (100%)	0	0	100	100
11	H	156/171 (91%)	143 (92%)	11 (7%)	2 (1%)	13	9
12	J	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	12	8
13	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	21	19
14	L	141/165 (86%)	123 (87%)	17 (12%)	1 (1%)	24	23
15	M	192/195 (98%)	183 (95%)	9 (5%)	0	100	100
16	N	184/187 (98%)	165 (90%)	13 (7%)	6 (3%)	4	1
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
18	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	143 (97%)	4 (3%)	1 (1%)	24	23
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	108 (92%)	8 (7%)	1 (1%)	19	16
23	U	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
24	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	4	1
25	W	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
26	X	80/92 (87%)	72 (90%)	8 (10%)	0	100	100
27	Y	140/241 (58%)	140 (100%)	0	0	100	100
28	Z	71/83 (86%)	59 (83%)	8 (11%)	4 (6%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
31	3	90/92 (98%)	89 (99%)	0	1 (1%)	16	11
32	I	68/162 (42%)	53 (78%)	14 (21%)	1 (2%)	11	7
All	All	3705/4431 (84%)	3451 (93%)	211 (6%)	43 (1%)	14	10

5 of 43 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	H	166	SER
14	L	80	ASP
16	N	154	LEU
16	N	184	ILE
28	Z	81	ARG

### 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%)	23	23
5	B	282/283 (100%)	261 (93%)	21 (7%)	15	14
6	C	193/193 (100%)	177 (92%)	16 (8%)	12	10
7	D	117/148 (79%)	112 (96%)	5 (4%)	32	36
8	E	152/156 (97%)	148 (97%)	4 (3%)	49	58
9	F	93/94 (99%)	92 (99%)	1 (1%)	76	84
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	132/138 (96%)	127 (96%)	5 (4%)	36	43
12	J	118/121 (98%)	111 (94%)	7 (6%)	21	21
13	K	106/106 (100%)	102 (96%)	4 (4%)	36	43
14	L	113/127 (89%)	109 (96%)	4 (4%)	39	47
15	M	158/159 (99%)	153 (97%)	5 (3%)	42	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	149/150 (99%)	145 (97%)	4 (3%)	48	57
17	O	93/94 (99%)	92 (99%)	1 (1%)	76	84
18	P	113/117 (97%)	111 (98%)	2 (2%)	62	71
19	Q	79/80 (99%)	76 (96%)	3 (4%)	36	43
20	R	117/122 (96%)	114 (97%)	3 (3%)	49	58
21	S	71/74 (96%)	71 (100%)	0	100	100
22	T	105/106 (99%)	101 (96%)	4 (4%)	36	43
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	50 (98%)	1 (2%)	58	67
25	W	130/130 (100%)	126 (97%)	4 (3%)	43	52
26	X	66/74 (89%)	62 (94%)	4 (6%)	20	20
27	Y	120/196 (61%)	108 (90%)	12 (10%)	8	6
28	Z	60/68 (88%)	60 (100%)	0	100	100
29	1	46/47 (98%)	45 (98%)	1 (2%)	55	64
30	2	42/46 (91%)	41 (98%)	1 (2%)	52	61
31	3	79/79 (100%)	79 (100%)	0	100	100
32	I	58/130 (45%)	58 (100%)	0	100	100
All	All	3093/3612 (86%)	2971 (96%)	122 (4%)	35	42

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	E	164	ASP
12	J	127	ILE
27	Y	154	ARG
9	F	12	LEU
11	H	170	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	143	ASN
18	P	118	GLN
30	2	16	ASN
15	M	170	ASN

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Mol	Chain	Res	Type
18	P	50	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	232 (8%)	34 (1%)
2	9	121/122 (99%)	14 (11%)	1 (0%)
3	4	0/8	-	-
All	All	2866/3052 (93%)	246 (8%)	35 (1%)

5 of 246 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	21	G
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1692	C
1	0	2761	A
1	0	1506	U
1	0	1684	A

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

7 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	14,22,23	0.98	2 (14%)	18,31,34	3.66	2 (11%)
1	OMG	0	2588	1,3	19,26,27	1.06	1 (5%)	22,38,41	2.48	4 (18%)
1	UR3	0	2619	1	13,22,23	0.90	1 (7%)	15,32,35	0.66	0
1	PSU	0	2621	1	16,21,22	1.67	3 (18%)	20,30,33	5.38	4 (20%)
1	1MA	0	628	1,35	16,25,26	0.95	1 (6%)	12,37,40	1.25	1 (8%)
3	PPU	4	76	1,3	17,26,41	0.67	0	16,38,60	1.08	1 (6%)
3	HFA	4	77	3	11,11,12	1.12	1 (9%)	13,13,15	1.06	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	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1,3	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,35	-	0/3/25/26	0/3/3/3
3	PPU	4	76	1,3	-	0/7/29/44	0/3/3/4
3	HFA	4	77	3	-	0/4/6/8	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.84	1.48	1.52
1	0	2619	UR3	C6-C5	-2.04	1.33	1.38
1	0	2587	OMU	C6-C5	-2.04	1.33	1.38
1	0	2587	OMU	C4-N3	2.41	1.37	1.33
1	0	2621	PSU	C2-N1	2.74	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	-16.99	114.75	128.41
1	0	2588	OMG	C5-C6-N1	-8.35	111.59	123.47
1	0	2621	PSU	C5-C4-N3	-8.27	114.70	125.36
1	0	628	1MA	C2-N3-C4	-3.68	110.88	116.51
1	0	2587	OMU	C5-C4-N3	-3.59	114.84	123.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	2	0
1	0	2619	UR3	1	0
3	4	77	HFA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 313 ligands modelled in this entry, 313 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	4	176:A	O3'	175:C	P	8.75

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2749/2922 (94%)	-0.08	127 (4%) 32 36	23, 45, 88, 147	0
2	9	122/122 (100%)	0.39	7 (5%) 24 26	40, 63, 89, 149	0
3	4	4/8 (50%)	-0.27	0 100 100	40, 45, 47, 48	0
4	A	237/240 (98%)	0.35	14 (5%) 22 25	27, 48, 83, 102	0
5	B	337/338 (99%)	0.20	11 (3%) 46 49	27, 50, 76, 88	0
6	C	246/246 (100%)	0.05	3 (1%) 79 81	24, 45, 68, 79	0
7	D	140/177 (79%)	1.79	45 (32%) 0 0	55, 93, 121, 129	0
8	E	172/178 (96%)	0.40	15 (8%) 10 11	41, 63, 83, 88	0
9	F	119/120 (99%)	0.72	11 (9%) 9 9	46, 69, 94, 106	0
10	G	29/348 (8%)	2.71	18 (62%) 0 0	67, 89, 97, 100	0
11	H	160/171 (93%)	0.49	19 (11%) 4 4	40, 58, 91, 98	0
12	J	142/145 (97%)	0.05	5 (3%) 44 47	34, 47, 69, 90	0
13	K	132/132 (100%)	0.02	3 (2%) 60 64	33, 44, 68, 78	0
14	L	145/165 (87%)	0.60	16 (11%) 5 5	26, 62, 107, 117	0
15	M	194/195 (99%)	0.27	6 (3%) 49 53	32, 44, 60, 69	0
16	N	186/187 (99%)	0.94	37 (19%) 1 1	44, 61, 107, 115	0
17	O	115/116 (99%)	0.24	2 (1%) 70 73	38, 53, 68, 77	0
18	P	143/149 (95%)	0.32	5 (3%) 44 47	36, 50, 63, 75	0
19	Q	95/96 (98%)	-0.05	2 (2%) 63 67	37, 46, 61, 72	0
20	R	150/155 (96%)	-0.08	2 (1%) 77 80	30, 43, 62, 71	0
21	S	81/85 (95%)	0.39	5 (6%) 20 23	39, 55, 75, 90	0
22	T	119/120 (99%)	0.67	13 (10%) 5 5	39, 53, 79, 104	0
23	U	53/66 (80%)	0.26	2 (3%) 40 44	40, 50, 69, 78	0
24	V	65/71 (91%)	1.93	17 (26%) 0 0	52, 72, 109, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	0.27	7 (4%) 33 37	37, 49, 69, 78	0
26	X	82/92 (89%)	0.56	9 (10%) 5 5	39, 54, 81, 98	0
27	Y	142/241 (58%)	-0.02	5 (3%) 44 47	28, 42, 64, 84	0
28	Z	73/83 (87%)	0.82	13 (17%) 1 1	46, 63, 80, 91	0
29	1	56/57 (98%)	-0.20	0 100 100	28, 33, 40, 48	0
30	2	46/50 (92%)	1.48	12 (26%) 0 0	34, 60, 89, 96	0
31	3	92/92 (100%)	0.23	4 (4%) 35 38	34, 54, 68, 80	0
32	I	70/162 (43%)	6.37	64 (91%) 0 0	105, 117, 137, 138	0
All	All	6650/7483 (88%)	0.28	499 (7%) 14 15	23, 50, 95, 149	0

The worst 5 of 499 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
32	I	88	GLY	22.4
24	V	1	THR	18.4
32	I	71	GLY	18.2
32	I	133	THR	17.3
32	I	96	PHE	17.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	HFA	4	77	11/12	0.97	0.16	37,39,42,43	0
1	OMU	0	2587	21/22	0.98	0.11	28,35,37,37	0
1	OMG	0	2588	24/25	0.98	0.13	28,32,36,37	0
3	PPU	4	76	24/38	0.98	0.10	35,39,41,43	0
1	1MA	0	628	23/24	0.98	0.15	30,32,34,39	0
1	UR3	0	2619	21/22	0.98	0.13	34,37,39,41	0
1	PSU	0	2621	20/21	0.98	0.08	28,31,38,39	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
37	SR	0	9500	1/1	0.01	0.64	179,179,179,179	0
33	MG	0	8024	1/1	0.42	1.11	92,92,92,92	0
33	MG	0	8055	1/1	0.48	0.26	102,102,102,102	0
38	CD	O	9205	1/1	0.51	0.23	183,183,183,183	0
35	NA	0	9169	1/1	0.58	0.57	96,96,96,96	0
37	SR	0	9547	1/1	0.63	0.79	194,194,194,194	0
33	MG	0	8052	1/1	0.64	0.23	88,88,88,88	0
35	NA	H	9122	1/1	0.65	0.20	80,80,80,80	0
35	NA	0	9185	1/1	0.66	0.28	50,50,50,50	0
35	NA	S	9112	1/1	0.67	0.43	68,68,68,68	0
35	NA	0	9129	1/1	0.69	0.22	70,70,70,70	0
33	MG	0	8108	1/1	0.70	0.17	111,111,111,111	0
35	NA	0	9174	1/1	0.71	0.33	62,62,62,62	0
33	MG	0	8022	1/1	0.71	1.19	103,103,103,103	0
35	NA	0	9157	1/1	0.71	0.13	44,44,44,44	0
35	NA	0	9182	1/1	0.71	0.26	78,78,78,78	0
33	MG	0	8061	1/1	0.74	0.10	60,60,60,60	0
35	NA	0	9125	1/1	0.74	1.04	93,93,93,93	0
35	NA	0	9173	1/1	0.74	0.26	66,66,66,66	0
35	NA	0	9168	1/1	0.76	0.38	63,63,63,63	0
35	NA	0	9184	1/1	0.76	0.23	75,75,75,75	0
35	NA	0	9118	1/1	0.76	0.44	60,60,60,60	0
35	NA	0	9164	1/1	0.76	0.25	59,59,59,59	0
35	NA	0	9116	1/1	0.76	0.22	44,44,44,44	0
35	NA	D	9151	1/1	0.78	0.13	61,61,61,61	0
33	MG	0	8089	1/1	0.78	0.17	58,58,58,58	0
33	MG	0	8101	1/1	0.79	0.25	78,78,78,78	0
33	MG	0	8082	1/1	0.79	0.32	89,89,89,89	0
33	MG	0	8050	1/1	0.79	0.19	74,74,74,74	0
35	NA	0	9127	1/1	0.80	0.19	45,45,45,45	0
33	MG	0	8059	1/1	0.80	0.49	61,61,61,61	0
35	NA	0	9152	1/1	0.80	0.22	66,66,66,66	0
37	SR	B	9521	1/1	0.80	0.18	165,165,165,165	0
35	NA	0	9126	1/1	0.80	0.31	54,54,54,54	0
35	NA	0	9171	1/1	0.81	0.23	56,56,56,56	0
33	MG	0	8014	1/1	0.81	0.27	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8084	1/1	0.82	0.34	76,76,76,76	0
34	K	0	9001	1/1	0.82	0.35	78,78,78,78	0
35	NA	0	9163	1/1	0.82	0.12	59,59,59,59	0
33	MG	0	8094	1/1	0.83	0.57	92,92,92,92	0
33	MG	0	8042	1/1	0.83	0.08	53,53,53,53	0
35	NA	R	9186	1/1	0.83	0.23	67,67,67,67	0
35	NA	9	9183	1/1	0.83	0.20	73,73,73,73	0
35	NA	0	9140	1/1	0.84	0.13	55,55,55,55	0
33	MG	0	8017	1/1	0.85	0.17	31,31,31,31	0
33	MG	0	8040	1/1	0.85	0.29	69,69,69,69	0
33	MG	0	8093	1/1	0.85	0.13	41,41,41,41	0
33	MG	0	8058	1/1	0.86	0.26	79,79,79,79	0
33	MG	0	8057	1/1	0.86	0.20	69,69,69,69	0
35	NA	0	9158	1/1	0.86	0.31	66,66,66,66	0
37	SR	0	9459	1/1	0.86	0.07	97,97,97,97	0
35	NA	0	9177	1/1	0.86	0.34	62,62,62,62	0
35	NA	0	9179	1/1	0.86	0.33	107,107,107,107	0
33	MG	0	8025	1/1	0.87	0.35	29,29,29,29	0
35	NA	0	9170	1/1	0.87	0.54	82,82,82,82	0
33	MG	0	8045	1/1	0.87	0.31	66,66,66,66	0
35	NA	0	9111	1/1	0.87	0.21	66,66,66,66	0
34	K	0	9003	1/1	0.87	0.23	80,80,80,80	0
33	MG	A	8065	1/1	0.87	0.14	79,79,79,79	0
35	NA	0	9172	1/1	0.87	0.67	71,71,71,71	0
33	MG	0	8047	1/1	0.87	0.29	89,89,89,89	0
37	SR	0	9484	1/1	0.87	0.09	123,123,123,123	0
35	NA	0	9181	1/1	0.87	0.17	52,52,52,52	0
33	MG	0	8085	1/1	0.87	0.30	65,65,65,65	0
33	MG	0	8107	1/1	0.88	0.17	63,63,63,63	0
37	SR	0	9532	1/1	0.88	0.10	123,123,123,123	0
35	NA	C	9104	1/1	0.89	0.17	27,27,27,27	0
35	NA	0	9167	1/1	0.89	0.09	50,50,50,50	0
35	NA	0	9166	1/1	0.89	0.07	59,59,59,59	0
33	MG	0	8113	1/1	0.89	0.11	43,43,43,43	0
37	SR	9	9588	1/1	0.89	0.15	126,126,126,126	0
36	CL	N	9307	1/1	0.89	0.15	55,55,55,55	0
35	NA	0	9150	1/1	0.90	0.18	42,42,42,42	0
35	NA	0	9108	1/1	0.90	0.14	33,33,33,33	0
37	SR	0	9539	1/1	0.90	0.26	134,134,134,134	0
35	NA	0	9141	1/1	0.90	0.09	60,60,60,60	0
33	MG	0	8092	1/1	0.90	0.65	68,68,68,68	0
33	MG	0	8103	1/1	0.90	0.16	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	9130	1/1	0.90	0.09	44,44,44,44	0
36	CL	B	9319	1/1	0.90	0.16	55,55,55,55	0
33	MG	0	8115	1/1	0.91	0.12	51,51,51,51	0
35	NA	0	9124	1/1	0.91	0.27	53,53,53,53	0
37	SR	0	9452	1/1	0.91	0.18	107,107,107,107	0
33	MG	0	8104	1/1	0.91	0.12	50,50,50,50	0
33	MG	0	8013	1/1	0.91	0.16	37,37,37,37	0
33	MG	0	8028	1/1	0.91	0.13	35,35,35,35	0
36	CL	J	9301	1/1	0.91	0.08	51,51,51,51	0
33	MG	0	8063	1/1	0.91	0.18	60,60,60,60	0
37	SR	A	9497	1/1	0.92	0.09	78,78,78,78	0
37	SR	0	9581	1/1	0.92	0.13	106,106,106,106	0
35	NA	0	9113	1/1	0.92	0.10	61,61,61,61	0
33	MG	0	8051	1/1	0.92	0.27	35,35,35,35	0
37	SR	0	9626	1/1	0.92	0.23	114,114,114,114	0
37	SR	0	9475	1/1	0.92	0.07	76,76,76,76	0
35	NA	0	9120	1/1	0.92	0.39	53,53,53,53	0
33	MG	0	8102	1/1	0.92	0.05	61,61,61,61	0
38	CD	Z	9203	1/1	0.92	0.06	57,57,57,57	0
33	MG	0	8083	1/1	0.93	0.05	50,50,50,50	0
35	NA	0	9178	1/1	0.93	0.23	51,51,51,51	0
33	MG	9	8095	1/1	0.93	0.21	49,49,49,49	0
33	MG	0	8114	1/1	0.93	0.40	76,76,76,76	0
36	CL	A	9309	1/1	0.93	0.09	57,57,57,57	0
37	SR	0	9490	1/1	0.93	0.09	89,89,89,89	0
37	SR	0	9590	1/1	0.93	0.05	91,91,91,91	0
37	SR	0	9517	1/1	0.93	0.05	113,113,113,113	0
33	MG	0	8002	1/1	0.93	0.06	45,45,45,45	0
37	SR	0	9468	1/1	0.93	0.07	108,108,108,108	0
33	MG	0	8046	1/1	0.93	0.05	41,41,41,41	0
33	MG	0	8021	1/1	0.93	0.20	53,53,53,53	0
35	NA	0	9165	1/1	0.94	0.17	42,42,42,42	0
35	NA	0	9149	1/1	0.94	0.14	42,42,42,42	0
33	MG	A	8066	1/1	0.94	0.13	56,56,56,56	0
33	MG	0	8054	1/1	0.94	0.18	39,39,39,39	0
35	NA	0	9102	1/1	0.94	0.31	58,58,58,58	0
33	MG	0	8080	1/1	0.94	0.28	48,48,48,48	0
33	MG	0	8039	1/1	0.94	0.15	80,80,80,80	0
37	SR	0	9465	1/1	0.94	0.05	93,93,93,93	0
33	MG	0	8099	1/1	0.94	0.15	62,62,62,62	0
33	MG	0	8072	1/1	0.94	0.25	69,69,69,69	0
37	SR	0	9522	1/1	0.94	0.03	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8019	1/1	0.94	0.12	45,45,45,45	0
35	NA	0	9136	1/1	0.94	0.15	33,33,33,33	0
35	NA	Q	9148	1/1	0.94	0.08	48,48,48,48	0
35	NA	0	9162	1/1	0.94	0.20	49,49,49,49	0
33	MG	0	8079	1/1	0.94	0.16	30,30,30,30	0
35	NA	0	9161	1/1	0.94	0.22	59,59,59,59	0
33	MG	0	8088	1/1	0.94	0.14	36,36,36,36	0
33	MG	0	8090	1/1	0.94	0.62	84,84,84,84	0
35	NA	0	9154	1/1	0.95	0.14	46,46,46,46	0
33	MG	0	8098	1/1	0.95	0.08	43,43,43,43	0
33	MG	0	8027	1/1	0.95	0.16	33,33,33,33	0
37	SR	F	9595	1/1	0.95	0.12	99,99,99,99	0
33	MG	0	8116	1/1	0.95	0.07	49,49,49,49	0
35	NA	0	9107	1/1	0.95	0.28	63,63,63,63	0
35	NA	M	9147	1/1	0.95	0.17	39,39,39,39	0
37	SR	0	9477	1/1	0.95	0.06	83,83,83,83	0
33	MG	0	8003	1/1	0.95	0.11	33,33,33,33	0
33	MG	0	8096	1/1	0.95	0.10	42,42,42,42	0
35	NA	0	9117	1/1	0.95	0.18	43,43,43,43	0
33	MG	0	8020	1/1	0.95	0.20	34,34,34,34	0
33	MG	0	8118	1/1	0.95	0.08	33,33,33,33	0
37	SR	0	9504	1/1	0.95	0.06	90,90,90,90	0
35	NA	R	9137	1/1	0.95	0.06	38,38,38,38	0
37	SR	0	9447	1/1	0.96	0.07	64,64,64,64	0
36	CL	L	9310	1/1	0.96	0.06	49,49,49,49	0
37	SR	0	9566	1/1	0.96	0.05	76,76,76,76	0
37	SR	A	9437	1/1	0.96	0.11	59,59,59,59	0
36	CL	0	9313	1/1	0.96	0.09	51,51,51,51	0
36	CL	0	9305	1/1	0.96	0.09	52,52,52,52	0
33	MG	0	8029	1/1	0.96	0.25	35,35,35,35	0
37	SR	0	9469	1/1	0.96	0.05	81,81,81,81	0
33	MG	0	8068	1/1	0.96	0.20	46,46,46,46	0
36	CL	0	9311	1/1	0.96	0.09	60,60,60,60	0
35	NA	0	9159	1/1	0.96	0.21	55,55,55,55	0
35	NA	0	9114	1/1	0.96	0.26	42,42,42,42	0
33	MG	0	8043	1/1	0.96	0.08	49,49,49,49	0
37	SR	0	9483	1/1	0.96	0.05	68,68,68,68	0
37	SR	0	9585	1/1	0.96	0.05	77,77,77,77	0
35	NA	0	9155	1/1	0.96	0.13	52,52,52,52	0
35	NA	0	9175	1/1	0.96	0.12	51,51,51,51	0
37	SR	0	9435	1/1	0.96	0.08	67,67,67,67	0
35	NA	0	9156	1/1	0.96	0.17	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8044	1/1	0.96	0.07	41,41,41,41	0
36	CL	0	9315	1/1	0.96	0.13	50,50,50,50	0
33	MG	Y	8109	1/1	0.96	0.09	38,38,38,38	0
33	MG	0	8076	1/1	0.96	0.16	56,56,56,56	0
37	SR	0	9455	1/1	0.96	0.07	78,78,78,78	0
33	MG	0	8009	1/1	0.96	0.15	32,32,32,32	0
33	MG	0	8001	1/1	0.96	0.20	23,23,23,23	0
36	CL	O	9308	1/1	0.96	0.10	61,61,61,61	0
35	NA	0	9143	1/1	0.96	0.07	36,36,36,36	0
37	SR	0	9505	1/1	0.96	0.08	79,79,79,79	0
35	NA	0	9139	1/1	0.96	0.12	41,41,41,41	0
36	CL	0	9322	1/1	0.96	0.09	53,53,53,53	0
33	MG	0	8031	1/1	0.96	0.04	44,44,44,44	0
35	NA	0	9110	1/1	0.97	0.12	44,44,44,44	0
33	MG	0	8037	1/1	0.97	0.09	37,37,37,37	0
35	NA	0	9132	1/1	0.97	0.12	45,45,45,45	0
37	SR	0	9601	1/1	0.97	0.06	107,107,107,107	0
37	SR	0	9433	1/1	0.97	0.12	64,64,64,64	0
36	CL	0	9316	1/1	0.97	0.17	71,71,71,71	0
37	SR	S	9470	1/1	0.97	0.12	87,87,87,87	0
36	CL	3	9304	1/1	0.97	0.09	54,54,54,54	0
33	MG	0	8117	1/1	0.97	0.18	39,39,39,39	0
33	MG	0	8112	1/1	0.97	0.07	41,41,41,41	0
35	NA	0	9106	1/1	0.97	0.10	37,37,37,37	0
37	SR	0	9560	1/1	0.97	0.05	91,91,91,91	0
36	CL	0	9314	1/1	0.97	0.14	45,45,45,45	0
35	NA	0	9160	1/1	0.97	0.09	35,35,35,35	0
35	NA	0	9134	1/1	0.97	0.14	48,48,48,48	0
37	SR	0	9570	1/1	0.97	0.06	86,86,86,86	0
33	MG	0	8106	1/1	0.97	0.06	43,43,43,43	0
33	MG	0	8091	1/1	0.97	0.04	47,47,47,47	0
35	NA	0	9115	1/1	0.97	0.11	36,36,36,36	0
37	SR	0	9506	1/1	0.97	0.06	61,61,61,61	0
37	SR	0	9480	1/1	0.97	0.06	85,85,85,85	0
37	SR	0	9467	1/1	0.97	0.04	74,74,74,74	0
36	CL	J	9321	1/1	0.97	0.08	57,57,57,57	0
33	MG	0	8036	1/1	0.97	0.19	56,56,56,56	0
35	NA	0	9131	1/1	0.97	0.17	44,44,44,44	0
37	SR	0	9466	1/1	0.97	0.05	80,80,80,80	0
33	MG	T	8073	1/1	0.97	0.14	40,40,40,40	0
33	MG	0	8060	1/1	0.97	0.11	76,76,76,76	0
37	SR	0	9405	1/1	0.97	0.07	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	CL	0	9317	1/1	0.97	0.06	45,45,45,45	0
37	SR	0	9442	1/1	0.97	0.11	59,59,59,59	0
35	NA	0	9101	1/1	0.97	0.24	46,46,46,46	0
37	SR	B	9458	1/1	0.97	0.09	68,68,68,68	0
33	MG	0	8041	1/1	0.97	0.12	53,53,53,53	0
33	MG	0	8032	1/1	0.97	0.09	41,41,41,41	0
34	K	0	9002	1/1	0.97	0.07	61,61,61,61	0
37	SR	0	9629	1/1	0.97	0.07	71,71,71,71	0
37	SR	0	9515	1/1	0.98	0.17	81,81,81,81	0
37	SR	0	9495	1/1	0.98	0.08	90,90,90,90	0
37	SR	0	9537	1/1	0.98	0.07	119,119,119,119	0
33	MG	0	8110	1/1	0.98	0.08	43,43,43,43	0
36	CL	R	9306	1/1	0.98	0.15	44,44,44,44	0
37	SR	H	9486	1/1	0.98	0.14	97,97,97,97	0
33	MG	0	8056	1/1	0.98	0.13	46,46,46,46	0
37	SR	0	9568	1/1	0.98	0.03	70,70,70,70	0
35	NA	J	9146	1/1	0.98	0.09	43,43,43,43	0
37	SR	0	9429	1/1	0.98	0.07	59,59,59,59	0
37	SR	0	9427	1/1	0.98	0.11	50,50,50,50	0
33	MG	0	8075	1/1	0.98	0.04	37,37,37,37	0
37	SR	0	9482	1/1	0.98	0.25	93,93,93,93	0
36	CL	0	9303	1/1	0.98	0.12	44,44,44,44	0
33	MG	0	8012	1/1	0.98	0.19	40,40,40,40	0
35	NA	R	9138	1/1	0.98	0.17	59,59,59,59	0
37	SR	0	9440	1/1	0.98	0.03	69,69,69,69	0
37	SR	0	9432	1/1	0.98	0.13	61,61,61,61	0
37	SR	0	9426	1/1	0.98	0.04	61,61,61,61	0
37	SR	0	9489	1/1	0.98	0.07	80,80,80,80	0
37	SR	1	9419	1/1	0.98	0.12	41,41,41,41	0
37	SR	0	9453	1/1	0.98	0.05	66,66,66,66	0
37	SR	0	9530	1/1	0.98	0.13	66,66,66,66	0
33	MG	0	8097	1/1	0.98	0.10	56,56,56,56	0
37	SR	0	9509	1/1	0.98	0.08	84,84,84,84	0
36	CL	Y	9320	1/1	0.98	0.08	39,39,39,39	0
35	NA	0	9105	1/1	0.98	0.19	38,38,38,38	0
37	SR	3	9439	1/1	0.98	0.06	57,57,57,57	0
37	SR	0	9434	1/1	0.98	0.09	60,60,60,60	0
33	MG	0	8005	1/1	0.98	0.09	28,28,28,28	0
37	SR	0	9417	1/1	0.98	0.09	55,55,55,55	0
37	SR	0	9508	1/1	0.98	0.04	82,82,82,82	0
33	MG	0	8074	1/1	0.98	0.20	31,31,31,31	0
37	SR	0	9420	1/1	0.98	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8004	1/1	0.98	0.12	33,33,33,33	0
37	SR	0	9457	1/1	0.98	0.06	56,56,56,56	0
35	NA	0	9135	1/1	0.98	0.17	43,43,43,43	0
37	SR	0	9431	1/1	0.98	0.07	61,61,61,61	0
37	SR	9	9503	1/1	0.98	0.07	104,104,104,104	0
37	SR	0	9464	1/1	0.98	0.05	73,73,73,73	0
33	MG	0	8038	1/1	0.99	0.27	27,27,27,27	0
33	MG	K	8069	1/1	0.99	0.28	22,22,22,22	0
37	SR	R	9418	1/1	0.99	0.12	50,50,50,50	0
36	CL	0	9312	1/1	0.99	0.13	48,48,48,48	0
37	SR	0	9425	1/1	0.99	0.12	54,54,54,54	0
37	SR	0	9443	1/1	0.99	0.06	54,54,54,54	0
37	SR	0	9450	1/1	0.99	0.06	65,65,65,65	0
37	SR	0	9423	1/1	0.99	0.04	56,56,56,56	0
37	SR	0	9406	1/1	0.99	0.14	32,32,32,32	0
37	SR	0	9441	1/1	0.99	0.06	62,62,62,62	0
37	SR	0	9451	1/1	0.99	0.07	62,62,62,62	0
37	SR	0	9438	1/1	0.99	0.06	59,59,59,59	0
37	SR	0	9454	1/1	0.99	0.05	65,65,65,65	0
37	SR	0	9422	1/1	0.99	0.09	52,52,52,52	0
37	SR	0	9545	1/1	0.99	0.03	70,70,70,70	0
37	SR	0	9449	1/1	0.99	0.06	60,60,60,60	0
33	MG	0	8026	1/1	0.99	0.20	33,33,33,33	0
36	CL	J	9302	1/1	0.99	0.09	51,51,51,51	0
37	SR	0	9529	1/1	0.99	0.05	89,89,89,89	0
33	MG	0	8015	1/1	0.99	0.07	31,31,31,31	0
33	MG	0	8030	1/1	0.99	0.09	34,34,34,34	0
38	CD	3	9204	1/1	0.99	0.05	57,57,57,57	0
37	SR	0	9414	1/1	0.99	0.10	57,57,57,57	0
37	SR	0	9461	1/1	0.99	0.04	69,69,69,69	0
37	SR	0	9411	1/1	0.99	0.15	42,42,42,42	0
33	MG	0	8067	1/1	0.99	0.08	38,38,38,38	0
37	SR	9	9481	1/1	0.99	0.04	80,80,80,80	0
37	SR	0	9430	1/1	0.99	0.09	47,47,47,47	0
35	NA	0	9123	1/1	0.99	0.08	38,38,38,38	0
37	SR	0	9462	1/1	0.99	0.10	64,64,64,64	0
37	SR	1	9460	1/1	0.99	0.07	47,47,47,47	0
35	NA	0	9128	1/1	0.99	0.09	40,40,40,40	0
33	MG	0	8008	1/1	0.99	0.15	23,23,23,23	0
37	SR	0	9498	1/1	0.99	0.03	58,58,58,58	0
38	CD	U	9201	1/1	0.99	0.07	58,58,58,58	0
37	SR	0	9534	1/1	0.99	0.16	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	9413	1/1	0.99	0.10	43,43,43,43	0
36	CL	M	9318	1/1	0.99	0.17	39,39,39,39	0
33	MG	0	8070	1/1	0.99	0.18	27,27,27,27	0
37	SR	0	9416	1/1	0.99	0.08	45,45,45,45	0
37	SR	0	9445	1/1	0.99	0.07	55,55,55,55	0
37	SR	0	9488	1/1	0.99	0.07	69,69,69,69	0
37	SR	0	9446	1/1	0.99	0.09	77,77,77,77	0
37	SR	0	9456	1/1	0.99	0.04	57,57,57,57	0
37	SR	0	9474	1/1	0.99	0.06	57,57,57,57	0
37	SR	0	9421	1/1	0.99	0.05	66,66,66,66	0
38	CD	1	9202	1/1	0.99	0.04	50,50,50,50	0
37	SR	0	9410	1/1	0.99	0.13	36,36,36,36	0
37	SR	0	9444	1/1	0.99	0.04	51,51,51,51	0
37	SR	0	9478	1/1	0.99	0.07	71,71,71,71	0
37	SR	0	9473	1/1	0.99	0.03	69,69,69,69	0
37	SR	L	9409	1/1	1.00	0.10	36,36,36,36	0
37	SR	0	9407	1/1	1.00	0.10	41,41,41,41	0
37	SR	0	9448	1/1	1.00	0.06	52,52,52,52	0
37	SR	0	9408	1/1	1.00	0.11	36,36,36,36	0
37	SR	A	9436	1/1	1.00	0.06	47,47,47,47	0
37	SR	0	9428	1/1	1.00	0.03	49,49,49,49	0
37	SR	0	9501	1/1	1.00	0.07	64,64,64,64	0
37	SR	0	9424	1/1	1.00	0.13	45,45,45,45	0
37	SR	0	9412	1/1	1.00	0.11	38,38,38,38	0
37	SR	0	9415	1/1	1.00	0.10	50,50,50,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.