



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:23 PM GMT

PDB ID : 1JJ2  
Title : Fully Refined Crystal Structure of the Haloarcula marismortui Large Ribosomal Subunit at 2.4 Angstrom Resolution  
Authors : Klein, D.J.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2001-07-03  
Resolution : 2.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

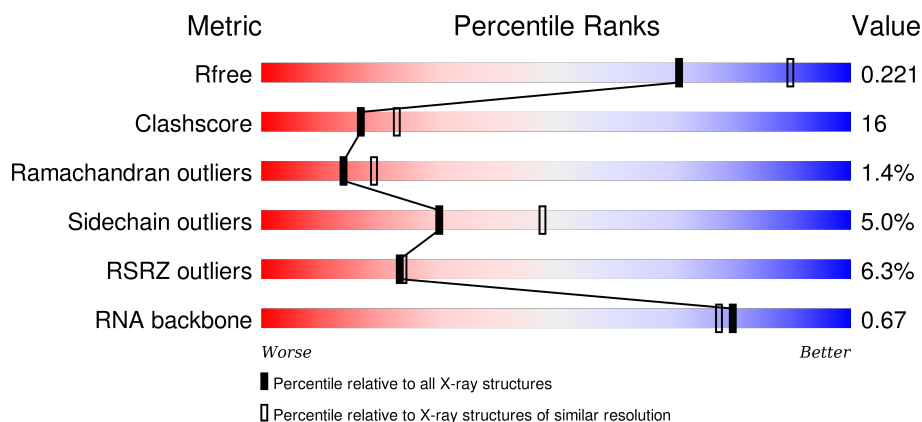
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)
RNA backbone	2183	1073 (2.90-1.90)

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  $\geq 3$ , 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>2%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>5%</div> <div> <div></div> <div>56%</div> <div>32%</div> <div>9%</div> <div>.</div> </div> </div>
3	A	239	<div> <div>9%</div> <div> <div></div> <div>62%</div> <div>31%</div> <div>6%</div> <div>.</div> </div> </div>
4	B	337	<div> <div>5%</div> <div> <div></div> <div>53%</div> <div>41%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	C	246	
6	D	176	
7	E	177	
8	F	119	
9	G	348	
10	H	167	
11	I	145	
12	J	132	
13	K	164	
14	L	194	
15	M	186	
16	N	115	
17	O	148	
18	P	95	
19	Q	154	
20	R	84	
21	S	119	
22	T	66	
23	U	70	
24	V	154	
25	W	91	
26	X	240	
27	Y	73	
28	Z	56	
29	1	48	

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Mol	Chain	Length	Quality of chain
30	2	92	 3% 62% 35% ..

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
31	MG	0	8060	-	-	-	X
33	NA	0	8302	-	-	-	X
33	NA	0	8303	-	-	-	X
33	NA	0	8305	-	-	-	X
33	NA	0	8314	-	-	-	X
33	NA	0	8320	-	-	-	X
33	NA	0	8321	-	-	-	X
33	NA	0	8325	-	-	-	X
33	NA	0	8327	-	-	-	X
33	NA	0	8331	-	-	-	X
33	NA	0	8340	-	-	-	X
33	NA	0	8350	-	-	-	X
33	NA	0	8361	-	-	-	X
33	NA	0	8362	-	-	-	X
33	NA	0	8364	-	-	-	X
33	NA	0	8366	-	-	-	X
33	NA	0	8371	-	-	-	X
33	NA	0	8372	-	-	-	X
33	NA	0	8374	-	-	-	X
33	NA	0	8376	-	-	-	X
33	NA	K	8380	-	-	-	X
33	NA	Q	8386	-	-	-	X

## 2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 98543 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	CONFLICT	GB 3377779

- Molecule 2 is a RNA chain called 5S RRNA.

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 protein called RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PRO	DELETION	UNP P20279
B	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	P	95	Total	C	N	O	0	0	0
			734	450	141	143			

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	S	119	Total	C	N	O	0	0	0
			949	568	180	201			

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	V	154	Total	C	N	O	S	0	0	0
			1195	737	209	243	6			

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.



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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	1	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	0	109	Total Mg 109 109	0	0
31	J	1	Total Mg 1 1	0	0
31	B	1	Total Mg 1 1	0	0
31	A	2	Total Mg 2 2	0	0
31	X	1	Total Mg 1 1	0	0
31	2	1	Total Mg 1 1	0	0
31	9	1	Total Mg 1 1	0	0
31	S	1	Total Mg 1 1	0	0

- Molecule 32 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	0	2	Total K 2 2	0	0

- Molecule 33 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	72	Total Na 72 72	0	0
33	P	1	Total Na 1 1	0	0
33	Q	2	Total Na 2 2	0	0
33	K	1	Total Na 1 1	0	0
33	H	2	Total Na 2 2	0	0
33	I	1	Total Na 1 1	0	0
33	C	1	Total Na 1 1	0	0
33	A	1	Total Na 1 1	0	0
33	R	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	2	Total 2	Na 2	0	0
33	L	1	Total 1	Na 1	0	0
33	S	1	Total 1	Na 1	0	0

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	10	Total 10	Cl 10	0	0
34	Q	1	Total 1	Cl 1	0	0
34	K	1	Total 1	Cl 1	0	0
34	B	1	Total 1	Cl 1	0	0
34	I	3	Total 3	Cl 3	0	0
34	A	1	Total 1	Cl 1	0	0
34	N	1	Total 1	Cl 1	0	0
34	X	1	Total 1	Cl 1	0	0
34	2	1	Total 1	Cl 1	0	0
34	L	1	Total 1	Cl 1	0	0
34	M	1	Total 1	Cl 1	0	0

- Molecule 35 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Z	1	Total 1	Cd 1	0	0
35	Y	1	Total 1	Cd 1	0	0
35	T	1	Total 1	Cd 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	2	1	Total	Cd	0	0
			1	1		
35	N	1	Total	Cd	0	0
			1	1		

- Molecule 36 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	5938	Total	O	0	0
			5938	5938		
36	9	135	Total	O	0	0
			135	135		
36	A	126	Total	O	0	0
			126	126		
36	B	150	Total	O	0	0
			150	150		
36	C	172	Total	O	0	0
			172	172		
36	D	53	Total	O	0	0
			53	53		
36	E	46	Total	O	0	0
			46	46		
36	F	28	Total	O	0	0
			28	28		
36	G	21	Total	O	0	0
			21	21		
36	H	74	Total	O	0	0
			74	74		
36	I	56	Total	O	0	0
			56	56		
36	J	62	Total	O	0	0
			62	62		
36	K	80	Total	O	0	0
			80	80		
36	L	127	Total	O	0	0
			127	127		
36	M	70	Total	O	0	0
			70	70		
36	N	43	Total	O	0	0
			43	43		
36	O	68	Total	O	0	0
			68	68		

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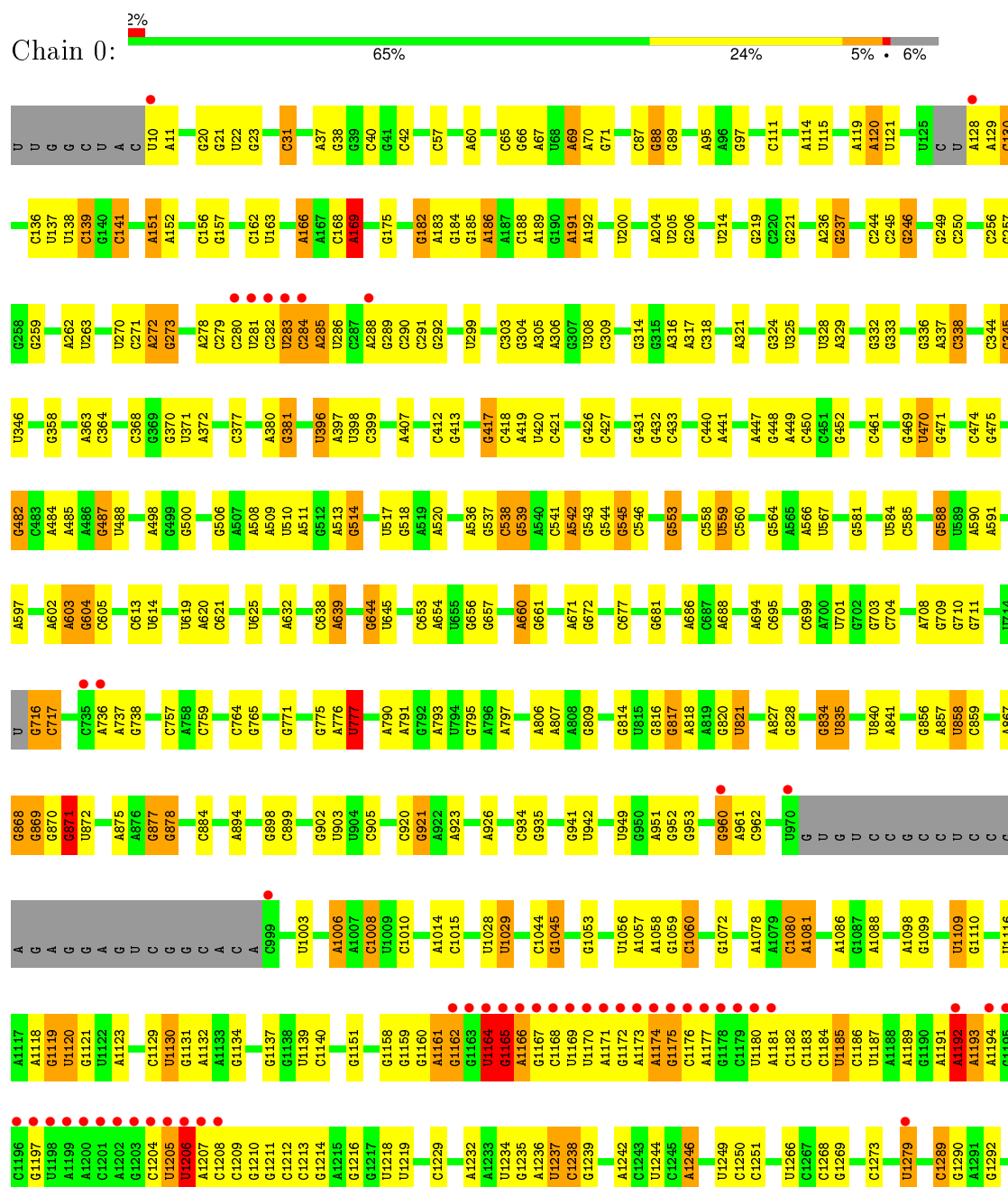
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	53	Total 53	O 53	0	0
36	Q	81	Total 81	O 81	0	0
36	R	32	Total 32	O 32	0	0
36	S	39	Total 39	O 39	0	0
36	T	25	Total 25	O 25	0	0
36	U	15	Total 15	O 15	0	0
36	V	67	Total 67	O 67	0	0
36	W	29	Total 29	O 29	0	0
36	X	99	Total 99	O 99	0	0
36	Y	39	Total 39	O 39	0	0
36	Z	53	Total 53	O 53	0	0
36	1	40	Total 40	O 40	0	0
36	2	72	Total 72	O 72	0	0

### 3 Residue-property plots

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

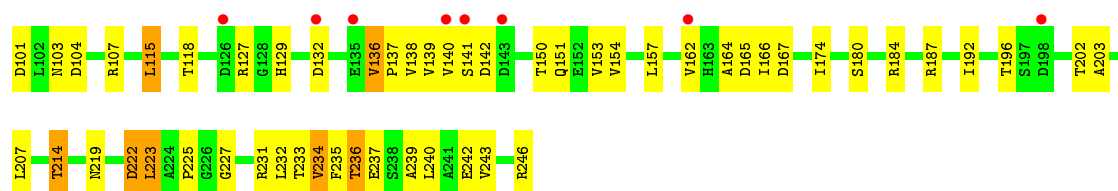
#### • Molecule 1: 23S rRNA



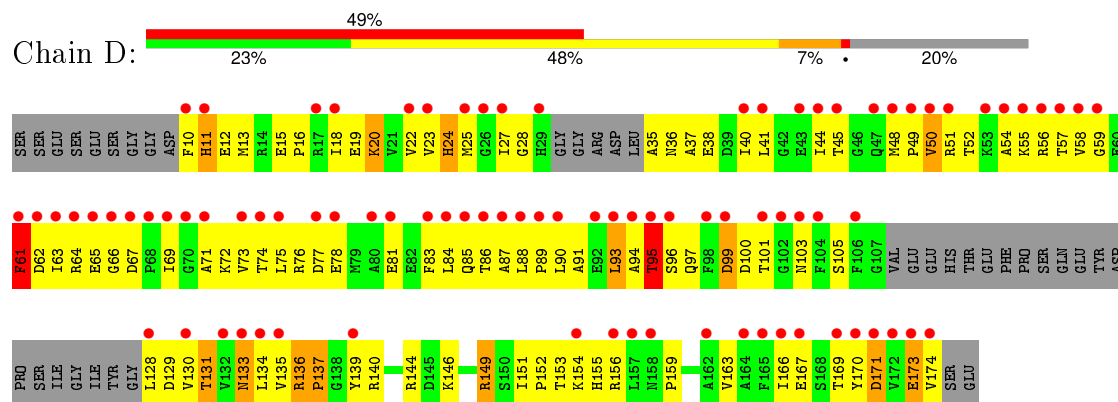
A2820	G2898	C2591	G2480	C2346	G2250	C	G2102	G1971	C1862	U1724	A1598	C1480	G1299
C2821	U2710	G2592	A2483	A2353	G2251	G	G2110	U1972	G1863	C1725	A1603	C1451	U1306
G2826	U2711	U2597	A2354	A2354	A2252	C	G2111	G1973	G1867	G1730	A1604	A1458	U1314
A2827	G2712	U2598	A2361	A2361	G2253	C	A2112	G1974	G1868	C1731	G1605	A1462	A1328
G2828	A2488	A2601	A2362	A2362	G2254	G	G2113	A1978	G1877	A1732	C1613	C1462	A1329
G2829	G2489	G2602	G2363	G2363	A2255	U	G2114	G1979	U1878	A1733	C1614	A1463	A1333
U2830	A2490	A2603	G2364	G2364	G2256	A	U2115	U1980	U1879	C1734	A1615	A1467	U1334
C2831	C2493	A2604	G2365	G2365	A2257	G	U2116	A1981	C1880	A1736	U1625	C1474	C1339
C2832	C2502	A2607	A2369	A2369	C2258	C	G2128	C1982	A1881	U1741	A1626	A1477	G1340
U2837	A2503	C2608	G2383	G2383	U2265	G	G2136	U1986	U1882	A1742	G1627	C1474	A1341
A2840	A2504	A2613	C2388	C2388	A2266	C	A	A1997	U1883	A1742	G1627	C1474	A1343
G2841	G2505	G2614	C2388	C2388	G2270	C	C	G2001	U1887	G1751	A1630	C1477	G1351
G2842	A2506	U2615	C2388	C2388	G2271	A	G	G2002	C1890	C1753	C1633	A1501	C1352
A2843	C2508	G2630	A2395	A2395	G2272	C	U	U2003	G1902	C1756	U1635	A1485	A1353
C2850	A2509	A2637	G2412	G2412	C2273	G	G	G2005	U1903	U1766	U1636	U1488	C1360
G2851	C2510	G2638	A2413	A2413	A2274	A	U	U2008	A1909	U1771	A1641	G1497	A1367
A2852	A2511	A2639	A2414	A2414	U2281	C	C	G2009	C1920	U1778	A1642	U1500	U1368
G2853	C2515	G2640	A2415	A2415	U2282	C	G	A2010	A1921	A1779	U1654	A1501	A1372
U2854	G2516	G2641	G2416	G2416	U2297	G	U	U2012	G1926	C1787	G1655	A1502	A1377
A2855	A2524	A2642	A2416	A2416	U2297	U	U	G2013	C1927	U1788	A1657	A1504	U1505
G2856	G2525	G2643	A2416	A2416	A2291	A	A	A2019	G1928	G1789	A1658	U1506	U1380
A2857	C2527	G2644	A2416	A2416	U2297	C	C	G2033	G1929	G1794	C1666	G1523	C1384
G2858	U2527	G2645	A2416	A2416	U2297	G	G	U2034	C1940	C1798	A1667	U1524	G1385
A2859	G2533	A2646	A2416	A2416	U2297	A	A	G2044	A1941	A1804	A1669	A1526	A1393
U2860	C2534	A2647	A2416	A2416	U2297	U	U	A2054	C1943	G1805	G1670	A1527	C1394
G2861	U2535	A2648	A2416	A2416	U2297	C	C	C2061	G1947	U1677	A1528	A1528	A1406
A2862	G2536	A2649	A2416	A2416	U2297	A	A	A2062	G1948	A1678	G1529	C1545	A1407
G2863	U2537	A2650	A2416	A2416	U2297	C	G	U2063	G1949	C1679	C1545	U1408	G1409
A2864	G2538	A2651	A2416	A2416	U2297	C	A	U2064	G1950	C1680	C1546	A1555	A1413
U2865	U2539	A2652	A2416	A2416	U2297	U	G	G2072	G1951	G1819	G1546	A1555	A1414
G2866	C2540	A2653	A2416	A2416	U2297	C	C	A2074	U	G1820	G1546	A1555	A1417
A2867	A2541	A2654	A2416	A2416	U2297	G	A	G2073	A	A1829	G1546	A1555	U1418
U2868	G2542	A2655	A2416	A2416	U2297	C	G	A2078	A	C1834	G1546	A1555	U1419
G2869	U2543	A2656	A2416	A2416	U2297	G	A	U2078	A	U1835	A1589	A1555	C1423
A2870	C2544	A2657	A2416	A2416	U2297	C	C	A2081	A	A1840	U	A1589	A1424
U2871	G2545	A2658	A2416	A2416	U2297	U	A	G2082	A	A1845	C1592	A1589	G1430
G2872	U2546	A2659	A2416	A2416	U2297	C	C	U2083	A	A1845	C1599	A1589	G1430
A2873	C2547	A2660	A2416	A2416	U2297	G	C	A2089	U	G1848	G1700	A1589	C1439
U2874	G2548	A2661	A2416	A2416	U2297	C	A	G2090	C	C1848	A1701	C1594	U1440
G2875	U2549	A2662	A2416	A2416	U2297	C	C	G2091	C	G1848	U1702	U1596	G1441
A2876	C2550	A2663	A2416	A2416	U2297	C	C	A2095	U	G1848	A1710	U1596	A1442
U2877	G2551	A2664	A2416	A2416	U2297	C	C	G2096	C	G1848	A1710	U1596	A1442
G2878	U2552	A2665	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
A2879	C2553	A2666	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
U2880	U2554	A2667	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
G2881	G2555	A2668	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
A2882	C2556	A2669	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
U2883	U2557	A2670	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
G2884	G2558	A2671	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
A2885	C2559	A2672	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
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G2887	C2561	A2674	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
A2888	U2562	A2675	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
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A2891	C2565	A2678	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
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A2903	C2577	A2690	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
U2904	U2578	A2691	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
G2905	G2579	A2692	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
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G2908	U2582	A2695	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
A2909	G2583	A2696	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
U2910	U2584	A2697	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
G2911	C2585	A2698	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
A2912	U2586	A2699	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
U2913	G2587	A2700	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
G2914	U2588	A2701	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
A2915	C2589	A2702	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
U2916	U2590	A2703	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
G2917	G2591	A2704	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
A2918	U2592	A2705	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
U2919	C2593	A2706	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
G2920	U2594	A2707	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
A2921	C2595	A2708	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
U2922	U2596	A2709	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
G2923	G2597	A2710	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
A2924	U2598	A2711	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
U2925	C2599	A2712	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
G2926	U2600	A2713	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
A2927	C2601	A2714	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
U2928	U2602	A2715	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
G2929	G2603	A2716	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
A2930	A2604	A2717	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
U2931	C2605	A2718	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
G2932	U2607	A2719	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	A1442
U2933	A2608	A2720	A2416	A2416	U2297	C	C	G2096	U	G1848	A1710	U1596	A1442
G2934	G2610	A2721	A2416	A2416	U2297	C	C	A2096	U	G1848	A1710	U1596	



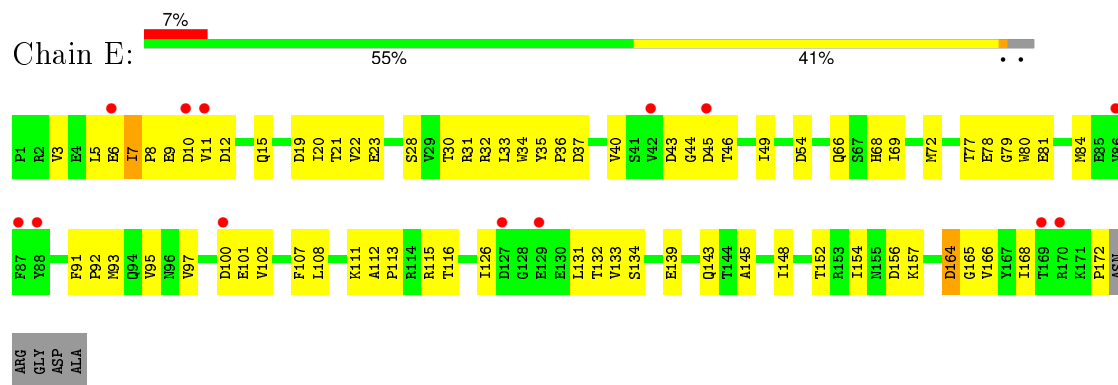




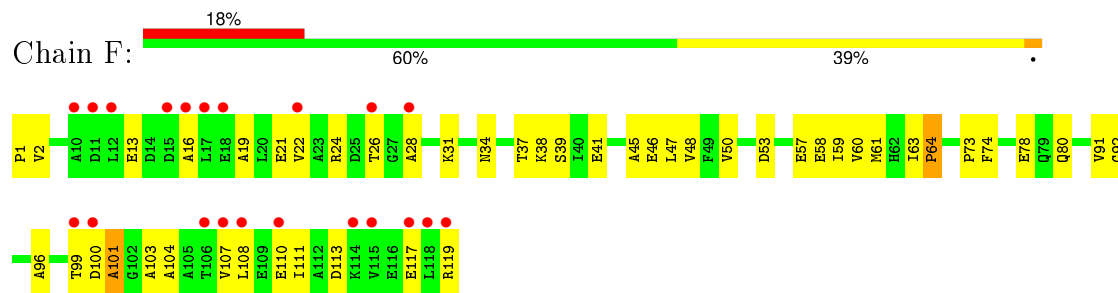
• Molecule 6: RIBOSOMAL PROTEIN L5



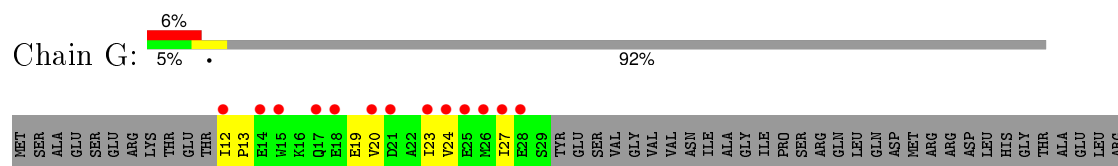
• Molecule 7: RIBOSOMAL PROTEIN L6



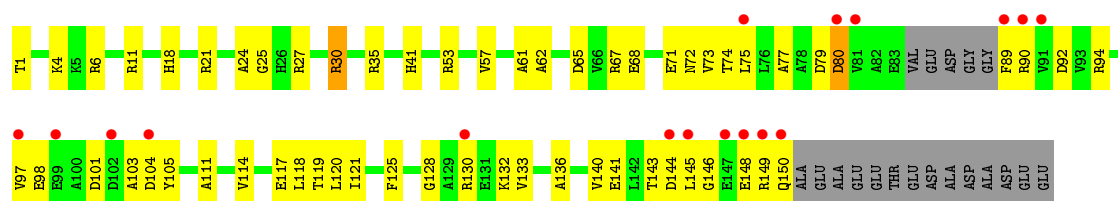
• Molecule 8: RIBOSOMAL PROTEIN L7AE



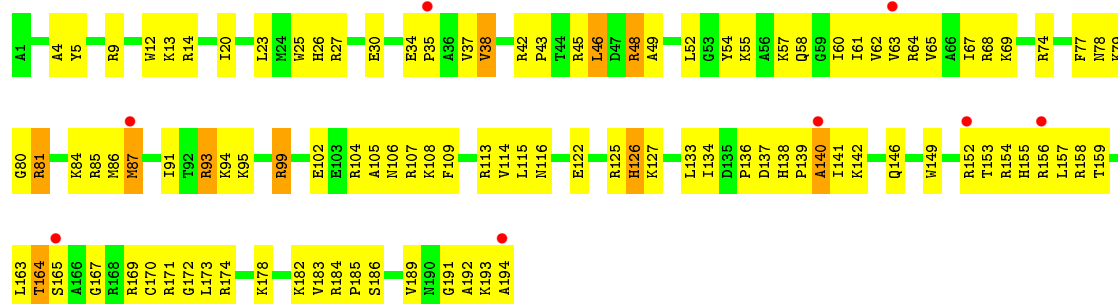
• Molecule 9: RIBOSOMAL PROTEIN L10



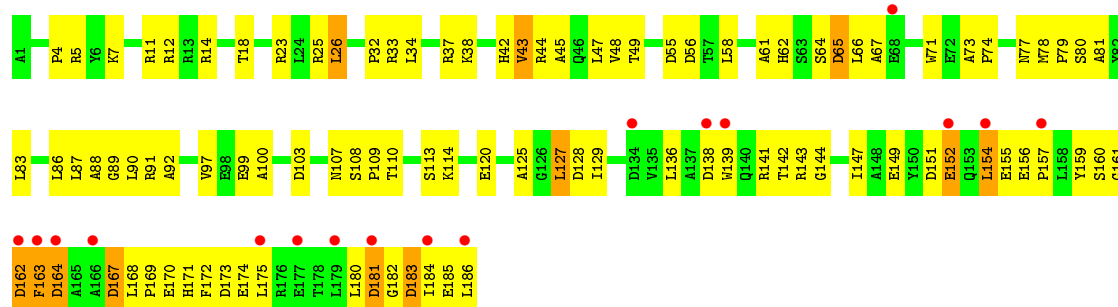




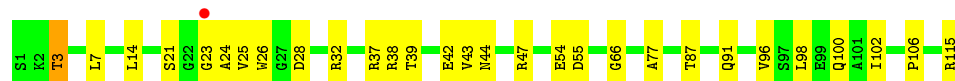
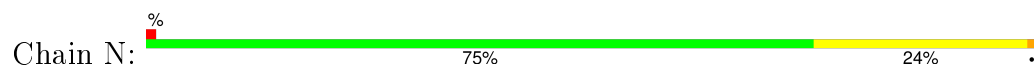
• Molecule 14: RIBOSOMAL PROTEIN L15E



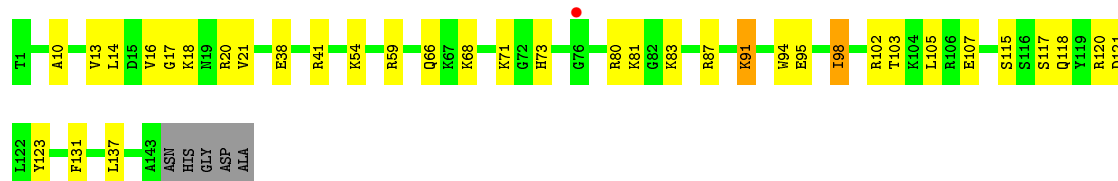
• Molecule 15: RIBOSOMAL PROTEIN L18



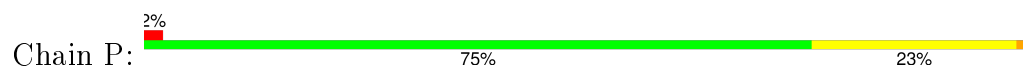
• Molecule 16: RIBOSOMAL PROTEIN L18E



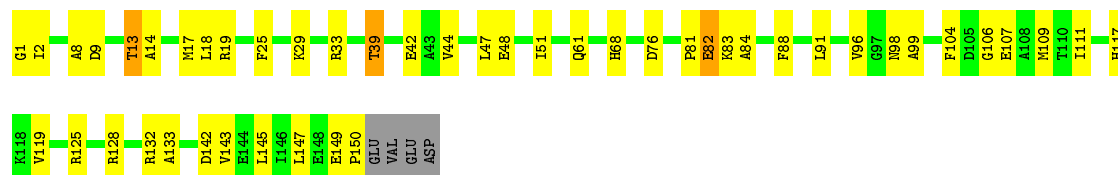
• Molecule 17: RIBOSOMAL PROTEIN L19E



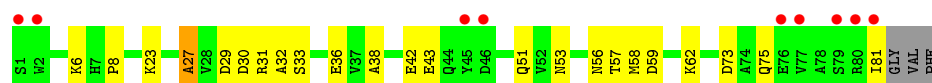
- Molecule 18: RIBOSOMAL PROTEIN L21E



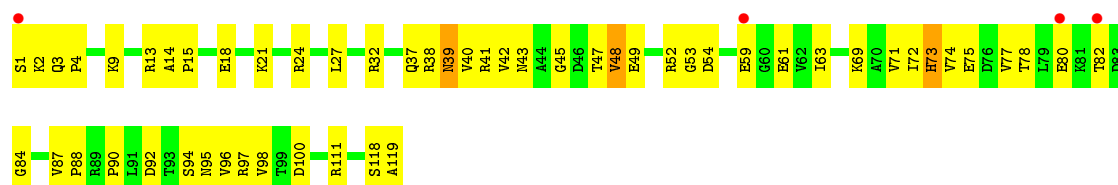
- Molecule 19: RIBOSOMAL PROTEIN L22



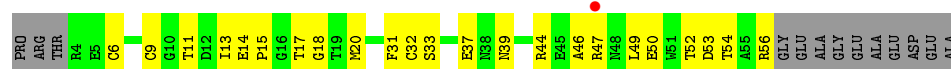
- Molecule 20: RIBOSOMAL PROTEIN L23



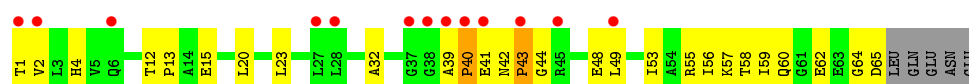
- Molecule 21: RIBOSOMAL PROTEIN L24



- Molecule 22: RIBOSOMAL PROTEIN L24E



- Molecule 23: RIBOSOMAL PROTEIN L29

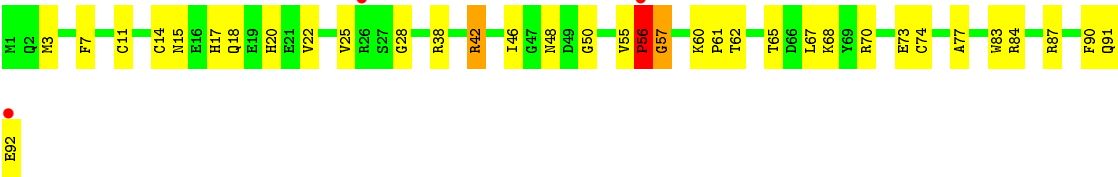


- Molecule 24: RIBOSOMAL PROTEIN L30





● Molecule 30: RIBOSOMAL PROTEIN L44E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.66Å 299.67Å 573.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.40 85.48 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (15.00-2.40) 90.6 (85.48-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.37 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.189 , 0.222 0.189 , 0.221	Depositor DCC
$R_{free}$ test set	6512 reflections (1.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	38.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 666819 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	98543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NA, MG, CD, K, CL

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	3/66076 (0.0%)	0.71	32/103052 (0.0%)
2	9	0.44	3/2905 (0.1%)	0.85	11/4528 (0.2%)
3	A	0.34	0/1787	0.66	0/2409
4	B	0.34	0/2689	0.64	0/3652
5	C	0.39	0/1883	0.67	0/2551
6	D	0.31	0/1111	0.59	0/1498
7	E	0.31	0/1382	0.57	0/1880
8	F	0.33	0/896	0.56	0/1219
9	G	0.25	0/241	0.47	0/324
10	H	0.38	0/1246	0.74	1/1686 (0.1%)
11	I	0.33	0/1135	0.61	0/1530
12	J	0.33	0/1003	0.65	0/1351
13	K	0.34	0/1126	0.68	0/1504
14	L	0.41	0/1633	0.71	1/2180 (0.0%)
15	M	0.29	0/1473	0.64	0/1999
16	N	0.32	0/873	0.61	1/1181 (0.1%)
17	O	0.33	0/1143	0.54	0/1521
18	P	0.35	0/748	0.68	0/1005
19	Q	0.35	0/1172	0.67	0/1578
20	R	0.32	0/648	0.59	1/875 (0.1%)
21	S	0.31	0/957	0.63	0/1289
22	T	0.32	0/417	0.58	0/562
23	U	0.29	0/502	0.54	0/675
24	V	0.33	0/1218	0.62	0/1655
25	W	0.32	0/664	0.60	0/895
26	X	0.34	0/1146	0.63	0/1536
27	Y	0.37	0/575	0.69	0/763
28	Z	0.42	0/437	0.67	0/578
29	1	0.34	0/398	0.54	0/527
30	2	0.38	0/771	0.62	0/1024
All	All	0.37	6/98255 (0.0%)	0.70	47/147027 (0.0%)



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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	1	62
2	9	0	2
All	All	1	64

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	9	3	A	C2'-O2'	-7.92	1.31	1.41
1	0	1206	U	P-OP2	6.22	1.59	1.49
2	9	3	A	O5'-C5'	6.21	1.54	1.44
1	0	1206	U	C3'-O3'	-5.28	1.34	1.42
1	0	1205	U	C3'-O3'	-5.23	1.34	1.42

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1165	G	O5'-P-OP1	-22.95	83.17	110.70
1	0	1164	U	OP1-P-O3'	-20.79	59.47	105.20
1	0	1165	G	O5'-P-OP2	-15.10	92.11	105.70
2	9	3	A	OP1-P-O3'	-13.36	75.82	105.20
1	0	1164	U	OP2-P-O3'	-13.28	75.98	105.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	191	A	Sidechain
1	0	22	U	Sidechain
1	0	221	G	Sidechain
1	0	246	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	59017	0	29807	760	0
2	9	2600	0	1326	78	0
3	A	1754	0	1763	109	0
4	B	2624	0	2533	176	0
5	C	1858	0	1816	105	0
6	D	1094	0	1085	130	0
7	E	1357	0	1266	79	0
8	F	885	0	854	59	0
9	G	240	0	231	18	0
10	H	1215	0	1215	150	0
11	I	1119	0	1098	62	0
12	J	993	0	1027	56	0
13	K	1114	0	1072	55	0
14	L	1605	0	1676	141	0
15	M	1444	0	1401	119	0
16	N	864	0	873	31	0
17	O	1133	0	1127	38	0
18	P	734	0	728	18	0
19	Q	1149	0	1122	49	0
20	R	641	0	605	21	0
21	S	949	0	923	52	0
22	T	410	0	364	31	0
23	U	499	0	511	28	0
24	V	1195	0	1137	91	0
25	W	654	0	653	44	0
26	X	1130	0	1133	52	0
27	Y	563	0	597	53	0
28	Z	430	0	426	22	0
29	1	393	0	406	32	0
30	2	755	0	728	36	0
31	0	109	0	0	0	0
31	2	1	0	0	0	0
31	9	1	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	J	1	0	0	0	0
31	S	1	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	X	1	0	0	0	0
32	0	2	0	0	0	0
33	0	72	0	0	0	0
33	9	2	0	0	0	0
33	A	1	0	0	0	0
33	C	1	0	0	0	0
33	H	2	0	0	0	0
33	I	1	0	0	0	0
33	K	1	0	0	0	0
33	L	1	0	0	0	0
33	P	1	0	0	0	0
33	Q	2	0	0	0	0
33	R	1	0	0	0	0
33	S	1	0	0	0	0
34	0	10	0	0	0	0
34	2	1	0	0	0	0
34	A	1	0	0	0	0
34	B	1	0	0	0	0
34	I	3	0	0	1	0
34	K	1	0	0	0	0
34	L	1	0	0	1	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	Q	1	0	0	0	0
34	X	1	0	0	0	0
35	2	1	0	0	0	0
35	N	1	0	0	0	0
35	T	1	0	0	0	0
35	Y	1	0	0	0	0
35	Z	1	0	0	0	0
36	0	5938	0	0	173	0
36	1	40	0	0	6	0
36	2	72	0	0	10	0
36	9	135	0	0	14	0
36	A	126	0	0	20	0
36	B	150	0	0	30	0
36	C	172	0	0	30	0
36	D	53	0	0	18	0
36	E	46	0	0	12	0
36	F	28	0	0	7	0
36	G	21	0	0	4	0
36	H	74	0	0	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	I	56	0	0	5	0
36	J	62	0	0	13	0
36	K	80	0	0	17	0
36	L	127	0	0	19	0
36	M	70	0	0	16	0
36	N	43	0	0	6	0
36	O	68	0	0	1	0
36	P	53	0	0	1	0
36	Q	81	0	0	9	0
36	R	32	0	0	5	0
36	S	39	0	0	5	0
36	T	25	0	0	6	0
36	U	15	0	0	4	0
36	V	67	0	0	10	0
36	W	29	0	0	3	0
36	X	99	0	0	15	0
36	Y	39	0	0	12	0
36	Z	53	0	0	1	0
All	All	98543	0	59503	2453	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 16.

The worst 5 of 2453 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.26	1.14
10:H:86:ARG:NH1	10:H:133:ILE:HG13	1.62	1.12
5:C:5:ILE:HD11	5:C:16:VAL:HG23	1.35	1.07
25:W:37:LEU:HD13	25:W:85:VAL:HG21	1.29	1.06
1:0:960:G:H4'	36:0:6956:HOH:O	1.54	1.06

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	
3	A	235/239 (98%)	216 (92%)	14 (6%)	5 (2%)	9	10
4	B	335/337 (99%)	314 (94%)	14 (4%)	7 (2%)	9	10
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/176 (76%)	97 (72%)	28 (21%)	9 (7%)	1	0
7	E	170/177 (96%)	161 (95%)	8 (5%)	1 (1%)	30	43
8	F	117/119 (98%)	106 (91%)	9 (8%)	2 (2%)	11	14
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	152/167 (91%)	135 (89%)	12 (8%)	5 (3%)	5	4
11	I	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	9	10
12	J	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	24	35
13	K	141/164 (86%)	121 (86%)	19 (14%)	1 (1%)	26	38
14	L	192/194 (99%)	181 (94%)	10 (5%)	1 (0%)	34	48
15	M	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	4	3
16	N	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	O	141/148 (95%)	138 (98%)	3 (2%)	0	100	100
18	P	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
19	Q	148/154 (96%)	143 (97%)	4 (3%)	1 (1%)	26	38
20	R	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
21	S	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
22	T	51/66 (77%)	48 (94%)	3 (6%)	0	100	100
23	U	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	5	4
24	V	152/154 (99%)	147 (97%)	4 (3%)	1 (1%)	26	38
25	W	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	7	7
26	X	140/240 (58%)	140 (100%)	0	0	100	100
27	Y	71/73 (97%)	64 (90%)	5 (7%)	2 (3%)	6	5
28	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	1	42/48 (88%)	42 (100%)	0	0	100	100
30	2	90/92 (98%)	86 (96%)	2 (2%)	2 (2%)	8	9
All	All	3633/4235 (86%)	3372 (93%)	209 (6%)	52 (1%)	14	19

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	139	ASP
6	D	93	LEU
6	D	95	THR
6	D	137	PRO
6	D	173	GLU

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	179/181 (99%)	166 (93%)	13 (7%)	17	27
4	B	282/282 (100%)	264 (94%)	18 (6%)	22	34
5	C	193/193 (100%)	179 (93%)	14 (7%)	17	27
6	D	117/147 (80%)	106 (91%)	11 (9%)	11	16
7	E	152/155 (98%)	148 (97%)	4 (3%)	54	74
8	F	92/92 (100%)	91 (99%)	1 (1%)	80	92
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	122/122 (100%)	109 (89%)	13 (11%)	8	11
11	I	118/121 (98%)	109 (92%)	9 (8%)	16	25
12	J	106/106 (100%)	103 (97%)	3 (3%)	51	72
13	K	112/126 (89%)	108 (96%)	4 (4%)	42	63
14	L	166/166 (100%)	157 (95%)	9 (5%)	27	43
15	M	149/149 (100%)	143 (96%)	6 (4%)	38	58
16	N	93/93 (100%)	91 (98%)	2 (2%)	60	79
17	O	113/116 (97%)	111 (98%)	2 (2%)	66	84
18	P	79/79 (100%)	75 (95%)	4 (5%)	29	46
19	Q	117/121 (97%)	114 (97%)	3 (3%)	54	74
20	R	71/73 (97%)	71 (100%)	0	100	100
21	S	105/105 (100%)	101 (96%)	4 (4%)	40	60
22	T	44/52 (85%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	U	51/56 (91%)	50 (98%)	1 (2%)	63	81
24	V	130/130 (100%)	122 (94%)	8 (6%)	23	35
25	W	66/73 (90%)	62 (94%)	4 (6%)	23	36
26	X	120/195 (62%)	110 (92%)	10 (8%)	14	21
27	Y	56/56 (100%)	52 (93%)	4 (7%)	18	28
28	Z	46/46 (100%)	46 (100%)	0	100	100
29	1	42/44 (96%)	41 (98%)	1 (2%)	57	76
30	2	79/79 (100%)	76 (96%)	3 (4%)	40	60
All	All	3027/3441 (88%)	2876 (95%)	151 (5%)	30	48

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	86	ARG
12	J	10	GLN
26	X	200	THR
10	H	129	ASN
11	I	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 87 such sidechains are listed below:

Mol	Chain	Res	Type
13	K	116	HIS
17	O	50	GLN
28	Z	28	HIS
14	L	26	HIS
15	M	21	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2747/2922 (94%)	239 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	5 (4%)
All	All	2868/3044 (94%)	255 (8%)	40 (1%)

5 of 255 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	11	A
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1856	C
2	9	23	U
1	0	1563	G
1	0	1942	A

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 232 ligands modelled in this entry, 232 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 ⓘ

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, 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	2754/2922 (94%)	-0.20	67 (2%) 62 61	17, 36, 79, 127	0
2	9	122/122 (100%)	-0.18	6 (4%) 33 34	31, 54, 78, 136	0
3	A	237/239 (99%)	0.45	22 (9%) 11 10	19, 38, 71, 92	0
4	B	337/337 (100%)	0.44	16 (4%) 35 36	21, 45, 71, 82	0
5	C	246/246 (100%)	0.38	12 (4%) 33 34	15, 35, 58, 70	0
6	D	140/176 (79%)	2.69	87 (62%) 0 0	43, 86, 105, 108	0
7	E	172/177 (97%)	0.66	13 (7%) 17 16	37, 59, 77, 81	0
8	F	119/119 (100%)	0.98	21 (17%) 2 2	37, 58, 83, 88	0
9	G	29/348 (8%)	2.70	21 (72%) 0 0	64, 79, 86, 91	0
10	H	156/167 (93%)	0.77	25 (16%) 3 2	30, 47, 75, 79	0
11	I	142/145 (97%)	0.30	6 (4%) 40 41	29, 42, 63, 84	0
12	J	132/132 (100%)	0.22	7 (5%) 30 30	27, 42, 61, 71	0
13	K	145/164 (88%)	0.77	17 (11%) 6 6	18, 54, 90, 102	0
14	L	194/194 (100%)	0.18	8 (4%) 41 42	19, 32, 50, 62	0
15	M	186/186 (100%)	0.67	17 (9%) 11 11	31, 50, 91, 103	0
16	N	115/115 (100%)	0.02	1 (0%) 85 85	27, 44, 60, 69	0
17	O	143/148 (96%)	0.19	1 (0%) 89 88	30, 44, 57, 64	0
18	P	95/95 (100%)	0.13	2 (2%) 67 66	25, 34, 50, 61	0
19	Q	150/154 (97%)	0.02	0 100 100	23, 36, 54, 63	0
20	R	81/84 (96%)	0.53	9 (11%) 7 7	31, 47, 68, 72	0
21	S	119/119 (100%)	0.47	4 (3%) 49 49	28, 45, 69, 81	0
22	T	53/66 (80%)	0.41	1 (1%) 70 69	33, 47, 63, 71	0
23	U	65/70 (92%)	1.73	13 (20%) 1 1	39, 59, 97, 101	0
24	V	154/154 (100%)	0.40	5 (3%) 51 51	27, 40, 57, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	82/91 (90%)	0.52	7 (8%) 13 13	35, 48, 73, 91	0
26	X	142/240 (59%)	0.05	5 (3%) 48 48	22, 35, 59, 74	0
27	Y	73/73 (100%)	0.64	9 (12%) 5 5	36, 49, 63, 77	0
28	Z	56/56 (100%)	0.27	0 100 100	17, 24, 32, 35	0
29	1	46/48 (95%)	0.58	7 (15%) 3 3	27, 49, 77, 86	0
30	2	92/92 (100%)	0.26	3 (3%) 50 50	23, 44, 59, 72	0
All	All	6577/7279 (90%)	0.21	412 (6%) 23 24	15, 41, 80, 136	0

The worst 5 of 412 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	U	1	THR	14.4
6	D	63	ILE	10.3
23	U	39	ALA	9.1
6	D	57	THR	7.9
23	U	40	PRO	7.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
33	NA	0	8320	1/1	0.99	0.29	31.60	38,38,38,38	0
33	NA	0	8350	1/1	0.93	0.35	29.76	36,36,36,36	0
33	NA	0	8371	1/1	0.76	0.36	23.72	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	NA	0	8372	1/1	0.92	0.43	23.09	54,54,54,54	0
33	NA	0	8362	1/1	0.94	0.34	18.39	51,51,51,51	0
33	NA	0	8327	1/1	0.92	0.27	17.22	38,38,38,38	0
33	NA	0	8340	1/1	0.90	0.26	15.56	47,47,47,47	0
33	NA	Q	8386	1/1	0.62	0.44	12.93	74,74,74,74	0
33	NA	0	8366	1/1	0.96	0.26	12.64	54,54,54,54	0
33	NA	0	8331	1/1	0.98	0.27	11.15	39,39,39,39	0
33	NA	0	8376	1/1	0.91	0.28	10.71	39,39,39,39	0
33	NA	0	8302	1/1	0.93	0.24	9.87	44,44,44,44	0
33	NA	0	8364	1/1	0.97	0.26	8.74	38,38,38,38	0
33	NA	0	8314	1/1	0.93	0.32	8.45	40,40,40,40	0
33	NA	0	8374	1/1	0.96	0.20	6.89	44,44,44,44	0
33	NA	0	8325	1/1	0.94	0.23	4.93	47,47,47,47	0
33	NA	0	8361	1/1	0.93	0.23	4.34	38,38,38,38	0
33	NA	K	8380	1/1	0.97	0.26	4.24	42,42,42,42	0
33	NA	0	8305	1/1	0.98	0.22	4.09	32,32,32,32	0
31	MG	0	8060	1/1	0.99	0.21	3.89	31,31,31,31	0
33	NA	0	8321	1/1	0.94	0.24	2.81	40,40,40,40	0
33	NA	0	8303	1/1	0.98	0.17	2.58	32,32,32,32	0
33	NA	9	8383	1/1	0.89	0.21	1.79	43,43,43,43	0
33	NA	0	8356	1/1	0.93	0.20	1.33	37,37,37,37	0
33	NA	0	8368	1/1	0.94	0.14	1.04	48,48,48,48	0
33	NA	0	8335	1/1	0.96	0.18	0.92	31,31,31,31	0
33	NA	0	8339	1/1	0.98	0.19	0.87	20,20,20,20	0
31	MG	0	8012	1/1	0.95	0.14	0.51	32,32,32,32	0
33	NA	0	8373	1/1	0.90	0.12	0.27	43,43,43,43	0
33	NA	C	8304	1/1	0.85	0.18	-0.09	30,30,30,30	0
33	NA	0	8365	1/1	0.96	0.18	-0.20	28,28,28,28	0
31	MG	0	8067	1/1	0.91	0.14	-0.24	34,34,34,34	0
33	NA	0	8324	1/1	0.95	0.13	-0.25	48,48,48,48	0
31	MG	0	8010	1/1	0.97	0.17	-0.35	24,24,24,24	0
31	MG	0	8007	1/1	0.98	0.17	-0.39	21,21,21,21	0
34	CL	I	8521	1/1	0.94	0.17	-0.39	47,47,47,47	0
34	CL	0	8516	1/1	0.99	0.14	-0.47	42,42,42,42	0
34	CL	L	8518	1/1	0.98	0.15	-0.50	32,32,32,32	0
33	NA	0	8381	1/1	0.98	0.12	-0.54	41,41,41,41	0
35	CD	Y	8403	1/1	0.99	0.14	-0.67	49,49,49,49	0
31	MG	0	8064	1/1	0.94	0.15	-0.72	26,26,26,26	0
33	NA	0	8378	1/1	0.97	0.17	-0.73	39,39,39,39	0
31	MG	0	8013	1/1	0.95	0.15	-0.75	22,22,22,22	0
33	NA	L	8347	1/1	0.97	0.14	-0.82	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8086	1/1	0.99	0.09	-0.90	33,33,33,33	0
31	MG	0	8015	1/1	0.98	0.18	-1.03	26,26,26,26	0
33	NA	0	8344	1/1	0.97	0.11	-1.11	24,24,24,24	0
33	NA	0	8382	1/1	0.94	0.10	-1.31	64,64,64,64	0
31	MG	0	8038	1/1	0.98	0.13	-1.38	22,22,22,22	0
33	NA	H	8309	1/1	0.99	0.10	-1.47	28,28,28,28	0
34	CL	0	8515	1/1	0.99	0.11	-1.54	48,48,48,48	0
33	NA	0	8332	1/1	0.97	0.12	-1.54	33,33,33,33	0
35	CD	T	8401	1/1	0.99	0.10	-1.62	49,49,49,49	0
33	NA	0	8310	1/1	0.94	0.11	-1.74	27,27,27,27	0
34	CL	B	8519	1/1	0.99	0.14	-1.78	33,33,33,33	0
35	CD	2	8404	1/1	0.99	0.09	-1.86	47,47,47,47	0
34	CL	0	8512	1/1	0.99	0.11	-1.86	34,34,34,34	0
31	MG	0	8054	1/1	0.98	0.16	-1.94	18,18,18,18	0
33	NA	I	8346	1/1	0.98	0.09	-2.02	34,34,34,34	0
33	NA	0	8353	1/1	0.99	0.14	-2.14	18,18,18,18	0
33	NA	0	8333	1/1	0.95	0.09	-2.19	23,23,23,23	0
31	MG	0	8004	1/1	0.99	0.13	-2.28	21,21,21,21	0
31	MG	0	8027	1/1	0.98	0.06	-2.39	37,37,37,37	0
33	NA	0	8317	1/1	0.96	0.10	-2.53	27,27,27,27	0
33	NA	0	8334	1/1	0.95	0.09	-2.54	33,33,33,33	0
34	CL	0	8505	1/1	0.98	0.11	-2.66	41,41,41,41	0
32	K	0	8201	1/1	0.95	0.14	-2.72	62,62,62,62	0
34	CL	N	8508	1/1	0.97	0.07	-2.75	52,52,52,52	0
31	MG	2	8078	1/1	0.98	0.10	-2.77	39,39,39,39	0
33	NA	P	8348	1/1	0.95	0.07	-2.80	32,32,32,32	0
31	MG	S	8073	1/1	0.98	0.06	-3.07	39,39,39,39	0
33	NA	A	8345	1/1	0.93	0.09	-3.18	46,46,46,46	0
31	MG	0	8091	1/1	0.96	0.10	-3.21	41,41,41,41	0
33	NA	S	8343	1/1	0.97	0.06	-3.27	29,29,29,29	0
31	MG	0	8003	1/1	0.98	0.11	-3.28	21,21,21,21	0
31	MG	0	8077	1/1	0.92	0.14	-3.29	23,23,23,23	0
31	MG	0	8057	1/1	0.98	0.12	-3.32	35,35,35,35	0
31	MG	0	8074	1/1	0.97	0.06	-3.40	36,36,36,36	0
31	MG	0	8096	1/1	0.97	0.10	-3.50	37,37,37,37	0
31	MG	0	8017	1/1	1.00	0.13	-3.61	12,12,12,12	0
31	MG	0	8112	1/1	0.98	0.10	-3.93	23,23,23,23	0
31	MG	0	8033	1/1	0.97	0.09	-4.00	20,20,20,20	0
35	CD	Z	8402	1/1	0.99	0.04	-4.10	37,37,37,37	0
31	MG	0	8008	1/1	0.99	0.10	-4.16	22,22,22,22	0
31	MG	X	8109	1/1	0.98	0.08	-4.18	25,25,25,25	0
31	MG	0	8080	1/1	0.94	0.07	-4.33	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8020	1/1	0.97	0.09	-4.47	24,24,24,24	0
31	MG	0	8110	1/1	0.99	0.10	-4.65	24,24,24,24	0
31	MG	B	8055	1/1	0.91	0.07	-4.80	40,40,40,40	0
31	MG	0	8084	1/1	0.98	0.07	-5.01	39,39,39,39	0
33	NA	Q	8337	1/1	0.96	0.07	-5.14	33,33,33,33	0
33	NA	0	8323	1/1	0.99	0.12	-5.40	31,31,31,31	0
31	MG	0	8056	1/1	0.98	0.04	-5.49	31,31,31,31	0
31	MG	A	8065	1/1	0.97	0.07	-5.63	24,24,24,24	0
31	MG	0	8108	1/1	0.97	0.07	-5.64	62,62,62,62	0
33	NA	0	8313	1/1	0.94	0.09	-5.93	48,48,48,48	0
31	MG	0	8001	1/1	0.98	0.11	-6.04	25,25,25,25	0
33	NA	0	8338	1/1	0.99	0.06	-6.32	36,36,36,36	0
31	MG	0	8107	1/1	0.96	0.03	-6.57	30,30,30,30	0
31	MG	0	8035	1/1	0.98	0.07	-6.62	36,36,36,36	0
31	MG	0	8044	1/1	0.98	0.09	-6.73	32,32,32,32	0
31	MG	0	8058	1/1	0.97	0.06	-6.73	27,27,27,27	0
34	CL	2	8504	1/1	0.98	0.06	-7.08	45,45,45,45	0
31	MG	0	8059	1/1	0.96	0.07	-7.65	25,25,25,25	0
31	MG	0	8053	1/1	0.99	0.07	-8.20	28,28,28,28	0
31	MG	0	8039	1/1	0.97	0.07	-8.73	32,32,32,32	0
31	MG	0	8018	1/1	0.97	0.06	-8.80	27,27,27,27	0
31	MG	0	8032	1/1	0.96	0.06	-8.82	23,23,23,23	0
31	MG	0	8021	1/1	0.99	0.09	-8.96	24,24,24,24	0
31	MG	0	8019	1/1	0.99	0.05	-9.13	23,23,23,23	0
31	MG	0	8006	1/1	0.94	0.07	-10.10	27,27,27,27	0
31	MG	0	8028	1/1	0.96	0.06	-11.38	25,25,25,25	0
31	MG	0	8071	1/1	0.94	0.04	-11.41	62,62,62,62	0
31	MG	0	8002	1/1	0.96	0.08	-12.77	26,26,26,26	0
31	MG	0	8052	1/1	0.98	0.06	-14.41	45,45,45,45	0
32	K	0	8202	1/1	0.99	0.08	-16.18	37,37,37,37	0
33	NA	0	8349	1/1	0.96	0.18	-	37,37,37,37	0
31	MG	0	8087	1/1	0.62	0.28	-	72,72,72,72	0
31	MG	0	8048	1/1	0.98	0.07	-	39,39,39,39	0
34	CL	K	8510	1/1	0.98	0.08	-	36,36,36,36	0
34	CL	I	8502	1/1	0.96	0.11	-	53,53,53,53	0
33	NA	9	8351	1/1	0.90	0.12	-	42,42,42,42	0
31	MG	0	8014	1/1	0.93	0.09	-	25,25,25,25	0
31	MG	0	8102	1/1	0.84	0.11	-	51,51,51,51	0
33	NA	0	8360	1/1	0.93	0.21	-	41,41,41,41	0
34	CL	A	8509	1/1	0.98	0.12	-	50,50,50,50	0
31	MG	0	8016	1/1	0.94	0.09	-	32,32,32,32	0
31	MG	0	8031	1/1	0.97	0.12	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8043	1/1	0.90	0.07	-	33,33,33,33	0
31	MG	0	8116	1/1	0.97	0.09	-	42,42,42,42	0
31	MG	0	8090	1/1	0.90	0.31	-	53,53,53,53	0
34	CL	0	8522	1/1	0.97	0.15	-	44,44,44,44	0
31	MG	0	8066	1/1	0.95	0.49	-	85,85,85,85	0
33	NA	0	8370	1/1	0.77	0.44	-	61,61,61,61	0
31	MG	0	8076	1/1	0.87	0.04	-	46,46,46,46	0
31	MG	A	8105	1/1	0.97	0.16	-	27,27,27,27	0
31	MG	0	8093	1/1	0.94	0.12	-	35,35,35,35	0
34	CL	0	8517	1/1	0.97	0.09	-	50,50,50,50	0
33	NA	0	8306	1/1	0.98	0.13	-	28,28,28,28	0
31	MG	0	8062	1/1	0.91	0.08	-	41,41,41,41	0
31	MG	0	8045	1/1	0.95	0.07	-	51,51,51,51	0
31	MG	0	8024	1/1	0.99	0.15	-	22,22,22,22	0
34	CL	I	8501	1/1	0.98	0.09	-	44,44,44,44	0
31	MG	0	8063	1/1	0.96	0.12	-	62,62,62,62	0
31	MG	0	8022	1/1	0.92	0.12	-	32,32,32,32	0
31	MG	0	8023	1/1	0.97	0.14	-	30,30,30,30	0
31	MG	0	8106	1/1	0.95	0.13	-	42,42,42,42	0
33	NA	0	8330	1/1	0.97	0.07	-	39,39,39,39	0
31	MG	0	8075	1/1	0.98	0.06	-	28,28,28,28	0
31	MG	0	8046	1/1	0.94	0.05	-	38,38,38,38	0
33	NA	0	8307	1/1	0.88	0.13	-	42,42,42,42	0
34	CL	X	8520	1/1	0.96	0.13	-	38,38,38,38	0
31	MG	0	8040	1/1	0.97	0.12	-	38,38,38,38	0
33	NA	0	8355	1/1	0.96	0.38	-	47,47,47,47	0
34	CL	0	8513	1/1	0.99	0.10	-	44,44,44,44	0
31	MG	0	8036	1/1	0.97	0.08	-	35,35,35,35	0
33	NA	0	8326	1/1	0.95	0.21	-	37,37,37,37	0
31	MG	0	8088	1/1	0.99	0.09	-	20,20,20,20	0
34	CL	Q	8506	1/1	0.97	0.12	-	40,40,40,40	0
34	CL	0	8503	1/1	0.98	0.17	-	40,40,40,40	0
31	MG	0	8100	1/1	0.96	0.06	-	64,64,64,64	0
33	NA	0	8358	1/1	0.92	0.35	-	74,74,74,74	0
33	NA	0	8363	1/1	0.88	0.32	-	52,52,52,52	0
31	MG	J	8069	1/1	0.94	0.13	-	46,46,46,46	0
31	MG	0	8083	1/1	0.98	0.07	-	30,30,30,30	0
31	MG	0	8082	1/1	0.94	0.17	-	56,56,56,56	0
31	MG	0	8029	1/1	0.98	0.09	-	35,35,35,35	0
31	MG	0	8047	1/1	0.87	0.10	-	54,54,54,54	0
31	MG	0	8009	1/1	0.97	0.14	-	24,24,24,24	0
33	NA	0	8342	1/1	0.96	0.22	-	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8030	1/1	0.99	0.07	-	22,22,22,22	0
31	MG	0	8099	1/1	0.93	0.24	-	44,44,44,44	0
31	MG	0	8114	1/1	0.97	0.09	-	35,35,35,35	0
31	MG	0	8049	1/1	0.84	0.12	-	56,56,56,56	0
31	MG	0	8101	1/1	0.88	0.30	-	48,48,48,48	0
33	NA	0	8352	1/1	0.98	0.12	-	40,40,40,40	0
33	NA	0	8316	1/1	0.97	0.22	-	35,35,35,35	0
31	MG	0	8042	1/1	0.97	0.10	-	29,29,29,29	0
33	NA	0	8384	1/1	0.82	0.14	-	52,52,52,52	0
31	MG	0	8113	1/1	0.86	0.13	-	36,36,36,36	0
31	MG	0	8061	1/1	0.97	0.13	-	32,32,32,32	0
33	NA	0	8367	1/1	0.97	0.26	-	45,45,45,45	0
31	MG	0	8041	1/1	0.97	0.10	-	33,33,33,33	0
35	CD	N	8405	1/1	0.98	0.08	-	71,71,71,71	0
33	NA	H	8322	1/1	0.86	0.26	-	52,52,52,52	0
31	MG	0	8092	1/1	0.98	0.10	-	66,66,66,66	0
34	CL	0	8511	1/1	0.98	0.10	-	37,37,37,37	0
31	MG	0	8111	1/1	0.99	0.12	-	32,32,32,32	0
34	CL	0	8514	1/1	0.98	0.20	-	36,36,36,36	0
33	NA	0	8301	1/1	0.97	0.09	-	33,33,33,33	0
31	MG	0	8068	1/1	0.94	0.04	-	44,44,44,44	0
31	MG	0	8115	1/1	0.95	0.07	-	36,36,36,36	0
33	NA	0	8319	1/1	0.96	0.13	-	29,29,29,29	0
31	MG	0	8117	1/1	0.92	0.17	-	36,36,36,36	0
31	MG	9	8095	1/1	0.80	0.15	-	69,69,69,69	0
31	MG	0	8104	1/1	0.94	0.13	-	45,45,45,45	0
33	NA	0	8328	1/1	0.99	0.12	-	28,28,28,28	0
33	NA	0	8336	1/1	0.96	0.06	-	37,37,37,37	0
33	NA	0	8308	1/1	0.89	0.18	-	42,42,42,42	0
33	NA	0	8369	1/1	0.92	0.22	-	40,40,40,40	0
31	MG	0	8070	1/1	0.84	0.15	-	40,40,40,40	0
31	MG	0	8051	1/1	0.94	0.09	-	56,56,56,56	0
31	MG	0	8034	1/1	0.89	0.09	-	31,31,31,31	0
33	NA	0	8341	1/1	0.94	0.11	-	37,37,37,37	0
33	NA	0	8329	1/1	0.80	0.14	-	48,48,48,48	0
31	MG	0	8037	1/1	0.97	0.07	-	35,35,35,35	0
31	MG	0	8005	1/1	0.99	0.12	-	24,24,24,24	0
33	NA	0	8379	1/1	0.97	0.45	-	48,48,48,48	0
31	MG	0	8085	1/1	0.93	0.07	-	35,35,35,35	0
31	MG	0	8081	1/1	0.96	0.11	-	39,39,39,39	0
33	NA	0	8315	1/1	0.95	0.17	-	30,30,30,30	0
33	NA	0	8375	1/1	0.99	0.21	-	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
31	MG	0	8025	1/1	0.98	0.10	-	36,36,36,36	0
33	NA	0	8357	1/1	0.94	0.08	-	39,39,39,39	0
33	NA	0	8311	1/1	0.89	0.15	-	48,48,48,48	0
31	MG	0	8050	1/1	0.76	0.12	-	56,56,56,56	0
33	NA	0	8377	1/1	0.94	0.23	-	50,50,50,50	0
31	MG	0	8026	1/1	0.97	0.15	-	26,26,26,26	0
33	NA	0	8385	1/1	0.92	0.40	-	48,48,48,48	0
31	MG	0	8079	1/1	0.95	0.16	-	19,19,19,19	0
33	NA	0	8318	1/1	0.92	0.25	-	49,49,49,49	0
31	MG	0	8103	1/1	0.78	0.23	-	54,54,54,54	0
31	MG	0	8098	1/1	0.95	0.07	-	27,27,27,27	0
31	MG	0	8011	1/1	0.98	0.10	-	23,23,23,23	0
33	NA	0	8359	1/1	0.96	0.26	-	39,39,39,39	0
33	NA	R	8312	1/1	0.93	0.09	-	26,26,26,26	0
34	CL	M	8507	1/1	0.99	0.08	-	45,45,45,45	0
31	MG	0	8094	1/1	0.92	0.09	-	59,59,59,59	0
31	MG	0	8089	1/1	0.91	0.06	-	51,51,51,51	0
31	MG	0	8097	1/1	0.96	0.07	-	30,30,30,30	0
33	NA	0	8354	1/1	0.98	0.16	-	25,25,25,25	0
31	MG	0	8072	1/1	0.81	0.09	-	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.