



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:00 AM GMT

PDB ID : 1YI2  
Title : Crystal Structure Of Erythromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui  
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2005-01-11  
Resolution : 2.65 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.

---

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

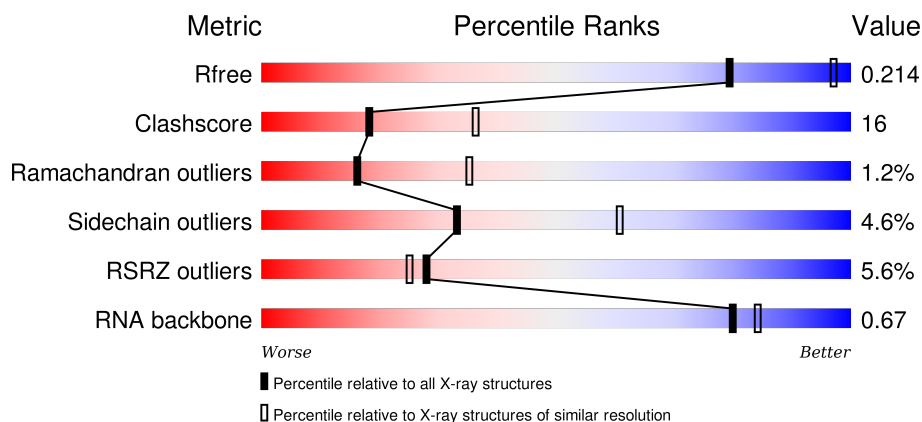
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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.




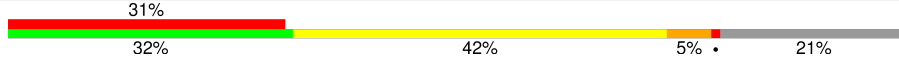


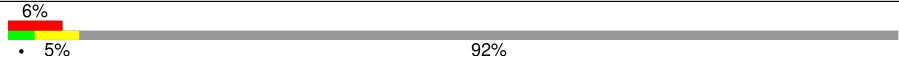
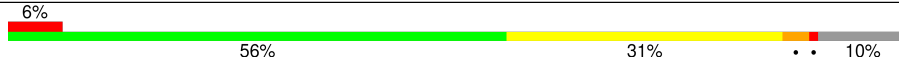

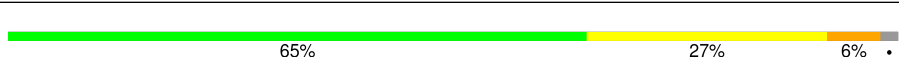
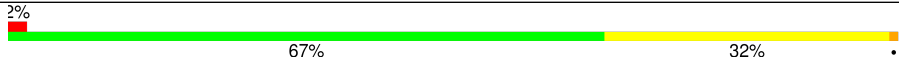
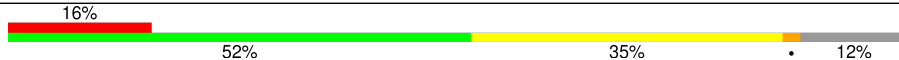
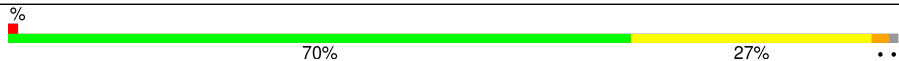
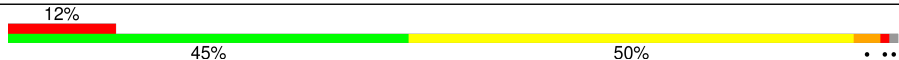


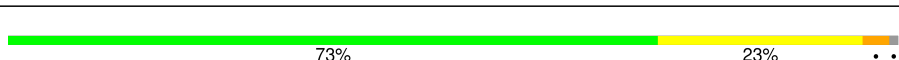
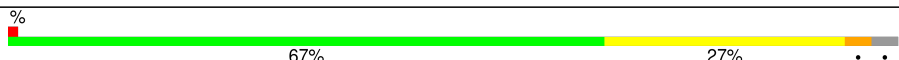
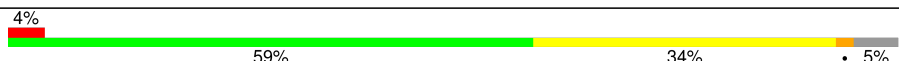
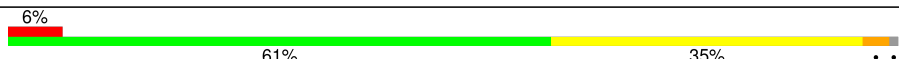

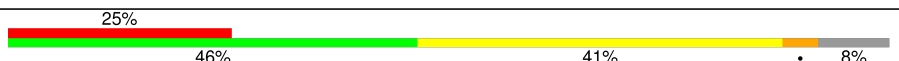
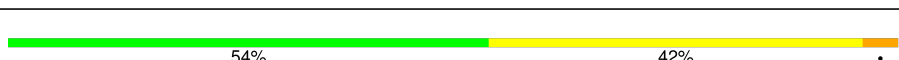
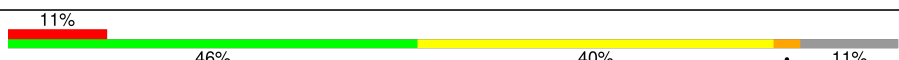
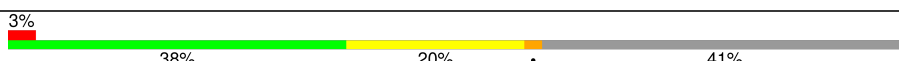

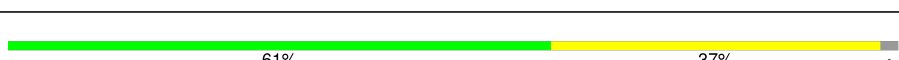
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)
RNA backbone	2183	1001 (3.08-2.24)

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>62%</div> <div>27%</div> <div>5%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>55%</div> <div>35%</div> <div>8%</div> <div></div> </div> </div>
3	A	240	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>31%</div> <div>5%</div> <div></div> </div> </div>
4	B	338	<div> <div>2%</div> <div> <div></div> <div>51%</div> <div>44%</div> <div></div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	
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	

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
30	2	50	
31	3	92	

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
32	ERY	0	9000	-	-	-	X
33	MG	0	8088	-	-	-	X
34	K	0	8401	-	-	-	X
35	NA	0	8502	-	-	-	X
35	NA	0	8510	-	-	-	X
35	NA	0	8514	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8525	-	-	-	X
35	NA	0	8526	-	-	-	X
35	NA	0	8532	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8540	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8566	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	0	8572	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	0	8574	-	-	-	X
35	NA	0	8576	-	-	-	X
35	NA	0	8577	-	-	-	X
35	NA	0	8578	-	-	-	X
35	NA	0	8582	-	-	-	X
35	NA	9	8583	-	-	-	X
35	NA	L	8580	-	-	-	X
35	NA	R	8586	-	-	-	X
36	CL	0	8815	-	-	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99086 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
			59020	26349	10873	19053	2745			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	628	1MA	A	MODIFIED RESIDUE	GB 55229667
0	2099	A	G	ENGINEERED	GB 55229667
0	2587	OMU	U	MODIFIED RESIDUE	GB 55229667
0	2588	OMG	G	MODIFIED RESIDUE	GB 55229667
0	2619	UR3	U	MODIFIED RESIDUE	GB 55229667
0	2621	PSU	U	MODIFIED RESIDUE	GB 55229667

- 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
			2599	1160	471	847	121			

- Molecule 3 is a protein called 50S ribosomal protein L2P.

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

- Molecule 4 is a protein called 50S ribosomal protein L3P.

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

- Molecule 5 is a protein called 50S ribosomal protein L4E.

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

- Molecule 6 is a protein called 50S ribosomal protein L5P.

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 50S ribosomal protein L6P.

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 50S ribosomal protein L7AE.

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

- Molecule 9 is a protein called ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG.

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 50S RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 11 is a protein called 50S RIBOSOMAL PROTEIN L11P.

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

- 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
			1558	942	332	283	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	13	GLU	LYS	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	S	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			

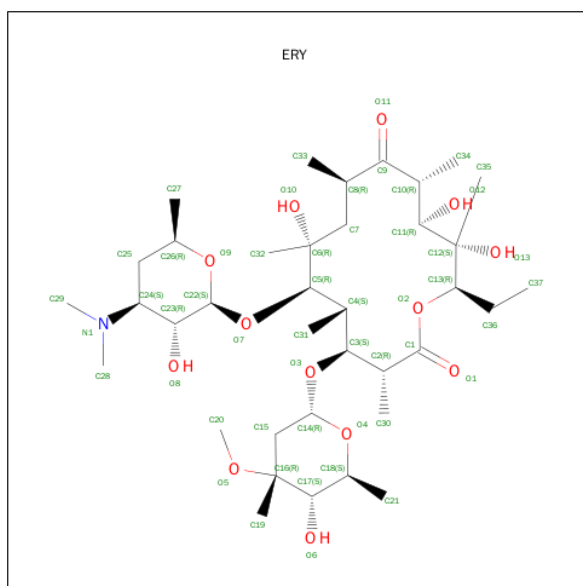
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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 ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	0	1	Total	C	N	O	0	0
			51	37	1	13		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	108	Total	Mg	0	0
			108	108		
33	Y	1	Total	Mg	0	0
			1	1		
33	K	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	1	Total	Mg	0	0
			1	1		
33	T	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	3	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	10	Total	Cl	0	0
			10	10		

*Continued on next page...*

*Continued from previous page...*

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5869	Total 5869	O 5869	0	0
38	9	138	Total 138	O 138	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	121	Total 121	O 121	0	0
38	B	151	Total 151	O 151	0	0
38	C	168	Total 168	O 168	0	0
38	D	50	Total 50	O 50	0	0
38	E	42	Total 42	O 42	0	0
38	F	28	Total 28	O 28	0	0
38	G	19	Total 19	O 19	0	0
38	H	71	Total 71	O 71	0	0
38	I	9	Total 9	O 9	0	0
38	J	55	Total 55	O 55	0	0
38	K	61	Total 61	O 61	0	0
38	L	81	Total 81	O 81	0	0
38	M	124	Total 124	O 124	0	0
38	N	67	Total 67	O 67	0	0
38	O	43	Total 43	O 43	0	0
38	P	66	Total 66	O 66	0	0
38	Q	49	Total 49	O 49	0	0
38	R	80	Total 80	O 80	0	0
38	S	37	Total 37	O 37	0	0
38	T	37	Total 37	O 37	0	0
38	U	27	Total 27	O 27	0	0

*Continued on next page...*

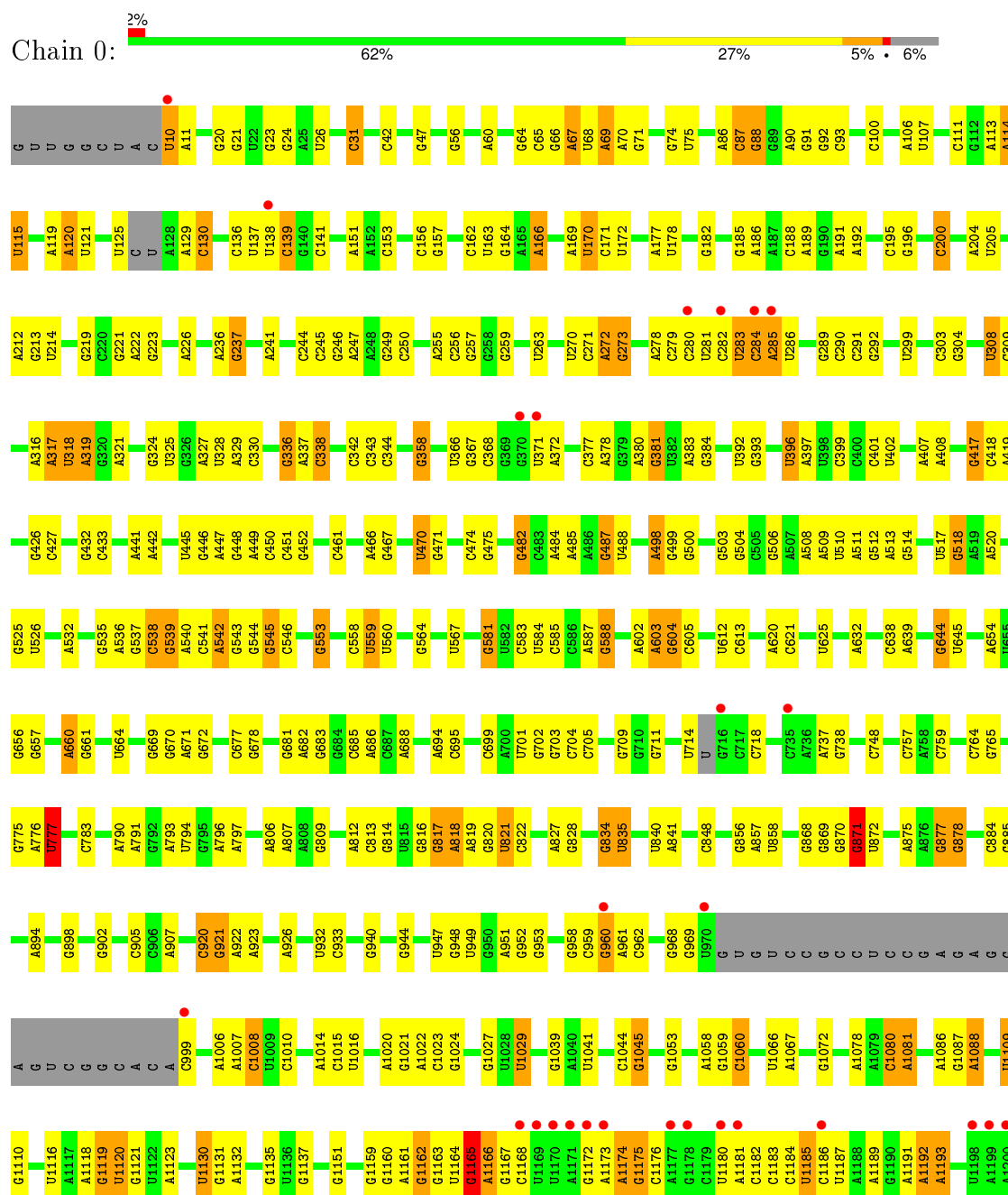
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	V	14	Total 14	O 14	0	0
38	W	73	Total 73	O 73	0	0
38	X	27	Total 27	O 27	0	0
38	Y	94	Total 94	O 94	0	0
38	Z	30	Total 30	O 30	0	0
38	1	54	Total 54	O 54	0	0
38	2	45	Total 45	O 45	0	0
38	3	78	Total 78	O 78	0	0

### 3 Residue-property plots

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

#### • Molecule 1: 23S Ribosomal RNA

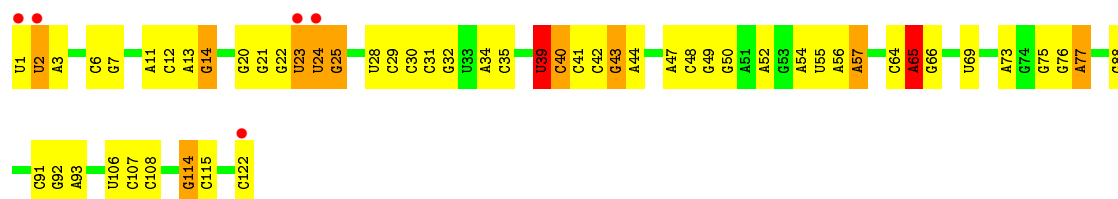


C2779	C2780	A2853	G2583	A2434	C2326	C	C	U	A2054	C1940	U1791	G1886	G1589	U1460	U1333	C1201		
G2781	U2781	A2864	C2534	C2443	G2338	C	G	A	A2054	A1941	C1798	C1687	G1592	U1461	U1334	A1202		
G2782	U2782	A	U2535	U2444	A	U	U	G	U2064	A1942		C1692	C1593	C1462	C1335	G1203		
A2783	C2536	C	C	U2445	C	C	C	A	G	C1943			C1594	A1470	G1340	C1204		
A2784	G2537	G	C	G2446	G	G	G	A	G	G1947	G1819	A1701	C1595	U1205	U1206	U1207		
G2785	U2541	U	A	G2453	A	U	U	U	C	G1948	G1820	U1702	U1596	C1474	C1341	C1208		
G2786	C2547	C	C	G2456	G2344	U	G	G	C	G1949	U1825	A1711	A1597	C1477	C1342	C1209		
C2787	C2548	U	U	U2457	A2345	G	G	G	G	G1950	C1826	A1712	A1598		C1343	C1209		
A2788	U2671	U	C	C2346	A2081	C	C	U	A	G1951				G1210	G1343	G1210		
U2791	C2676	U	U	A2353	A2089	U	U	A	A	U	A1829	A1717	A1603	G1351	G1351	C1213		
A2792	A2553	C	U	A2354	A2090	U	C	A	A	A	C1830		G1604	A1482	A1352	C1214		
G2793	U2680	C	C	G2355	G2091	A	A	A	C	C		U1722	G1605	C1483	C1353	G1215		
G2794	C2681	U	G	A2356	G2092	G	G	A	G	U	C1834	U1723	A1606	U1488	A1215	G1216		
C2795	C2682	C	C	A2467	G2093	A	A	A	C	A	U1835	U1724	A1607		C1360			
U2796	U2563	U	U	U2468	A2095	G	G	U	U	U	A1840	C1725	G1613	A1494	G1363	C1229		
A2800	G2564	C	C	A2469	A2096	U	U	A	A	G	A1845	G1730	G1614	A1496	A1230	U1234		
A2801	C2565	U	C	C2359	A2096	A	C	C	C	C	U1846	C1731	A1615	G1497	A1372	U1235		
U2807	G2570	U	U	C2360	A2101	C	C	C	C	C	A1847	A1732	C1617	U1500	A1375	G1236		
A2811	U2577	U	C	A2361	G2102	C	C	C	C	C	A1848	A1733	A1624	U1503	G1376	U1237		
G2812	C2578	U	C	G2362	A2103	G	C	C	C	U	G1849	C1734	G1625	U1504	C1377	U1238		
A2813	U2579	U	C	G2363	C2104	G	G	C	C	U	U1850	C1735	A1626	A1505	G1378	G1239		
G2814	U2580	U	C	G2364	G2110	C	C	C	C	U	G1851	A1736	U1506	U1506	U1380			
G2815	U2581	U	C	G2365	G2110	G	C	C	C	C	A1852		G1627					
C2821	U2582	U	C	A2369	G1970	C	C	C	C	U	C1853	U1741	A1630	G1391	A1242	A1242		
U2825	U2583	U	C	A2370	G1971	U	U	U	U	U	C1856	A1742	A1630	C1243	C1243	C1243		
G2826	U2584	U	C	U2372	U2115	U	U	A	A	A			A1515	A1392	U1244	U1244		
G2827	U2585	U	C	U2373	U2116	C	C	C	C	U	C1857	G1751	C1633	A1393	G1245	G1245		
U2828	U2586	U	C	U2374	C2132	C	C	C	C	U	C1861	G1752	G1634	C1394	A1246	A1246		
C2831	U2587	U	C	U2375	A2135	G	G	C	C	U	C1862	G1753	U1524	G1398	C1250	C1250		
G2832	U2588	U	C	U2376	A2136	G	C	C	C	U	C1863	A1754	U1525	A1399	C1251	C1251		
U2833	U2589	U	C	U2377	G2270	C	C	C	C	U	G1867	G1755	A1527	A1406	A1252	A1252		
G2834	U2590	U	C	U2378	G2271	C	C	C	C	U	G1868	G1756	G1529	A1407	C1253	C1253		
C2835	U2591	U	C	U2379	G2272	C	C	C	C	U								
G2836	U2592	U	C	U2380	A2265	C	C	C	C	U	G1877	U1761	G1641	G1415	U1266	U1266		
U2837	U2593	U	C	U2381	A2266	C	C	C	C	U	C1878	C1762	A1642	G1416	C1267	C1267		
C2838	U2594	U	C	U2382	C2269	C	C	C	C	U	U1879	C1763	C1643	G1417	C1268	G1268		
G2839	U2595	U	C	U2383	G2270	C	C	C	C	U	C1880	U1766	U1654	U1418	G1269	G1269		
U2840	U2596	U	C	U2384	G2271	C	C	C	C	U	C1881	A1767	U1654	U1419				
C2841	U2597	U	C	U2385	G2272	C	C	C	C	U	C1882	C1768	A1656	C1545	C1273	C1273		
G2842	U2598	U	C	U2386	G2273	C	C	C	C	U	C1887	C1769	A1657	U1422	A1278	A1278		
U2843	U2599	U	C	U2387	G2274	C	C	C	C	U	U1887	U1770	C1553	C1423	U1279	U1279		
C2844	U2600	U	C	U2388	C2281	C	C	C	C	U		U1771	C1554	A1424				
G2845	U2601	U	C	U2389	A2291	C	C	C	C	U	G1877	C1772	C1554	A1427	A1287	A1287		
U2846	U2602	U	C	U2390	A2300	C	C	C	C	U	U1879	G1773	U1654	A1434	U1288	U1288		
C2847	U2603	U	C	U2391	A2301	C	C	C	C	U	C1880	G1773	A1666	A1435	C1289	C1289		
G2848	U2604	U	C	U2392	A2302	C	C	C	C	U	C1881	G1774	U1668	C1436	G1290	G1290		
U2849	U2605	U	C	U2393	C2309	C	C	C	C	U	A1904	U1775	U1668	U1437	G1295	G1295		
C2850	U2606	U	C	U2394	C2313	C	C	C	C	U	U1905	G1775	U1668	U1438	U1298	U1298		
G2851	U2607	U	C	U2395	C2314	C	C	C	C	U	A1919	G1776	U1668	U1439	G1299	G1299		
U2852	U2608	U	C	U2396	C2315	C	C	C	C	U	C1920	A1778	U1668	U1440	U1314	U1314		
C2853	U2609	U	C	U2397	C2316	C	C	C	C	U	A1921	G1779	U1668	U1441	C1451	C1451		
G2854	U2610	U	C	U2398	C2317	C	C	C	C	U	G1925	A1783	C1675	U1442				
U2855	U2611	U	C	U2399	C2318	C	C	C	C	U	G1926	U1784	C1676	A1442				
C2856	U2612	U	C	U2400	C2319	C	C	C	C	U	A1927	C1787	A1682					
G2857	U2613	U	C	U2401	C2320	C	C	C	C	U	A1930	U1788	A1683					
U2858	U2614	U	C	U2402	C2321	C	C	C	C	U	A1931	C1790	A1684					
C2859	U2615	U	C	U2403	C2322	C	C	C	C	U								
G2860	U2616	U	C	U2404	C2323	C	C	C	C	U								
U2861	U2617	U	C	U2405	C2324	C	C	C	C	U								
C2862	U2618	U	C	U2406	C2325	C	C	C	C	U								
G2863	U2619	U	C	U2407	C2326	C	C	C	C	U								
U2864	U2620	U	C	U2408	C2327	C	C	C	C	U								
C2865	U2621	U	C	U2409	C2328	C	C	C	C	U								
G2866	U2622	U	C	U2410	C2329	C	C	C	C	U								
U2867	U2623	U	C	U2411	C2330	C	C	C	C	U								
C2868	U2624	U	C	U2412	C2331	C	C	C	C	U								
G2869	U2625	U	C	U2413	C2332	C	C	C	C	U								
U2870	U2626	U	C	U2414	C2333	C	C	C	C	U								
C2871	U2627	U	C	U2415	C2334	C	C	C	C	U								
G2872	U2628	U	C	U2416	C2335	C	C	C	C	U								
U2873	U2629	U	C	U2417	C2336	C	C	C	C	U								
C2874	U2630	U	C	U2418	C2337	C	C	C	C	U								
G2875	U2631	U	C	U2419	C2338	C	C	C	C	U								
U2876	U2632	U	C	U2420	C2339	C	C	C	C	U								
C2877	U2633	U	C	U2421	C2340	C	C	C	C	U								
G2878	U2634	U	C	U2422	C2341	C	C	C	C	U								
U2879	U2635	U	C	U2423	C2342	C	C	C	C	U								
C2880	U2636	U	C	U2424	C2343	C	C	C	C	U								
G2881	U2637	U	C	U2425	C2344	C	C	C	C	U								
U2882	U2638	U	C	U2426	C2345	C	C	C	C	U								
C2883	U2639	U	C	U2427	C2346	C	C	C	C	U								
G2884	U2640	U	C	U2428	C2347	C	C	C	C	U								
U2885	U2641	U	C	U2429	C2348	C	C	C	C	U								
C2886	U2642	U	C	U2430	C2349	C	C	C	C	U								
G2887	U2643	U	C	U2431	C2350	C	C	C	C	U								
U2888	U2644	U	C	U2432	C2351	C	C	C	C	U								
C2889	U2645	U	C	U2433	C2352	C	C	C	C	U								
G2890	U2646	U	C	U2434	C2353	C	C	C	C	U								
U2891	U2647	U	C	U2435	C2354	C	C	C	C	U								
C2892	U2648	U	C	U2436	C2355	C	C	C	C	U								
G2893	U2649	U	C	U2437	C2356	C	C	C	C	U								
U2894	U2650	U	C	U2438	C2357	C	C	C	C	U								
C2895	U2651	U	C	U2439	C2358	C	C	C	C	U								
G2896	U2652	U	C	U2440	C2359	C	C	C	C	U								
U2897	U2653	U	C	U2441	C2360	C	C	C	C	U								
C2898	U2654	U	C	U2442	C2361	C	C	C	C	U								
G2899	U2655	U	C	U2443	C2362	C	C	C	C	U								
U2900	U2656	U	C	U2444	C2363	C	C	C	C	U								

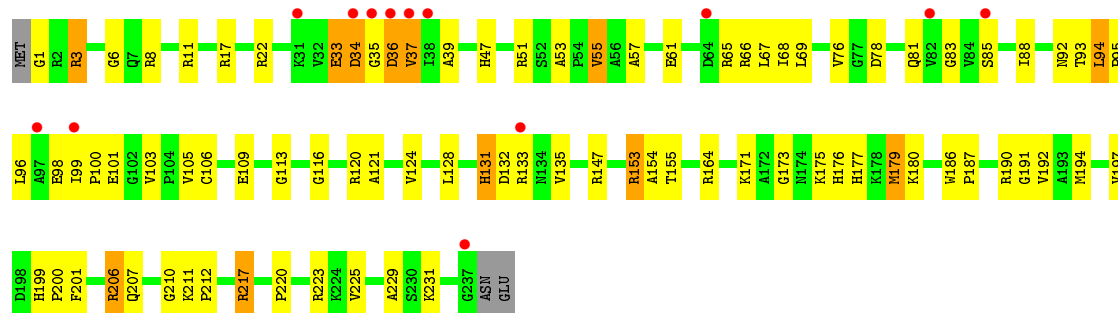




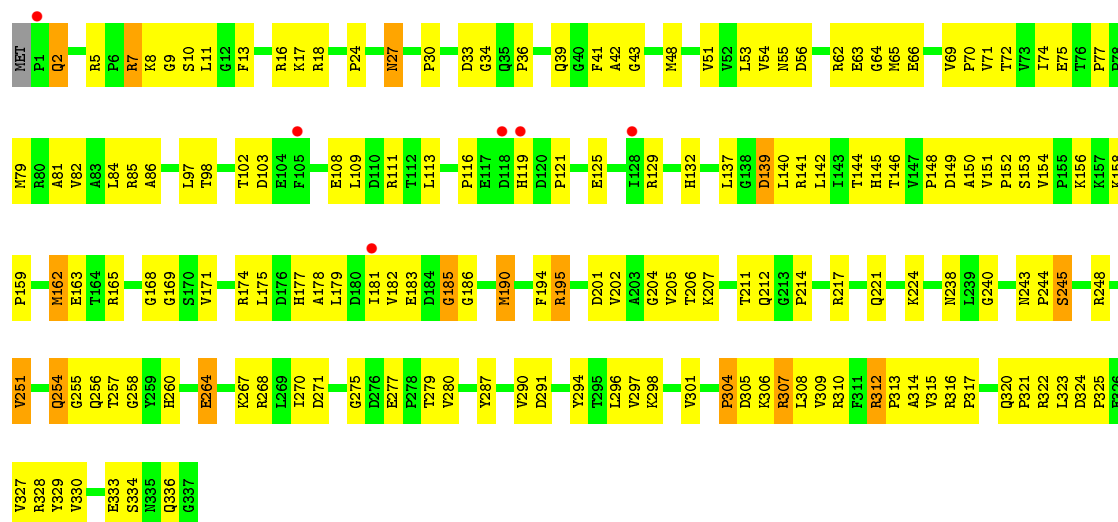
• Molecule 2: 5S Ribosomal RNA



• Molecule 3: 50S ribosomal protein L2P

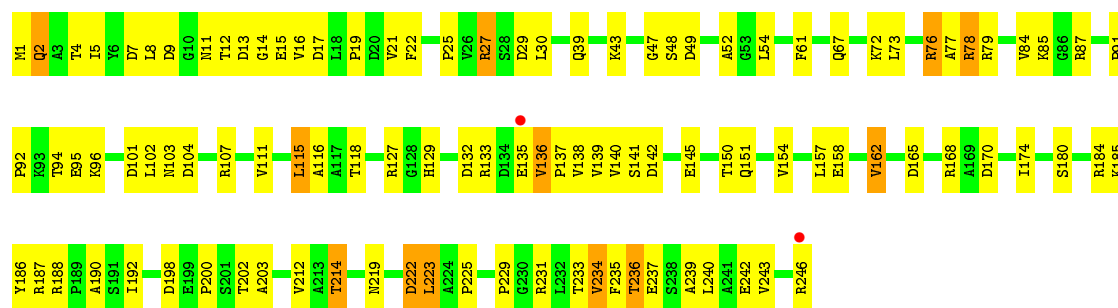


• Molecule 4: 50S ribosomal protein L3P

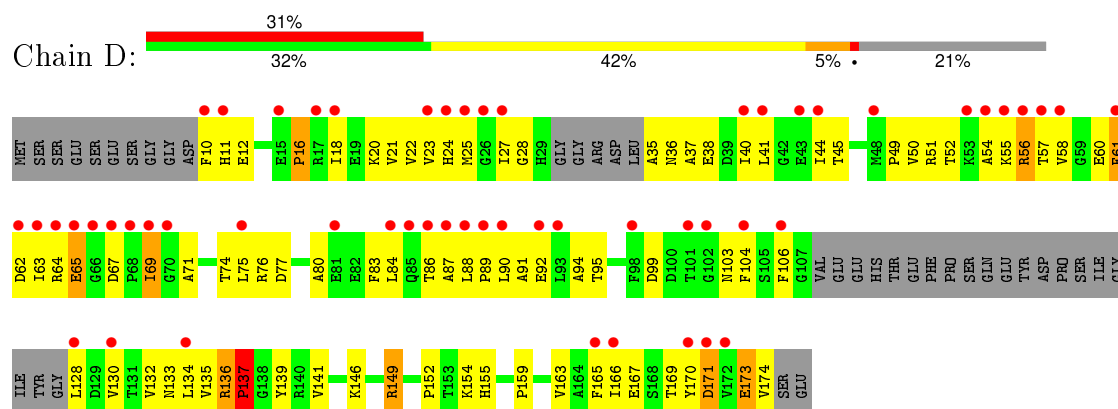


• Molecule 5: 50S ribosomal protein L4E

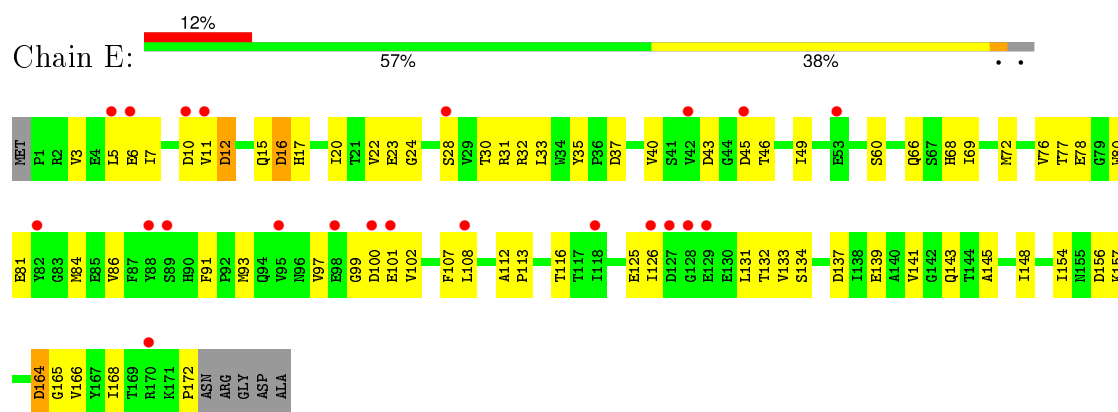




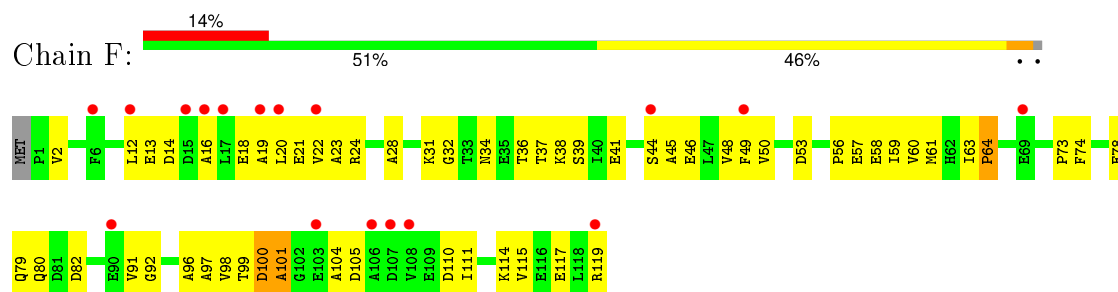
• Molecule 6: 50S ribosomal protein L5P



• Molecule 7: 50S ribosomal protein L6P



• Molecule 8: 50S ribosomal protein L7AE

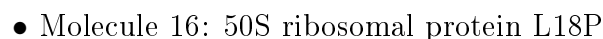


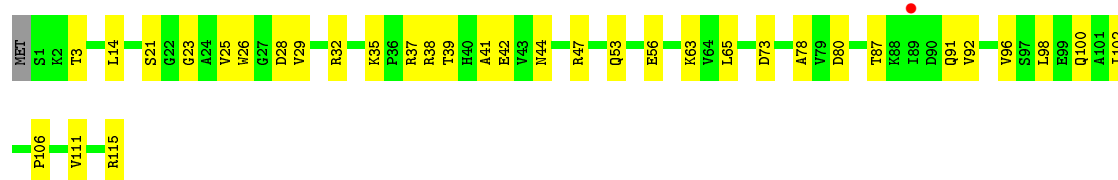
• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



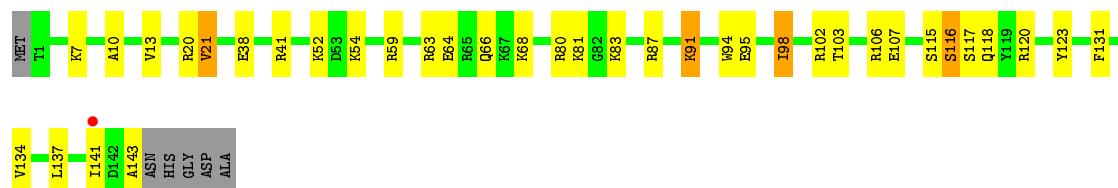


- Molecule 14: 50S ribosomal protein L15P





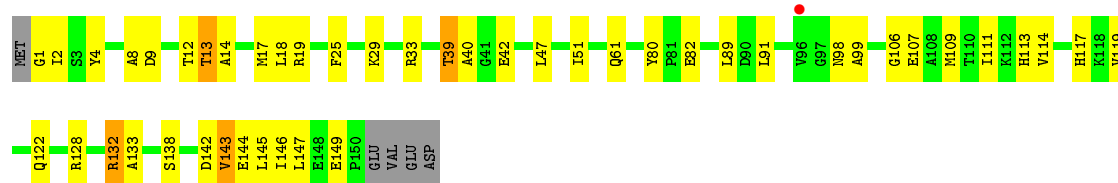
- Molecule 18: 50S ribosomal protein L19E



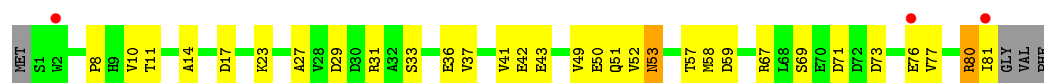
- Molecule 19: 50S ribosomal protein L21e



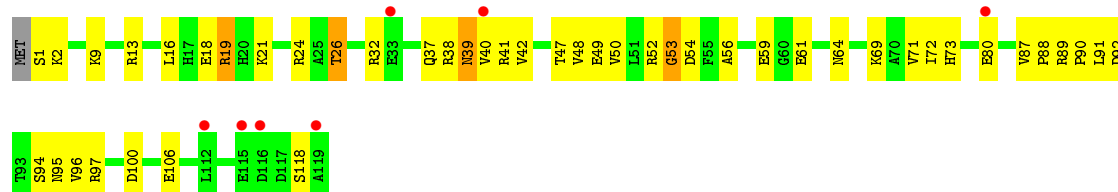
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

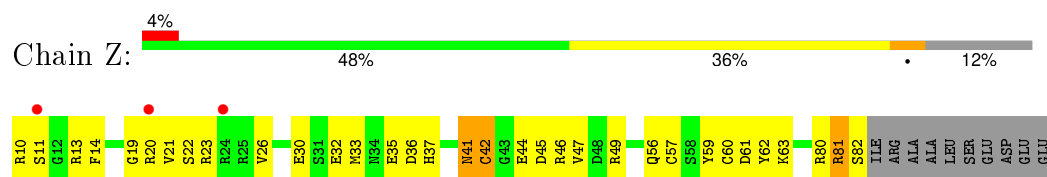


- Molecule 22: 50S ribosomal protein L24P

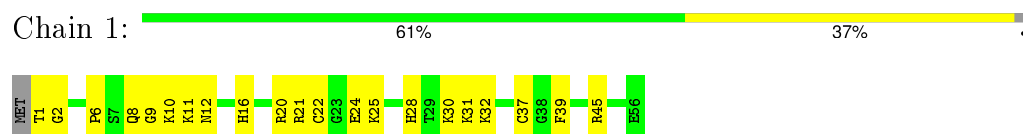




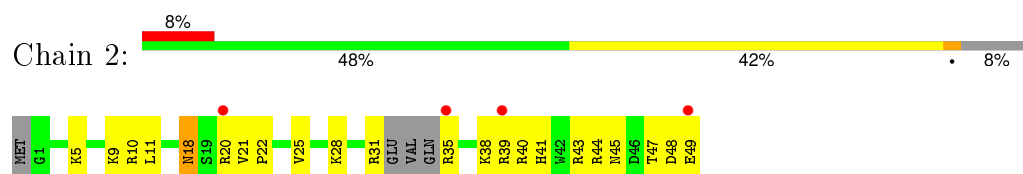
- Molecule 28: 50S ribosomal protein L37Ae



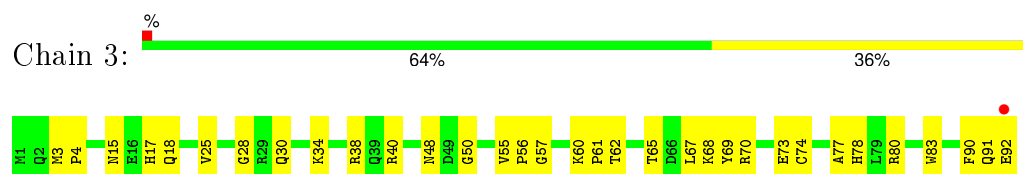
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.44Å 299.99Å 574.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 49.81 – 2.65	Depositor EDS
% Data completeness (in resolution range)	94.4 (30.00-2.65) 94.5 (49.81-2.65)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.65Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.176 , 0.214 0.177 , 0.214	Depositor DCC
$R_{free}$ test set	4878 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	52.1	Xtriage
Anisotropy	0.185	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 51.6	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 495739 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99086	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	0	0.36	0/65957	0.69	23/102867 (0.0%)
2	9	0.33	0/2904	0.70	2/4526 (0.0%)
3	A	0.32	0/1786	0.64	0/2408
4	B	0.32	0/2690	0.64	0/3652
5	C	0.37	0/1884	0.64	0/2551
6	D	0.31	0/1111	0.55	0/1498
7	E	0.31	0/1382	0.57	0/1880
8	F	0.31	0/901	0.55	0/1224
9	G	0.27	0/241	0.45	0/324
10	H	0.39	0/1302	0.66	1/1743 (0.1%)
11	I	0.30	0/526	0.54	0/716
12	J	0.35	0/1136	0.61	0/1530
13	K	0.33	0/1001	0.68	0/1347
14	L	0.32	0/1130	0.64	0/1509
15	M	0.33	0/1582	0.62	0/2117
16	N	0.29	0/1474	0.61	0/1999
17	O	0.33	0/874	0.59	0/1181
18	P	0.33	0/1147	0.53	0/1528
19	Q	0.35	0/749	0.69	0/1005
20	R	0.34	0/1172	0.63	0/1578
21	S	0.33	0/648	0.57	1/875 (0.1%)
22	T	0.30	0/958	0.62	0/1289
23	U	0.33	0/417	0.55	0/562
24	V	0.29	0/502	0.55	0/675
25	W	0.34	0/1219	0.62	0/1655
26	X	0.34	0/664	0.59	0/895
27	Y	0.35	0/1146	0.62	0/1536
28	Z	0.33	0/589	0.65	0/787
29	1	0.38	0/438	0.63	0/578
30	2	0.33	0/401	0.54	0/529
31	3	0.37	0/771	0.58	0/1024
All	All	0.35	0/98702	0.67	27/147588 (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	45
2	9	0	2
All	All	1	47

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1563	G	C2'-C3'-O3'	9.25	129.85	109.50
1	0	1942	A	C5'-C4'-C3'	7.55	128.08	116.00
2	9	39	U	N1-C1'-C2'	7.02	123.12	114.00
1	0	871	G	C5'-C4'-O4'	-6.90	100.82	109.10
1	0	1504	A	C1'-O4'-C4'	-6.19	104.95	109.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	0	1563	G	C3'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	221	G	Sidechain
1	0	26	U	Sidechain
1	0	270	U	Sidechain
1	0	396	U	Sidechain
1	0	470	U	Sidechain

## 5.2 Too-close contacts [i](#)

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	59020	0	29810	809	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	9	2599	0	1325	63	0
3	A	1753	0	1766	111	0
4	B	2625	0	2533	172	0
5	C	1859	0	1816	122	0
6	D	1094	0	1085	92	0
7	E	1357	0	1266	74	0
8	F	890	0	843	60	0
9	G	240	0	231	19	0
10	H	1282	0	1292	70	0
11	I	519	0	500	57	0
12	J	1120	0	1098	55	0
13	K	992	0	1031	53	0
14	L	1118	0	1076	61	0
15	M	1558	0	1566	58	0
16	N	1445	0	1401	112	0
17	O	865	0	873	29	0
18	P	1136	0	1123	41	0
19	Q	735	0	729	22	0
20	R	1149	0	1122	52	0
21	S	641	0	605	25	0
22	T	950	0	923	45	0
23	U	410	0	364	28	0
24	V	499	0	511	33	0
25	W	1196	0	1137	97	0
26	X	654	0	653	48	0
27	Y	1130	0	1133	62	0
28	Z	578	0	539	27	0
29	1	431	0	426	30	0
30	2	396	0	413	32	0
31	3	755	0	728	29	0
32	0	51	0	67	0	0
33	0	108	0	0	0	0
33	2	1	0	0	0	0
33	3	1	0	0	0	0
33	9	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
33	T	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	2	0	0	0	0
35	0	71	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
35	T	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	1	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	1	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5869	0	0	162	0
38	1	54	0	0	2	0
38	2	45	0	0	6	0
38	3	78	0	0	10	0
38	9	138	0	0	9	0
38	A	121	0	0	16	0
38	B	151	0	0	20	0
38	C	168	0	0	27	0
38	D	50	0	0	17	0
38	E	42	0	0	11	0
38	F	28	0	0	8	0
38	G	19	0	0	1	0
38	H	71	0	0	17	0
38	I	9	0	0	4	0
38	J	55	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	K	61	0	0	11	0
38	L	81	0	0	23	0
38	M	124	0	0	12	0
38	N	67	0	0	13	0
38	O	43	0	0	6	0
38	P	66	0	0	2	0
38	Q	49	0	0	6	0
38	R	80	0	0	7	0
38	S	37	0	0	5	0
38	T	37	0	0	6	0
38	U	27	0	0	4	0
38	V	14	0	0	3	0
38	W	73	0	0	11	0
38	X	27	0	0	9	0
38	Y	94	0	0	14	0
38	Z	30	0	0	1	0
All	All	99086	0	59985	2356	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 2356 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)
10:H:172:GLU:HB2	38:H:8591:HOH:O	1.34	1.21
1:O:1160:G:H5'	1:O:1161:A:H5'	1.24	1.17
5:C:236:THR:HG22	5:C:239:ALA:H	1.04	1.16
10:H:174:LEU:HA	38:H:8571:HOH:O	1.50	1.11
2:9:6:C:H5"	16:N:37:ARG:NH1	1.66	1.10

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	235/240 (98%)	213 (91%)	20 (8%)	2 (1%)	21	44
4	B	335/338 (99%)	300 (90%)	30 (9%)	5 (2%)	13	28
5	C	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	39	65
6	D	134/177 (76%)	98 (73%)	27 (20%)	9 (7%)	1	1
7	E	170/178 (96%)	160 (94%)	10 (6%)	0	100	100
8	F	117/120 (98%)	101 (86%)	12 (10%)	4 (3%)	5	9
9	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	15	33
11	I	68/162 (42%)	53 (78%)	15 (22%)	0	100	100
12	J	140/145 (97%)	130 (93%)	5 (4%)	5 (4%)	4	8
13	K	130/132 (98%)	119 (92%)	10 (8%)	1 (1%)	24	47
14	L	141/165 (86%)	121 (86%)	19 (14%)	1 (1%)	26	51
15	M	192/195 (98%)	178 (93%)	14 (7%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	6	13
17	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
18	P	141/149 (95%)	133 (94%)	7 (5%)	1 (1%)	26	51
19	Q	93/96 (97%)	86 (92%)	7 (8%)	0	100	100
20	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
21	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
22	T	117/120 (98%)	109 (93%)	7 (6%)	1 (1%)	21	44
23	U	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	V	63/71 (89%)	56 (89%)	5 (8%)	2 (3%)	5	10
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	15	33
26	X	80/92 (87%)	71 (89%)	9 (11%)	0	100	100
27	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
28	Z	71/83 (86%)	60 (84%)	7 (10%)	4 (6%)	2	3
29	1	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
30	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
31	3	90/92 (98%)	85 (94%)	4 (4%)	1 (1%)	17	38
All	All	3705/4437 (84%)	3374 (91%)	285 (8%)	46 (1%)	16	35

5 of 46 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	34	ASP
6	D	173	GLU
8	F	101	ALA
14	L	80	ASP
16	N	154	LEU

### 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	179/182 (98%)	167 (93%)	12 (7%)	20	41
4	B	282/283 (100%)	265 (94%)	17 (6%)	24	47
5	C	193/193 (100%)	175 (91%)	18 (9%)	11	23
6	D	117/148 (79%)	111 (95%)	6 (5%)	29	55
7	E	152/156 (97%)	147 (97%)	5 (3%)	45	73
8	F	93/94 (99%)	91 (98%)	2 (2%)	60	84
9	G	27/283 (10%)	26 (96%)	1 (4%)	41	69
10	H	134/145 (92%)	128 (96%)	6 (4%)	34	61
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	106 (90%)	12 (10%)	9	19
13	K	106/106 (100%)	103 (97%)	3 (3%)	51	79
14	L	113/127 (89%)	109 (96%)	4 (4%)	43	71
15	M	158/159 (99%)	152 (96%)	6 (4%)	40	68
16	N	149/150 (99%)	144 (97%)	5 (3%)	44	72
17	O	93/94 (99%)	91 (98%)	2 (2%)	60	84
18	P	113/117 (97%)	109 (96%)	4 (4%)	43	71
19	Q	79/80 (99%)	74 (94%)	5 (6%)	22	44
20	R	117/122 (96%)	112 (96%)	5 (4%)	35	63
21	S	71/74 (96%)	68 (96%)	3 (4%)	36	64

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	T	105/106 (99%)	99 (94%)	6 (6%)	25	49
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	39	67
25	W	130/130 (100%)	125 (96%)	5 (4%)	40	68
26	X	66/74 (89%)	63 (96%)	3 (4%)	34	61
27	Y	120/196 (61%)	113 (94%)	7 (6%)	25	48
28	Z	60/68 (88%)	59 (98%)	1 (2%)	68	88
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	57	82
31	3	79/79 (100%)	78 (99%)	1 (1%)	76	91
All	All	3095/3619 (86%)	2953 (95%)	142 (5%)	33	61

5 of 142 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	114	ASP
13	K	7	ASP
26	X	72	VAL
10	H	172	GLU
12	J	79	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	24	GLN
19	Q	16	ASN
30	2	18	ASN
15	M	26	GLN
16	N	40	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2746/2922 (93%)	240 (8%)	35 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2867/3044 (94%)	256 (8%)	36 (1%)



5 of 256 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 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1563	G
1	0	2761	A
1	0	1450	C
1	0	1692	C

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

5 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	12,22,23	0.97	1 (8%)	19,31,34	3.15	2 (10%)
1	OMG	0	2588	1	17,26,27	1.04	1 (5%)	21,38,41	2.51	3 (14%)
1	UR3	0	2619	1	12,22,23	0.92	0	16,32,35	0.79	0
1	PSU	0	2621	1	13,21,22	1.55	2 (15%)	18,30,33	6.12	3 (16%)
1	1MA	0	628	1	14,25,26	0.94	1 (7%)	15,37,40	1.22	1 (6%)

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	-	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	-	0/3/25/26	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.62	1.48	1.52
1	0	2587	OMU	C4-N3	2.29	1.37	1.33
1	0	628	1MA	C6-N6	2.54	1.33	1.29
1	0	2621	PSU	C4-N3	2.72	1.38	1.33
1	0	2588	OMG	C6-N1	3.22	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.50	114.62	128.33
1	0	2588	OMG	C5-C6-N1	-8.70	111.70	123.59
1	0	628	1MA	C2-N3-C4	-3.67	110.72	116.40
1	0	2587	OMU	C5-C4-N3	-3.24	114.81	123.12
1	0	2588	OMG	N3-C2-N1	-2.22	124.06	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2588	OMG	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 232 ligands modelled in this entry, 231 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
32	ERY	0	9000	-	53,53,53	1.15	3 (5%)	82,82,82	0.97	3 (3%)

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
32	ERY	0	9000	-	-	0/72/107/107	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9000	ERY	C2-C3	2.07	1.60	1.55
32	0	9000	ERY	C7-C6	2.29	1.58	1.54
32	0	9000	ERY	C6-C5	2.78	1.61	1.55

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9000	ERY	C3-C2-C1	-2.63	104.71	109.86
32	0	9000	ERY	C25-C24-C23	-2.42	106.50	110.03
32	0	9000	ERY	C6-C5-C4	-2.26	110.94	114.11

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 ⓘ

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	2749/2922 (94%)	-0.43	46 (1%) 73 72	26, 49, 94, 152	0
2	9	122/122 (100%)	-0.38	5 (4%) 41 39	40, 65, 90, 154	0
3	A	237/240 (98%)	0.24	13 (5%) 29 26	31, 54, 88, 109	0
4	B	337/338 (99%)	0.06	6 (1%) 71 70	30, 58, 83, 92	0
5	C	246/246 (100%)	-0.06	2 (0%) 87 87	26, 48, 73, 82	0
6	D	140/177 (79%)	1.90	55 (39%) 0 0	56, 101, 125, 132	0
7	E	172/178 (96%)	0.81	22 (12%) 5 3	49, 71, 90, 94	0
8	F	119/120 (99%)	0.82	17 (14%) 4 2	51, 76, 95, 111	0
9	G	29/348 (8%)	2.72	22 (75%) 0 0	77, 93, 102, 105	0
10	H	160/177 (90%)	0.26	11 (6%) 20 17	39, 59, 92, 99	0
11	I	70/162 (43%)	4.29	63 (90%) 0 0	109, 122, 139, 141	0
12	J	142/145 (97%)	0.01	0 100 100	38, 53, 75, 95	0
13	K	132/132 (100%)	-0.07	2 (1%) 76 75	34, 55, 75, 86	0
14	L	145/165 (87%)	0.68	26 (17%) 2 1	27, 68, 109, 122	0
15	M	194/195 (99%)	-0.15	1 (0%) 91 92	35, 46, 61, 70	0
16	N	186/187 (99%)	0.64	23 (12%) 5 4	41, 64, 108, 119	0
17	O	115/116 (99%)	0.05	1 (0%) 85 86	39, 57, 74, 78	0
18	P	143/149 (95%)	0.15	1 (0%) 89 89	41, 58, 71, 80	0
19	Q	95/96 (98%)	-0.07	0 100 100	38, 46, 62, 76	0
20	R	150/155 (96%)	-0.11	1 (0%) 89 89	35, 48, 67, 77	0
21	S	81/85 (95%)	0.20	3 (3%) 45 44	47, 63, 83, 88	0
22	T	119/120 (99%)	0.45	7 (5%) 26 23	40, 61, 85, 97	0
23	U	53/66 (80%)	0.24	1 (1%) 70 69	46, 59, 76, 86	0
24	V	65/71 (91%)	1.65	18 (27%) 1 0	58, 77, 114, 118	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	-0.17	0 <span>100</span> <span>100</span>	35, 50, 67, 78	0
26	X	82/92 (89%)	0.52	10 (12%) <span>5</span> <span>4</span>	48, 61, 85, 101	0
27	Y	142/241 (58%)	0.10	7 (4%) <span>33</span> <span>31</span>	28, 47, 71, 89	0
28	Z	73/83 (87%)	0.18	3 (4%) <span>41</span> <span>39</span>	52, 64, 80, 95	0
29	1	56/57 (98%)	-0.46	0 <span>100</span> <span>100</span>	29, 36, 42, 52	0
30	2	46/50 (92%)	0.39	4 (8%) <span>13</span> <span>9</span>	37, 61, 87, 102	0
31	3	92/92 (100%)	0.25	1 (1%) <span>82</span> <span>82</span>	37, 56, 70, 83	0
All	All	6646/7481 (88%)	0.03	371 (5%) <span>28</span> <span>25</span>	26, 55, 99, 154	0

The worst 5 of 371 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	128	THR	13.3
24	V	1	THR	11.1
11	I	91	PHE	9.4
24	V	39	ALA	8.9
11	I	88	GLN	8.5

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

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
1	PSU	0	2621	20/21	0.99	0.14	-	28,31,35,36	0
1	OMU	0	2587	21/22	0.99	0.12	-	35,37,40,43	0
1	UR3	0	2619	21/22	0.99	0.12	-	35,37,41,45	0
1	1MA	0	628	23/24	0.99	0.15	-	30,33,34,36	0
1	OMG	0	2588	24/25	0.98	0.14	-	34,36,38,40	0

## 6.3 Carbohydrates [i](#)

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
35	NA	L	8580	1/1	0.92	0.69	40.89	60,60,60,60	0
35	NA	0	8574	1/1	0.98	0.53	36.87	65,65,65,65	0
35	NA	0	8556	1/1	0.95	0.37	23.19	44,44,44,44	0
35	NA	R	8586	1/1	0.61	0.74	21.44	87,87,87,87	0
35	NA	0	8561	1/1	0.91	0.28	20.39	58,58,58,58	0
35	NA	0	8571	1/1	0.83	0.28	19.60	58,58,58,58	0
35	NA	0	8578	1/1	0.97	0.37	19.47	52,52,52,52	0
35	NA	0	8572	1/1	0.91	0.34	14.89	64,64,64,64	0
35	NA	0	8535	1/1	0.91	0.25	13.55	49,49,49,49	0
35	NA	0	8564	1/1	0.85	0.25	13.51	49,49,49,49	0
36	CL	0	8815	1/1	0.94	0.24	13.31	81,81,81,81	0
35	NA	0	8562	1/1	0.88	0.27	13.16	63,63,63,63	0
35	NA	0	8573	1/1	0.95	0.39	12.94	58,58,58,58	0
35	NA	9	8583	1/1	0.86	0.28	11.85	58,58,58,58	0
35	NA	0	8510	1/1	0.88	0.29	11.11	45,45,45,45	0
35	NA	0	8540	1/1	0.88	0.37	11.08	52,52,52,52	0
35	NA	0	8521	1/1	0.97	0.28	8.86	57,57,57,57	0
35	NA	0	8532	1/1	0.91	0.23	8.68	40,40,40,40	0
35	NA	0	8502	1/1	0.95	0.20	6.89	56,56,56,56	0
34	K	0	8401	1/1	0.94	0.19	6.42	75,75,75,75	0
35	NA	0	8525	1/1	0.98	0.21	6.28	59,59,59,59	0
33	MG	0	8088	1/1	0.90	0.19	6.23	38,38,38,38	0
32	ERY	0	9000	51/51	0.90	0.24	5.50	69,75,79,80	0
35	NA	0	8550	1/1	0.96	0.20	5.19	47,47,47,47	0
35	NA	0	8568	1/1	0.87	0.17	5.07	76,76,76,76	0
35	NA	0	8526	1/1	0.84	0.27	4.39	55,55,55,55	0
35	NA	0	8577	1/1	0.95	0.18	3.27	62,62,62,62	0
35	NA	0	8566	1/1	0.86	0.23	2.97	59,59,59,59	0
35	NA	0	8576	1/1	0.96	0.18	2.92	52,52,52,52	0
35	NA	0	8565	1/1	0.93	0.44	2.49	46,46,46,46	0
35	NA	0	8582	1/1	0.86	0.18	2.06	80,80,80,80	0
35	NA	0	8514	1/1	0.92	0.17	2.06	40,40,40,40	0
35	NA	0	8527	1/1	0.93	0.14	0.26	45,45,45,45	0
33	MG	0	8060	1/1	0.98	0.15	0.23	42,42,42,42	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	C	8504	1/1	0.84	0.18	0.21	46,46,46,46	0
35	NA	0	8523	1/1	0.96	0.17	0.08	38,38,38,38	0
35	NA	0	8524	1/1	0.95	0.15	-0.01	62,62,62,62	0
35	NA	0	8503	1/1	0.99	0.15	-0.07	39,39,39,39	0
35	NA	M	8547	1/1	0.96	0.14	-0.11	33,33,33,33	0
35	NA	0	8539	1/1	0.93	0.14	-0.13	28,28,28,28	0
33	MG	3	8078	1/1	0.98	0.12	-0.49	47,47,47,47	0
33	MG	0	8086	1/1	0.98	0.12	-0.68	48,48,48,48	0
36	CL	M	8818	1/1	0.99	0.14	-0.69	48,48,48,48	0
35	NA	0	8531	1/1	0.95	0.13	-0.81	40,40,40,40	0
37	CD	U	8701	1/1	0.99	0.11	-0.82	67,67,67,67	0
35	NA	Q	8548	1/1	0.91	0.16	-0.94	47,47,47,47	0
36	CL	O	8808	1/1	0.98	0.14	-0.97	72,72,72,72	0
35	NA	J	8546	1/1	0.95	0.14	-1.04	55,55,55,55	0
33	MG	0	8015	1/1	0.99	0.12	-1.29	35,35,35,35	0
35	NA	R	8537	1/1	0.94	0.12	-1.34	42,42,42,42	0
36	CL	J	8821	1/1	0.97	0.13	-1.45	55,55,55,55	0
37	CD	Z	8703	1/1	0.99	0.09	-1.51	63,63,63,63	0
33	MG	0	8044	1/1	0.97	0.10	-1.53	49,49,49,49	0
33	MG	0	8013	1/1	0.98	0.15	-1.63	45,45,45,45	0
36	CL	0	8816	1/1	0.97	0.10	-1.66	60,60,60,60	0
37	CD	1	8702	1/1	0.99	0.08	-1.77	63,63,63,63	0
37	CD	3	8704	1/1	0.99	0.07	-1.87	62,62,62,62	0
35	NA	0	8517	1/1	0.91	0.09	-2.03	46,46,46,46	0
36	CL	B	8819	1/1	0.99	0.12	-2.13	54,54,54,54	0
35	NA	0	8533	1/1	0.92	0.09	-2.21	38,38,38,38	0
33	MG	0	8064	1/1	0.96	0.10	-2.26	34,34,34,34	0
33	MG	0	8033	1/1	0.96	0.12	-2.37	32,32,32,32	0
35	NA	0	8505	1/1	0.96	0.12	-2.42	33,33,33,33	0
33	MG	T	8073	1/1	0.95	0.12	-2.44	61,61,61,61	0
36	CL	L	8810	1/1	0.96	0.09	-2.45	60,60,60,60	0
33	MG	0	8018	1/1	0.99	0.11	-2.47	45,45,45,45	0
33	MG	A	8065	1/1	0.99	0.10	-2.52	42,42,42,42	0
36	CL	3	8804	1/1	0.89	0.09	-2.54	63,63,63,63	0
33	MG	0	8070	1/1	0.93	0.08	-2.55	50,50,50,50	0
35	NA	A	8545	1/1	0.98	0.09	-2.64	50,50,50,50	0
35	NA	0	8553	1/1	0.97	0.10	-2.67	30,30,30,30	0
33	MG	0	8056	1/1	0.98	0.10	-2.72	53,53,53,53	0
33	MG	B	8055	1/1	0.98	0.07	-2.74	52,52,52,52	0
33	MG	0	8057	1/1	0.96	0.12	-2.83	49,49,49,49	0
33	MG	0	8106	1/1	0.98	0.06	-2.93	42,42,42,42	0
36	CL	0	8805	1/1	0.94	0.11	-2.95	63,63,63,63	0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8074	1/1	0.99	0.05	-3.01	38,38,38,38	0
36	CL	0	8812	1/1	0.99	0.09	-3.13	54,54,54,54	0
33	MG	0	8080	1/1	0.98	0.10	-3.23	46,46,46,46	0
35	NA	H	8509	1/1	0.97	0.06	-3.67	34,34,34,34	0
35	NA	R	8538	1/1	0.95	0.07	-3.71	57,57,57,57	0
33	MG	0	8096	1/1	0.93	0.07	-3.74	45,45,45,45	0
34	K	0	8402	1/1	0.99	0.11	-3.85	59,59,59,59	0
33	MG	0	8058	1/1	0.99	0.09	-3.85	44,44,44,44	0
33	MG	0	8111	1/1	0.96	0.10	-4.19	34,34,34,34	0
33	MG	0	8017	1/1	0.99	0.04	-4.20	25,25,25,25	0
33	MG	0	8054	1/1	0.99	0.11	-4.31	32,32,32,32	0
33	MG	0	8021	1/1	0.99	0.10	-4.33	35,35,35,35	0
33	MG	0	8003	1/1	0.99	0.15	-4.39	32,32,32,32	0
33	MG	0	8020	1/1	0.99	0.09	-4.40	36,36,36,36	0
33	MG	0	8084	1/1	0.98	0.07	-4.52	48,48,48,48	0
33	MG	0	8038	1/1	0.99	0.10	-4.67	32,32,32,32	0
33	MG	0	8004	1/1	0.99	0.05	-4.74	27,27,27,27	0
35	NA	0	8544	1/1	0.98	0.05	-4.77	32,32,32,32	0
33	MG	0	8008	1/1	0.99	0.07	-4.89	33,33,33,33	0
33	MG	0	8012	1/1	0.99	0.09	-5.12	34,34,34,34	0
33	MG	0	8032	1/1	0.99	0.05	-5.37	39,39,39,39	0
33	MG	0	8010	1/1	0.98	0.09	-5.38	37,37,37,37	0
33	MG	0	8101	1/1	0.95	0.09	-5.77	58,58,58,58	0
33	MG	0	8019	1/1	0.99	0.06	-6.01	37,37,37,37	0
33	MG	0	8053	1/1	0.96	0.07	-6.05	45,45,45,45	0
35	NA	0	8520	1/1	0.98	0.10	-6.35	37,37,37,37	0
35	NA	T	8543	1/1	0.97	0.08	-6.38	39,39,39,39	0
33	MG	0	8067	1/1	0.98	0.10	-6.39	49,49,49,49	0
33	MG	0	8107	1/1	0.93	0.06	-6.44	68,68,68,68	0
33	MG	0	8001	1/1	0.99	0.08	-6.71	33,33,33,33	0
33	MG	0	8077	1/1	0.98	0.09	-7.35	30,30,30,30	0
35	NA	0	8567	1/1	0.90	0.09	-7.93	50,50,50,50	0
33	MG	0	8007	1/1	0.98	0.07	-8.42	27,27,27,27	0
33	MG	0	8006	1/1	0.96	0.06	-8.74	38,38,38,38	0
33	MG	0	8014	1/1	0.97	0.06	-9.41	34,34,34,34	0
33	MG	0	8052	1/1	0.98	0.07	-10.30	58,58,58,58	0
33	MG	0	8071	1/1	0.97	0.06	-10.40	72,72,72,72	0
33	MG	0	8091	1/1	0.98	0.06	-10.57	59,59,59,59	0
33	MG	0	8109	1/1	0.99	0.09	-11.42	23,23,23,23	0
33	MG	0	8022	1/1	0.99	0.08	-12.36	41,41,41,41	0
33	MG	0	8035	1/1	0.97	0.03	-12.48	49,49,49,49	0
33	MG	Y	8108	1/1	0.97	0.07	-12.87	40,40,40,40	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8002	1/1	0.98	0.05	-13.79	33,33,33,33	0
33	MG	0	8079	1/1	0.99	0.11	-	30,30,30,30	0
33	MG	0	8089	1/1	0.98	0.13	-	56,56,56,56	0
33	MG	0	8072	1/1	0.98	0.08	-	56,56,56,56	0
36	CL	J	8802	1/1	0.96	0.09	-	63,63,63,63	0
33	MG	0	8039	1/1	0.99	0.05	-	50,50,50,50	0
33	MG	0	8048	1/1	0.96	0.10	-	71,71,71,71	0
35	NA	S	8512	1/1	0.95	0.22	-	22,22,22,22	0
33	MG	0	8066	1/1	0.92	0.16	-	96,96,96,96	0
33	MG	0	8026	1/1	0.99	0.10	-	29,29,29,29	0
35	NA	0	8536	1/1	0.99	0.08	-	47,47,47,47	0
33	MG	0	8050	1/1	0.89	0.09	-	71,71,71,71	0
35	NA	0	8530	1/1	0.98	0.18	-	49,49,49,49	0
36	CL	N	8807	1/1	0.94	0.15	-	63,63,63,63	0
33	MG	0	8061	1/1	0.97	0.10	-	40,40,40,40	0
35	NA	0	8534	1/1	0.96	0.06	-	44,44,44,44	0
35	NA	0	8575	1/1	0.99	0.23	-	50,50,50,50	0
33	MG	0	8082	1/1	0.90	0.16	-	64,64,64,64	0
35	NA	0	8560	1/1	0.95	0.50	-	50,50,50,50	0
33	MG	0	8009	1/1	1.00	0.07	-	33,33,33,33	0
33	MG	0	8047	1/1	0.93	0.19	-	77,77,77,77	0
35	NA	0	8508	1/1	0.93	0.21	-	68,68,68,68	0
35	NA	H	8522	1/1	0.95	0.16	-	56,56,56,56	0
33	MG	0	8036	1/1	0.99	0.07	-	35,35,35,35	0
35	NA	0	8528	1/1	0.98	0.44	-	49,49,49,49	0
33	MG	0	8112	1/1	0.84	0.18	-	47,47,47,47	0
33	MG	0	8113	1/1	0.94	0.08	-	51,51,51,51	0
33	MG	0	8093	1/1	0.94	0.08	-	48,48,48,48	0
33	MG	0	8043	1/1	0.90	0.06	-	49,49,49,49	0
33	MG	0	8024	1/1	0.97	0.08	-	23,23,23,23	0
33	MG	0	8100	1/1	0.95	0.09	-	69,69,69,69	0
33	MG	0	8040	1/1	0.97	0.12	-	61,61,61,61	0
36	CL	A	8809	1/1	0.99	0.18	-	66,66,66,66	0
33	MG	0	8110	1/1	0.97	0.07	-	41,41,41,41	0
33	MG	0	8085	1/1	0.87	0.10	-	50,50,50,50	0
33	MG	0	8037	1/1	1.00	0.04	-	45,45,45,45	0
35	NA	0	8558	1/1	0.86	0.74	-	102,102,102,102	0
33	MG	0	8099	1/1	0.90	0.18	-	55,55,55,55	0
33	MG	0	8115	1/1	0.94	0.09	-	55,55,55,55	0
33	MG	0	8051	1/1	0.95	0.08	-	71,71,71,71	0
33	MG	0	8116	1/1	0.99	0.07	-	37,37,37,37	0
33	MG	0	8049	1/1	0.84	0.20	-	74,74,74,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	CD	O	8705	1/1	0.98	0.09	-	74,74,74,74	0
33	MG	0	8092	1/1	0.85	0.46	-	83,83,83,83	0
33	MG	0	8097	1/1	0.97	0.10	-	36,36,36,36	0
33	MG	0	8104	1/1	0.91	0.12	-	53,53,53,53	0
35	NA	0	8563	1/1	0.85	0.31	-	63,63,63,63	0
35	NA	0	8554	1/1	0.99	0.17	-	41,41,41,41	0
35	NA	0	8542	1/1	0.85	0.25	-	52,52,52,52	0
33	MG	0	8063	1/1	0.96	0.10	-	68,68,68,68	0
33	MG	0	8025	1/1	0.96	0.08	-	46,46,46,46	0
35	NA	0	8516	1/1	0.94	0.31	-	51,51,51,51	0
33	MG	0	8090	1/1	0.94	0.24	-	60,60,60,60	0
35	NA	0	8581	1/1	0.85	0.19	-	51,51,51,51	0
33	MG	0	8083	1/1	0.97	0.06	-	41,41,41,41	0
35	NA	0	8541	1/1	0.90	0.14	-	53,53,53,53	0
33	MG	0	8005	1/1	0.99	0.10	-	30,30,30,30	0
33	MG	0	8030	1/1	0.99	0.12	-	29,29,29,29	0
33	MG	0	8114	1/1	0.91	0.13	-	55,55,55,55	0
33	MG	0	8045	1/1	0.94	0.13	-	60,60,60,60	0
35	NA	0	8585	1/1	0.90	0.39	-	53,53,53,53	0
33	MG	0	8075	1/1	0.96	0.06	-	44,44,44,44	0
33	MG	0	8029	1/1	0.99	0.12	-	49,49,49,49	0
36	CL	0	8822	1/1	0.94	0.48	-	83,83,83,83	0
36	CL	0	8803	1/1	0.95	0.14	-	59,59,59,59	0
33	MG	0	8062	1/1	0.95	0.09	-	66,66,66,66	0
35	NA	0	8555	1/1	0.95	0.40	-	72,72,72,72	0
35	NA	0	8513	1/1	0.93	0.12	-	54,54,54,54	0
33	MG	0	8023	1/1	0.99	0.08	-	39,39,39,39	0
35	NA	0	8559	1/1	0.91	0.28	-	64,64,64,64	0
35	NA	0	8584	1/1	0.82	0.17	-	54,54,54,54	0
35	NA	9	8551	1/1	0.79	0.27	-	39,39,39,39	0
33	MG	0	8081	1/1	0.96	0.10	-	53,53,53,53	0
35	NA	0	8552	1/1	0.89	0.39	-	57,57,57,57	0
35	NA	0	8570	1/1	0.89	0.36	-	63,63,63,63	0
33	MG	0	8102	1/1	0.95	0.11	-	55,55,55,55	0
35	NA	0	8579	1/1	0.94	0.17	-	58,58,58,58	0
35	NA	0	8519	1/1	0.99	0.10	-	36,36,36,36	0
33	MG	0	8016	1/1	0.96	0.13	-	35,35,35,35	0
36	CL	0	8813	1/1	0.98	0.16	-	57,57,57,57	0
35	NA	0	8549	1/1	0.95	0.13	-	46,46,46,46	0
33	MG	K	8069	1/1	0.94	0.11	-	57,57,57,57	0
33	MG	0	8031	1/1	0.99	0.06	-	34,34,34,34	0
33	MG	0	8041	1/1	0.97	0.16	-	69,69,69,69	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8094	1/1	0.98	0.10	-	72,72,72,72	0
33	MG	0	8087	1/1	0.76	0.21	-	63,63,63,63	0
33	MG	2	8076	1/1	0.88	0.12	-	53,53,53,53	0
33	MG	0	8098	1/1	0.97	0.07	-	34,34,34,34	0
33	MG	0	8028	1/1	0.96	0.08	-	37,37,37,37	0
35	NA	0	8529	1/1	0.21	0.30	-	76,76,76,76	0
36	CL	0	8817	1/1	0.97	0.15	-	63,63,63,63	0
35	NA	0	8506	1/1	0.96	0.45	-	42,42,42,42	0
33	MG	0	8105	1/1	0.96	0.19	-	54,54,54,54	0
35	NA	0	8518	1/1	0.97	0.17	-	39,39,39,39	0
36	CL	J	8801	1/1	0.98	0.17	-	65,65,65,65	0
33	MG	0	8046	1/1	0.91	0.07	-	43,43,43,43	0
35	NA	0	8511	1/1	0.84	0.09	-	58,58,58,58	0
35	NA	0	8507	1/1	0.93	0.31	-	54,54,54,54	0
33	MG	0	8034	1/1	0.98	0.08	-	34,34,34,34	0
33	MG	0	8103	1/1	0.92	0.15	-	67,67,67,67	0
33	MG	0	8011	1/1	0.99	0.12	-	25,25,25,25	0
33	MG	0	8059	1/1	0.99	0.05	-	33,33,33,33	0
35	NA	0	8515	1/1	0.96	0.14	-	48,48,48,48	0
35	NA	0	8569	1/1	0.81	0.30	-	57,57,57,57	0
36	CL	0	8811	1/1	0.98	0.10	-	54,54,54,54	0
33	MG	9	8095	1/1	0.96	0.09	-	72,72,72,72	0
33	MG	0	8027	1/1	0.97	0.10	-	49,49,49,49	0
36	CL	Y	8820	1/1	0.96	0.09	-	46,46,46,46	0
35	NA	0	8557	1/1	0.91	0.08	-	60,60,60,60	0
33	MG	0	8042	1/1	0.96	0.13	-	40,40,40,40	0
33	MG	0	8068	1/1	0.95	0.09	-	68,68,68,68	0
36	CL	0	8814	1/1	0.98	0.08	-	48,48,48,48	0
35	NA	0	8501	1/1	0.98	0.20	-	35,35,35,35	0
36	CL	R	8806	1/1	0.96	0.09	-	50,50,50,50	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.