



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 08:26 am GMT

PDB ID : 1YHQ  
Title : Crystal Structure Of Azithromycin Bound To The G2099A Mutant 50S Ribosomal Subunit Of Haloarcula Marismortui  
Authors : Tu, D.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2005-01-10  
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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

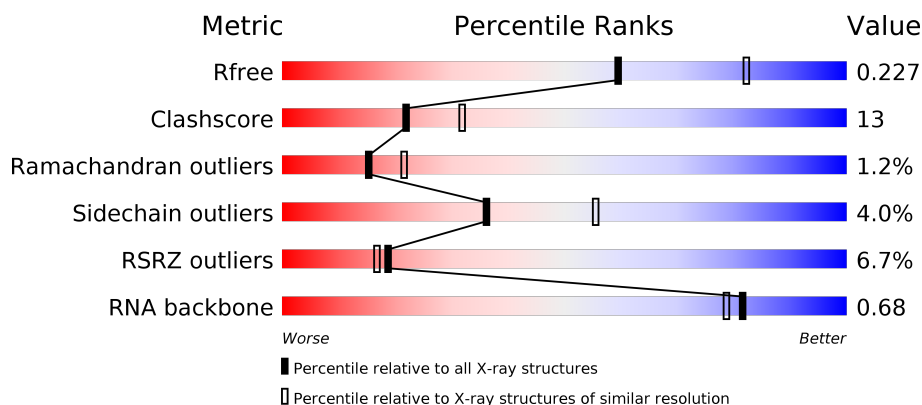
# 1 Overall quality at a glance

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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)
RNA backbone	2435	1034 (2.86-1.94)

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>3%</div> <div>65% 24% 6%</div> </div>
2	9	122	<div> <div>5%</div> <div>60% 30% 10%</div> </div>
3	A	240	<div> <div>5%</div> <div>63% 30% 5%</div> </div>
4	B	338	<div> <div>3%</div> <div>60% 36%</div> </div>

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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	194	
16	N	187	
17	O	116	
18	P	149	
19	Q	96	
20	R	155	
21	S	85	
22	T	120	
23	U	66	
24	V	71	
25	W	154	
26	X	92	
27	Y	241	
28	Z	83	
29	1	57	

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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
35	NA	0	8517	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8523	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8534	-	-	-	X
35	NA	0	8535	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8550	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8568	-	-	-	X
35	NA	0	8571	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	R	8575	-	-	-	X
36	CL	M	8818	-	-	-	X
37	SR	0	8903	-	-	-	X
37	SR	0	8969	-	-	-	X
37	SR	0	8992	-	-	-	X
37	SR	A	8929	-	-	-	X
37	SR	B	8987	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99116 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			

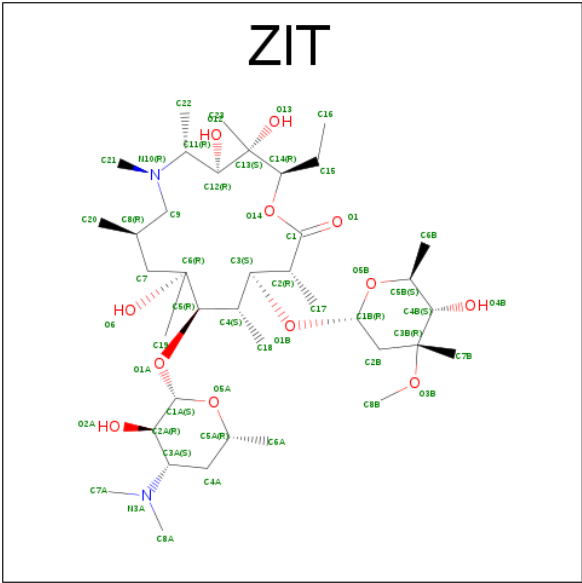
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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 AZITHROMYCIN (three-letter code: ZIT) (formula: C<sub>38</sub>H<sub>72</sub>N<sub>2</sub>O<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
32	0	1	Total	C	N	O	0	0
			52	38	2	12		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	86	Total	Mg	0	0
			86	86		
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	2	Total	Mg	0	0
			2	2		
33	T	1	Total	Mg	0	0
			1	1		
33	9	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	65	Total Na 65 65	0	0
35	J	1	Total Na 1 1	0	0
35	Q	1	Total Na 1 1	0	0
35	H	1	Total Na 1 1	0	0
35	C	1	Total Na 1 1	0	0
35	R	2	Total Na 2 2	0	0
35	9	2	Total Na 2 2	0	0
35	S	1	Total Na 1 1	0	0
35	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	0	10	Total Cl 10 10	0	0
36	J	3	Total Cl 3 3	0	0
36	B	1	Total Cl 1 1	0	0
36	A	1	Total Cl 1 1	0	0
36	N	1	Total Cl 1 1	0	0
36	O	1	Total Cl 1 1	0	0
36	R	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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 STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	0	94	Total 94	Sr 94	0	0
37	1	2	Total 2	Sr 2	0	0
37	H	1	Total 1	Sr 1	0	0
37	B	2	Total 2	Sr 2	0	0
37	3	1	Total 1	Sr 1	0	0
37	A	3	Total 3	Sr 3	0	0
37	R	1	Total 1	Sr 1	0	0
37	9	2	Total 2	Sr 2	0	0
37	S	1	Total 1	Sr 1	0	0
37	F	1	Total 1	Sr 1	0	0

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

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5845	Total 5845	O 5845	0	0
39	9	145	Total 145	O 145	0	0
39	A	118	Total 118	O 118	0	0
39	B	151	Total 151	O 151	0	0
39	C	176	Total 176	O 176	0	0
39	D	49	Total 49	O 49	0	0
39	E	40	Total 40	O 40	0	0
39	F	26	Total 26	O 26	0	0
39	G	18	Total 18	O 18	0	0
39	H	72	Total 72	O 72	0	0
39	I	8	Total 8	O 8	0	0
39	J	59	Total 59	O 59	0	0
39	K	58	Total 58	O 58	0	0
39	L	72	Total 72	O 72	0	0
39	M	124	Total 124	O 124	0	0
39	N	61	Total 61	O 61	0	0
39	O	38	Total 38	O 38	0	0

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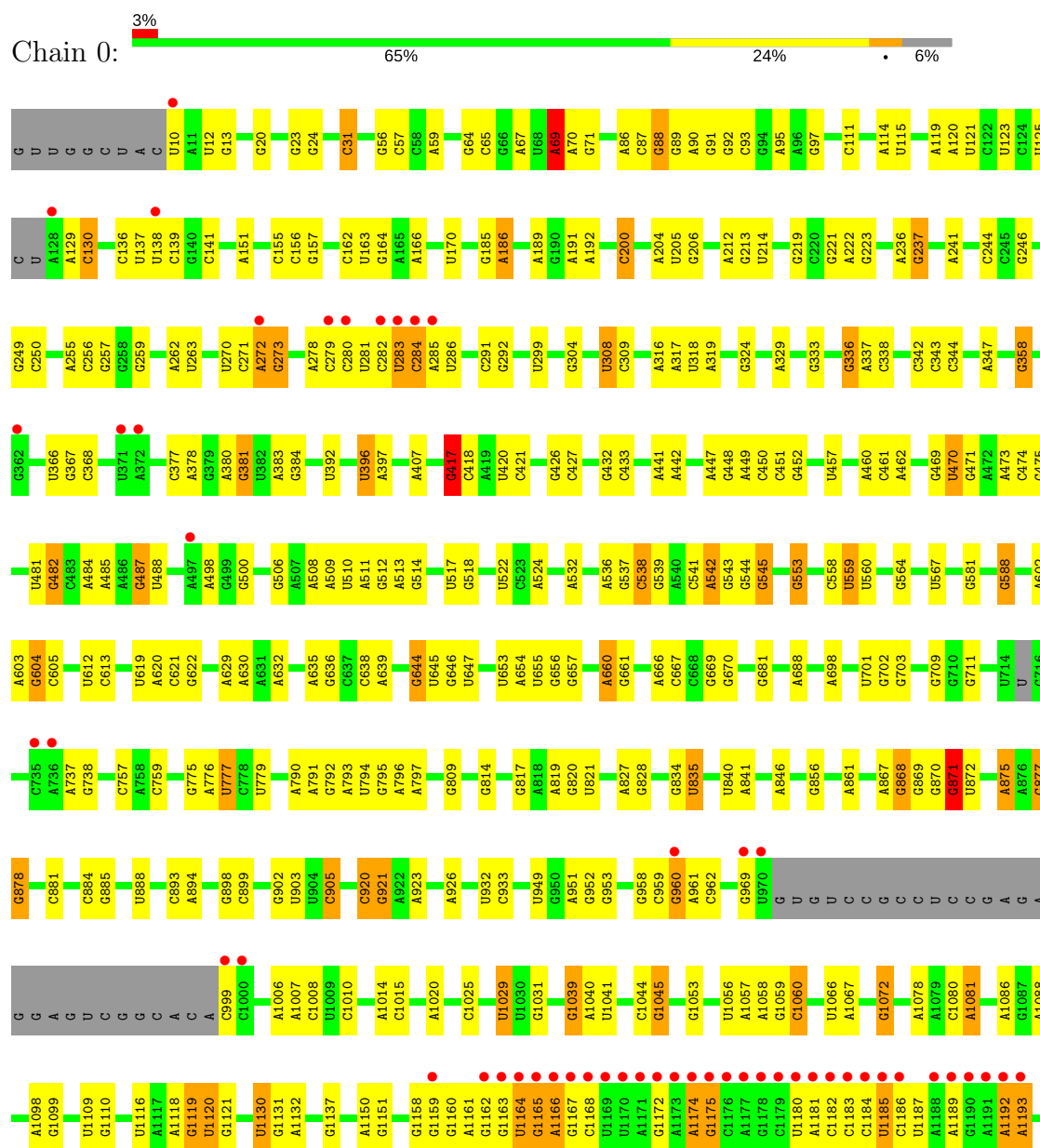
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	66	Total 66	O 66	0	0
39	Q	53	Total 53	O 53	0	0
39	R	87	Total 87	O 87	0	0
39	S	32	Total 32	O 32	0	0
39	T	41	Total 41	O 41	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	24	Total 24	O 24	0	0
39	Y	95	Total 95	O 95	0	0
39	Z	32	Total 32	O 32	0	0
39	1	50	Total 50	O 50	0	0
39	2	44	Total 44	O 44	0	0
39	3	71	Total 71	O 71	0	0

### 3 Residue-property plots [i](#)

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

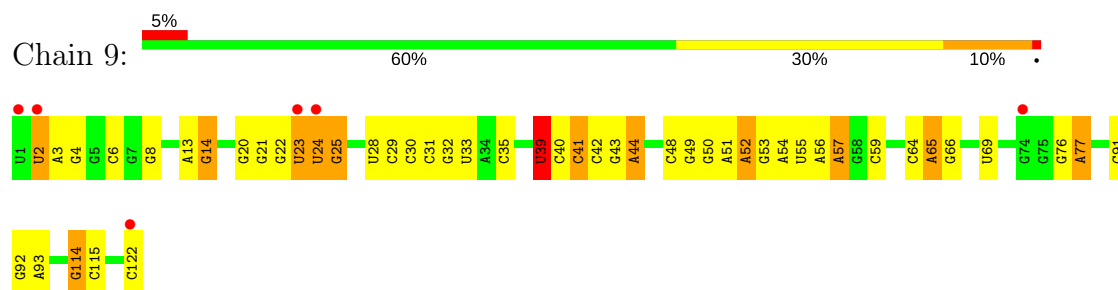
#### • Molecule 1: 23S Ribosomal RNA



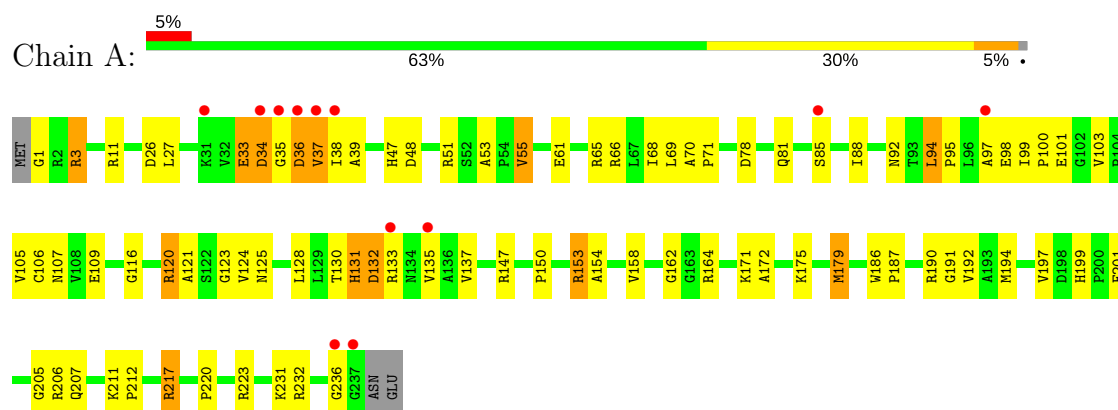
G2884	C2780	A2649	U2527	U2435	C2309	A	G	G2014	G1753	U1625	G1452	G1300	C1196
G2781	U2761	U2652	C2533	G2442	C2313	C	A	A2015	A1754	A1626	G1458	U1304	G1197
A2783	G2782	A2653	C2534	C2443	G2317	A	U	G1927	A1755	G1627	A1458	C1305	A1199
C2787	C2787	U2661	G2537	U2444	G2317	U	U	C1940	C1762	A1630	A1470	U1306	C1201
U2791	U2791	A2664	U2541	U2445	C2317	A	C	A1941	U1766	G1634	C1474	A1308	C1202
A2792	A2792	A	C2542	G2453	A2321	A	A	C1943	U1767	A1641	C1477	U1314	G1203
C2793	C2793	U	G2543	A2456	A2326	U	C	A1642	C1768	A1642	C1477	U1314	C1204
A2902	G2794	G2667	G2544	U2457	C2326	A	U	A1653	C1769	G1484	G1484	A1328	U1205
C2903	U2796	G2670	C2547	G2462	G2336	C	U	G1946	G1773	G1497	G1497	U1333	A1207
A2906	A2800	U2671	C2548	G2466	G2337	U	A	G1947	U1766	U1654	G1497	C1334	C1208
C2907	U2807	U2672	C2552	A2465	G2338	A	G	G1948	A1767	G1655	G1497	C1335	C1209
A2908	G2808	U2673	A2553	A2467	A	C	U	G1949	C1768	A1656	U1500	C1335	G1210
C2909	U2809	U2674	C2559	A2468	C	U	G	G1950	C1769	A1657	U1500	C1335	G1211
C2911	G2810	C2676	U2563	C2472	A	C	U	G1951	A1779	A1658	U1503	C1342	C1212
C2912	A2811	C2682	G2564	C2476	C	C	A	U	G1777	A1778	U1504	C1343	G1216
A2913	A2812	A	C2565	U2477	C	G	G	A	A1779	A1658	U1504	C1343	G1217
A2914	A2813	A2694	C2570	U2478	G	U	A	A	G1777	A1658	U1504	C1343	U1218
G	G2814	A2697	G2578	U2479	C2346	U	C	A	C1786	A1658	U1504	C1343	U1219
C	A2815	G2698	U2578	A2483	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2816	C2712	U2586	A2484	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
A	A2817	G2717	U2587	A2485	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	A2818	C2718	U2588	A2486	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	A2819	U2719	U2589	A2487	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	A2820	G2720	U2590	A2488	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
A	C2825	U2721	U2591	A2489	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
G	G2826	G2722	U2592	A2490	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	A2827	U2723	U2593	A2491	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2828	G2724	U2594	A2492	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
A	C2831	U2725	U2595	A2493	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	A2840	G2726	U2596	A2494	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2842	U2727	U2597	A2495	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
A	A2851	G2728	U2598	A2496	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	A2852	U2729	U2599	A2497	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2862	G2730	U2600	A2498	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	A2863	U2731	U2601	A2499	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2864	G2732	U2602	A2500	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	U2865	U2733	U2603	A2501	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2866	G2734	U2604	A2502	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	U2867	U2735	U2605	A2503	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2868	G2736	U2606	A2504	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2884	G2752	U2622	A2520	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2898	G2766	U2636	A2534	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2906	G2774	U2644	A2542	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2908	G2776	U2646	A2544	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2910	G2778	U2648	A2546	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2912	G2780	U2650	A2548	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2914	G2782	U2652	A2550	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	U2915	U2783	U2653	A2551	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2916	G2784	U2654	A2552	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2918	G2786	U2656	A2554	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	G2924	G2792	U2662	A2560	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
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C	U2929	U2797	U2667	A2565	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	G2930	G2798	U2668	A2566	A2346	U	C	A	C1787	A1658	U1504	C1343	U1219
C	U2931	U2799	U2669	A2567	A2346	U	C	A	C17				



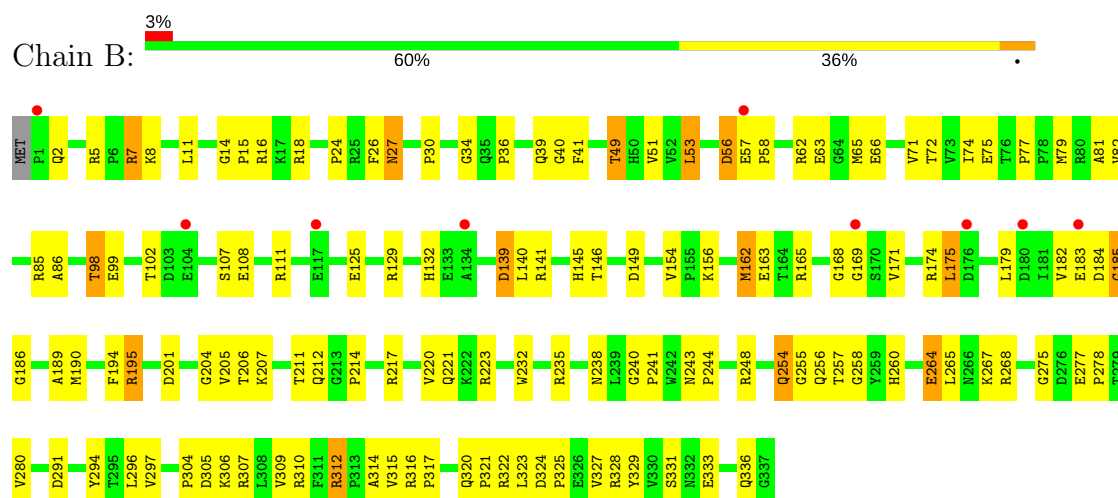
- Molecule 2: 5S Ribosomal RNA



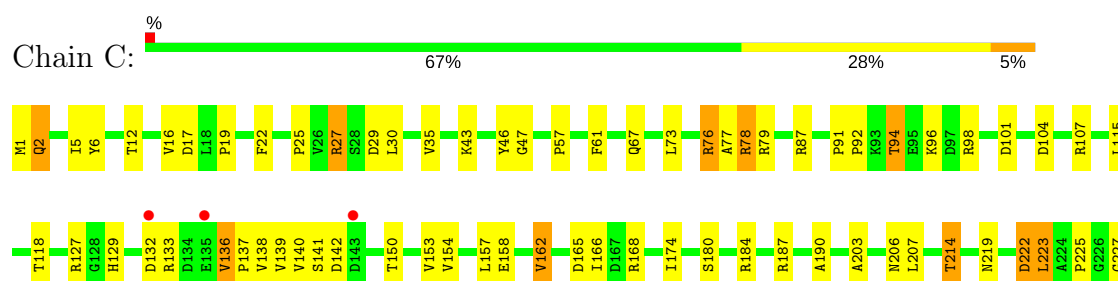
- Molecule 3: 50S ribosomal protein L2P

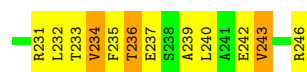


- Molecule 4: 50S ribosomal protein L3P

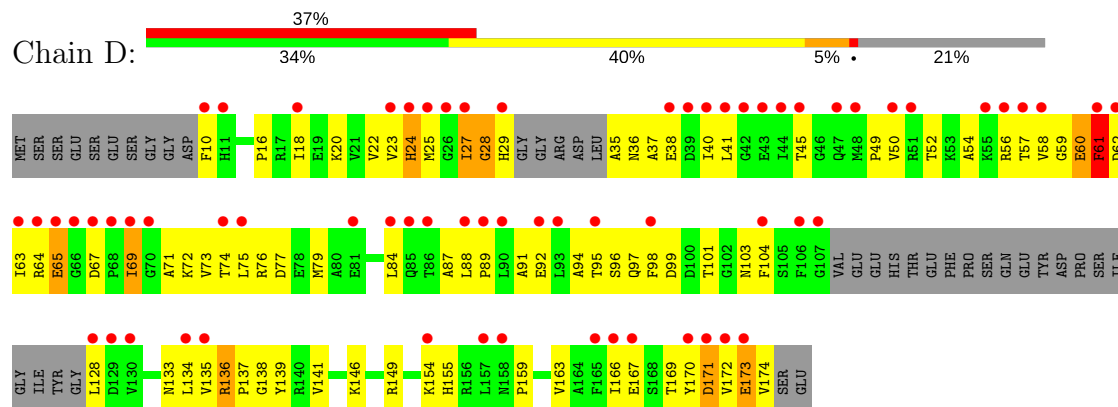


- Molecule 5: 50S ribosomal protein L4E

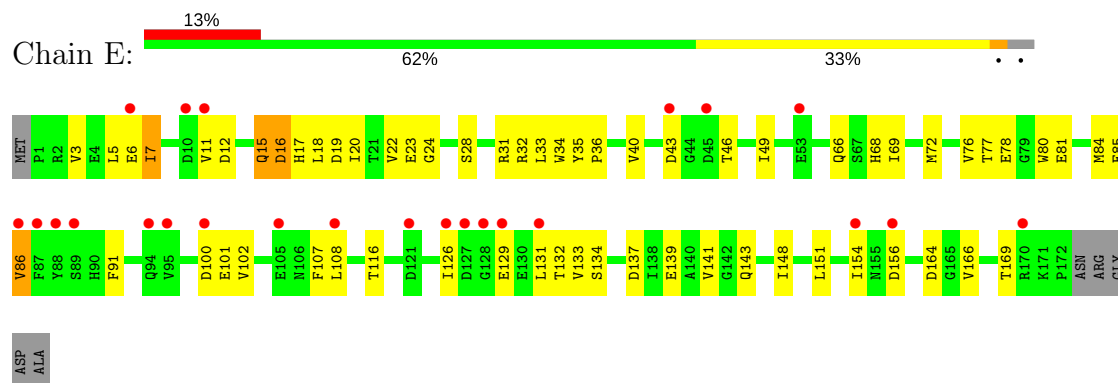




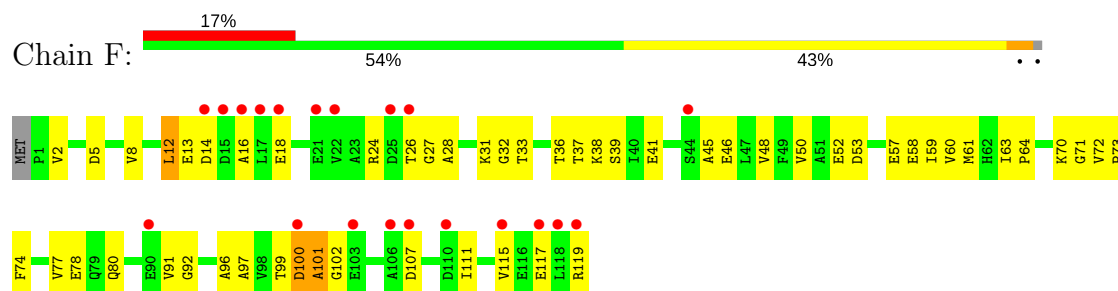
• Molecule 6: 50S ribosomal protein L5P



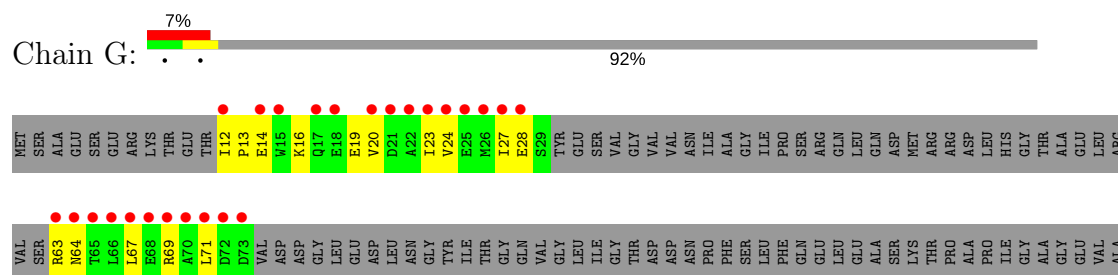
• Molecule 7: 50S ribosomal protein L6P



• Molecule 8: 50S ribosomal protein L7AE



• Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG



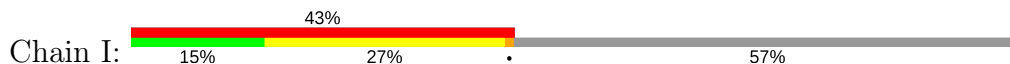
[illegible]

- Molecule 10: 50S RIBOSOMAL PROTEIN L10E



THR	GLY	ALA	GLY	ALA	ASP	ARG	VAL	D114	A119	F120	G121	K122	I123	R129	Y140	C141	E144	D145	A146	V149	K150	E151	R154	R155	A156	Y157	T161	P162	R165	I166	K167	V168	E169	R170	G171	E172	E173	L174	LEU	ILE	ALA						
Met	SR	ASP	R4	P5	A6	P15	Y22	T23	T24	K30	I31	A32	Q33	Q40	A43	V48	Q49	T50	T57	V58	Q59	L60	R61	H62	L65	E66	R69	L70	S71	A72	L76	E79	L80	G81	E82	E83	G84	P85	Y86	K87	N88	T89	L90	R91	K102	G1N	ALA

- Molecule 11: 50S RIBOSOMAL PROTEIN L11P



A120	A121	E122	V123	V124	G125	T126	C127	T128	S129	L130	G131	V132	T133	I134	E135		GLY	GLU	ASN	PRO	ARG	GLU	PHE	LYS	GLU	ARG	ILE	ASP	ALA	GLY	GLN	TYR	ASP	ASP	VAL	VAL	PHE	ALA	ALA	ALA	PHE	ASP	GLY	THR	GLU	VAL	PRO	VAL	THR	VAL	LYS	TYR	ASP	ASP	GLY			
SER	PHE	GLU	ILE	GLU	GLU	G66	V67	F68	P69	T70	A71	E72	L73	I74	K75	D76	E77	A78	G79	E81	H82	G83	S84	G85	E86	P87	O88	E89	B90	F91	V92	A93	D94	L95	S96	V97	D98	Q99	V100	K101	I102	I103	A104	E105	G106	K107	H108	P109	D110	L111	L112	S113	V114	D115	L116	T117	N118	R119
MET	ALA	THR	ILE	GLU	VAL	LEU	VAL	PRO	GLY	GLY	GLU	ALA	ASN	PRO	GLY	GLU	PRO	PRO	LEU	PRO	GLY	GLU	LEU	GLY	PRO	THR	PRO	VAL	ASP	VAL	GLN	ALA	VAL	GLN	GLU	ILE	ASN	ASP	GLN	THR	ALA	ALA	PHE	ASP	GLY	THR	GLU	VAL	PRO	VAL	THR	VAL	LYS	TYR	ASP	ASP	GLY	

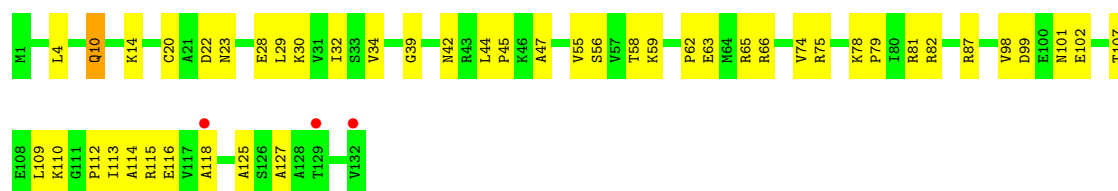
- Molecule 12: 50S ribosomal protein L13P



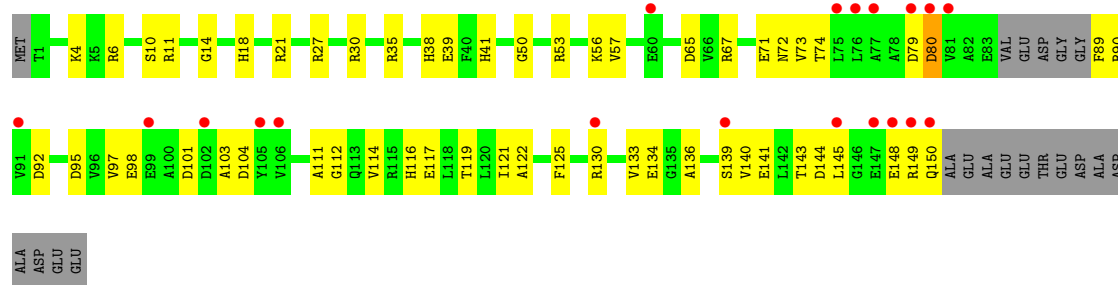
N107	P108	Y109	D110	I127	K128	F129	V130	T131	L132	G133	S136	K143	T144	W145	MET	SER	VAL	A4	E5	F6	D7	D13	A14	R15	I18	M19	V26	V36	E42	V45	I46	T47	G48	O52	I53	T63	G64	Y69	F70	Y71	P72	K73	R74	P75	D76	G77	I78	F79	K80	R81	T82	P88	H89	K90	R93	G94	Y101	R102	V103	Y104	L105	G106
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	----	----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------

- Molecule 13: 50S ribosomal protein L14P

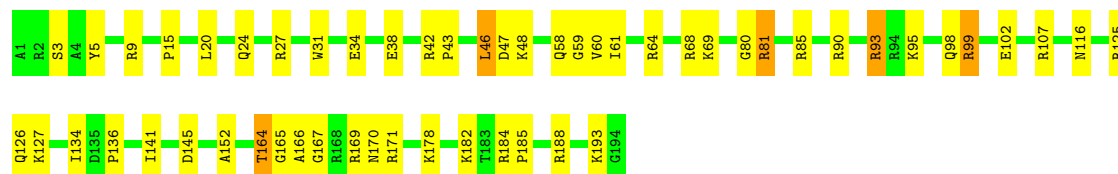




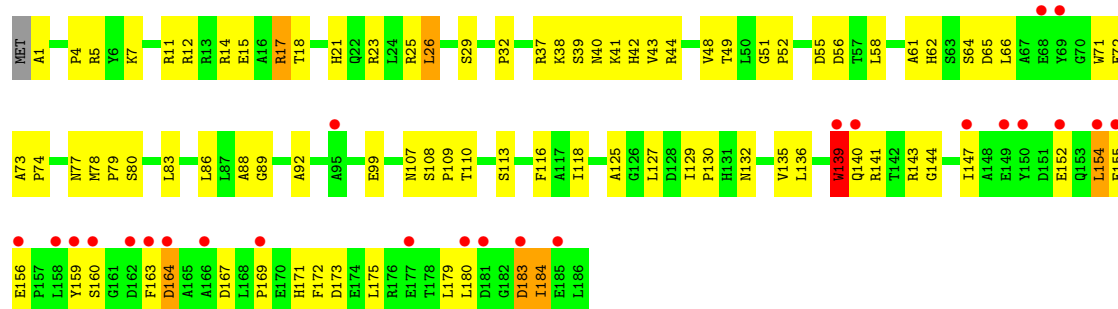
• Molecule 14: 50S ribosomal protein L15P



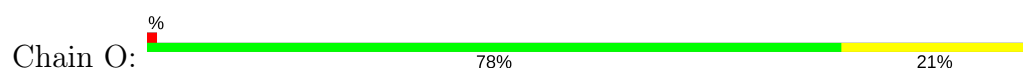
• Molecule 15: 50S Ribosomal Protein L15E



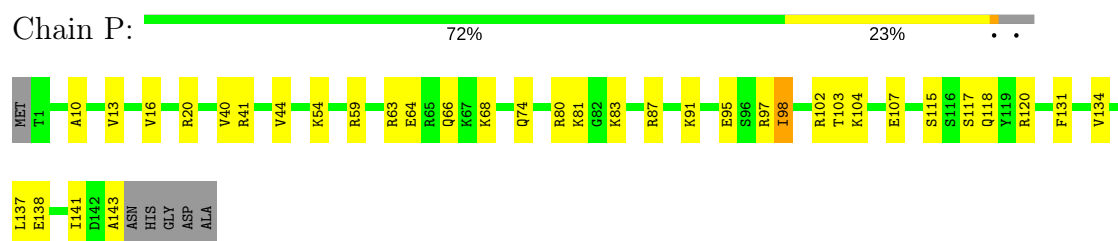
• Molecule 16: 50S ribosomal protein L18P



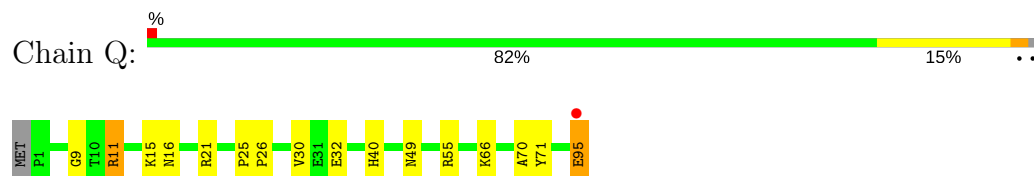
• Molecule 17: 50S ribosomal protein L18e



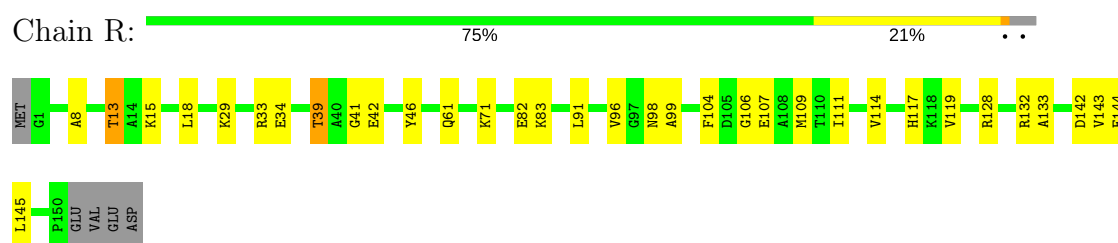
- Molecule 18: 50S ribosomal protein L19E



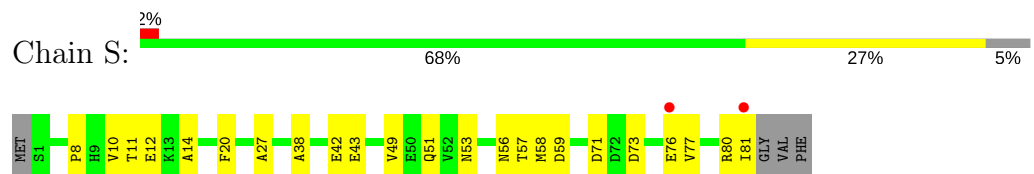
- Molecule 19: 50S ribosomal protein L21e



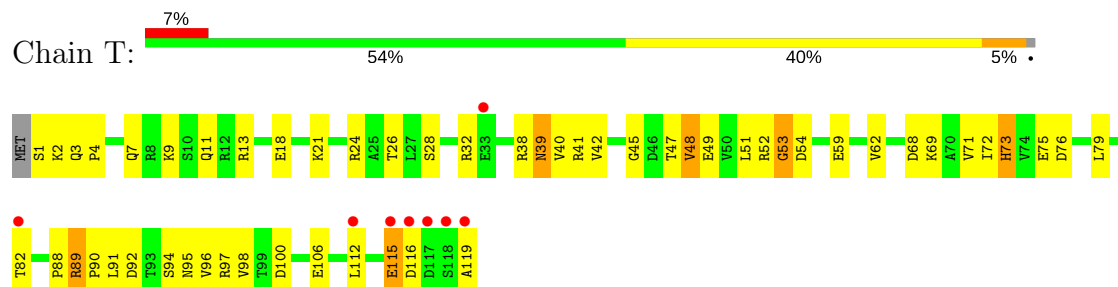
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

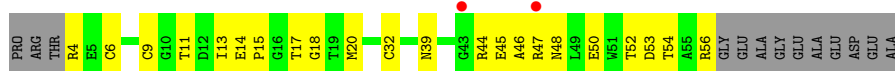


- Molecule 22: 50S ribosomal protein L24P

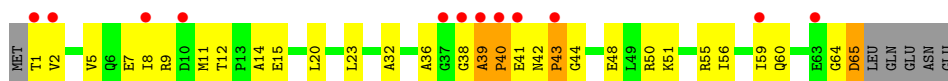


- Molecule 23: 50S ribosomal protein L24E

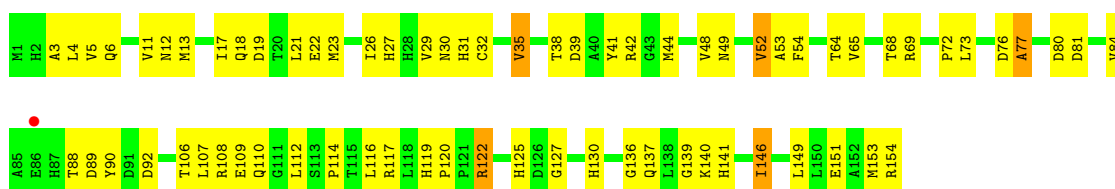




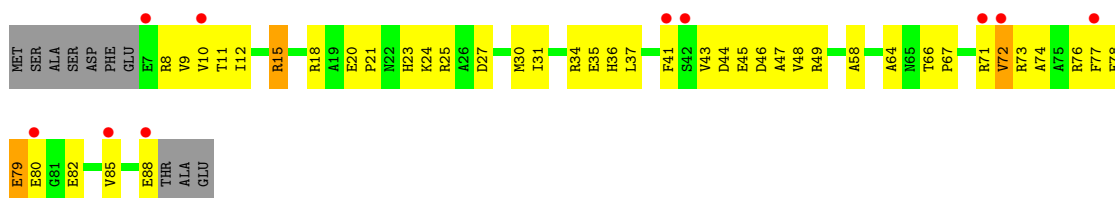
- Molecule 24: 50S ribosomal protein L29P



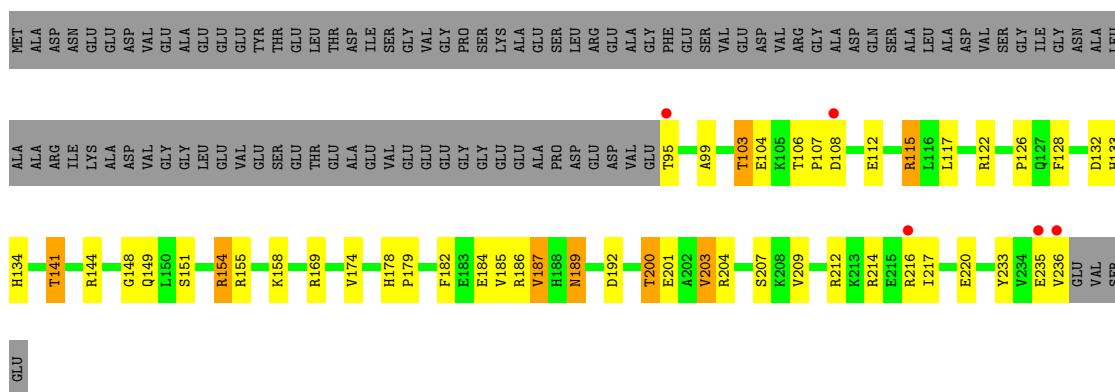
- Molecule 25: 50S ribosomal protein L30P



- Molecule 26: 50S ribosomal protein L31e

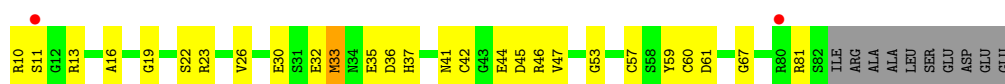


- Molecule 27: 50S ribosomal protein L32E



- Molecule 28: 50S ribosomal protein L37Ae





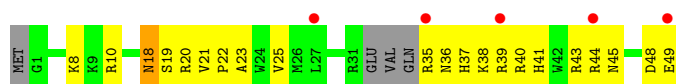
- Molecule 29: 50S ribosomal protein L37e

Chain 1: 70% 28%



- Molecule 30: 50S ribosomal protein L39e

Chain 2: 10% 50% 40% 8%



- Molecule 31: 50S ribosomal protein L44E

Chain 3: 2% 68% 32%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.08Å 298.91Å 574.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.40 49.82 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.2 (29.96-2.40) 90.2 (49.82-2.40)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.190 , 0.229 0.190 , 0.227	Depositor DCC
$R_{free}$ test set	6150 reflections (0.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, ZIT, 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	0.35	0/65957	0.69	25/102867 (0.0%)
2	9	0.32	0/2904	0.70	1/4526 (0.0%)
3	A	0.33	0/1786	0.66	0/2408
4	B	0.31	0/2690	0.64	0/3652
5	C	0.37	0/1884	0.64	0/2551
6	D	0.29	0/1111	0.53	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	0.47	0/324
10	H	0.35	0/1302	0.65	0/1743
11	I	0.28	0/526	0.48	0/716
12	J	0.34	0/1136	0.59	0/1530
13	K	0.33	0/1001	0.65	0/1347
14	L	0.32	0/1130	0.64	0/1509
15	M	0.33	0/1582	0.61	0/2117
16	N	0.28	0/1474	0.60	0/1999
17	O	0.32	0/874	0.59	0/1181
18	P	0.32	0/1147	0.53	0/1528
19	Q	0.34	0/749	0.69	0/1005
20	R	0.34	0/1172	0.64	0/1578
21	S	0.32	0/648	0.58	1/875 (0.1%)
22	T	0.30	0/958	0.62	0/1289
23	U	0.32	0/417	0.53	0/562
24	V	0.29	0/502	0.53	0/675
25	W	0.33	0/1219	0.62	0/1655
26	X	0.31	0/664	0.56	0/895
27	Y	0.34	0/1146	0.62	0/1536
28	Z	0.34	0/589	0.64	0/787
29	1	0.40	0/438	0.64	0/578
30	2	0.33	0/401	0.55	0/529
31	3	0.36	0/771	0.58	0/1024
All	All	0.34	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	0	53
2	9	0	2
All	All	0	55

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	1942	A	C5'-C4'-C3'	8.34	129.34	116.00
1	0	871	G	C5'-C4'-O4'	-7.87	99.66	109.10
2	9	39	U	N1-C1'-C2'	6.90	122.97	114.00
1	0	1979	G	C2'-C3'-O3'	6.61	124.27	113.70
1	0	1504	A	C1'-O4'-C4'	-6.48	104.71	109.90

There are no chirality outliers.

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	221	G	Sidechain
1	0	246	G	Sidechain
1	0	270	U	Sidechain
1	0	324	G	Sidechain
1	0	333	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	59020	0	29808	686	0
2	9	2599	0	1325	53	0
3	A	1753	0	1766	109	0
4	B	2625	0	2533	125	0
5	C	1859	0	1816	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1094	0	1085	91	0
7	E	1357	0	1266	55	0
8	F	890	0	843	51	0
9	G	240	0	231	18	0
10	H	1282	0	1292	53	0
11	I	519	0	500	47	0
12	J	1120	0	1098	58	0
13	K	992	0	1031	56	0
14	L	1118	0	1076	52	0
15	M	1558	0	1566	63	0
16	N	1445	0	1401	100	0
17	O	865	0	873	30	0
18	P	1136	0	1123	34	0
19	Q	735	0	728	14	0
20	R	1149	0	1122	41	0
21	S	641	0	605	20	0
22	T	950	0	923	51	0
23	U	410	0	364	24	0
24	V	499	0	511	35	0
25	W	1196	0	1137	88	0
26	X	654	0	653	42	0
27	Y	1130	0	1133	58	0
28	Z	578	0	539	19	0
29	1	431	0	426	22	0
30	2	396	0	413	25	0
31	3	755	0	728	24	0
32	0	52	0	72	0	0
33	0	86	0	0	0	0
33	9	1	0	0	0	0
33	A	2	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	65	0	0	0	0
35	9	2	0	0	0	0
35	C	1	0	0	0	0
35	H	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	R	2	0	0	0	0
35	S	1	0	0	0	0
36	0	10	0	0	0	0
36	3	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	J	3	0	0	2	0
36	L	1	0	0	0	0
36	M	1	0	0	0	0
36	N	1	0	0	0	0
36	O	1	0	0	0	0
36	R	1	0	0	0	0
36	Y	1	0	0	0	0
37	0	94	0	0	0	0
37	1	2	0	0	0	0
37	3	1	0	0	0	0
37	9	2	0	0	0	0
37	A	3	0	0	0	0
37	B	2	0	0	0	0
37	F	1	0	0	0	0
37	H	1	0	0	0	0
37	R	1	0	0	0	0
37	S	1	0	0	0	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5845	0	0	120	0
39	1	50	0	0	2	0
39	2	44	0	0	3	0
39	3	71	0	0	5	0
39	9	145	0	0	4	0
39	A	118	0	0	19	0
39	B	151	0	0	25	0
39	C	176	0	0	24	0
39	D	49	0	0	19	0
39	E	40	0	0	5	0
39	F	26	0	0	7	0
39	G	18	0	0	2	0
39	H	72	0	0	12	0
39	I	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	J	59	0	0	2	0
39	K	58	0	0	7	0
39	L	72	0	0	15	0
39	M	124	0	0	8	0
39	N	61	0	0	12	0
39	O	38	0	0	6	0
39	P	66	0	0	4	0
39	Q	53	0	0	4	0
39	R	87	0	0	7	0
39	S	32	0	0	3	0
39	T	41	0	0	4	0
39	U	28	0	0	3	0
39	V	12	0	0	2	0
39	W	68	0	0	7	0
39	X	24	0	0	8	0
39	Y	95	0	0	13	0
39	Z	32	0	0	2	0
All	All	99116	0	59987	2007	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 2007 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:O:1160:G:H5'	1:O:1161:A:H5'	1.18	1.10
26:X:37:LEU:HD13	26:X:85:VAL:HG21	1.32	1.09
5:C:236:THR:HG22	5:C:239:ALA:H	1.10	1.06
6:D:25:MET:HE3	6:D:37:ALA:HB1	1.34	1.04
1:O:1242:A:H5'	12:J:82:THR:HG23	1.39	1.04

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%)	218 (93%)	13 (6%)	4 (2%)	11	13
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	8	9
5	C	244/246 (99%)	226 (93%)	18 (7%)	0	100	100
6	D	134/177 (76%)	103 (77%)	20 (15%)	11 (8%)	1	0
7	E	170/178 (96%)	163 (96%)	7 (4%)	0	100	100
8	F	117/120 (98%)	104 (89%)	10 (8%)	3 (3%)	6	6
9	G	25/348 (7%)	25 (100%)	0	0	100	100
10	H	156/177 (88%)	143 (92%)	13 (8%)	0	100	100
11	I	68/162 (42%)	49 (72%)	17 (25%)	2 (3%)	5	5
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	13	18
13	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
14	L	141/165 (86%)	124 (88%)	16 (11%)	1 (1%)	25	37
15	M	192/194 (99%)	181 (94%)	11 (6%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	6	6
17	O	113/116 (97%)	110 (97%)	3 (3%)	0	100	100
18	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
19	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
20	R	148/155 (96%)	142 (96%)	6 (4%)	0	100	100
21	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100
22	T	117/120 (98%)	111 (95%)	5 (4%)	1 (1%)	20	29
23	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
24	V	63/71 (89%)	58 (92%)	2 (3%)	3 (5%)	2	1
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	14	19
26	X	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
27	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
28	Z	71/83 (86%)	61 (86%)	7 (10%)	3 (4%)	3	2
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	7	7
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	3705/4436 (84%)	3437 (93%)	223 (6%)	45 (1%)	15	21

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	LEU
3	A	37	VAL
6	D	171	ASP
8	F	101	ALA
12	J	5	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	179/182 (98%)	167 (93%)	12 (7%)	19	30
4	B	282/283 (100%)	268 (95%)	14 (5%)	28	45
5	C	193/193 (100%)	175 (91%)	18 (9%)	10	15
6	D	117/148 (79%)	113 (97%)	4 (3%)	42	63
7	E	152/156 (97%)	147 (97%)	5 (3%)	43	64
8	F	93/94 (99%)	92 (99%)	1 (1%)	78	90
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	39	59
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	110 (93%)	8 (7%)	18	29
13	K	106/106 (100%)	105 (99%)	1 (1%)	82	92
14	L	113/127 (89%)	110 (97%)	3 (3%)	50	71
15	M	158/158 (100%)	151 (96%)	7 (4%)	33	51
16	N	149/150 (99%)	145 (97%)	4 (3%)	50	71
17	O	93/94 (99%)	91 (98%)	2 (2%)	57	76
18	P	113/117 (97%)	112 (99%)	1 (1%)	82	92
19	Q	79/80 (99%)	76 (96%)	3 (4%)	38	58
20	R	117/122 (96%)	115 (98%)	2 (2%)	66	82
21	S	71/74 (96%)	69 (97%)	2 (3%)	49	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	T	105/106 (99%)	100 (95%)	5 (5%)	30	47
23	U	44/52 (85%)	44 (100%)	0	100	100
24	V	51/57 (90%)	49 (96%)	2 (4%)	37	56
25	W	130/130 (100%)	125 (96%)	5 (4%)	38	58
26	X	66/74 (89%)	59 (89%)	7 (11%)	8	11
27	Y	120/196 (61%)	111 (92%)	9 (8%)	16	24
28	Z	60/68 (88%)	58 (97%)	2 (3%)	43	64
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	54	74
31	3	79/79 (100%)	79 (100%)	0	100	100
All	All	3095/3618 (86%)	2972 (96%)	123 (4%)	36	55

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	H	91	ARG
14	L	35	ARG
27	Y	141	THR
10	H	157	TYR
12	J	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
15	M	26	GLN
18	P	66	GLN
30	2	16	ASN
15	M	58	GLN
16	N	93	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	226 (8%)	0
2	9	121/122 (99%)	16 (13%)	0
All	All	2866/3044 (94%)	242 (8%)	0



5 of 242 RNA backbone outliers are listed below:

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

There are no RNA pucker outliers to report.

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

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	14,22,23	1.01	1 (7%)	18,31,34	3.68	2 (11%)
1	OMG	0	2588	1	18,26,27	1.06	1 (5%)	22,38,41	2.49	4 (18%)
1	UR3	0	2619	1	14,22,23	0.76	0	16,32,35	0.74	0
1	PSU	0	2621	1	16,21,22	1.57	3 (18%)	20,30,33	6.08	4 (20%)
1	1MA	0	628	1	16,25,26	1.05	1 (6%)	13,37,40	1.17	1 (7%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-4.72	1.48	1.52
1	0	2587	OMU	C4-N3	2.60	1.37	1.33
1	0	2621	PSU	C2-N1	2.65	1.43	1.38
1	0	2621	PSU	C4-N3	2.72	1.38	1.33
1	0	628	1MA	C6-N6	2.82	1.33	1.27

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-19.09	114.67	128.40
1	0	2621	PSU	C5-C4-N3	-12.90	114.85	125.43
1	0	2588	OMG	C5-C6-N1	-8.46	111.44	123.48
1	0	628	1MA	C2-N3-C4	-3.65	110.81	116.41
1	0	2587	OMU	C5-C4-N3	-3.47	114.84	123.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 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	ZIT	0	9500	-	54,54,54	1.35	7 (12%)	81,83,83	1.06	4 (4%)

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	ZIT	0	9500	-	-	0/72/107/107	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZIT	O5A-C1A	2.02	1.46	1.41
32	0	9500	ZIT	O6-C6	2.04	1.48	1.44
32	0	9500	ZIT	C13-C12	2.22	1.61	1.55
32	0	9500	ZIT	C6-C5	2.31	1.60	1.55
32	0	9500	ZIT	O13-C13	2.58	1.48	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZIT	C9-N10-C11	-2.96	106.97	112.26
32	0	9500	ZIT	C4A-C3A-C2A	-2.24	106.90	110.07
32	0	9500	ZIT	O6-C6-C7	2.08	113.87	108.37
32	0	9500	ZIT	C7-C8-C9	2.66	116.14	112.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.46	92 (3%) 47 45	15, 38, 82, 157	0
2	9	122/122 (100%)	-0.12	6 (4%) 30 29	32, 58, 80, 139	0
3	A	237/240 (98%)	0.24	12 (5%) 29 27	19, 40, 75, 96	0
4	B	337/338 (99%)	0.18	9 (2%) 55 52	21, 47, 73, 84	0
5	C	246/246 (100%)	-0.14	3 (1%) 79 77	17, 36, 60, 69	0
6	D	140/177 (79%)	2.12	66 (47%) 0 0	51, 88, 114, 122	0
7	E	172/178 (96%)	0.86	24 (13%) 3 3	39, 61, 80, 84	0
8	F	119/120 (99%)	0.80	20 (16%) 2 1	38, 62, 88, 103	0
9	G	29/348 (8%)	3.20	25 (86%) 0 0	71, 87, 93, 95	0
10	H	160/177 (90%)	0.43	15 (9%) 9 8	31, 50, 83, 91	0
11	I	70/162 (43%)	6.91	70 (100%) 0 0	122, 135, 154, 155	0
12	J	142/145 (97%)	0.06	4 (2%) 53 51	29, 44, 65, 88	0
13	K	132/132 (100%)	-0.10	3 (2%) 61 58	24, 43, 65, 77	0
14	L	145/165 (87%)	0.59	19 (13%) 4 3	18, 56, 101, 115	0
15	M	194/194 (100%)	0.02	0 100 100	21, 33, 49, 56	0
16	N	186/187 (99%)	0.72	25 (13%) 4 3	34, 55, 102, 112	0
17	O	115/116 (99%)	0.03	1 (0%) 84 82	30, 45, 61, 69	0
18	P	143/149 (95%)	-0.05	0 100 100	30, 44, 57, 68	0
19	Q	95/96 (98%)	-0.04	1 (1%) 80 79	30, 37, 54, 68	0
20	R	150/155 (96%)	-0.15	0 100 100	25, 38, 58, 66	0
21	S	81/85 (95%)	0.11	2 (2%) 58 55	34, 50, 71, 81	0
22	T	119/120 (99%)	0.40	8 (6%) 19 17	29, 47, 76, 103	0
23	U	53/66 (80%)	0.28	2 (3%) 41 40	35, 48, 66, 78	0
24	V	65/71 (91%)	1.45	12 (18%) 1 1	43, 62, 107, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	154/154 (100%)	-0.03	1 (0%) 89 87	29, 43, 58, 69	0
26	X	82/92 (89%)	0.54	10 (12%) 5 4	37, 50, 78, 94	0
27	Y	142/241 (58%)	0.13	5 (3%) 44 43	21, 36, 59, 80	0
28	Z	73/83 (87%)	0.06	2 (2%) 55 52	35, 51, 68, 86	0
29	1	56/57 (98%)	-0.44	0 100 100	18, 24, 32, 43	0
30	2	46/50 (92%)	0.48	5 (10%) 6 5	26, 51, 75, 89	0
31	3	92/92 (100%)	0.22	2 (2%) 62 59	26, 48, 62, 77	0
All	All	6646/7480 (88%)	0.06	444 (6%) 19 17	15, 43, 89, 157	0

The worst 5 of 444 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	74	ILE	15.4
11	I	91	PHE	15.2
11	I	66	GLY	14.4
11	I	128	THR	14.2
11	I	88	GLN	13.8

## 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	OMU	0	2587	21/22	0.98	0.12	-	26,28,29,32	0
1	UR3	0	2619	21/22	0.98	0.13	-	29,33,35,41	0
1	PSU	0	2621	20/21	0.98	0.13	-	22,25,33,33	0
1	1MA	0	628	23/24	0.98	0.15	-	22,24,25,28	0
1	OMG	0	2588	24/25	0.98	0.12	-	23,27,29,30	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	0	8555	1/1	0.82	0.49	93.70	43,43,43,43	0
35	NA	0	8542	1/1	0.85	0.43	32.60	51,51,51,51	0
35	NA	0	8563	1/1	0.84	0.39	21.85	56,56,56,56	0
35	NA	0	8565	1/1	0.89	0.29	21.02	46,46,46,46	0
37	SR	B	8987	1/1	0.14	0.48	14.67	189,189,189,189	0
35	NA	0	8553	1/1	0.93	0.23	14.40	48,48,48,48	0
37	SR	0	8969	1/1	0.97	0.25	13.74	115,115,115,115	0
35	NA	0	8550	1/1	0.92	0.21	12.73	41,41,41,41	0
35	NA	0	8564	1/1	0.86	0.37	12.07	55,55,55,55	0
35	NA	0	8517	1/1	0.94	0.21	11.56	36,36,36,36	0
35	NA	0	8562	1/1	0.72	0.27	10.20	59,59,59,59	0
35	NA	0	8560	1/1	0.98	0.36	9.84	54,54,54,54	0
35	NA	0	8521	1/1	0.87	0.24	9.60	55,55,55,55	0
35	NA	0	8571	1/1	0.55	0.25	7.35	79,79,79,79	0
37	SR	0	8903	1/1	0.99	0.17	6.41	41,41,41,41	0
35	NA	0	8528	1/1	0.98	0.20	6.38	32,32,32,32	0
35	NA	9	8572	1/1	0.89	0.29	6.06	59,59,59,59	0
37	SR	0	8992	1/1	0.97	0.22	5.02	111,111,111,111	0
35	NA	0	8568	1/1	0.91	0.24	4.60	42,42,42,42	0
35	NA	0	8535	1/1	0.94	0.26	4.20	40,40,40,40	0
37	SR	A	8929	1/1	0.68	0.25	4.05	123,123,123,123	0
35	NA	0	8547	1/1	0.94	0.19	3.81	42,42,42,42	0
35	NA	0	8559	1/1	0.92	0.15	2.69	51,51,51,51	0
35	NA	0	8527	1/1	0.95	0.17	2.49	31,31,31,31	0
35	NA	0	8534	1/1	0.95	0.15	2.43	29,29,29,29	0
35	NA	0	8523	1/1	0.93	0.16	2.29	31,31,31,31	0
35	NA	R	8575	1/1	0.90	0.21	2.22	73,73,73,73	0
36	CL	M	8818	1/1	0.97	0.23	2.16	36,36,36,36	0
37	SR	0	8991	1/1	0.79	0.15	1.94	167,167,167,167	0
35	NA	M	8539	1/1	0.95	0.18	1.60	28,28,28,28	0
35	NA	0	8530	1/1	0.97	0.16	1.53	37,37,37,37	0
35	NA	0	8556	1/1	0.94	0.22	1.31	37,37,37,37	0
35	NA	0	8552	1/1	0.96	0.14	0.98	48,48,48,48	0
35	NA	0	8515	1/1	0.97	0.17	0.48	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8508	1/1	0.92	0.13	0.20	40,40,40,40	0
37	SR	0	8959	1/1	0.86	0.17	0.19	132,132,132,132	0
37	SR	0	8975	1/1	0.94	0.13	0.08	99,99,99,99	0
33	MG	A	8051	1/1	0.97	0.17	-0.01	55,55,55,55	0
35	NA	0	8569	1/1	0.91	0.13	-0.02	61,61,61,61	0
36	CL	0	8812	1/1	0.99	0.13	-0.20	39,39,39,39	0
32	ZIT	0	9500	52/52	0.95	0.14	-0.35	28,38,42,44	0
36	CL	J	8821	1/1	0.92	0.17	-0.36	52,52,52,52	0
35	NA	Q	8540	1/1	0.98	0.17	-0.37	39,39,39,39	0
35	NA	C	8503	1/1	0.92	0.14	-0.38	29,29,29,29	0
35	NA	0	8504	1/1	0.95	0.13	-0.50	26,26,26,26	0
35	NA	0	8557	1/1	0.92	0.12	-0.57	54,54,54,54	0
37	SR	0	8993	1/1	0.69	0.10	-0.73	143,143,143,143	0
37	SR	H	8972	1/1	0.84	0.12	-0.76	112,112,112,112	0
35	NA	0	8519	1/1	0.99	0.15	-0.78	36,36,36,36	0
37	SR	R	8912	1/1	0.95	0.12	-0.79	77,77,77,77	0
33	MG	0	8047	1/1	0.98	0.13	-0.84	46,46,46,46	0
35	NA	0	8520	1/1	0.98	0.09	-0.98	50,50,50,50	0
37	SR	0	8985	1/1	0.94	0.11	-1.02	104,104,104,104	0
36	CL	0	8815	1/1	0.95	0.11	-1.04	47,47,47,47	0
35	NA	0	8512	1/1	0.97	0.11	-1.05	36,36,36,36	0
33	MG	0	8044	1/1	0.97	0.15	-1.10	40,40,40,40	0
35	NA	0	8537	1/1	0.99	0.13	-1.28	32,32,32,32	0
38	CD	U	8701	1/1	0.99	0.09	-1.35	55,55,55,55	0
37	SR	0	8947	1/1	0.83	0.10	-1.46	148,148,148,148	0
37	SR	0	8922	1/1	0.55	0.12	-1.47	161,161,161,161	0
35	NA	J	8538	1/1	0.95	0.10	-1.50	48,48,48,48	0
36	CL	O	8808	1/1	0.97	0.10	-1.52	54,54,54,54	0
37	SR	0	8981	1/1	0.94	0.11	-1.52	141,141,141,141	0
38	CD	Z	8703	1/1	0.98	0.08	-1.53	44,44,44,44	0
36	CL	0	8816	1/1	0.98	0.11	-1.57	53,53,53,53	0
33	MG	0	8009	1/1	0.98	0.13	-1.63	26,26,26,26	0
35	NA	0	8513	1/1	0.94	0.13	-1.70	33,33,33,33	0
33	MG	0	8084	1/1	0.95	0.04	-1.70	36,36,36,36	0
33	MG	0	8008	1/1	0.97	0.12	-1.77	26,26,26,26	0
33	MG	A	8050	1/1	0.96	0.13	-1.82	33,33,33,33	0
36	CL	B	8819	1/1	0.98	0.09	-1.85	46,46,46,46	0
33	MG	0	8058	1/1	0.99	0.08	-1.92	26,26,26,26	0
37	SR	0	8964	1/1	0.90	0.09	-1.92	109,109,109,109	0
37	SR	A	8930	1/1	0.96	0.05	-2.11	82,82,82,82	0
33	MG	0	8011	1/1	0.99	0.09	-2.15	24,24,24,24	0
33	MG	T	8057	1/1	0.94	0.08	-2.42	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
33	MG	0	8028	1/1	0.98	0.11	-2.45	19,19,19,19	0
38	CD	3	8704	1/1	0.99	0.07	-2.57	53,53,53,53	0
37	SR	0	8970	1/1	0.81	0.09	-2.61	109,109,109,109	0
37	SR	0	8984	1/1	0.96	0.10	-2.63	98,98,98,98	0
37	SR	0	8943	1/1	0.86	0.09	-2.67	108,108,108,108	0
37	SR	F	9005	1/1	0.91	0.05	-2.74	106,106,106,106	0
35	NA	0	8533	1/1	0.97	0.08	-2.78	50,50,50,50	0
33	MG	0	8070	1/1	0.96	0.10	-3.02	36,36,36,36	0
33	MG	0	8045	1/1	0.97	0.09	-3.08	29,29,29,29	0
33	MG	0	8003	1/1	0.97	0.11	-3.23	23,23,23,23	0
37	SR	0	8918	1/1	0.99	0.12	-3.50	66,66,66,66	0
33	MG	0	8041	1/1	0.98	0.10	-3.68	18,18,18,18	0
33	MG	0	8052	1/1	0.95	0.09	-3.72	23,23,23,23	0
37	SR	3	8932	1/1	0.99	0.07	-3.74	58,58,58,58	0
37	SR	0	8936	1/1	0.99	0.09	-3.74	67,67,67,67	0
33	MG	0	8025	1/1	0.94	0.08	-3.80	24,24,24,24	0
33	MG	Y	8086	1/1	0.97	0.11	-3.82	35,35,35,35	0
33	MG	0	8062	1/1	0.89	0.08	-3.94	46,46,46,46	0
33	MG	0	8075	1/1	0.97	0.07	-4.06	31,31,31,31	0
37	SR	0	8904	1/1	0.99	0.08	-4.23	34,34,34,34	0
33	MG	0	8065	1/1	0.95	0.07	-4.27	45,45,45,45	0
36	CL	3	8804	1/1	0.97	0.09	-4.29	47,47,47,47	0
35	NA	0	8558	1/1	0.98	0.08	-4.53	46,46,46,46	0
33	MG	0	8014	1/1	0.99	0.09	-4.56	25,25,25,25	0
33	MG	0	8043	1/1	0.98	0.09	-4.58	46,46,46,46	0
36	CL	0	8805	1/1	0.97	0.09	-4.58	45,45,45,45	0
33	MG	0	8012	1/1	0.98	0.07	-4.59	13,13,13,13	0
33	MG	B	8042	1/1	0.97	0.05	-4.60	52,52,52,52	0
34	K	0	8402	1/1	0.99	0.09	-4.84	46,46,46,46	0
37	SR	1	8913	1/1	0.98	0.07	-4.84	70,70,70,70	0
38	CD	1	8702	1/1	0.99	0.06	-4.90	44,44,44,44	0
33	MG	0	8001	1/1	0.99	0.08	-5.57	25,25,25,25	0
33	MG	0	8034	1/1	0.98	0.08	-5.64	35,35,35,35	0
33	MG	0	8029	1/1	0.92	0.08	-5.97	40,40,40,40	0
33	MG	0	8088	1/1	0.98	0.05	-6.93	29,29,29,29	0
33	MG	0	8013	1/1	0.99	0.04	-6.97	24,24,24,24	0
33	MG	0	8040	1/1	0.93	0.09	-6.98	78,78,78,78	0
33	MG	0	8015	1/1	0.98	0.09	-7.69	31,31,31,31	0
33	MG	0	8002	1/1	0.97	0.08	-7.69	27,27,27,27	0
33	MG	0	8087	1/1	0.99	0.08	-9.06	26,26,26,26	0
33	MG	0	8006	1/1	0.99	0.06	-9.12	30,30,30,30	0
37	SR	0	8902	1/1	0.99	0.07	-9.12	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	MG	0	8004	1/1	0.98	0.05	-9.82	22,22,22,22	0
37	SR	0	8945	1/1	0.98	0.04	-9.98	92,92,92,92	0
37	SR	0	8910	1/1	0.96	0.04	-10.59	80,80,80,80	0
37	SR	0	8949	1/1	0.95	0.05	-11.20	93,93,93,93	0
37	SR	0	8978	1/1	0.96	0.05	-13.07	82,82,82,82	0
37	SR	0	8948	1/1	0.97	0.07	-14.93	69,69,69,69	0
37	SR	A	8977	1/1	0.89	0.07	-	143,143,143,143	0
37	SR	0	8955	1/1	0.59	0.37	-	169,169,169,169	0
33	MG	0	8007	1/1	0.97	0.10	-	24,24,24,24	0
35	NA	0	8574	1/1	0.85	0.44	-	48,48,48,48	0
35	NA	0	8511	1/1	0.96	0.11	-	59,59,59,59	0
33	MG	0	8032	1/1	0.99	0.08	-	36,36,36,36	0
33	MG	0	8053	1/1	0.93	0.09	-	58,58,58,58	0
33	MG	0	8022	1/1	0.93	0.15	-	30,30,30,30	0
33	MG	0	8021	1/1	0.97	0.09	-	28,28,28,28	0
35	NA	0	8549	1/1	0.95	0.47	-	74,74,74,74	0
33	MG	0	8079	1/1	0.89	0.08	-	40,40,40,40	0
33	MG	0	8073	1/1	0.86	0.19	-	76,76,76,76	0
35	NA	0	8551	1/1	0.93	0.20	-	39,39,39,39	0
35	NA	0	8505	1/1	0.98	0.14	-	33,33,33,33	0
37	SR	0	8958	1/1	0.96	0.07	-	83,83,83,83	0
33	MG	0	8081	1/1	0.70	0.20	-	55,55,55,55	0
37	SR	0	8960	1/1	0.73	0.09	-	128,128,128,128	0
37	SR	0	8944	1/1	0.72	0.16	-	146,146,146,146	0
33	MG	0	8072	1/1	0.97	0.09	-	37,37,37,37	0
33	MG	0	8082	1/1	0.90	0.23	-	44,44,44,44	0
37	SR	0	8920	1/1	0.95	0.08	-	96,96,96,96	0
37	SR	0	8921	1/1	0.98	0.07	-	66,66,66,66	0
37	SR	0	8927	1/1	0.80	0.12	-	133,133,133,133	0
37	SR	B	8950	1/1	0.90	0.06	-	90,90,90,90	0
35	NA	0	8570	1/1	0.97	0.09	-	35,35,35,35	0
36	CL	N	8807	1/1	0.98	0.12	-	46,46,46,46	0
33	MG	0	8061	1/1	0.97	0.12	-	23,23,23,23	0
37	SR	0	9008	1/1	0.95	0.07	-	83,83,83,83	0
33	MG	0	8019	1/1	0.96	0.07	-	22,22,22,22	0
37	SR	0	8946	1/1	0.93	0.09	-	87,87,87,87	0
36	CL	Y	8820	1/1	0.97	0.17	-	35,35,35,35	0
37	SR	0	8907	1/1	0.99	0.11	-	33,33,33,33	0
37	SR	0	8937	1/1	0.96	0.09	-	94,94,94,94	0
33	MG	0	8024	1/1	0.92	0.09	-	53,53,53,53	0
35	NA	0	8522	1/1	0.91	0.28	-	46,46,46,46	0
37	SR	0	8963	1/1	0.91	0.06	-	103,103,103,103	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
37	SR	0	8999	1/1	0.94	0.04	-	78,78,78,78	0
33	MG	0	8068	1/1	0.97	0.15	-	48,48,48,48	0
33	MG	0	8071	1/1	0.86	0.36	-	54,54,54,54	0
35	NA	S	8510	1/1	0.94	0.17	-	24,24,24,24	0
35	NA	0	8573	1/1	0.88	0.09	-	55,55,55,55	0
33	MG	0	8083	1/1	0.95	0.08	-	41,41,41,41	0
35	NA	0	8506	1/1	0.79	0.18	-	50,50,50,50	0
37	SR	0	8905	1/1	0.99	0.23	-	48,48,48,48	0
33	MG	0	8067	1/1	0.96	0.09	-	29,29,29,29	0
35	NA	0	8531	1/1	0.94	0.06	-	29,29,29,29	0
37	SR	0	9007	1/1	0.91	0.27	-	154,154,154,154	0
37	SR	0	8962	1/1	0.80	0.19	-	139,139,139,139	0
33	MG	0	8010	1/1	0.98	0.09	-	29,29,29,29	0
37	SR	0	8917	1/1	0.97	0.09	-	90,90,90,90	0
33	MG	0	8038	1/1	0.92	0.12	-	65,65,65,65	0
37	SR	0	8973	1/1	0.90	0.11	-	113,113,113,113	0
33	MG	0	8037	1/1	0.79	0.22	-	77,77,77,77	0
36	CL	0	8813	1/1	0.98	0.14	-	45,45,45,45	0
33	MG	0	8076	1/1	0.94	0.08	-	28,28,28,28	0
33	MG	0	8036	1/1	0.94	0.10	-	36,36,36,36	0
35	NA	0	8536	1/1	0.72	0.14	-	46,46,46,46	0
37	SR	0	8911	1/1	0.97	0.08	-	65,65,65,65	0
35	NA	0	8548	1/1	0.78	0.09	-	50,50,50,50	0
33	MG	0	8048	1/1	0.99	0.07	-	33,33,33,33	0
37	SR	0	9000	1/1	0.79	0.18	-	150,150,150,150	0
33	MG	0	8077	1/1	0.96	0.08	-	26,26,26,26	0
33	MG	0	8090	1/1	0.98	0.09	-	49,49,49,49	0
33	MG	0	8018	1/1	0.99	0.13	-	38,38,38,38	0
33	MG	0	8016	1/1	0.96	0.06	-	35,35,35,35	0
33	MG	0	8023	1/1	0.98	0.06	-	24,24,24,24	0
33	MG	0	8069	1/1	0.78	0.17	-	58,58,58,58	0
37	SR	0	8956	1/1	0.92	0.06	-	127,127,127,127	0
37	SR	0	8971	1/1	0.75	0.09	-	158,158,158,158	0
35	NA	0	8561	1/1	0.87	0.55	-	62,62,62,62	0
37	SR	9	8980	1/1	0.65	0.20	-	162,162,162,162	0
37	SR	0	8990	1/1	0.93	0.10	-	106,106,106,106	0
33	MG	0	8046	1/1	0.93	0.10	-	25,25,25,25	0
36	CL	J	8802	1/1	0.97	0.09	-	51,51,51,51	0
37	SR	0	8967	1/1	0.97	0.04	-	116,116,116,116	0
37	SR	0	8938	1/1	0.97	0.05	-	147,147,147,147	0
33	MG	9	8074	1/1	0.75	0.10	-	64,64,64,64	0
35	NA	0	8554	1/1	0.76	0.31	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8507	1/1	0.93	0.10	-	27,27,27,27	0
33	MG	0	8093	1/1	0.94	0.09	-	29,29,29,29	0
37	SR	0	8957	1/1	0.67	0.33	-	176,176,176,176	0
37	SR	0	8979	1/1	0.49	0.29	-	184,184,184,184	0
38	CD	O	8705	1/1	0.99	0.06	-	58,58,58,58	0
37	SR	0	8995	1/1	0.95	0.07	-	112,112,112,112	0
33	MG	0	8017	1/1	0.94	0.21	-	26,26,26,26	0
37	SR	0	8906	1/1	0.99	0.10	-	40,40,40,40	0
37	SR	0	8988	1/1	0.82	0.10	-	149,149,149,149	0
33	MG	0	8027	1/1	0.95	0.04	-	32,32,32,32	0
35	NA	0	8502	1/1	0.95	0.18	-	43,43,43,43	0
37	SR	0	8909	1/1	1.00	0.08	-	70,70,70,70	0
35	NA	0	8501	1/1	0.99	0.19	-	26,26,26,26	0
37	SR	0	8982	1/1	0.91	0.19	-	152,152,152,152	0
35	NA	0	8524	1/1	0.98	0.20	-	31,31,31,31	0
37	SR	0	8931	1/1	0.96	0.06	-	86,86,86,86	0
33	MG	0	8049	1/1	0.96	0.11	-	64,64,64,64	0
36	CL	0	8814	1/1	0.97	0.11	-	40,40,40,40	0
33	MG	0	8089	1/1	0.95	0.19	-	37,37,37,37	0
36	CL	0	8811	1/1	0.97	0.11	-	45,45,45,45	0
33	MG	0	8031	1/1	0.89	0.09	-	41,41,41,41	0
37	SR	S	8961	1/1	0.89	0.09	-	113,113,113,113	0
37	SR	0	8933	1/1	0.94	0.14	-	108,108,108,108	0
36	CL	0	8803	1/1	0.99	0.16	-	41,41,41,41	0
37	SR	0	8965	1/1	0.92	0.05	-	109,109,109,109	0
33	MG	0	8092	1/1	0.96	0.09	-	47,47,47,47	0
33	MG	0	8080	1/1	0.88	0.08	-	53,53,53,53	0
35	NA	0	8526	1/1	0.95	0.10	-	36,36,36,36	0
37	SR	0	8928	1/1	0.72	0.11	-	112,112,112,112	0
35	NA	0	8525	1/1	0.67	0.21	-	65,65,65,65	0
35	NA	0	8529	1/1	0.97	0.09	-	32,32,32,32	0
33	MG	K	8054	1/1	0.97	0.10	-	34,34,34,34	0
37	SR	0	8942	1/1	0.96	0.06	-	110,110,110,110	0
37	SR	0	8983	1/1	0.71	0.15	-	149,149,149,149	0
37	SR	0	8935	1/1	0.99	0.13	-	60,60,60,60	0
36	CL	0	8817	1/1	0.99	0.08	-	46,46,46,46	0
37	SR	1	8952	1/1	0.99	0.06	-	62,62,62,62	0
35	NA	0	8566	1/1	0.97	0.15	-	44,44,44,44	0
37	SR	0	8901	1/1	0.99	0.05	-	71,71,71,71	0
33	MG	0	8039	1/1	0.89	0.13	-	60,60,60,60	0
35	NA	0	8514	1/1	0.92	0.16	-	41,41,41,41	0
33	MG	0	8056	1/1	0.94	0.17	-	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
35	NA	0	8567	1/1	0.87	0.31	-	53,53,53,53	0
35	NA	0	8546	1/1	0.93	0.25	-	63,63,63,63	0
36	CL	A	8809	1/1	0.97	0.23	-	52,52,52,52	0
33	MG	0	8064	1/1	0.99	0.04	-	34,34,34,34	0
37	SR	0	8940	1/1	0.97	0.05	-	66,66,66,66	0
37	SR	0	8976	1/1	0.43	0.25	-	159,159,159,159	0
33	MG	0	8066	1/1	0.83	0.11	-	47,47,47,47	0
37	SR	0	8994	1/1	0.94	0.27	-	168,168,168,168	0
37	SR	0	8919	1/1	0.77	0.16	-	169,169,169,169	0
37	SR	0	9004	1/1	0.61	0.23	-	176,176,176,176	0
36	CL	L	8810	1/1	0.96	0.08	-	43,43,43,43	0
33	MG	0	8091	1/1	0.98	0.12	-	42,42,42,42	0
35	NA	0	8516	1/1	0.96	0.14	-	44,44,44,44	0
37	SR	0	8951	1/1	0.85	0.05	-	137,137,137,137	0
33	MG	0	8055	1/1	0.99	0.11	-	29,29,29,29	0
37	SR	0	8916	1/1	0.91	0.06	-	95,95,95,95	0
37	SR	0	9006	1/1	-0.01	0.99	-	200,200,200,200	0
35	NA	0	8509	1/1	0.90	0.15	-	47,47,47,47	0
37	SR	0	9002	1/1	0.63	0.17	-	162,162,162,162	0
35	NA	H	8518	1/1	0.73	0.23	-	66,66,66,66	0
37	SR	0	8989	1/1	0.87	0.18	-	148,148,148,148	0
37	SR	0	8998	1/1	0.84	0.13	-	133,133,133,133	0
33	MG	0	8063	1/1	0.91	0.19	-	71,71,71,71	0
37	SR	0	8924	1/1	0.88	0.13	-	123,123,123,123	0
33	MG	0	8078	1/1	0.97	0.09	-	40,40,40,40	0
33	MG	0	8020	1/1	0.97	0.12	-	37,37,37,37	0
37	SR	0	8996	1/1	0.17	0.59	-	185,185,185,185	0
33	MG	0	8060	1/1	0.94	0.07	-	45,45,45,45	0
33	MG	0	8030	1/1	0.86	0.24	-	48,48,48,48	0
36	CL	J	8801	1/1	0.94	0.11	-	49,49,49,49	0
37	SR	0	8986	1/1	0.59	0.81	-	169,169,169,169	0
37	SR	0	8966	1/1	0.96	0.03	-	89,89,89,89	0
33	MG	0	8026	1/1	0.99	0.07	-	28,28,28,28	0
35	NA	9	8543	1/1	0.90	0.24	-	41,41,41,41	0
33	MG	0	8033	1/1	0.97	0.07	-	32,32,32,32	0
37	SR	0	8997	1/1	0.89	0.56	-	171,171,171,171	0
37	SR	0	8968	1/1	0.76	0.09	-	142,142,142,142	0
34	K	0	8401	1/1	0.93	0.11	-	58,58,58,58	0
37	SR	0	8926	1/1	0.94	0.06	-	95,95,95,95	0
37	SR	0	8908	1/1	0.97	0.09	-	71,71,71,71	0
37	SR	0	8915	1/1	0.96	0.06	-	85,85,85,85	0
35	NA	0	8544	1/1	0.89	0.20	-	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
37	SR	0	8953	1/1	0.96	0.07	-	121,121,121,121	0
37	SR	0	8941	1/1	0.93	0.05	-	90,90,90,90	0
33	MG	0	8035	1/1	0.95	0.07	-	52,52,52,52	0
37	SR	0	8925	1/1	0.99	0.06	-	75,75,75,75	0
33	MG	0	8059	1/1	0.99	0.04	-	27,27,27,27	0
33	MG	0	8085	1/1	0.73	0.12	-	90,90,90,90	0
36	CL	R	8806	1/1	0.97	0.16	-	40,40,40,40	0
35	NA	0	8545	1/1	0.99	0.13	-	29,29,29,29	0
37	SR	0	8939	1/1	0.91	0.09	-	108,108,108,108	0
36	CL	0	8822	1/1	0.98	0.15	-	48,48,48,48	0
37	SR	0	9001	1/1	0.36	0.26	-	160,160,160,160	0
37	SR	0	8923	1/1	0.98	0.08	-	78,78,78,78	0
37	SR	0	8914	1/1	0.97	0.10	-	88,88,88,88	0
33	MG	0	8005	1/1	0.98	0.10	-	23,23,23,23	0
35	NA	R	8532	1/1	0.93	0.09	-	37,37,37,37	0
37	SR	9	9003	1/1	0.90	0.08	-	141,141,141,141	0
35	NA	0	8541	1/1	0.88	0.15	-	41,41,41,41	0
37	SR	0	8934	1/1	0.96	0.12	-	116,116,116,116	0
37	SR	0	8974	1/1	0.56	0.20	-	159,159,159,159	0
37	SR	0	8954	1/1	0.95	0.11	-	88,88,88,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.