



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:38 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 validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

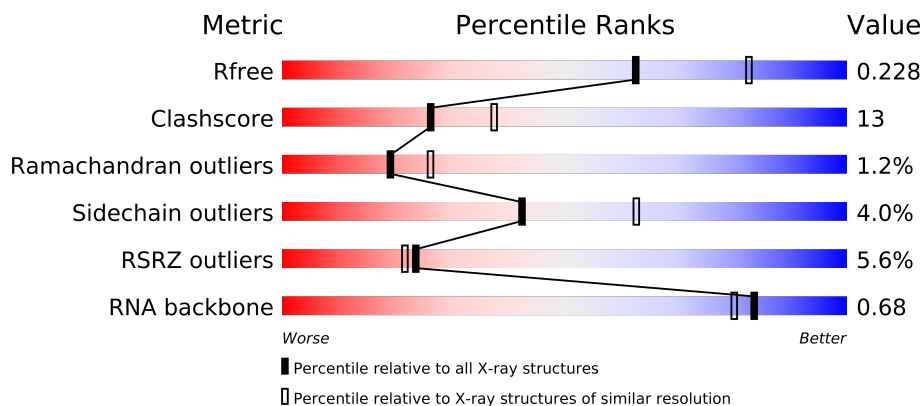
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	0	2922	
2	9	122	
3	A	240	
4	B	338	
5	C	246	
6	D	177	
7	E	178	
8	F	120	
9	G	348	
10	H	177	
11	I	162	

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

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
33	MG	0	8030	-	X
33	MG	0	8037	-	X
33	MG	0	8063	-	X
33	MG	0	8068	-	X
33	MG	0	8071	-	X
33	MG	0	8073	-	X
33	MG	0	8081	-	X
33	MG	0	8085	-	X
33	MG	0	8089	-	X
35	NA	0	8505	-	X
35	NA	0	8506	-	X
35	NA	0	8508	-	X
35	NA	0	8509	-	X
35	NA	0	8514	-	X
35	NA	0	8516	-	X
35	NA	0	8517	-	X
35	NA	0	8521	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
35	NA	0	8522	-	X
35	NA	0	8524	-	X
35	NA	0	8525	-	X
35	NA	0	8528	-	X
35	NA	0	8536	-	X
35	NA	0	8542	-	X
35	NA	0	8547	-	X
35	NA	0	8549	-	X
35	NA	0	8550	-	X
35	NA	0	8551	-	X
35	NA	0	8552	-	X
35	NA	0	8553	-	X
35	NA	0	8554	-	X
35	NA	0	8555	-	X
35	NA	0	8556	-	X
35	NA	0	8560	-	X
35	NA	0	8561	-	X
35	NA	0	8562	-	X
35	NA	0	8563	-	X
35	NA	0	8564	-	X
35	NA	0	8565	-	X
35	NA	0	8567	-	X
35	NA	0	8568	-	X
35	NA	0	8571	-	X
35	NA	0	8574	-	X
35	NA	9	8572	-	X
35	NA	R	8575	-	X
36	CL	0	8822	-	X
37	SR	0	8903	-	X
37	SR	0	8905	-	X
37	SR	0	8919	-	X
37	SR	0	8955	-	X
37	SR	0	8957	-	X
37	SR	0	8962	-	X
37	SR	0	8969	-	X
37	SR	0	8974	-	X
37	SR	0	8976	-	X
37	SR	0	8979	-	X
37	SR	0	8982	-	X
37	SR	0	8986	-	X
37	SR	0	8989	-	X
37	SR	0	8992	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
37	SR	0	8994	-	X
37	SR	0	8996	-	X
37	SR	0	8997	-	X
37	SR	0	9000	-	X
37	SR	0	9001	-	X
37	SR	0	9002	-	X
37	SR	0	9004	-	X
37	SR	0	9006	-	X
37	SR	0	9007	-	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 hydrogen and 0 are deuterium.

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			

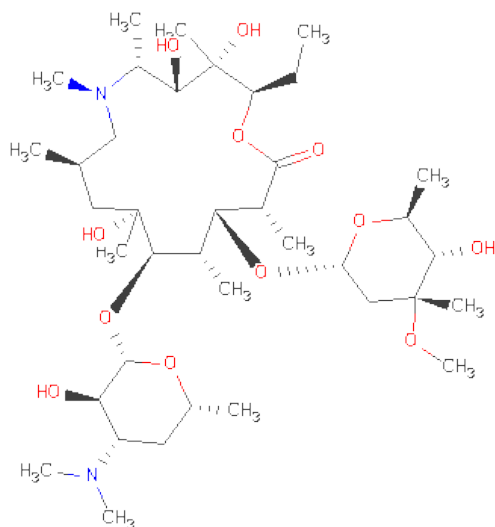
- Molecule 30 is a protein called 50S ribosomal protein L39e.

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: $C_{38}H_{72}N_2O_{12}$).



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	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

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

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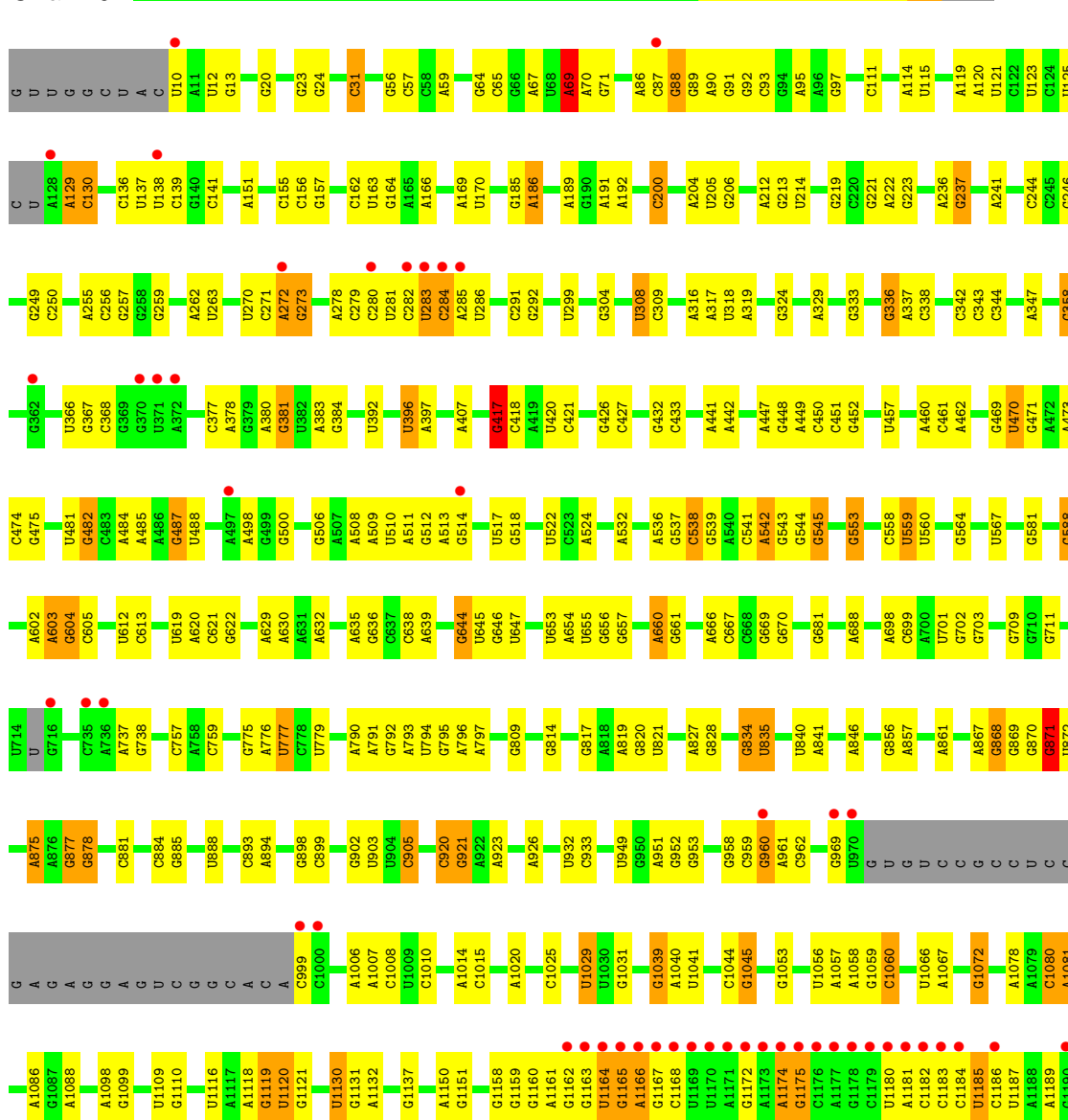
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	66	Total 66	O 66	0	0
39	Q	53	Total 53	O 53	0	0
39	R	87	Total 87	O 87	0	0
39	S	32	Total 32	O 32	0	0
39	T	41	Total 41	O 41	0	0
39	U	28	Total 28	O 28	0	0
39	V	12	Total 12	O 12	0	0
39	W	68	Total 68	O 68	0	0
39	X	24	Total 24	O 24	0	0
39	Y	95	Total 95	O 95	0	0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

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.

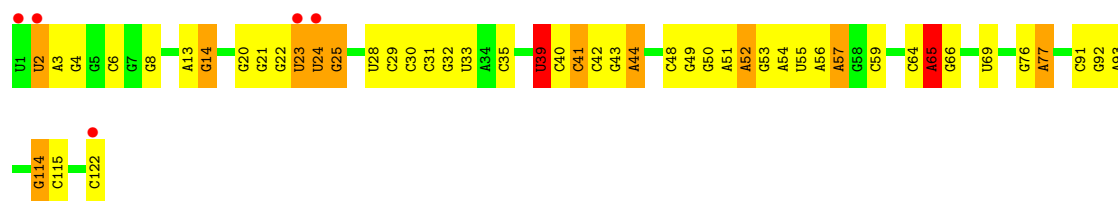
• Molecule 1: 23S Ribosomal RNA

Chain 0:

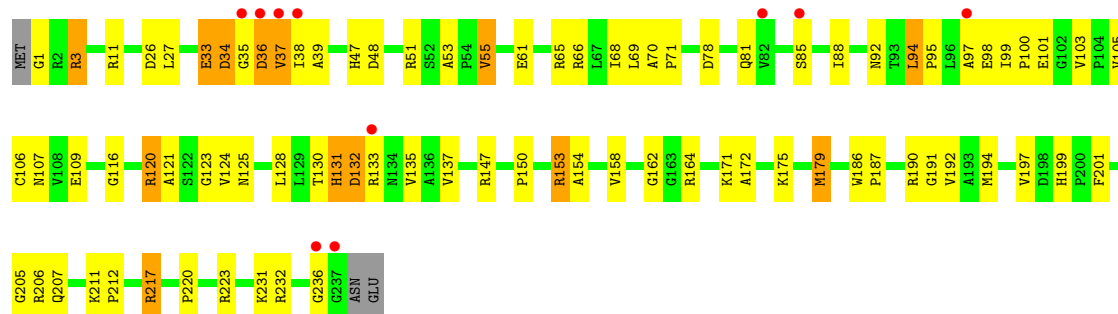


C2867	U2756	G2634	G2516	G2421	U2590	C	G	G2005	U1740	A1603	A1427	C1289	A1191
C2868	A2761	A2635	A2521	U2422	A2291	C	U	U2008	U1741	G1604	A1439	G1290	A1192
G2869	C2762	C2636	G2524	G2426	A2300	A	C	G	A1742	G1605	U1440	A1291	A1193
G2876	A2768	G2638	G2525	G2427	A2301	C	C	C	G1752	A1615	G1441	G1295	A1194
G2877	C2769	C2637	G2526	G2428	A2302	A	C	U2012	C1753	U1625	A1442	G1299	G1196
U2878	G2770	G2642	U2527	U2435	C2309	C	G	G2013	A1754	A1626	G1452	G1300	G1197
A2879		G2643	G2533	G2442	C2313	A	U	G2014	G1755	A1627	U1458	U1304	U1198
			G2534	U2444	G2316	C	U	U2015	G1756	A1627	A1470	C1305	C1201
			G2535	U2445	G2317	A	U	G2016	C1762	A1630	A1474	U1306	A1202
			G2536	G2446	C2320	C	U	G2017	U1766	A1634	U1477	U1307	G1203
			G2537	G2447	A2321	A	C	C2031	A1767	U1634	C1477	A1308	G1204
			G2538	G2448	A2322	A	C	G2032	C1768	A1642	C1477	U1314	U1205
			U2541	G2453	A2323	U	C	G2033	C1769	A1642	C1477	U1314	U1206
			C2542	G2454	C2324	U	C	U2034	U1773	A1642	C1477	U1314	U1207
			G2543	A2456	C2325	A	C	C2035	G1773	A1642	C1477	U1314	U1208
			G2544	U2457	C2326	U	C	G2036	G1774	A1642	C1477	U1314	U1209
			U2545	G2458	G2336	U	C	G2044	G1775	A1642	C1477	U1314	U1210
			C2547	A2462	G2337	A	C	A2054	A1777	A1642	C1477	U1314	G1211
			G2548	G2463	G2338	C	C	U2064	A1778	A1642	C1477	U1314	G1212
			G2549	A2464	A	C	C	G2072	A1779	A1642	C1477	U1314	G1212
			C2552	A2465	C	C	C	G2073	C1786	A1642	C1477	U1314	G1212
			A2553	A2466	A	C	C	A2074	C1787	A1642	C1477	U1314	G1212
				A2467	C	C	C	U2081	C1788	A1642	C1477	U1314	G1212
				A2468	C	C	C	G2089	C1789	A1642	C1477	U1314	G1212
					C	C	C	G2090	C1790	A1642	C1477	U1314	G1212
					A	C	C	G2091	C1791	A1642	C1477	U1314	G1212
					C	C	C	A2096	C1792	A1642	C1477	U1314	G1212
					C	C	C	A2101	C1793	A1642	C1477	U1314	G1212
					C	C	C	G2102	C1794	A1642	C1477	U1314	G1212
					C	C	C	G2103	C1795	A1642	C1477	U1314	G1212
					C	C	C	G2104	C1796	A1642	C1477	U1314	G1212
					C	C	C	G2110	C1797	A1642	C1477	U1314	G1212
					C	C	C	G2111	C1798	A1642	C1477	U1314	G1212
					C	C	C	G2112	C1799	A1642	C1477	U1314	G1212
					C	C	C	G2113	C1800	A1642	C1477	U1314	G1212
					C	C	C	G2114	C1801	A1642	C1477	U1314	G1212
					C	C	C	G2115	C1802	A1642	C1477	U1314	G1212
					C	C	C	G2116	C1803	A1642	C1477	U1314	G1212
					C	C	C	G2117	C1804	A1642	C1477	U1314	G1212
					C	C	C	G2118	C1805	A1642	C1477	U1314	G1212
					C	C	C	G2119	C1806	A1642	C1477	U1314	G1212
					C	C	C	G2120	C1807	A1642	C1477	U1314	G1212
					C	C	C	G2121	C1808	A1642	C1477	U1314	G1212
					C	C	C	G2122	C1809	A1642	C1477	U1314	G1212
					C	C	C	G2123	C1810	A1642	C1477	U1314	G1212
					C	C	C	G2124	C1811	A1642	C1477	U1314	G1212
					C	C	C	G2125	C1812	A1642	C1477	U1314	G1212
					C	C	C	G2126	C1813	A1642	C1477	U1314	G1212
					C	C	C	G2127	C1814	A1642	C1477	U1314	G1212
					C	C	C	G2128	C1815	A1642	C1477	U1314	G1212
					C	C	C	G2129	C1816	A1642	C1477	U1314	G1212
					C	C	C	G2130	C1817	A1642	C1477	U1314	G1212
					C	C	C	G2131	C1818	A1642	C1477	U1314	G1212
					C	C	C	G2132	C1819	A1642	C1477	U1314	G1212
					C	C	C	G2133	C1820	A1642	C1477	U1314	G1212
					C	C	C	G2134	C1821	A1642	C1477	U1314	G1212
					C	C	C	G2135	C1822	A1642	C1477	U1314	G1212
					C	C	C	G2136	C1823	A1642	C1477	U1314	G1212
					C	C	C	G2137	C1824	A1642	C1477	U1314	G1212
					C	C	C	G2138	C1825	A1642	C1477	U1314	G1212
					C	C	C	G2139	C1826	A1642	C1477	U1314	G1212
					C	C	C	G2140	C1827	A1642	C1477	U1314	G1212
					C	C	C	G2141	C1828	A1642	C1477	U1314	G1212
					C	C	C	G2142	C1829	A1642	C1477	U1314	G1212
					C	C	C	G2143	C1830	A1642	C1477	U1314	G1212
					C	C	C	G2144	C1831	A1642	C1477	U1314	G1212
					C	C	C	G2145	C1832	A1642	C1477	U1314	G1212
					C	C	C	G2146	C1833	A1642	C1477	U1314	G1212
					C	C	C	G2147	C1834	A1642	C1477	U1314	G1212
					C	C	C	G2148	C1835	A1642	C1477	U1314	G1212
					C	C	C	G2149	C1836	A1642	C1477	U1314	G1212
					C	C	C	G2150	C1837	A1642	C1477	U1314	G1212
					C	C	C	G2151	C1838	A1642	C1477	U1314	G1212
					C	C	C	G2152	C1839	A1642	C1477	U1314	G1212
					C	C	C	G2153	C1840	A1642	C1477	U1314	G1212
					C	C	C	G2154	C1841	A1642	C1477	U1314	G1212
					C	C	C	G2155	C1842	A1642	C1477	U1314	G1212
					C	C	C	G2156	C1843	A1642	C1477	U1314	G1212
					C	C	C	G2157	C1844	A1642	C1477	U1314	G1212
					C	C	C	G2158	C1845	A1642	C1477	U1314	G1212
					C	C	C	G2159	C1846	A1642	C1477	U1314	G1212
					C	C	C	G2160	C1847	A1642	C1477	U1314	G1212
					C	C	C	G2161	C1848	A1642	C1477	U1314	G1212
					C	C	C	G2162	C1849	A1642	C1477	U1314	G1212
					C	C	C	G2163	C1850	A1642	C1477	U1314	G1212
					C	C	C	G2164	C1851	A1642	C1477	U1314	G1212
					C	C	C	G2165	C1852	A1642	C1477	U1314	G1212
					C	C	C	G2166	C1853	A1642	C1477	U1314	G1212
					C	C	C	G2167	C1854	A1642	C1477	U1314	G1212
					C	C	C	G2168	C1855	A1642	C1477	U1314	G1212
					C	C	C	G2169	C1856	A1642	C1477	U1314	G1212
					C	C	C	G2170	C1857	A1642	C1477	U1314	G1212
					C	C	C	G2171	C1858	A1642	C1477	U1314	G1212
					C	C	C	G2172	C1859	A1642	C1477	U1314	G1212
					C	C	C	G2173	C1860	A1642	C1477	U1314	G1212
					C	C	C	G2174	C1861	A1642	C1477	U1314	G1212
					C	C	C	G2175	C1862	A1642	C1477	U1314	G1212
					C	C	C	G2176	C1863	A1642	C1477	U1314	G1212
					C	C	C	G2177	C1864	A1642	C1477	U1314	G1212
					C	C	C	G2178	C1865	A1642	C1477	U1314	G1212
					C	C	C	G2179	C1866	A1642	C1477	U1314	G1212
					C	C	C	G2180	C1867	A1642	C1477	U1314	G1212
					C	C	C	G2181	C1868	A1642	C1477	U1314	G1212
					C	C	C	G2182	C1869	A1642	C1477	U1314	G1212
					C	C	C	G2183	C1870	A1642	C1477	U1314	G1212
					C	C	C	G2184	C1871	A1642	C1477	U1314	G1212
					C	C	C	G2185	C1872	A1642	C1477	U1314	G1212
					C	C	C	G2186	C1873	A1642	C1477	U1314	G1212
					C	C	C	G2187	C1874	A1642	C1477	U1314	G1212
					C	C	C	G2188	C1875	A1642	C1477	U1314	G1212
					C	C	C	G2189	C1876	A1642	C1477	U1314	G1212
					C	C	C	G2190	C1877	A1642	C1477	U1314	G1212
					C	C	C	G2191	C1878	A1642	C1477	U1314	G1212
					C	C	C	G2192	C1879	A1642	C1477	U1314	G1212
					C	C	C	G2193	C1880	A1642	C1477	U1314	G1212
					C	C	C	G2194	C1881	A1642	C1477	U1314	G1212
					C	C	C	G2195	C1882	A1642	C1477	U1314	G1212
					C	C	C	G2196	C1883	A1642	C1477	U1314	G1212
					C	C	C	G2197	C1884	A1642	C1477	U1314	G1212
					C	C	C	G2198	C1885	A1642	C1477	U1314	G1212
					C	C	C	G2199	C1886	A1642	C1477	U1314	G1212
					C	C	C	G2200	C1887	A1642	C1477	U1314	G1212
					C	C	C	G2201	C1888	A1642	C1477	U1314	G1212
					C	C	C	G2202	C1889	A1642	C1477	U1314	G1212
					C	C	C	G2203	C1890	A1642	C1477	U1314	G1212
					C	C	C	G2204	C1891	A1642	C1477		

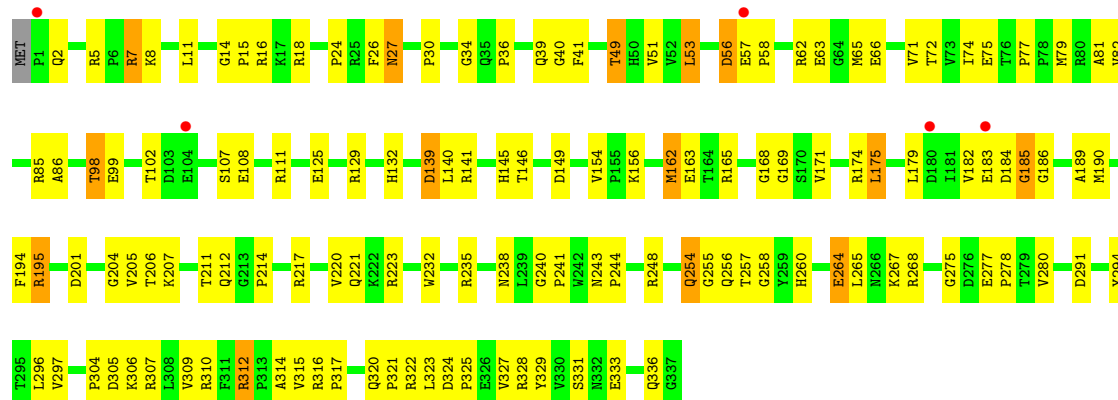
- Molecule 2: 5S Ribosomal RNA

Chain 9: 

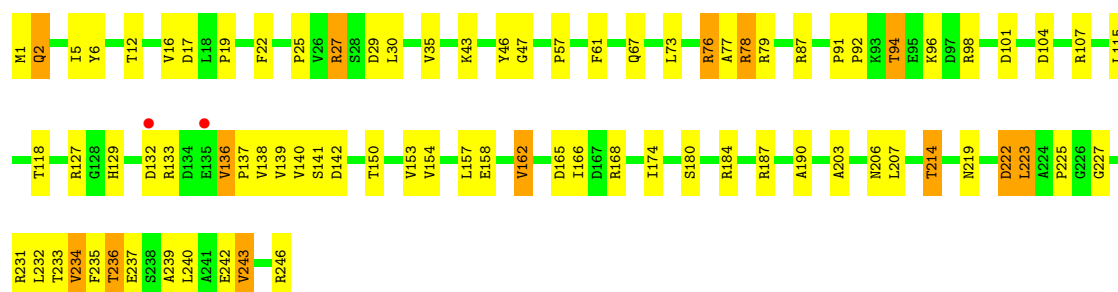
- Molecule 3: 50S ribosomal protein L2P

Chain A: 

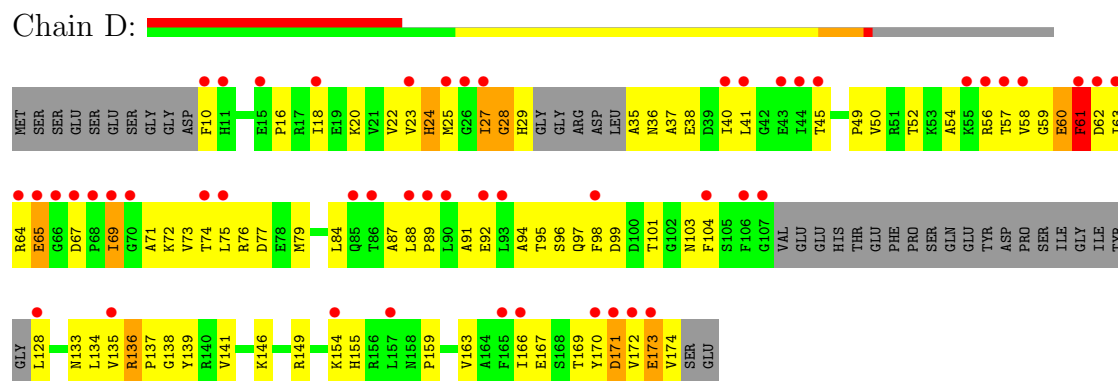
- Molecule 4: 50S ribosomal protein L3P

Chain B: 

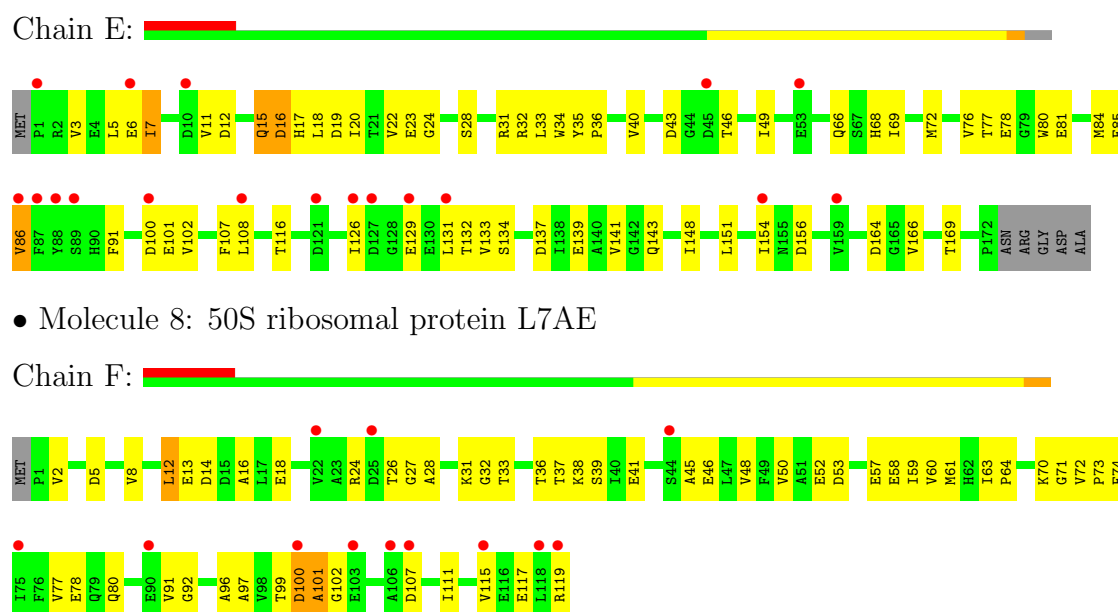
- Molecule 5: 50S ribosomal protein L4E

Chain C: 

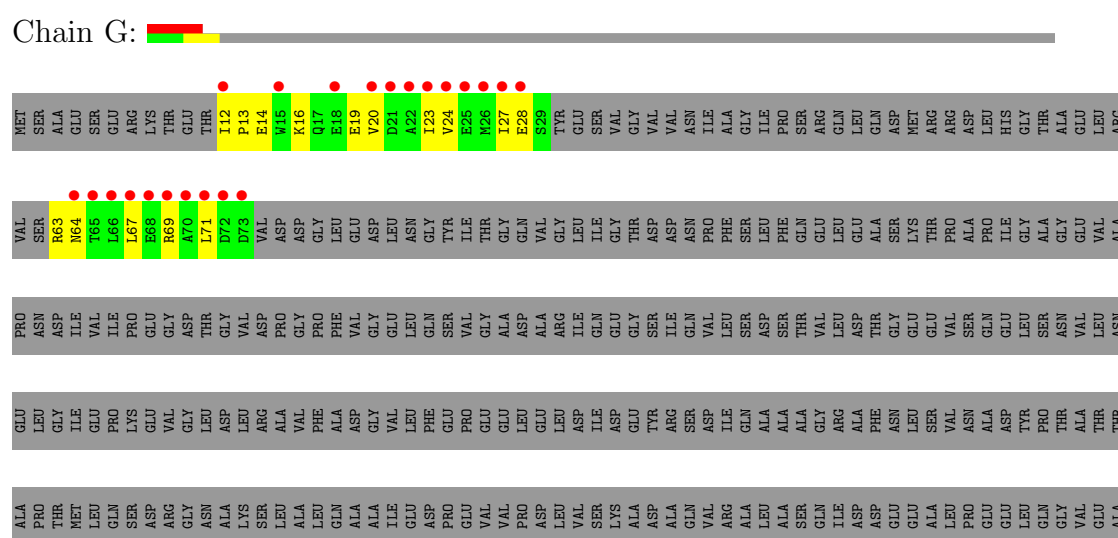
- Molecule 6: 50S ribosomal protein L5P



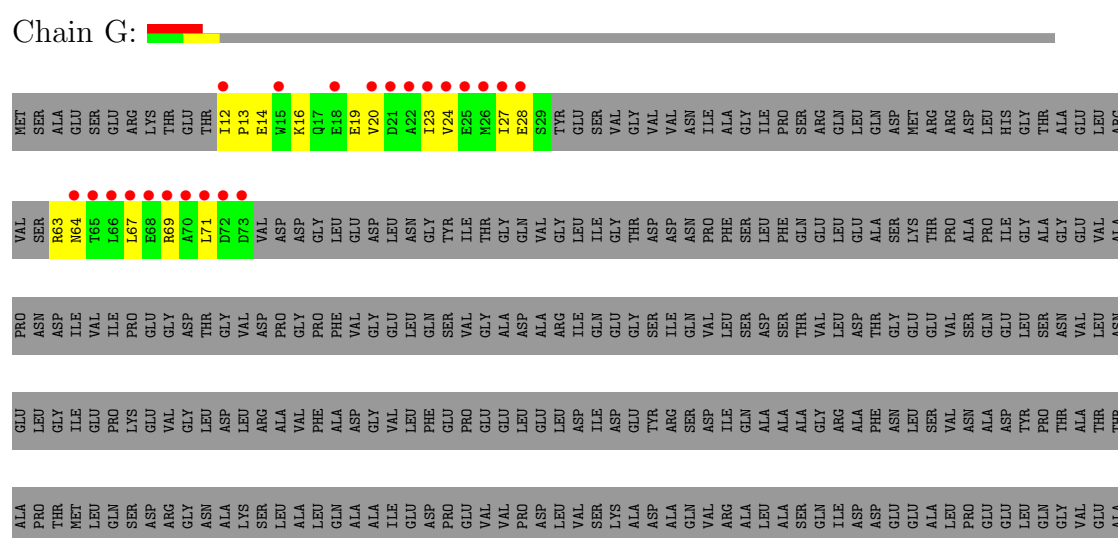
- Molecule 7: 50S ribosomal protein L6P

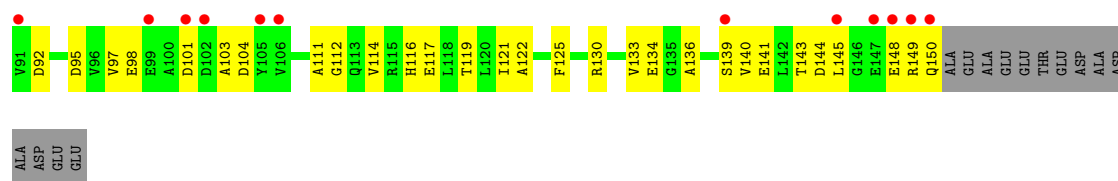


- Molecule 8: 50S ribosomal protein L7AE



- Molecule 9: ACIDIC RIBOSOMAL PROTEIN P0 HOMOLOG





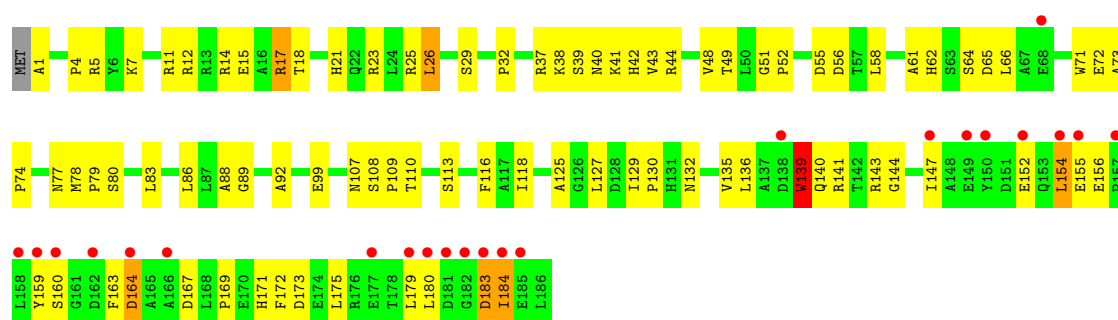
• Molecule 15: 50S Ribosomal Protein L15E

Chain M:



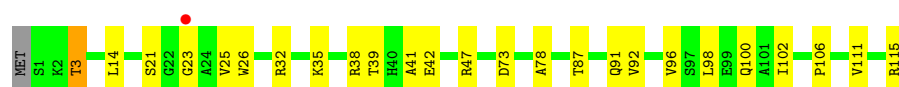
• Molecule 16: 50S ribosomal protein L18P

Chain N:



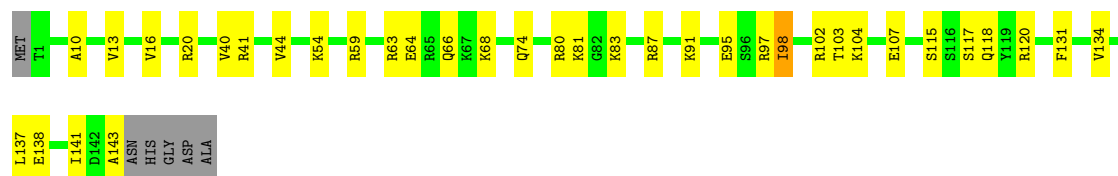
• Molecule 17: 50S ribosomal protein L18e

Chain O:



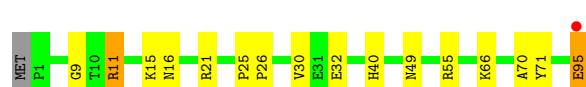
• Molecule 18: 50S ribosomal protein L19E

Chain P:



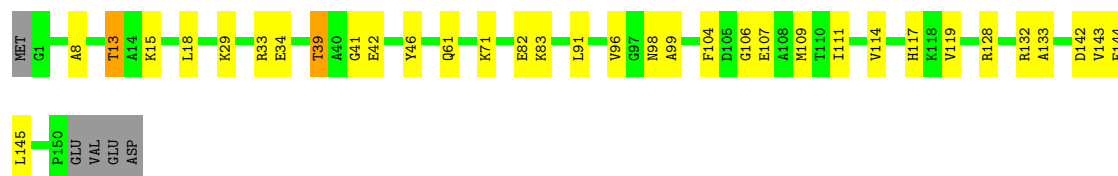
• Molecule 19: 50S ribosomal protein L21e

Chain Q:



- Molecule 20: 50S ribosomal protein L22P

Chain R:



- Molecule 21: 50S ribosomal protein L23P

Chain S:



- Molecule 22: 50S ribosomal protein L24P

Chain T:



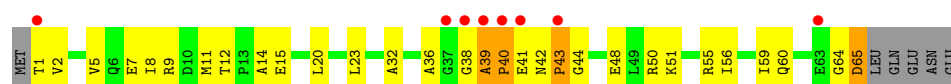
- Molecule 23: 50S ribosomal protein L24E

Chain U:



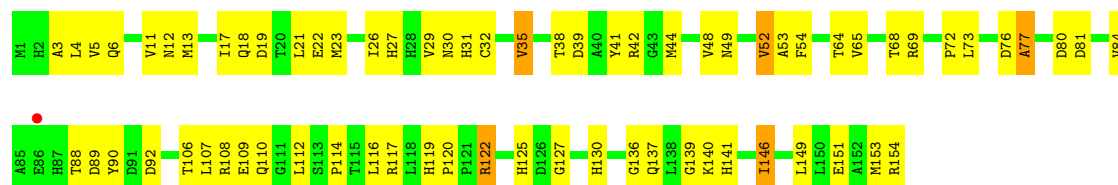
- Molecule 24: 50S ribosomal protein L29P

Chain V:



- Molecule 25: 50S ribosomal protein L30P

Chain W:



- Molecule 26: 50S ribosomal protein L31e

Chain X:

4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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) 90.1 (49.82-2.40)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.190 , 0.229 0.191 , 0.228	Depositor DCC
R_{free} test set	6150 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 634402 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	99116	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2625	0	2533	125	0
5	C	1859	0	1816	97	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	H	72	0	0	12	0
39	I	8	0	0	2	0
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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 2007 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:0:1160:G:H5'	1:0:1161: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
1:0:1242:A:H5'	12:J:82:THR:HG23	1.39	1.04

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	235/240 (98%)	218 (93%)	13 (6%)	4 (2%)	14	17
4	B	335/338 (99%)	314 (94%)	14 (4%)	7 (2%)	11	12
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%)	8	8
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%)	7	6
12	J	140/145 (97%)	130 (93%)	8 (6%)	2 (1%)	16	22
13	K	130/132 (98%)	122 (94%)	8 (6%)	0	100	100
14	L	141/165 (86%)	124 (88%)	16 (11%)	1 (1%)	30	43
15	M	192/194 (99%)	181 (94%)	11 (6%)	0	100	100
16	N	184/187 (98%)	166 (90%)	13 (7%)	5 (3%)	8	7
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%)	25	35
23	U	51/66 (77%)	49 (96%)	2 (4%)	0	100	100
24	V	63/71 (89%)	58 (92%)	2 (3%)	3 (5%)	4	2
25	W	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	18	24
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%)	4	3
29	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
30	2	42/50 (84%)	40 (95%)	1 (2%)	1 (2%)	9	9
31	3	90/92 (98%)	85 (94%)	5 (6%)	0	100	100
All	All	3705/4436 (84%)	3437 (93%)	223 (6%)	45 (1%)	19	26

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%)	23	35
4	B	282/283 (100%)	268 (95%)	14 (5%)	34	51
5	C	193/193 (100%)	175 (91%)	18 (9%)	13	19
6	D	117/148 (79%)	113 (97%)	4 (3%)	49	70
7	E	152/156 (97%)	147 (97%)	5 (3%)	50	71
8	F	93/94 (99%)	92 (99%)	1 (1%)	84	94
9	G	27/283 (10%)	27 (100%)	0	100	100
10	H	134/145 (92%)	129 (96%)	5 (4%)	45	66
11	I	58/130 (45%)	58 (100%)	0	100	100
12	J	118/121 (98%)	110 (93%)	8 (7%)	22	34
13	K	106/106 (100%)	105 (99%)	1 (1%)	87	96
14	L	113/127 (89%)	110 (97%)	3 (3%)	57	78
15	M	158/158 (100%)	151 (96%)	7 (4%)	39	58
16	N	149/150 (99%)	145 (97%)	4 (3%)	57	78
17	O	93/94 (99%)	91 (98%)	2 (2%)	64	83
18	P	113/117 (97%)	112 (99%)	1 (1%)	87	96
19	Q	79/80 (99%)	76 (96%)	3 (4%)	44	65
20	R	117/122 (96%)	115 (98%)	2 (2%)	73	89
21	S	71/74 (96%)	69 (97%)	2 (3%)	56	77
22	T	105/106 (99%)	100 (95%)	5 (5%)	35	53
23	U	44/52 (85%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	V	51/57 (90%)	49 (96%)	2 (4%)	43	64
25	W	130/130 (100%)	125 (96%)	5 (4%)	44	65
26	X	66/74 (89%)	59 (89%)	7 (11%)	10	14
27	Y	120/196 (61%)	111 (92%)	9 (8%)	19	29
28	Z	60/68 (88%)	58 (97%)	2 (3%)	50	71
29	1	46/47 (98%)	46 (100%)	0	100	100
30	2	42/46 (91%)	41 (98%)	1 (2%)	61	81
31	3	79/79 (100%)	79 (100%)	0	100	100
All	All	3095/3618 (86%)	2972 (96%)	123 (4%)	42	63

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%)	34 (1%)
2	9	121/122 (99%)	16 (13%)	1 (0%)
All	All	2866/3044 (94%)	242 (8%)	35 (1%)

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

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1377	C
1	0	1856	C
1	0	2761	A
1	0	1684	A
1	0	1685	A

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	20,22,23	0.76	1 (5%)	24,31,34	0.77	0
1	OMG	0	2588	1	24,26,27	0.82	0	32,38,41	5.10	3 (9%)
1	UR3	0	2619	1	20,22,23	0.79	1 (5%)	23,32,35	0.85	0
1	PSU	0	2621	1	19,21,22	1.12	2 (10%)	23,30,33	0.99	1 (4%)
1	1MA	0	628	1	23,25,26	0.82	0	32,37,40	1.00	1 (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
1	OMU	0	2587	1	-	0/8/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	0	2588	1	-	0/10/27/28	0/1/3/3
1	UR3	0	2619	1	-	0/6/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/8/25/26	0/2/2/2
1	1MA	0	628	1	-	1/8/25/26	0/1/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	3.13	1.43	1.37
1	0	2621	PSU	C6-N1	2.36	1.34	1.32
1	0	2587	OMU	P-OP1	2.20	1.49	1.46
1	0	2619	UR3	P-OP1	2.15	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2588	OMG	C6-C5-N7	-28.26	130.34	134.14
1	0	2588	OMG	C6-N1-C2	3.33	125.33	119.51
1	0	628	1MA	C2-N3-C4	-3.17	110.81	116.23
1	0	2588	OMG	C2-N3-C4	-2.29	111.88	115.09
1	0	2621	PSU	C5-C4-N3	-2.20	114.85	118.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	1.30	5 (9%)	83,83,83	1.13	5 (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
32	ZIT	0	9500	-	-	0/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	ZIT	C22-C11	3.40	1.58	1.52
32	0	9500	ZIT	C13-C14	2.88	1.60	1.54
32	0	9500	ZIT	O13-C13	2.39	1.48	1.44
32	0	9500	ZIT	C13-C12	2.07	1.61	1.55
32	0	9500	ZIT	C6-C5	2.03	1.60	1.55

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	ZIT	C12-C11-N10	-4.07	105.83	110.02
32	0	9500	ZIT	C9-N10-C11	-2.93	106.97	112.06
32	0	9500	ZIT	C7-C8-C9	2.62	116.14	112.24
32	0	9500	ZIT	C4A-C3A-C2A	-2.25	106.90	110.12
32	0	9500	ZIT	O6-C6-C7	2.05	113.87	108.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2754/2922 (94%)	-0.22	91 (3%) 44 42	15, 38, 82, 157	0
2	9	122/122 (100%)	0.11	5 (4%) 35 33	32, 58, 80, 139	0
3	A	237/240 (98%)	0.07	10 (4%) 35 32	19, 40, 75, 96	0
4	B	337/338 (99%)	0.05	5 (1%) 70 69	21, 47, 73, 84	0
5	C	246/246 (100%)	-0.21	2 (0%) 83 82	17, 36, 60, 69	0
6	D	140/177 (79%)	1.77	50 (35%) 1 0	51, 88, 114, 122	0
7	E	172/178 (96%)	0.73	18 (10%) 7 6	39, 61, 80, 84	0
8	F	119/120 (99%)	0.66	12 (10%) 7 7	38, 62, 88, 103	0
9	G	29/348 (8%)	2.56	22 (75%) 0 0	71, 87, 93, 95	0
10	H	160/177 (90%)	0.28	10 (6%) 19 18	31, 50, 83, 91	0
11	I	70/162 (43%)	6.09	70 (100%) 0 0	122, 135, 154, 155	0
12	J	142/145 (97%)	0.00	3 (2%) 60 58	29, 44, 65, 88	0
13	K	132/132 (100%)	-0.23	1 (0%) 83 82	24, 43, 65, 77	0
14	L	145/165 (87%)	0.46	19 (13%) 4 4	18, 56, 101, 115	0
15	M	194/194 (100%)	-0.18	0 100 100	21, 33, 49, 56	0
16	N	186/187 (99%)	0.60	23 (12%) 5 4	34, 55, 102, 112	0
17	O	115/116 (99%)	-0.03	1 (0%) 81 81	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%)	-0.14	1 (1%) 77 77	30, 37, 54, 68	0
20	R	150/155 (96%)	-0.24	0 100 100	25, 38, 58, 66	0
21	S	81/85 (95%)	0.08	3 (3%) 39 38	34, 50, 71, 81	0
22	T	119/120 (99%)	0.32	5 (4%) 35 32	29, 47, 76, 103	0
23	U	53/66 (80%)	0.17	1 (1%) 64 61	35, 48, 66, 78	0
24	V	65/71 (91%)	1.14	8 (12%) 5 4	43, 62, 107, 113	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	154/154 (100%)	-0.12	1 (0%) 86 86	29, 43, 58, 69	0
26	X	82/92 (89%)	0.51	8 (9%) 8 7	37, 50, 78, 94	0
27	Y	142/241 (58%)	0.02	5 (3%) 42 40	21, 36, 59, 80	0
28	Z	73/83 (87%)	0.01	2 (2%) 52 49	35, 51, 68, 86	0
29	1	56/57 (98%)	-0.62	0 100 100	18, 24, 32, 43	0
30	2	46/50 (92%)	0.43	5 (10%) 6 6	26, 51, 75, 89	0
31	3	92/92 (100%)	0.12	1 (1%) 77 77	26, 48, 62, 77	0
All	All	6651/7480 (88%)	0.09	382 (5%) 24 21	15, 43, 89, 157	0

The worst 5 of 382 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	I	74	ILE	14.7
11	I	66	GLY	13.7
11	I	128	THR	13.6
11	I	91	PHE	13.2
11	I	88	GLN	12.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	UR3	0	2619	21/22	0.12	0.90	29,33,35,41	0
1	1MA	0	628	23/24	0.13	0.33	22,24,25,28	0
1	OMU	0	2587	21/22	0.10	-0.96	26,28,29,32	0
1	PSU	0	2621	20/21	0.12	-1.23	22,25,33,33	0
1	OMG	0	2588	24/25	0.11	-1.26	23,27,29,30	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
37	SR	0	9006	1/1	0.87	168.33	200,200,200,200	0
37	SR	0	8996	1/1	0.54	127.59	185,185,185,185	0
35	NA	0	8549	1/1	0.52	87.66	74,74,74,74	0
37	SR	0	8997	1/1	0.43	70.79	171,171,171,171	0
37	SR	0	8955	1/1	0.33	59.40	169,169,169,169	0
35	NA	0	8555	1/1	0.38	50.73	43,43,43,43	0
35	NA	0	8561	1/1	0.47	32.75	62,62,62,62	0
35	NA	0	8542	1/1	0.32	31.97	51,51,51,51	0
37	SR	0	9007	1/1	0.24	28.93	154,154,154,154	0
33	MG	0	8073	1/1	0.15	24.27	76,76,76,76	0
37	SR	0	8976	1/1	0.23	22.54	159,159,159,159	0
35	NA	0	8565	1/1	0.25	22.33	46,46,46,46	0
35	NA	0	8552	1/1	0.29	19.82	48,48,48,48	0
37	SR	0	8957	1/1	0.32	19.09	176,176,176,176	0
35	NA	9	8572	1/1	0.36	18.56	59,59,59,59	0
35	NA	0	8564	1/1	0.39	16.91	55,55,55,55	0
37	SR	0	8994	1/1	0.31	16.62	168,168,168,168	0
35	NA	0	8556	1/1	0.47	16.31	37,37,37,37	0
35	NA	0	8525	1/1	0.18	16.22	65,65,65,65	0
33	MG	0	8089	1/1	0.24	15.98	37,37,37,37	0
33	MG	0	8037	1/1	0.20	15.91	77,77,77,77	0
33	MG	0	8071	1/1	0.27	15.79	54,54,54,54	0
35	NA	0	8551	1/1	0.25	15.57	39,39,39,39	0
33	MG	0	8030	1/1	0.19	15.52	48,48,48,48	0
35	NA	0	8528	1/1	0.21	13.12	32,32,32,32	0
35	NA	0	8554	1/1	0.24	13.04	52,52,52,52	0
37	SR	B	8987	1/1	0.43	12.92	189,189,189,189	0
35	NA	0	8574	1/1	0.35	12.73	48,48,48,48	0
35	NA	0	8516	1/1	0.16	12.72	44,44,44,44	0
35	NA	0	8506	1/1	0.23	12.58	50,50,50,50	0
36	CL	0	8822	1/1	0.16	12.25	48,48,48,48	0
35	NA	0	8521	1/1	0.25	11.23	55,55,55,55	0
35	NA	0	8550	1/1	0.21	10.44	41,41,41,41	0
35	NA	0	8517	1/1	0.15	10.20	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8563	1/1	0.27	9.73	56,56,56,56	0
35	NA	0	8567	1/1	0.21	9.53	53,53,53,53	0
37	SR	0	8979	1/1	0.31	9.40	184,184,184,184	0
37	SR	0	8974	1/1	0.24	9.19	159,159,159,159	0
37	SR	0	8969	1/1	0.22	9.00	115,115,115,115	0
35	NA	0	8522	1/1	0.23	8.80	46,46,46,46	0
35	NA	0	8560	1/1	0.37	8.63	54,54,54,54	0
35	NA	0	8524	1/1	0.19	8.61	31,31,31,31	0
37	SR	0	8982	1/1	0.18	8.45	152,152,152,152	0
35	NA	0	8509	1/1	0.14	8.26	47,47,47,47	0
33	MG	0	8063	1/1	0.15	8.11	71,71,71,71	0
33	MG	0	8081	1/1	0.17	7.26	55,55,55,55	0
37	SR	0	8986	1/1	0.73	7.11	169,169,169,169	0
37	SR	0	8903	1/1	0.16	7.01	41,41,41,41	0
35	NA	0	8568	1/1	0.24	6.98	42,42,42,42	0
35	NA	0	8553	1/1	0.18	6.76	48,48,48,48	0
35	NA	0	8514	1/1	0.18	6.43	41,41,41,41	0
37	SR	0	8992	1/1	0.22	6.07	111,111,111,111	0
35	NA	0	8562	1/1	0.17	5.99	59,59,59,59	0
37	SR	0	9000	1/1	0.17	5.69	150,150,150,150	0
35	NA	0	8547	1/1	0.19	5.07	42,42,42,42	0
37	SR	0	8905	1/1	0.20	5.00	48,48,48,48	0
35	NA	0	8571	1/1	0.19	4.99	79,79,79,79	0
33	MG	0	8068	1/1	0.13	4.28	48,48,48,48	0
35	NA	0	8508	1/1	0.16	4.08	40,40,40,40	0
37	SR	0	9001	1/1	0.16	4.05	160,160,160,160	0
35	NA	0	8505	1/1	0.15	3.86	33,33,33,33	0
37	SR	0	8919	1/1	0.14	3.81	169,169,169,169	0
37	SR	0	8962	1/1	0.13	3.71	139,139,139,139	0
35	NA	R	8575	1/1	0.20	3.14	73,73,73,73	0
33	MG	0	8085	1/1	0.13	3.00	90,90,90,90	0
37	SR	A	8929	1/1	0.21	2.83	123,123,123,123	0
37	SR	0	8989	1/1	0.16	2.81	148,148,148,148	0
37	SR	0	9002	1/1	0.17	2.76	162,162,162,162	0
35	NA	0	8536	1/1	0.12	2.50	46,46,46,46	0
37	SR	0	9004	1/1	0.22	2.33	176,176,176,176	0
37	SR	0	8983	1/1	0.15	1.85	149,149,149,149	0
35	NA	0	8501	1/1	0.13	1.60	26,26,26,26	0
33	MG	0	8090	1/1	0.12	1.49	49,49,49,49	0
35	NA	0	8544	1/1	0.13	1.38	49,49,49,49	0
35	NA	0	8559	1/1	0.12	1.38	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	M	8818	1/1	0.19	1.32	36,36,36,36	0
33	MG	0	8056	1/1	0.14	1.23	49,49,49,49	0
37	SR	0	8991	1/1	0.13	1.17	167,167,167,167	0
35	NA	0	8557	1/1	0.15	1.15	54,54,54,54	0
37	SR	0	8998	1/1	0.13	1.11	133,133,133,133	0
37	SR	0	8922	1/1	0.12	0.99	161,161,161,161	0
35	NA	0	8569	1/1	0.13	0.97	61,61,61,61	0
33	MG	0	8082	1/1	0.17	0.72	44,44,44,44	0
33	MG	0	8017	1/1	0.15	0.69	26,26,26,26	0
33	MG	0	8069	1/1	0.17	0.68	58,58,58,58	0
35	NA	0	8523	1/1	0.12	0.57	31,31,31,31	0
35	NA	M	8539	1/1	0.15	0.56	28,28,28,28	0
35	NA	0	8546	1/1	0.20	0.54	63,63,63,63	0
35	NA	S	8510	1/1	0.16	0.47	24,24,24,24	0
33	MG	0	8018	1/1	0.12	0.39	38,38,38,38	0
35	NA	H	8518	1/1	0.18	0.39	66,66,66,66	0
33	MG	0	8047	1/1	0.12	0.27	46,46,46,46	0
33	MG	0	8008	1/1	0.13	0.26	26,26,26,26	0
35	NA	0	8530	1/1	0.13	0.15	37,37,37,37	0
37	SR	9	8980	1/1	0.13	0.15	162,162,162,162	0
33	MG	0	8038	1/1	0.13	0.00	65,65,65,65	0
32	ZIT	0	9500	52/52	0.13	-0.07	28,38,42,44	0
37	SR	0	8959	1/1	0.13	-0.14	132,132,132,132	0
36	CL	A	8809	1/1	0.16	-0.15	52,52,52,52	0
33	MG	0	8049	1/1	0.11	-0.19	64,64,64,64	0
36	CL	R	8806	1/1	0.11	-0.27	40,40,40,40	0
35	NA	0	8515	1/1	0.13	-0.30	30,30,30,30	0
35	NA	0	8535	1/1	0.15	-0.36	40,40,40,40	0
37	SR	0	8985	1/1	0.11	-0.36	104,104,104,104	0
33	MG	A	8051	1/1	0.14	-0.36	55,55,55,55	0
37	SR	0	8944	1/1	0.11	-0.40	146,146,146,146	0
33	MG	0	8022	1/1	0.13	-0.43	30,30,30,30	0
35	NA	0	8566	1/1	0.14	-0.51	44,44,44,44	0
37	SR	H	8972	1/1	0.12	-0.52	112,112,112,112	0
35	NA	0	8527	1/1	0.11	-0.52	31,31,31,31	0
37	SR	0	8933	1/1	0.10	-0.59	108,108,108,108	0
35	NA	0	8573	1/1	0.10	-0.65	55,55,55,55	0
37	SR	0	8993	1/1	0.10	-0.67	143,143,143,143	0
33	MG	0	8020	1/1	0.10	-0.73	37,37,37,37	0
37	SR	R	8912	1/1	0.11	-0.81	77,77,77,77	0
36	CL	Y	8820	1/1	0.10	-0.82	35,35,35,35	0
35	NA	0	8520	1/1	0.08	-0.86	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	CL	0	8803	1/1	0.12	-0.90	41,41,41,41	0
33	MG	0	8031	1/1	0.11	-0.90	41,41,41,41	0
33	MG	0	8080	1/1	0.09	-0.95	53,53,53,53	0
34	K	0	8401	1/1	0.10	-0.96	58,58,58,58	0
37	SR	0	8947	1/1	0.09	-1.00	148,148,148,148	0
35	NA	0	8502	1/1	0.11	-1.02	43,43,43,43	0
33	MG	0	8032	1/1	0.10	-1.02	36,36,36,36	0
38	CD	U	8701	1/1	0.09	-1.03	55,55,55,55	0
37	SR	0	8975	1/1	0.10	-1.04	99,99,99,99	0
35	NA	C	8503	1/1	0.09	-1.06	29,29,29,29	0
33	MG	0	8061	1/1	0.11	-1.07	23,23,23,23	0
35	NA	0	8513	1/1	0.11	-1.10	33,33,33,33	0
35	NA	9	8543	1/1	0.19	-1.16	41,41,41,41	0
37	SR	0	8927	1/1	0.11	-1.19	133,133,133,133	0
37	SR	0	8954	1/1	0.11	-1.22	88,88,88,88	0
35	NA	0	8541	1/1	0.12	-1.23	41,41,41,41	0
33	MG	0	8009	1/1	0.12	-1.25	26,26,26,26	0
36	CL	0	8813	1/1	0.10	-1.27	45,45,45,45	0
36	CL	0	8811	1/1	0.08	-1.29	45,45,45,45	0
33	MG	0	8084	1/1	0.04	-1.34	36,36,36,36	0
36	CL	J	8821	1/1	0.10	-1.34	52,52,52,52	0
36	CL	0	8812	1/1	0.09	-1.38	39,39,39,39	0
33	MG	0	8011	1/1	0.09	-1.39	24,24,24,24	0
37	SR	0	8907	1/1	0.09	-1.39	33,33,33,33	0
37	SR	A	8977	1/1	0.08	-1.39	143,143,143,143	0
33	MG	0	8053	1/1	0.09	-1.41	58,58,58,58	0
33	MG	0	8041	1/1	0.10	-1.42	18,18,18,18	0
36	CL	O	8808	1/1	0.08	-1.43	54,54,54,54	0
37	SR	0	8981	1/1	0.10	-1.43	141,141,141,141	0
35	NA	J	8538	1/1	0.08	-1.44	48,48,48,48	0
33	MG	0	8036	1/1	0.08	-1.61	36,36,36,36	0
33	MG	0	8005	1/1	0.12	-1.64	23,23,23,23	0
33	MG	0	8058	1/1	0.08	-1.65	26,26,26,26	0
37	SR	A	8930	1/1	0.06	-1.67	82,82,82,82	0
33	MG	0	8092	1/1	0.09	-1.69	47,47,47,47	0
33	MG	A	8050	1/1	0.11	-1.70	33,33,33,33	0
35	NA	Q	8540	1/1	0.10	-1.70	39,39,39,39	0
36	CL	0	8814	1/1	0.08	-1.75	40,40,40,40	0
37	SR	0	8964	1/1	0.08	-1.76	109,109,109,109	0
36	CL	0	8816	1/1	0.09	-1.77	53,53,53,53	0
37	SR	0	8934	1/1	0.10	-1.78	116,116,116,116	0
38	CD	Z	8703	1/1	0.07	-1.89	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8512	1/1	0.09	-1.91	36,36,36,36	0
33	MG	0	8035	1/1	0.06	-1.92	52,52,52,52	0
38	CD	3	8704	1/1	0.07	-1.93	53,53,53,53	0
35	NA	0	8526	1/1	0.08	-1.94	36,36,36,36	0
35	NA	0	8529	1/1	0.07	-1.98	32,32,32,32	0
33	MG	0	8028	1/1	0.09	-1.98	19,19,19,19	0
37	SR	0	8939	1/1	0.07	-2.00	108,108,108,108	0
37	SR	0	8918	1/1	0.11	-2.06	66,66,66,66	0
35	NA	0	8533	1/1	0.08	-2.09	50,50,50,50	0
35	NA	0	8534	1/1	0.10	-2.10	29,29,29,29	0
36	CL	J	8802	1/1	0.06	-2.15	51,51,51,51	0
33	MG	T	8057	1/1	0.07	-2.17	51,51,51,51	0
35	NA	R	8532	1/1	0.07	-2.22	37,37,37,37	0
37	SR	0	8911	1/1	0.06	-2.25	65,65,65,65	0
37	SR	0	8917	1/1	0.08	-2.26	90,90,90,90	0
33	MG	0	8040	1/1	0.10	-2.34	78,78,78,78	0
37	SR	0	8940	1/1	0.04	-2.36	66,66,66,66	0
38	CD	O	8705	1/1	0.05	-2.38	58,58,58,58	0
35	NA	0	8504	1/1	0.09	-2.46	26,26,26,26	0
36	CL	J	8801	1/1	0.06	-2.49	49,49,49,49	0
35	NA	0	8548	1/1	0.09	-2.50	50,50,50,50	0
37	SR	0	8984	1/1	0.08	-2.54	98,98,98,98	0
33	MG	0	8043	1/1	0.11	-2.55	46,46,46,46	0
33	MG	0	8055	1/1	0.09	-2.57	29,29,29,29	0
33	MG	0	8062	1/1	0.08	-2.61	46,46,46,46	0
36	CL	B	8819	1/1	0.06	-2.63	46,46,46,46	0
33	MG	0	8045	1/1	0.09	-2.64	29,29,29,29	0
33	MG	0	8024	1/1	0.09	-2.66	53,53,53,53	0
36	CL	0	8805	1/1	0.07	-2.71	45,45,45,45	0
33	MG	0	8034	1/1	0.10	-2.74	35,35,35,35	0
37	SR	0	8999	1/1	0.04	-2.76	78,78,78,78	0
37	SR	F	9005	1/1	0.06	-2.81	106,106,106,106	0
37	SR	0	8943	1/1	0.08	-2.81	108,108,108,108	0
37	SR	0	8960	1/1	0.09	-2.82	128,128,128,128	0
37	SR	0	8973	1/1	0.07	-2.82	113,113,113,113	0
37	SR	0	8990	1/1	0.10	-2.83	106,106,106,106	0
34	K	0	8402	1/1	0.08	-2.90	46,46,46,46	0
37	SR	0	8908	1/1	0.07	-2.95	71,71,71,71	0
33	MG	0	8070	1/1	0.08	-2.98	36,36,36,36	0
33	MG	0	8003	1/1	0.10	-3.02	23,23,23,23	0
37	SR	0	8925	1/1	0.08	-3.05	75,75,75,75	0
37	SR	S	8961	1/1	0.09	-3.08	113,113,113,113	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
33	MG	B	8042	1/1	0.07	-3.09	52,52,52,52	0
35	NA	0	8537	1/1	0.09	-3.10	32,32,32,32	0
37	SR	0	8923	1/1	0.07	-3.12	78,78,78,78	0
33	MG	0	8039	1/1	0.11	-3.16	60,60,60,60	0
37	SR	0	8970	1/1	0.08	-3.18	109,109,109,109	0
37	SR	0	8937	1/1	0.07	-3.19	94,94,94,94	0
35	NA	0	8519	1/1	0.11	-3.21	36,36,36,36	0
37	SR	0	8953	1/1	0.06	-3.26	121,121,121,121	0
37	SR	0	8936	1/1	0.08	-3.26	67,67,67,67	0
37	SR	0	8904	1/1	0.06	-3.27	34,34,34,34	0
33	MG	0	8077	1/1	0.06	-3.29	26,26,26,26	0
37	SR	0	8942	1/1	0.06	-3.34	110,110,110,110	0
37	SR	0	8924	1/1	0.12	-3.34	123,123,123,123	0
36	CL	0	8817	1/1	0.09	-3.42	46,46,46,46	0
33	MG	0	8014	1/1	0.08	-3.42	25,25,25,25	0
33	MG	0	8001	1/1	0.08	-3.49	25,25,25,25	0
33	MG	0	8066	1/1	0.09	-3.50	47,47,47,47	0
37	SR	9	9003	1/1	0.07	-3.56	141,141,141,141	0
36	CL	0	8815	1/1	0.08	-3.58	47,47,47,47	0
33	MG	0	8010	1/1	0.08	-3.58	29,29,29,29	0
33	MG	0	8065	1/1	0.06	-3.63	45,45,45,45	0
33	MG	0	8044	1/1	0.10	-3.66	40,40,40,40	0
33	MG	0	8052	1/1	0.07	-3.67	23,23,23,23	0
37	SR	3	8932	1/1	0.06	-3.69	58,58,58,58	0
37	SR	0	8956	1/1	0.07	-3.70	127,127,127,127	0
35	NA	0	8507	1/1	0.08	-3.83	27,27,27,27	0
33	MG	0	8083	1/1	0.05	-3.90	41,41,41,41	0
36	CL	L	8810	1/1	0.07	-3.92	43,43,43,43	0
38	CD	1	8702	1/1	0.04	-3.94	44,44,44,44	0
33	MG	K	8054	1/1	0.07	-3.96	34,34,34,34	0
33	MG	0	8048	1/1	0.08	-4.06	33,33,33,33	0
33	MG	0	8079	1/1	0.07	-4.08	40,40,40,40	0
33	MG	0	8075	1/1	0.06	-4.17	31,31,31,31	0
33	MG	9	8074	1/1	0.09	-4.20	64,64,64,64	0
37	SR	0	8968	1/1	0.07	-4.41	142,142,142,142	0
33	MG	0	8025	1/1	0.06	-4.49	24,24,24,24	0
33	MG	0	8012	1/1	0.05	-4.51	13,13,13,13	0
37	SR	0	8958	1/1	0.07	-4.55	83,83,83,83	0
37	SR	1	8913	1/1	0.06	-4.56	70,70,70,70	0
37	SR	0	8971	1/1	0.09	-4.60	158,158,158,158	0
36	CL	N	8807	1/1	0.09	-4.70	46,46,46,46	0
33	MG	0	8015	1/1	0.08	-4.78	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	B	8950	1/1	0.05	-5.01	90,90,90,90	0
35	NA	0	8511	1/1	0.09	-5.07	59,59,59,59	0
37	SR	0	8941	1/1	0.05	-5.12	90,90,90,90	0
37	SR	0	8915	1/1	0.05	-5.22	85,85,85,85	0
33	MG	0	8029	1/1	0.07	-5.27	40,40,40,40	0
37	SR	0	8935	1/1	0.11	-5.44	60,60,60,60	0
33	MG	0	8016	1/1	0.06	-5.51	35,35,35,35	0
37	SR	0	8914	1/1	0.08	-5.53	88,88,88,88	0
33	MG	0	8078	1/1	0.07	-5.57	40,40,40,40	0
33	MG	Y	8086	1/1	0.08	-5.79	35,35,35,35	0
33	MG	0	8007	1/1	0.08	-5.80	24,24,24,24	0
37	SR	0	8909	1/1	0.07	-5.82	70,70,70,70	0
37	SR	0	8967	1/1	0.03	-5.83	116,116,116,116	0
37	SR	0	8995	1/1	0.07	-5.89	112,112,112,112	0
33	MG	0	8093	1/1	0.07	-5.94	29,29,29,29	0
37	SR	0	8920	1/1	0.06	-5.94	96,96,96,96	0
33	MG	0	8046	1/1	0.08	-6.05	25,25,25,25	0
33	MG	0	8019	1/1	0.07	-6.09	22,22,22,22	0
33	MG	0	8023	1/1	0.06	-6.20	24,24,24,24	0
33	MG	0	8002	1/1	0.07	-6.20	27,27,27,27	0
37	SR	0	8926	1/1	0.05	-6.45	95,95,95,95	0
35	NA	0	8558	1/1	0.06	-6.55	46,46,46,46	0
33	MG	0	8033	1/1	0.06	-6.55	32,32,32,32	0
35	NA	0	8570	1/1	0.07	-6.61	35,35,35,35	0
37	SR	0	8916	1/1	0.05	-6.87	95,95,95,95	0
33	MG	0	8088	1/1	0.04	-6.96	29,29,29,29	0
33	MG	0	8006	1/1	0.06	-6.99	30,30,30,30	0
33	MG	0	8076	1/1	0.07	-7.32	28,28,28,28	0
37	SR	0	8938	1/1	0.05	-7.35	147,147,147,147	0
33	MG	0	8027	1/1	0.04	-7.36	32,32,32,32	0
37	SR	0	9008	1/1	0.06	-7.44	83,83,83,83	0
33	MG	0	8004	1/1	0.04	-7.48	22,22,22,22	0
33	MG	0	8026	1/1	0.05	-7.50	28,28,28,28	0
33	MG	0	8013	1/1	0.04	-7.62	24,24,24,24	0
37	SR	1	8952	1/1	0.05	-7.67	62,62,62,62	0
37	SR	0	8951	1/1	0.05	-7.70	137,137,137,137	0
33	MG	0	8021	1/1	0.08	-7.82	28,28,28,28	0
37	SR	0	8921	1/1	0.07	-7.91	66,66,66,66	0
36	CL	3	8804	1/1	0.04	-8.09	47,47,47,47	0
37	SR	0	8948	1/1	0.06	-8.19	69,69,69,69	0
37	SR	0	8946	1/1	0.07	-8.26	87,87,87,87	0
33	MG	0	8059	1/1	0.04	-8.45	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
37	SR	0	8928	1/1	0.09	-8.56	112,112,112,112	0
37	SR	0	8901	1/1	0.04	-8.77	71,71,71,71	0
37	SR	0	8906	1/1	0.09	-8.81	40,40,40,40	0
37	SR	0	8978	1/1	0.04	-8.85	82,82,82,82	0
35	NA	0	8545	1/1	0.07	-8.92	29,29,29,29	0
33	MG	0	8067	1/1	0.05	-9.05	29,29,29,29	0
37	SR	0	8910	1/1	0.04	-9.18	80,80,80,80	0
37	SR	0	8945	1/1	0.04	-9.18	92,92,92,92	0
33	MG	0	8087	1/1	0.05	-9.35	26,26,26,26	0
37	SR	0	8966	1/1	0.03	-9.58	89,89,89,89	0
37	SR	0	8949	1/1	0.04	-9.67	93,93,93,93	0
33	MG	0	8060	1/1	0.06	-9.97	45,45,45,45	0
33	MG	0	8064	1/1	0.03	-10.03	34,34,34,34	0
37	SR	0	8931	1/1	0.04	-10.78	86,86,86,86	0
37	SR	0	8988	1/1	0.06	-12.50	149,149,149,149	0
33	MG	0	8072	1/1	0.06	-15.67	37,37,37,37	0
35	NA	0	8531	1/1	0.05	-23.85	29,29,29,29	0
37	SR	0	8902	1/1	0.04	-26.60	49,49,49,49	0
33	MG	0	8091	1/1	0.09	-28.00	42,42,42,42	0
37	SR	0	8965	1/1	0.05	-40.41	109,109,109,109	0
37	SR	0	8963	1/1	0.05	-93.00	103,103,103,103	0

6.5 Other polymers ⓘ

There are no such residues in this entry.