



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 05:31 PM BST

PDB ID : 3CCS
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482A
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 2.95 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

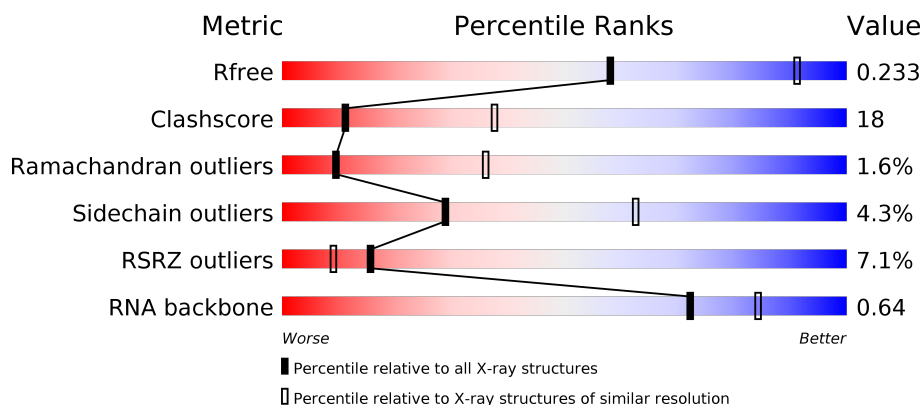
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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 respectively. 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	A	240	<div> <div>3%</div> <div> <div></div> <div>66%</div> <div>28%</div> <div>• •</div> </div> </div>
2	B	338	<div> <div>62%</div> <div>33%</div> <div>•</div> </div>
3	C	246	<div> <div>73%</div> <div>24%</div> <div>•</div> </div>
4	D	177	<div> <div>29%</div> <div>51%</div> <div>25%</div> <div>•</div> <div>21%</div> </div>

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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1	57	
28	2	50	
29	3	92	

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Mol	Chain	Length	Quality of chain
30	0	2923	
31	9	122	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CL	0	8812	-	-	X	-
33	CL	Y	8820	-	-	X	-
34	SR	0	8982	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	0	9007	-	-	-	X
35	NA	0	8528	-	-	-	X
37	CD	3	8704	-	-	-	X
37	CD	Z	8703	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99121 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 protein called 50S ribosomal protein L2P.

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

- Molecule 2 is a protein called 50S ribosomal protein L3P.

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

- Molecule 3 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 4 is a protein called 50S ribosomal protein L5P.

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

- Molecule 5 is a protein called 50S ribosomal protein L6P.

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

- Molecule 6 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 7 is a protein called 50S ribosomal protein L10E.

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

- Molecule 8 is a protein called 50S ribosomal protein L10e.

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

- Molecule 9 is a protein called 50S ribosomal protein L11P.

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

- Molecule 10 is a protein called 50S ribosomal protein L13P.

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

- Molecule 11 is a protein called 50S ribosomal protein L14P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	132	Total	C	N	O	S	0	0	0
			994	609	189	192	4			

- Molecule 12 is a protein called 50S ribosomal protein L15P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	194	Total	C	N	O	S	0	0	0
			1558	943	333	281	1			

- Molecule 14 is a protein called 50S ribosomal protein L18P.

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

- Molecule 15 is a protein called 50S ribosomal protein L18e.

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

- Molecule 16 is a protein called 50S ribosomal protein L19e.

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

- Molecule 17 is a protein called 50S ribosomal protein L21e.

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

- Molecule 18 is a protein called 50S ribosomal protein L22P.

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

- Molecule 19 is a protein called 50S ribosomal protein L23P.

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

- Molecule 20 is a protein called 50S ribosomal protein L24P.

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

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

- Molecule 22 is a protein called 50S ribosomal protein L29P.

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

- Molecule 23 is a protein called 50S ribosomal protein L30P.

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

- Molecule 24 is a protein called 50S ribosomal protein L31e.

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

- Molecule 25 is a protein called 50S ribosomal protein L32e.

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

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59019	26349	10873	19052	2745			

- Molecule 31 is a RNA chain called 5S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

- Molecule 32 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	86	Total	Mg	0	0
			86	86		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	10	Total 10	Cl 10	0	0
33	J	3	Total 3	Cl 3	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

- Molecule 34 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	92	Total 92	Sr 92	0	0
34	1	2	Total 2	Sr 2	0	0
34	H	1	Total 1	Sr 1	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	2	Total 2	Sr 2	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	3	Total 3	Sr 3	0	0
34	L	1	Total 1	Sr 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	S	1	Total 1	Sr 1	0	0
34	F	1	Total 1	Sr 1	0	0

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

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

- Molecule 36 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

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

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	119	Total 119	O 119	0	0
38	B	152	Total 152	O 152	0	0
38	C	185	Total 185	O 185	0	0
38	D	42	Total 42	O 42	0	0
38	E	43	Total 43	O 43	0	0
38	F	26	Total 26	O 26	0	0
38	G	19	Total 19	O 19	0	0
38	H	65	Total 65	O 65	0	0
38	I	8	Total 8	O 8	0	0
38	J	53	Total 53	O 53	0	0
38	K	58	Total 58	O 58	0	0
38	L	85	Total 85	O 85	0	0
38	M	127	Total 127	O 127	0	0
38	N	59	Total 59	O 59	0	0
38	O	39	Total 39	O 39	0	0

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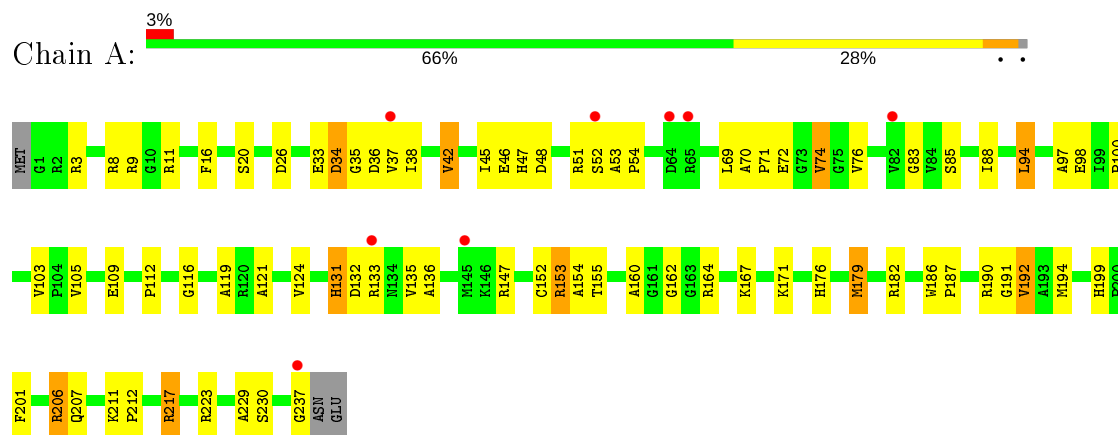
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	P	67	Total 67	O 67	0	0
38	Q	48	Total 48	O 48	0	0
38	R	77	Total 77	O 77	0	0
38	S	30	Total 30	O 30	0	0
38	T	36	Total 36	O 36	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	67	Total 67	O 67	0	0
38	X	21	Total 21	O 21	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	31	Total 31	O 31	0	0
38	1	59	Total 59	O 59	0	0
38	2	43	Total 43	O 43	0	0
38	3	70	Total 70	O 70	0	0
38	0	5904	Total 5904	O 5904	0	0
38	9	149	Total 149	O 149	0	0

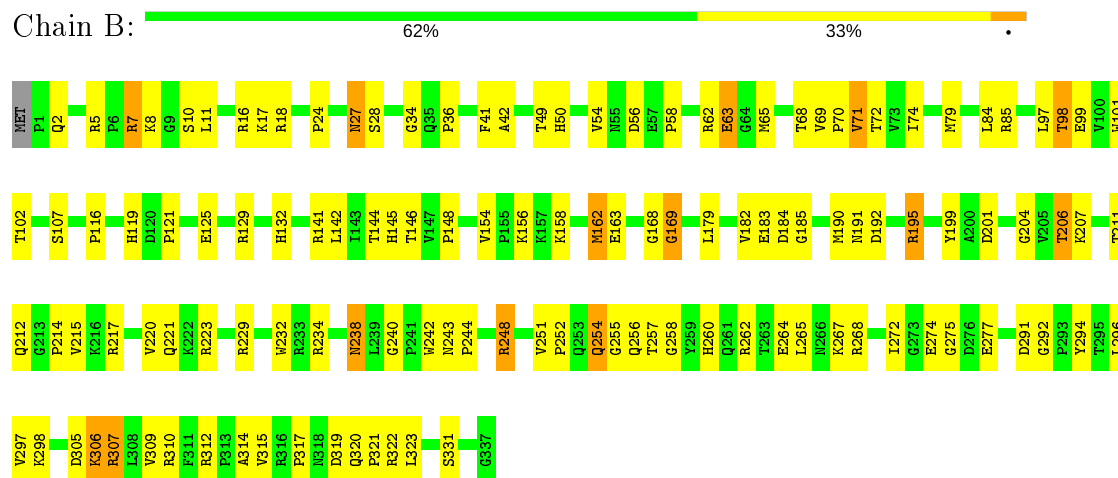
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

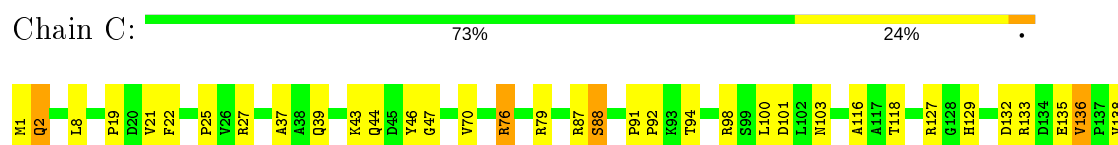
• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P

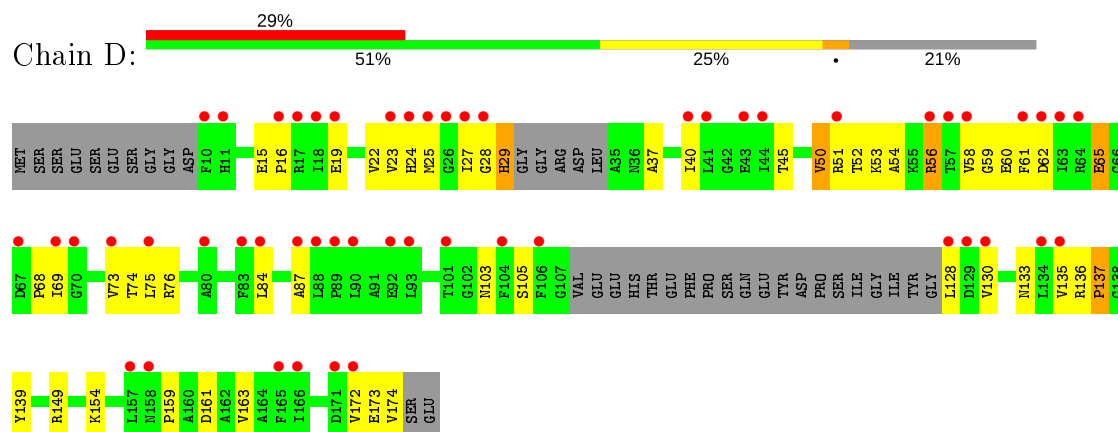


• Molecule 3: 50S ribosomal protein L4P

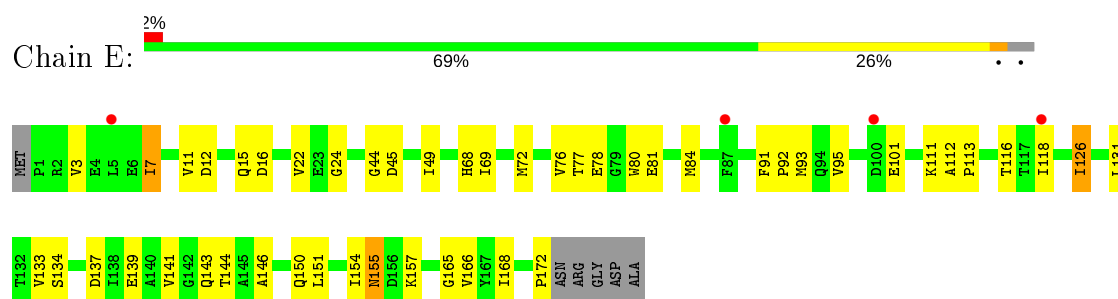




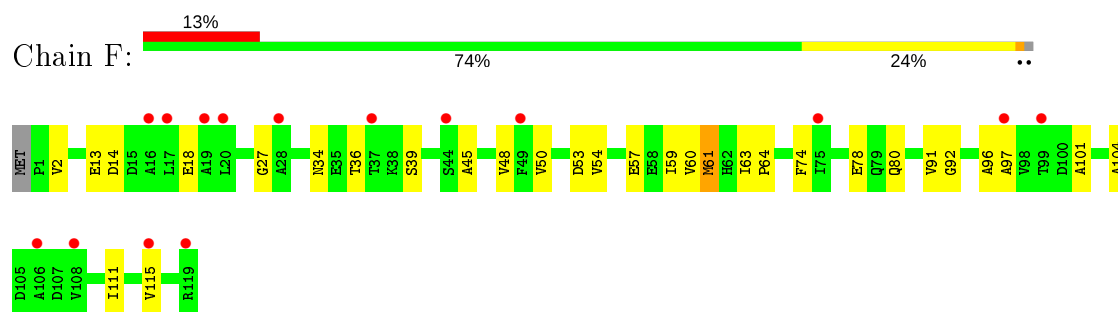
• Molecule 4: 50S ribosomal protein L5P



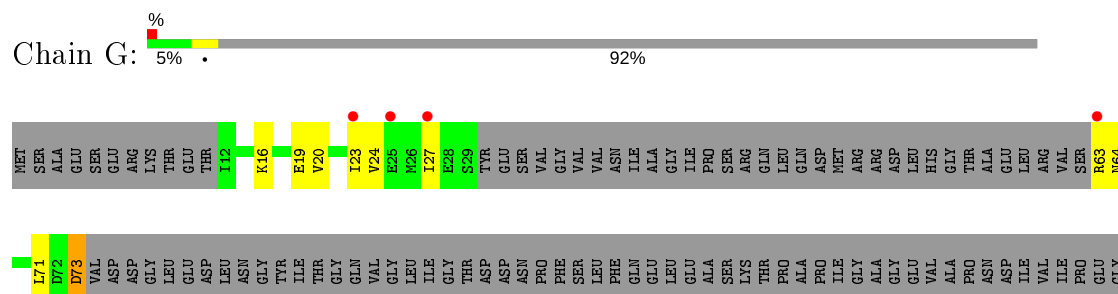
• Molecule 5: 50S ribosomal protein L6P

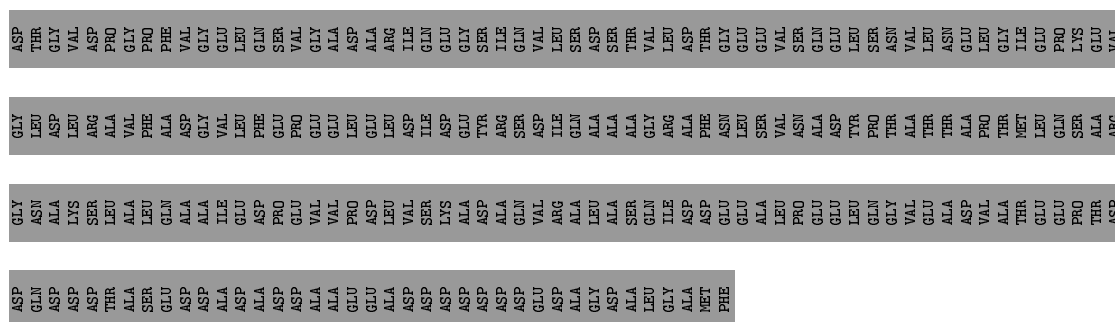


• Molecule 6: 50S ribosomal protein L7Ae

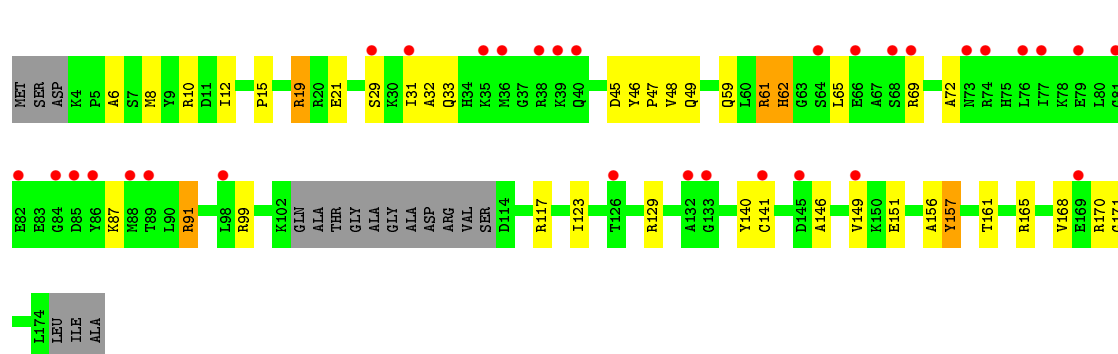


• Molecule 7: 50S ribosomal protein L10E

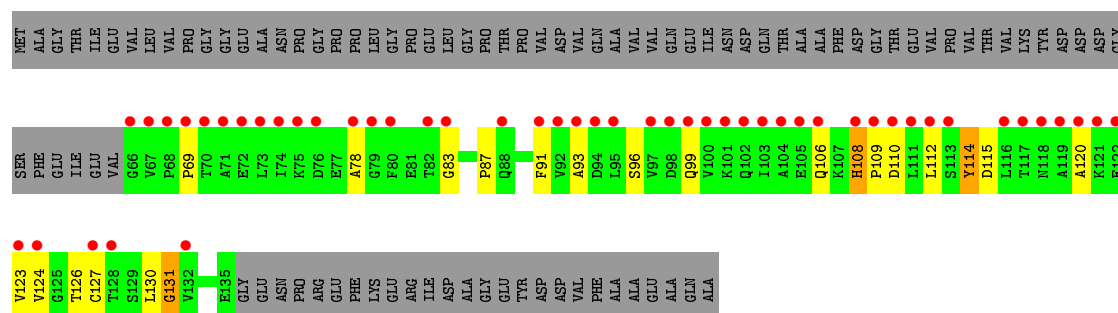




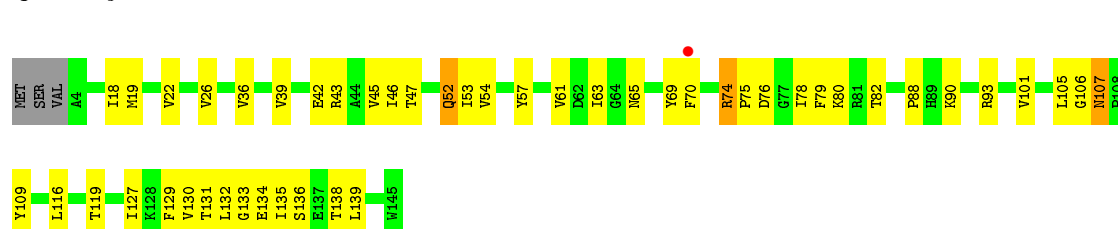
• Molecule 8: 50S ribosomal protein L10e



• Molecule 9: 50S ribosomal protein L11P

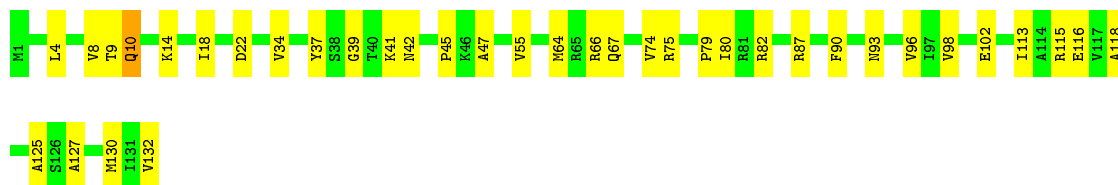


• Molecule 10: 50S ribosomal protein L13P



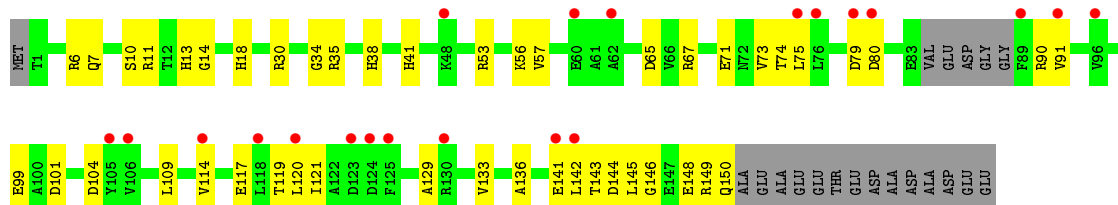
• Molecule 11: 50S ribosomal protein L14P

Chain K:  72% 27% .



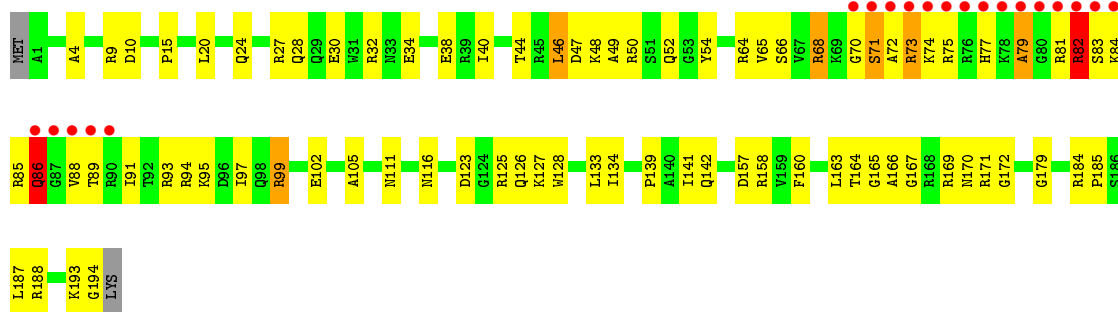
- Molecule 12: 50S ribosomal protein L15P

Chain L:  13% 60% 28% 12%



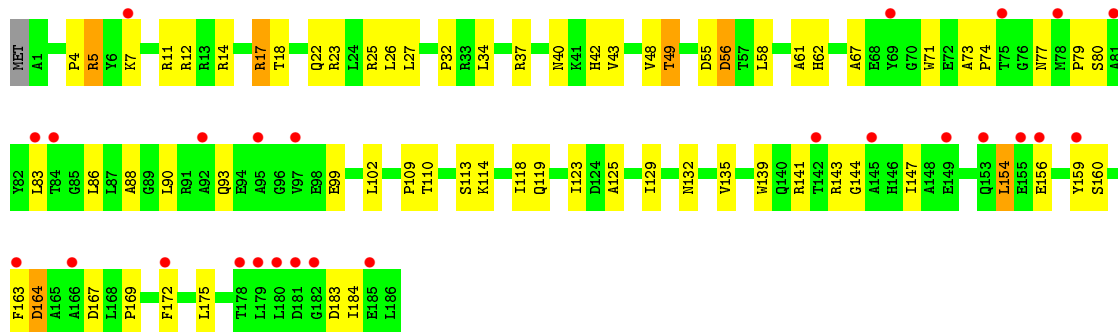
- Molecule 13: 50S ribosomal protein L15e

Chain M:  10% 58% 37% . .




- Molecule 14: 50S ribosomal protein L18P

Chain N:  14% 63% 33% . .



- Molecule 15: 50S ribosomal protein L18e

Chain O:  78% 21% ..



- Molecule 16: 50S ribosomal protein L19e

Chain P:  70% 23% . .



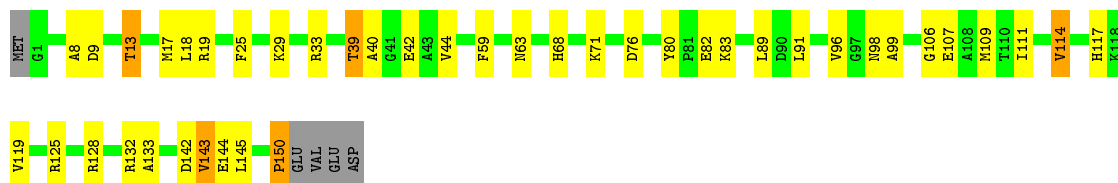
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  73% 25% ..



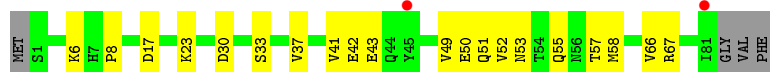
- Molecule 18: 50S ribosomal protein L22P

Chain R:  70% 24% . .



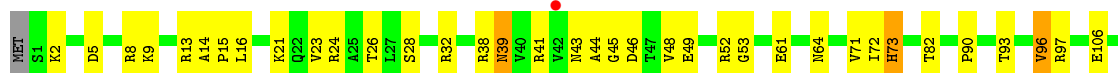
- Molecule 19: 50S ribosomal protein L23P

Chain S:  72% 24% 5%



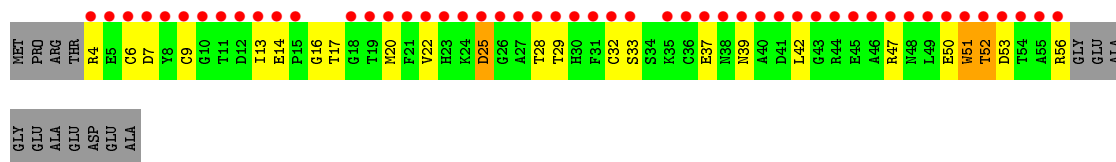
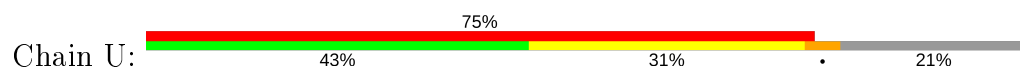
- Molecule 20: 50S ribosomal protein L24P

Chain T:  68% 29% . .

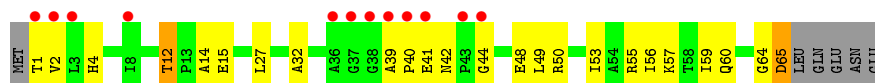




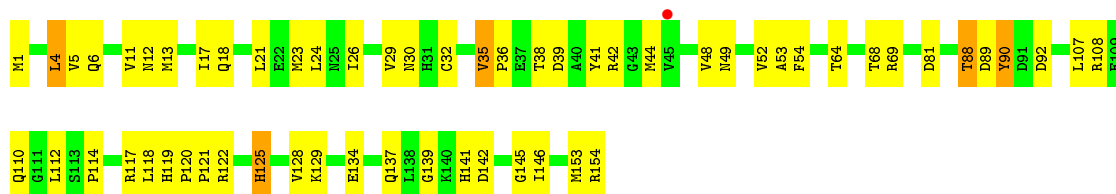
- Molecule 21: 50S ribosomal protein L24e



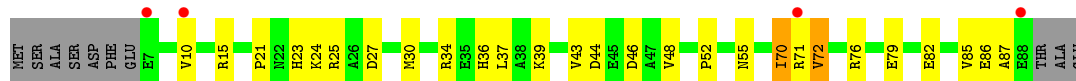
- Molecule 22: 50S ribosomal protein L29P



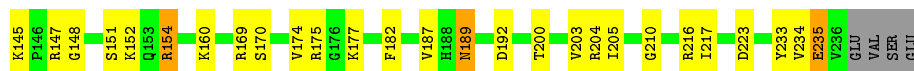
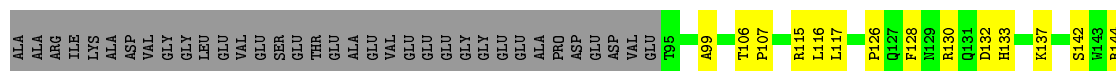
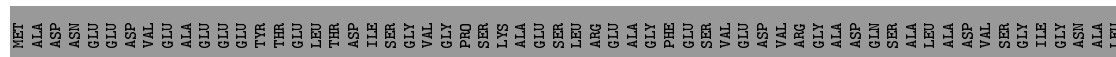
- Molecule 23: 50S ribosomal protein L30P



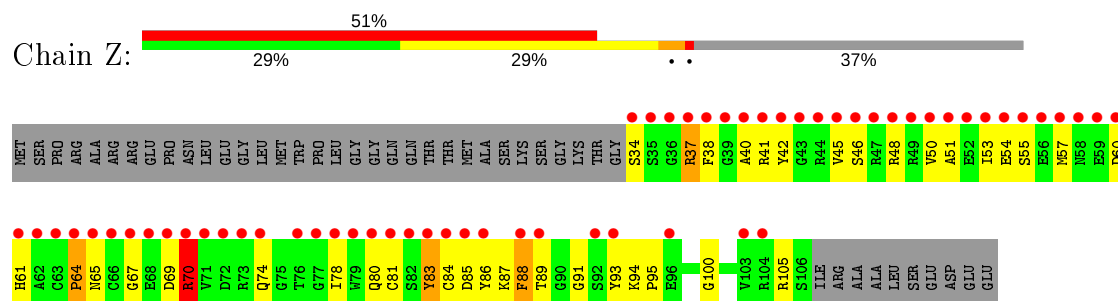
- Molecule 24: 50S ribosomal protein L31e



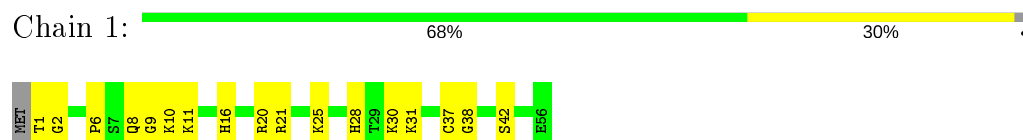
- Molecule 25: 50S ribosomal protein L32e



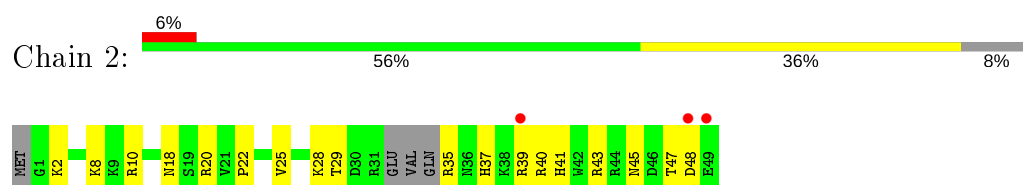
- Molecule 26: 50S ribosomal protein L37Ae



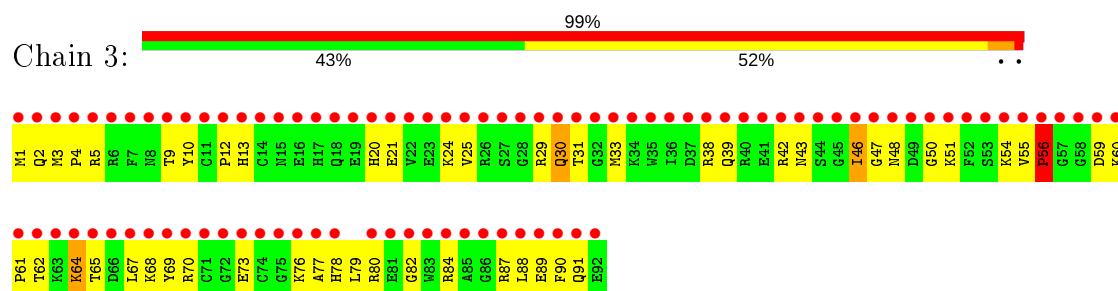
- Molecule 27: 50S ribosomal protein L37e



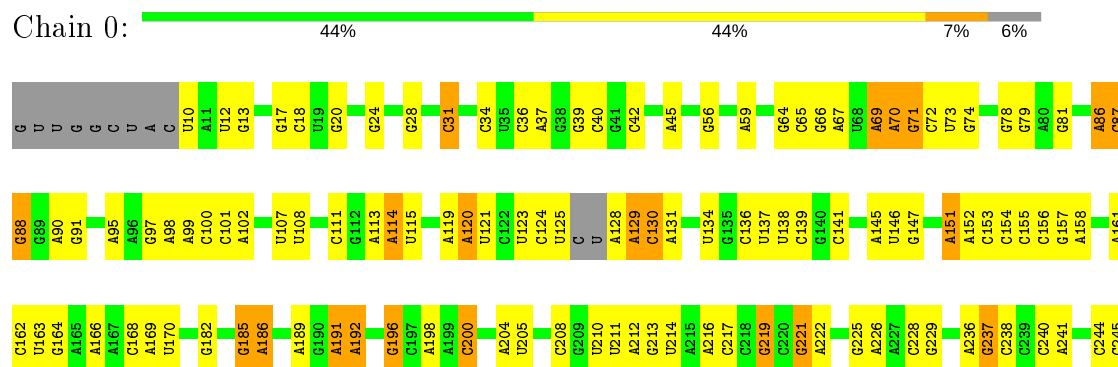
- Molecule 28: 50S ribosomal protein L39e



- Molecule 29: 50S ribosomal protein L44E

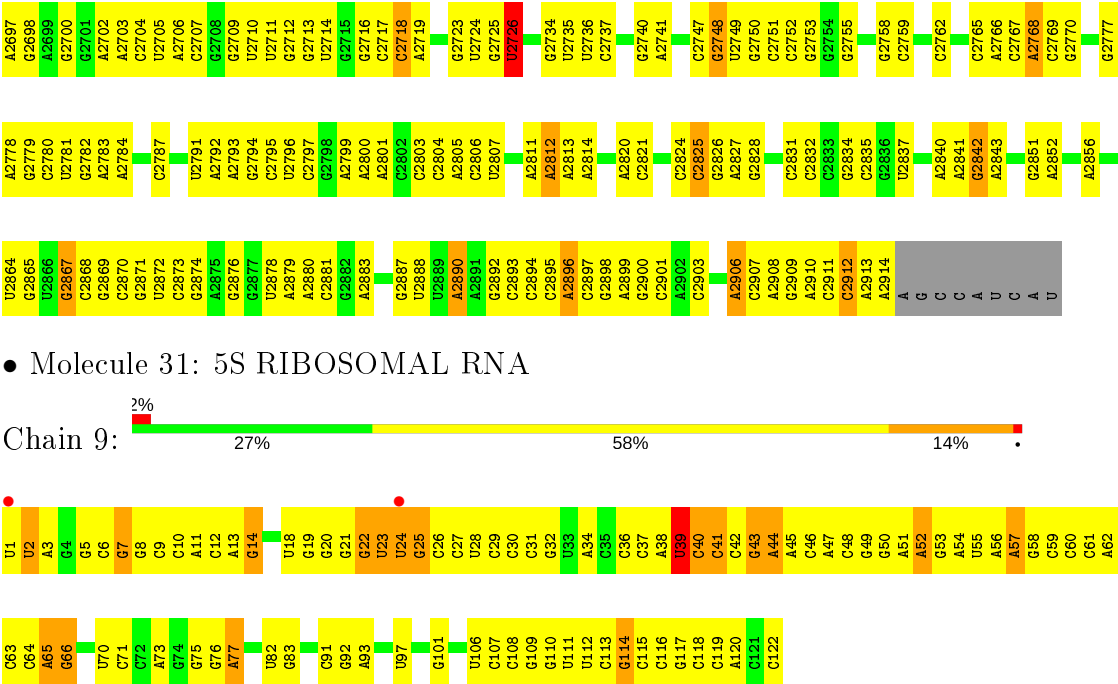


- Molecule 30: 23S RIBOSOMAL RNA



G1398	U1314	G1226	G1162	G1059	A	G902	G814	G717	G644	C558	U392	G315	G246
A1399	G1315	C1229	G1163	C1060	G	U903	U815	C713	U645	U599	G393	A316	A247
U1405	G1317	A1230	G1165	C1061	A	U904	G817	C719	U646	U560	U396	U317	A248
A1406	A1318		A1166	U1066	G	C905	A818	G724	U647	G561	G320	A319	C250
A1407		U1234	G1167	A1067	A	A912	A819	C725		A562	U398	G320	
U1408	A1321	G1235	C1168	U1068	G	G918	G820	C726	G652	G564	C399	G324	C254
G1409	G1322	A1236	U1169	U1069	U	U919	U821	C727	U653	U488		U325	A255
G1410		U1237	U1170	C	C	C920	C822	C728	U654	U567	A407	U326	C256
	G1325	G1238	A1171	G1073	G	G921	U823		U655	G496	A408	U328	G257
	G1326	G1239	G1172	G1074	G	A922	U827	U734	U656	G497	A410	A329	G258
A1413	G1327		A1173	G1075	C	A923	A827	C735	G657	G498	A411	C330	G259
U1419	A1242		A1174	G1076	A	G924	G834	C736	G658	G499	A412		U283
C1420	C1243		G1175		C	G925	U835	A737	A659	G500	C412	U284	G264
C1421	U1244		A1176	A1081	A	A926	G836	C738	A660	G506	G413	U265	U265
C1422	C1245		A1177		C999	U932	U840	G744	G661	U582		G333	
C1423	A1246			G1084	G1000	C933	U841	G745	U662	U584	G416	U335	C271
A1424	C1394	A1247	U1180	A1085	U1003		U842	A746	C663	U585	G417	G336	A272
G1425	C1395	A1248	A1181	A1086	G1004	A939	A844	A747	U664	C586	A418	A337	G273
C1426	U1336	U1249	C1182	A1087	U1005	G940	U845	G748		A587	A419	C338	G274
A1427	G1337		C1183	A1088	A1006	G941	A846	C749	G669	U589	U420	A339	G275
C1428	G1338		U1185	U1089	A1007	U942	C849	U750	A671	A590	C421		C276
U1429	G1339	C1254	U1186	U1090	C1008	U943	U850	U751	G672	A591	U424	C342	
G1430	G1340	A1255	C1187	A1091	A943	A944	C851	C759	G677	G592	C343	C344	C279
	A1341		A1188	A1092	G945	U946	C852	G760	G678	U517	G345		C280
A1434	C1342	G1260	A1189	A1093	U946	U947	C853	A761		G518	U346	U347	U281
U1435	G1343	U1266	G1190	A1094	U947	U948	U854	C762	G681	U595	A347	A348	C282
C1436	C1344	C1267	A1191	A1095	U947	U949	U855	C763	U682	A521	C348		U283
A1345	U1346	G1268	A1192	A1096	U948	U950	G856	C764	A683	C596	A442	U284	C284
C1439	U1347	G1269	A1193	C1015	U949	G951	A857	G765	G684	C597	U445	A352	A285
U1440		U1270	U1109	U1016	G950	A951	U858		G685	G525	G446	C353	U286
G1441	U1350		G1110	U1017	A952	G953		G775	C686	U526	A447		C287
A1442	G1351	C1273	U1197	A1018	G952	G952	A867	A776	G687	U527	G448	U358	A288
	A1352		A1116	C1019	G953	A957	G868	C777	A688	G604	A449	U359	G289
U1446	C1353	A1278	A1117	G1020	A957		G869	U778			C450	C361	C290
U1447		U1279	A1118	G1021		G870	G871	U779	A693	U611	C451	C362	C291
C1451	U1359	A1280	C1201	A1022			U872		A694	U612	A452	C363	C292
G1452	C1360	A1287	A1202	C1025	G960	A961		A790	C695	U613	A453	U371	A293
G1453	C1361	U1287	G1203	U1026	C962	C962		A791	C696	U614	U454	A372	C294
U1454	U1362	G1288	C1204	G1027	C963	C963	A875	G792	C697	U615	U455	G373	C303
C1455	G1363	C1289	U1205	U1028	G964	A965	G876	A793	A698	A536	U456	U374	C302
C1456	G1364		U1130	U1029	A965		G877		C699	G537	A459	G375	G304
U1457	C1365	A1294	G1131	U1029	A965		G878	A797	A700	C538	A460	C376	A305
		G1295	C1208	A1132		G969	C879		U701	C539	C461	C377	A306
U1461	A1372	A1296	C1209	G1039	G969	U970	C880		G702	A540	A462	U378	G307
C1462		G1299	G1210	U1042	G	U	G881	G800	G703	U549	A463	A379	U308
C1469	G1375	G1300	G1213	C1043	U	G	A882	U801	G704	A542	U464	G471	C309
A1470	C1376		G1214	C1044	G	G	U883	G802	C705	G543	A466	A472	G310
C1471	G1377	U1304	A1215	G1045	U	U	G884	C803	G706	G544	G467	G380	C311
C1472	G1378	C1305	G1216	C1051	C	C	G885	G804	C707	G545	U468	A381	U312
C1473	A1379	U1306	G1217	C1052	C	C	U886	A806	A708	C546	G469	G379	G313
C1474	C1384	A1307	U1218	G1053	G	G	A887	A807	G709	U470	A470	A380	U314
		A1308	U1219	G1054	C	C	A888	A808	G710	A549	G471	A381	C311
C1477	A1309	U1220	U1220	G1055	C	U	A889	G809	G711	C550	A472	G381	U310
U1478	C1394	G1221	G1056	G1055	U	U	G890	G810	G711	C553	A473	G382	C311
C1395	G1311	G1311	U1056	U1056	C	C	G891	C811	U	G539	G479	G390	U312
C1396	G1312	G1312	U1057	U1057	C	C	G892	A812	G714	C557	G480	U391	G314
A1482	C1397	A1313	A1058	A1058	G	G	G893	C813	G716				





● Molecule 31: 5S RIBOSOMAL RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.24Å 299.19Å 575.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.95 85.59 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.95) 91.7 (85.59-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.238 0.177 , 0.233	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 79.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99121	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, 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	A	0.34	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.39	0/1885	0.65	0/2552
4	D	0.33	0/1111	0.57	0/1498
5	E	0.34	0/1382	0.56	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.32	0/241	0.47	0/324
8	H	0.33	0/1302	0.62	0/1743
9	I	0.32	0/526	0.54	0/716
10	J	0.39	0/1136	0.61	0/1530
11	K	0.37	0/1004	0.66	0/1351
12	L	0.34	0/1130	0.61	0/1509
13	M	0.40	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.61	0/1999
15	O	0.37	0/874	0.62	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.64	0/1005
18	R	1.27	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.36	0/648	0.59	0/875
20	T	0.34	0/958	0.66	0/1289
21	U	0.45	0/417	0.60	0/562
22	V	0.34	0/502	0.53	0/675
23	W	0.38	0/1219	0.65	0/1655
24	X	0.36	0/664	0.61	0/895
25	Y	0.38	0/1146	0.62	0/1536
26	Z	0.43	0/584	0.63	0/781
27	1	0.47	0/438	0.64	0/578
28	2	0.36	0/401	0.61	0/529
29	3	0.46	0/771	0.60	0/1024
30	0	0.42	0/65956	0.68	7/102865 (0.0%)
31	9	0.32	0/2904	0.67	1/4526 (0.0%)
All	All	0.42	7/98700 (0.0%)	0.67	14/147584 (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
18	R	1	0
23	W	0	1
30	0	0	34
All	All	1	35

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.15	2.85	1.50
18	R	150	PRO	CA-C	-18.51	1.15	1.52
18	R	150	PRO	CG-CD	13.84	1.96	1.50
18	R	150	PRO	C-O	11.87	1.47	1.23
18	R	150	PRO	N-CA	11.57	1.67	1.47

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.43	55.92	112.00
18	R	150	PRO	N-CA-C	-19.45	61.53	112.10
18	R	150	PRO	CA-N-CD	12.27	128.88	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.27	100.34	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	196	G	Sidechain
30	0	221	G	Sidechain
30	0	324	G	Sidechain
30	0	333	G	Sidechain
23	W	90	TYR	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	A	1753	0	1766	85	0
2	B	2625	0	2533	108	0
3	C	1860	0	1813	63	0
4	D	1094	0	1085	37	0
5	E	1357	0	1266	39	0
6	F	890	0	843	19	0
7	G	240	0	231	8	0
8	H	1282	0	1292	33	0
9	I	519	0	500	14	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	34	0
12	L	1118	0	1076	38	0
13	M	1558	0	1573	95	0
14	N	1445	0	1401	73	0
15	O	865	0	873	22	0
16	P	1136	0	1123	34	0
17	Q	735	0	729	28	0
18	R	1149	0	1122	41	0
19	S	641	0	605	15	0
20	T	950	0	924	36	0
21	U	410	0	368	26	0
22	V	499	0	511	21	0
23	W	1196	0	1137	58	0
24	X	654	0	653	20	0
25	Y	1130	0	1133	39	0
26	Z	573	0	535	50	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	732	57	0
30	0	59019	0	29809	1661	0
31	9	2599	0	1325	127	0
32	0	86	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	10	0	0	3	0
33	3	1	0	0	1	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	2	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	2	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	L	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	65	0	0	0	0
35	9	2	0	0	0	0
35	B	1	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
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	0	1	0	0	0	0
36	M	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5904	0	0	251	0
38	1	59	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	43	0	0	2	0
38	3	70	0	0	3	0
38	9	149	0	0	10	0
38	A	119	0	0	7	0
38	B	152	0	0	16	0
38	C	185	0	0	18	0
38	D	42	0	0	4	0
38	E	43	0	0	1	0
38	F	26	0	0	1	0
38	G	19	0	0	1	0
38	H	65	0	0	4	0
38	I	8	0	0	1	0
38	J	53	0	0	1	0
38	K	58	0	0	3	0
38	L	85	0	0	9	0
38	M	127	0	0	13	0
38	N	59	0	0	2	0
38	O	39	0	0	2	0
38	P	67	0	0	3	0
38	Q	48	0	0	1	0
38	R	77	0	0	2	0
38	S	30	0	0	2	0
38	T	36	0	0	3	0
38	U	28	0	0	4	0
38	V	13	0	0	2	0
38	W	67	0	0	3	0
38	X	21	0	0	2	0
38	Y	100	0	0	5	0
38	Z	31	0	0	7	0
All	All	99121	0	59922	2675	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 18.

The worst 5 of 2675 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)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.41
30:0:871:G:C8	30:0:871:G:H5'	1.77	1.19
10:J:82:THR:HG23	30:0:1242:A:H5'	1.23	1.16
30:0:1165:G:H1'	30:0:1174:A:H1'	1.17	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.19	1.13

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	
1	A	235/240 (98%)	202 (86%)	27 (12%)	6 (3%)	5	24
2	B	335/338 (99%)	309 (92%)	17 (5%)	9 (3%)	5	23
3	C	244/246 (99%)	222 (91%)	20 (8%)	2 (1%)	19	53
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	4	20
5	E	170/178 (96%)	157 (92%)	12 (7%)	1 (1%)	25	60
6	F	117/120 (98%)	106 (91%)	7 (6%)	4 (3%)	3	17
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	12	41
9	I	68/162 (42%)	52 (76%)	12 (18%)	4 (6%)	1	7
10	J	140/145 (97%)	131 (94%)	8 (6%)	1 (1%)	22	56
11	K	130/132 (98%)	121 (93%)	8 (6%)	1 (1%)	19	53
12	L	141/165 (86%)	120 (85%)	21 (15%)	0	100	100
13	M	192/196 (98%)	179 (93%)	9 (5%)	4 (2%)	7	29
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	6	28
15	O	113/116 (97%)	107 (95%)	6 (5%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	85 (91%)	7 (8%)	1 (1%)	14	46
18	R	148/155 (96%)	140 (95%)	7 (5%)	1 (1%)	22	56
19	S	79/85 (93%)	74 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	117/120 (98%)	107 (92%)	8 (7%)	2 (2%)	9	34
21	U	51/67 (76%)	42 (82%)	8 (16%)	1 (2%)	7	30
22	V	63/71 (89%)	58 (92%)	5 (8%)	0	100	100
23	W	152/154 (99%)	140 (92%)	10 (7%)	2 (1%)	12	41
24	X	80/92 (87%)	74 (92%)	4 (5%)	2 (2%)	5	25
25	Y	140/241 (58%)	137 (98%)	3 (2%)	0	100	100
26	Z	71/116 (61%)	58 (82%)	8 (11%)	5 (7%)	1	4
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	39 (93%)	2 (5%)	1 (2%)	6	26
29	3	90/92 (98%)	74 (82%)	13 (14%)	3 (3%)	4	18
All	All	3705/4472 (83%)	3359 (91%)	286 (8%)	60 (2%)	9	36

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	ASP
1	A	37	VAL
1	A	74	VAL
4	D	65	GLU
4	D	137	PRO

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	
1	A	179/182 (98%)	171 (96%)	8 (4%)	27	61
2	B	282/283 (100%)	264 (94%)	18 (6%)	17	47
3	C	193/193 (100%)	182 (94%)	11 (6%)	20	52
4	D	117/148 (79%)	110 (94%)	7 (6%)	19	50
5	E	152/156 (97%)	148 (97%)	4 (3%)	46	75
6	F	93/94 (99%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	66
8	H	134/145 (92%)	126 (94%)	8 (6%)	19	50
9	I	58/130 (45%)	56 (97%)	2 (3%)	37	69
10	J	118/121 (98%)	113 (96%)	5 (4%)	30	63
11	K	106/106 (100%)	104 (98%)	2 (2%)	57	81
12	L	113/127 (89%)	108 (96%)	5 (4%)	28	62
13	M	158/160 (99%)	148 (94%)	10 (6%)	18	48
14	N	149/150 (99%)	144 (97%)	5 (3%)	37	69
15	O	93/94 (99%)	92 (99%)	1 (1%)	73	89
16	P	113/117 (97%)	107 (95%)	6 (5%)	22	55
17	Q	79/80 (99%)	78 (99%)	1 (1%)	69	87
18	R	117/122 (96%)	114 (97%)	3 (3%)	46	75
19	S	71/74 (96%)	70 (99%)	1 (1%)	67	86
20	T	105/106 (99%)	99 (94%)	6 (6%)	20	52
21	U	44/53 (83%)	41 (93%)	3 (7%)	16	45
22	V	51/57 (90%)	49 (96%)	2 (4%)	32	65
23	W	130/130 (100%)	124 (95%)	6 (5%)	27	60
24	X	66/74 (89%)	61 (92%)	5 (8%)	13	39
25	Y	120/196 (61%)	115 (96%)	5 (4%)	30	63
26	Z	60/94 (64%)	57 (95%)	3 (5%)	24	57
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	77
29	3	79/79 (100%)	76 (96%)	3 (4%)	33	66
All	All	3095/3646 (85%)	2963 (96%)	132 (4%)	29	62

5 of 132 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	46	ILE
13	M	68	ARG
25	Y	189	ASN
10	J	74	ARG
12	L	99	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 80 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	93	GLN
17	Q	16	ASN
27	1	28	HIS
14	N	107	ASN
16	P	66	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	250 (9%)	21 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	269 (9%)	23 (0%)

5 of 269 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1474	C
31	9	43	G
30	0	1377	C
30	0	1506	U

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
30	PSU	0	2621	30	17,21,22	1.66	3 (17%)	20,30,33	5.46	4 (20%)
30	OMG	0	2588	30	18,26,27	1.03	2 (11%)	20,38,41	2.62	4 (20%)
30	1MA	0	628	30,35	15,25,26	0.77	0	15,37,40	1.42	1 (6%)
30	UR3	0	2619	30	14,22,23	0.76	0	15,32,35	0.55	0
30	OMU	0	2587	30	14,22,23	0.99	1 (7%)	14,31,34	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
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/7/27/28	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.31	1.47	1.52
30	0	2588	OMG	C6-N1	3.28	1.38	1.33
30	0	2621	PSU	C4-N3	2.70	1.37	1.33
30	0	2587	OMU	C4-N3	2.45	1.37	1.33
30	0	2621	PSU	C2-N1	2.35	1.42	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.30	114.68	128.43
30	0	2621	PSU	C4-N3-C2	14.37	127.28	115.14
30	0	2588	OMG	C5-C6-N1	-8.66	111.59	123.43
30	0	2621	PSU	C5-C4-N3	-8.19	114.81	125.36
30	0	2588	OMG	C6-N1-C2	5.90	125.31	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2621	PSU	1	0
30	0	2588	OMG	1	0
30	0	2587	OMU	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 305 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	237/240 (98%)	-0.14	8 (3%) 45 29	36, 71, 108, 128	0
2	B	337/338 (99%)	-0.45	0 100 100	38, 67, 98, 112	0
3	C	246/246 (100%)	-0.38	0 100 100	32, 56, 80, 91	0
4	D	140/177 (79%)	1.53	52 (37%) 0 0	89, 121, 144, 151	0
5	E	172/178 (96%)	-0.07	4 (2%) 60 43	57, 83, 104, 113	0
6	F	119/120 (99%)	0.50	15 (12%) 3 2	64, 88, 121, 131	0
7	G	29/348 (8%)	1.11	4 (13%) 2 1	92, 107, 116, 118	0
8	H	160/177 (90%)	0.89	31 (19%) 1 0	65, 89, 118, 127	0
9	I	70/162 (43%)	3.64	50 (71%) 0 0	145, 162, 177, 179	0
10	J	142/145 (97%)	-0.38	1 (0%) 87 76	47, 63, 86, 105	0
11	K	132/132 (100%)	-0.38	0 100 100	45, 63, 91, 100	0
12	L	145/165 (87%)	0.55	21 (14%) 2 1	41, 88, 131, 140	0
13	M	194/196 (98%)	0.25	20 (10%) 6 4	37, 53, 115, 122	0
14	N	186/187 (99%)	0.65	26 (13%) 2 1	70, 90, 134, 139	0
15	O	115/116 (99%)	-0.37	0 100 100	46, 64, 81, 87	0
16	P	143/149 (95%)	-0.30	0 100 100	48, 67, 85, 96	0
17	Q	95/96 (98%)	-0.17	1 (1%) 80 65	57, 69, 89, 97	0
18	R	150/155 (96%)	-0.50	0 100 100	39, 56, 79, 95	0
19	S	81/85 (95%)	-0.28	2 (2%) 57 40	52, 70, 89, 104	0
20	T	119/120 (99%)	-0.03	5 (4%) 36 23	48, 67, 95, 125	0
21	U	53/67 (79%)	4.50	50 (94%) 0 0	112, 125, 131, 134	0
22	V	65/71 (91%)	0.92	12 (18%) 1 0	51, 83, 131, 135	0
23	W	154/154 (100%)	-0.34	1 (0%) 89 78	45, 62, 79, 92	0
24	X	82/92 (89%)	0.03	4 (4%) 29 18	54, 72, 95, 109	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.60	0 100 100	30, 53, 78, 97	0
26	Z	73/116 (62%)	7.40	59 (80%) 0 0	111, 130, 139, 142	0
27	1	56/57 (98%)	-0.51	0 100 100	30, 39, 47, 65	0
28	2	46/50 (92%)	-0.22	3 (6%) 18 11	39, 72, 104, 110	0
29	3	92/92 (100%)	8.50	91 (98%) 0 0	123, 135, 142, 148	0
30	0	2749/2923 (94%)	-0.63	10 (0%) 92 84	25, 58, 106, 183	0
31	9	122/122 (100%)	-0.81	2 (1%) 72 55	51, 90, 111, 159	0
All	All	6646/7517 (88%)	-0.00	472 (7%) 16 9	25, 66, 129, 183	0

The worst 5 of 472 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	58	ASN	25.7
29	3	39	GLN	21.9
29	3	41	GLU	19.7
29	3	47	GLY	18.8
29	3	35	TRP	18.8

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
30	PSU	0	2621	20/21	0.98	0.18	39,41,53,53	0
30	OMG	0	2588	24/25	0.98	0.12	41,43,46,50	0
30	1MA	0	628	23/24	0.98	0.14	38,44,47,47	0
30	UR3	0	2619	21/22	0.98	0.13	47,49,51,54	0
30	OMU	0	2587	21/22	0.98	0.11	43,47,50,51	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
33	CL	3	8804	1/1	0.25	0.20	128,128,128,128	0
35	NA	0	8528	1/1	0.51	0.67	76,76,76,76	0
34	SR	0	8979	1/1	0.53	0.19	196,196,196,196	0
34	SR	0	9006	1/1	0.57	0.98	200,200,200,200	0
35	NA	J	8538	1/1	0.58	0.15	78,78,78,78	0
35	NA	0	8563	1/1	0.59	0.12	117,117,117,117	0
32	MG	0	8040	1/1	0.59	0.39	86,86,86,86	0
34	SR	0	8988	1/1	0.61	0.08	173,173,173,173	0
35	NA	0	8570	1/1	0.66	0.09	61,61,61,61	0
35	NA	0	8511	1/1	0.67	0.08	81,81,81,81	0
34	SR	0	8991	1/1	0.67	0.08	180,180,180,180	0
34	SR	0	8982	1/1	0.68	1.93	200,200,200,200	0
34	SR	0	9004	1/1	0.71	0.84	200,200,200,200	0
35	NA	0	8506	1/1	0.72	0.20	83,83,83,83	0
34	SR	0	9001	1/1	0.75	0.13	177,177,177,177	0
32	MG	A	8051	1/1	0.76	0.25	94,94,94,94	0
35	NA	0	8525	1/1	0.77	0.16	75,75,75,75	0
37	CD	Z	8703	1/1	0.78	0.46	200,200,200,200	0
35	NA	B	8552	1/1	0.78	0.28	89,89,89,89	0
37	CD	3	8704	1/1	0.78	0.66	200,200,200,200	0
34	SR	0	8977	1/1	0.80	0.07	200,200,200,200	0
32	MG	0	8089	1/1	0.80	0.25	65,65,65,65	0
34	SR	0	8959	1/1	0.80	0.27	200,200,200,200	0
34	SR	0	9007	1/1	0.80	1.77	200,200,200,200	0
34	SR	0	8938	1/1	0.80	0.08	183,183,183,183	0
34	SR	0	9002	1/1	0.82	0.12	193,193,193,193	0
35	NA	0	8562	1/1	0.83	0.97	82,82,82,82	0
35	NA	0	8535	1/1	0.83	0.29	67,67,67,67	0
34	SR	3	8999	1/1	0.84	0.28	187,187,187,187	0
35	NA	0	8509	1/1	0.84	0.13	69,69,69,69	0
34	SR	0	8962	1/1	0.84	0.09	172,172,172,172	0
32	MG	0	8071	1/1	0.84	0.12	60,60,60,60	0
33	CL	J	8801	1/1	0.84	0.12	95,95,95,95	0
34	SR	0	8992	1/1	0.84	0.23	159,159,159,159	0
35	NA	0	8502	1/1	0.85	0.12	69,69,69,69	0
35	NA	H	8518	1/1	0.85	0.42	91,91,91,91	0
32	MG	0	8075	1/1	0.85	0.05	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8951	1/1	0.85	0.10	155,155,155,155	0
34	SR	0	8928	1/1	0.86	0.04	137,137,137,137	0
35	NA	Q	8540	1/1	0.86	0.11	79,79,79,79	0
32	MG	0	8081	1/1	0.86	0.17	88,88,88,88	0
34	SR	0	8985	1/1	0.86	0.06	164,164,164,164	0
34	SR	0	8957	1/1	0.86	0.34	200,200,200,200	0
34	SR	0	8953	1/1	0.86	0.55	200,200,200,200	0
34	SR	0	8994	1/1	0.86	0.48	200,200,200,200	0
35	NA	0	8555	1/1	0.87	0.42	52,52,52,52	0
34	SR	9	8980	1/1	0.87	0.15	183,183,183,183	0
35	NA	0	8560	1/1	0.87	0.56	118,118,118,118	0
34	SR	0	8919	1/1	0.87	0.09	168,168,168,168	0
35	NA	0	8548	1/1	0.88	0.12	56,56,56,56	0
34	SR	0	8989	1/1	0.88	0.20	178,178,178,178	0
35	NA	0	8545	1/1	0.88	0.80	58,58,58,58	0
34	SR	0	8993	1/1	0.89	0.08	167,167,167,167	0
32	MG	0	8056	1/1	0.89	0.06	57,57,57,57	0
34	SR	9	9003	1/1	0.89	0.10	187,187,187,187	0
32	MG	0	8067	1/1	0.89	0.11	35,35,35,35	0
35	NA	0	8508	1/1	0.89	0.47	52,52,52,52	0
32	MG	9	8074	1/1	0.89	0.07	87,87,87,87	0
35	NA	0	8536	1/1	0.90	0.17	64,64,64,64	0
34	SR	0	8976	1/1	0.90	0.29	193,193,193,193	0
35	NA	0	8544	1/1	0.90	0.19	79,79,79,79	0
32	MG	0	8080	1/1	0.90	0.75	83,83,83,83	0
35	NA	0	8551	1/1	0.90	0.46	63,63,63,63	0
32	MG	0	8030	1/1	0.90	0.47	90,90,90,90	0
34	SR	0	8944	1/1	0.90	0.07	172,172,172,172	0
34	SR	3	8932	1/1	0.90	0.23	178,178,178,178	0
34	SR	0	8975	1/1	0.90	0.14	149,149,149,149	0
34	SR	0	8954	1/1	0.91	0.12	108,108,108,108	0
35	NA	0	8565	1/1	0.91	1.10	78,78,78,78	0
34	SR	0	8983	1/1	0.91	0.33	197,197,197,197	0
35	NA	9	8543	1/1	0.91	0.21	61,61,61,61	0
36	K	0	8401	1/1	0.91	0.63	139,139,139,139	0
34	SR	0	8946	1/1	0.91	0.20	137,137,137,137	0
35	NA	0	8522	1/1	0.91	0.14	82,82,82,82	0
35	NA	0	8566	1/1	0.92	0.30	63,63,63,63	0
34	SR	0	8971	1/1	0.92	0.06	192,192,192,192	0
33	CL	O	8808	1/1	0.92	0.17	86,86,86,86	0
34	SR	0	8996	1/1	0.92	0.52	200,200,200,200	0
34	SR	H	8972	1/1	0.92	0.10	164,164,164,164	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8031	1/1	0.92	0.39	83,83,83,83	0
34	SR	L	8969	1/1	0.92	0.29	200,200,200,200	0
36	K	M	8402	1/1	0.92	0.19	87,87,87,87	0
33	CL	0	8805	1/1	0.92	0.17	98,98,98,98	0
35	NA	S	8510	1/1	0.93	0.03	44,44,44,44	0
35	NA	0	8567	1/1	0.93	0.25	78,78,78,78	0
35	NA	0	8547	1/1	0.93	0.99	67,67,67,67	0
34	SR	9	8978	1/1	0.93	0.06	157,157,157,157	0
32	MG	0	8053	1/1	0.93	0.05	63,63,63,63	0
35	NA	0	8526	1/1	0.93	0.15	46,46,46,46	0
33	CL	B	8819	1/1	0.93	0.22	69,69,69,69	0
32	MG	0	8059	1/1	0.93	0.09	51,51,51,51	0
33	CL	0	8815	1/1	0.93	0.22	89,89,89,89	0
35	NA	0	8530	1/1	0.93	0.44	74,74,74,74	0
34	SR	0	8915	1/1	0.93	0.08	126,126,126,126	0
35	NA	0	8542	1/1	0.93	0.53	58,58,58,58	0
34	SR	A	8930	1/1	0.93	0.15	142,142,142,142	0
32	MG	0	8063	1/1	0.93	0.30	116,116,116,116	0
35	NA	0	8553	1/1	0.93	0.28	89,89,89,89	0
35	NA	0	8521	1/1	0.93	0.45	64,64,64,64	0
34	SR	B	8987	1/1	0.93	0.62	200,200,200,200	0
34	SR	0	8997	1/1	0.93	0.15	189,189,189,189	0
33	CL	J	8802	1/1	0.93	0.06	67,67,67,67	0
32	MG	0	8061	1/1	0.93	0.17	36,36,36,36	0
33	CL	N	8807	1/1	0.94	0.22	87,87,87,87	0
35	NA	0	8558	1/1	0.94	0.20	58,58,58,58	0
34	SR	0	8968	1/1	0.94	0.06	177,177,177,177	0
34	SR	0	8922	1/1	0.94	0.17	168,168,168,168	0
34	SR	0	8939	1/1	0.94	0.04	144,144,144,144	0
35	NA	0	8550	1/1	0.94	0.26	71,71,71,71	0
32	MG	0	8066	1/1	0.94	0.18	69,69,69,69	0
35	NA	0	8568	1/1	0.94	0.33	54,54,54,54	0
35	NA	0	8546	1/1	0.94	0.74	94,94,94,94	0
32	MG	0	8055	1/1	0.94	0.06	62,62,62,62	0
35	NA	0	8557	1/1	0.94	0.06	65,65,65,65	0
34	SR	0	8917	1/1	0.94	0.16	114,114,114,114	0
32	MG	0	8019	1/1	0.94	0.19	29,29,29,29	0
35	NA	0	8569	1/1	0.94	0.18	50,50,50,50	0
35	NA	0	8573	1/1	0.94	0.13	73,73,73,73	0
32	MG	0	8044	1/1	0.94	0.05	58,58,58,58	0
32	MG	0	8082	1/1	0.94	0.23	76,76,76,76	0
32	MG	A	8050	1/1	0.94	0.05	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8527	1/1	0.94	0.28	72,72,72,72	0
32	MG	0	8028	1/1	0.94	0.17	34,34,34,34	0
32	MG	0	8006	1/1	0.94	0.12	44,44,44,44	0
35	NA	0	8571	1/1	0.94	0.12	79,79,79,79	0
35	NA	0	8564	1/1	0.95	0.43	69,69,69,69	0
35	NA	9	8572	1/1	0.95	0.27	88,88,88,88	0
32	MG	0	8060	1/1	0.95	0.06	53,53,53,53	0
32	MG	0	8091	1/1	0.95	0.11	56,56,56,56	0
34	SR	0	8947	1/1	0.95	0.26	200,200,200,200	0
32	MG	0	8092	1/1	0.95	0.08	76,76,76,76	0
35	NA	0	8519	1/1	0.95	0.15	52,52,52,52	0
34	SR	0	8920	1/1	0.95	0.05	127,127,127,127	0
32	MG	0	8090	1/1	0.95	0.17	97,97,97,97	0
34	SR	0	8965	1/1	0.95	0.06	134,134,134,134	0
32	MG	0	8036	1/1	0.95	0.10	48,48,48,48	0
35	NA	C	8503	1/1	0.95	0.17	46,46,46,46	0
34	SR	A	8929	1/1	0.95	0.11	139,139,139,139	0
35	NA	0	8533	1/1	0.95	0.09	70,70,70,70	0
34	SR	0	8963	1/1	0.95	0.06	133,133,133,133	0
35	NA	0	8537	1/1	0.95	0.15	50,50,50,50	0
37	CD	U	8701	1/1	0.95	0.45	200,200,200,200	0
33	CL	Y	8820	1/1	0.95	0.07	52,52,52,52	0
32	MG	Y	8086	1/1	0.95	0.07	50,50,50,50	0
34	SR	S	8961	1/1	0.95	0.09	128,128,128,128	0
34	SR	0	8943	1/1	0.95	0.13	84,84,84,84	0
34	SR	0	8956	1/1	0.95	0.12	169,169,169,169	0
32	MG	0	8026	1/1	0.95	0.08	50,50,50,50	0
35	NA	0	8574	1/1	0.95	0.58	60,60,60,60	0
34	SR	0	9000	1/1	0.95	0.07	183,183,183,183	0
32	MG	0	8083	1/1	0.95	0.10	55,55,55,55	0
32	MG	0	8020	1/1	0.95	0.16	41,41,41,41	0
32	MG	0	8021	1/1	0.95	0.09	33,33,33,33	0
34	SR	0	8966	1/1	0.96	0.09	105,105,105,105	0
33	CL	J	8821	1/1	0.96	0.10	77,77,77,77	0
33	CL	L	8810	1/1	0.96	0.05	64,64,64,64	0
34	SR	0	8937	1/1	0.96	0.15	113,113,113,113	0
35	NA	0	8514	1/1	0.96	0.29	55,55,55,55	0
35	NA	0	8529	1/1	0.96	0.11	48,48,48,48	0
34	SR	B	8950	1/1	0.96	0.16	130,130,130,130	0
32	MG	0	8010	1/1	0.96	0.13	72,72,72,72	0
33	CL	0	8816	1/1	0.96	0.43	85,85,85,85	0
32	MG	0	8068	1/1	0.96	0.09	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8513	1/1	0.96	0.41	68,68,68,68	0
35	NA	0	8561	1/1	0.96	0.31	65,65,65,65	0
32	MG	0	8085	1/1	0.96	0.17	76,76,76,76	0
35	NA	0	8515	1/1	0.96	0.15	32,32,32,32	0
32	MG	0	8064	1/1	0.96	0.18	45,45,45,45	0
34	SR	0	8967	1/1	0.96	0.04	131,131,131,131	0
32	MG	0	8087	1/1	0.96	0.09	38,38,38,38	0
34	SR	0	8908	1/1	0.96	0.11	85,85,85,85	0
34	SR	0	8960	1/1	0.96	0.02	151,151,151,151	0
34	SR	0	8941	1/1	0.96	0.11	114,114,114,114	0
34	SR	0	8955	1/1	0.96	0.07	200,200,200,200	0
34	SR	0	8970	1/1	0.96	0.05	125,125,125,125	0
32	MG	0	8033	1/1	0.96	0.06	63,63,63,63	0
32	MG	0	8039	1/1	0.96	0.19	84,84,84,84	0
34	SR	0	8927	1/1	0.96	0.06	181,181,181,181	0
32	MG	0	8052	1/1	0.96	0.09	44,44,44,44	0
34	SR	0	8933	1/1	0.96	0.04	135,135,135,135	0
32	MG	0	8073	1/1	0.96	0.07	72,72,72,72	0
35	NA	0	8517	1/1	0.96	0.09	38,38,38,38	0
32	MG	0	8093	1/1	0.96	0.06	36,36,36,36	0
35	NA	0	8520	1/1	0.97	0.10	56,56,56,56	0
32	MG	0	8058	1/1	0.97	0.06	18,18,18,18	0
32	MG	0	8047	1/1	0.97	0.31	66,66,66,66	0
32	MG	0	8077	1/1	0.97	0.08	48,48,48,48	0
34	SR	0	8931	1/1	0.97	0.09	111,111,111,111	0
32	MG	B	8042	1/1	0.97	0.07	69,69,69,69	0
32	MG	0	8003	1/1	0.97	0.17	38,38,38,38	0
34	SR	0	8958	1/1	0.97	0.07	116,116,116,116	0
32	MG	0	8002	1/1	0.97	0.10	40,40,40,40	0
33	CL	0	8822	1/1	0.97	0.42	88,88,88,88	0
32	MG	0	8062	1/1	0.97	0.17	56,56,56,56	0
34	SR	0	8942	1/1	0.97	0.09	124,124,124,124	0
32	MG	0	8065	1/1	0.97	0.06	42,42,42,42	0
35	NA	0	8554	1/1	0.97	0.86	69,69,69,69	0
34	SR	0	8974	1/1	0.97	0.06	166,166,166,166	0
33	CL	0	8814	1/1	0.97	0.16	79,79,79,79	0
34	SR	0	8984	1/1	0.97	0.09	119,119,119,119	0
32	MG	0	8041	1/1	0.97	0.16	36,36,36,36	0
32	MG	0	8079	1/1	0.97	0.20	66,66,66,66	0
32	MG	0	8045	1/1	0.97	0.10	31,31,31,31	0
35	NA	0	8524	1/1	0.97	0.69	73,73,73,73	0
35	NA	M	8539	1/1	0.97	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8914	1/1	0.98	0.27	133,133,133,133	0
32	MG	0	8038	1/1	0.98	0.08	74,74,74,74	0
32	MG	0	8025	1/1	0.98	0.10	37,37,37,37	0
32	MG	0	8076	1/1	0.98	0.06	40,40,40,40	0
32	MG	0	8069	1/1	0.98	0.10	102,102,102,102	0
35	NA	0	8541	1/1	0.98	0.23	64,64,64,64	0
34	SR	0	8949	1/1	0.98	0.15	117,117,117,117	0
34	SR	0	9008	1/1	0.98	0.14	92,92,92,92	0
35	NA	0	8559	1/1	0.98	0.17	77,77,77,77	0
32	MG	0	8043	1/1	0.98	0.13	52,52,52,52	0
35	NA	0	8549	1/1	0.98	0.85	56,56,56,56	0
34	SR	R	8912	1/1	0.98	0.19	95,95,95,95	0
32	MG	T	8057	1/1	0.98	0.07	65,65,65,65	0
35	NA	0	8534	1/1	0.98	0.13	50,50,50,50	0
32	MG	0	8024	1/1	0.98	0.16	62,62,62,62	0
34	SR	0	8973	1/1	0.98	0.16	146,146,146,146	0
32	MG	0	8072	1/1	0.98	0.06	59,59,59,59	0
34	SR	0	8926	1/1	0.98	0.14	122,122,122,122	0
33	CL	0	8803	1/1	0.98	0.09	60,60,60,60	0
34	SR	F	9005	1/1	0.98	0.07	147,147,147,147	0
33	CL	0	8817	1/1	0.98	0.14	72,72,72,72	0
32	MG	0	8032	1/1	0.98	0.04	52,52,52,52	0
34	SR	0	8945	1/1	0.98	0.09	105,105,105,105	0
32	MG	0	8001	1/1	0.98	0.11	36,36,36,36	0
32	MG	0	8027	1/1	0.98	0.12	47,47,47,47	0
35	NA	0	8505	1/1	0.98	0.66	53,53,53,53	0
32	MG	0	8005	1/1	0.98	0.21	42,42,42,42	0
33	CL	0	8812	1/1	0.98	0.05	61,61,61,61	0
34	SR	0	8986	1/1	0.98	1.04	200,200,200,200	0
32	MG	0	8012	1/1	0.98	0.16	25,25,25,25	0
34	SR	0	8910	1/1	0.98	0.09	108,108,108,108	0
34	SR	0	8995	1/1	0.98	0.19	150,150,150,150	0
34	SR	0	8911	1/1	0.98	0.13	88,88,88,88	0
32	MG	0	8035	1/1	0.98	0.10	66,66,66,66	0
32	MG	0	8078	1/1	0.98	0.26	65,65,65,65	0
35	NA	0	8523	1/1	0.98	0.14	54,54,54,54	0
35	NA	0	8512	1/1	0.98	0.15	56,56,56,56	0
34	SR	0	8901	1/1	0.99	0.18	66,66,66,66	0
34	SR	0	8990	1/1	0.99	0.14	137,137,137,137	0
34	SR	0	8935	1/1	0.99	0.11	103,103,103,103	0
37	CD	O	8705	1/1	0.99	0.08	100,100,100,100	0
34	SR	0	8934	1/1	0.99	0.13	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8023	1/1	0.99	0.17	28,28,28,28	0
33	CL	A	8809	1/1	0.99	0.15	104,104,104,104	0
34	SR	0	8998	1/1	0.99	0.18	178,178,178,178	0
34	SR	0	8948	1/1	0.99	0.10	115,115,115,115	0
34	SR	0	8905	1/1	0.99	0.25	72,72,72,72	0
33	CL	0	8811	1/1	0.99	0.20	81,81,81,81	0
32	MG	0	8070	1/1	0.99	0.17	66,66,66,66	0
34	SR	0	8936	1/1	0.99	0.11	95,95,95,95	0
32	MG	0	8088	1/1	0.99	0.10	35,35,35,35	0
35	NA	0	8531	1/1	0.99	0.06	39,39,39,39	0
32	MG	0	8009	1/1	0.99	0.24	34,34,34,34	0
32	MG	0	8013	1/1	0.99	0.06	28,28,28,28	0
35	NA	0	8556	1/1	0.99	0.80	71,71,71,71	0
34	SR	0	8981	1/1	0.99	0.13	161,161,161,161	0
32	MG	0	8007	1/1	0.99	0.18	36,36,36,36	0
32	MG	0	8022	1/1	0.99	0.20	33,33,33,33	0
34	SR	0	8924	1/1	0.99	0.20	124,124,124,124	0
32	MG	0	8046	1/1	0.99	0.10	45,45,45,45	0
34	SR	0	8918	1/1	0.99	0.12	85,85,85,85	0
34	SR	0	8916	1/1	0.99	0.05	105,105,105,105	0
32	MG	0	8018	1/1	0.99	0.24	33,33,33,33	0
32	MG	0	8048	1/1	0.99	0.24	29,29,29,29	0
32	MG	0	8008	1/1	0.99	0.13	31,31,31,31	0
32	MG	0	8014	1/1	0.99	0.17	37,37,37,37	0
33	CL	M	8818	1/1	0.99	0.05	49,49,49,49	0
33	CL	0	8813	1/1	0.99	0.07	60,60,60,60	0
35	NA	0	8516	1/1	0.99	0.19	39,39,39,39	0
32	MG	0	8037	1/1	0.99	0.21	77,77,77,77	0
32	MG	0	8017	1/1	0.99	0.17	40,40,40,40	0
32	MG	0	8049	1/1	0.99	0.23	64,64,64,64	0
32	MG	K	8054	1/1	0.99	0.17	57,57,57,57	0
33	CL	R	8806	1/1	0.99	0.14	58,58,58,58	0
32	MG	0	8016	1/1	0.99	0.17	40,40,40,40	0
35	NA	R	8532	1/1	0.99	0.11	50,50,50,50	0
34	SR	0	8907	1/1	0.99	0.13	63,63,63,63	0
34	SR	0	8925	1/1	0.99	0.13	98,98,98,98	0
34	SR	0	8940	1/1	0.99	0.09	93,93,93,93	0
32	MG	0	8004	1/1	0.99	0.12	29,29,29,29	0
34	SR	1	8913	1/1	0.99	0.06	95,95,95,95	0
32	MG	0	8011	1/1	0.99	0.22	25,25,25,25	0
35	NA	0	8575	1/1	0.99	0.23	103,103,103,103	0
35	NA	0	8507	1/1	0.99	0.24	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8084	1/1	0.99	0.14	35,35,35,35	0
34	SR	0	8902	1/1	0.99	0.15	68,68,68,68	0
34	SR	0	8964	1/1	0.99	0.12	134,134,134,134	0
34	SR	0	8921	1/1	0.99	0.13	83,83,83,83	0
35	NA	0	8501	1/1	0.99	0.16	39,39,39,39	0
34	SR	0	8906	1/1	1.00	0.21	67,67,67,67	0
35	NA	0	8504	1/1	1.00	0.12	40,40,40,40	0
37	CD	1	8702	1/1	1.00	0.10	61,61,61,61	0
32	MG	0	8029	1/1	1.00	0.13	59,59,59,59	0
34	SR	0	8904	1/1	1.00	0.20	57,57,57,57	0
34	SR	1	8952	1/1	1.00	0.15	90,90,90,90	0
34	SR	0	8909	1/1	1.00	0.14	93,93,93,93	0
34	SR	0	8923	1/1	1.00	0.13	109,109,109,109	0
32	MG	0	8034	1/1	1.00	0.07	50,50,50,50	0
32	MG	0	8015	1/1	1.00	0.13	45,45,45,45	0
34	SR	0	8903	1/1	1.00	0.19	57,57,57,57	0

6.5 Other polymers

There are no such residues in this entry.