



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 12:15 pm BST

PDB ID : 3CCR
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488C. Density for anisomycin is visible but not included in the model.
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-26
Resolution : 3.00 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 : 2.11
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) : 2.11

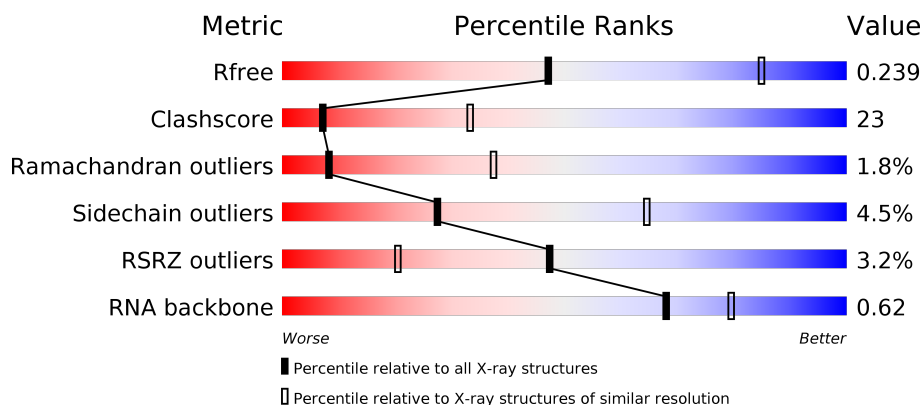
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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	 62% 33% . .
2	B	338	 58% 37% .
3	C	246	 68% 27% 5%
4	D	177	 8% 42% 35% .. 21%

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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	3	8804	-	-	X	-
33	CL	B	8819	-	-	X	-
33	CL	M	8818	-	-	X	-
34	SR	0	8957	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8997	-	-	-	X
34	SR	0	9004	-	-	-	X
34	SR	0	9006	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8563	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99120 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
			59018	26348	10871	19054	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	84	Total	Mg	0	0
			84	84		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	3	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	9	Total 9	Cl 9	0	0
33	J	3	Total 3	Cl 3	0	0
33	K	1	Total 1	Cl 1	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	93	Total 93	Sr 93	0	0
34	1	2	Total 2	Sr 2	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	3	Total 3	Sr 3	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	66	Total 66	Na 66	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	2	Total 2	Na 2	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
37	Z	1	Total 1	Cd 1	0	0
37	1	1	Total 1	Cd 1	0	0

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	121	Total	O	0	0
			121	121		
38	B	145	Total	O	0	0
			145	145		
38	C	166	Total	O	0	0
			166	166		
38	D	46	Total	O	0	0
			46	46		
38	E	43	Total	O	0	0
			43	43		
38	F	31	Total	O	0	0
			31	31		
38	G	17	Total	O	0	0
			17	17		
38	H	72	Total	O	0	0
			72	72		
38	I	5	Total	O	0	0
			5	5		
38	J	52	Total	O	0	0
			52	52		
38	K	52	Total	O	0	0
			52	52		
38	L	81	Total	O	0	0
			81	81		
38	M	133	Total	O	0	0
			133	133		
38	N	56	Total	O	0	0
			56	56		
38	O	41	Total	O	0	0
			41	41		
38	P	63	Total	O	0	0
			63	63		
38	Q	52	Total	O	0	0
			52	52		

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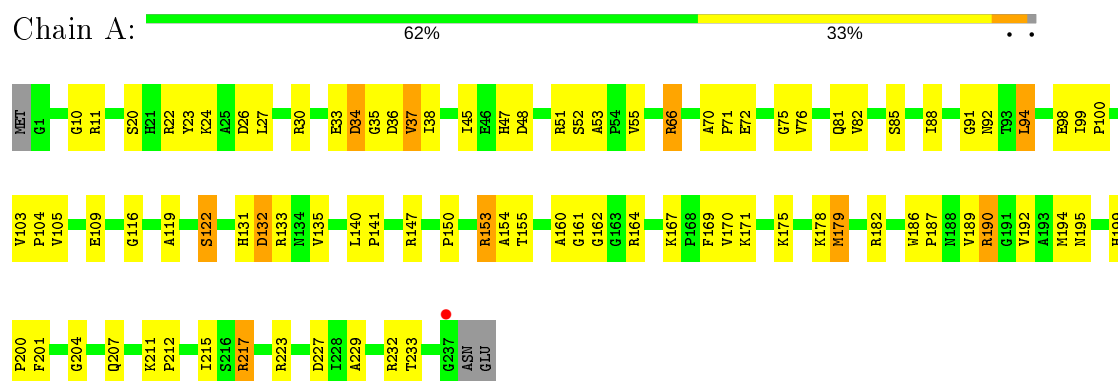
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	R	75	Total 75	O 75	0	0
38	S	37	Total 37	O 37	0	0
38	T	40	Total 40	O 40	0	0
38	U	28	Total 28	O 28	0	0
38	V	15	Total 15	O 15	0	0
38	W	69	Total 69	O 69	0	0
38	X	22	Total 22	O 22	0	0
38	Y	100	Total 100	O 100	0	0
38	Z	28	Total 28	O 28	0	0
38	1	61	Total 61	O 61	0	0
38	2	45	Total 45	O 45	0	0
38	3	76	Total 76	O 76	0	0
38	0	5897	Total 5897	O 5897	0	0
38	9	154	Total 154	O 154	0	0

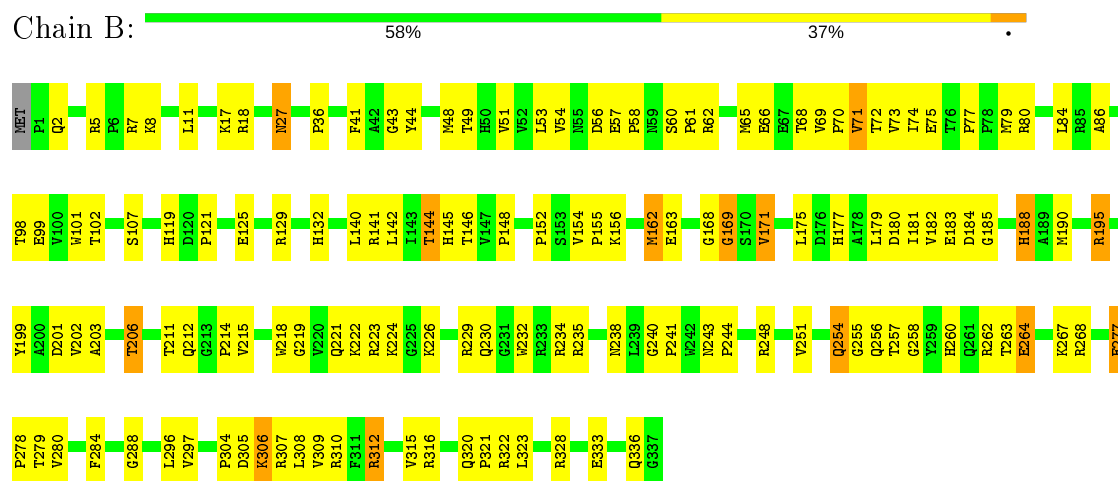
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

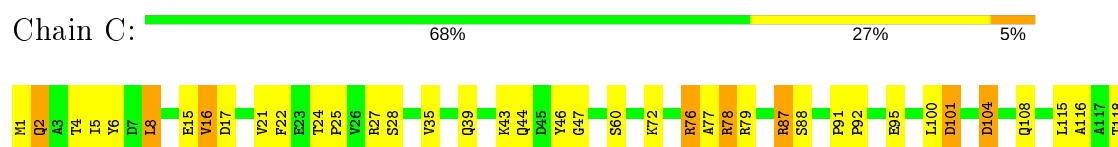
• Molecule 1: 50S ribosomal protein L2P

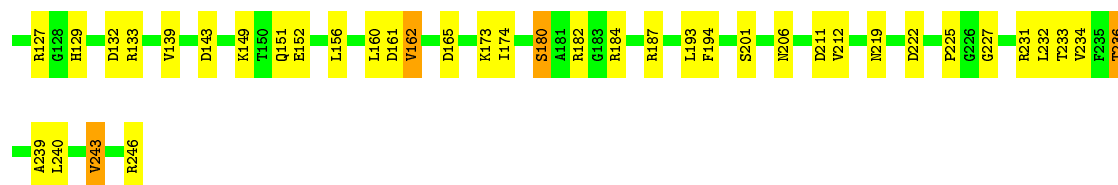


• Molecule 2: 50S ribosomal protein L3P

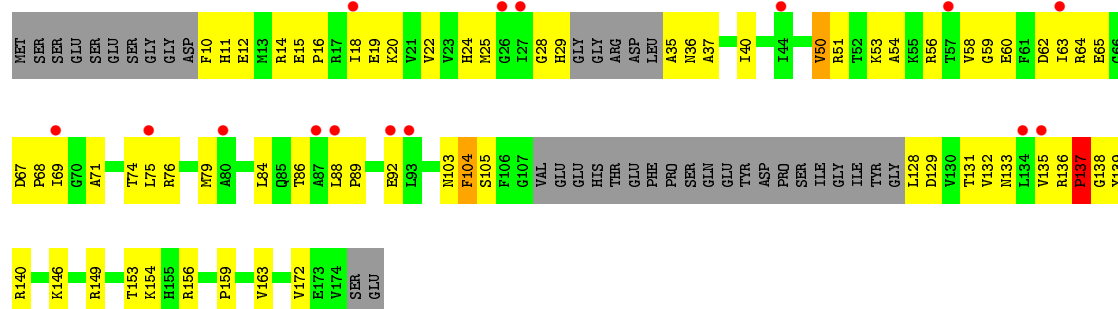
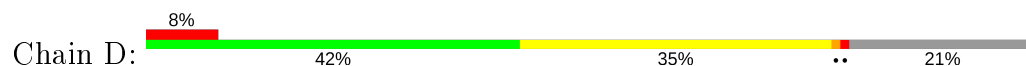


• Molecule 3: 50S ribosomal protein L4P

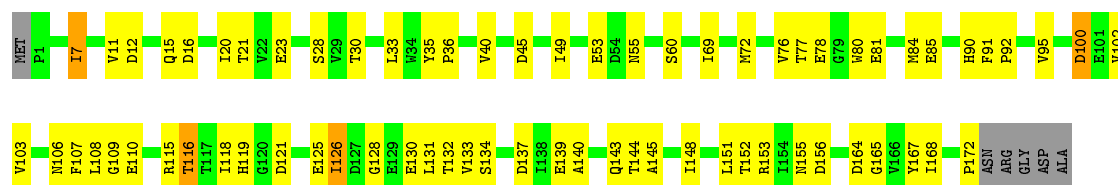




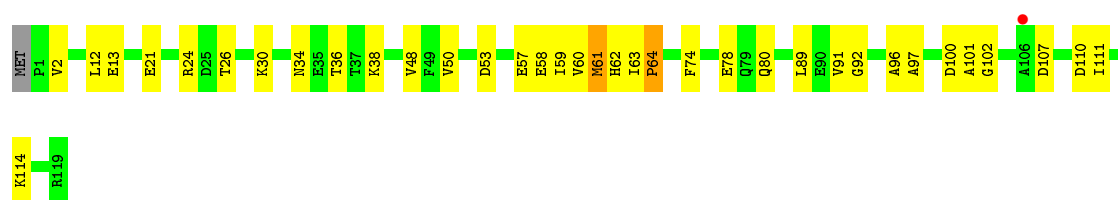
• Molecule 4: 50S ribosomal protein L5P



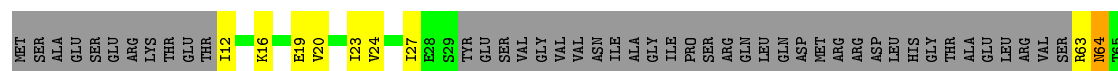
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae



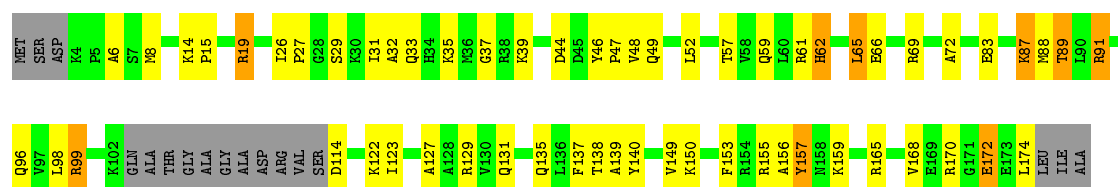
• Molecule 7: 50S ribosomal protein L10E





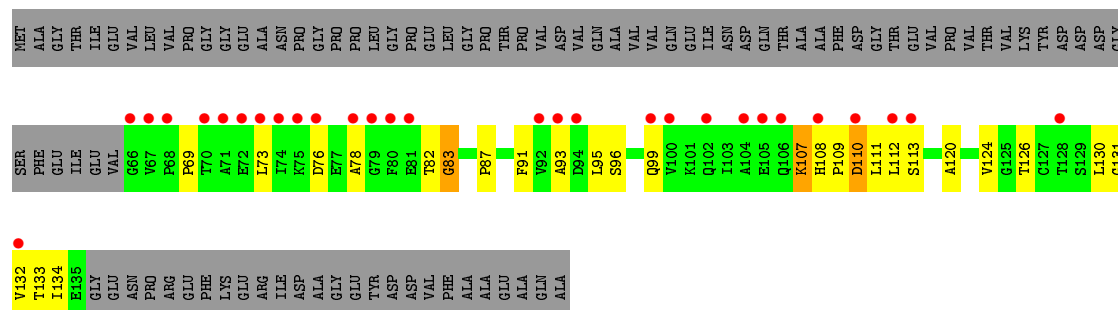
• Molecule 8: 50S ribosomal protein L10e

Chain H: 57% 28% 5% 10%



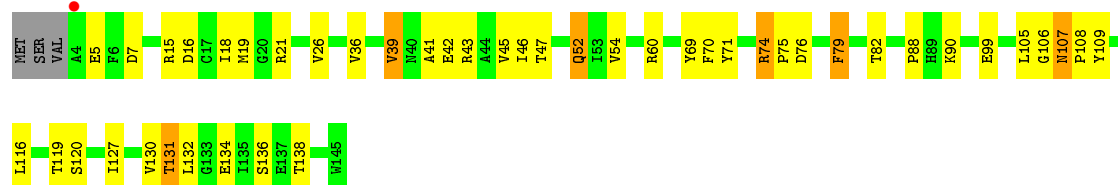
• Molecule 9: 50S ribosomal protein L11P

Chain I: 18% 27% 15% 57%



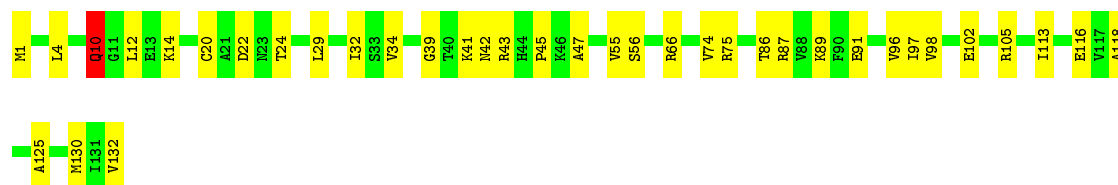
• Molecule 10: 50S ribosomal protein L13P

Chain J: 67% 27% 6%

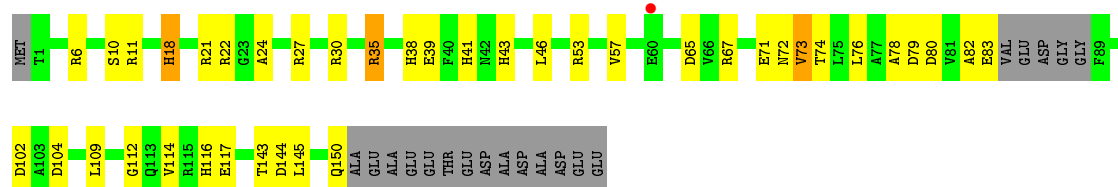


• Molecule 11: 50S ribosomal protein L14P

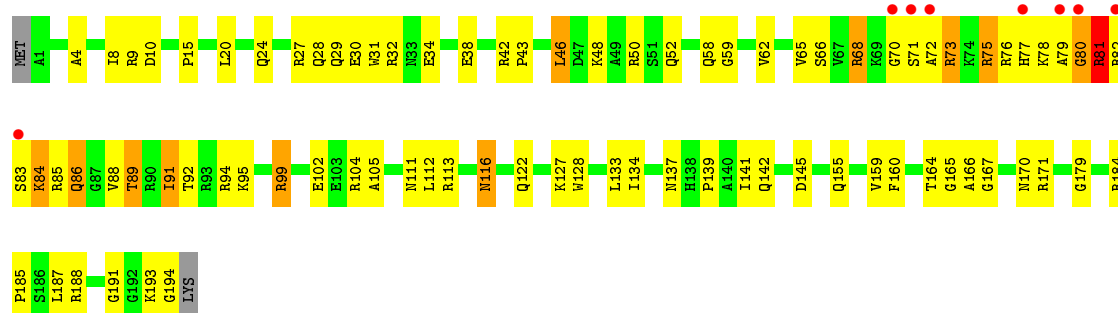
Chain K: 72% 27% 1%



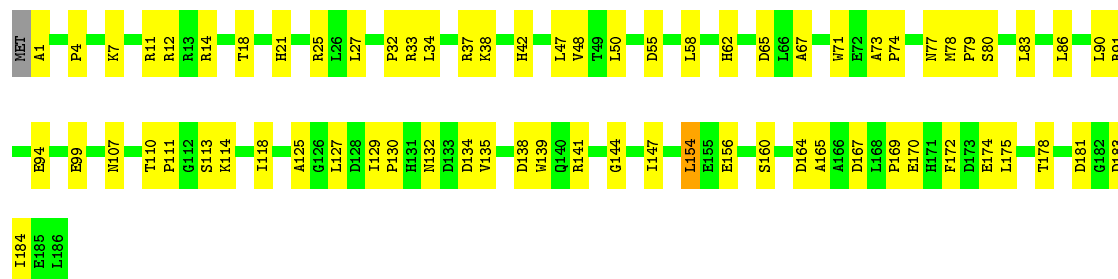
- Molecule 12: 50S ribosomal protein L15P



- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P

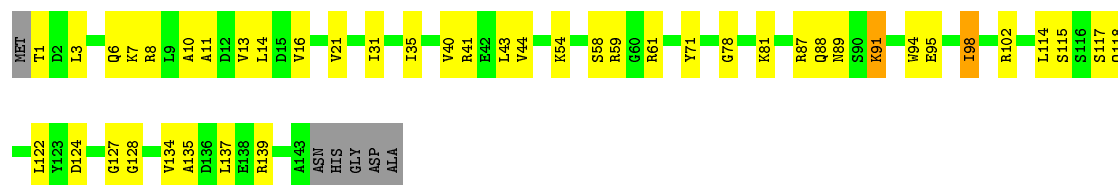


- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e

Chain P:  66% 28%



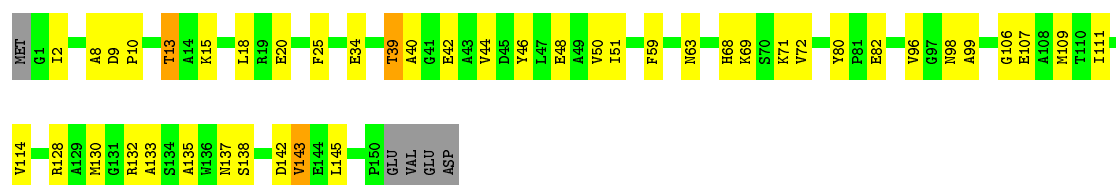
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  69% 27%



- Molecule 18: 50S ribosomal protein L22P

Chain R:  68% 26%



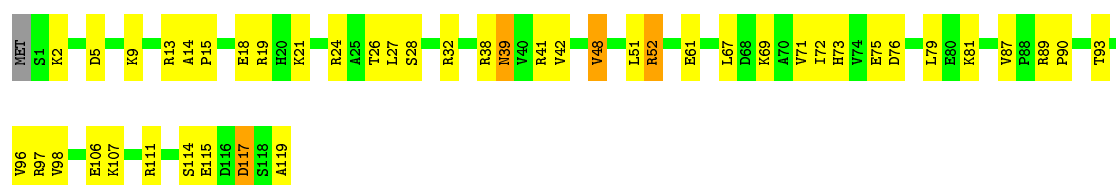
- Molecule 19: 50S ribosomal protein L23P

Chain S:  67% 28% 5%



- Molecule 20: 50S ribosomal protein L24P

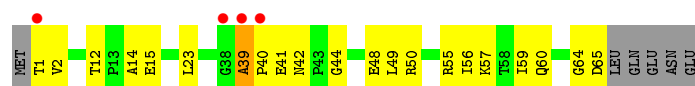
Chain T:  62% 34%



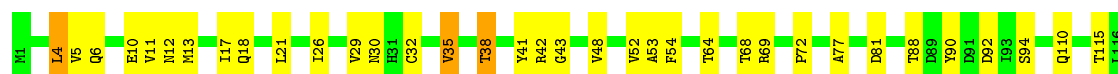
- Molecule 21: 50S ribosomal protein L24e

Chain U:  48% 39% 37% 21%

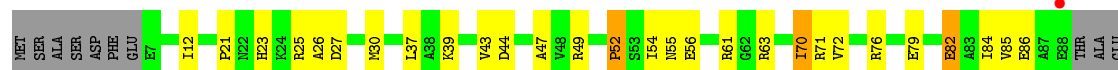
- Molecule 22: 50S ribosomal protein L29P



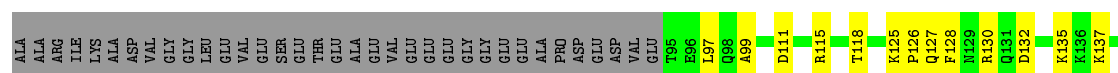
- Molecule 23: 50S ribosomal protein L30P



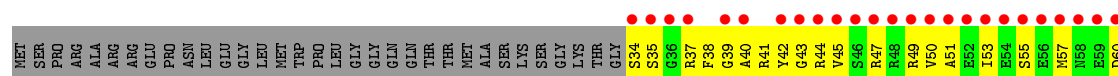
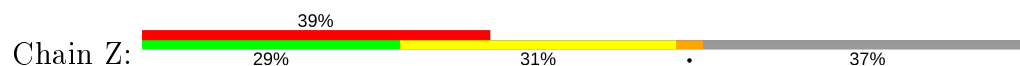
- Molecule 24: 50S ribosomal protein L31e



- Molecule 25: 50S ribosomal protein L32e



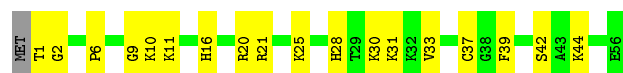
- Molecule 26: 50S ribosomal protein L37Ae





- Molecule 27: 50S ribosomal protein L37e

Chain 1: 67% 32%



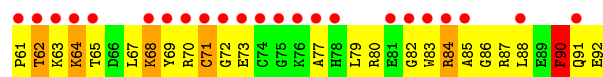
- Molecule 28: 50S ribosomal protein L39e

Chain 2: 2% 60% 30% 8%



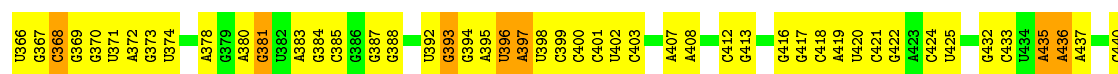
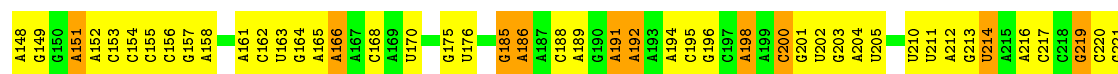
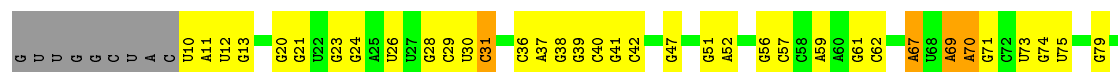
- Molecule 29: 50S ribosomal protein L44E

Chain 3: 34% 77% 57% 9%



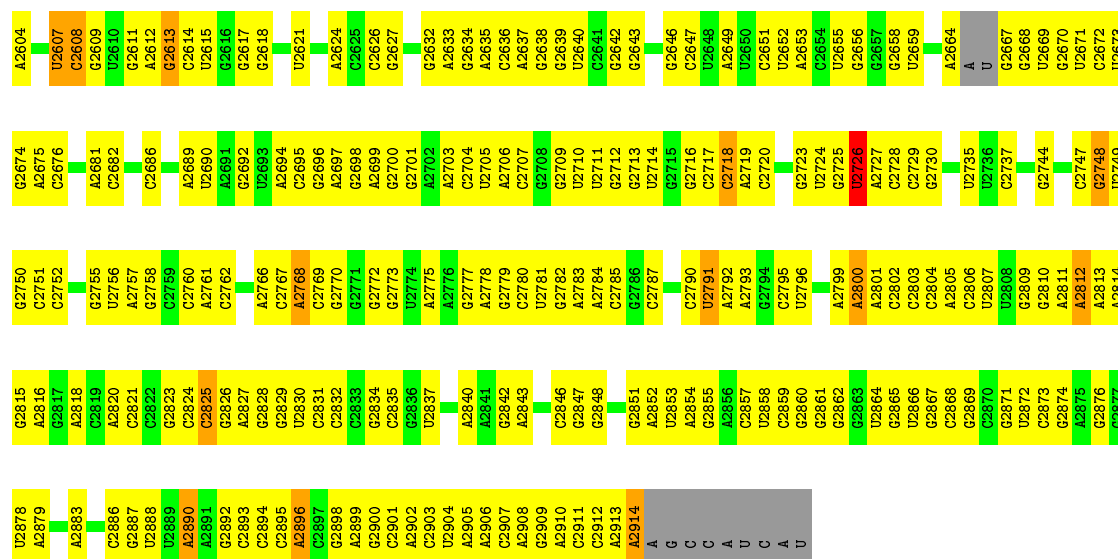
- Molecule 30: 23S RIBOSOMAL RNA

Chain 0: 34% 54% 6% 6%

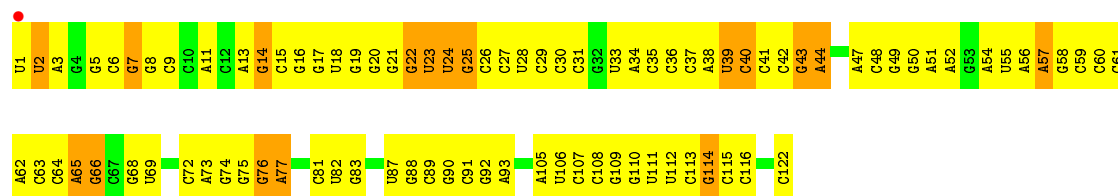


G1475	U1405	C1251	G1186	G1112	C1025	G964	G887	G814	C735	G670	A591	G514	A441
A1476	A1406	C1251	U1187	U1115	U1026	A965	U888	U815	A736	A671	A591	U517	A442
C1477	A1407	C1256	A1188	U1116	G1027	U966	C889	G816	A737	G672	C594	U517	C443
G1478	U1408	C1266	U1189	U1117	U1028	U967	C890	G817	U518	U675	C594	G518	C444
A1485	G1410	G1260	A1191	A1117	U1029	G968	G894	A818	C741	U676	C594	A519	U445
			A1192	A1118	U1030	G969	G895	A819	G742	C676	C594	A520	G446
			A1193	U1119	G1031	U970	A896	G820	G743	C677	C594	A521	A447
			U1120	G1121	A1032	G	C896	G821	G744	C678	C594	A522	G448
			C1127	U1041	U	U	A897	C822	G745	U678	C594	U523	A449
			U1128	U	U	U	G898	G823	G746	C679	C594	C523	C450
			U1129	C	C	C	C899	G824	A746	U680	C594	C451	A451
			U1130	U	U	U	G902	U825	G747	A603	C594	A532	A452
			G1131	U	U	U	U903	U826	C748	G604	C594	U533	G453
			A1132	C	C	C	U904	A827	C749	C605	C594	G534	A454
			A1133	U	U	U	G905	G828	A750	U611	C594	G535	U457
			G1134	U	U	U	C906	G829	U751	U612	C594	A536	G458
			C1137	U	U	U	U907	G830	U752	U613	C594	G537	A459
			U1138	C	C	C	G908	G831	U753	U614	C594	C538	A460
			G1139	U	U	U	G909	U832	C754	U615	C594	G539	C461
			U1140	U	U	U	G910	U833	C755	U616	C594	A540	A462
			A1150	C	C	C	G911	G834	C756	A682	C594	C541	A466
			G1151	U	U	U	A912	U835	C757	A683	C594	G542	G467
			A1154	U	U	U	A913	C838	C758	A684	C594	A543	U468
			U1155	G	G	G	A916	C839	C759	C685	C594	G544	U469
			C1156	A	A	A	U917	U840	A765	A686	C594	G545	C462
			C1157	U	U	U	C920	A841	A766	G687	C594	A546	A470
			U1158	C	C	C	G921	C842	A767	C688	C594	A547	
			G1159	U	U	U	A922	U843	G772	C689	C594	A548	
			G1160	U	U	U	A923	A844	C773	U701	C594	A549	A473
			A1161	C	C	C	G924	C845	C774	U702	C594	A550	C474
			C1162	U	U	U	A925	U846	C775	G703	C594	A551	A477
			U1163	U	U	U	A926	C847	A776	C704	C594	A552	A478
			G1164	C	C	C	U927	U848	U777	C705	C594	G553	G479
			U1165	A	A	A	G928	C849	C778	C706	C594	C556	
			A1166	U	U	U	G929	U850	A780	A630	C594	C557	G482
			C1167	U	U	U	A929	U851	C781	C707	C594	C558	C483
			U1168	C	C	C	G930	U852	C782	A708	C594	U560	A484
			C1169	U	U	U	G931	U853	A783	C709	C594	U561	A485
			U1170	U	U	U	A932	U854	C784	G710	C594	A562	A486
			A1171	C	C	C	G933	U855	A785	C711	C594	C563	G487
			C1172	U	U	U	A934	U856	C786	C712	C594	G564	U488
			U1173	U	U	U	G935	U857	A787	U713	C594	G564	
			A1174	C	C	C	A936	U858	C788	U	C594	U567	C491
			G1175	U	U	U	G937	U859	A789	C717	C594	G568	C492
			C1176	U	U	U	U942	C860	C790	C718	C594	A569	U493
			U1177	U	U	U	U943	U861	C791	U714	C594	C571	C494
			C1178	U	U	U	A944	U862	C792	A721	C594	G577	A495
			U1179	U	U	U	G945	U863	C793	G724	C594	G577	G496
			A1180	U	U	U	U946	U864	C794	C725	C594	G577	A497
			C1181	U	U	U	A947	U865	C795	C726	C594	G577	A498
			U1182	U	U	U	G948	U866	A796	A659	C594	G577	G499
			G1183	U	U	U	U949	U867	C796	U581	C594	G577	G500
			C1184	U	U	U	G950	U868	C797	C727	C594	G577	G501
			U1185	U	U	U	A951	U869	C798	G661	C594	G577	G502
				U	U	U	G952	U870	C799	U582	C594	G577	G503
				U	U	U	A953	U871	C800	C728	C594	G577	G504
				U	U	U	G954	U872	U801	U662	C594	G577	G505
				U	U	U	A955	U873	G802	U663	C594	G577	G506
				U	U	U	G956	U874	U802	C729	C594	G577	A507
				U	U	U	A957	U875	U803	U664	C594	G577	A508
				U	U	U	G958	U876	U804	U665	C594	G577	A509
				U	U	U	A959	U877	U805	A656	C594	G577	U510
				U	U	U	G960	U878	U806	A657	C594	G577	A511
				U	U	U	A961	U879	U807	G669	C594	G577	A512
				U	U	U	G962	U880	U808	U669	C594	G577	A513
				U	U	U	A963	U881	U809	U670	C594	G577	A514
				U	U	U	G964	U882	U810	U671	C594	G577	A515
				U	U	U	A965	U883	U811	U672	C594	G577	A516
				U	U	U	G966	U884	U812	U673	C594	G577	A517
				U	U	U	A967	U885	U813	U674	C594	G577	A518
				U	U	U	G968	U886	U814	U675	C594	G577	A519
				U	U	U	A969	U887	U815	U676	C594	G577	A520
				U	U	U	G970	U888	U816	U677	C594	G577	A521
				U	U	U	A971	U889	U817	U678	C594	G577	A522
				U	U	U	G972	U890	U818	U679	C594	G577	A523
				U	U	U	A973	U891	U819	U680	C594	G577	A524
				U	U	U	G974	U892	U820	U681	C594	G577	A525
				U	U	U	A975	U893	U821	U682	C594	G577	A526
				U	U	U	G976	U894	U822	U683	C594	G577	A527
				U	U	U	A977	U895	U823	U684	C594	G577	A528
				U	U	U	G978	U896	U824	U685	C594	G577	A529
				U	U	U	A979	U897	U825	U686	C594	G577	A530
				U	U	U	G980	U898	U826	U687	C594	G577	A531
				U	U	U	A981	U899	U827	U688	C594	G577	A532
				U	U	U	G982	U900	U828	U689	C594	G577	A533
				U	U	U	A983	U901	U829	U690	C594	G577	A534
				U	U	U	G984	U902	U830	U691	C594	G577	A535
				U	U	U	A985	U903	U831	U692	C594	G577	A536
				U	U	U	G986	U904	U832	U693	C594	G577	A537
				U	U	U	A987	U905	U833	U694	C594	G577	A538
				U	U	U	G988	U906	U834	U695	C594	G577	A539
				U	U	U	A989	U907	U835	U696	C594	G577	A540
				U	U	U	G990	U908	U836	U697	C594	G577	A541
				U	U	U	A991	U909	U837	U698	C594	G577	A542
				U	U	U	G992	U910	U838	U699	C594	G577	A543
				U	U	U	A993	U911	U839	U700	C594	G577	A544
				U	U	U	G994	U912	U840	U701	C594	G577	A545
				U	U	U	A995	U913	U841	U702	C594	G577	A546
				U	U	U	G996	U914	U842	U703	C594	G577	A547
				U	U	U	A997	U915	U843	U704	C594	G577	A548
				U	U	U	G998	U916	U844	U705	C594	G577	A549
				U	U	U	A999	U917	U845	U706	C594	G577	A550
				U	U	U	G1000	U918	U846	U707	C594	G577	A551
				U	U	U	A1001	U919	U847	U708	C594	G577	A552
				U	U	U	G1002	U920	U848	U709	C594	G577	A553
				U	U	U	A1003	U921	U849	U710	C594	G577	A554
				U	U	U	G1004	U922	U850	U711	C594	G577	A555
				U	U	U	A1005	U923	U851	U712	C594	G577	A556
				U	U	U	G1006	U924	U852	U713	C594	G577	A557
				U	U	U	A1007	U925	U853	U714	C594	G577	A558
				U	U	U	G1008	U926	U854	U	C594	G577	A559
				U	U	U	A1009	U927	U855	C715	C594	G577	A560
				U	U	U	G1010	U928	U856	C716	C594	G577	A561
				U	U	U	A1011	U929	U857	C717	C594	G577	A562
				U	U	U	G1012	U930	U858	C718	C594	G577	A563
				U	U	U	A1013	U931	U859	C719	C594	G577	A564
				U	U	U	G1014	U932	U860	C720	C594	G577	A565
				U	U	U	A1015	U933	U861	C721	C594	G577	A566
				U	U	U	G1016	U934	U862	C722	C594	G577	A567
				U	U	U	A1017	U935	U863	C723	C594	G577	A568
				U	U	U	G1018	U936	U864	C724	C594	G577	A569
				U	U	U	A1019	U937	U865	C725	C594	G577	A570
				U	U	U	G1020	U938	U866	C726	C594	G577	A571
				U	U								





● 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	212.41Å 299.52Å 574.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 3.00 85.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	77.8 (49.81-3.00) 77.4 (85.66-2.40)	Depositor EDS
R_{merge}	0.14	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}	0.180 , 0.247 0.177 , 0.239	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 82.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.09% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, 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	0.65	0/2408
2	B	0.34	0/2690	0.64	0/3652
3	C	0.38	0/1885	0.65	0/2552
4	D	0.32	0/1111	0.56	0/1498
5	E	0.34	0/1382	0.59	0/1880
6	F	0.34	0/901	0.58	0/1224
7	G	0.33	0/241	0.48	0/324
8	H	0.34	0/1302	0.65	0/1743
9	I	0.31	0/526	0.51	0/716
10	J	0.38	0/1136	0.62	0/1530
11	K	0.36	0/1004	0.67	0/1351
12	L	0.33	0/1130	0.62	0/1509
13	M	0.38	0/1582	0.63	0/2116
14	N	0.32	0/1474	0.63	0/1999
15	O	0.37	0/874	0.60	0/1181
16	P	0.34	0/1147	0.53	0/1528
17	Q	0.33	0/749	0.69	0/1005
18	R	0.37	0/1172	0.63	0/1578
19	S	0.38	0/648	0.60	0/875
20	T	0.34	0/958	0.66	1/1289 (0.1%)
21	U	0.45	0/417	0.67	0/562
22	V	0.32	0/502	0.55	0/675
23	W	0.36	0/1219	0.64	0/1655
24	X	0.35	0/664	0.61	0/895
25	Y	0.36	0/1146	0.62	0/1536
26	Z	0.45	0/584	0.63	0/781
27	1	0.43	0/438	0.57	0/578
28	2	0.35	0/401	0.60	0/529
29	3	0.48	0/771	0.66	0/1024
30	0	0.41	0/65954	0.68	4/102862 (0.0%)
31	9	0.35	0/2904	0.68	0/4526
All	All	0.39	0/98698	0.67	5/147581 (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
23	W	0	1
30	0	0	18
31	9	0	1
All	All	0	20

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	1819	G	C5'-C4'-C3'	5.99	125.59	116.00
30	0	871	G	C5'-C4'-O4'	-5.85	102.08	109.10
30	0	1504	A	C1'-O4'-C4'	-5.36	105.62	109.90
20	T	52	ARG	N-CA-C	5.08	124.73	111.00
30	0	2726	U	N1-C1'-C2'	5.01	120.52	114.00

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	214	U	Sidechain
30	0	324	G	Sidechain
30	0	393	G	Sidechain
30	0	435	A	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	97	0
2	B	2625	0	2532	127	0
3	C	1860	0	1813	70	0
4	D	1094	0	1085	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1357	0	1266	55	0
6	F	890	0	843	27	0
7	G	240	0	231	11	0
8	H	1282	0	1292	55	0
9	I	519	0	500	26	0
10	J	1120	0	1098	44	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	29	0
13	M	1558	0	1573	98	0
14	N	1445	0	1401	59	0
15	O	865	0	873	32	0
16	P	1136	0	1123	44	0
17	Q	735	0	729	21	0
18	R	1149	0	1122	37	0
19	S	641	0	605	16	0
20	T	950	0	924	33	0
21	U	410	0	368	38	0
22	V	499	0	511	19	0
23	W	1196	0	1137	52	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	44	0
26	Z	573	0	535	64	0
27	1	431	0	426	20	0
28	2	396	0	413	21	0
29	3	755	0	732	90	0
30	0	59018	0	29810	2239	0
31	9	2599	0	1325	161	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	3	1	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	9	0	0	2	0
33	3	1	0	0	3	0
33	A	1	0	0	1	0
33	B	1	0	0	2	0
33	J	3	0	0	2	0
33	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	L	1	0	0	1	0
33	M	1	0	0	2	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	0	0
34	0	93	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	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	C	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	2	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	5897	0	0	323	0
38	1	61	0	0	3	0
38	2	45	0	0	1	0
38	3	76	0	0	7	0
38	9	154	0	0	11	0
38	A	121	0	0	3	0
38	B	145	0	0	20	0
38	C	166	0	0	13	0
38	D	46	0	0	7	0
38	E	43	0	0	4	0
38	F	31	0	0	1	0
38	G	17	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	72	0	0	10	0
38	I	5	0	0	2	0
38	J	52	0	0	4	0
38	K	52	0	0	3	0
38	L	81	0	0	4	0
38	M	133	0	0	12	0
38	N	56	0	0	6	0
38	O	41	0	0	2	0
38	P	63	0	0	5	0
38	Q	52	0	0	1	0
38	R	75	0	0	2	0
38	S	37	0	0	0	0
38	T	40	0	0	3	0
38	U	28	0	0	5	0
38	V	15	0	0	1	0
38	W	69	0	0	7	0
38	X	22	0	0	4	0
38	Y	100	0	0	5	0
38	Z	28	0	0	5	0
All	All	99120	0	59922	3377	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 23.

The worst 5 of 3377 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)
30:0:871:G:C8	30:0:871:G:H5'	1.74	1.22
30:0:1160:G:H5'	30:0:1161:A:C5'	1.70	1.20
30:0:1160:G:C5'	30:0:1161:A:H5'	1.73	1.18
30:0:1278:A:H4'	30:0:1279:U:C4	1.81	1.16
13:M:171:ARG:HD3	30:0:156:C:H5''	1.15	1.13

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	
1	A	235/240 (98%)	200 (85%)	30 (13%)	5 (2%)	7	33
2	B	335/338 (99%)	305 (91%)	23 (7%)	7 (2%)	7	33
3	C	244/246 (99%)	216 (88%)	26 (11%)	2 (1%)	19	57
4	D	134/177 (76%)	105 (78%)	23 (17%)	6 (4%)	2	14
5	E	170/178 (96%)	158 (93%)	11 (6%)	1 (1%)	25	64
6	F	117/120 (98%)	97 (83%)	16 (14%)	4 (3%)	3	20
7	G	25/348 (7%)	22 (88%)	3 (12%)	0	100	100
8	H	156/177 (88%)	139 (89%)	16 (10%)	1 (1%)	25	64
9	I	68/162 (42%)	49 (72%)	16 (24%)	3 (4%)	2	15
10	J	140/145 (97%)	128 (91%)	10 (7%)	2 (1%)	11	43
11	K	130/132 (98%)	120 (92%)	9 (7%)	1 (1%)	19	57
12	L	141/165 (86%)	116 (82%)	22 (16%)	3 (2%)	7	33
13	M	192/196 (98%)	171 (89%)	17 (9%)	4 (2%)	7	33
14	N	184/187 (98%)	163 (89%)	17 (9%)	4 (2%)	6	31
15	O	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
16	P	141/149 (95%)	133 (94%)	8 (6%)	0	100	100
17	Q	93/96 (97%)	86 (92%)	5 (5%)	2 (2%)	6	31
18	R	148/155 (96%)	138 (93%)	9 (6%)	1 (1%)	22	60
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
21	U	51/67 (76%)	44 (86%)	6 (12%)	1 (2%)	7	34
22	V	63/71 (89%)	58 (92%)	4 (6%)	1 (2%)	9	40
23	W	152/154 (99%)	142 (93%)	9 (6%)	1 (1%)	22	60
24	X	80/92 (87%)	72 (90%)	6 (8%)	2 (2%)	5	28
25	Y	140/241 (58%)	132 (94%)	7 (5%)	1 (1%)	22	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	55 (78%)	12 (17%)	4 (6%)	2	10
27	1	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	64 (71%)	17 (19%)	9 (10%)	0	2
All	All	3705/4472 (83%)	3292 (89%)	348 (9%)	65 (2%)	8	37

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	206	THR
2	B	306	LYS
4	D	137	PRO
6	F	61	MET
6	F	101	ALA

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%)	170 (95%)	9 (5%)	24	60
2	B	282/283 (100%)	263 (93%)	19 (7%)	16	49
3	C	193/193 (100%)	180 (93%)	13 (7%)	16	49
4	D	117/148 (79%)	110 (94%)	7 (6%)	19	53
5	E	152/156 (97%)	146 (96%)	6 (4%)	32	69
6	F	93/94 (99%)	92 (99%)	1 (1%)	73	90
7	G	27/282 (10%)	25 (93%)	2 (7%)	13	44
8	H	134/145 (92%)	124 (92%)	10 (8%)	13	43
9	I	58/130 (45%)	57 (98%)	1 (2%)	60	85
10	J	118/121 (98%)	109 (92%)	9 (8%)	13	43
11	K	106/106 (100%)	103 (97%)	3 (3%)	43	77
12	L	113/127 (89%)	106 (94%)	7 (6%)	18	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	147 (93%)	11 (7%)	15	47
14	N	149/150 (99%)	146 (98%)	3 (2%)	55	83
15	O	93/94 (99%)	93 (100%)	0	100	100
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	85
17	Q	79/80 (99%)	74 (94%)	5 (6%)	18	51
18	R	117/122 (96%)	113 (97%)	4 (3%)	37	72
19	S	71/74 (96%)	70 (99%)	1 (1%)	67	88
20	T	105/106 (99%)	98 (93%)	7 (7%)	16	49
21	U	44/53 (83%)	43 (98%)	1 (2%)	50	80
22	V	51/57 (90%)	51 (100%)	0	100	100
23	W	130/130 (100%)	126 (97%)	4 (3%)	40	75
24	X	66/74 (89%)	61 (92%)	5 (8%)	13	43
25	Y	120/196 (61%)	117 (98%)	3 (2%)	47	79
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	73 (92%)	6 (8%)	13	43
All	All	3095/3646 (85%)	2955 (96%)	140 (4%)	27	64

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	99	ARG
11	K	24	THR
24	X	82	GLU
8	H	157	TYR
10	J	52	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	116	HIS
16	P	50	GLN
28	2	45	ASN
13	M	24	GLN

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Mol	Chain	Res	Type
13	M	137	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	243 (8%)	22 (0%)
31	9	121/122 (99%)	19 (15%)	2 (1%)
All	All	2866/3045 (94%)	262 (9%)	24 (0%)

5 of 262 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 24 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	871	G
30	0	1237	U
31	9	43	G
30	0	877	G
30	0	1080	C

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	UR3	0	2619	30	14,22,23	0.70	0	15,32,35	0.56	0

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	1.65	3 (17%)	20,30,33	5.40	4 (20%)
30	OMG	0	2588	30	18,26,27	1.12	2 (11%)	20,38,41	2.58	4 (20%)
30	OMU	0	2587	30,35	14,22,23	0.98	1 (7%)	14,31,34	1.17	1 (7%)
30	1MA	0	628	30,35	15,25,26	0.78	0	15,37,40	1.39	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	UR3	0	2619	30	-	0/5/25/26	0/2/2/2
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	OMU	0	2587	30,35	-	0/7/27/28	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-5.19	1.47	1.52
30	0	2588	OMG	C6-N1	3.72	1.39	1.33
30	0	2587	OMU	C4-N3	2.72	1.37	1.33
30	0	2621	PSU	C4-N3	2.67	1.37	1.33
30	0	2621	PSU	C2-N1	2.59	1.43	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	-17.23	114.73	128.43
30	0	2621	PSU	C4-N3-C2	14.24	127.16	115.14
30	0	2588	OMG	C5-C6-N1	-8.58	111.69	123.43
30	0	2621	PSU	C5-C4-N3	-8.09	114.94	125.36
30	0	2588	OMG	C6-N1-C2	5.76	125.08	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2621	PSU	2	0
30	0	2587	OMU	2	0
30	0	628	1MA	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates 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%)	-0.60	1 (0%) 92 79	29, 65, 98, 115	0
2	B	337/338 (99%)	-0.73	0 100 100	31, 59, 87, 97	0
3	C	246/246 (100%)	-0.82	0 100 100	23, 47, 69, 80	0
4	D	140/177 (79%)	0.45	15 (10%) 6 2	74, 109, 132, 140	0
5	E	172/178 (96%)	-0.64	0 100 100	50, 74, 97, 103	0
6	F	119/120 (99%)	-0.30	1 (0%) 86 65	50, 73, 106, 113	0
7	G	29/348 (8%)	0.08	0 100 100	75, 96, 105, 109	0
8	H	160/177 (90%)	-0.49	0 100 100	48, 67, 99, 109	0
9	I	70/162 (43%)	1.80	29 (41%) 0 0	134, 152, 167, 169	0
10	J	142/145 (97%)	-0.79	1 (0%) 87 69	40, 58, 75, 97	0
11	K	132/132 (100%)	-0.87	0 100 100	39, 55, 81, 86	0
12	L	145/165 (87%)	-0.24	1 (0%) 87 69	35, 72, 113, 129	0
13	M	194/196 (98%)	-0.51	8 (4%) 37 14	31, 46, 99, 106	0
14	N	186/187 (99%)	-0.33	0 100 100	60, 80, 126, 132	0
15	O	115/116 (99%)	-0.86	0 100 100	43, 56, 74, 80	0
16	P	143/149 (95%)	-0.75	0 100 100	40, 59, 79, 85	0
17	Q	95/96 (98%)	-0.71	0 100 100	44, 56, 72, 88	0
18	R	150/155 (96%)	-0.83	0 100 100	33, 49, 70, 83	0
19	S	81/85 (95%)	-0.67	1 (1%) 79 54	40, 62, 82, 92	0
20	T	119/120 (99%)	-0.55	0 100 100	40, 59, 87, 116	0
21	U	53/67 (79%)	2.66	32 (60%) 0 0	107, 117, 125, 126	0
22	V	65/71 (91%)	-0.02	4 (6%) 20 7	47, 74, 118, 123	0
23	W	154/154 (100%)	-0.69	0 100 100	39, 54, 73, 87	0
24	X	82/92 (89%)	-0.45	1 (1%) 79 54	46, 65, 94, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.88	0 100 100	30, 49, 71, 92	0
26	Z	73/116 (62%)	3.62	45 (61%) 0 0	98, 116, 126, 130	0
27	1	56/57 (98%)	-0.78	0 100 100	28, 36, 43, 48	0
28	2	46/50 (92%)	-0.57	1 (2%) 62 33	31, 66, 97, 104	0
29	3	92/92 (100%)	4.21	71 (77%) 0 0	104, 119, 130, 134	0
30	0	2749/2923 (94%)	-0.83	2 (0%) 95 89	23, 51, 96, 175	0
31	9	122/122 (100%)	-0.97	1 (0%) 86 65	45, 75, 103, 154	0
All	All	6646/7517 (88%)	-0.53	214 (3%) 47 20	23, 57, 116, 175	0

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	Z	46	SER	17.2
26	Z	58	ASN	13.1
29	3	39	GLN	12.1
26	Z	36	GLY	11.6
29	3	34	LYS	11.4

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. 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	OMG	0	2588	24/25	0.98	0.13	39,41,42,45	0
30	UR3	0	2619	21/22	0.98	0.14	39,43,45,48	0
30	1MA	0	628	23/24	0.98	0.14	31,36,38,38	0
30	PSU	0	2621	20/21	0.98	0.18	40,43,44,44	0
30	OMU	0	2587	21/22	0.98	0.12	41,44,50,50	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. 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
34	SR	0	9006	1/1	0.31	0.83	180,180,180,180	0
35	NA	0	8557	1/1	0.41	0.08	59,59,59,59	0
34	SR	0	9004	1/1	0.44	1.01	200,200,200,200	0
34	SR	0	8985	1/1	0.45	0.12	182,182,182,182	0
35	NA	0	8567	1/1	0.50	0.30	68,68,68,68	0
35	NA	0	8563	1/1	0.53	0.68	65,65,65,65	0
34	SR	0	8971	1/1	0.54	0.11	170,170,170,170	0
34	SR	0	8997	1/1	0.54	0.83	194,194,194,194	0
33	CL	J	8802	1/1	0.54	0.08	76,76,76,76	0
34	SR	0	9001	1/1	0.55	0.08	166,166,166,166	0
34	SR	0	8959	1/1	0.56	0.28	200,200,200,200	0
34	SR	0	8974	1/1	0.57	0.14	164,164,164,164	0
34	SR	0	8957	1/1	0.57	0.73	200,200,200,200	0
34	SR	0	8979	1/1	0.61	0.18	198,198,198,198	0
35	NA	0	8553	1/1	0.62	0.33	70,70,70,70	0
35	NA	0	8528	1/1	0.63	0.91	83,83,83,83	0
34	SR	0	8986	1/1	0.63	0.45	200,200,200,200	0
34	SR	0	8975	1/1	0.64	0.11	171,171,171,171	0
34	SR	0	8962	1/1	0.67	0.08	179,179,179,179	0
34	SR	0	8977	1/1	0.72	0.11	181,181,181,181	0
32	MG	0	8091	1/1	0.73	0.07	58,58,58,58	0
37	CD	U	8701	1/1	0.74	0.35	200,200,200,200	0
34	SR	0	8998	1/1	0.75	0.30	184,184,184,184	0
34	SR	0	8922	1/1	0.75	0.29	169,169,169,169	0
34	SR	9	8980	1/1	0.75	0.14	182,182,182,182	0
36	K	0	8401	1/1	0.75	0.15	156,156,156,156	0
34	SR	0	8919	1/1	0.76	0.32	200,200,200,200	0
34	SR	0	8960	1/1	0.76	0.05	152,152,152,152	0
34	SR	0	8982	1/1	0.78	1.88	200,200,200,200	0
33	CL	0	8814	1/1	0.78	0.18	72,72,72,72	0
34	SR	0	8969	1/1	0.78	0.31	192,192,192,192	0
32	MG	0	8063	1/1	0.78	0.22	86,86,86,86	0
35	NA	0	8518	1/1	0.79	0.26	75,75,75,75	0
35	NA	0	8559	1/1	0.79	0.46	122,122,122,122	0
34	SR	0	8973	1/1	0.80	0.14	112,112,112,112	0
34	SR	0	8944	1/1	0.80	0.08	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8967	1/1	0.81	0.05	133,133,133,133	0
35	NA	0	8566	1/1	0.81	0.32	62,62,62,62	0
34	SR	0	8988	1/1	0.81	0.13	170,170,170,170	0
35	NA	0	8571	1/1	0.82	0.17	46,46,46,46	0
34	SR	0	9007	1/1	0.82	0.24	179,179,179,179	0
35	NA	0	8556	1/1	0.82	0.44	63,63,63,63	0
34	SR	0	8968	1/1	0.82	0.15	177,177,177,177	0
34	SR	3	8932	1/1	0.82	0.09	158,158,158,158	0
35	NA	9	8572	1/1	0.82	0.17	71,71,71,71	0
35	NA	0	8573	1/1	0.82	0.28	55,55,55,55	0
34	SR	0	8947	1/1	0.83	0.30	194,194,194,194	0
35	NA	0	8535	1/1	0.83	0.20	64,64,64,64	0
32	MG	A	8051	1/1	0.83	0.22	101,101,101,101	0
34	SR	0	8931	1/1	0.83	0.07	110,110,110,110	0
33	CL	0	8815	1/1	0.83	0.09	87,87,87,87	0
35	NA	0	8541	1/1	0.83	0.24	54,54,54,54	0
34	SR	0	9002	1/1	0.83	0.06	157,157,157,157	0
34	SR	0	8946	1/1	0.85	0.12	123,123,123,123	0
34	SR	0	8955	1/1	0.85	0.17	200,200,200,200	0
35	NA	0	8548	1/1	0.85	0.12	68,68,68,68	0
35	NA	0	8515	1/1	0.86	0.15	44,44,44,44	0
32	MG	0	8081	1/1	0.86	0.32	80,80,80,80	0
35	NA	0	8564	1/1	0.86	0.34	57,57,57,57	0
35	NA	0	8546	1/1	0.86	0.47	80,80,80,80	0
34	SR	A	8993	1/1	0.86	0.08	159,159,159,159	0
37	CD	Z	8703	1/1	0.86	0.28	200,200,200,200	0
35	NA	0	8507	1/1	0.86	0.16	32,32,32,32	0
34	SR	0	8989	1/1	0.86	0.18	200,200,200,200	0
32	MG	2	8060	1/1	0.86	0.10	35,35,35,35	0
35	NA	0	8525	1/1	0.87	0.25	85,85,85,85	0
32	MG	0	8093	1/1	0.87	0.05	28,28,28,28	0
34	SR	B	8987	1/1	0.87	0.39	200,200,200,200	0
34	SR	0	8953	1/1	0.88	0.07	200,200,200,200	0
35	NA	0	8562	1/1	0.88	0.53	89,89,89,89	0
35	NA	0	8530	1/1	0.88	0.37	49,49,49,49	0
34	SR	0	8942	1/1	0.88	0.07	130,130,130,130	0
34	SR	0	8915	1/1	0.88	0.07	118,118,118,118	0
34	SR	0	8964	1/1	0.88	0.08	129,129,129,129	0
34	SR	0	8939	1/1	0.88	0.08	152,152,152,152	0
35	NA	0	8545	1/1	0.88	0.24	33,33,33,33	0
34	SR	0	8991	1/1	0.88	0.35	193,193,193,193	0
33	CL	3	8804	1/1	0.89	0.19	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8071	1/1	0.89	0.13	31,31,31,31	0
37	CD	3	8704	1/1	0.89	0.71	200,200,200,200	0
35	NA	0	8570	1/1	0.89	0.07	25,25,25,25	0
34	SR	0	8928	1/1	0.89	0.09	146,146,146,146	0
35	NA	0	8549	1/1	0.90	0.17	77,77,77,77	0
32	MG	0	8047	1/1	0.90	0.15	67,67,67,67	0
34	SR	0	8976	1/1	0.90	0.23	197,197,197,197	0
35	NA	0	8522	1/1	0.90	0.21	45,45,45,45	0
32	MG	B	8042	1/1	0.90	0.08	56,56,56,56	0
32	MG	0	8036	1/1	0.90	0.05	37,37,37,37	0
32	MG	0	8069	1/1	0.90	0.19	55,55,55,55	0
35	NA	0	8552	1/1	0.90	0.26	58,58,58,58	0
34	SR	0	8981	1/1	0.91	0.13	157,157,157,157	0
32	MG	0	8052	1/1	0.91	0.04	51,51,51,51	0
35	NA	0	8505	1/1	0.91	1.13	53,53,53,53	0
34	SR	0	8965	1/1	0.91	0.07	127,127,127,127	0
34	SR	9	9003	1/1	0.91	0.09	177,177,177,177	0
34	SR	0	8956	1/1	0.91	0.05	151,151,151,151	0
32	MG	0	8032	1/1	0.91	0.05	27,27,27,27	0
32	MG	0	8050	1/1	0.91	0.08	52,52,52,52	0
34	SR	3	8999	1/1	0.91	0.28	172,172,172,172	0
32	MG	0	8075	1/1	0.92	0.09	83,83,83,83	0
34	SR	F	9005	1/1	0.92	0.09	131,131,131,131	0
32	MG	0	8049	1/1	0.92	0.38	74,74,74,74	0
35	NA	0	8565	1/1	0.92	0.94	70,70,70,70	0
34	SR	0	8984	1/1	0.92	0.07	105,105,105,105	0
35	NA	0	8509	1/1	0.92	0.14	54,54,54,54	0
34	SR	0	9000	1/1	0.92	0.31	200,200,200,200	0
32	MG	0	8068	1/1	0.92	0.11	49,49,49,49	0
32	MG	K	8054	1/1	0.92	0.15	40,40,40,40	0
32	MG	0	8046	1/1	0.92	0.13	26,26,26,26	0
35	NA	0	8519	1/1	0.92	0.27	51,51,51,51	0
34	SR	0	8937	1/1	0.93	0.17	100,100,100,100	0
32	MG	0	8016	1/1	0.93	0.22	48,48,48,48	0
32	MG	0	8010	1/1	0.93	0.17	24,24,24,24	0
34	SR	0	8994	1/1	0.93	0.24	200,200,200,200	0
35	NA	0	8511	1/1	0.93	0.09	48,48,48,48	0
33	CL	L	8810	1/1	0.93	0.10	64,64,64,64	0
35	NA	0	8521	1/1	0.93	0.20	53,53,53,53	0
32	MG	0	8039	1/1	0.94	0.18	71,71,71,71	0
35	NA	0	8547	1/1	0.94	0.67	47,47,47,47	0
33	CL	J	8821	1/1	0.94	0.11	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8560	1/1	0.94	0.76	74,74,74,74	0
34	SR	0	8970	1/1	0.94	0.04	131,131,131,131	0
35	NA	J	8538	1/1	0.94	0.08	49,49,49,49	0
34	SR	0	8910	1/1	0.94	0.08	99,99,99,99	0
32	MG	0	8037	1/1	0.94	0.17	76,76,76,76	0
32	MG	0	8088	1/1	0.94	0.16	35,35,35,35	0
32	MG	0	8033	1/1	0.94	0.13	40,40,40,40	0
35	NA	0	8544	1/1	0.94	0.11	41,41,41,41	0
33	CL	N	8807	1/1	0.94	0.35	99,99,99,99	0
35	NA	R	8532	1/1	0.94	0.14	37,37,37,37	0
34	SR	0	8916	1/1	0.94	0.10	114,114,114,114	0
33	CL	Y	8820	1/1	0.94	0.11	47,47,47,47	0
34	SR	0	8927	1/1	0.94	0.20	196,196,196,196	0
35	NA	0	8506	1/1	0.95	0.51	58,58,58,58	0
35	NA	0	8526	1/1	0.95	0.13	33,33,33,33	0
34	SR	0	8983	1/1	0.95	0.27	191,191,191,191	0
33	CL	K	8812	1/1	0.95	0.07	48,48,48,48	0
34	SR	0	8914	1/1	0.95	0.20	105,105,105,105	0
35	NA	0	8508	1/1	0.95	0.56	61,61,61,61	0
32	MG	0	8082	1/1	0.95	0.12	66,66,66,66	0
32	MG	0	8065	1/1	0.95	0.12	50,50,50,50	0
33	CL	0	8803	1/1	0.95	0.14	69,69,69,69	0
33	CL	R	8806	1/1	0.95	0.11	47,47,47,47	0
32	MG	0	8062	1/1	0.95	0.20	57,57,57,57	0
35	NA	0	8504	1/1	0.95	0.09	27,27,27,27	0
34	SR	0	8945	1/1	0.95	0.06	107,107,107,107	0
32	MG	0	8080	1/1	0.95	0.28	68,68,68,68	0
33	CL	0	8822	1/1	0.95	0.60	97,97,97,97	0
35	NA	0	8501	1/1	0.96	0.14	43,43,43,43	0
35	NA	0	8561	1/1	0.96	0.36	57,57,57,57	0
35	NA	0	8554	1/1	0.96	0.55	65,65,65,65	0
35	NA	Q	8540	1/1	0.96	0.11	67,67,67,67	0
32	MG	0	8004	1/1	0.96	0.18	21,21,21,21	0
33	CL	0	8817	1/1	0.96	0.20	69,69,69,69	0
33	CL	0	8816	1/1	0.96	0.39	94,94,94,94	0
34	SR	0	8917	1/1	0.96	0.10	109,109,109,109	0
32	MG	B	8043	1/1	0.96	0.11	53,53,53,53	0
34	SR	0	8972	1/1	0.96	0.10	150,150,150,150	0
34	SR	0	8943	1/1	0.96	0.09	72,72,72,72	0
35	NA	S	8510	1/1	0.96	0.04	26,26,26,26	0
35	NA	0	8527	1/1	0.96	0.15	54,54,54,54	0
32	MG	0	8041	1/1	0.96	0.31	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	SR	0	8990	1/1	0.96	0.15	125,125,125,125	0
35	NA	0	8513	1/1	0.96	0.34	66,66,66,66	0
35	NA	0	8533	1/1	0.96	0.08	53,53,53,53	0
33	CL	J	8801	1/1	0.96	0.13	71,71,71,71	0
34	SR	0	8996	1/1	0.96	0.22	199,199,199,199	0
32	MG	3	8090	1/1	0.96	0.12	80,80,80,80	0
35	NA	M	8539	1/1	0.96	0.09	32,32,32,32	0
35	NA	0	8574	1/1	0.96	0.35	54,54,54,54	0
35	NA	0	8516	1/1	0.96	0.08	20,20,20,20	0
32	MG	0	8035	1/1	0.96	0.10	61,61,61,61	0
32	MG	0	8040	1/1	0.96	0.21	54,54,54,54	0
34	SR	A	8929	1/1	0.96	0.04	117,117,117,117	0
34	SR	0	8948	1/1	0.97	0.08	103,103,103,103	0
35	NA	0	8536	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8020	1/1	0.97	0.14	29,29,29,29	0
34	SR	0	8995	1/1	0.97	0.14	140,140,140,140	0
32	MG	0	8055	1/1	0.97	0.10	45,45,45,45	0
32	MG	0	8089	1/1	0.97	0.17	59,59,59,59	0
35	NA	0	8550	1/1	0.97	0.27	47,47,47,47	0
32	MG	0	8029	1/1	0.97	0.07	68,68,68,68	0
32	MG	0	8025	1/1	0.97	0.10	30,30,30,30	0
34	SR	0	8924	1/1	0.97	0.17	133,133,133,133	0
32	MG	0	8064	1/1	0.97	0.06	33,33,33,33	0
32	MG	Y	8086	1/1	0.97	0.06	37,37,37,37	0
33	CL	A	8809	1/1	0.97	0.35	100,100,100,100	0
32	MG	T	8057	1/1	0.97	0.04	63,63,63,63	0
34	SR	0	8920	1/1	0.97	0.05	106,106,106,106	0
35	NA	0	8529	1/1	0.97	0.18	41,41,41,41	0
35	NA	0	8534	1/1	0.97	0.18	37,37,37,37	0
32	MG	0	8083	1/1	0.97	0.12	71,71,71,71	0
32	MG	0	8027	1/1	0.97	0.12	26,26,26,26	0
32	MG	0	8067	1/1	0.98	0.13	32,32,32,32	0
32	MG	0	8021	1/1	0.98	0.11	25,25,25,25	0
34	SR	0	8940	1/1	0.98	0.11	77,77,77,77	0
34	SR	0	8963	1/1	0.98	0.05	123,123,123,123	0
32	MG	0	8078	1/1	0.98	0.23	51,51,51,51	0
34	SR	0	8926	1/1	0.98	0.09	109,109,109,109	0
34	SR	S	8961	1/1	0.98	0.05	126,126,126,126	0
32	MG	0	8002	1/1	0.98	0.08	29,29,29,29	0
35	NA	0	8555	1/1	0.98	0.34	50,50,50,50	0
32	MG	0	8018	1/1	0.98	0.14	34,34,34,34	0
32	MG	0	8092	1/1	0.98	0.02	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8005	1/1	0.98	0.22	34,34,34,34	0
35	NA	R	8575	1/1	0.98	0.34	89,89,89,89	0
32	MG	0	8024	1/1	0.98	0.12	96,96,96,96	0
35	NA	0	8551	1/1	0.98	0.15	55,55,55,55	0
34	SR	0	8908	1/1	0.98	0.13	77,77,77,77	0
32	MG	0	8053	1/1	0.98	0.05	45,45,45,45	0
32	MG	0	8014	1/1	0.98	0.19	21,21,21,21	0
32	MG	0	8009	1/1	0.98	0.21	24,24,24,24	0
32	MG	0	8087	1/1	0.98	0.09	26,26,26,26	0
34	SR	0	8936	1/1	0.98	0.08	87,87,87,87	0
32	MG	0	8034	1/1	0.98	0.13	53,53,53,53	0
34	SR	0	8901	1/1	0.98	0.14	63,63,63,63	0
32	MG	0	8006	1/1	0.98	0.13	20,20,20,20	0
34	SR	B	8950	1/1	0.98	0.16	113,113,113,113	0
34	SR	0	8958	1/1	0.98	0.07	114,114,114,114	0
34	SR	0	8921	1/1	0.98	0.09	75,75,75,75	0
37	CD	O	8705	1/1	0.98	0.08	93,93,93,93	0
34	SR	0	8923	1/1	0.98	0.12	85,85,85,85	0
36	K	M	8402	1/1	0.98	0.11	60,60,60,60	0
34	SR	0	8992	1/1	0.98	0.08	130,130,130,130	0
35	NA	0	8568	1/1	0.98	0.10	38,38,38,38	0
34	SR	0	8951	1/1	0.98	0.09	139,139,139,139	0
34	SR	0	8938	1/1	0.98	0.07	164,164,164,164	0
34	SR	0	8941	1/1	0.98	0.18	122,122,122,122	0
32	MG	0	8073	1/1	0.98	0.06	51,51,51,51	0
35	NA	0	8542	1/1	0.98	0.16	51,51,51,51	0
34	SR	0	8935	1/1	0.98	0.09	87,87,87,87	0
35	NA	0	8520	1/1	0.98	0.10	39,39,39,39	0
35	NA	0	8558	1/1	0.98	0.22	44,44,44,44	0
32	MG	0	8023	1/1	0.98	0.18	24,24,24,24	0
34	SR	0	8911	1/1	0.98	0.06	79,79,79,79	0
32	MG	0	8017	1/1	0.98	0.10	20,20,20,20	0
32	MG	0	8066	1/1	0.98	0.31	75,75,75,75	0
34	SR	0	8909	1/1	0.98	0.13	89,89,89,89	0
34	SR	0	8918	1/1	0.99	0.09	71,71,71,71	0
32	MG	0	8019	1/1	0.99	0.15	23,23,23,23	0
32	MG	0	8038	1/1	0.99	0.05	61,61,61,61	0
32	MG	0	8084	1/1	0.99	0.14	24,24,24,24	0
32	MG	0	8072	1/1	0.99	0.08	47,47,47,47	0
32	MG	0	8030	1/1	0.99	0.34	86,86,86,86	0
32	MG	0	8070	1/1	0.99	0.10	40,40,40,40	0
32	MG	0	8077	1/1	0.99	0.10	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	8045	1/1	0.99	0.10	24,24,24,24	0
32	MG	0	8044	1/1	0.99	0.14	52,52,52,52	0
35	NA	0	8512	1/1	0.99	0.08	36,36,36,36	0
32	MG	0	8056	1/1	0.99	0.08	75,75,75,75	0
34	SR	0	8905	1/1	0.99	0.23	62,62,62,62	0
32	MG	0	8085	1/1	0.99	0.12	67,67,67,67	0
34	SR	0	9008	1/1	0.99	0.17	97,97,97,97	0
32	MG	0	8012	1/1	0.99	0.14	15,15,15,15	0
34	SR	0	8902	1/1	0.99	0.16	67,67,67,67	0
34	SR	0	8966	1/1	0.99	0.07	97,97,97,97	0
32	MG	0	8061	1/1	0.99	0.18	19,19,19,19	0
35	NA	0	8524	1/1	0.99	0.40	54,54,54,54	0
32	MG	0	8048	1/1	0.99	0.21	20,20,20,20	0
32	MG	0	8058	1/1	0.99	0.06	22,22,22,22	0
33	CL	B	8819	1/1	0.99	0.15	59,59,59,59	0
33	CL	M	8818	1/1	0.99	0.05	39,39,39,39	0
33	CL	0	8813	1/1	0.99	0.03	46,46,46,46	0
34	SR	A	8930	1/1	0.99	0.07	125,125,125,125	0
32	MG	0	8013	1/1	0.99	0.04	24,24,24,24	0
32	MG	0	8031	1/1	0.99	0.23	52,52,52,52	0
32	MG	0	8001	1/1	0.99	0.12	26,26,26,26	0
32	MG	0	8079	1/1	0.99	0.11	36,36,36,36	0
35	NA	0	8502	1/1	0.99	0.05	56,56,56,56	0
34	SR	0	8934	1/1	0.99	0.09	99,99,99,99	0
34	SR	1	8913	1/1	0.99	0.11	100,100,100,100	0
32	MG	0	8022	1/1	0.99	0.12	17,17,17,17	0
35	NA	0	8569	1/1	0.99	0.20	67,67,67,67	0
32	MG	0	8003	1/1	0.99	0.17	22,22,22,22	0
35	NA	0	8517	1/1	0.99	0.15	21,21,21,21	0
32	MG	0	8015	1/1	0.99	0.13	25,25,25,25	0
34	SR	0	8933	1/1	0.99	0.07	126,126,126,126	0
35	NA	0	8523	1/1	0.99	0.11	51,51,51,51	0
34	SR	0	8949	1/1	0.99	0.05	102,102,102,102	0
35	NA	0	8514	1/1	0.99	0.19	17,17,17,17	0
32	MG	9	8074	1/1	0.99	0.05	63,63,63,63	0
35	NA	9	8543	1/1	0.99	0.11	38,38,38,38	0
33	CL	0	8811	1/1	0.99	0.38	79,79,79,79	0
35	NA	C	8503	1/1	0.99	0.17	45,45,45,45	0
32	MG	0	8008	1/1	0.99	0.14	26,26,26,26	0
33	CL	O	8808	1/1	0.99	0.11	87,87,87,87	0
32	MG	0	8076	1/1	0.99	0.11	27,27,27,27	0
32	MG	0	8059	1/1	0.99	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8531	1/1	0.99	0.10	15,15,15,15	0
33	CL	0	8805	1/1	0.99	0.14	70,70,70,70	0
34	SR	0	8925	1/1	0.99	0.15	94,94,94,94	0
34	SR	0	8906	1/1	1.00	0.20	64,64,64,64	0
34	SR	0	8903	1/1	1.00	0.13	46,46,46,46	0
32	MG	0	8028	1/1	1.00	0.13	19,19,19,19	0
35	NA	0	8537	1/1	1.00	0.17	29,29,29,29	0
34	SR	1	8952	1/1	1.00	0.11	72,72,72,72	0
32	MG	0	8011	1/1	1.00	0.21	24,24,24,24	0
32	MG	0	8007	1/1	1.00	0.19	18,18,18,18	0
34	SR	0	8907	1/1	1.00	0.12	40,40,40,40	0
34	SR	0	8904	1/1	1.00	0.17	58,58,58,58	0
37	CD	1	8702	1/1	1.00	0.13	61,61,61,61	0
34	SR	0	8954	1/1	1.00	0.12	103,103,103,103	0
32	MG	0	8026	1/1	1.00	0.04	27,27,27,27	0
34	SR	R	8912	1/1	1.00	0.12	86,86,86,86	0
34	SR	9	8978	1/1	1.00	0.07	125,125,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.