



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 16, 2017 – 08:27 PM EDT

PDB ID : 3CCQ
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U
Authors : Blaha, G.; Gurel, G.
Deposited on : unknown
Resolution : 2.90 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

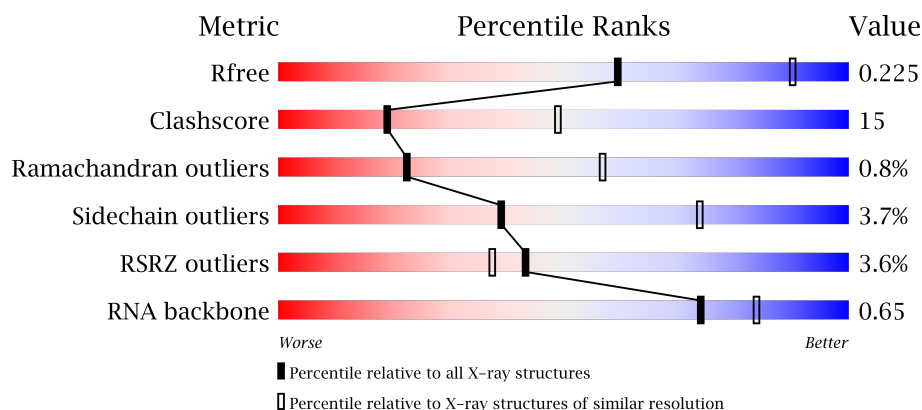
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (2.90-2.90)
RNA backbone	2435	1004 (3.20-2.60)

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. 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>71% 25% . .</div> </div>
2	B	338	<div> <div>.%</div> <div>68% 29% .</div> </div>
3	C	246	<div> <div>2%</div> <div>72% 26% .</div> </div>
4	D	177	<div> <div>28%</div> <div>40% 37% . 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
32	MG	0	8009	-	-	-	X
32	MG	0	8014	-	-	-	X
32	MG	0	8028	-	-	-	X
32	MG	0	8041	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8084	-	-	-	X
32	MG	0	8085	-	-	-	X
32	MG	A	8051	-	-	-	X
34	SR	0	8903	-	-	-	X
34	SR	0	8904	-	-	-	X
34	SR	0	8949	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8521	-	-	-	X
35	NA	0	8527	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8530	-	-	-	X
35	NA	0	8542	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8547	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8556	-	-	-	X
35	NA	0	8559	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8563	-	-	-	X
35	NA	0	8564	-	-	-	X
35	NA	0	8565	-	-	-	X
35	NA	0	8567	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	R	8575	-	-	-	X
37	K	0	8401	-	-	-	X
37	K	0	8402	-	-	-	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	10870	19055	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	87	Total	Mg	0	0
			87	87		
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	1	Total	Mg	0	0
			1	1		
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	9	Total Cl 9 9	0	0
33	J	3	Total Cl 3 3	0	0
33	Q	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	93	Total Sr 93 93	0	0
34	1	2	Total Sr 2 2	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	3	Total Sr 3 3	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	S	1	Total Sr 1 1	0	0

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

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

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

- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	O	1	Total	Cd	0	0
			1	1		
36	Z	1	Total	Cd	0	0
			1	1		
36	1	1	Total	Cd	0	0
			1	1		
36	3	1	Total	Cd	0	0
			1	1		
36	U	1	Total	Cd	0	0
			1	1		

- Molecule 37 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
37	0	2	Total K 2 2	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	168	Total O 168 168	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	17	Total O 17 17	0	0
38	H	65	Total O 65 65	0	0
38	I	5	Total O 5 5	0	0
38	J	56	Total O 56 56	0	0
38	K	60	Total O 60 60	0	0
38	L	82	Total O 82 82	0	0
38	M	123	Total O 123 123	0	0
38	N	59	Total O 59 59	0	0
38	O	47	Total O 47 47	0	0
38	P	59	Total O 59 59	0	0
38	Q	47	Total O 47 47	0	0
38	R	76	Total O 76 76	0	0
38	S	33	Total O 33 33	0	0

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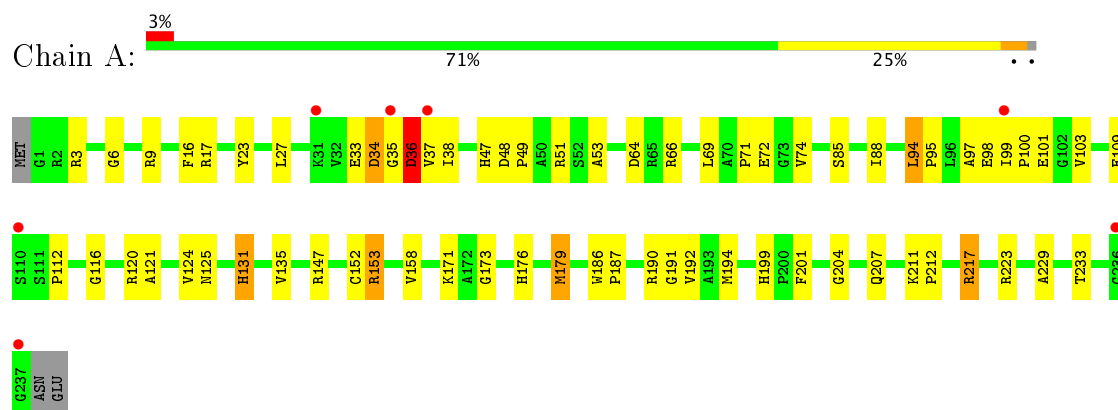
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	12	Total 12	O 12	0	0
38	W	66	Total 66	O 66	0	0
38	X	28	Total 28	O 28	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	31	Total 31	O 31	0	0
38	1	54	Total 54	O 54	0	0
38	2	43	Total 43	O 43	0	0
38	3	68	Total 68	O 68	0	0
38	0	5950	Total 5950	O 5950	0	0
38	9	148	Total 148	O 148	0	0

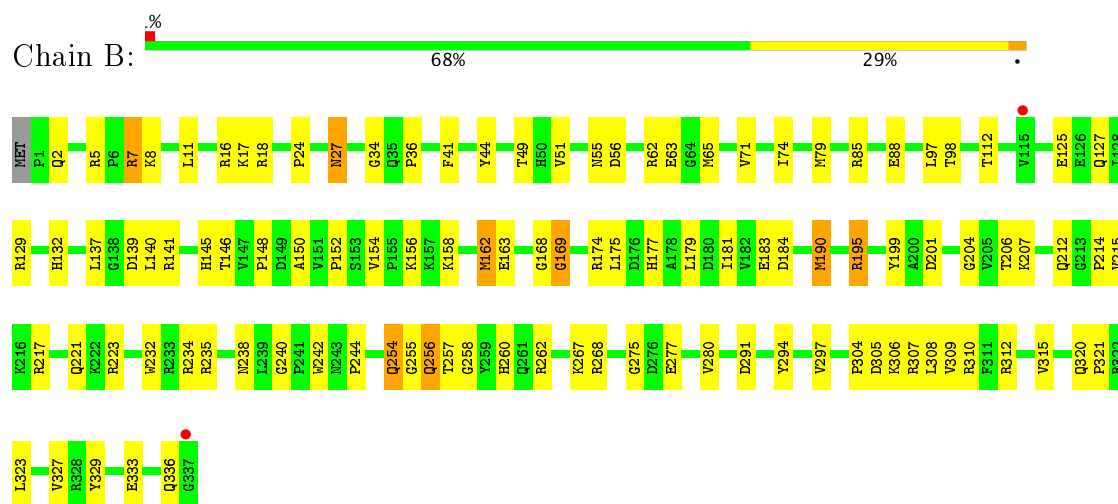
3 Residue-property plots [i](#)

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

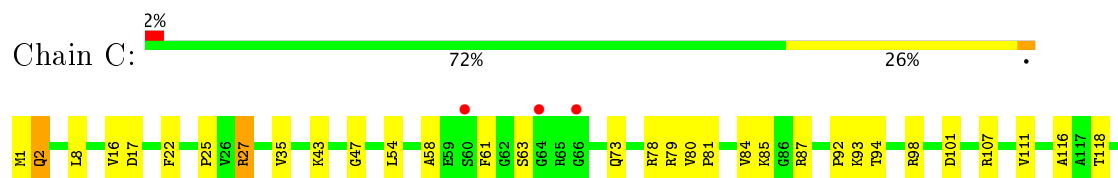
- Molecule 1: 50S ribosomal protein L2P

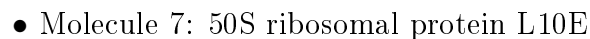
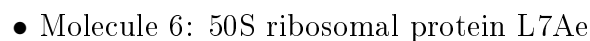
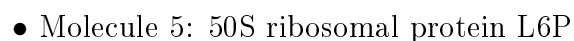
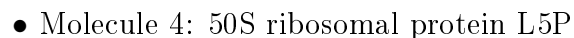


- Molecule 2: 50S ribosomal protein L3P



- Molecule 3: 50S ribosomal protein L4P





PRO	GLU	GLY	ASP	THR	GLY	VAL	ASP	PRO	GLY	PRO	GLY	PHE	VAL	GLY	GLU	LEU	GLN	SER	VAL	GLY	ALA	ASP	ALA	ARG	ILE	GLN	GLU	GLY	SER	TYR	ILE	ARG	SER	GLN	VAL	LEU	SER	GLN	ALA	ASP	THR	VAL	LEU	ASP	THR	GLY	GLU	VAL	GLU	SER	ASN	VAL	LEU	ASN	GLY	LEU	GLY	ILE	PRO	GLN			
LYS	GLU	VAL	GLY	LEU	ASP	LEU	ASP	ARG	LEU	ALA	VAL	PHE	ALA	ASP	GLY	VAL	LEU	PHE	GLU	PRO	GLU	VAL	VAL	LEU	ASP	ILE	ASP	GLU	GLY	TYR	ASP	ARG	SER	GLN	VAL	ASP	ILE	ALA	GLN	ALA	GLY	ARG	ALA	ASP	PHE	ASN	LEU	SER	VAL	GLU	ASN	VAL	THR	THR	THR	ALA	PRO	THR	MET	ILE	GLU	PRO	GLN
SER	ALA	ARG	GLY	ASN	ALA	LYS	ASP	LEU	SER	LEU	ALA	GLN	ALA	ALA	ILE	ALA	ASP	ALA	ASP	PRO	GLU	VAL	VAL	GLU	VAL	SER	LYS	ASP	ASP	ASP	ALA	GLN	VAL	ASP	ARG	ALA	GLY	ILE	ASP	GLU	GLY	LEU	PRO	GLU	LEU	TYR	GLY	GLN	VAL	VAL	GLU	ASN	GLY	ASP	THR	ALA	ALA	THR	GLY	GLU	GLU		
PRO	THR	ASP	ASP	GLN	ASP	ASP	ASP	THR	ASP	THR	ALA	SER	GLU	ASP	ASP	ALA	ASP	ALA	ASP	ASP	ALA	VAL	GLU	GLU	ASP	ALA	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLU	ASP	ASP	GLY	ALA	GLY	ILE	ASP	GLU	GLY	LEU	LEU	SER	ASN	VAL	THR	THR	THR	ALA	ASP	THR	ALA	THR	GLY	GLU	GLU	PRO	PHE		

• Molecule 8: 50S ribosomal protein L10e



MET	ALA	SER	ASP	ARG	VAL	P5	D114	P15	I123	R19	E21	Y22	T26	G28	S29	K30	I31	A32	K39	Q40	Y46	P47	V48	L52	Q59	L60	R61	H62	G63	S64	L65	E66	R69	A72	H73	R74	K87	R91	R99	E100	M101	K102	GLN	ALA	THR	GLY	ALA	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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• Molecule 9: 50S ribosomal protein L11P



MET	ALA	GLY	THR	ILE	GLU	VAL	LEU	VAL	PRO	GLY	GLY	ALA	ASN	PRO	GLY	PRO	PRO	LEU	GLY	PRO	THR	VAL	ASP	VAL	GLN	VAL	VAL	GLN	GLU	ILE	ASN	ASP	GLN	THR	ALA	ALA	PHE	ASP	GLY	THR	GLU	VAL	PRO	VAL	THR	VAL	VAL	LYS	TYR	ASP	ASP	GLY																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
SER	PHE	GLU	ILE	GLU	VAL	G66	V67	P68	P69	T70	A71	L73	I74	K75	D76	E77	A78	G79	F80	E81	T82	G83	S84	G85	E86	P87	Q88	E89	D90	F91	V92	A93	D94	V97	D98	Q99	V100	K101	Q102	I103	A104	E105	Q106	K107	H108	P109	D110	L111	L112	S113	Y114	A120	K121	V124	G125																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
T126	C127	T128	S129	L130	G131	V132	T133	I134	E135	GLY	GLU	ASN	PRO	ARG	GLU	PHE	LYS	GLU	ARG	ILE	ASP	ALA	GLY	GLU	TYR	ASP	ASP	VAL	PHE	ALA	ALA	ALA	GLU	ALA	GLN	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												

• Molecule 10: 50S ribosomal protein L13P



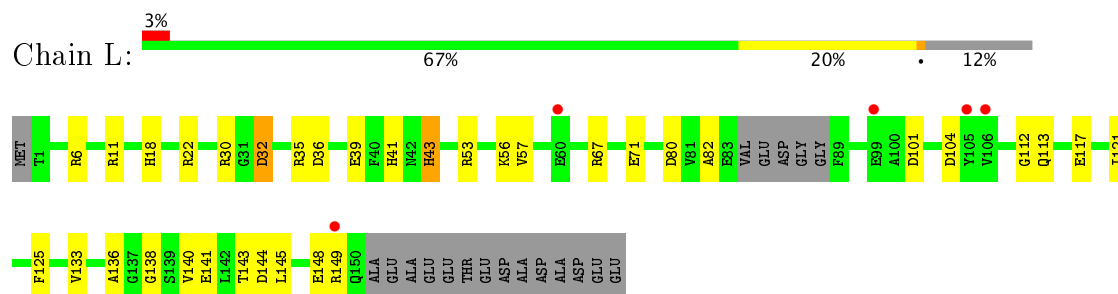
MET	SER	VAL	A4	E5	I18	M19	V39	N40	A41	E42	V45	I46	S33	T47	Q52	I53	V54	R60	Y69	P70	R74	P75	D76	G77	I78	F79	T82	P88	H89	K90	L105	G106	M107	P108	Y109	L121	I127	V130	T131	L132	S136	E137	T138	W145
-----	-----	-----	----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------

• Molecule 11: 50S ribosomal protein L14P

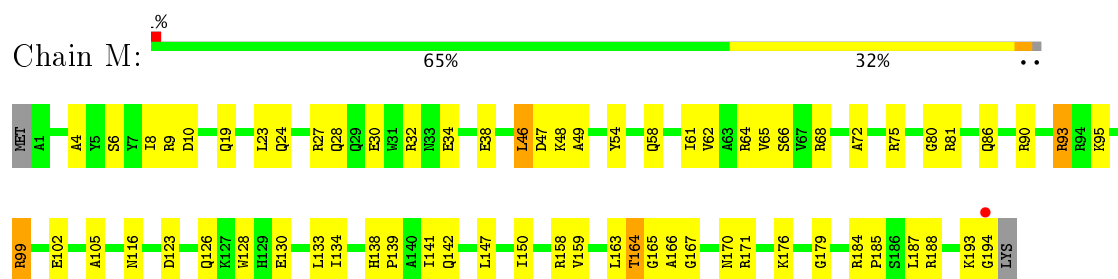


H1	L4	D7	Q10	K14	C20	L29	I32	S33	V34	G39	T40	K41	N42	P45	R46	A47	V55	S56	E63	M64	R65	R66	Q67	V74	R75	K78	P79	I80	R81	R87	V88	K89	V98	E102	I113	E116	V117	A118	A125	S126	
A127	M130	I131	V132																																						

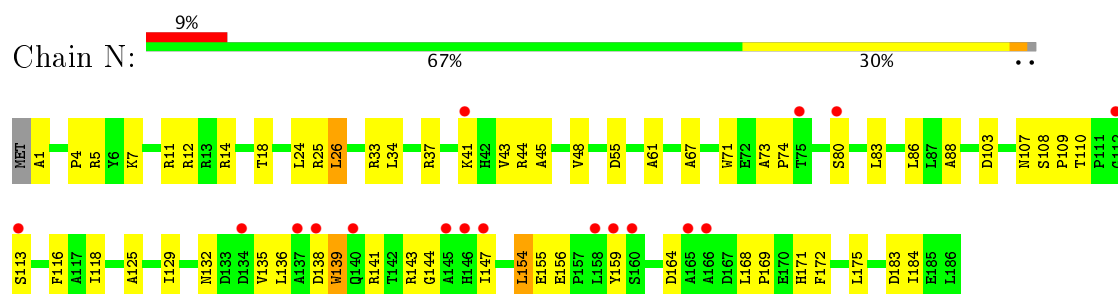
- Molecule 12: 50S ribosomal protein L15P



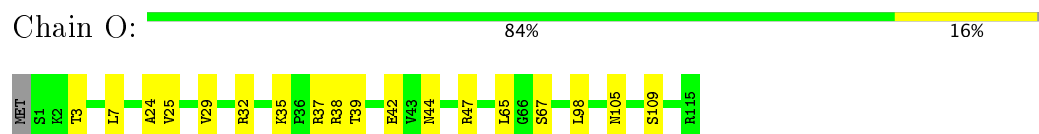
- Molecule 13: 50S ribosomal protein L15e



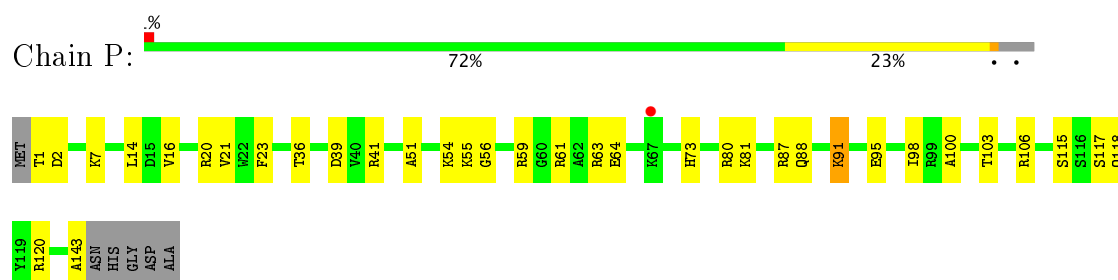
- Molecule 14: 50S ribosomal protein L18P



- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e



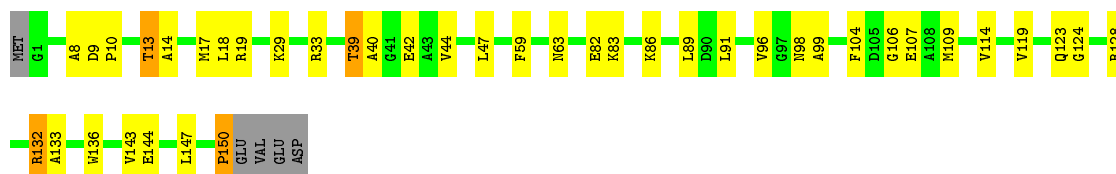
- Molecule 17: 50S ribosomal protein L21e

Chain Q:  72% 25% ..




- Molecule 18: 50S ribosomal protein L22P

Chain R:  70% 24% . .




- Molecule 19: 50S ribosomal protein L23P

Chain S:  2% 75% 20% 5%



- Molecule 20: 50S ribosomal protein L24P

Chain T:  3% 80% 18% ..



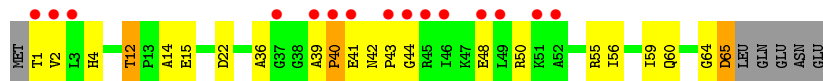
- Molecule 21: 50S ribosomal protein L24e

Chain U:  0% 51% 27% 21%



- Molecule 22: 50S ribosomal protein L29P

Chain V:  21% 61% 27% 8%



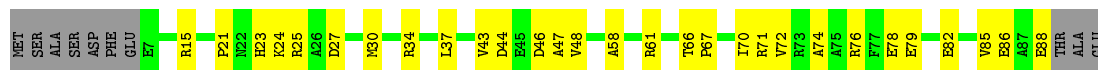
- Molecule 23: 50S ribosomal protein L30P

Chain W:  57% 42%

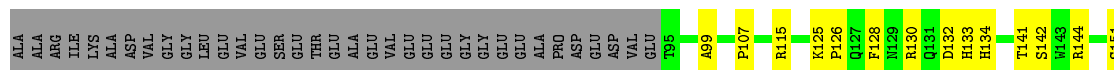




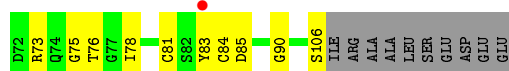
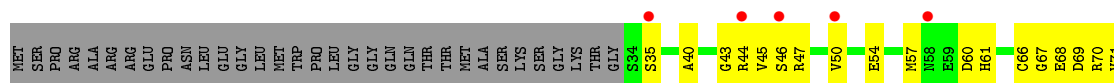
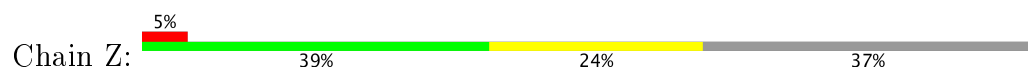
- Molecule 24: 50S ribosomal protein L31e



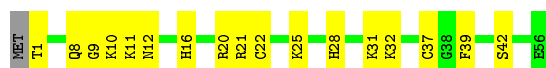
- Molecule 25: 50S ribosomal protein L32e



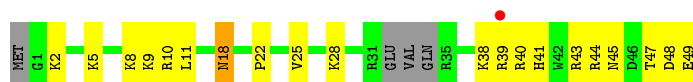
- Molecule 26: 50S ribosomal protein L37Ae



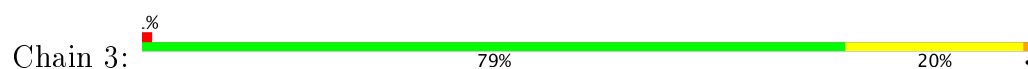
- Molecule 27: 50S ribosomal protein L37e



- Molecule 28: 50S ribosomal protein L39e

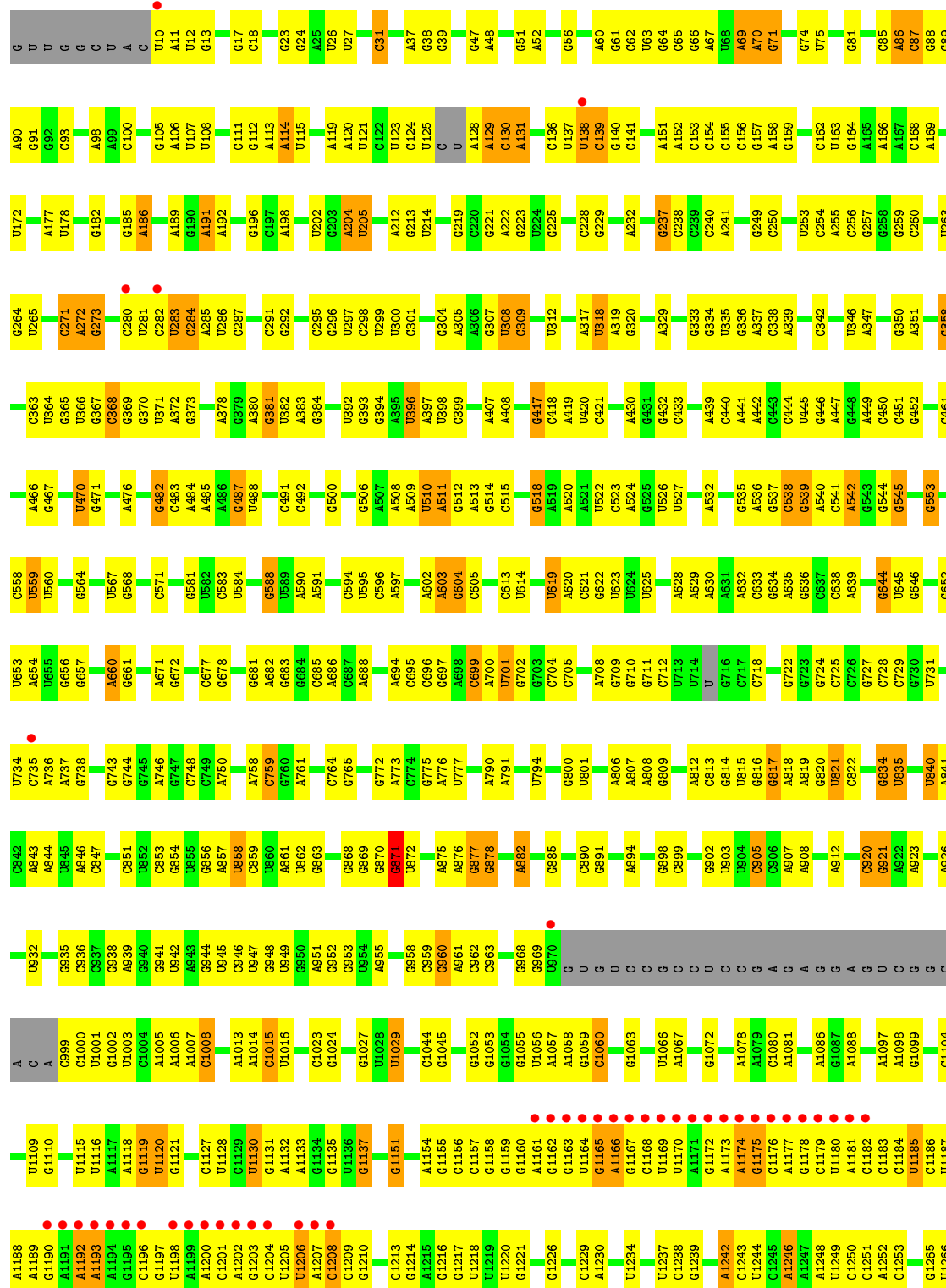


- Molecule 29: 50S ribosomal protein L44E

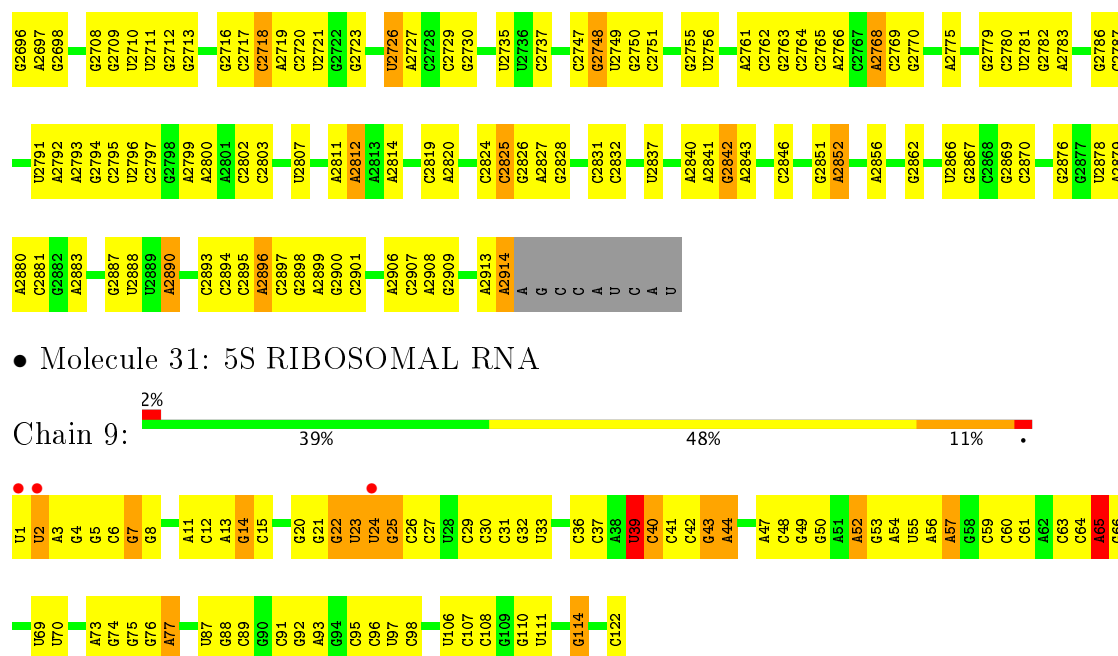




• Molecule 30: 23S RIBOSOMAL RNA



C2503	C2502	G2412	A2321	G	C2105	G2000	A1909	U1825	C1731	G1555	C1456	U1359	C1267
C2504	A2503	G2413	C2326	C	C2106	G2001	A1915	C1826	A1732	A1559	C1457	C1360	C1268
C2505	G2504	A2414	A2238	G	G2110	C2002	U1915	A1829	C1733	U	C1366	C1366	G1269
C2506	G2507	G2415	C2239	G	G2111	U2003	C1916	U1829	C1735	C1561	C1474	C1372	C1273
C2507	G2508	G2416	U2240	G	A2112	U2004	A1919	C1834	A1736	U1562	C1477	A1372	A1278
C2508	C2509	U2419	C2241	U	C2113	G2005	C1920	U1835	U1741	C1563	U1478	C1377	U1279
A2600	C2510	G2420	U2242	A	C2114	C2006	A1921	U1836	A1742	C1564	C1479	C1378	C1289
C2602	G2511	G2421	A2244	C	U2115	A2007	A1922	U1837	U1743	C1565	C1482	U1379	C1290
G2603	C2512	U2422	C2245	C	U2116	U2008	A1923	U1838	U1744	C1566	C1483	U1380	A1291
A2604	G2513	G2426	C2246	C	C2119	G2009	G1925	U1839	U1748	A1573	C1484	U1381	A1294
U2607	U2514	C2426	C2247	G	U2120	A2011	G1926	A1840	U1749	C1574	A1486	U1382	A1296
C2608	C2515	C2426	C2248	G	G2121	U2012	A1927	C1841	C1751	C1575	A1487	U1383	A1297
C2609	C2516	C2426	C2249	C	C2122	G2013	A1930	U1842	G1752	G1576	U1488	U1384	G1295
U2610	G2517	C2426	C2250	U	G2128	A2022	A1931	A1845	A1756	U1577	U1489	A1296	A1296
C2613	C2518	C2426	C2251	G	U2133	C2026	U1939	G1849	A1759	A1581	A1492	U1387	U1297
C2614	G2519	C2426	A2252	G	G2134	U2027	A1942	C1853	C1760	C1586	C1495	U1388	G1300
C2615	C2520	C2426	C2253	C	U2135	U2028	C1943	G1854	U1761	U1587	A1496	A1393	U1304
U2616	U2521	C2426	C2254	G	G2136	U2029	C1944	C1855	C1762	G1588	G1497	C1394	C1305
C2627	U2531	C2450	G2256	C	A	U2030	G1947	A1857	C1763	G1589	U1500	C1395	U1306
C2632	A2532	G2451	C2257	C	G	U2031	G1948	A1858	C1764	C1592	U1501	C1396	A1307
A2633	C2533	G2452	A2258	A	U	G2044	G1949	C1861	U1766	C1593	U1502	C1397	A1308
G2634	C2534	G2453	U2265	C	C	A2054	G1950	C1862	A1767	C1594	A1503	G1398	U1309
C2635	C2535	C2454	A2266	C	G	U2055	G1951	C1863	C1768	C1595	A1504	U1399	U1310
C2636	G2536	U2444	C2269	C	U	C	U	C1864	U1769	C1596	A1505	C1407	U1314
C2637	C2537	U2445	G2270	A	C	U2063	U	C1865	C1770	U1597	U1511	U1408	G1315
C2638	G2538	G2446	C2271	G	C	U2064	A	C1866	U1771	C1598	G1512	G1409	G1316
U2643	U2540	C2462	G2272	C	C	A2067	C	U1867	C1772	C1602	U1513	A1413	A1317
C2644	C2541	G2465	C2273	A	C	U2068	U	U1871	G1773	A1603	A1515	A1414	G1318
A2649	C2542	A2467	A2274	A	G	G2069	C	C1872	G1774	G1604	U1516	G1415	G1319
C2651	G2543	C2468	G2275	C	U	U2070	G	G1873	A1778	G1605	G1416	G1417	C1320
U2652	U2544	A2469	U2276	A	C	C2071	U	U1881	C1779	C1622	U1524	C1423	G1322
C2658	C2545	C2472	U2277	G	U	G2072	C	U1882	C1792	C1623	A1526	A1427	G1325
A2664	A2553	C2476	C2281	U	C	U2073	U	G1883	G1795	U1624	A1527	C1428	C1331
U	U2563	C2477	U2282	C	A	A2074	C	A1884	U1796	U1625	A1528	G1433	G1339
C2667	C2564	C2478	A2291	A	C	U2075	U	A1885	A1797	A1626	G1529	A1434	G1340
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C2671	A2566	C2482	U2297	U	A	A2081	U	U1887	G1799	A1630	C1538	G1441	G1344
C2672	C2567	U2483	C2299	C	U	G2082	G	C1889	C1803	A1631	U1539	G1442	U1350
C2673	U2568	C2484	A2300	U	A	A2083	U	A1890	A1804	C1632	G1543	U1443	G1351
C2676	C2569	U2485	A2301	C	C	C2087	G	U1891	G1805	G1633	U1544	U1444	U1352
A2680	U2570	C2488	C2302	C	U	C2088	G	U1892	C1806	C1634	U1545	U1445	C1353
C2681	C2571	G2489	A2303	C	G	A2089	U	C1893	C1807	C1635	G1546	U1446	U1354
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C2687	C2591	C2495	C2309	C	A	A2101	U	U1903	C1818	C1639	C1558	C1455	C1362
C2688	U2592	C2496	A2311	G	U	G2102	C	A1904	C1819	C1640	C1559	C1456	C1363
C2689	C2593	C2497	C2312	C	C	C2103	C	U1905	G1820	C1641	C1560	C1457	C1364
C2690	U2594	C2498	C2313	U	C	C2104	U	C1906	C1821	C1642	C1561	C1458	C1365
C2691	C2595	C2499	C2314	A	U	C	C	C1907	C1822	C1643	C1562	C1459	C1366
C2692	C2596	C2500	C2315	C	A	C	C	C1908	C1823	C1644	C1563	C1460	C1367
C2693	U2597	C2501	C2316	U	C	C	C	C1909	C1824	C1645	C1564	C1461	C1368
C2694	C2598	C2502	C2317	G	U	C	C	C1910	C1825	C1646	C1565	C1462	C1369
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C2725	U2529	C2533	C2348	C	C	C	C	C1941	C1856	C1677	C1596	C1493	C1400
C2726	C2530	C2534	C2349	C	C	C	C	C1942	C1857	C1678	C1597	C1494	C1401
C2727	C2531	C2535	C2350	C	C	C	C	C1943	C1858	C1679	C1598	C1495	C1402
C2728	U2532	C2536	C2351	C	C	C	C	C1944	C1859	C1680	C1599	C1496	C1403
C2729	C2533	C2537	C2352	C	C	C	C	C1945	C1860	C1681	C1600	C1497	C1404
C2730	C2534	C2538	C2353	C	C	C	C	C1946	C1861	C1682	C1601	C1498	C1405
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C2735	C2539	C2543	C2358	C	C	C	C	C1951	C1866	C1687	C1606	C1503	C1410
C2736	C2540	C2544	C2359	C	C	C	C	C1952	C1867	C1688	C1607	C1504	C1411
C2737	U2541	C2545	C2360	C	C	C	C	C1953	C1868	C1689	C1608	C1505	C1412
C2738	C2542	C2546	C2361	C	C	C	C	C1954	C1869	C1690	C1609	C1506	C1413
C2739	C2543	C2547	C2362	C	C	C	C	C1955	C1870	C1691	C1610	C1507	C1414
C2740	U2544	C2548	C2363	C	C	C	C	C1956	C1871	C1692	C1611	C1508	C1415
C2741	C2545	C2549	C2364	C	C	C	C	C1957	C1872	C1693	C1612	C1509	C1416
C2742	C2546	C2550	C2365	C	C	C	C	C1958	C1873	C1694	C1		



• 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	212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 85.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.90) 98.2 (85.65-2.41)	Depositor EDS
R_{merge}	0.17	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}	0.186 , 0.233 0.182 , 0.225	Depositor DCC
R_{free} test set	3843 reflections (0.99%)	DCC
Wilson B-factor (Å ²)	61.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 82.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 1.50% 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	0.33	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.32	0/1111	0.56	1/1498 (0.1%)
5	E	0.33	0/1382	0.57	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.33	0/241	0.51	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.61	0/1530
11	K	0.34	0/1004	0.66	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.36	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.61	0/1999
15	O	0.35	0/874	0.59	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.09	6/1578 (0.4%)
19	S	0.33	0/648	0.54	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.32	0/417	0.57	0/562
22	V	0.32	0/502	0.54	0/675
23	W	0.36	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.37	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.63	0/781
27	1	0.39	0/438	0.62	0/578
28	2	0.34	0/401	0.58	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.39	0/65954	0.68	9/102862 (0.0%)
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.40	7/98698 (0.0%)	0.67	17/147581 (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
18	R	1	0
23	W	0	1
30	0	0	32
31	9	0	3
All	All	1	36

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	27.45	2.87	1.50
18	R	150	PRO	CA-C	-18.11	1.16	1.52
18	R	150	PRO	CG-CD	13.90	1.96	1.50
18	R	150	PRO	C-O	11.92	1.47	1.23
18	R	150	PRO	N-CA	11.35	1.66	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.81	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.28	128.89	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.52	99.75	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	202	U	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	48	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	66	0
2	B	2625	0	2533	94	0
3	C	1860	0	1813	53	0
4	D	1094	0	1085	52	0
5	E	1357	0	1266	36	0
6	F	890	0	843	30	0
7	G	240	0	231	11	0
8	H	1282	0	1292	41	0
9	I	519	0	500	21	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	33	0
13	M	1558	0	1573	59	0
14	N	1445	0	1401	54	0
15	O	865	0	873	18	0
16	P	1136	0	1123	30	0
17	Q	735	0	729	26	0
18	R	1149	0	1122	32	0
19	S	641	0	605	10	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	17	0
23	W	1196	0	1137	66	0
24	X	654	0	653	22	0
25	Y	1130	0	1133	33	0
26	Z	573	0	531	21	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	728	17	0
30	0	59018	0	29809	1329	0
31	9	2599	0	1325	97	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	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	9	0	0	3	0
33	3	1	0	0	0	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	1	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	Q	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	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	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	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	5950	0	0	203	0
38	1	54	0	0	3	0
38	2	43	0	0	1	0
38	3	68	0	0	6	0
38	9	148	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	112	0	0	5	0
38	B	142	0	0	14	0
38	C	168	0	0	13	0
38	D	45	0	0	4	0
38	E	42	0	0	4	0
38	F	26	0	0	1	0
38	G	17	0	0	1	0
38	H	65	0	0	5	0
38	I	5	0	0	0	0
38	J	56	0	0	2	0
38	K	60	0	0	5	0
38	L	82	0	0	8	0
38	M	123	0	0	2	0
38	N	59	0	0	3	0
38	O	47	0	0	4	0
38	P	59	0	0	2	0
38	Q	47	0	0	2	0
38	R	76	0	0	1	0
38	S	33	0	0	0	0
38	T	36	0	0	4	0
38	U	26	0	0	2	0
38	V	12	0	0	1	0
38	W	66	0	0	6	0
38	X	28	0	0	3	0
38	Y	97	0	0	7	0
38	Z	31	0	0	4	0
All	All	99120	0	59910	2191	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 15.

The worst 5 of 2191 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	1.44
30:0:871:G:C8	30:0:871:G:H5'	1.75	1.21
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.12
31:9:56:A:H2'	31:9:57:A:H5''	1.21	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.79	1.11

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%)	213 (91%)	18 (8%)	4 (2%)	11	36
2	B	335/338 (99%)	309 (92%)	22 (7%)	4 (1%)	15	46
3	C	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
4	D	134/177 (76%)	107 (80%)	22 (16%)	5 (4%)	4	16
5	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
6	F	117/120 (98%)	104 (89%)	9 (8%)	4 (3%)	4	18
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	145 (93%)	11 (7%)	0	100	100
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	12	39
10	J	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	8	30
13	M	192/196 (98%)	182 (95%)	10 (5%)	0	100	100
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	8	29
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
19	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
20	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	20	54
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	5	19
23	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	25	60
24	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	14	43
25	Y	140/241 (58%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	62 (87%)	8 (11%)	1 (1%)	13	41
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	37 (88%)	5 (12%)	0	100	100
29	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4472 (83%)	3416 (92%)	258 (7%)	31 (1%)	22	57

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ASP
1	A	37	VAL
6	F	101	ALA
14	N	154	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	171 (96%)	8 (4%)	32	66
2	B	282/283 (100%)	268 (95%)	14 (5%)	28	62
3	C	193/193 (100%)	180 (93%)	13 (7%)	19	48
4	D	117/148 (79%)	113 (97%)	4 (3%)	42	76
5	E	152/156 (97%)	148 (97%)	4 (3%)	51	83
6	F	93/94 (99%)	91 (98%)	2 (2%)	57	86
7	G	27/282 (10%)	26 (96%)	1 (4%)	39	74
8	H	134/145 (92%)	128 (96%)	6 (4%)	32	66
9	I	58/130 (45%)	56 (97%)	2 (3%)	42	76
10	J	118/121 (98%)	110 (93%)	8 (7%)	18	47
11	K	106/106 (100%)	103 (97%)	3 (3%)	49	82
12	L	113/127 (89%)	108 (96%)	5 (4%)	33	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	151 (96%)	7 (4%)	33	67
14	N	149/150 (99%)	147 (99%)	2 (1%)	73	93
15	O	93/94 (99%)	92 (99%)	1 (1%)	78	94
16	P	113/117 (97%)	111 (98%)	2 (2%)	64	89
17	Q	79/80 (99%)	75 (95%)	4 (5%)	28	62
18	R	117/122 (96%)	112 (96%)	5 (4%)	33	68
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	101 (96%)	4 (4%)	38	73
21	U	44/53 (83%)	42 (96%)	2 (4%)	32	66
22	V	51/57 (90%)	48 (94%)	3 (6%)	23	55
23	W	130/130 (100%)	127 (98%)	3 (2%)	56	85
24	X	66/74 (89%)	63 (96%)	3 (4%)	32	66
25	Y	120/196 (61%)	116 (97%)	4 (3%)	43	77
26	Z	60/94 (64%)	59 (98%)	1 (2%)	66	89
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	54	84
29	3	79/79 (100%)	78 (99%)	1 (1%)	73	93
All	All	3095/3646 (85%)	2982 (96%)	113 (4%)	39	74

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	173	GLU
11	K	10	GLN
24	X	46	ASP
9	I	110	ASP
10	J	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	88	GLN
27	1	28	HIS
13	M	137	ASN

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Mol	Chain	Res	Type
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	22 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	23 (0%)

5 of 260 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	1246	A
30	0	1377	C
30	0	2718	C
30	0	1352	A
30	0	1474	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	OMU	0	2587	30	14,22,23	0.98	1 (7%)	18,31,34	3.69	2 (11%)
30	OMG	0	2588	30	18,26,27	1.05	1 (5%)	22,38,41	2.46	5 (22%)
30	UR3	0	2619	30	14,22,23	0.73	0	16,32,35	0.75	0
30	PSU	0	2621	30	16,21,22	1.58	3 (18%)	20,30,33	6.13	5 (25%)
30	1MA	0	628	30,35	16,25,26	1.06	1 (6%)	13,37,40	1.25	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	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	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'	-4.88	1.48	1.52
30	0	2621	PSU	C2-N1	2.26	1.42	1.38
30	0	2621	PSU	C4-N3	2.61	1.37	1.33
30	0	2587	OMU	C4-N3	2.64	1.37	1.33
30	0	628	1MA	C6-N6	2.71	1.33	1.27

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-19.11	114.66	128.40
30	0	2621	PSU	C5-C4-N3	-13.03	114.74	125.43
30	0	2588	OMG	C5-C6-N1	-8.30	111.66	123.48
30	0	628	1MA	C2-N3-C4	-3.78	110.61	116.41
30	0	2587	OMU	C5-C4-N3	-3.56	114.63	123.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	237/240 (98%)	-0.22	7 (2%) 51 44	34, 56, 94, 116	0
2	B	337/338 (99%)	-0.42	2 (0%) 89 88	34, 58, 89, 99	0
3	C	246/246 (100%)	-0.24	4 (1%) 72 70	32, 51, 75, 87	0
4	D	140/177 (79%)	1.64	50 (35%) 0 0	69, 106, 134, 144	0
5	E	172/178 (96%)	-0.10	9 (5%) 28 23	49, 73, 97, 102	0
6	F	119/120 (99%)	-0.01	6 (5%) 30 25	52, 76, 109, 124	0
7	G	29/348 (8%)	0.52	2 (6%) 18 13	79, 103, 110, 113	0
8	H	160/177 (90%)	-0.34	2 (1%) 77 76	53, 73, 107, 111	0
9	I	70/162 (43%)	3.81	49 (70%) 0 0	137, 155, 173, 175	0
10	J	142/145 (97%)	-0.65	0 100 100	43, 57, 77, 99	0
11	K	132/132 (100%)	-0.62	0 100 100	39, 54, 79, 83	0
12	L	145/165 (87%)	0.33	5 (3%) 46 39	32, 71, 123, 134	0
13	M	194/196 (98%)	-0.48	1 (0%) 90 90	35, 49, 64, 71	0
14	N	186/187 (99%)	0.24	17 (9%) 10 7	51, 74, 121, 131	0
15	O	115/116 (99%)	-0.49	0 100 100	44, 61, 78, 85	0
16	P	143/149 (95%)	-0.42	1 (0%) 87 86	47, 61, 74, 83	0
17	Q	95/96 (98%)	-0.49	0 100 100	44, 55, 72, 85	0
18	R	150/155 (96%)	-0.50	0 100 100	37, 51, 73, 84	0
19	S	81/85 (95%)	-0.05	2 (2%) 58 53	49, 64, 87, 97	0
20	T	119/120 (99%)	-0.17	3 (2%) 58 53	42, 62, 92, 121	0
21	U	53/67 (79%)	0.01	1 (1%) 67 64	51, 64, 83, 91	0
22	V	65/71 (91%)	1.07	15 (23%) 1 0	53, 76, 130, 134	0
23	W	154/154 (100%)	-0.69	0 100 100	41, 56, 74, 88	0
24	X	82/92 (89%)	-0.31	0 100 100	49, 66, 91, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	-0.51	1 (0%) 87 86	34, 48, 72, 94	0
26	Z	73/116 (62%)	0.19	6 (8%) 12 9	59, 77, 92, 101	0
27	1	56/57 (98%)	-0.24	0 100 100	33, 39, 48, 56	0
28	2	46/50 (92%)	-0.14	1 (2%) 62 59	41, 69, 102, 114	0
29	3	92/92 (100%)	-0.13	1 (1%) 80 79	43, 65, 78, 91	0
30	0	2749/2923 (94%)	-0.32	51 (1%) 67 64	28, 51, 95, 171	0
31	9	122/122 (100%)	-0.23	3 (2%) 58 53	45, 72, 95, 154	0
All	All	6646/7517 (88%)	-0.20	239 (3%) 43 37	28, 57, 106, 175	0

The worst 5 of 239 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	71	ALA	15.4
9	I	74	ILE	13.1
31	9	1	U	12.2
22	V	1	THR	11.9
9	I	72	GLU	11.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
30	1MA	0	628	23/24	0.98	0.18	-	33,37,38,39	0
30	OMG	0	2588	24/25	0.99	0.14	-	36,39,42,43	0
30	OMU	0	2587	21/22	0.99	0.13	-	38,40,44,45	0
30	PSU	0	2621	20/21	0.98	0.18	-	34,35,47,48	0
30	UR3	0	2619	21/22	0.98	0.15	-	42,44,47,47	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
35	NA	0	8565	1/1	0.87	1.24	97.52	79,79,79,79	0
35	NA	0	8547	1/1	0.91	0.70	73.51	80,80,80,80	0
35	NA	0	8562	1/1	0.69	1.31	72.93	78,78,78,78	0
35	NA	0	8560	1/1	0.19	0.89	36.93	101,101,101,101	0
37	K	0	8401	1/1	0.41	0.78	30.06	128,128,128,128	0
35	NA	0	8564	1/1	0.93	0.39	27.90	68,68,68,68	0
35	NA	0	8555	1/1	0.96	0.81	25.22	75,75,75,75	0
35	NA	9	8572	1/1	0.96	0.89	21.13	81,81,81,81	0
35	NA	0	8559	1/1	0.92	0.29	16.79	91,91,91,91	0
35	NA	0	8528	1/1	0.65	0.55	13.46	66,66,66,66	0
35	NA	0	8553	1/1	0.98	0.46	12.64	65,65,65,65	0
32	MG	0	8085	1/1	0.98	0.53	12.56	97,97,97,97	0
34	SR	B	8987	1/1	0.80	0.56	10.79	200,200,200,200	0
35	NA	0	8521	1/1	0.91	0.39	9.53	61,61,61,61	0
35	NA	0	8542	1/1	0.96	0.45	9.03	49,49,49,49	0
35	NA	0	8567	1/1	0.88	0.36	8.01	76,76,76,76	0
35	NA	0	8556	1/1	0.96	0.82	7.68	64,64,64,64	0
34	SR	0	8903	1/1	1.00	0.19	7.63	59,59,59,59	0
32	MG	A	8051	1/1	0.93	0.65	7.37	70,70,70,70	0
35	NA	0	8546	1/1	0.84	0.40	7.31	65,65,65,65	0
32	MG	0	8047	1/1	0.96	0.32	6.31	51,51,51,51	0
35	NA	0	8527	1/1	0.81	0.27	5.82	71,71,71,71	0
35	NA	0	8563	1/1	0.69	0.28	4.99	88,88,88,88	0
34	SR	0	8949	1/1	0.98	0.16	4.90	122,122,122,122	0
35	NA	R	8575	1/1	0.93	0.25	4.29	99,99,99,99	0
32	MG	0	8014	1/1	0.95	0.20	3.99	33,33,33,33	0
32	MG	0	8009	1/1	0.98	0.25	3.75	36,36,36,36	0
35	NA	0	8530	1/1	0.74	0.32	3.55	59,59,59,59	0
37	K	0	8402	1/1	0.98	0.25	3.53	76,76,76,76	0
32	MG	0	8041	1/1	0.96	0.21	3.23	29,29,29,29	0
34	SR	0	8904	1/1	0.99	0.18	3.08	65,65,65,65	0
32	MG	0	8028	1/1	0.98	0.16	2.27	26,26,26,26	0
32	MG	0	8084	1/1	0.99	0.15	2.17	33,33,33,33	0
35	NA	M	8539	1/1	0.99	0.18	1.97	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	A	8929	1/1	0.92	0.23	1.84	144,144,144,144	0
35	NA	0	8537	1/1	0.95	0.18	1.65	38,38,38,38	0
34	SR	0	8918	1/1	0.99	0.15	1.59	80,80,80,80	0
32	MG	0	8003	1/1	0.96	0.19	1.54	45,45,45,45	0
32	MG	0	8004	1/1	1.00	0.19	1.41	32,32,32,32	0
34	SR	0	8944	1/1	0.79	0.14	1.21	169,169,169,169	0
35	NA	0	8558	1/1	0.97	0.23	1.14	49,49,49,49	0
32	MG	0	8088	1/1	0.98	0.21	1.12	52,52,52,52	0
34	SR	R	8912	1/1	0.99	0.17	0.80	92,92,92,92	0
34	SR	0	8985	1/1	0.90	0.13	0.72	134,134,134,134	0
32	MG	0	8044	1/1	0.92	0.16	0.60	50,50,50,50	0
32	MG	K	8054	1/1	0.99	0.16	0.39	46,46,46,46	0
35	NA	C	8503	1/1	0.97	0.21	0.28	36,36,36,36	0
35	NA	0	8519	1/1	0.96	0.20	0.28	43,43,43,43	0
35	NA	0	8515	1/1	0.94	0.20	0.26	41,41,41,41	0
35	NA	0	8504	1/1	0.88	0.18	0.22	44,44,44,44	0
32	MG	0	8053	1/1	0.95	0.20	0.15	47,47,47,47	0
32	MG	0	8011	1/1	0.92	0.23	0.08	25,25,25,25	0
35	NA	0	8568	1/1	0.79	0.21	0.02	52,52,52,52	0
35	NA	J	8538	1/1	0.83	0.18	-0.02	56,56,56,56	0
32	MG	0	8034	1/1	0.98	0.16	-0.07	46,46,46,46	0
32	MG	0	8010	1/1	0.99	0.22	-0.15	45,45,45,45	0
32	MG	0	8015	1/1	0.99	0.13	-0.20	30,30,30,30	0
34	SR	0	8992	1/1	0.88	0.15	-0.21	136,136,136,136	0
36	CD	Z	8703	1/1	0.99	0.13	-0.35	75,75,75,75	0
34	SR	0	8972	1/1	0.90	0.14	-0.54	146,146,146,146	0
33	CL	J	8821	1/1	0.95	0.14	-0.63	67,67,67,67	0
36	CD	1	8702	1/1	0.99	0.13	-0.66	67,67,67,67	0
32	MG	0	8002	1/1	0.97	0.15	-0.67	36,36,36,36	0
32	MG	0	8067	1/1	0.83	0.16	-0.75	40,40,40,40	0
34	SR	0	8975	1/1	0.91	0.14	-0.77	130,130,130,130	0
35	NA	0	8517	1/1	0.99	0.15	-0.93	31,31,31,31	0
32	MG	0	8062	1/1	0.91	0.15	-1.12	59,59,59,59	0
35	NA	Q	8540	1/1	0.78	0.11	-1.14	64,64,64,64	0
35	NA	0	8569	1/1	0.93	0.15	-1.15	48,48,48,48	0
36	CD	3	8704	1/1	1.00	0.10	-1.17	74,74,74,74	0
35	NA	0	8520	1/1	0.95	0.07	-1.19	49,49,49,49	0
32	MG	T	8057	1/1	0.94	0.12	-1.22	60,60,60,60	0
32	MG	0	8058	1/1	1.00	0.10	-1.22	22,22,22,22	0
32	MG	0	8043	1/1	0.99	0.06	-1.23	52,52,52,52	0
34	SR	1	8913	1/1	0.97	0.14	-1.41	95,95,95,95	0
32	MG	0	8025	1/1	0.98	0.12	-1.42	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8936	1/1	0.91	0.11	-1.42	94,94,94,94	0
34	SR	F	9005	1/1	0.99	0.08	-1.45	133,133,133,133	0
34	SR	0	8902	1/1	0.99	0.17	-1.55	66,66,66,66	0
36	CD	U	8701	1/1	0.99	0.10	-1.57	63,63,63,63	0
34	SR	0	8935	1/1	0.99	0.09	-1.62	79,79,79,79	0
35	NA	0	8534	1/1	0.97	0.14	-1.65	44,44,44,44	0
35	NA	0	8533	1/1	0.95	0.10	-1.68	55,55,55,55	0
33	CL	L	8810	1/1	0.94	0.09	-1.84	68,68,68,68	0
32	MG	0	8045	1/1	0.92	0.09	-1.92	44,44,44,44	0
33	CL	O	8808	1/1	0.91	0.08	-1.93	70,70,70,70	0
32	MG	0	8012	1/1	0.98	0.14	-2.02	18,18,18,18	0
35	NA	0	8557	1/1	0.82	0.06	-2.02	53,53,53,53	0
34	SR	0	8969	1/1	0.94	0.12	-2.02	159,159,159,159	0
33	CL	M	8818	1/1	0.96	0.09	-2.03	40,40,40,40	0
32	MG	0	8008	1/1	1.00	0.09	-2.10	28,28,28,28	0
32	MG	0	8050	1/1	0.97	0.09	-2.13	32,32,32,32	0
32	MG	0	8016	1/1	0.96	0.14	-2.26	48,48,48,48	0
33	CL	0	8813	1/1	0.93	0.09	-2.26	66,66,66,66	0
35	NA	0	8523	1/1	0.96	0.09	-2.51	50,50,50,50	0
33	CL	0	8816	1/1	0.99	0.08	-2.53	79,79,79,79	0
33	CL	3	8804	1/1	0.98	0.06	-2.60	63,63,63,63	0
35	NA	0	8512	1/1	0.94	0.15	-2.69	52,52,52,52	0
32	MG	0	8056	1/1	0.93	0.11	-2.89	47,47,47,47	0
34	SR	A	8930	1/1	0.99	0.06	-2.98	97,97,97,97	0
32	MG	0	8079	1/1	0.97	0.11	-2.98	51,51,51,51	0
34	SR	0	8948	1/1	0.99	0.10	-3.14	92,92,92,92	0
33	CL	0	8812	1/1	0.98	0.06	-3.18	58,58,58,58	0
35	NA	0	8507	1/1	0.98	0.11	-3.20	37,37,37,37	0
34	SR	0	8943	1/1	0.96	0.04	-3.33	124,124,124,124	0
33	CL	0	8805	1/1	0.98	0.06	-3.47	67,67,67,67	0
32	MG	0	8006	1/1	0.93	0.10	-3.62	32,32,32,32	0
32	MG	0	8021	1/1	0.97	0.05	-3.62	40,40,40,40	0
32	MG	Y	8086	1/1	0.99	0.08	-3.72	44,44,44,44	0
32	MG	0	8001	1/1	0.96	0.11	-3.88	33,33,33,33	0
32	MG	0	8052	1/1	0.98	0.07	-3.98	56,56,56,56	0
32	MG	0	8013	1/1	0.97	0.06	-4.46	25,25,25,25	0
32	MG	0	8065	1/1	0.98	0.06	-4.68	57,57,57,57	0
35	NA	B	8552	1/1	0.98	0.10	-5.15	83,83,83,83	0
34	SR	0	8970	1/1	0.99	0.01	-6.07	123,123,123,123	0
32	MG	0	8075	1/1	0.93	0.03	-6.54	42,42,42,42	0
34	SR	0	8945	1/1	0.97	0.07	-6.57	106,106,106,106	0
34	SR	0	8910	1/1	0.98	0.04	-7.09	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	8984	1/1	0.98	0.03	-9.15	121,121,121,121	0
33	CL	B	8819	1/1	0.98	0.09	-9.73	58,58,58,58	0
32	MG	0	8029	1/1	0.99	0.15	-	49,49,49,49	0
32	MG	0	8089	1/1	0.93	0.17	-	72,72,72,72	0
34	SR	0	8955	1/1	0.68	0.21	-	199,199,199,199	0
34	SR	9	8978	1/1	0.99	0.08	-	135,135,135,135	0
34	SR	0	8967	1/1	0.99	0.06	-	133,133,133,133	0
35	NA	0	8536	1/1	0.91	0.24	-	61,61,61,61	0
33	CL	0	8815	1/1	0.91	0.12	-	77,77,77,77	0
32	MG	0	8035	1/1	0.96	0.10	-	54,54,54,54	0
35	NA	0	8561	1/1	0.94	0.22	-	68,68,68,68	0
34	SR	0	8927	1/1	0.90	0.09	-	153,153,153,153	0
32	MG	0	8092	1/1	0.89	0.18	-	53,53,53,53	0
33	CL	0	8822	1/1	0.97	0.45	-	81,81,81,81	0
34	SR	0	8954	1/1	0.97	0.10	-	109,109,109,109	0
34	SR	0	9002	1/1	0.92	0.29	-	177,177,177,177	0
35	NA	0	8531	1/1	0.97	0.06	-	40,40,40,40	0
32	MG	0	8033	1/1	0.94	0.09	-	55,55,55,55	0
34	SR	0	8966	1/1	0.95	0.10	-	107,107,107,107	0
32	MG	0	8063	1/1	0.98	0.14	-	80,80,80,80	0
32	MG	0	8020	1/1	0.97	0.07	-	40,40,40,40	0
34	SR	0	8923	1/1	0.98	0.11	-	101,101,101,101	0
32	MG	0	8078	1/1	0.98	0.27	-	69,69,69,69	0
32	MG	0	8024	1/1	0.97	0.12	-	49,49,49,49	0
35	NA	0	8550	1/1	0.86	0.96	-	57,57,57,57	0
34	SR	0	8941	1/1	0.98	0.14	-	108,108,108,108	0
32	MG	0	8080	1/1	0.99	0.12	-	75,75,75,75	0
35	NA	0	8549	1/1	0.91	0.51	-	52,52,52,52	0
35	NA	0	8509	1/1	0.70	0.92	-	85,85,85,85	0
32	MG	0	8073	1/1	0.99	0.34	-	73,73,73,73	0
32	MG	0	8083	1/1	0.91	0.10	-	60,60,60,60	0
34	SR	0	8997	1/1	0.84	0.84	-	200,200,200,200	0
34	SR	0	8914	1/1	0.98	0.32	-	120,120,120,120	0
34	SR	0	8920	1/1	0.97	0.08	-	135,135,135,135	0
33	CL	0	8814	1/1	0.94	0.21	-	72,72,72,72	0
32	MG	0	8023	1/1	0.98	0.10	-	37,37,37,37	0
34	SR	0	8905	1/1	1.00	0.27	-	61,61,61,61	0
32	MG	0	8018	1/1	1.00	0.24	-	40,40,40,40	0
32	MG	B	8042	1/1	0.99	0.07	-	44,44,44,44	0
34	SR	0	8938	1/1	0.98	0.02	-	147,147,147,147	0
32	MG	0	8072	1/1	0.81	0.18	-	63,63,63,63	0
33	CL	0	8803	1/1	0.95	0.10	-	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8036	1/1	0.94	0.12	-	56,56,56,56	0
35	NA	0	8501	1/1	0.87	0.08	-	40,40,40,40	0
34	SR	0	8991	1/1	0.64	0.07	-	199,199,199,199	0
33	CL	Y	8820	1/1	0.97	0.04	-	48,48,48,48	0
32	MG	0	8069	1/1	0.98	0.30	-	73,73,73,73	0
35	NA	0	8524	1/1	0.97	0.25	-	58,58,58,58	0
34	SR	0	8981	1/1	0.98	0.34	-	178,178,178,178	0
34	SR	0	8982	1/1	0.73	2.26	-	200,200,200,200	0
34	SR	0	8933	1/1	0.98	0.16	-	139,139,139,139	0
34	SR	0	8921	1/1	0.96	0.15	-	96,96,96,96	0
32	MG	9	8074	1/1	0.84	0.09	-	86,86,86,86	0
34	SR	0	8989	1/1	0.92	0.16	-	168,168,168,168	0
33	CL	A	8809	1/1	0.91	0.11	-	80,80,80,80	0
32	MG	0	8066	1/1	0.92	0.18	-	70,70,70,70	0
32	MG	0	8059	1/1	0.99	0.07	-	57,57,57,57	0
34	SR	0	9006	1/1	-0.20	2.27	-	200,200,200,200	0
35	NA	0	8571	1/1	0.82	0.16	-	76,76,76,76	0
32	MG	0	8060	1/1	0.94	0.08	-	53,53,53,53	0
34	SR	0	8947	1/1	0.54	0.51	-	200,200,200,200	0
34	SR	0	8906	1/1	0.99	0.23	-	64,64,64,64	0
35	NA	0	8573	1/1	0.88	0.35	-	73,73,73,73	0
33	CL	N	8807	1/1	0.93	0.17	-	69,69,69,69	0
35	NA	0	8514	1/1	0.98	0.50	-	56,56,56,56	0
32	MG	0	8070	1/1	0.95	0.12	-	46,46,46,46	0
34	SR	0	8998	1/1	0.82	0.19	-	173,173,173,173	0
32	MG	0	8064	1/1	0.99	0.18	-	44,44,44,44	0
32	MG	0	8082	1/1	0.95	0.78	-	89,89,89,89	0
32	MG	0	8077	1/1	0.93	0.06	-	45,45,45,45	0
32	MG	0	8037	1/1	0.93	0.14	-	88,88,88,88	0
34	SR	3	8999	1/1	0.98	0.10	-	110,110,110,110	0
34	SR	0	8963	1/1	0.96	0.17	-	112,112,112,112	0
34	SR	0	8926	1/1	0.98	0.17	-	108,108,108,108	0
34	SR	0	8916	1/1	1.00	0.03	-	120,120,120,120	0
34	SR	0	8958	1/1	0.96	0.06	-	122,122,122,122	0
34	SR	0	8901	1/1	0.94	0.08	-	91,91,91,91	0
34	SR	0	8951	1/1	0.90	0.04	-	148,148,148,148	0
32	MG	0	8039	1/1	0.92	0.27	-	76,76,76,76	0
34	SR	0	9001	1/1	0.81	0.08	-	173,173,173,173	0
34	SR	S	8961	1/1	0.94	0.06	-	121,121,121,121	0
32	MG	0	8022	1/1	0.97	0.21	-	44,44,44,44	0
34	SR	0	8931	1/1	0.99	0.07	-	113,113,113,113	0
34	SR	0	8957	1/1	0.97	0.14	-	195,195,195,195	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	SR	0	9000	1/1	0.94	0.07	-	176,176,176,176	0
34	SR	0	8973	1/1	0.94	0.05	-	130,130,130,130	0
35	NA	0	8544	1/1	0.86	0.17	-	67,67,67,67	0
33	CL	0	8817	1/1	0.99	0.15	-	67,67,67,67	0
32	MG	0	8040	1/1	0.96	0.21	-	96,96,96,96	0
32	MG	0	8055	1/1	0.94	0.16	-	53,53,53,53	0
34	SR	0	8939	1/1	0.97	0.09	-	149,149,149,149	0
32	MG	0	8076	1/1	0.99	0.08	-	40,40,40,40	0
32	MG	0	8049	1/1	0.88	0.30	-	69,69,69,69	0
35	NA	0	8506	1/1	0.69	0.16	-	64,64,64,64	0
32	MG	0	8091	1/1	0.93	0.07	-	57,57,57,57	0
34	SR	0	8956	1/1	0.99	0.06	-	155,155,155,155	0
35	NA	0	8522	1/1	0.90	1.14	-	79,79,79,79	0
32	MG	0	8019	1/1	0.99	0.20	-	28,28,28,28	0
34	SR	0	8907	1/1	1.00	0.15	-	56,56,56,56	0
34	SR	0	8911	1/1	0.99	0.08	-	85,85,85,85	0
32	MG	0	8026	1/1	0.97	0.08	-	35,35,35,35	0
33	CL	J	8802	1/1	0.95	0.21	-	75,75,75,75	0
34	SR	0	8908	1/1	0.96	0.08	-	116,116,116,116	0
34	SR	0	8990	1/1	0.99	0.10	-	139,139,139,139	0
35	NA	0	8570	1/1	0.91	0.09	-	52,52,52,52	0
32	MG	0	8017	1/1	0.98	0.19	-	52,52,52,52	0
35	NA	0	8535	1/1	0.83	0.53	-	61,61,61,61	0
35	NA	0	8526	1/1	0.93	0.08	-	47,47,47,47	0
34	SR	0	8942	1/1	0.93	0.08	-	122,122,122,122	0
34	SR	0	9004	1/1	0.96	0.30	-	200,200,200,200	0
34	SR	0	8962	1/1	0.53	0.19	-	169,169,169,169	0
33	CL	Q	8811	1/1	0.93	0.15	-	82,82,82,82	0
34	SR	0	8994	1/1	0.75	0.43	-	200,200,200,200	0
34	SR	0	8940	1/1	0.98	0.07	-	97,97,97,97	0
34	SR	3	8932	1/1	0.99	0.14	-	76,76,76,76	0
35	NA	0	8525	1/1	0.29	0.25	-	92,92,92,92	0
34	SR	0	9008	1/1	0.95	0.17	-	95,95,95,95	0
34	SR	9	9003	1/1	0.94	0.09	-	171,171,171,171	0
34	SR	0	8934	1/1	0.98	0.25	-	134,134,134,134	0
34	SR	0	8993	1/1	0.74	0.10	-	176,176,176,176	0
32	MG	0	8046	1/1	0.96	0.14	-	43,43,43,43	0
34	SR	0	8928	1/1	0.93	0.06	-	135,135,135,135	0
32	MG	0	8038	1/1	0.90	0.15	-	70,70,70,70	0
32	MG	0	8081	1/1	0.90	0.23	-	73,73,73,73	0
35	NA	0	8518	1/1	0.85	0.59	-	88,88,88,88	0
35	NA	0	8566	1/1	0.98	0.12	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8048	1/1	0.98	0.24	-	33,33,33,33	0
34	SR	0	8971	1/1	0.96	0.07	-	171,171,171,171	0
35	NA	0	8513	1/1	0.98	0.21	-	54,54,54,54	0
32	MG	0	8068	1/1	0.98	0.08	-	51,51,51,51	0
32	MG	0	8005	1/1	0.99	0.23	-	35,35,35,35	0
34	SR	0	8995	1/1	0.94	0.15	-	136,136,136,136	0
32	MG	0	8087	1/1	0.92	0.12	-	51,51,51,51	0
34	SR	0	8960	1/1	0.83	0.10	-	141,141,141,141	0
35	NA	0	8541	1/1	0.98	0.18	-	75,75,75,75	0
34	SR	0	8968	1/1	0.94	0.03	-	160,160,160,160	0
32	MG	0	8090	1/1	0.99	0.10	-	65,65,65,65	0
33	CL	J	8801	1/1	0.99	0.07	-	79,79,79,79	0
34	SR	A	8977	1/1	0.83	0.06	-	160,160,160,160	0
34	SR	0	8917	1/1	0.96	0.10	-	107,107,107,107	0
34	SR	0	9007	1/1	0.97	0.67	-	200,200,200,200	0
35	NA	0	8508	1/1	0.98	0.20	-	35,35,35,35	0
34	SR	9	8980	1/1	0.93	0.15	-	175,175,175,175	0
35	NA	0	8529	1/1	0.92	0.15	-	39,39,39,39	0
34	SR	0	8988	1/1	0.93	0.05	-	158,158,158,158	0
32	MG	0	8030	1/1	0.98	0.30	-	68,68,68,68	0
35	NA	0	8574	1/1	0.89	0.26	-	59,59,59,59	0
32	MG	0	8093	1/1	0.95	0.08	-	42,42,42,42	0
34	SR	0	8925	1/1	1.00	0.08	-	86,86,86,86	0
34	SR	B	8950	1/1	0.98	0.14	-	116,116,116,116	0
35	NA	0	8516	1/1	0.96	0.11	-	45,45,45,45	0
36	CD	O	8705	1/1	0.99	0.06	-	118,118,118,118	0
32	MG	0	8061	1/1	0.99	0.23	-	37,37,37,37	0
32	MG	0	8031	1/1	0.91	0.11	-	62,62,62,62	0
35	NA	0	8505	1/1	0.93	0.86	-	48,48,48,48	0
34	SR	0	8959	1/1	0.91	0.37	-	163,163,163,163	0
34	SR	1	8952	1/1	0.98	0.15	-	89,89,89,89	0
32	MG	0	8027	1/1	0.99	0.11	-	51,51,51,51	0
35	NA	0	8551	1/1	0.94	0.38	-	52,52,52,52	0
32	MG	0	8032	1/1	0.99	0.05	-	44,44,44,44	0
34	SR	0	8996	1/1	0.78	1.20	-	200,200,200,200	0
32	MG	0	8007	1/1	0.99	0.15	-	32,32,32,32	0
35	NA	0	8548	1/1	0.74	0.26	-	58,58,58,58	0
35	NA	R	8532	1/1	0.96	0.11	-	58,58,58,58	0
34	SR	0	8909	1/1	0.99	0.15	-	88,88,88,88	0
35	NA	S	8510	1/1	0.81	0.48	-	64,64,64,64	0
34	SR	0	8924	1/1	0.34	0.09	-	154,154,154,154	0
32	MG	0	8071	1/1	0.97	0.10	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	NA	0	8545	1/1	0.88	0.26	-	47,47,47,47	0
35	NA	0	8502	1/1	0.72	0.15	-	66,66,66,66	0
34	SR	0	8983	1/1	0.98	0.24	-	170,170,170,170	0
34	SR	0	8915	1/1	0.92	0.08	-	121,121,121,121	0
35	NA	0	8511	1/1	0.75	0.29	-	69,69,69,69	0
34	SR	0	8986	1/1	0.78	0.42	-	200,200,200,200	0
34	SR	0	8979	1/1	0.76	0.13	-	200,200,200,200	0
34	SR	0	8919	1/1	0.97	0.07	-	170,170,170,170	0
35	NA	0	8554	1/1	0.90	1.00	-	65,65,65,65	0
34	SR	0	8964	1/1	0.99	0.09	-	131,131,131,131	0
34	SR	0	8937	1/1	0.98	0.27	-	112,112,112,112	0
34	SR	0	8976	1/1	0.88	0.28	-	194,194,194,194	0
34	SR	0	8922	1/1	0.88	0.47	-	161,161,161,161	0
34	SR	0	8953	1/1	0.96	0.13	-	144,144,144,144	0
34	SR	0	8946	1/1	0.91	0.22	-	123,123,123,123	0
33	CL	R	8806	1/1	0.99	0.17	-	57,57,57,57	0
35	NA	9	8543	1/1	0.77	0.11	-	74,74,74,74	0
34	SR	0	8974	1/1	0.87	0.24	-	165,165,165,165	0
34	SR	0	8965	1/1	0.93	0.09	-	132,132,132,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.