



# wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 04:21 PM GMT

PDB ID : 3CCU  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation G2482C  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 2.80 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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

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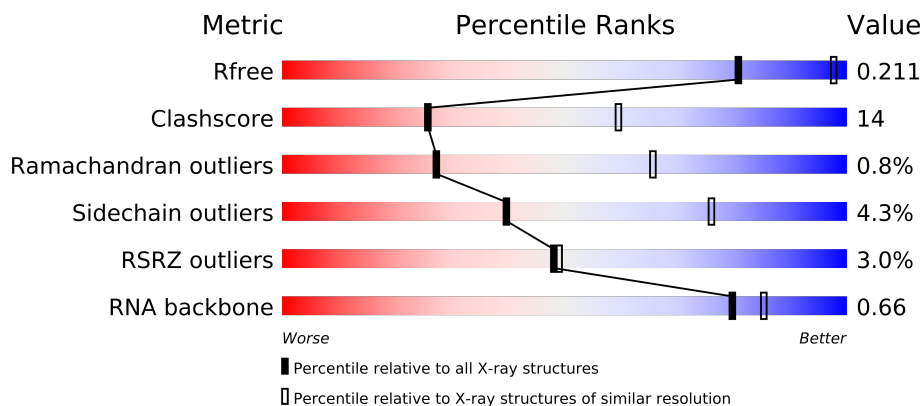
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)
RNA backbone	1838	1076 (3.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	

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

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

Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8004	-	X
32	MG	0	8005	-	X
32	MG	0	8007	-	X
32	MG	0	8009	-	X
32	MG	0	8014	-	X
32	MG	0	8015	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8019	-	X
32	MG	0	8028	-	X
32	MG	0	8029	-	X
32	MG	0	8030	-	X
32	MG	0	8037	-	X
32	MG	0	8038	-	X
32	MG	0	8039	-	X
32	MG	0	8041	-	X
32	MG	0	8045	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8047	-	X
32	MG	0	8048	-	X
32	MG	0	8049	-	X
32	MG	0	8061	-	X
32	MG	0	8063	-	X
32	MG	0	8066	-	X
32	MG	0	8069	-	X
32	MG	0	8070	-	X
32	MG	0	8071	-	X
32	MG	0	8076	-	X
32	MG	0	8078	-	X
32	MG	0	8081	-	X
32	MG	0	8082	-	X
32	MG	0	8085	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
34	NA	0	8501	-	X
34	NA	0	8502	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8507	-	X
34	NA	0	8508	-	X
34	NA	0	8509	-	X
34	NA	0	8511	-	X
34	NA	0	8512	-	X
34	NA	0	8514	-	X
34	NA	0	8522	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8530	-	X
34	NA	0	8535	-	X
34	NA	0	8536	-	X
34	NA	0	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8546	-	X
34	NA	0	8547	-	X
34	NA	0	8548	-	X
34	NA	0	8549	-	X
34	NA	0	8550	-	X
34	NA	0	8552	-	X
34	NA	0	8553	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X
34	NA	0	8557	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X
34	NA	0	8561	-	X
34	NA	0	8562	-	X
34	NA	0	8563	-	X
34	NA	0	8564	-	X
34	NA	0	8565	-	X
34	NA	0	8566	-	X
34	NA	0	8567	-	X
34	NA	0	8569	-	X
34	NA	0	8573	-	X
34	NA	0	8574	-	X
34	NA	0	8575	-	X
34	NA	9	8572	-	X
34	NA	H	8518	-	X
35	CL	0	8822	-	X
36	SR	0	8903	-	X
36	SR	0	8904	-	X
36	SR	0	8905	-	X
36	SR	0	8909	-	X
36	SR	0	8914	-	X
36	SR	0	8924	-	X
36	SR	0	8925	-	X
36	SR	0	8926	-	X
36	SR	0	8937	-	X
36	SR	0	8938	-	X
36	SR	0	8946	-	X
36	SR	0	8947	-	X
36	SR	0	8959	-	X
36	SR	0	8969	-	X
36	SR	0	8976	-	X
36	SR	0	8982	-	X
36	SR	0	8983	-	X
36	SR	0	8989	-	X
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	0	9000	-	X
36	SR	0	9001	-	X
36	SR	0	9004	-	X
36	SR	0	9007	-	X
36	SR	9	9003	-	X
36	SR	B	8987	-	X
36	SR	J	8986	-	X

## 2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99119 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a 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
			59017	26348	10871	19053	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	Y	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	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	9	2	Total	Mg	0	0
			2	2		

- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	2	Total K 2 2	0	0

- Molecule 34 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	H	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0

- Molecule 35 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	9	Total Cl 9 9	0	0
35	J	3	Total Cl 3 3	0	0
35	K	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Y	1	Total 1	Cl 1	0	0
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	92	Total 92	Sr 92	0	0
36	J	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	3	Total 3	Sr 3	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 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 1	Cd 1	0	0
37	U	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5933	Total 5933	O 5933	0	0
38	9	144	Total 144	O 144	0	0
38	A	110	Total 110	O 110	0	0
38	B	144	Total 144	O 144	0	0
38	C	178	Total 178	O 178	0	0
38	D	45	Total 45	O 45	0	0
38	E	43	Total 43	O 43	0	0
38	F	27	Total 27	O 27	0	0
38	G	17	Total 17	O 17	0	0
38	H	69	Total 69	O 69	0	0
38	I	6	Total 6	O 6	0	0
38	J	53	Total 53	O 53	0	0
38	K	56	Total 56	O 56	0	0
38	L	92	Total 92	O 92	0	0
38	M	129	Total 129	O 129	0	0
38	N	63	Total 63	O 63	0	0
38	O	40	Total 40	O 40	0	0

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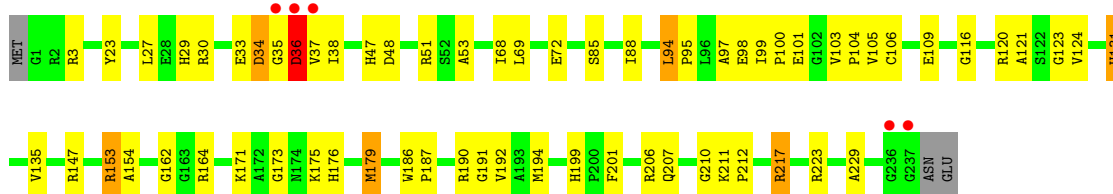
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	P	66	Total 66	O 66	0	0
38	Q	46	Total 46	O 46	0	0
38	R	76	Total 76	O 76	0	0
38	S	39	Total 39	O 39	0	0
38	T	35	Total 35	O 35	0	0
38	U	28	Total 28	O 28	0	0
38	V	13	Total 13	O 13	0	0
38	W	69	Total 69	O 69	0	0
38	X	27	Total 27	O 27	0	0
38	Y	91	Total 91	O 91	0	0
38	Z	25	Total 25	O 25	0	0
38	1	56	Total 56	O 56	0	0
38	2	38	Total 38	O 38	0	0
38	3	65	Total 65	O 65	0	0

### 3 Residue-property plots

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

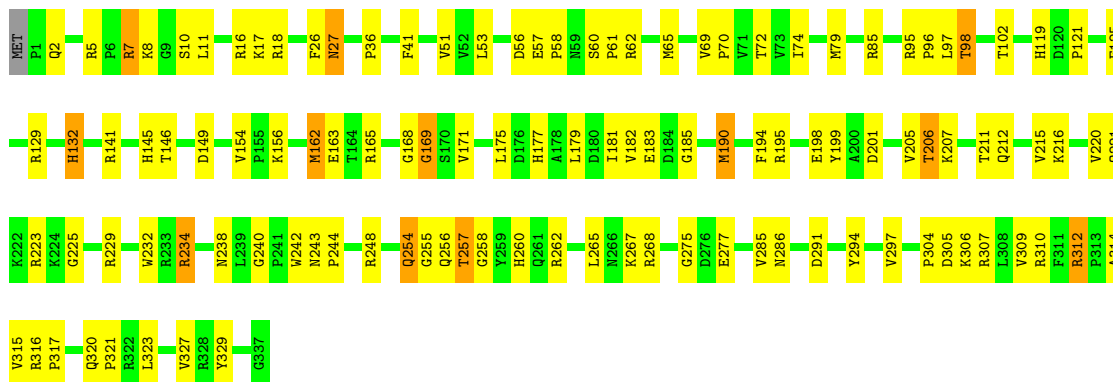
- Molecule 1: 50S ribosomal protein L2P

Chain A: 



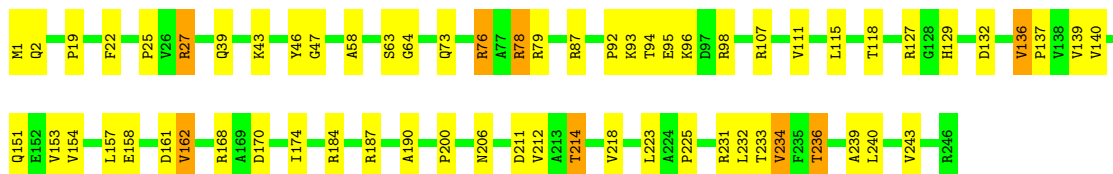
- Molecule 2: 50S ribosomal protein L3P

Chain B: 



- Molecule 3: 50S ribosomal protein L4P

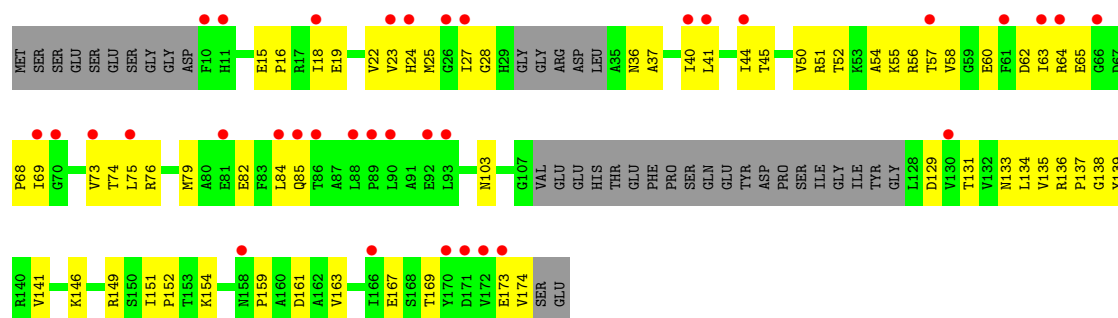
Chain C: 



- Molecule 4: 50S ribosomal protein L5P

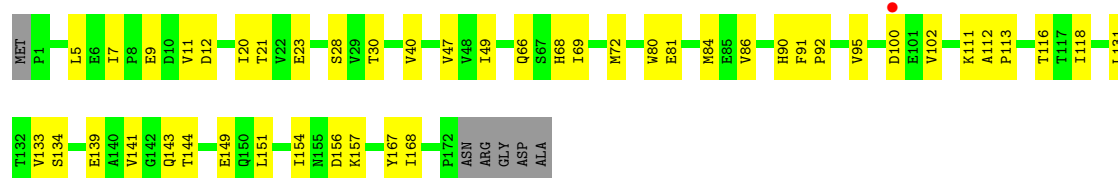
Chain D: 





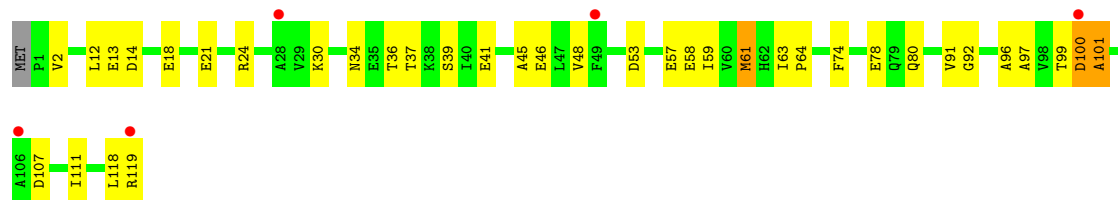
- Molecule 5: 50S ribosomal protein L6P

Chain E: 



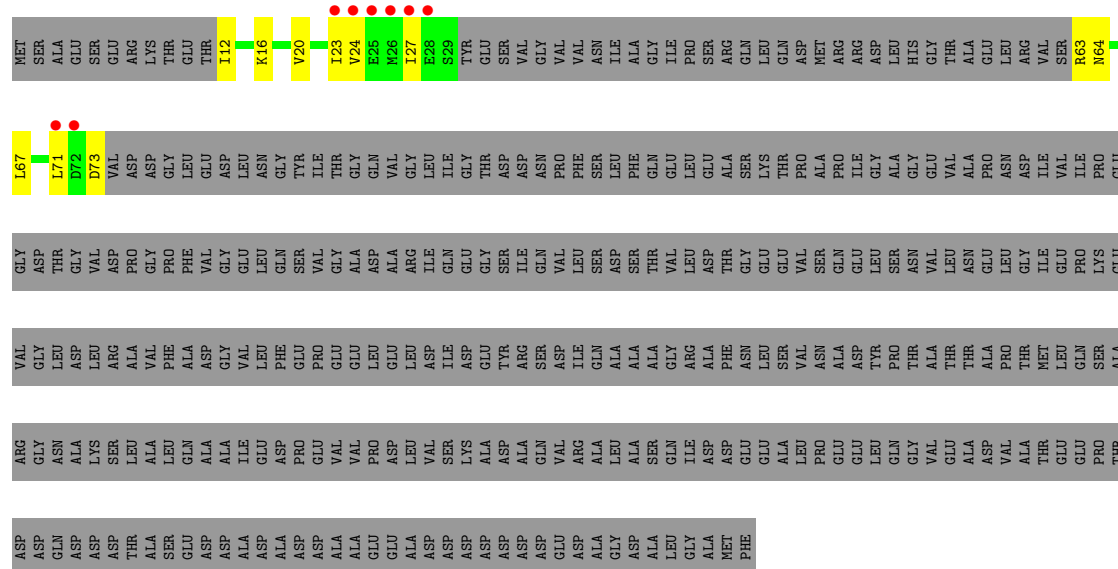
- Molecule 6: 50S ribosomal protein L7Ae

Chain F: 



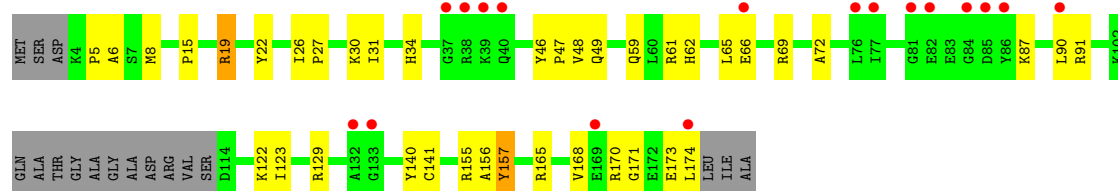
- Molecule 7: 50S ribosomal protein L10E

Chain G:



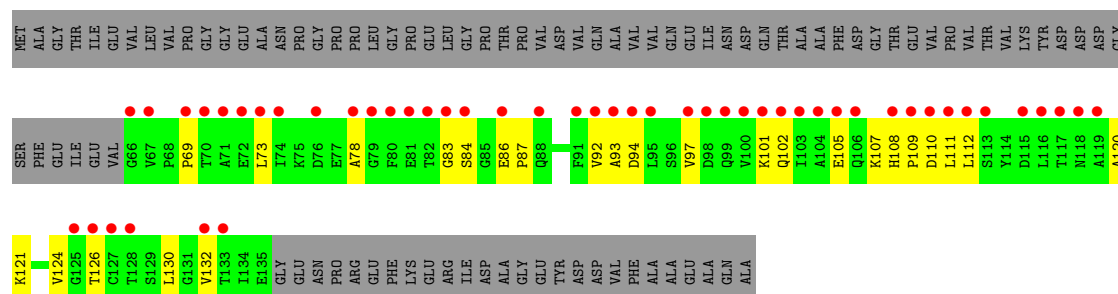
- Molecule 8: 50S ribosomal protein L10e

Chain H: 



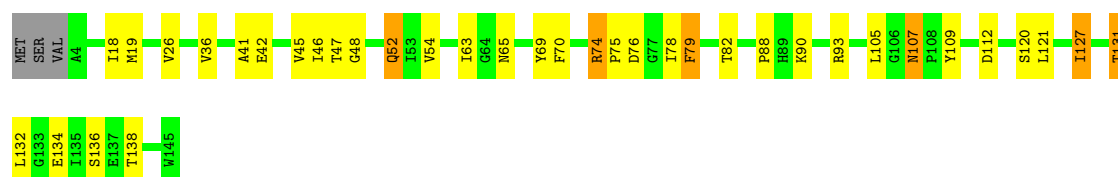
- Molecule 9: 50S ribosomal protein L11P

Chain I: 



- Molecule 10: 50S ribosomal protein L13P

Chain J: 



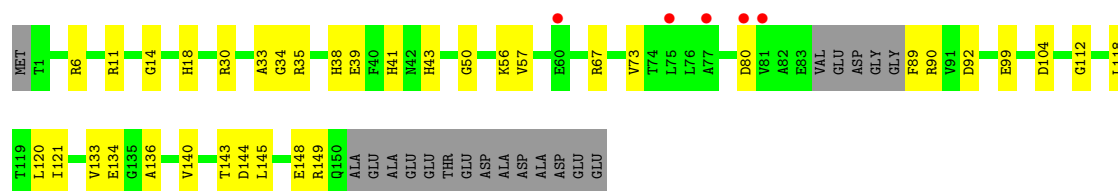
- Molecule 11: 50S ribosomal protein L14P

Chain K: 



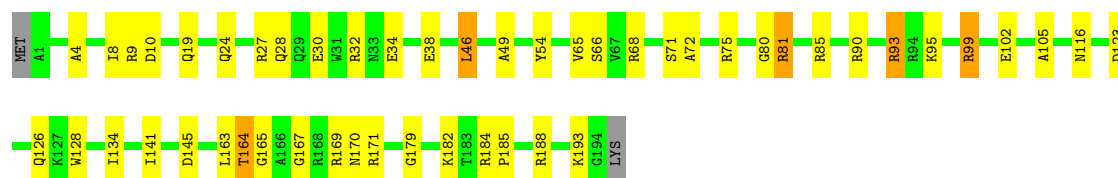
- Molecule 12: 50S ribosomal protein L15P

Chain L: 



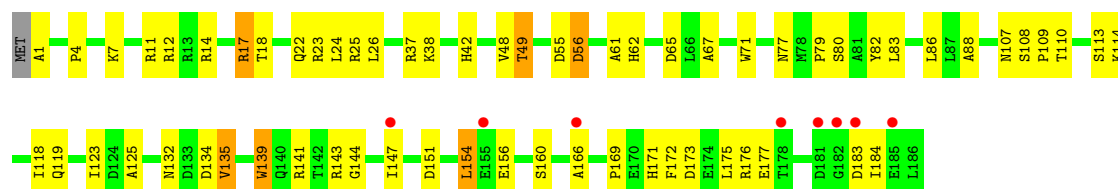
- Molecule 13: 50S ribosomal protein L15e

Chain M:



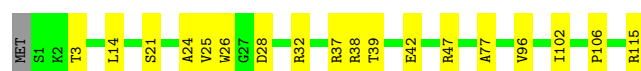
- Molecule 14: 50S ribosomal protein L18P

Chain N:



- Molecule 15: 50S ribosomal protein L18e

Chain O:



- Molecule 16: 50S ribosomal protein L19e

Chain P:



- Molecule 17: 50S ribosomal protein L21e

Chain Q:



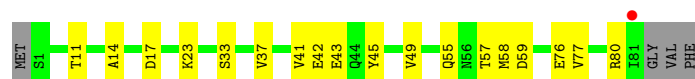
- Molecule 18: 50S ribosomal protein L22P

Chain R:



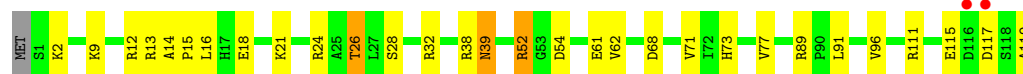
- Molecule 19: 50S ribosomal protein L23P

Chain S:



- Molecule 20: 50S ribosomal protein L24P

Chain T: 



- Molecule 21: 50S ribosomal protein L24e

Chain U: 



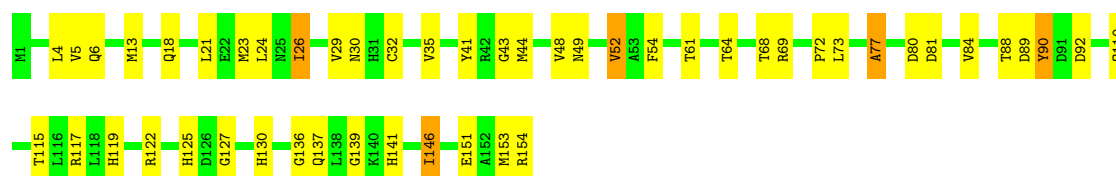
- Molecule 22: 50S ribosomal protein L29P

Chain V: 



- Molecule 23: 50S ribosomal protein L30P

Chain W: 



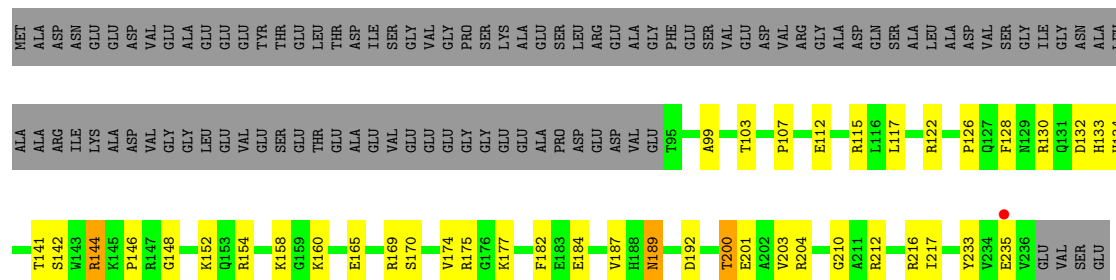
- Molecule 24: 50S ribosomal protein L31e

Chain X: 



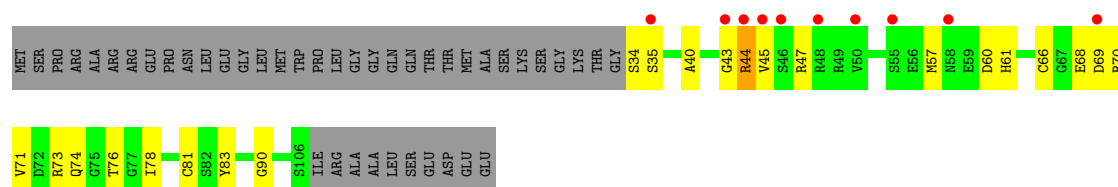
- Molecule 25: 50S ribosomal protein L32e

Chain Y: 



- Molecule 26: 50S ribosomal protein L37Ae

Chain Z: 



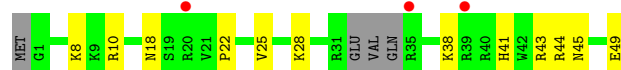
- Molecule 27: 50S ribosomal protein L37e

Chain 1:



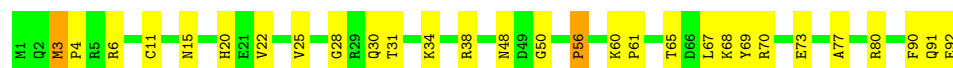
- Molecule 28: 50S ribosomal protein L39e

Chain 2:



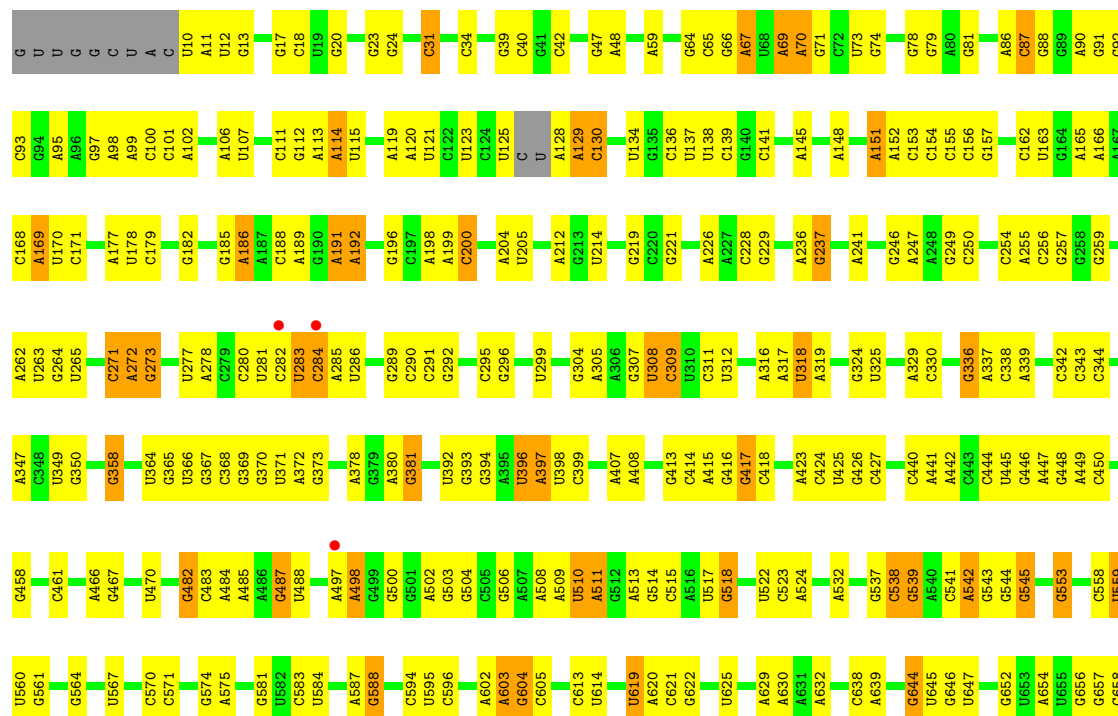
- Molecule 29: 50S ribosomal protein L44E

Chain 3:

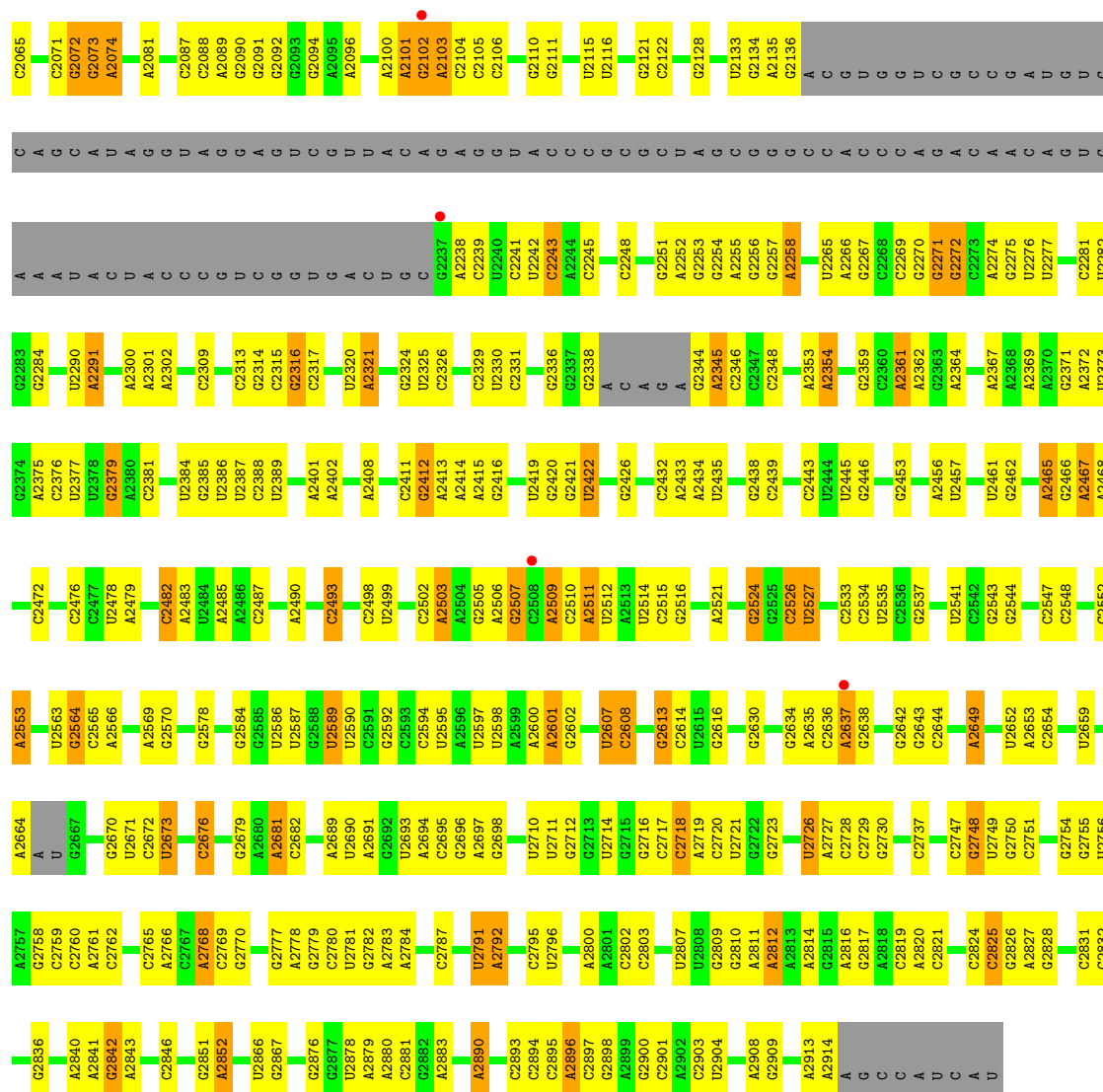


- Molecule 30: 23S RIBOSOMAL RNA

Chain 0:

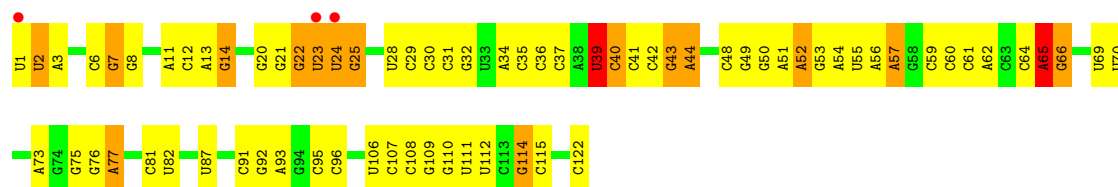


A	C1769	G1681	G1589	C1477	G1391	G1299	G1210	U1149	U1028	G958	A861	A761	A859
U	U1770	A1682	G1592	U1478	A1392	G1300	G1211	A1150	U1029	C959	G861	G761	A860
G	U1771	A1683	C1593	G1481	A1393	U1304	C1212	G1151	U1041	G860	G765	G764	G661
A	C1772	A1684	C1594	G1482	A1394	U1305	C1213	A1154	U1042	G869	G766	G765	G669
C	G1773	A1685	C1595	C1483	C1395	U1306	A1215	G1155	C1043	G870	G775	G775	G670
C	G1774	C1686	U1596	G1484	C1396	A1307	G1216	C1156	C1044	G871	A776	A776	A671
U1864	A1778	C1687	A1597	A1492	C1397	A1308	G1217	C1157	G1045	G869	U777	U777	G672
C1965	A1779	C1692	A1598	A1493	G1398	U1309	U1218	G1158	U1062	U970	A875	A875	C677
U1966	A1780	A1693	U1503	A1494	A1399	U1310	U1219	G1159	G1063	G	A876	A876	C677
U1967	A1783	A1603	A1504	A1495	C1400	U1311	U1220	G1160	U1063	U	G877	G877	A791
A1968	U1784	G1597	A1505	A1496	G1401	G1312	G1221	A1161	U1064	G	G878	G878	A791
A1969	C1787	C1700	A1506	G1497	A1406	A1313	G1226	G1162	A1068	U	C884	U794	G682
A1970	U1788	A1701	A1507	A1497	A1407	A1321	C1229	G1163	G1069	C	G885	G795	G683
U1971	U1789	U1702	C1513	U1503	U1408	G1322	C1229	U1164	C1060	C	G886	G796	G684
A1972	C1790	G1705	A1514	A1504	G1409	A1230	A1231	A1166	U1066	G	U888	A797	G685
C1973	U1791	G1706	A1515	U1505	C1410	G1325	A1232	G1167	A1067	C	U889	G800	A686
G1974	C1798	G1707	U1516	U1506	A1413	A1328	A1233	U1169	G1072	U	A895	U801	C687
G1975	A1315	C1715	G1622	U1511	A1414	G1329	U1234	U1170	A1073	C	C896	G802	G688
G1976	G1806	C1716	C1623	G1512	A1415	A1330	G1235	G1171	G1074	C	G897	A812	G689
U1977	C1818	G1723	A1625	C1514	G1416	U1333	A1236	G1172	C1080	G	A694	A813	A694
U1978	C1819	U1722	U1626	A1515	U1417	C1334	U1237	A1173	A1081	A	C695	U815	C695
U1979	G1820	C1725	G1627	U1516	U1418	U1334	U1238	A1174	A1082	G	G696	G816	G696
U2004	G1821	U1726	A1632	G1520	U1419	G1339	A1242	G1175	A1087	G	G697	G817	G709
G2005	G1822	C1727	C1633	C1521	U1422	G1340	A1243	C1176	G1087	A	A698	A818	G710
G2006	C1823	U1728	G1634	A1522	A1424	A1342	U1244	C1177	A1088	G	C699	A819	G711
G2007	C1824	C1729	U1635	G1523	A1425	C1343	C1245	C1178	A700	U	U701	G820	G712
G2008	U1825	G1730	U1636	U1524	G1426	G1344	A1246	U1180	A1097	C	G702	U821	U713
G2009	C1826	C1731	A1637	G1525	A1427	U1350	A1247	A1181	A1098	G	G	C822	U714
A1921	A1829	A1732	A1641	A1527	A1434	G1351	U1249	U1182	C1104	C	A912	U823	U
A1922	C1830	C1734	A1642	A1528	U1435	A1352	C1260	U1185	A	A	C920	A827	G716
A1923	C1834	C1735	G1649	G1529	C1436	C1353	C1261	C1186	U1109	A	A922	C828	C717
A1924	U1835	U1835	C1650	C1537	A1437	C1360	G1260	U1187	G1110	C999	A923	U834	G718
A1925	U1836	U1740	C1651	U1537	G1438	C1361	U1266	U1188	U1116	U1003	A926	U835	C725
A1926	U1837	U1741	C1652	U1545	C1439	C1362	C1267	A1189	A1117	C1004	U932	U840	G730
A1927	U1838	A1742	A1653	C1545	U1440	G1363	G1268	A1190	A1118	U1005	U933	A841	G734
A1928	U1839	U1746	U1654	A1559	A1442	G1364	G1269	A1191	G1119	A1006	C933	U848	C735
A1929	C1841	A1747	G1655	U	G1443	C1365	U1279	A1192	U1120	A1007	G940	C848	A736
A1930	U1845	A1748	A1656	U1561	G1444	C1366	C1273	U1193	G1121	C1008	G941	C851	A737
A1931	U1846	G1752	A1657	C1562	U1445	C1372	U1278	C1195	U1122	U1009	U942	U852	G738
A1932	U1847	A1755	A1658	C1563	U1446	C1373	U1279	C1196	G1129	A943	U945	C853	C741
A1933	U1848	G1756	A1659	C1564	C1450	C1374	U1279	U1198	C1129	U944	U946	G856	G744
A1934	U1849	U1757	A1660	C1565	C1451	C1375	A1287	A1199	U1130	U945	U947	G857	C759
A1935	U1850	U1758	C1666	C1566	G1452	C1376	U1288	A1200	G1131	U946	U948	U858	U860
A1936	U1851	A1759	U1668	C1567	G1453	C1377	U1289	A1201	A1132	U1016	G949	C859	
A1937	U1852	U1760	C1574	A1573	U1457	A1381	A1291	A1202	G1135	A1020	G950	G856	
A1938	C1853	U1761	C1575	C1576	U1458	U1382	G1382	A1203	U1136	A1021	G951	G857	
A1939	C1854	C1762	U1577	U1577	U1463	U1383	A1291	C1204	G1137	A1022	G952	G858	
A1940	G1855	C1763	C1578	U1577	C1464	C1384	A1291	U1205	U1138	U1026	G953	U1139	
A1941	C1856	U1766	A1578	G1586	C1464	C1385	A1291	U1206	G1139	C1025	G954	U1140	
A1942	A1857	U1767	C1579	U1587	C1474	C1386	A1291	A1207	C1140	U1026	U954	U1140	
A1943	U1858	C1768	C1580	G1588	C1474	G1387	U1298	C1208		G1027			



• Molecule 31: 5S RIBOSOMAL RNA

Chain 9:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	211.76Å 299.27Å 574.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.99 – 2.80 85.47 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.3 (49.99-2.80) 93.0 (85.47-2.40)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.179 , 0.223 0.172 , 0.211	Depositor DCC
$R_{free}$ test set	4047 reflections (0.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.1	Xtriage
Anisotropy	0.234	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 667168 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99119	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

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

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



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, 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	0.65	0/2408
2	B	0.33	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.63	0/2552
4	D	0.32	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.58	0/1880
6	F	0.33	0/901	0.57	0/1224
7	G	0.30	0/241	0.48	0/324
8	H	0.33	0/1302	0.61	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.59	0/1530
11	K	0.35	0/1004	0.67	0/1351
12	L	0.32	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.62	0/1999
15	O	0.33	0/874	0.58	0/1181
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.34	0/749	0.66	0/1005
18	R	1.26	7/1172 (0.6%)	1.10	6/1578 (0.4%)
19	S	0.33	0/648	0.57	0/875
20	T	0.33	0/958	0.64	1/1289 (0.1%)
21	U	0.34	0/417	0.57	0/562
22	V	0.31	0/502	0.51	0/675
23	W	0.34	0/1219	0.62	0/1655
24	X	0.34	0/664	0.60	0/895
25	Y	0.36	0/1146	0.63	0/1536
26	Z	0.35	0/584	0.59	0/781
27	1	0.39	0/438	0.61	0/578
28	2	0.34	0/401	0.59	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.37	0/65953	0.69	16/102860 (0.0%)
31	9	0.31	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98697 (0.0%)	0.67	24/147579 (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	1	34
31	9	0	3
All	All	2	38

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	27.61	2.88	1.50
18	R	150	PRO	CA-C	-17.92	1.17	1.52
18	R	150	PRO	CG-CD	13.88	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.29	1.66	1.47

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.50	55.74	112.00
18	R	150	PRO	N-CA-C	-19.33	61.84	112.10
18	R	150	PRO	CA-N-CD	12.33	128.96	111.70
18	R	150	PRO	N-CA-CB	10.99	116.49	103.30
30	0	2482	C	C2'-C3'-O3'	9.28	129.92	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA
30	0	2482	C	C3'

5 of 38 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	221	G	Sidechain
30	0	246	G	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
23	W	90	TYR	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	71	0
2	B	2625	0	2533	100	0
3	C	1860	0	1813	58	0
4	D	1094	0	1085	44	0
5	E	1357	0	1266	32	0
6	F	890	0	843	30	0
7	G	240	0	231	9	0
8	H	1282	0	1292	33	0
9	I	519	0	500	23	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	35	0
12	L	1118	0	1076	28	0
13	M	1558	0	1573	45	0
14	N	1445	0	1401	57	0
15	O	865	0	873	19	0
16	P	1136	0	1123	18	0
17	Q	735	0	729	16	0
18	R	1149	0	1122	38	0
19	S	641	0	605	16	0
20	T	950	0	924	22	0
21	U	410	0	364	19	0
22	V	499	0	511	14	0
23	W	1196	0	1137	48	0
24	X	654	0	653	16	0
25	Y	1130	0	1133	38	0
26	Z	573	0	531	21	0
27	1	431	0	426	23	0
28	2	396	0	413	14	0
29	3	755	0	728	25	0
30	0	59017	0	29810	1217	0
31	9	2599	0	1325	89	0
32	0	84	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	2	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	H	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	9	0	0	1	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	3	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	92	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	3	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	J	1	0	0	0	0
36	R	1	0	0	0	0
36	S	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	5933	0	0	188	0
38	1	56	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	38	0	0	0	0
38	3	65	0	0	4	0
38	9	144	0	0	9	0
38	A	110	0	0	6	0
38	B	144	0	0	18	0
38	C	178	0	0	14	0
38	D	45	0	0	3	0
38	E	43	0	0	2	0
38	F	27	0	0	2	0
38	G	17	0	0	0	0
38	H	69	0	0	8	0
38	I	6	0	0	0	0
38	J	53	0	0	2	0
38	K	56	0	0	3	0
38	L	92	0	0	6	0
38	M	129	0	0	4	0
38	N	63	0	0	6	0
38	O	40	0	0	2	0
38	P	66	0	0	1	0
38	Q	46	0	0	1	0
38	R	76	0	0	2	0
38	S	39	0	0	4	0
38	T	35	0	0	3	0
38	U	28	0	0	3	0
38	V	13	0	0	0	0
38	W	69	0	0	5	0
38	X	27	0	0	2	0
38	Y	91	0	0	10	0
38	Z	25	0	0	3	0
All	All	99119	0	59911	2035	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 2035 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.43
30:0:1160:G:C5'	30:0:1161:A:H5'	1.74	1.16
31:9:56:A:H2'	31:9:57:A:H5''	1.20	1.16
30:0:1160:G:H5'	30:0:1161:A:C5'	1.77	1.14
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.14

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%)	212 (90%)	19 (8%)	4 (2%)	14	42
2	B	335/338 (99%)	307 (92%)	24 (7%)	4 (1%)	19	54
3	C	244/246 (99%)	224 (92%)	20 (8%)	0	100	100
4	D	134/177 (76%)	110 (82%)	20 (15%)	4 (3%)	7	22
5	E	170/178 (96%)	162 (95%)	8 (5%)	0	100	100
6	F	117/120 (98%)	106 (91%)	8 (7%)	3 (3%)	8	26
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	144 (92%)	10 (6%)	2 (1%)	18	51
9	I	68/162 (42%)	52 (76%)	15 (22%)	1 (2%)	15	46
10	J	140/145 (97%)	129 (92%)	10 (7%)	1 (1%)	30	69
11	K	130/132 (98%)	122 (94%)	7 (5%)	1 (1%)	27	65
12	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	30	69
13	M	192/196 (98%)	184 (96%)	7 (4%)	1 (0%)	38	76
14	N	184/187 (98%)	168 (91%)	12 (6%)	4 (2%)	10	32
15	O	113/116 (97%)	111 (98%)	2 (2%)	0	100	100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	141 (95%)	7 (5%)	0	100	100
19	S	79/85 (93%)	75 (95%)	4 (5%)	0	100	100
20	T	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	3 (5%)	0	100	100
23	W	152/154 (99%)	150 (99%)	0	2 (1%)	18	51
24	X	80/92 (87%)	74 (92%)	5 (6%)	1 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y	140/241 (58%)	140 (100%)	0	0	100	100
26	Z	71/116 (61%)	63 (89%)	7 (10%)	1 (1%)	16	49
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	21	57
All	All	3705/4472 (83%)	3453 (93%)	221 (6%)	31 (1%)	27	65

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
6	F	101	ALA
8	H	19	ARG
12	L	149	ARG

### 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%)	169 (94%)	10 (6%)	30	64
2	B	282/283 (100%)	267 (95%)	15 (5%)	32	67
3	C	193/193 (100%)	178 (92%)	15 (8%)	18	45
4	D	117/148 (79%)	112 (96%)	5 (4%)	40	76
5	E	152/156 (97%)	148 (97%)	4 (3%)	59	90
6	F	93/94 (99%)	92 (99%)	1 (1%)	84	98
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	81
8	H	134/145 (92%)	130 (97%)	4 (3%)	53	87
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	95
10	J	118/121 (98%)	108 (92%)	10 (8%)	15	41
11	K	106/106 (100%)	102 (96%)	4 (4%)	44	80
12	L	113/127 (89%)	108 (96%)	5 (4%)	39	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	149 (94%)	9 (6%)	29	64
14	N	149/150 (99%)	141 (95%)	8 (5%)	31	66
15	O	93/94 (99%)	92 (99%)	1 (1%)	84	98
16	P	113/117 (97%)	111 (98%)	2 (2%)	71	94
17	Q	79/80 (99%)	75 (95%)	4 (5%)	33	69
18	R	117/122 (96%)	114 (97%)	3 (3%)	59	90
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	97 (92%)	8 (8%)	19	46
21	U	44/53 (83%)	43 (98%)	1 (2%)	63	92
22	V	51/57 (90%)	49 (96%)	2 (4%)	43	80
23	W	130/130 (100%)	126 (97%)	4 (3%)	52	86
24	X	66/74 (89%)	57 (86%)	9 (14%)	5	16
25	Y	120/196 (61%)	115 (96%)	5 (4%)	40	77
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%)	61	91
29	3	79/79 (100%)	77 (98%)	2 (2%)	60	90
All	All	3095/3646 (85%)	2961 (96%)	134 (4%)	40	76

5 of 134 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	93	ARG
13	M	10	ASP
24	X	72	VAL
10	J	112	ASP
11	K	98	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	107	ASN
18	R	94	ASN
28	2	18	ASN
14	N	132	ASN

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Mol	Chain	Res	Type
16	P	118	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	236 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	254 (8%)	31 (1%)

5 of 254 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 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1246	A
30	0	1474	C
30	0	2761	A
30	0	1352	A
30	0	1506	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	OMU	0	2587	30	20,22,23	0.76	1 (5%)	24,31,34	0.76	0
30	OMG	0	2588	30	24,26,27	0.80	1 (4%)	32,38,41	5.04	3 (9%)
30	UR3	0	2619	30	20,22,23	0.70	0	23,32,35	0.87	0
30	PSU	0	2621	30	19,21,22	1.15	3 (15%)	23,30,33	1.09	2 (8%)
30	1MA	0	628	30	23,25,26	0.83	0	32,37,40	0.89	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/8/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/10/27/28	0/1/3/3
30	UR3	0	2619	30	-	0/6/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/8/25/26	0/2/2/2
30	1MA	0	628	30	-	1/8/25/26	0/1/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	2.94	1.43	1.37
30	0	2587	OMU	P-OP1	2.44	1.49	1.46
30	0	2621	PSU	C6-N1	2.22	1.34	1.32
30	0	2588	OMG	P-OP1	2.11	1.49	1.46
30	0	2621	PSU	P-OP1	2.03	1.49	1.46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-27.89	130.38	134.14
30	0	2588	OMG	C6-N1-C2	3.25	125.19	119.51
30	0	628	1MA	C2-N3-C4	-3.22	110.72	116.23
30	0	2588	OMG	C2-N3-C4	-2.34	111.80	115.09
30	0	2621	PSU	C5-C4-N3	-2.21	114.84	118.86

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	0	628	1MA	C2'-C1'-N9-C8

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 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.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	-0.57	5 (2%) 60 61	22, 48, 85, 107	0
2	B	337/338 (99%)	-0.75	0 100 100	24, 49, 78, 90	0
3	C	246/246 (100%)	-0.73	0 100 100	20, 40, 64, 79	0
4	D	140/177 (79%)	1.08	35 (25%) 1 1	61, 98, 123, 132	0
5	E	172/178 (96%)	-0.44	1 (0%) 86 88	43, 66, 86, 91	0
6	F	119/120 (99%)	0.06	5 (4%) 35 35	44, 67, 97, 113	0
7	G	29/348 (8%)	0.91	8 (27%) 1 1	77, 94, 103, 104	0
8	H	160/177 (90%)	0.36	17 (10%) 7 6	48, 69, 99, 104	0
9	I	70/162 (43%)	3.44	50 (71%) 0 0	128, 145, 162, 163	0
10	J	142/145 (97%)	-0.74	0 100 100	32, 47, 68, 90	0
11	K	132/132 (100%)	-0.98	0 100 100	30, 44, 67, 73	0
12	L	145/165 (87%)	-0.18	5 (3%) 43 44	25, 62, 112, 124	0
13	M	194/196 (98%)	-0.89	0 100 100	26, 39, 55, 63	0
14	N	186/187 (99%)	-0.22	8 (4%) 34 34	39, 63, 111, 120	0
15	O	115/116 (99%)	-0.67	0 100 100	33, 51, 68, 72	0
16	P	143/149 (95%)	-0.78	0 100 100	33, 49, 65, 73	0
17	Q	95/96 (98%)	-0.73	0 100 100	35, 45, 62, 79	0
18	R	150/155 (96%)	-0.87	0 100 100	27, 42, 62, 77	0
19	S	81/85 (95%)	-0.57	1 (1%) 75 76	38, 54, 74, 87	0
20	T	119/120 (99%)	-0.59	2 (1%) 67 68	37, 52, 80, 109	0
21	U	53/67 (79%)	-0.63	0 100 100	37, 50, 68, 78	0
22	V	65/71 (91%)	0.76	7 (10%) 6 5	47, 68, 117, 122	0
23	W	154/154 (100%)	-0.65	0 100 100	32, 47, 63, 77	0
24	X	82/92 (89%)	-0.43	3 (3%) 39 39	41, 57, 82, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.90	1 (0%) 84 85	21, 40, 63, 86	0
26	Z	73/116 (62%)	0.47	10 (13%) 4 3	53, 72, 85, 95	0
27	1	56/57 (98%)	-0.84	0 100 100	22, 28, 36, 44	0
28	2	46/50 (92%)	-0.30	3 (6%) 18 17	30, 56, 84, 98	0
29	3	92/92 (100%)	-0.55	0 100 100	33, 56, 68, 81	0
30	0	2754/2923 (94%)	-0.57	37 (1%) 74 75	19, 42, 86, 163	0
31	9	122/122 (100%)	-0.58	3 (2%) 54 55	34, 64, 87, 144	0
All	All	6651/7517 (88%)	-0.47	201 (3%) 48 49	19, 48, 97, 163	0

The worst 5 of 201 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	1	THR	12.9
22	V	39	ALA	11.5
9	I	74	ILE	9.9
4	D	63	ILE	8.8
9	I	104	ALA	8.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
30	UR3	0	2619	21/22	0.13	1.51	33,36,38,41	0
30	OMU	0	2587	21/22	0.11	0.72	29,31,32,35	0
30	1MA	0	628	23/24	0.13	0.01	23,27,29,31	0
30	OMG	0	2588	24/25	0.12	-0.31	29,31,34,35	0
30	PSU	0	2621	20/21	0.12	-0.73	22,26,37,37	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8561	1/1	0.56	106.80	76,76,76,76	0
34	NA	0	8562	1/1	0.41	100.45	78,78,78,78	0
36	SR	0	8997	1/1	0.39	75.37	196,196,196,196	0
34	NA	0	8566	1/1	0.51	71.28	43,43,43,43	0
36	SR	0	9007	1/1	0.36	57.42	187,187,187,187	0
35	CL	0	8822	1/1	0.24	37.75	78,78,78,78	0
36	SR	B	8987	1/1	0.98	37.50	200,200,200,200	0
34	NA	0	8574	1/1	0.46	33.97	65,65,65,65	0
34	NA	0	8549	1/1	0.49	33.42	50,50,50,50	0
34	NA	0	8555	1/1	0.51	29.61	54,54,54,54	0
34	NA	0	8563	1/1	0.62	29.58	74,74,74,74	0
34	NA	0	8522	1/1	0.35	28.13	73,73,73,73	0
32	MG	0	8049	1/1	0.28	27.91	65,65,65,65	0
36	SR	J	8986	1/1	0.87	25.75	200,200,200,200	0
34	NA	9	8572	1/1	0.53	24.93	93,93,93,93	0
34	NA	0	8502	1/1	0.33	23.87	62,62,62,62	0
34	NA	0	8554	1/1	0.37	23.49	59,59,59,59	0
34	NA	0	8505	1/1	0.33	21.94	36,36,36,36	0
36	SR	0	8994	1/1	0.41	21.53	200,200,200,200	0
34	NA	0	8564	1/1	0.29	20.58	61,61,61,61	0
34	NA	0	8512	1/1	0.33	19.71	50,50,50,50	0
34	NA	0	8535	1/1	0.20	19.67	47,47,47,47	0
36	SR	0	8982	1/1	0.41	19.17	178,178,178,178	0
32	MG	0	8038	1/1	0.16	19.00	65,65,65,65	0
32	MG	0	8037	1/1	0.22	18.17	92,92,92,92	0
34	NA	0	8546	1/1	0.82	17.81	69,69,69,69	0
36	SR	0	8996	1/1	0.43	17.23	200,200,200,200	0
34	NA	0	8556	1/1	0.76	17.11	44,44,44,44	0
34	NA	0	8565	1/1	0.24	16.95	66,66,66,66	0
34	NA	0	8548	1/1	0.23	15.41	56,56,56,56	0
34	NA	0	8524	1/1	0.23	15.31	39,39,39,39	0
34	NA	0	8560	1/1	0.37	14.44	74,74,74,74	0
34	NA	0	8509	1/1	0.15	14.43	56,56,56,56	0
36	SR	0	9000	1/1	0.21	14.30	160,160,160,160	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8536	1/1	0.16	13.90	47,47,47,47	0
36	SR	0	8925	1/1	0.11	13.86	83,83,83,83	0
34	NA	0	8573	1/1	0.27	12.34	64,64,64,64	0
32	MG	0	8078	1/1	0.32	11.87	50,50,50,50	0
34	NA	0	8542	1/1	0.27	10.76	48,48,48,48	0
34	NA	0	8525	1/1	0.26	9.33	71,71,71,71	0
34	NA	0	8559	1/1	0.17	8.93	73,73,73,73	0
34	NA	0	8557	1/1	0.11	8.70	56,56,56,56	0
34	NA	0	8511	1/1	0.19	8.69	59,59,59,59	0
34	NA	0	8508	1/1	0.21	8.50	43,43,43,43	0
36	SR	0	8914	1/1	0.24	8.48	106,106,106,106	0
36	SR	0	8924	1/1	0.16	8.33	139,139,139,139	0
34	NA	0	8547	1/1	0.22	8.21	43,43,43,43	0
36	SR	0	8983	1/1	0.23	8.17	169,169,169,169	0
33	K	0	8401	1/1	0.60	7.30	132,132,132,132	0
32	MG	0	8063	1/1	0.27	7.22	78,78,78,78	0
32	MG	0	8017	1/1	0.23	7.14	32,32,32,32	0
36	SR	0	8937	1/1	0.17	7.00	100,100,100,100	0
34	NA	0	8514	1/1	0.27	7.00	42,42,42,42	0
32	MG	0	8041	1/1	0.20	6.89	25,25,25,25	0
36	SR	0	8903	1/1	0.14	6.84	46,46,46,46	0
32	MG	0	8029	1/1	0.14	6.74	37,37,37,37	0
32	MG	0	8048	1/1	0.20	6.63	19,19,19,19	0
34	NA	0	8553	1/1	0.24	6.55	68,68,68,68	0
32	MG	A	8051	1/1	0.44	6.25	62,62,62,62	0
36	SR	0	8905	1/1	0.23	6.11	52,52,52,52	0
36	SR	0	9001	1/1	0.17	5.86	158,158,158,158	0
34	NA	0	8552	1/1	0.26	5.80	56,56,56,56	0
36	SR	0	8989	1/1	0.17	5.78	177,177,177,177	0
32	MG	0	8069	1/1	0.58	5.65	99,99,99,99	0
34	NA	0	8569	1/1	0.25	5.51	65,65,65,65	0
32	MG	0	8070	1/1	0.17	5.44	45,45,45,45	0
32	MG	0	8014	1/1	0.17	5.39	21,21,21,21	0
34	NA	0	8507	1/1	0.17	5.31	31,31,31,31	0
32	MG	0	8045	1/1	0.13	5.24	28,28,28,28	0
36	SR	0	8947	1/1	0.20	4.78	170,170,170,170	0
32	MG	0	8085	1/1	0.13	4.71	76,76,76,76	0
36	SR	0	8976	1/1	0.22	4.41	185,185,185,185	0
36	SR	0	8926	1/1	0.13	4.40	114,114,114,114	0
32	MG	0	8039	1/1	0.19	4.33	70,70,70,70	0
32	MG	0	8071	1/1	0.16	4.23	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	H	8518	1/1	0.38	4.22	86,86,86,86	0
32	MG	0	8018	1/1	0.17	4.18	29,29,29,29	0
34	NA	0	8506	1/1	0.14	4.16	56,56,56,56	0
32	MG	0	8030	1/1	0.23	4.12	60,60,60,60	0
32	MG	0	8009	1/1	0.18	4.11	18,18,18,18	0
36	SR	0	8969	1/1	0.16	3.91	158,158,158,158	0
32	MG	0	8066	1/1	0.18	3.88	44,44,44,44	0
34	NA	0	8544	1/1	0.12	3.76	60,60,60,60	0
32	MG	0	8082	1/1	0.15	3.62	77,77,77,77	0
32	MG	0	8007	1/1	0.18	3.58	29,29,29,29	0
34	NA	0	8575	1/1	0.23	3.57	86,86,86,86	0
34	NA	0	8541	1/1	0.18	3.41	53,53,53,53	0
34	NA	0	8550	1/1	0.16	3.39	51,51,51,51	0
36	SR	0	8938	1/1	0.12	3.35	158,158,158,158	0
32	MG	0	8028	1/1	0.16	3.30	22,22,22,22	0
32	MG	0	8015	1/1	0.13	3.25	24,24,24,24	0
32	MG	0	8047	1/1	0.21	3.20	38,38,38,38	0
36	SR	0	9004	1/1	0.39	3.10	200,200,200,200	0
36	SR	0	8904	1/1	0.16	2.91	48,48,48,48	0
34	NA	0	8567	1/1	0.17	2.90	77,77,77,77	0
34	NA	0	8501	1/1	0.13	2.87	31,31,31,31	0
36	SR	0	8992	1/1	0.16	2.87	136,136,136,136	0
32	MG	0	8005	1/1	0.21	2.74	31,31,31,31	0
32	MG	0	8019	1/1	0.16	2.68	24,24,24,24	0
36	SR	0	8909	1/1	0.14	2.53	77,77,77,77	0
32	MG	0	8081	1/1	0.13	2.53	64,64,64,64	0
36	SR	9	9003	1/1	0.15	2.53	157,157,157,157	0
34	NA	0	8530	1/1	0.16	2.33	46,46,46,46	0
32	MG	0	8061	1/1	0.19	2.33	22,22,22,22	0
36	SR	0	8946	1/1	0.16	2.30	110,110,110,110	0
32	MG	0	8004	1/1	0.17	2.25	22,22,22,22	0
36	SR	0	8959	1/1	0.13	2.23	157,157,157,157	0
32	MG	0	8076	1/1	0.14	2.07	38,38,38,38	0
32	MG	0	8079	1/1	0.14	1.99	48,48,48,48	0
34	NA	0	8527	1/1	0.15	1.94	53,53,53,53	0
36	SR	0	8915	1/1	0.12	1.93	110,110,110,110	0
34	NA	0	8533	1/1	0.14	1.93	45,45,45,45	0
34	NA	0	8551	1/1	0.14	1.92	40,40,40,40	0
32	MG	0	8008	1/1	0.13	1.91	19,19,19,19	0
32	MG	0	8064	1/1	0.14	1.88	36,36,36,36	0
34	NA	0	8558	1/1	0.17	1.86	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8020	1/1	0.11	1.77	37,37,37,37	0
34	NA	0	8528	1/1	0.13	1.76	35,35,35,35	0
32	MG	0	8022	1/1	0.13	1.76	30,30,30,30	0
34	NA	0	8568	1/1	0.18	1.72	36,36,36,36	0
36	SR	0	8991	1/1	0.14	1.54	183,183,183,183	0
32	MG	0	8024	1/1	0.14	1.36	55,55,55,55	0
32	MG	0	8006	1/1	0.13	1.35	25,25,25,25	0
32	MG	9	8074	1/1	0.12	1.32	62,62,62,62	0
32	MG	0	8011	1/1	0.17	1.27	20,20,20,20	0
32	MG	0	8060	1/1	0.13	1.26	52,52,52,52	0
36	SR	0	9002	1/1	0.12	1.25	173,173,173,173	0
36	SR	0	8985	1/1	0.11	1.04	115,115,115,115	0
32	MG	0	8003	1/1	0.14	1.00	28,28,28,28	0
34	NA	0	8537	1/1	0.11	0.98	34,34,34,34	0
36	SR	R	8912	1/1	0.17	0.97	78,78,78,78	0
32	MG	0	8080	1/1	0.11	0.94	66,66,66,66	0
32	MG	0	8067	1/1	0.15	0.89	31,31,31,31	0
36	SR	0	8990	1/1	0.14	0.84	124,124,124,124	0
32	MG	0	8055	1/1	0.15	0.83	35,35,35,35	0
36	SR	0	8972	1/1	0.19	0.78	163,163,163,163	0
36	SR	0	8933	1/1	0.17	0.66	136,136,136,136	0
36	SR	3	8932	1/1	0.12	0.62	67,67,67,67	0
36	SR	0	8988	1/1	0.14	0.60	159,159,159,159	0
34	NA	0	8504	1/1	0.13	0.60	30,30,30,30	0
36	SR	0	8918	1/1	0.11	0.49	74,74,74,74	0
32	MG	0	8090	1/1	0.12	0.47	70,70,70,70	0
36	SR	0	8908	1/1	0.12	0.47	92,92,92,92	0
37	CD	1	8702	1/1	0.11	0.46	59,59,59,59	0
36	SR	0	8906	1/1	0.17	0.45	48,48,48,48	0
36	SR	0	8984	1/1	0.10	0.44	111,111,111,111	0
32	MG	0	8062	1/1	0.15	0.32	37,37,37,37	0
34	NA	0	8545	1/1	0.15	0.27	38,38,38,38	0
32	MG	0	8046	1/1	0.13	0.23	33,33,33,33	0
34	NA	0	8571	1/1	0.10	0.21	72,72,72,72	0
36	SR	0	8981	1/1	0.12	0.10	156,156,156,156	0
32	MG	0	8026	1/1	0.10	0.07	32,32,32,32	0
36	SR	0	8944	1/1	0.10	-0.09	167,167,167,167	0
32	MG	0	8084	1/1	0.10	-0.12	31,31,31,31	0
36	SR	0	8974	1/1	0.18	-0.13	160,160,160,160	0
34	NA	J	8538	1/1	0.14	-0.33	51,51,51,51	0
34	NA	0	8523	1/1	0.11	-0.35	41,41,41,41	0
32	MG	0	8068	1/1	0.10	-0.38	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	A	8929	1/1	0.11	-0.42	123,123,123,123	0
36	SR	B	8950	1/1	0.11	-0.44	121,121,121,121	0
36	SR	0	8993	1/1	0.11	-0.46	170,170,170,170	0
32	MG	0	8012	1/1	0.14	-0.62	15,15,15,15	0
32	MG	B	8043	1/1	0.09	-0.63	38,38,38,38	0
35	CL	R	8806	1/1	0.10	-0.68	38,38,38,38	0
34	NA	0	8570	1/1	0.09	-0.68	43,43,43,43	0
32	MG	0	8016	1/1	0.13	-0.68	46,46,46,46	0
36	SR	A	8977	1/1	0.11	-0.69	159,159,159,159	0
36	SR	0	8957	1/1	0.09	-0.73	187,187,187,187	0
36	SR	0	8968	1/1	0.08	-0.74	165,165,165,165	0
36	SR	0	8953	1/1	0.13	-0.76	140,140,140,140	0
34	NA	C	8503	1/1	0.11	-0.76	31,31,31,31	0
32	MG	0	8023	1/1	0.10	-0.81	24,24,24,24	0
34	NA	0	8521	1/1	0.12	-0.81	52,52,52,52	0
36	SR	0	8907	1/1	0.10	-0.81	54,54,54,54	0
34	NA	0	8520	1/1	0.09	-0.86	47,47,47,47	0
32	MG	0	8072	1/1	0.12	-0.87	48,48,48,48	0
32	MG	B	8042	1/1	0.07	-0.87	50,50,50,50	0
36	SR	0	8922	1/1	0.13	-0.93	150,150,150,150	0
35	CL	O	8808	1/1	0.11	-0.93	58,58,58,58	0
32	MG	0	8088	1/1	0.12	-0.95	30,30,30,30	0
36	SR	0	8917	1/1	0.10	-0.95	103,103,103,103	0
32	MG	0	8058	1/1	0.08	-1.01	18,18,18,18	0
34	NA	M	8539	1/1	0.09	-1.04	26,26,26,26	0
36	SR	0	8956	1/1	0.06	-1.07	130,130,130,130	0
36	SR	0	8948	1/1	0.10	-1.10	94,94,94,94	0
36	SR	0	8927	1/1	0.09	-1.11	136,136,136,136	0
32	MG	0	8036	1/1	0.07	-1.12	33,33,33,33	0
36	SR	0	8911	1/1	0.07	-1.18	74,74,74,74	0
35	CL	0	8811	1/1	0.08	-1.26	62,62,62,62	0
32	MG	0	8065	1/1	0.09	-1.38	38,38,38,38	0
35	CL	J	8801	1/1	0.07	-1.38	66,66,66,66	0
32	MG	0	8001	1/1	0.10	-1.43	33,33,33,33	0
32	MG	9	8040	1/1	0.09	-1.44	69,69,69,69	0
32	MG	K	8054	1/1	0.09	-1.47	34,34,34,34	0
32	MG	0	8035	1/1	0.09	-1.50	49,49,49,49	0
36	SR	A	8930	1/1	0.06	-1.51	96,96,96,96	0
35	CL	J	8821	1/1	0.06	-1.53	60,60,60,60	0
32	MG	T	8057	1/1	0.11	-1.53	59,59,59,59	0
32	MG	0	8010	1/1	0.09	-1.53	44,44,44,44	0
36	SR	0	8979	1/1	0.09	-1.54	200,200,200,200	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8529	1/1	0.05	-1.55	30,30,30,30	0
35	CL	J	8802	1/1	0.06	-1.59	55,55,55,55	0
36	SR	0	8916	1/1	0.09	-1.61	101,101,101,101	0
37	CD	3	8704	1/1	0.06	-1.63	66,66,66,66	0
34	NA	S	8510	1/1	0.08	-1.63	29,29,29,29	0
34	NA	9	8543	1/1	0.12	-1.68	42,42,42,42	0
32	MG	0	8032	1/1	0.07	-1.71	38,38,38,38	0
36	SR	0	8998	1/1	0.11	-1.72	148,148,148,148	0
36	SR	0	8958	1/1	0.08	-1.72	101,101,101,101	0
36	SR	0	8939	1/1	0.05	-1.76	128,128,128,128	0
34	NA	Q	8540	1/1	0.07	-1.84	48,48,48,48	0
37	CD	O	8705	1/1	0.07	-1.88	80,80,80,80	0
37	CD	U	8701	1/1	0.07	-1.91	48,48,48,48	0
36	SR	0	8964	1/1	0.06	-2.08	118,118,118,118	0
37	CD	Z	8703	1/1	0.06	-2.12	79,79,79,79	0
35	CL	M	8818	1/1	0.05	-2.17	34,34,34,34	0
36	SR	0	8943	1/1	0.05	-2.22	94,94,94,94	0
34	NA	0	8531	1/1	0.08	-2.26	44,44,44,44	0
34	NA	0	8515	1/1	0.07	-2.30	32,32,32,32	0
36	SR	0	8936	1/1	0.07	-2.32	84,84,84,84	0
36	SR	0	9008	1/1	0.12	-2.33	84,84,84,84	0
36	SR	0	8934	1/1	0.08	-2.37	104,104,104,104	0
36	SR	0	8975	1/1	0.05	-2.37	124,124,124,124	0
36	SR	F	9005	1/1	0.06	-2.39	118,118,118,118	0
32	MG	0	8077	1/1	0.06	-2.46	32,32,32,32	0
36	SR	0	8919	1/1	0.11	-2.47	159,159,159,159	0
32	MG	0	8053	1/1	0.05	-2.48	52,52,52,52	0
34	NA	0	8519	1/1	0.11	-2.49	37,37,37,37	0
36	SR	0	8902	1/1	0.12	-2.51	57,57,57,57	0
36	SR	0	8921	1/1	0.09	-2.52	82,82,82,82	0
36	SR	0	8935	1/1	0.09	-2.62	73,73,73,73	0
35	CL	N	8807	1/1	0.07	-2.63	57,57,57,57	0
32	MG	0	8073	1/1	0.07	-2.71	65,65,65,65	0
36	SR	0	8941	1/1	0.11	-2.81	99,99,99,99	0
35	CL	3	8804	1/1	0.05	-2.85	57,57,57,57	0
35	CL	0	8816	1/1	0.07	-2.86	66,66,66,66	0
35	CL	K	8812	1/1	0.06	-2.90	39,39,39,39	0
36	SR	0	8954	1/1	0.07	-2.92	94,94,94,94	0
32	MG	0	8056	1/1	0.09	-2.96	48,48,48,48	0
36	SR	0	8940	1/1	0.09	-2.97	85,85,85,85	0
36	SR	S	8961	1/1	0.08	-3.02	116,116,116,116	0
35	CL	L	8810	1/1	0.06	-3.03	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	A	8050	1/1	0.08	-3.06	34,34,34,34	0
34	NA	0	8513	1/1	0.09	-3.10	42,42,42,42	0
32	MG	0	8087	1/1	0.10	-3.13	29,29,29,29	0
34	NA	0	8517	1/1	0.10	-3.13	28,28,28,28	0
36	SR	3	8999	1/1	0.05	-3.16	94,94,94,94	0
36	SR	9	8978	1/1	0.05	-3.17	133,133,133,133	0
32	MG	0	8021	1/1	0.07	-3.19	29,29,29,29	0
32	MG	0	8052	1/1	0.06	-3.22	39,39,39,39	0
36	SR	9	8980	1/1	0.09	-3.24	168,168,168,168	0
36	SR	0	8910	1/1	0.06	-3.27	93,93,93,93	0
36	SR	0	8945	1/1	0.07	-3.37	97,97,97,97	0
33	K	0	8402	1/1	0.07	-3.38	69,69,69,69	0
34	NA	0	8516	1/1	0.09	-3.47	27,27,27,27	0
36	SR	0	8951	1/1	0.06	-3.51	138,138,138,138	0
32	MG	0	8031	1/1	0.07	-3.55	59,59,59,59	0
36	SR	0	8960	1/1	0.04	-3.58	135,135,135,135	0
34	NA	R	8532	1/1	0.06	-3.60	37,37,37,37	0
36	SR	0	8942	1/1	0.07	-3.65	108,108,108,108	0
35	CL	0	8817	1/1	0.05	-3.66	50,50,50,50	0
36	SR	0	8971	1/1	0.04	-3.82	150,150,150,150	0
35	CL	0	8813	1/1	0.04	-3.88	49,49,49,49	0
35	CL	A	8809	1/1	0.05	-3.91	63,63,63,63	0
35	CL	0	8803	1/1	0.08	-3.94	46,46,46,46	0
32	MG	0	8044	1/1	0.07	-3.94	40,40,40,40	0
35	CL	0	8805	1/1	0.05	-3.95	50,50,50,50	0
36	SR	1	8913	1/1	0.07	-3.99	76,76,76,76	0
36	SR	1	8952	1/1	0.10	-4.05	73,73,73,73	0
32	MG	0	8059	1/1	0.07	-4.17	44,44,44,44	0
35	CL	Y	8820	1/1	0.05	-4.17	35,35,35,35	0
32	MG	0	8089	1/1	0.10	-4.28	43,43,43,43	0
32	MG	0	8002	1/1	0.08	-4.28	25,25,25,25	0
32	MG	0	8083	1/1	0.04	-4.31	48,48,48,48	0
36	SR	0	8995	1/1	0.12	-4.44	133,133,133,133	0
36	SR	0	8962	1/1	0.10	-4.47	168,168,168,168	0
34	NA	0	8534	1/1	0.09	-4.50	37,37,37,37	0
32	MG	0	8075	1/1	0.05	-4.54	45,45,45,45	0
34	NA	0	8526	1/1	0.02	-4.63	36,36,36,36	0
36	SR	0	8928	1/1	0.07	-4.64	127,127,127,127	0
32	MG	0	8025	1/1	0.07	-4.64	22,22,22,22	0
36	SR	0	8970	1/1	0.04	-4.77	118,118,118,118	0
32	MG	0	8093	1/1	0.08	-4.79	29,29,29,29	0
36	SR	0	8965	1/1	0.04	-5.22	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	0	8815	1/1	0.04	-5.26	61,61,61,61	0
35	CL	0	8814	1/1	0.08	-5.67	48,48,48,48	0
32	MG	Y	8086	1/1	0.08	-5.69	34,34,34,34	0
36	SR	0	8920	1/1	0.03	-6.07	108,108,108,108	0
36	SR	0	8955	1/1	0.05	-6.11	187,187,187,187	0
36	SR	0	8967	1/1	0.04	-6.13	127,127,127,127	0
36	SR	0	8931	1/1	0.07	-6.14	98,98,98,98	0
36	SR	0	8923	1/1	0.04	-6.46	104,104,104,104	0
36	SR	0	8966	1/1	0.06	-6.84	100,100,100,100	0
35	CL	B	8819	1/1	0.04	-7.05	44,44,44,44	0
36	SR	0	8949	1/1	0.06	-7.06	99,99,99,99	0
32	MG	0	8027	1/1	0.04	-7.32	29,29,29,29	0
32	MG	0	8033	1/1	0.06	-7.44	35,35,35,35	0
32	MG	0	8034	1/1	0.04	-8.22	36,36,36,36	0
32	MG	0	8013	1/1	0.03	-8.91	22,22,22,22	0
32	MG	0	8091	1/1	0.03	-11.44	48,48,48,48	0
36	SR	0	8901	1/1	0.08	-12.95	74,74,74,74	0
32	MG	0	8092	1/1	0.05	-39.00	51,51,51,51	0
36	SR	0	9006	1/1	2.26	-	200,200,200,200	0
36	SR	0	8963	1/1	0.07	-	167,167,167,167	0
36	SR	0	8973	1/1	0.07	-	124,124,124,124	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.