



wwPDB X-ray Structure Validation Summary Report

May 8, 2014 – 03:22 AM EDT

PDB ID : 3CC7
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2487U
Authors : Blaha, G.; Gurel, G.
Deposited on : 2008-02-25
Resolution : 2.70 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

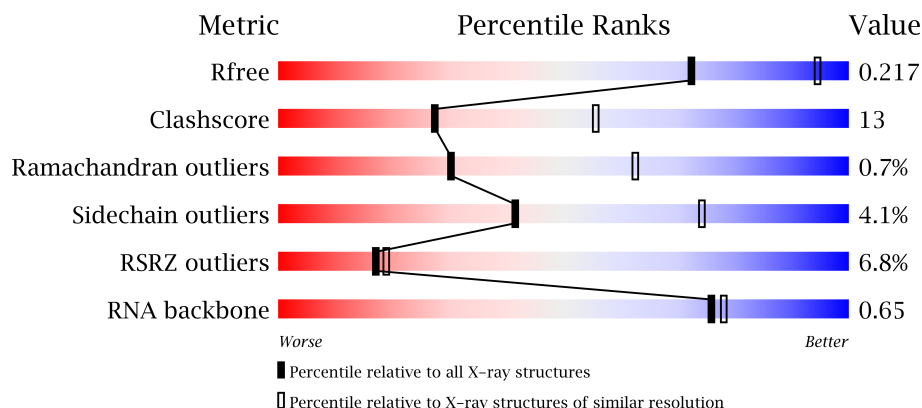
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable22978
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) : stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.70 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	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)
RNA backbone	1838	1042 (3.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	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	8001	-	X
32	MG	0	8009	-	X
32	MG	0	8017	-	X
32	MG	0	8018	-	X
32	MG	0	8024	-	X
32	MG	0	8030	-	X
32	MG	0	8031	-	X
32	MG	0	8037	-	X
32	MG	0	8039	-	X
32	MG	0	8040	-	X
32	MG	0	8041	-	X
32	MG	0	8047	-	X
32	MG	0	8049	-	X
32	MG	0	8061	-	X
32	MG	0	8062	-	X
32	MG	0	8063	-	X
32	MG	0	8069	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
32	MG	0	8071	-	X
32	MG	0	8078	-	X
32	MG	0	8079	-	X
32	MG	0	8081	-	X
32	MG	0	8083	-	X
32	MG	0	8090	-	X
32	MG	A	8051	-	X
33	K	0	8401	-	X
34	NA	0	8502	-	X
34	NA	0	8505	-	X
34	NA	0	8506	-	X
34	NA	0	8511	-	X
34	NA	0	8512	-	X
34	NA	0	8513	-	X
34	NA	0	8514	-	X
34	NA	0	8517	-	X
34	NA	0	8519	-	X
34	NA	0	8521	-	X
34	NA	0	8522	-	X
34	NA	0	8524	-	X
34	NA	0	8525	-	X
34	NA	0	8526	-	X
34	NA	0	8527	-	X
34	NA	0	8535	-	X
34	NA	0	8541	-	X
34	NA	0	8542	-	X
34	NA	0	8544	-	X
34	NA	0	8545	-	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	8551	-	X
34	NA	0	8552	-	X
34	NA	0	8553	-	X
34	NA	0	8554	-	X
34	NA	0	8555	-	X
34	NA	0	8556	-	X
34	NA	0	8558	-	X
34	NA	0	8559	-	X
34	NA	0	8560	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
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	8568	-	X
34	NA	0	8569	-	X
34	NA	0	8571	-	X
34	NA	0	8574	-	X
34	NA	9	8572	-	X
34	NA	R	8575	-	X
35	CL	0	8822	-	X
36	SR	0	8905	-	X
36	SR	0	8906	-	X
36	SR	0	8907	-	X
36	SR	0	8914	-	X
36	SR	0	8919	-	X
36	SR	0	8922	-	X
36	SR	0	8934	-	X
36	SR	0	8947	-	X
36	SR	0	8955	-	X
36	SR	0	8959	-	X
36	SR	0	8962	-	X
36	SR	0	8974	-	X
36	SR	0	8976	-	X
36	SR	0	8979	-	X
36	SR	0	8982	-	X
36	SR	0	8985	-	X
36	SR	0	8989	-	X
36	SR	0	8991	-	X
36	SR	0	8992	-	X
36	SR	0	8994	-	X
36	SR	0	8996	-	X
36	SR	0	8997	-	X
36	SR	0	8998	-	X
36	SR	0	9004	-	X
36	SR	0	9006	-	X
36	SR	0	9007	-	X
36	SR	9	8980	-	X
36	SR	B	8987	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
36	SR	J	8986	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 99122 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
			59020	26349	10872	19054	2745			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	2	Total	Mg	0	0
			2	2		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is 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	C	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	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	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	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
35	Y	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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	93	Total 93	Sr 93	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	2	Total 2	Sr 2	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
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	5951	Total O 5951 5951	0	0
38	A	111	Total O 111 111	0	0
38	B	153	Total O 153 153	0	0
38	C	165	Total O 165 165	0	0
38	D	46	Total O 46 46	0	0
38	E	44	Total O 44 44	0	0
38	F	23	Total O 23 23	0	0
38	G	19	Total O 19 19	0	0
38	H	71	Total O 71 71	0	0
38	I	10	Total O 10 10	0	0
38	J	54	Total O 54 54	0	0
38	K	56	Total O 56 56	0	0
38	L	80	Total O 80 80	0	0
38	M	130	Total O 130 130	0	0
38	N	59	Total O 59 59	0	0
38	O	41	Total O 41 41	0	0
38	P	61	Total O 61 61	0	0
38	Q	51	Total O 51 51	0	0
38	R	78	Total O 78 78	0	0
38	S	33	Total O 33 33	0	0
38	T	37	Total O 37 37	0	0

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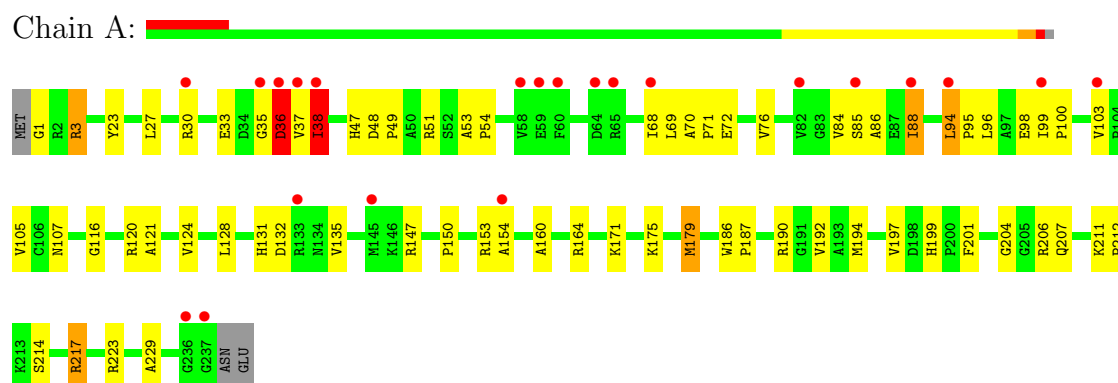
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	U	25	Total 25	O 25	0	0
38	V	11	Total 11	O 11	0	0
38	W	63	Total 63	O 63	0	0
38	X	28	Total 28	O 28	0	0
38	Y	91	Total 91	O 91	0	0
38	Z	28	Total 28	O 28	0	0
38	1	52	Total 52	O 52	0	0
38	2	37	Total 37	O 37	0	0
38	3	68	Total 68	O 68	0	0
38	9	147	Total 147	O 147	0	0

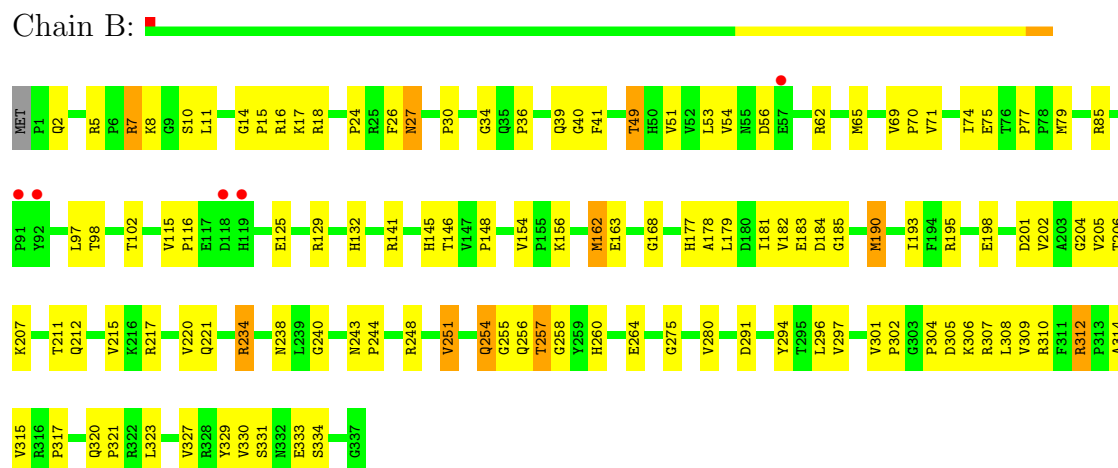
3 Residue-property plots

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.

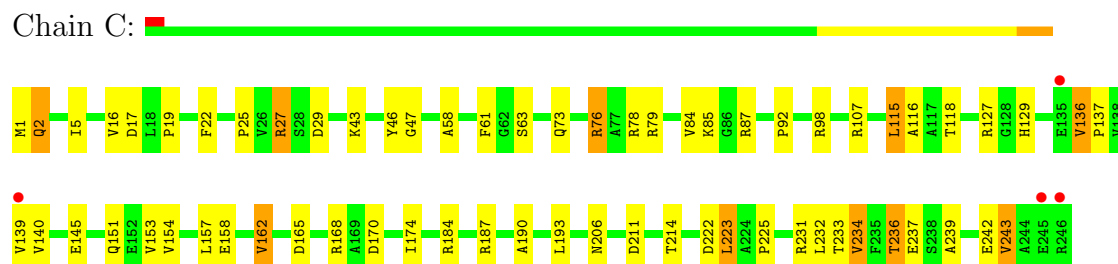
• Molecule 1: 50S ribosomal protein L2P



• Molecule 2: 50S ribosomal protein L3P

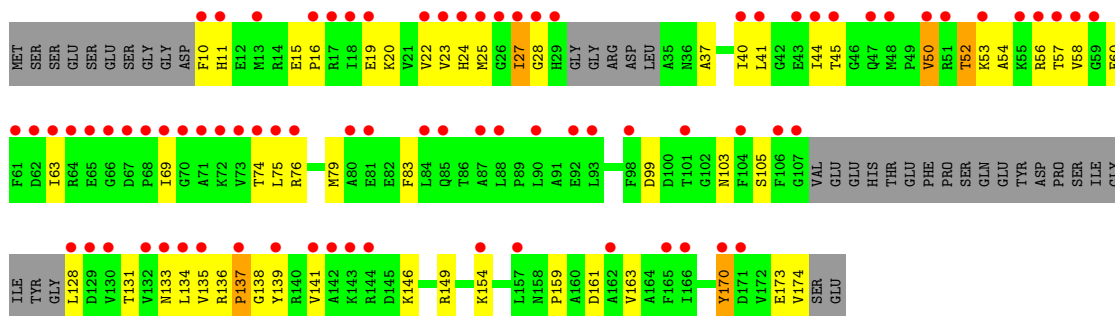


• Molecule 3: 50S ribosomal protein L4P



- Molecule 4: 50S ribosomal protein L5P

Chain D:



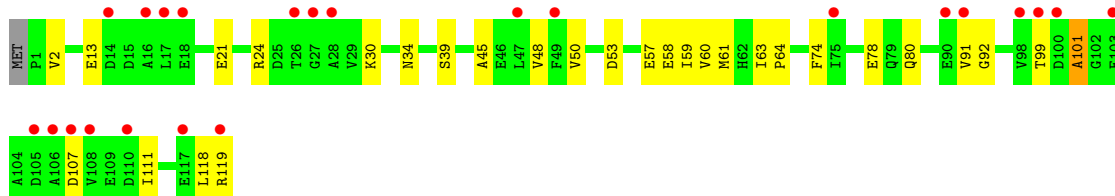
- Molecule 5: 50S ribosomal protein L6P

Chain E:



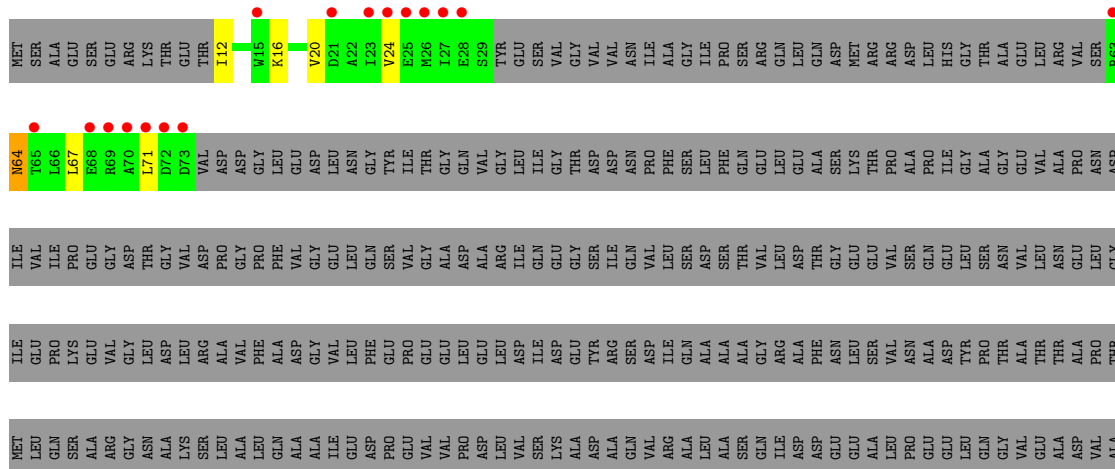
- Molecule 6: 50S ribosomal protein L7Ae

Chain F:



- Molecule 7: 50S ribosomal protein L10E

Chain G:



- Molecule 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:



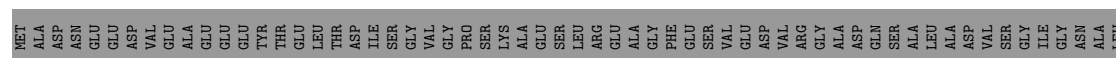
- Molecule 24: 50S ribosomal protein L31e

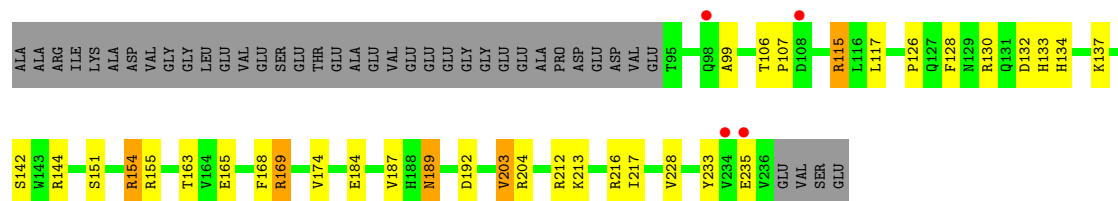
Chain X:



- Molecule 25: 50S ribosomal protein L32e

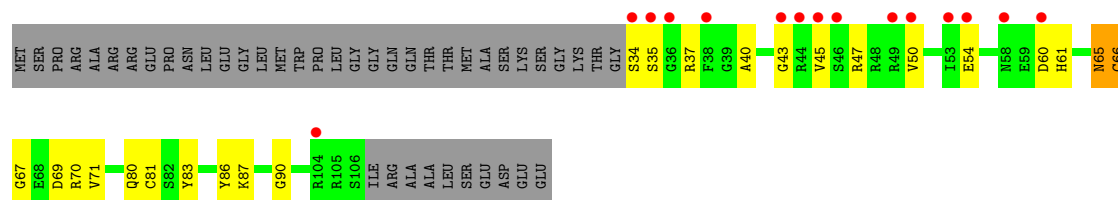
Chain Y:





• Molecule 26: 50S ribosomal protein L37Ae

Chain Z:



• Molecule 27: 50S ribosomal protein L37e

Chain 1:



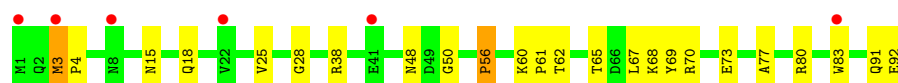
• Molecule 28: 50S ribosomal protein L39e

Chain 2:



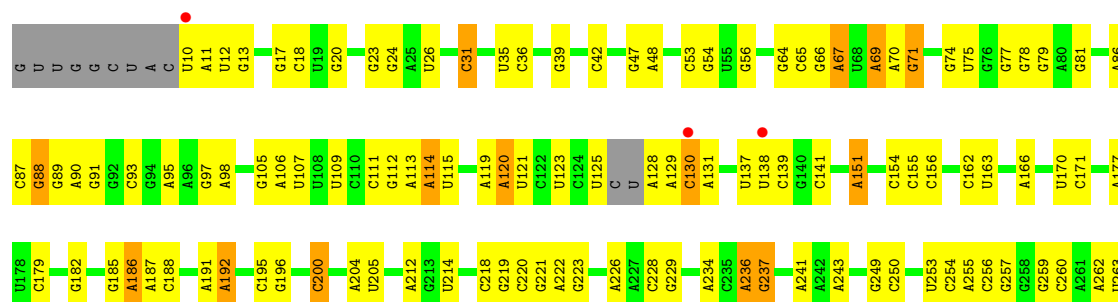
• Molecule 29: 50S ribosomal protein L44E

Chain 3:

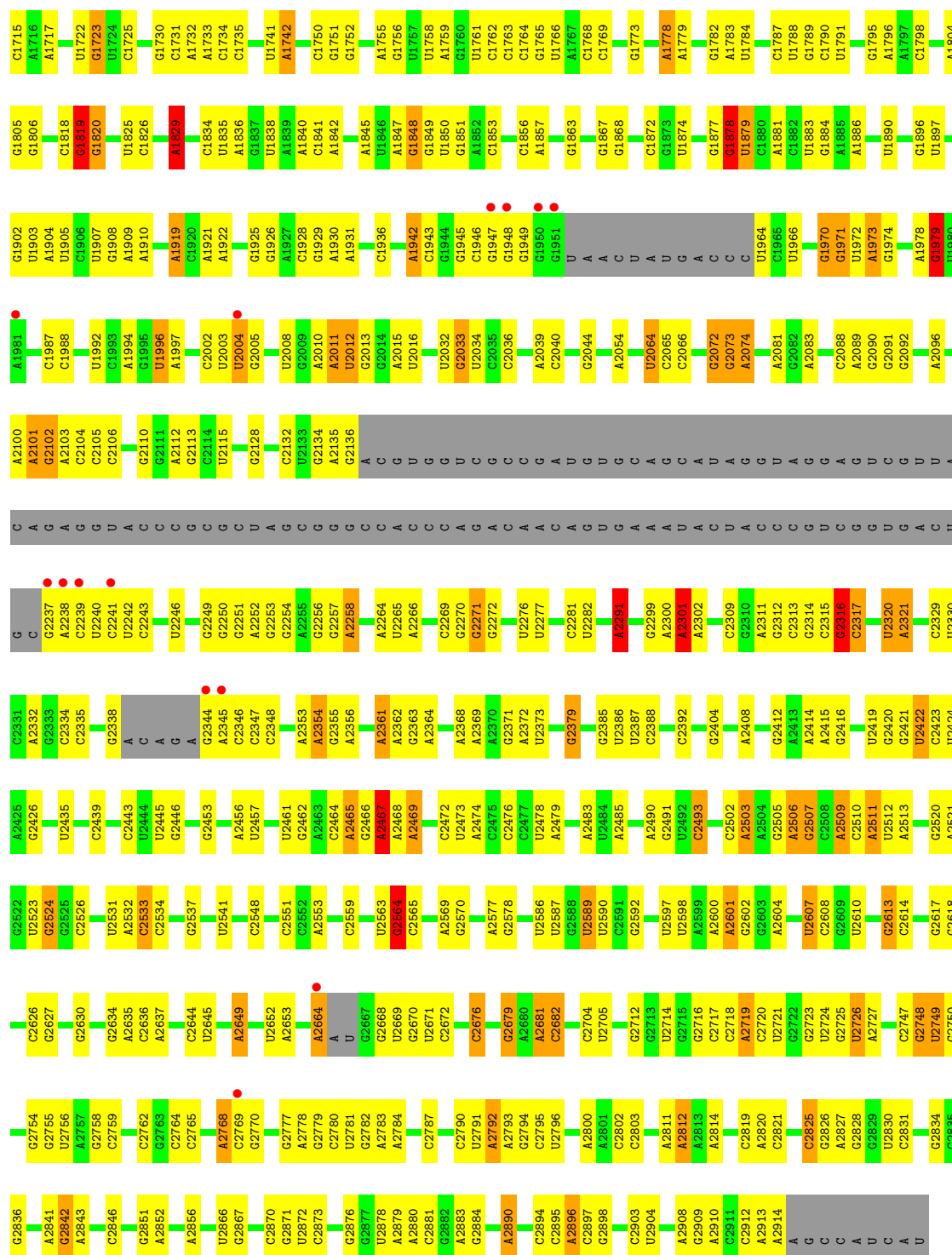


• Molecule 30: 23S ribosomal RNA

Chain 0:

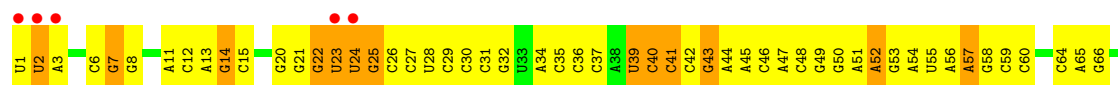


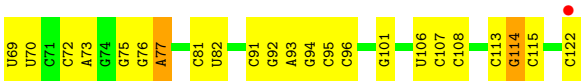
C1613	G1512	A1308	G1214	G1151	C1044	A961	G869	C764	A660	G537	A441	G345	G264
G1614	A1515	G1311	A1215	C1156	G1045	C962	G870	G765	A661	C538	A442	U346	U265
A1615	G1416	G1312	G1216	C1157	G1045	C963	U872	G775	G667	G539	C443	A347	G269
C1617	C1517	A1313	C1229	G1158	C1051	G968	A875	U777	G668	A540	U445	G350	U270
U1625	G1520	A1314	A1230	G1159	G1052	G969	A876	A790	G669	C541	U446	G358	A271
A1626	U1419	G1311	U1234	G1160	G1053	U970	G877	G790	A671	A542	A447	A272	G273
A1627	G1420	A1321	G1235	A1161	G1054	G	G878	A791	G670	G543	G448	C383	C278
A1628	C1421	G1322	A1236	G1162	G1055	U	A882	G792	A671	G544	U364	U364	A279
A1629	U1524	G1323	U1237	G1163	U1056	U	U883	G793	G677	G545	C451	G365	C280
A1630	C1423	G1324	C1238	G1164	A1057	G	U886	G794	G678	G553	G452	U366	U281
A1631	U1525	A1328	G1239	G1165	A1058	C	A886	A796	G681	C558	A453	C387	C282
A1632	A1427	G1329	U1242	G1166	G1059	G	G889	A797	G682	U559	U454	G389	U283
A1633	U1428	A1330	A1243	G1167	C1060	C	G892	G800	A683	U560	G458	G370	U284
A1634	G1432	C1331	C1243	G1168	G1063	C	G898	U801	G684	G564	A372	A285	U286
A1635	U1433	G1332	U1244	G1169	G1063	C	G902	A806	G685	U567	A461	U371	G289
A1636	U1434	C1333	C1245	G1170	U1066	U	U903	A807	A686	U582	A462	G373	C290
C1536	C1435	G1334	A1246	G1171	A1067	C	U904	A808	G687	U583	A466	G378	C291
U1548	U1440	U1335	U1249	G1172	A1067	C	G905	G816	G688	C582	G467	U392	G292
U1549	U1441	U1336	C1250	G1173	G1071	G	U906	G817	G689	U584	U468	G381	A293
U1550	A1442	G1337	A1251	G1174	G1072	A	A907	A818	G690	G588	U470	U382	C294
U1551	G1443	C1341	A1252	G1175	G1073	A	U908	G819	G691	C594	G482	C295	G295
U1552	G1444	C1342	C1253	G1176	G1074	G	A909	G820	G692	U595	G483	C296	U297
U1553	G1445	C1343	G1260	G1177	G1075	G	A912	G821	G693	C596	U484	C297	U298
U1554	U1446	C1344	A1261	G1178	G1076	A	U910	G822	G694	A602	U485	U300	U299
U1555	U1447	U1345	C1262	G1179	G1077	G	A912	G823	G695	A603	G486	C301	C302
U1556	U1448	U1346	A1263	G1180	A1078	G	U912	G824	G696	U604	U487	G303	G304
U1557	C1451	C1360	C1264	G1181	A1079	U	A912	U825	G697	G613	A497	U308	U308
U1558	U1456	C1366	C1265	G1182	A1080	C	U912	U826	G698	U614	A498	C309	C309
U1559	U1457	C1367	C1266	G1183	A1081	C	C920	G834	G699	U619	A407	A316	A316
U1560	U1458	C1368	C1267	G1184	A1082	C	C921	G835	G716	G621	A408	A317	A317
U1561	U1459	C1369	C1268	G1185	A1083	C	U922	G836	G717	G622	A409	U318	U318
U1562	U1460	C1370	C1269	G1186	A1084	C	A923	G837	G718	U623	A412	A319	A319
U1563	U1461	C1371	C1270	G1187	A1085	C	U924	G838	G719	U624	C413	A327	A327
U1564	U1462	C1372	C1271	G1188	A1086	C	U925	G839	G720	U625	A511	U328	U328
U1565	U1463	C1373	C1272	G1189	A1087	C	U926	G840	G721	U626	A512	A329	A329
U1566	U1464	C1374	C1273	G1190	A1088	C	U927	G841	G722	U627	A513	C330	C330
U1567	U1465	C1375	C1274	G1191	A1089	C	U928	G842	G723	U628	A514	A331	A331
U1568	U1466	C1376	C1275	G1192	A1090	C	U929	G843	G724	U629	U510	G332	G332
U1569	U1467	C1377	C1276	G1193	A1091	C	U930	G844	G725	U630	G517	G333	G333
U1570	U1468	C1378	C1277	G1194	A1092	C	U931	G845	G726	U631	G518	G334	G334
U1571	U1469	C1379	C1278	G1195	A1093	C	U932	G846	G727	U632	G519	G335	G335
U1572	U1470	C1380	C1279	G1196	A1094	C	U933	G847	G728	U633	G520	G336	G336
U1573	U1471	C1381	C1280	G1197	A1095	C	U934	G848	G729	U634	G521	G337	G337
U1574	U1472	C1382	C1281	G1198	A1096	C	U935	G849	G730	U635	G522	G338	G338
U1575	U1473	C1383	C1282	G1199	A1097	C	U936	G850	G731	U636	G523	C339	C339
U1576	U1474	C1384	C1283	G1200	A1098	C	U937	G851	G732	U637	G524	C340	C340
U1577	U1475	C1385	C1284	G1201	A1099	C	U938	G852	G733	U638	G525	C341	C341
U1578	U1476	C1386	C1285	G1202	A1100	C	U939	G853	G734	U639	G526	C342	C342
U1579	U1477	C1387	C1286	G1203	A1101	C	U940	G854	G735	U640	G527	C343	C343
U1580	U1478	C1388	C1287	G1204	A1102	C	U941	G855	G736	U641	G528	C344	C344
U1581	U1479	C1389	C1288	G1205	A1103	C	U942	G856	G737	U642	G529	C345	C345
U1582	U1480	C1390	C1289	G1206	A1104	C	U943	G857	G738	U643	G530	C346	C346
U1583	U1481	C1391	C1290	G1207	A1105	C	U944	G858	G739	U644	G531	C347	C347
U1584	U1482	C1392	C1291	G1208	A1106	C	U945	G859	G740	U645	G532	C348	C348
U1585	U1483	C1393	C1292	G1209	A1107	C	U946	G860	G741	U646	G533	C349	C349
U1586	U1484	C1394	C1293	G1210	A1108	C	U947	G861	G742	U647	G534	C350	C350
U1587	U1485	C1395	C1294	G1211	A1109	C	U948	G862	G743	U648	G535	C351	C351
U1588	U1486	C1396	C1295	G1212	A1110	C	U949	G863	G744	U649	G536	C352	C352
U1589	U1487	C1397	C1296	G1213	A1111	C	U950	G864	G745	U650	G537	C353	C353
U1590	U1488	C1398	C1297	G1214	A1112	C	U951	G865	G746	U651	G538	C354	C354
U1591	U1489	C1399	C1298	G1215	A1113	C	U952	G866	G747	U652	G539	C355	C355
U1592	U1490	C1400	C1299	G1216	A1114	C	U953	G867	G748	U653	G540	C356	C356
U1593	U1491	C1401	C1300	G1217	A1115	C	U954	G868	G749	U654	G541	C357	C357
U1594	U1492	C1402	U1293	G1218	A1116	C	U955	G869	G750	U655	G542	C358	C358
U1595	U1493	C1403	U1294	G1219	A1117	C	U956	G870	G751	U656	G543	C359	C359
U1596	U1494	C1404	U1295	G1220	A1118	C	U957	G871	G752	U657	G544	C360	C360
U1597	U1495	C1405	U1296	G1221	A1119	C	U958	G872	G753	U658	G545	C361	C361
U1598	U1496	C1406	U1297	G1222	A1120	C	U959	G873	G754	U659	G546	C362	C362
U1599	U1497	C1407	U1298	G1223	A1121	C	U960	G874	G755	U660	G547	C363	C363
U1600	U1498	C1408	U1299	G1224	A1122	C	U961	G875	G756	U661	G548	C364	C364
U1601	U1499	C1409	U1300	G1225	A1123	C	U962	G876	G757	U662	G549	C365	C365
U1602	U1500	C1410	U1301	G1226	A1124	C	U963	G877	G758	U663	G550	C366	C366
U1603	U1501	C1411	U1302	G1227	A1125	C	U964	G878	G759	U664	G551	C367	C367
U1604	U1502	C1412	U1303	G1228	A1126	C	U965	G879	G760	U665	G552	C368	C368
U1605	U1503	C1413	U1304	G1229	A1127	C	U966	G880	G761	U666	G553	C369	C369
U1606	U1504	C1414	U1305	G1230	A1128	C	U967	G881	G762	U667	G554	C370	C370
U1607	U1505	C1415	U1306	G1231	A1129	C	U968	G882	G763	U668	G555	C371	C371
U1608	U1506	C1416	U1307	G1232	A1130	C	U969	G883	G764	U669	G556	C372	C372
U1609	U1507	C1417	U1308	G1233	A1131	C	U970	G884	G765	U670	G557	C373	C373
U1610	U1508	C1418	U1309	G1234	A1132	C	U971	G885	G766	U671	G558	C374	C374
U1611	U1509	C1419	U1310	G1235	A1133	C	U972	G886	G767	U672	G559	C375	C375
U1612	U1510	C1420	U1311	G1236	A1134	C	U973	G887	G768	U673	G560	C376	C376
U1613	U1511	C1421	U1312	G1237	A1135	C	U974	G888	G769	U674	G561	C377	C377
U1614	U1512	C1422	U1313	G1238	A1136	C	U975	G889	G770	U675	G562	C378	C378
U1615	U1513	C1423	U1314	G1239	A1137	C	U976	G890	G771	U676	G563	C379	C379
U1616	U1514	C1424	U1315	G1240	A1138	C	U977	G891	G772	U677	G564	C380	C380
U1617	U1515	C1425	U1316	G1241	A1139	C	U978	G892	G773	U678	G565	C381	C381
U1618	U1516	C1426	U1317	G1242	A1140	C	U979	G893	G774	U679	G566	C382	C382
U1619	U1517	C1427	U1318	G1243	A1141	C	U980	G894	G775	U680	G567	C383	C383
U1620	U1518	C1428	U1319	G1244	A1142	C	U981	G895	G776	U681	G568	C384	C384
U1621	U1519	C1429	U1320	G1245	A1143	C	U982	G896	G777	U682	G569	C385	C385
U1622	U1520	C1430	U1321	G1246	A1144	C	U983	G897	G778	U683	G570	C386	C386
U1623	U1521	C1431	U1322	G1247	A1145	C	U984	G898	G779	U684	G571	C387	C387
U1624	U1522	C1432	U1323	G1248	A1146	C	U985	G899	G780	U685	G572	C388	C388
U1625	U1523	C1433	U1324	G1249	A1147	C	U986	G900	G781	U686	G573	C389	C389
U1626	U1524	C1434	U1325	G1250	A1148	C	U987	G901	G782	U687	G574	C390	C390
U1627	U1525	C1435	U1326	G1251	A1149	C	U988	G902	G783	U688	G575	C391	C391
U1628	U1526	C1436	U1327	G1252	A1150	C	U989	G903	G784	U689			



• 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, α , β , γ	212.83Å 299.90Å 576.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.83 – 2.70 85.81 – 2.41	Depositor EDS
% Data completeness (in resolution range)	92.7 (49.83-2.70) 90.8 (85.81-2.41)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.184 , 0.226 0.175 , 0.217	Depositor DCC
R_{free} test set	4705 reflections (0.98%)	DCC
Wilson B-factor (Å ²)	47.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.2	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	3 of 667281 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, OMG, CL, SR, NA, K, 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	0.32	0/1786	0.64	0/2408
2	B	0.32	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.31	0/1111	0.55	0/1498
5	E	0.32	0/1382	0.56	0/1880
6	F	0.32	0/901	0.57	0/1224
7	G	0.31	0/241	0.48	0/324
8	H	0.32	0/1302	0.63	0/1743
9	I	0.29	0/526	0.51	0/716
10	J	0.35	0/1136	0.59	0/1530
11	K	0.33	0/1004	0.65	0/1351
12	L	0.33	0/1130	0.63	0/1509
13	M	0.34	0/1582	0.62	0/2116
14	N	0.29	0/1474	0.61	0/1999
15	O	0.34	0/874	0.59	1/1181 (0.1%)
16	P	0.32	0/1147	0.52	0/1528
17	Q	0.35	0/749	0.68	0/1005
18	R	1.26	7/1172 (0.6%)	1.11	6/1578 (0.4%)
19	S	0.31	0/648	0.57	0/875
20	T	0.33	0/958	0.62	1/1289 (0.1%)
21	U	0.34	0/417	0.55	0/562
22	V	0.31	0/502	0.52	0/675
23	W	0.34	0/1219	0.64	0/1655
24	X	0.34	0/664	0.58	0/895
25	Y	0.36	0/1146	0.60	0/1536
26	Z	0.35	0/584	0.60	0/781
27	1	0.37	0/438	0.61	0/578
28	2	0.34	0/401	0.55	0/529
29	3	0.36	0/771	0.57	0/1024
30	0	0.36	0/65957	0.68	17/102867 (0.0%)
31	9	0.32	0/2904	0.68	1/4526 (0.0%)
All	All	0.38	7/98701 (0.0%)	0.67	26/147586 (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
30	0	0	42
31	9	0	1
All	All	1	43

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	27.34	2.86	1.50
18	R	150	PRO	CA-C	-18.21	1.16	1.52
18	R	150	PRO	CG-CD	13.97	1.96	1.50
18	R	150	PRO	C-O	11.88	1.47	1.23
18	R	150	PRO	N-CA	11.28	1.66	1.47

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.83	112.00
18	R	150	PRO	N-CA-C	-19.39	61.69	112.10
18	R	150	PRO	CA-N-CD	12.31	128.94	111.70
18	R	150	PRO	N-CA-CB	10.98	116.48	103.30
18	R	150	PRO	CA-C-O	-8.51	99.77	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 43 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	221	G	Sidechain
30	0	26	U	Sidechain
30	0	396	U	Sidechain
30	0	458	G	Sidechain
30	0	48	A	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	75	0
2	B	2625	0	2533	92	0
3	C	1860	0	1813	57	0
4	D	1094	0	1085	40	0
5	E	1357	0	1266	23	0
6	F	890	0	843	26	0
7	G	240	0	231	7	0
8	H	1282	0	1292	37	0
9	I	519	0	500	15	0
10	J	1120	0	1098	30	0
11	K	994	0	1027	36	0
12	L	1118	0	1076	22	0
13	M	1558	0	1573	42	0
14	N	1445	0	1401	45	0
15	O	865	0	873	15	0
16	P	1136	0	1123	28	0
17	Q	735	0	729	14	0
18	R	1149	0	1122	34	0
19	S	641	0	605	11	0
20	T	950	0	924	19	0
21	U	410	0	364	19	0
22	V	499	0	511	17	0
23	W	1196	0	1137	55	0
24	X	654	0	653	24	0
25	Y	1130	0	1133	36	0
26	Z	573	0	531	16	0
27	1	431	0	426	22	0
28	2	396	0	413	19	0
29	3	755	0	728	20	0
30	0	59020	0	29806	1142	0
31	9	2599	0	1325	101	0
32	0	85	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	2	0	0	0	0

Continued on next page...

Continued from previous page...

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	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	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	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	93	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	2	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	5951	0	0	153	0
38	1	52	0	0	3	0
38	2	37	0	0	2	0
38	3	68	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	9	147	0	0	8	0
38	A	111	0	0	5	0
38	B	153	0	0	14	0
38	C	165	0	0	11	0
38	D	46	0	0	2	0
38	E	44	0	0	2	0
38	F	23	0	0	1	0
38	G	19	0	0	0	0
38	H	71	0	0	6	0
38	I	10	0	0	2	0
38	J	54	0	0	1	0
38	K	56	0	0	3	0
38	L	80	0	0	6	0
38	M	130	0	0	5	0
38	N	59	0	0	5	0
38	O	41	0	0	3	0
38	P	61	0	0	1	0
38	Q	51	0	0	2	0
38	R	78	0	0	3	0
38	S	33	0	0	2	0
38	T	37	0	0	2	0
38	U	25	0	0	3	0
38	V	11	0	0	0	0
38	W	63	0	0	4	0
38	X	28	0	0	1	0
38	Y	91	0	0	6	0
38	Z	28	0	0	3	0
All	All	99122	0	59907	1937	0

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

The worst 5 of 1937 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	1.44
30:0:1160:G:C5'	30:0:1161:A:H5'	1.81	1.10
31:9:56:A:H2'	31:9:57:A:H5''	1.33	1.08
30:0:871:G:C8	30:0:871:G:H5'	1.87	1.07
18:R:150:PRO:CG	18:R:150:PRO:C	2.22	1.07

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%)	18 (8%)	5 (2%)	11	27
2	B	335/338 (99%)	306 (91%)	26 (8%)	3 (1%)	25	55
3	C	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
4	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	10	25
5	E	170/178 (96%)	161 (95%)	9 (5%)	0	100	100
6	F	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	25	55
7	G	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
8	H	156/177 (88%)	149 (96%)	6 (4%)	1 (1%)	33	66
9	I	68/162 (42%)	55 (81%)	10 (15%)	3 (4%)	4	8
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	125 (96%)	5 (4%)	0	100	100
12	L	141/165 (86%)	127 (90%)	13 (9%)	1 (1%)	30	62
13	M	192/196 (98%)	182 (95%)	9 (5%)	1 (0%)	38	70
14	N	184/187 (98%)	168 (91%)	13 (7%)	3 (2%)	14	35
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	141 (100%)	0	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	140 (95%)	8 (5%)	0	100	100
19	S	79/85 (93%)	78 (99%)	1 (1%)	0	100	100
20	T	117/120 (98%)	110 (94%)	6 (5%)	1 (1%)	25	55
21	U	51/67 (76%)	47 (92%)	4 (8%)	0	100	100
22	V	63/71 (89%)	60 (95%)	2 (3%)	1 (2%)	14	35
23	W	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
24	X	80/92 (87%)	73 (91%)	6 (8%)	1 (1%)	18	43
25	Y	140/241 (58%)	138 (99%)	2 (1%)	0	100	100
26	Z	71/116 (61%)	61 (86%)	8 (11%)	2 (3%)	8	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	41 (98%)	1 (2%)	0	100	100
29	3	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	21	49
All	All	3705/4472 (83%)	3458 (93%)	220 (6%)	27 (1%)	30	62

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	37	VAL
14	N	154	LEU
14	N	183	ASP
14	N	184	ILE

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%)	38	70
2	B	282/283 (100%)	265 (94%)	17 (6%)	27	56
3	C	193/193 (100%)	178 (92%)	15 (8%)	18	40
4	D	117/148 (79%)	109 (93%)	8 (7%)	22	48
5	E	152/156 (97%)	147 (97%)	5 (3%)	50	81
6	F	93/94 (99%)	93 (100%)	0	100	100
7	G	27/282 (10%)	26 (96%)	1 (4%)	45	78
8	H	134/145 (92%)	127 (95%)	7 (5%)	32	63
9	I	58/130 (45%)	57 (98%)	1 (2%)	73	94
10	J	118/121 (98%)	112 (95%)	6 (5%)	33	64
11	K	106/106 (100%)	103 (97%)	3 (3%)	56	86
12	L	113/127 (89%)	111 (98%)	2 (2%)	71	93
13	M	158/160 (99%)	150 (95%)	8 (5%)	33	64
14	N	149/150 (99%)	144 (97%)	5 (3%)	49	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	93/94 (99%)	91 (98%)	2 (2%)	64	90
16	P	113/117 (97%)	108 (96%)	5 (4%)	39	71
17	Q	79/80 (99%)	77 (98%)	2 (2%)	60	89
18	R	117/122 (96%)	113 (97%)	4 (3%)	49	81
19	S	71/74 (96%)	70 (99%)	1 (1%)	78	95
20	T	105/106 (99%)	99 (94%)	6 (6%)	29	58
21	U	44/53 (83%)	43 (98%)	1 (2%)	63	90
22	V	51/57 (90%)	50 (98%)	1 (2%)	68	92
23	W	130/130 (100%)	126 (97%)	4 (3%)	52	83
24	X	66/74 (89%)	60 (91%)	6 (9%)	14	30
25	Y	120/196 (61%)	114 (95%)	6 (5%)	34	66
26	Z	60/94 (64%)	59 (98%)	1 (2%)	73	94
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	61	89
29	3	79/79 (100%)	77 (98%)	2 (2%)	60	89
All	All	3095/3646 (85%)	2967 (96%)	128 (4%)	41	74

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	91	ARG
12	L	35	ARG
25	Y	115	ARG
8	H	169	GLU
10	J	107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	73	HIS
27	1	16	HIS
13	M	137	ASN
14	N	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	239 (8%)	0
31	9	121/122 (99%)	16 (13%)	0
All	All	2866/3045 (94%)	255 (8%)	0

5 of 255 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

There are no RNA pucker outliers to report.

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	1.46	2 (10%)	24,31,34	0.75	0
30	OMG	0	2588	30	24,26,27	0.90	0	33,38,41	5.31	4 (12%)
30	UR3	0	2619	30	20,22,23	1.49	1 (5%)	23,32,35	0.79	0
30	PSU	0	2621	30	19,21,22	1.50	2 (10%)	23,30,33	0.99	0
30	1MA	0	628	30,34	23,25,26	0.95	2 (8%)	32,37,40	0.97	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	0/3/3/3
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	30,34	-	1/8/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2619	UR3	C5-C4	5.81	1.43	1.37
30	0	2587	OMU	C5-C4	5.50	1.43	1.37
30	0	2621	PSU	C5-C1'	-4.98	1.47	1.52
30	0	628	1MA	C6-N6	2.23	1.33	1.29
30	0	2587	OMU	P-OP1	2.16	1.49	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2588	OMG	C6-C5-N7	-28.81	130.26	134.14
30	0	2588	OMG	C6-N1-C2	8.53	125.02	120.20
30	0	628	1MA	C2-N3-C4	-3.46	110.60	116.23
30	0	2588	OMG	C2-N3-C4	-2.89	111.84	115.30
30	0	2588	OMG	C5-C4-N3	2.11	128.50	126.07

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, 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%)	0.39	22 (9%) 9 9	26, 50, 86, 109	0
2	B	337/338 (99%)	0.00	5 (1%) 70 75	28, 51, 79, 93	0
3	C	246/246 (100%)	0.17	4 (1%) 68 74	21, 43, 69, 77	0
4	D	140/177 (79%)	2.42	80 (57%) 0 0	56, 98, 124, 134	0
5	E	172/178 (96%)	0.75	16 (9%) 9 9	43, 66, 87, 91	0
6	F	119/120 (99%)	0.92	23 (19%) 2 2	47, 70, 99, 114	0
7	G	29/348 (8%)	2.09	16 (55%) 0 0	75, 93, 103, 106	0
8	H	160/177 (90%)	0.35	7 (4%) 33 37	34, 54, 92, 100	0
9	I	70/162 (43%)	4.57	61 (87%) 0 0	129, 145, 162, 163	0
10	J	142/145 (97%)	0.00	1 (0%) 84 89	34, 48, 70, 91	0
11	K	132/132 (100%)	0.26	3 (2%) 57 64	31, 49, 72, 78	0
12	L	145/165 (87%)	1.21	40 (27%) 1 1	24, 63, 111, 125	0
13	M	194/196 (98%)	-0.07	2 (1%) 79 83	28, 40, 55, 64	0
14	N	186/187 (99%)	0.79	28 (15%) 3 3	39, 61, 111, 121	0
15	O	115/116 (99%)	0.24	2 (1%) 67 73	36, 51, 69, 79	0
16	P	143/149 (95%)	0.38	4 (2%) 50 56	37, 53, 67, 76	0
17	Q	95/96 (98%)	0.00	1 (1%) 77 82	33, 43, 59, 76	0
18	R	150/155 (96%)	-0.12	0 100 100	30, 43, 62, 77	0
19	S	81/85 (95%)	0.76	6 (7%) 14 15	38, 57, 78, 89	0
20	T	119/120 (99%)	0.58	10 (8%) 11 12	37, 54, 86, 111	0
21	U	53/67 (79%)	0.35	1 (1%) 64 70	40, 54, 72, 80	0
22	V	65/71 (91%)	1.92	24 (36%) 1 1	51, 71, 116, 122	0
23	W	154/154 (100%)	-0.07	0 100 100	32, 48, 64, 77	0
24	X	82/92 (89%)	0.20	1 (1%) 75 81	39, 58, 83, 100	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	142/241 (58%)	0.13	4 (2%) 50 56	23, 43, 66, 86	0
26	Z	73/116 (62%)	0.89	15 (20%) 1 2	49, 67, 83, 95	0
27	1	56/57 (98%)	-0.24	0 100 100	25, 31, 39, 47	0
28	2	46/50 (92%)	0.30	2 (4%) 34 38	31, 59, 88, 100	0
29	3	92/92 (100%)	0.56	6 (6%) 18 21	33, 55, 68, 83	0
30	0	2754/2923 (94%)	-0.00	77 (2%) 50 56	19, 42, 87, 162	0
31	9	122/122 (100%)	0.17	6 (4%) 28 31	35, 61, 85, 146	0
All	All	6651/7517 (88%)	0.30	467 (7%) 17 17	19, 49, 98, 163	0

The worst 5 of 467 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	63	ILE	14.7
22	V	1	THR	13.4
9	I	66	GLY	11.5
9	I	74	ILE	11.2
9	I	112	LEU	10.3

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

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
30	UR3	0	2619	21/22	0.16	1.69	34,37,39,43	0
30	1MA	0	628	23/24	0.17	0.99	22,25,28,28	0
30	OMU	0	2587	21/22	0.13	-0.30	29,32,34,36	0
30	PSU	0	2621	20/21	0.14	-1.27	24,26,33,33	0
30	OMG	0	2588	24/25	0.14	-1.62	28,32,34,36	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
36	SR	0	9006	1/1	1.03	179.20	200,200,200,200	0
34	NA	0	8554	1/1	0.63	165.77	63,63,63,63	0
36	SR	0	8997	1/1	0.58	143.85	190,190,190,190	0
34	NA	0	8505	1/1	0.77	89.24	45,45,45,45	0
34	NA	0	8561	1/1	0.39	78.83	68,68,68,68	0
36	SR	0	8982	1/1	0.73	69.38	189,189,189,189	0
32	MG	0	8030	1/1	0.34	54.94	60,60,60,60	0
36	SR	J	8986	1/1	1.95	49.94	200,200,200,200	0
32	MG	0	8040	1/1	0.50	45.02	84,84,84,84	0
32	MG	0	8031	1/1	0.37	41.45	55,55,55,55	0
34	NA	0	8574	1/1	0.50	41.44	61,61,61,61	0
36	SR	0	9007	1/1	0.54	34.44	200,200,200,200	0
34	NA	0	8565	1/1	0.35	29.65	57,57,57,57	0
32	MG	0	8037	1/1	0.32	25.44	89,89,89,89	0
34	NA	0	8555	1/1	0.50	24.45	61,61,61,61	0
34	NA	0	8547	1/1	0.49	23.75	51,51,51,51	0
36	SR	0	8994	1/1	0.47	23.65	198,198,198,198	0
34	NA	0	8562	1/1	0.35	23.47	62,62,62,62	0
36	SR	0	8955	1/1	0.25	20.21	189,189,189,189	0
32	MG	0	8081	1/1	0.22	20.01	64,64,64,64	0
34	NA	0	8525	1/1	0.28	19.77	79,79,79,79	0
34	NA	0	8542	1/1	0.31	18.93	42,42,42,42	0
34	NA	0	8558	1/1	0.39	18.74	44,44,44,44	0
34	NA	0	8566	1/1	0.32	18.63	58,58,58,58	0
36	SR	0	8996	1/1	0.44	17.70	200,200,200,200	0
34	NA	0	8549	1/1	0.32	17.35	58,58,58,58	0
32	MG	0	8071	1/1	0.21	17.28	53,53,53,53	0
36	SR	B	8987	1/1	0.48	17.00	200,200,200,200	0
36	SR	0	8934	1/1	0.22	16.70	108,108,108,108	0
32	MG	0	8047	1/1	0.33	15.01	44,44,44,44	0
36	SR	0	8919	1/1	0.19	14.53	173,173,173,173	0
34	NA	0	8513	1/1	0.31	13.72	45,45,45,45	0
34	NA	0	8546	1/1	0.63	12.96	77,77,77,77	0
34	NA	0	8511	1/1	0.26	12.67	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8571	1/1	0.33	12.23	73,73,73,73	0
36	SR	0	8962	1/1	0.29	11.97	164,164,164,164	0
32	MG	0	8049	1/1	0.31	11.52	65,65,65,65	0
36	SR	0	8976	1/1	0.36	11.28	194,194,194,194	0
34	NA	0	8524	1/1	0.34	10.87	41,41,41,41	0
34	NA	0	8567	1/1	0.35	10.68	65,65,65,65	0
34	NA	9	8572	1/1	0.42	10.64	64,64,64,64	0
34	NA	0	8548	1/1	0.25	10.57	59,59,59,59	0
34	NA	0	8553	1/1	0.22	10.35	67,67,67,67	0
36	SR	0	8998	1/1	0.29	10.27	171,171,171,171	0
36	SR	0	8989	1/1	0.23	10.09	168,168,168,168	0
34	NA	0	8559	1/1	0.19	10.06	71,71,71,71	0
32	MG	0	8024	1/1	0.23	9.70	61,61,61,61	0
36	SR	0	8914	1/1	0.24	9.55	107,107,107,107	0
34	NA	0	8506	1/1	0.26	9.24	66,66,66,66	0
34	NA	0	8545	1/1	0.18	9.18	38,38,38,38	0
34	NA	0	8527	1/1	0.27	8.99	43,43,43,43	0
33	K	0	8401	1/1	0.19	8.84	88,88,88,88	0
34	NA	0	8535	1/1	0.22	8.68	46,46,46,46	0
36	SR	0	8992	1/1	0.23	8.52	125,125,125,125	0
35	CL	0	8822	1/1	0.30	8.31	74,74,74,74	0
34	NA	0	8544	1/1	0.20	8.23	64,64,64,64	0
36	SR	0	8922	1/1	0.29	8.17	160,160,160,160	0
32	MG	0	8069	1/1	0.39	7.48	65,65,65,65	0
32	MG	A	8051	1/1	0.27	7.48	72,72,72,72	0
34	NA	0	8502	1/1	0.22	7.23	55,55,55,55	0
34	NA	0	8560	1/1	0.33	7.23	92,92,92,92	0
36	SR	0	9004	1/1	0.41	7.20	200,200,200,200	0
34	NA	0	8552	1/1	0.29	7.09	59,59,59,59	0
34	NA	0	8568	1/1	0.24	6.84	53,53,53,53	0
34	NA	0	8569	1/1	0.28	6.37	53,53,53,53	0
34	NA	0	8551	1/1	0.21	5.99	47,47,47,47	0
32	MG	0	8062	1/1	0.26	5.98	47,47,47,47	0
32	MG	0	8079	1/1	0.20	5.71	50,50,50,50	0
34	NA	0	8564	1/1	0.28	5.66	63,63,63,63	0
34	NA	0	8521	1/1	0.20	5.57	54,54,54,54	0
32	MG	0	8083	1/1	0.31	5.40	55,55,55,55	0
34	NA	R	8575	1/1	0.29	5.30	82,82,82,82	0
34	NA	0	8517	1/1	0.20	5.20	31,31,31,31	0
34	NA	0	8522	1/1	0.33	5.16	58,58,58,58	0
32	MG	0	8063	1/1	0.17	5.14	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8905	1/1	0.25	4.71	54,54,54,54	0
34	NA	0	8526	1/1	0.31	4.55	46,46,46,46	0
36	SR	0	8947	1/1	0.27	4.53	178,178,178,178	0
36	SR	0	8991	1/1	0.23	4.52	188,188,188,188	0
32	MG	0	8018	1/1	0.18	4.45	36,36,36,36	0
34	NA	0	8519	1/1	0.20	4.26	36,36,36,36	0
32	MG	0	8041	1/1	0.19	4.13	19,19,19,19	0
34	NA	0	8541	1/1	0.22	4.08	50,50,50,50	0
32	MG	0	8009	1/1	0.21	3.94	19,19,19,19	0
34	NA	0	8556	1/1	0.45	3.93	41,41,41,41	0
36	SR	9	8980	1/1	0.14	3.89	177,177,177,177	0
36	SR	0	8974	1/1	0.24	3.83	166,166,166,166	0
32	MG	0	8017	1/1	0.23	3.79	23,23,23,23	0
32	MG	0	8001	1/1	0.18	3.61	29,29,29,29	0
36	SR	0	8907	1/1	0.21	3.58	53,53,53,53	0
32	MG	0	8090	1/1	0.20	3.57	55,55,55,55	0
34	NA	0	8512	1/1	0.19	3.47	38,38,38,38	0
34	NA	0	8550	1/1	0.21	3.29	55,55,55,55	0
36	SR	0	8979	1/1	0.21	3.04	199,199,199,199	0
34	NA	0	8514	1/1	0.19	2.83	41,41,41,41	0
36	SR	0	8906	1/1	0.20	2.69	52,52,52,52	0
34	NA	0	8563	1/1	0.21	2.52	65,65,65,65	0
32	MG	0	8061	1/1	0.18	2.46	29,29,29,29	0
36	SR	0	8959	1/1	0.23	2.35	159,159,159,159	0
32	MG	0	8078	1/1	0.19	2.32	43,43,43,43	0
36	SR	0	8985	1/1	0.17	2.16	118,118,118,118	0
32	MG	0	8039	1/1	0.18	2.01	64,64,64,64	0
34	NA	0	8509	1/1	0.14	1.96	50,50,50,50	0
36	SR	0	8957	1/1	0.17	1.79	188,188,188,188	0
36	SR	0	8904	1/1	0.17	1.51	49,49,49,49	0
34	NA	0	8518	1/1	0.26	1.42	65,65,65,65	0
36	SR	0	8903	1/1	0.16	1.41	45,45,45,45	0
34	NA	0	8570	1/1	0.15	1.37	44,44,44,44	0
32	MG	0	8068	1/1	0.16	1.17	64,64,64,64	0
32	MG	0	8005	1/1	0.19	1.03	29,29,29,29	0
32	MG	0	8012	1/1	0.18	0.99	22,22,22,22	0
32	MG	0	8048	1/1	0.17	0.93	27,27,27,27	0
32	MG	0	8011	1/1	0.19	0.83	24,24,24,24	0
32	MG	0	8019	1/1	0.16	0.74	20,20,20,20	0
32	MG	0	8029	1/1	0.14	0.66	52,52,52,52	0
34	NA	R	8532	1/1	0.18	0.61	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8082	1/1	0.19	0.51	56,56,56,56	0
35	CL	0	8816	1/1	0.17	0.46	54,54,54,54	0
33	K	0	8402	1/1	0.17	0.38	62,62,62,62	0
34	NA	0	8530	1/1	0.16	0.20	47,47,47,47	0
32	MG	0	8015	1/1	0.13	0.00	27,27,27,27	0
36	SR	0	8990	1/1	0.16	-0.04	113,113,113,113	0
32	MG	0	8085	1/1	0.15	-0.11	73,73,73,73	0
34	NA	0	8504	1/1	0.15	-0.12	33,33,33,33	0
35	CL	J	8801	1/1	0.15	-0.13	54,54,54,54	0
32	MG	0	8004	1/1	0.15	-0.18	21,21,21,21	0
36	SR	R	8912	1/1	0.15	-0.33	73,73,73,73	0
32	MG	0	8006	1/1	0.14	-0.36	23,23,23,23	0
36	SR	0	8981	1/1	0.15	-0.40	153,153,153,153	0
34	NA	0	8528	1/1	0.13	-0.41	40,40,40,40	0
36	SR	0	8972	1/1	0.15	-0.49	112,112,112,112	0
36	SR	0	8944	1/1	0.14	-0.51	161,161,161,161	0
35	CL	J	8821	1/1	0.15	-0.54	59,59,59,59	0
32	MG	0	8080	1/1	0.12	-0.60	66,66,66,66	0
34	NA	0	8520	1/1	0.12	-0.61	54,54,54,54	0
36	SR	0	8927	1/1	0.13	-0.65	150,150,150,150	0
34	NA	0	8573	1/1	0.14	-0.67	69,69,69,69	0
35	CL	N	8807	1/1	0.20	-0.73	68,68,68,68	0
32	MG	0	8084	1/1	0.11	-0.76	27,27,27,27	0
36	SR	0	8983	1/1	0.14	-0.78	177,177,177,177	0
36	SR	0	8963	1/1	0.14	-0.82	105,105,105,105	0
35	CL	O	8808	1/1	0.14	-0.83	62,62,62,62	0
32	MG	0	8076	1/1	0.13	-0.85	32,32,32,32	0
36	SR	0	9002	1/1	0.13	-0.87	175,175,175,175	0
36	SR	0	8956	1/1	0.09	-0.88	128,128,128,128	0
36	SR	F	9005	1/1	0.09	-0.95	122,122,122,122	0
34	NA	0	8501	1/1	0.13	-1.01	24,24,24,24	0
34	NA	0	8523	1/1	0.14	-1.05	29,29,29,29	0
34	NA	0	8557	1/1	0.10	-1.11	68,68,68,68	0
32	MG	0	8003	1/1	0.14	-1.13	26,26,26,26	0
32	MG	0	8010	1/1	0.15	-1.15	23,23,23,23	0
35	CL	0	8815	1/1	0.11	-1.17	58,58,58,58	0
34	NA	0	8515	1/1	0.13	-1.17	35,35,35,35	0
34	NA	C	8503	1/1	0.13	-1.23	31,31,31,31	0
37	CD	Z	8703	1/1	0.09	-1.26	71,71,71,71	0
34	NA	J	8538	1/1	0.10	-1.27	57,57,57,57	0
34	NA	9	8543	1/1	0.12	-1.29	47,47,47,47	0
36	SR	0	8993	1/1	0.09	-1.34	165,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
36	SR	0	8921	1/1	0.12	-1.43	84,84,84,84	0
36	SR	A	8977	1/1	0.08	-1.50	158,158,158,158	0
36	SR	0	8943	1/1	0.11	-1.52	104,104,104,104	0
36	SR	0	8909	1/1	0.12	-1.54	75,75,75,75	0
37	CD	U	8701	1/1	0.07	-1.68	51,51,51,51	0
35	CL	L	8810	1/1	0.11	-1.71	50,50,50,50	0
36	SR	0	8953	1/1	0.15	-1.72	143,143,143,143	0
32	MG	0	8008	1/1	0.11	-1.73	23,23,23,23	0
32	MG	0	8053	1/1	0.09	-1.75	53,53,53,53	0
36	SR	0	8917	1/1	0.12	-1.76	95,95,95,95	0
36	SR	0	8937	1/1	0.15	-1.78	103,103,103,103	0
34	NA	0	8537	1/1	0.10	-1.79	32,32,32,32	0
37	CD	3	8704	1/1	0.07	-1.81	64,64,64,64	0
35	CL	A	8809	1/1	0.15	-1.82	60,60,60,60	0
36	SR	0	8935	1/1	0.11	-1.82	68,68,68,68	0
32	MG	0	8064	1/1	0.14	-1.85	43,43,43,43	0
32	MG	0	8046	1/1	0.13	-1.85	28,28,28,28	0
32	MG	B	8043	1/1	0.07	-1.91	48,48,48,48	0
34	NA	0	8533	1/1	0.10	-1.91	55,55,55,55	0
32	MG	0	8055	1/1	0.14	-1.97	30,30,30,30	0
32	MG	0	8025	1/1	0.12	-1.99	31,31,31,31	0
36	SR	3	8932	1/1	0.10	-2.00	67,67,67,67	0
35	CL	J	8802	1/1	0.06	-2.07	56,56,56,56	0
35	CL	0	8811	1/1	0.10	-2.08	58,58,58,58	0
34	NA	0	8508	1/1	0.11	-2.10	39,39,39,39	0
37	CD	O	8705	1/1	0.07	-2.11	83,83,83,83	0
32	MG	0	8092	1/1	0.11	-2.11	51,51,51,51	0
36	SR	0	8925	1/1	0.11	-2.14	84,84,84,84	0
32	MG	B	8042	1/1	0.07	-2.14	47,47,47,47	0
36	SR	0	8918	1/1	0.12	-2.15	76,76,76,76	0
32	MG	Y	8086	1/1	0.10	-2.16	33,33,33,33	0
32	MG	0	8045	1/1	0.11	-2.29	39,39,39,39	0
36	SR	3	8999	1/1	0.06	-2.30	93,93,93,93	0
32	MG	0	8073	1/1	0.11	-2.43	79,79,79,79	0
32	MG	0	8007	1/1	0.13	-2.67	27,27,27,27	0
36	SR	0	8939	1/1	0.09	-2.71	146,146,146,146	0
36	SR	A	8929	1/1	0.10	-2.77	113,113,113,113	0
36	SR	0	9000	1/1	0.11	-2.83	157,157,157,157	0
36	SR	9	9003	1/1	0.16	-2.84	169,169,169,169	0
35	CL	0	8812	1/1	0.06	-2.85	40,40,40,40	0
34	NA	0	8507	1/1	0.13	-2.85	40,40,40,40	0
34	NA	0	8516	1/1	0.12	-2.98	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
35	CL	0	8805	1/1	0.10	-2.99	58,58,58,58	0
32	MG	0	8060	1/1	0.11	-3.00	54,54,54,54	0
32	MG	0	8016	1/1	0.14	-3.01	43,43,43,43	0
35	CL	R	8806	1/1	0.11	-3.03	42,42,42,42	0
37	CD	1	8702	1/1	0.07	-3.13	53,53,53,53	0
32	MG	T	8057	1/1	0.10	-3.15	58,58,58,58	0
36	SR	0	8940	1/1	0.09	-3.18	70,70,70,70	0
32	MG	0	8075	1/1	0.10	-3.18	49,49,49,49	0
36	SR	0	8954	1/1	0.08	-3.24	94,94,94,94	0
36	SR	0	8965	1/1	0.08	-3.26	117,117,117,117	0
32	MG	9	8074	1/1	0.11	-3.29	74,74,74,74	0
34	NA	M	8539	1/1	0.08	-3.29	33,33,33,33	0
36	SR	0	8975	1/1	0.07	-3.39	120,120,120,120	0
36	SR	0	8933	1/1	0.11	-3.43	127,127,127,127	0
36	SR	0	8911	1/1	0.06	-3.49	74,74,74,74	0
36	SR	0	8968	1/1	0.08	-3.49	146,146,146,146	0
32	MG	0	8028	1/1	0.11	-3.53	18,18,18,18	0
35	CL	0	8814	1/1	0.11	-3.54	48,48,48,48	0
32	MG	0	8020	1/1	0.09	-3.63	38,38,38,38	0
36	SR	0	8969	1/1	0.11	-3.64	134,134,134,134	0
32	MG	A	8050	1/1	0.08	-3.65	24,24,24,24	0
32	MG	0	8066	1/1	0.12	-3.66	57,57,57,57	0
32	MG	0	8058	1/1	0.06	-3.69	25,25,25,25	0
32	MG	0	8093	1/1	0.10	-3.76	29,29,29,29	0
36	SR	0	8960	1/1	0.07	-3.77	141,141,141,141	0
36	SR	0	8931	1/1	0.07	-3.81	94,94,94,94	0
36	SR	0	8941	1/1	0.11	-3.86	113,113,113,113	0
32	MG	0	8021	1/1	0.07	-3.90	31,31,31,31	0
35	CL	B	8819	1/1	0.10	-3.92	50,50,50,50	0
36	SR	0	8946	1/1	0.13	-3.99	102,102,102,102	0
32	MG	0	8070	1/1	0.10	-4.02	40,40,40,40	0
35	CL	M	8818	1/1	0.07	-4.10	33,33,33,33	0
32	MG	0	8035	1/1	0.10	-4.11	62,62,62,62	0
35	CL	3	8804	1/1	0.09	-4.13	53,53,53,53	0
32	MG	0	8014	1/1	0.12	-4.15	19,19,19,19	0
36	SR	0	9008	1/1	0.13	-4.18	85,85,85,85	0
36	SR	0	8978	1/1	0.05	-4.29	108,108,108,108	0
36	SR	0	8973	1/1	0.09	-4.30	121,121,121,121	0
36	SR	0	8967	1/1	0.06	-4.39	116,116,116,116	0
36	SR	0	8964	1/1	0.06	-4.50	110,110,110,110	0
36	SR	0	8926	1/1	0.09	-4.51	107,107,107,107	0
36	SR	0	8966	1/1	0.08	-4.51	100,100,100,100	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
34	NA	0	8529	1/1	0.04	-4.54	38,38,38,38	0
34	NA	Q	8540	1/1	0.07	-4.59	41,41,41,41	0
36	SR	1	8913	1/1	0.07	-4.61	78,78,78,78	0
36	SR	0	9001	1/1	0.09	-4.64	171,171,171,171	0
32	MG	0	8067	1/1	0.11	-4.65	26,26,26,26	0
35	CL	0	8803	1/1	0.08	-4.67	50,50,50,50	0
32	MG	0	8038	1/1	0.10	-4.74	68,68,68,68	0
36	SR	0	8928	1/1	0.07	-4.85	125,125,125,125	0
32	MG	0	8023	1/1	0.08	-4.86	18,18,18,18	0
36	SR	A	8930	1/1	0.05	-4.87	100,100,100,100	0
36	SR	0	8902	1/1	0.13	-4.95	58,58,58,58	0
36	SR	0	8908	1/1	0.08	-5.07	80,80,80,80	0
36	SR	0	8923	1/1	0.08	-5.14	85,85,85,85	0
36	SR	0	8958	1/1	0.08	-5.21	86,86,86,86	0
32	MG	0	8022	1/1	0.10	-5.22	32,32,32,32	0
36	SR	0	8970	1/1	0.06	-5.25	115,115,115,115	0
36	SR	0	8949	1/1	0.09	-5.30	90,90,90,90	0
32	MG	0	8087	1/1	0.13	-5.31	31,31,31,31	0
34	NA	0	8534	1/1	0.11	-5.35	25,25,25,25	0
36	SR	0	8951	1/1	0.04	-5.38	132,132,132,132	0
32	MG	0	8072	1/1	0.11	-5.66	53,53,53,53	0
36	SR	0	8920	1/1	0.05	-5.72	113,113,113,113	0
36	SR	0	8936	1/1	0.08	-5.74	84,84,84,84	0
32	MG	0	8065	1/1	0.09	-5.90	47,47,47,47	0
32	MG	0	8077	1/1	0.07	-5.97	35,35,35,35	0
35	CL	0	8817	1/1	0.09	-6.19	50,50,50,50	0
34	NA	0	8531	1/1	0.07	-6.26	41,41,41,41	0
32	MG	0	8013	1/1	0.07	-6.48	24,24,24,24	0
32	MG	0	8056	1/1	0.12	-6.52	41,41,41,41	0
36	SR	0	8988	1/1	0.11	-6.53	158,158,158,158	0
32	MG	0	8036	1/1	0.07	-6.59	49,49,49,49	0
34	NA	0	8536	1/1	0.08	-6.60	44,44,44,44	0
32	MG	0	8002	1/1	0.09	-6.69	21,21,21,21	0
35	CL	0	8813	1/1	0.07	-6.75	44,44,44,44	0
36	SR	0	8945	1/1	0.06	-6.82	105,105,105,105	0
36	SR	0	8984	1/1	0.07	-6.99	105,105,105,105	0
32	MG	0	8088	1/1	0.09	-7.00	34,34,34,34	0
36	SR	0	8910	1/1	0.06	-7.03	84,84,84,84	0
32	MG	0	8044	1/1	0.06	-7.06	46,46,46,46	0
36	SR	0	8924	1/1	0.09	-7.17	134,134,134,134	0
32	MG	0	8027	1/1	0.09	-7.63	39,39,39,39	0
32	MG	0	8052	1/1	0.06	-7.66	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
32	MG	0	8026	1/1	0.08	-7.74	27,27,27,27	0
32	MG	0	8033	1/1	0.04	-7.78	51,51,51,51	0
36	SR	0	8995	1/1	0.08	-8.11	117,117,117,117	0
36	SR	B	8950	1/1	0.08	-8.16	101,101,101,101	0
36	SR	0	8971	1/1	0.10	-8.40	165,165,165,165	0
36	SR	0	8942	1/1	0.07	-8.66	115,115,115,115	0
36	SR	0	8901	1/1	0.08	-8.76	73,73,73,73	0
36	SR	0	8915	1/1	0.06	-9.38	115,115,115,115	0
36	SR	0	8948	1/1	0.08	-10.12	77,77,77,77	0
32	MG	0	8034	1/1	0.08	-10.28	36,36,36,36	0
36	SR	1	8952	1/1	0.07	-11.75	74,74,74,74	0
35	CL	Y	8820	1/1	0.09	-12.30	38,38,38,38	0
32	MG	K	8054	1/1	0.07	-15.61	37,37,37,37	0
34	NA	S	8510	1/1	0.11	-16.06	34,34,34,34	0
32	MG	0	8032	1/1	0.05	-16.12	36,36,36,36	0
36	SR	0	8938	1/1	0.05	-17.34	139,139,139,139	0
32	MG	0	8059	1/1	0.07	-17.67	35,35,35,35	0
32	MG	0	8089	1/1	0.13	-24.33	40,40,40,40	0
36	SR	0	8916	1/1	0.06	-24.72	98,98,98,98	0
32	MG	0	8091	1/1	0.11	-51.00	54,54,54,54	0
36	SR	S	8961	1/1	0.06	-	113,113,113,113	0

6.5 Other polymers ⓘ

There are no such residues in this entry.