



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 04:39 PM UTC

PDB ID : 3CCJ / pdb\_00003ccj  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation C2534U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

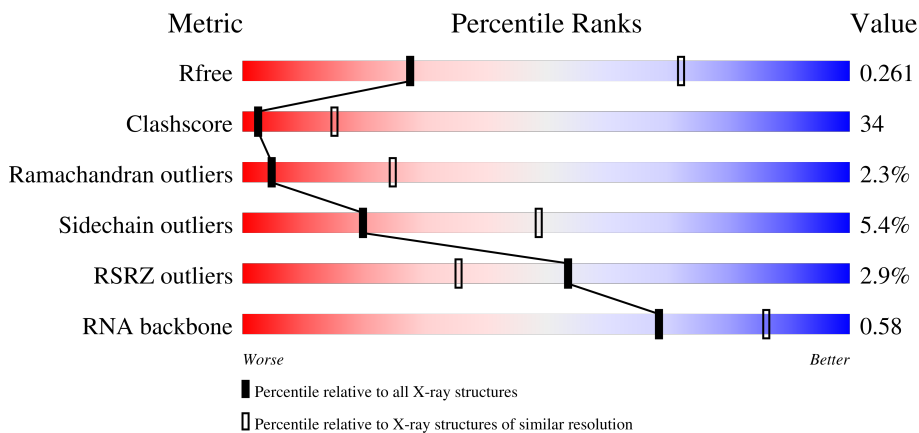
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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.



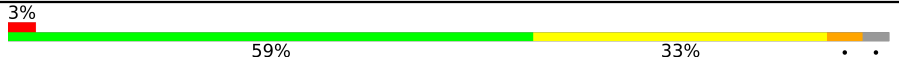

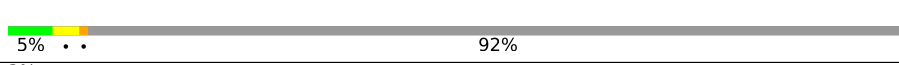

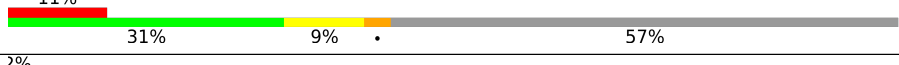
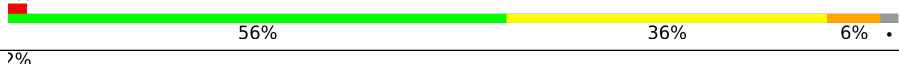
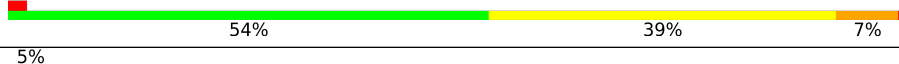
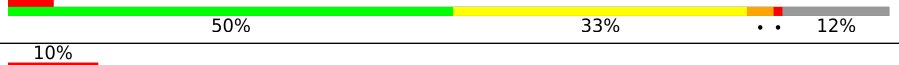



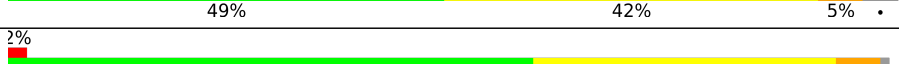
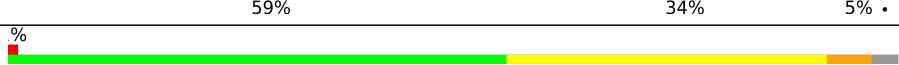
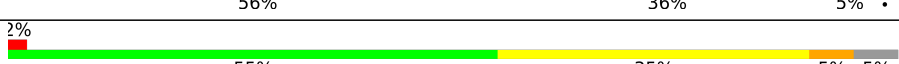

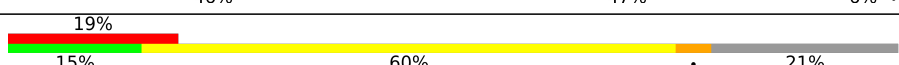


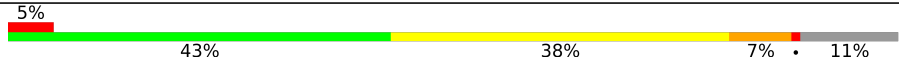
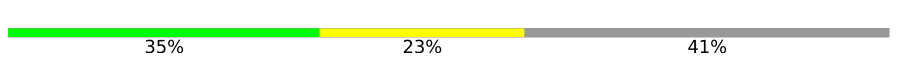


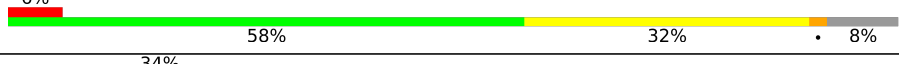
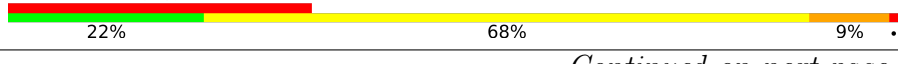

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	
2	B	338	
3	C	246	
4	D	177	


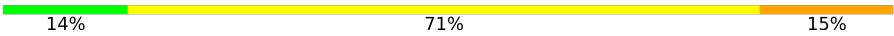
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Mol	Chain	Length	Quality of chain
5	E	178	
6	F	120	
7	G	348	
8	H	177	
9	I	162	
10	J	145	
11	K	132	
12	L	165	
13	M	196	
14	N	187	
15	O	116	
16	P	149	
17	Q	96	
18	R	155	
19	S	85	
20	T	120	
21	U	67	
22	V	71	
23	W	154	
24	X	92	
25	Y	241	
26	Z	116	
27	1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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	CL	0	8812	-	-	X	-
33	CL	0	8813	-	-	X	-
33	CL	3	8804	-	-	X	-
33	CL	J	8801	-	-	X	-
33	CL	M	8818	-	-	X	-
33	CL	N	8807	-	-	X	-
35	NA	0	8518	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8574	-	-	-	X
37	CD	3	8704	-	-	-	X

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99122 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2P.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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 (CCD ID: MG) (formula: Mg).

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

- Molecule 33 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	B	1	Total Cl 1 1	0	0
33	J	4	Total Cl 4 4	0	0
33	L	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	Q	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	0	8	Total Cl 8 8	0	0

- Molecule 34 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	A	2	Total Sr 2 2	0	0
34	B	2	Total Sr 2 2	0	0
34	F	1	Total Sr 1 1	0	0
34	J	1	Total Sr 1 1	0	0
34	R	1	Total Sr 1 1	0	0
34	S	1	Total Sr 1 1	0	0
34	1	2	Total Sr 2 2	0	0
34	2	1	Total Sr 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	3	2	Total 2	Sr 2	0	0
34	0	93	Total 93	Sr 93	0	0
34	9	2	Total 2	Sr 2	0	0

- Molecule 35 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	J	1	Total 1	Na 1	0	0
35	L	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	R	3	Total 3	Na 3	0	0
35	S	1	Total 1	Na 1	0	0
35	0	63	Total 63	Na 63	0	0
35	9	2	Total 2	Na 2	0	0

- Molecule 36 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 38 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	122	Total O 122 122	0	0
38	B	158	Total O 158 158	0	0
38	C	176	Total O 176 176	0	0
38	D	51	Total O 51 51	0	0
38	E	51	Total O 51 51	0	0
38	F	27	Total O 27 27	0	0
38	G	15	Total O 15 15	0	0
38	H	73	Total O 73 73	0	0
38	I	3	Total O 3 3	0	0
38	J	55	Total O 55 55	0	0
38	K	61	Total O 61 61	0	0
38	L	99	Total O 99 99	0	0
38	M	148	Total O 148 148	0	0
38	N	56	Total O 56 56	0	0
38	O	42	Total O 42 42	0	0

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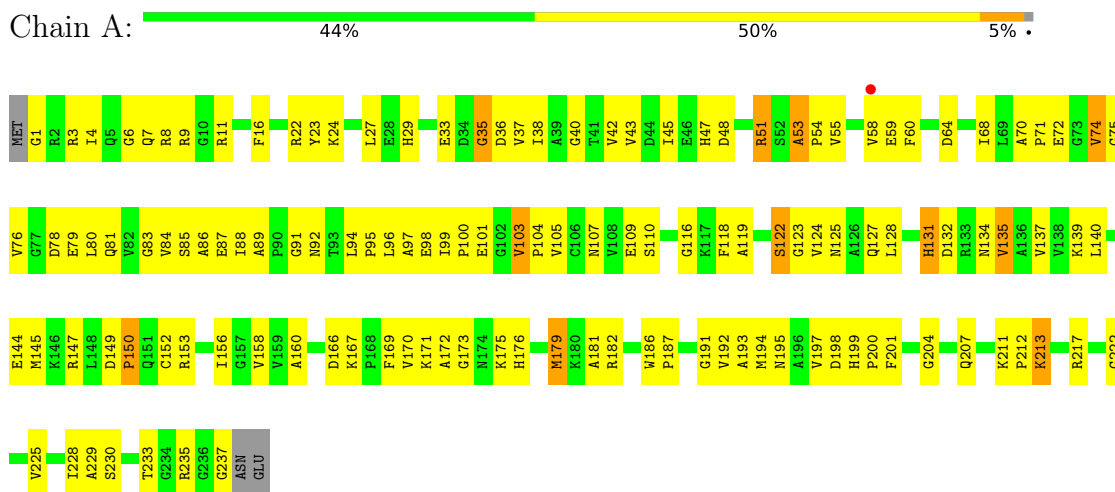
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	P	56	Total O 56 56	0	0
38	Q	58	Total O 58 58	0	0
38	R	78	Total O 78 78	0	0
38	S	37	Total O 37 37	0	0
38	T	41	Total O 41 41	0	0
38	U	34	Total O 34 34	0	0
38	V	10	Total O 10 10	0	0
38	W	71	Total O 71 71	0	0
38	X	28	Total O 28 28	0	0
38	Y	102	Total O 102 102	0	0
38	Z	33	Total O 33 33	0	0
38	1	53	Total O 53 53	0	0
38	2	48	Total O 48 48	0	0
38	3	80	Total O 80 80	0	0
38	0	5813	Total O 5813 5813	0	0
38	9	144	Total O 144 144	0	0

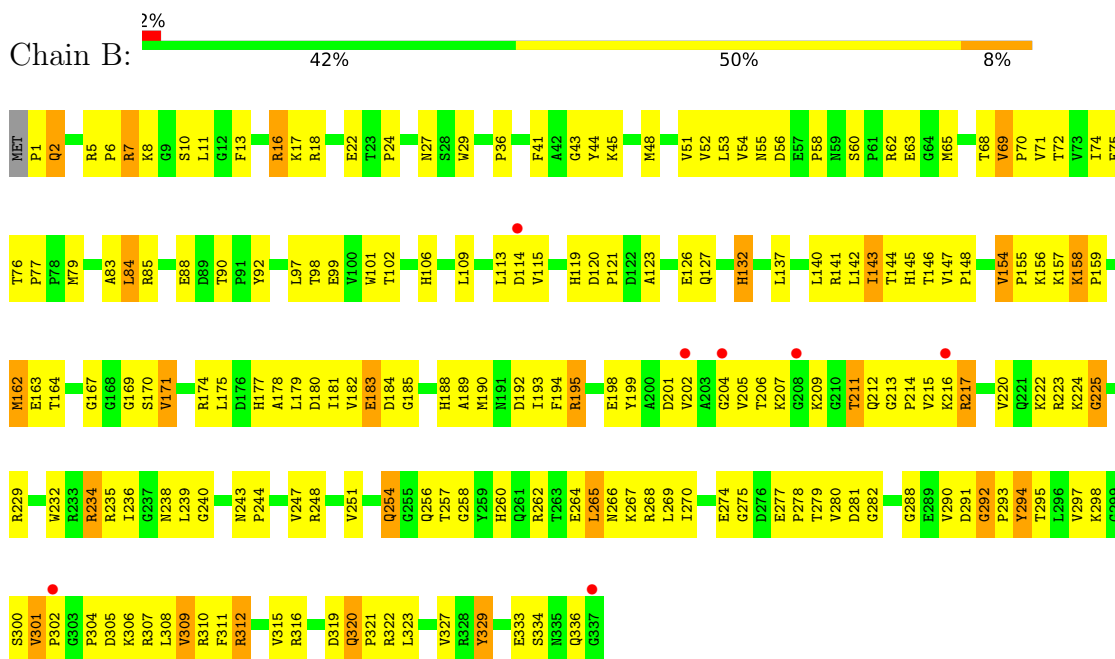
### 3 Residue-property plots i

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

#### • Molecule 1: 50S ribosomal protein L2P

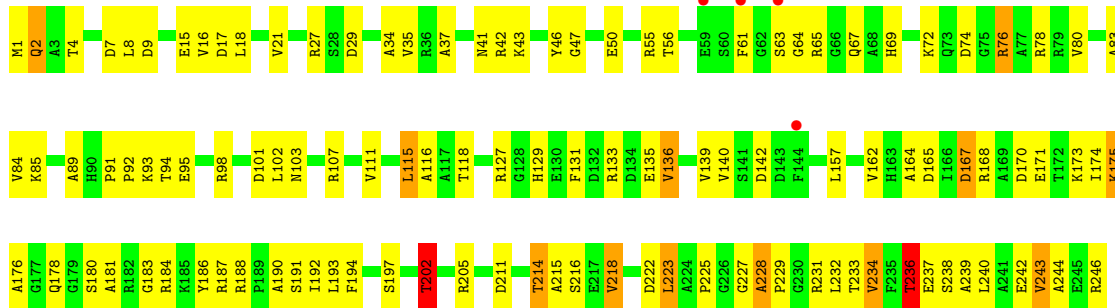


#### • Molecule 2: 50S ribosomal protein L3P



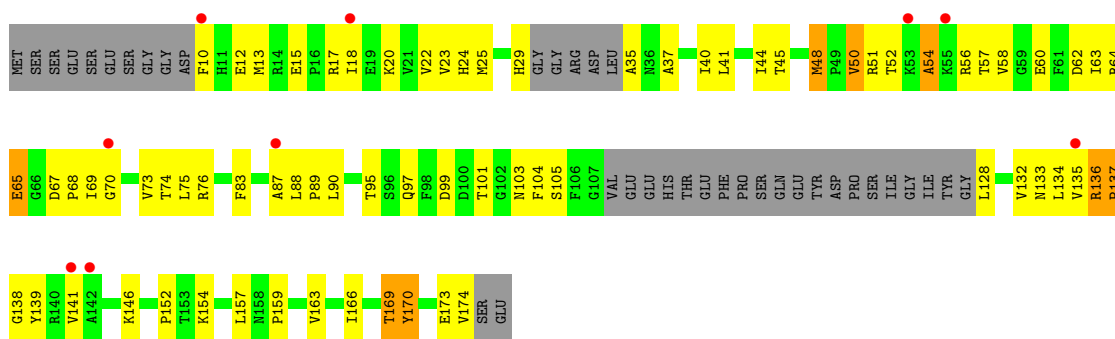
#### • Molecule 3: 50S ribosomal protein L4P

Chain C: 



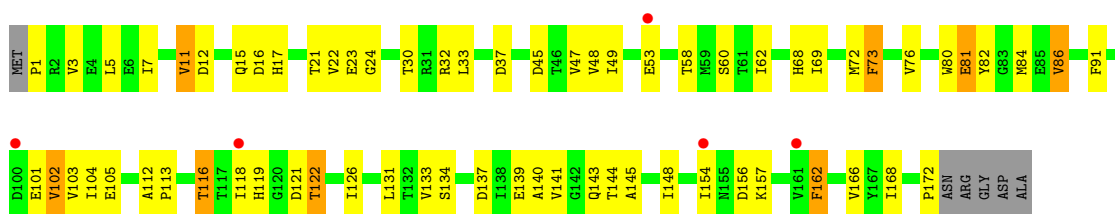
• Molecule 4: 50S ribosomal protein L5P

Chain D: 



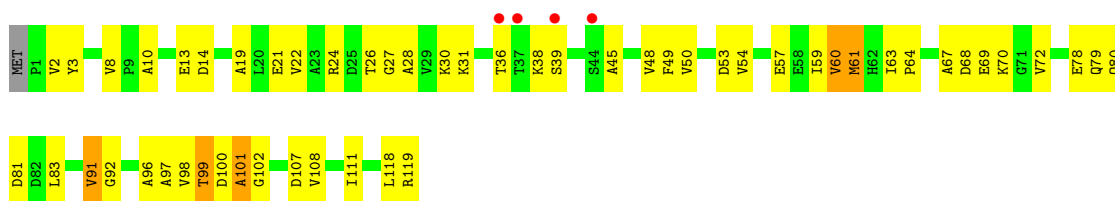
• Molecule 5: 50S ribosomal protein L6P

Chain E: 



• Molecule 6: 50S ribosomal protein L7Ae

Chain F: 



• Molecule 7: 50S ribosomal protein L10E

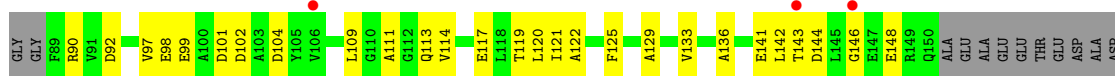




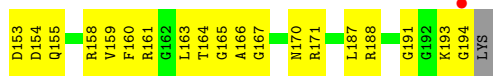
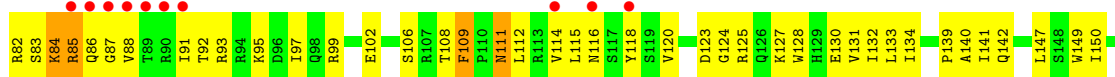
- Molecule 11: 50S ribosomal protein L14P



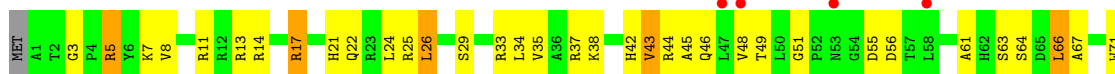
- Molecule 12: 50S ribosomal protein L15P

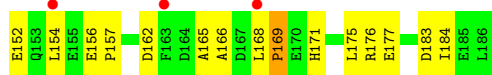
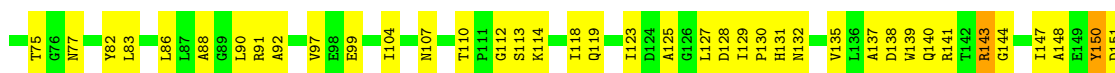


- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P

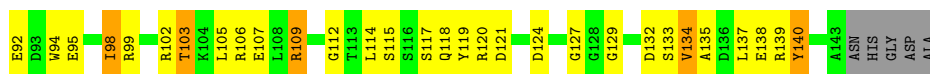
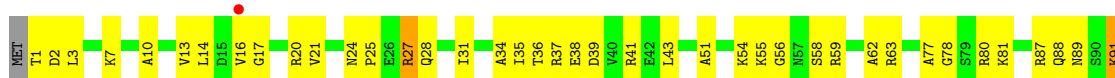




- Molecule 15: 50S ribosomal protein L18e



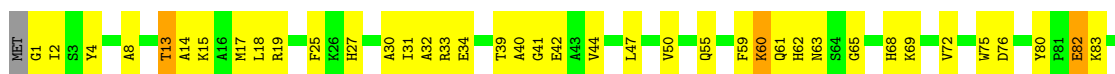
- Molecule 16: 50S ribosomal protein L19e



- Molecule 17: 50S ribosomal protein L21e

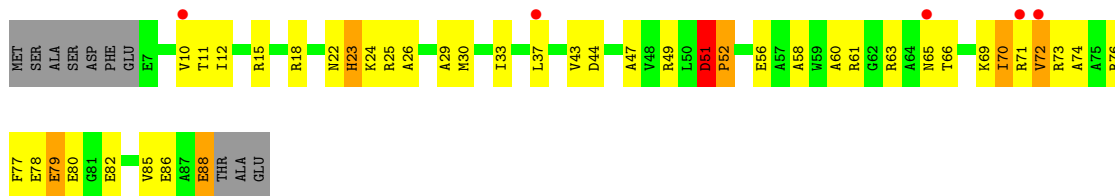


- Molecule 18: 50S ribosomal protein L22P

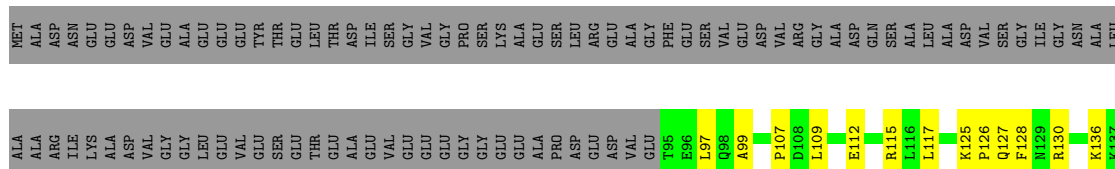
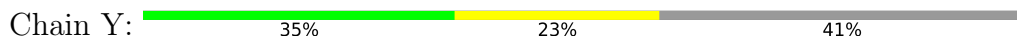


- Molecule 19: 50S ribosomal protein L23P

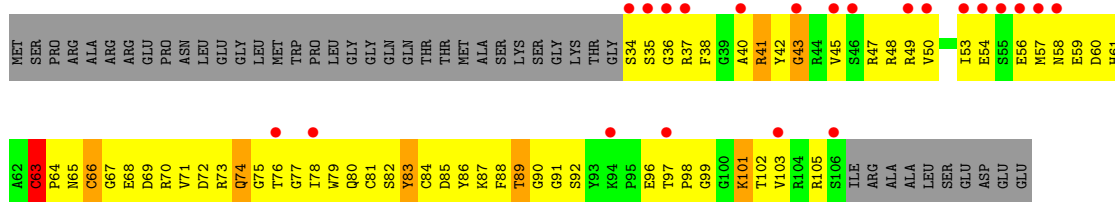




• Molecule 25: 50S ribosomal protein L32e



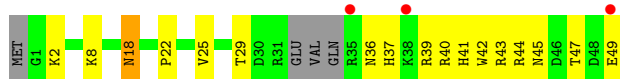
• Molecule 26: 50S ribosomal protein L37Ae



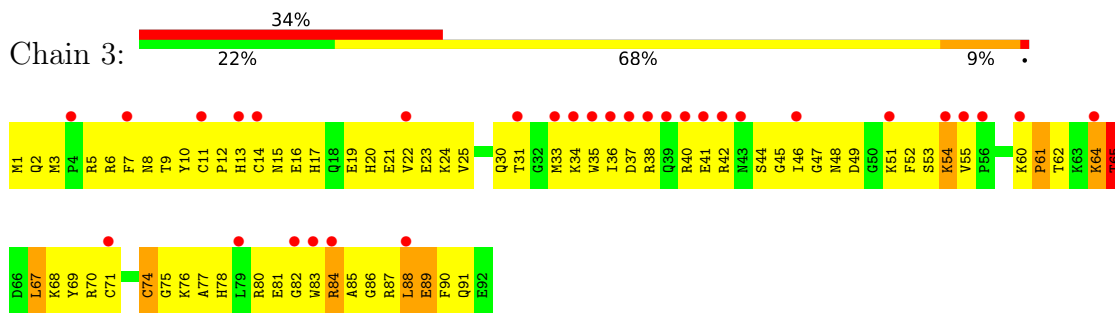
• Molecule 27: 50S ribosomal protein L37e



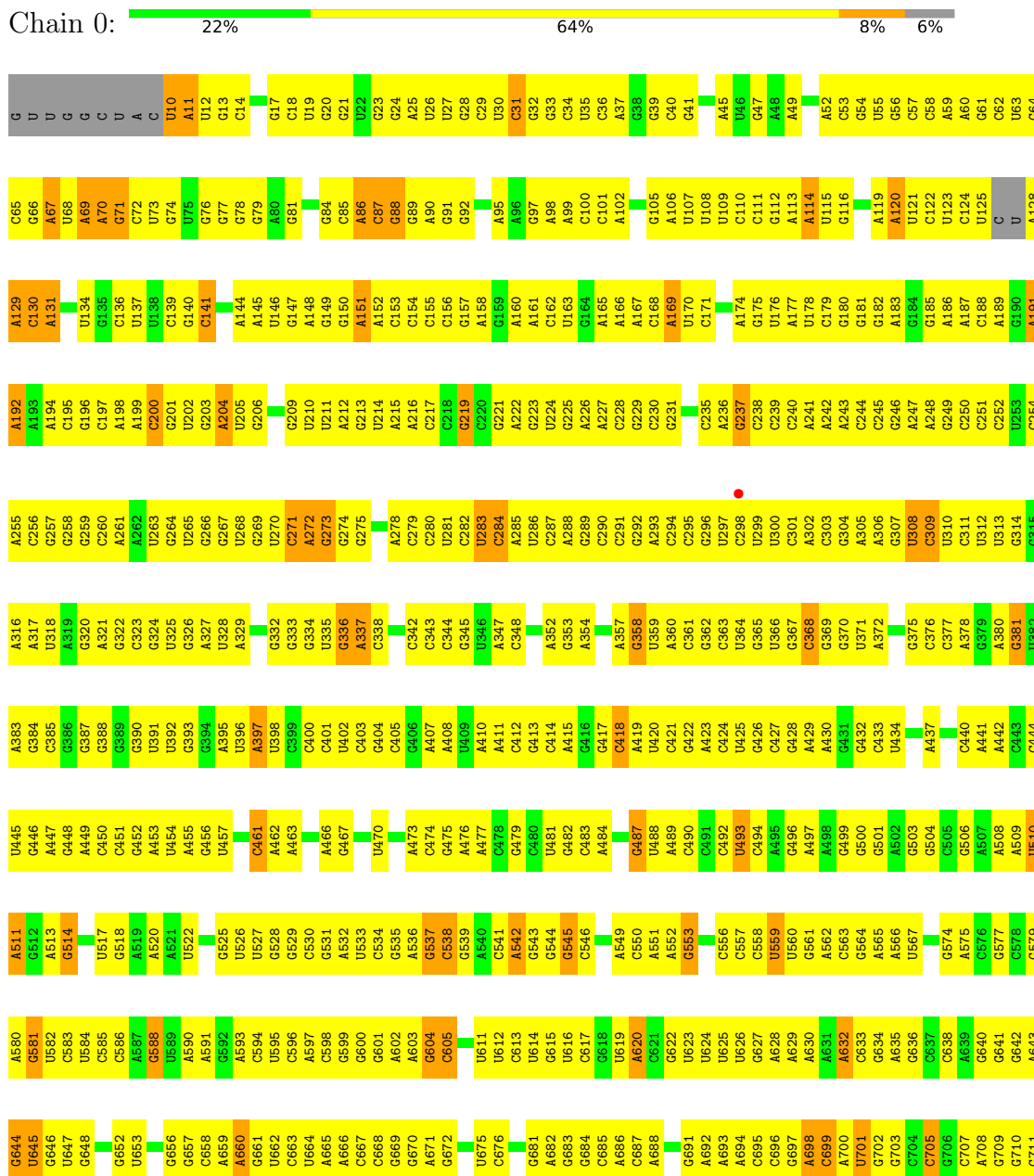
• Molecule 28: 50S ribosomal protein L39e



• Molecule 29: 50S ribosomal protein L44E

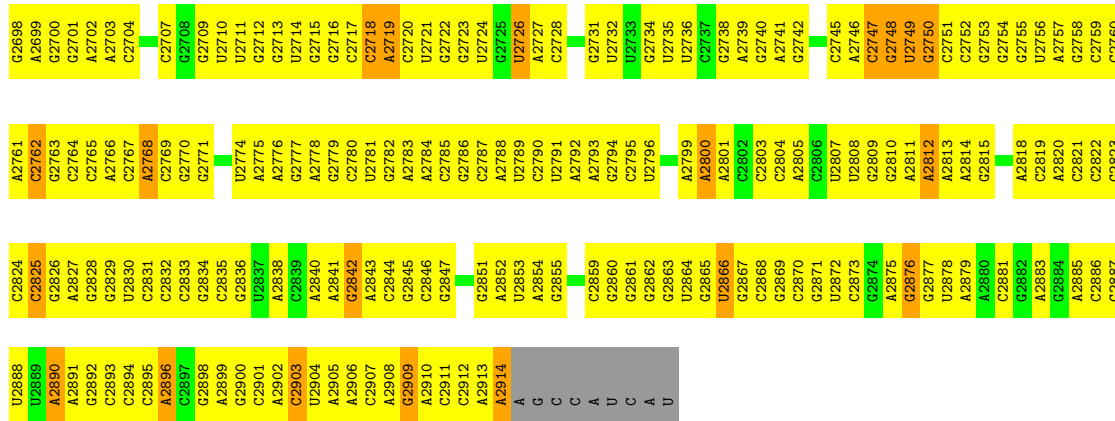


● Molecule 30: 23S RIBOSOMAL RNA



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A1660	A1598	C1472	G1331	G1194	U1130	G1055	G	G928	G856	A791	U
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A1664	C1602	A1476	U1335	U1266	G1137	G1059	G	C934	U860	G795	C719
A1665	G1603	A1477	U1336	C1267	G1138	A1060	C	G935	A861	A796	C720
A1666	U1604	U1478	G1337	G1268	U1139	G1061	A	C936	U862	A797	A721
A1667	G1605	A1479	U1338	C1269	C1140	A1062	C	C937	G863	G798	C722
A1668	A1606	G1480	G1339	U1270	U1141	G1063	A	G938	U864	C799	G723
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A1670	G1608	A1482	C1343	U1205	U1066	A1067	C1000	G940	U867	U801	C725
A1671	C1609	A1483	G1344	A1206	C1146	A1067	U1001	G941	G868	G802	G726
A1672	G1610	G1484	A1345	U1207	C1147	A1068	U1002	G942	G869	C803	G727
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A1674	A1612	C1420	U1347	C1275	U1149	A1070	U1004	G944	G871	G805	U731
A1675	C1613	C1421	U1347	U1278	A1150	G1071	A1005	U945	U872	A806	U732
A1676	G1614	U1422	U1347	G1279	G1151	G1072	A1006	C946	A807	A807	C733
A1677	A1615	C1423	U1350	U1280	A1152	A1073	U1007	U947	A808	A808	U733
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A1680	G1618	A1426	C1353	U1282	G1155	G1076	U1010	G950	G878	C811	A736
A1681	G1619	A1427	G1354	A1287	C1156	G1077	C1011	A951	G879	A812	A737
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A1685	C1623	A1434	C1360	G1292	A1160	A1081	C1015	A955	U883	G816	A746
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A1688	A1626	A1437	G1363	G1295	G1163	C1084	A1018	G958	U888	A819	C749
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A1690	G1628	U1439	C1365	U1297	C1165	A1086	A1020	G960	C890	U821	A750
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A1692	A1630	G1441	U1367	G1299	G1167	A1088	A1022	C962	U823	U823	G752
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A1694	C1632	G1443	G1370	U1301	U1169	G1089	G1024	G964	U895	U895	G754
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A1698	G1636	U1447	C1374	C1305	A1173	G1099	U1028	G968	U831	U831	G760
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A1700	U1638	G1449	G1376	G1240	G1175	G1100	U1030	U970	G902	G834	G771
A1701	U1639	C1450	C1377	U1309	C1176	U1101	G1031	G	U903	C834	G771
A1702	C1640	C1451	G1378	U1310	A1177	C1102	A1032	U	U904	U835	A776
A1703	A1641	G1452	A1379	G1311	G1178	C1103	C1033	G	C905	A766	U777
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A1709	G1647	A1458	G1386	G1319	U1184	U1115	A1040	C	U845	U845	U777
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A1713	G1651	C1464	A1390	G1323	A1188	G1119	G1044	C	C849	C849	C783
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G2641	G2574	A2506	U2441	U2373	G2313	U2247	C2125	U2057	A1994	A1930	G1863	U1791	G1727
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G2656	G2579	A2511	G2446	U2378	C2318	A2252	G2132	U2063	U1999	G1935	G1868	A1737	C1738
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G2692	G2623	A2553	G2491	C	C	C2295	C	G2110	C2037	U1972	A1912	U1770	C1769
G2693	A2624	U2554	U2492	C	C	C2296	C	A2112	C2037	A1973	C1913	U1771	U1770
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G2698	G2630	A2559	A2497	C	C	A2301	C	U2117	C2041	A1978	C1917	U1850	A1775
G2699	U2631	C2560	U2498	C	C	A2302	C	A2118	G2044	G1979	U1917	G1851	A1775
G2700	G2632	U2561	A2499	C	C	A2303	C	C2119	U1980	G1979	U1918	A1852	A1778
G2701	U2633	G2562	U2500	C	C	A2304	C	U2120	A1981	U1980	A1919	A1852	A1779
G2702	U2634	U2563	A2501	C	C	A2305	C	U2121	C2047	A1981	C1920	C1853	A1780
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G2705	U2637	C2566	U2504	C	C	U2308	C	U2120	U2051	C1987	A1924	A1857	U1784
G2706	A2637	U2567	U2505	C	C	U2309	C	G2121	G2053	C1988	G1926	A1858	U1784
G2707	U2638	G2568	U2506	C	C	C2309	C	G2122	G2053	C1988	G1926	A1859	U1784



• Molecule 31: 5S RIBOSOMAL RNA



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.01Å 299.25Å 573.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.30 50.00 – 3.30	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-3.30) 90.5 (50.00-3.30)	Depositor EDS
$R_{merge}$	0.18	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.208 , 0.287 0.184 , 0.261	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.9	Xtrriage
Anisotropy	0.112	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 122.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	99122	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.71% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, CD, NA, SR, OMU, 1MA, MG, PSU, UR3, OMG, K

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	0.47	0/1786	1.05	11/2408 (0.5%)
2	B	0.49	0/2690	1.07	26/3652 (0.7%)
3	C	0.54	0/1885	1.06	11/2552 (0.4%)
4	D	0.43	0/1111	1.00	6/1498 (0.4%)
5	E	0.44	0/1382	0.95	4/1880 (0.2%)
6	F	0.44	0/901	1.02	4/1224 (0.3%)
7	G	0.43	0/241	1.00	1/324 (0.3%)
8	H	0.43	0/1302	1.01	7/1743 (0.4%)
9	I	0.43	0/526	0.98	1/716 (0.1%)
10	J	0.51	0/1136	1.02	6/1530 (0.4%)
11	K	0.48	0/1004	1.08	8/1351 (0.6%)
12	L	0.40	0/1130	0.97	6/1509 (0.4%)
13	M	0.53	1/1582 (0.1%)	1.03	8/2116 (0.4%)
14	N	0.41	0/1474	1.08	14/1999 (0.7%)
15	O	0.48	0/874	0.99	4/1181 (0.3%)
16	P	0.47	0/1147	0.96	5/1528 (0.3%)
17	Q	0.47	0/749	1.10	6/1005 (0.6%)
18	R	1.33	7/1172 (0.6%)	1.43	12/1578 (0.8%)
19	S	0.44	0/648	0.88	2/875 (0.2%)
20	T	0.47	0/958	1.02	2/1289 (0.2%)
21	U	0.58	0/417	1.09	2/562 (0.4%)
22	V	0.44	0/502	0.98	1/675 (0.1%)
23	W	0.55	0/1219	1.07	9/1655 (0.5%)
24	X	0.51	0/664	1.05	4/895 (0.4%)
25	Y	0.50	0/1146	1.01	3/1536 (0.2%)
26	Z	0.46	0/584	1.04	4/781 (0.5%)
27	1	0.54	0/438	0.96	3/578 (0.5%)
28	2	0.47	0/401	0.90	0/529
29	3	0.54	0/771	1.05	5/1024 (0.5%)
30	0	0.43	0/65957	0.62	11/102867 (0.0%)
31	9	0.40	0/2904	0.60	0/4526
All	All	0.47	8/98701 (0.0%)	0.76	186/147586 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
23	W	0	1
30	0	0	19
All	All	1	20

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.19	2.85	1.49
18	R	150	PRO	CA-C	-17.63	1.16	1.52
18	R	150	PRO	CG-CD	13.59	1.97	1.50
18	R	150	PRO	N-CA	13.15	1.66	1.47
18	R	150	PRO	C-O	11.79	1.47	1.23

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-28.56	55.84	110.10
18	R	150	PRO	N-CA-C	-20.16	61.71	112.10
18	R	150	PRO	N-CA-CB	12.31	116.54	103.00
18	R	150	PRO	CA-N-CD	11.91	128.68	112.00
1	A	53	ALA	CA-C-N	9.23	129.32	119.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	493	U	Sidechain
30	0	788	A	Sidechain
30	0	862	U	Sidechain
30	0	882	A	Sidechain
23	W	90	TYR	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	125	0
2	B	2625	0	2533	178	0
3	C	1860	0	1813	100	0
4	D	1094	0	1085	72	0
5	E	1357	0	1266	53	0
6	F	890	0	843	40	0
7	G	240	0	231	18	0
8	H	1282	0	1292	63	0
9	I	519	0	500	24	0
10	J	1120	0	1098	63	0
11	K	994	0	1027	60	0
12	L	1118	0	1076	56	0
13	M	1558	0	1573	121	0
14	N	1445	0	1401	74	0
15	O	865	0	873	49	0
16	P	1136	0	1123	66	0
17	Q	735	0	729	32	0
18	R	1149	0	1122	59	0
19	S	641	0	605	30	0
20	T	950	0	924	57	0
21	U	410	0	368	59	0
22	V	499	0	511	27	0
23	W	1196	0	1137	82	0
24	X	654	0	653	43	0
25	Y	1130	0	1133	71	0
26	Z	573	0	534	86	0
27	1	431	0	426	28	0
28	2	396	0	413	20	0
29	3	755	0	732	138	0
30	0	59020	0	29802	3480	0
31	9	2599	0	1325	195	0
32	0	85	0	0	0	0
32	9	2	0	0	0	0
32	A	2	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	0	8	0	0	6	0
33	3	1	0	0	4	0
33	A	1	0	0	0	0
33	B	1	0	0	1	0
33	J	4	0	0	4	0
33	L	1	0	0	0	0
33	M	1	0	0	2	0
33	N	1	0	0	2	0
33	O	1	0	0	1	0
33	Q	1	0	0	1	0
33	R	1	0	0	0	0
33	Y	1	0	0	1	0
34	0	93	0	0	0	0
34	1	2	0	0	0	0
34	2	1	0	0	0	0
34	3	2	0	0	0	0
34	9	2	0	0	0	0
34	A	2	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	J	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	63	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	L	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	3	0	0	0	0
35	S	1	0	0	0	0
36	0	1	0	0	0	0
36	M	1	0	0	0	0
37	1	1	0	0	0	0
37	3	1	0	0	0	0
37	O	1	0	0	0	0
37	U	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5813	0	0	458	0
38	1	53	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	2	48	0	0	0	0
38	3	80	0	0	12	0
38	9	144	0	0	18	0
38	A	122	0	0	13	0
38	B	158	0	0	20	0
38	C	176	0	0	16	0
38	D	51	0	0	7	0
38	E	51	0	0	3	0
38	F	27	0	0	2	0
38	G	15	0	0	1	0
38	H	73	0	0	2	0
38	I	3	0	0	0	0
38	J	55	0	0	4	0
38	K	61	0	0	6	0
38	L	99	0	0	11	0
38	M	148	0	0	15	0
38	N	56	0	0	7	0
38	O	42	0	0	3	0
38	P	56	0	0	4	0
38	Q	58	0	0	5	0
38	R	78	0	0	1	0
38	S	37	0	0	3	0
38	T	41	0	0	3	0
38	U	34	0	0	4	0
38	V	10	0	0	2	0
38	W	71	0	0	4	0
38	X	28	0	0	1	0
38	Y	102	0	0	8	0
38	Z	33	0	0	7	0
All	All	99122	0	59914	5107	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

The worst 5 of 5107 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.97	1.43
30:0:871:G:C8	30:0:871:G:H5'	1.74	1.22
31:9:29:C:H2'	31:9:30:C:H5'	1.21	1.17
14:N:37:ARG:NH1	31:9:6:C:H5''	1.59	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:9:56:A:H2'	31:9:57:A:H5''	1.23	1.16

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	235/240 (98%)	198 (84%)	28 (12%)	9 (4%)	2	16
2	B	335/338 (99%)	287 (86%)	42 (12%)	6 (2%)	6	29
3	C	244/246 (99%)	211 (86%)	29 (12%)	4 (2%)	7	31
4	D	134/177 (76%)	109 (81%)	22 (16%)	3 (2%)	5	26
5	E	170/178 (96%)	152 (89%)	16 (9%)	2 (1%)	10	37
6	F	117/120 (98%)	102 (87%)	11 (9%)	4 (3%)	3	18
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	139 (89%)	14 (9%)	3 (2%)	6	28
9	I	68/162 (42%)	56 (82%)	10 (15%)	2 (3%)	3	21
10	J	140/145 (97%)	125 (89%)	12 (9%)	3 (2%)	5	26
11	K	130/132 (98%)	107 (82%)	21 (16%)	2 (2%)	8	32
12	L	141/165 (86%)	112 (79%)	25 (18%)	4 (3%)	4	21
13	M	192/196 (98%)	165 (86%)	22 (12%)	5 (3%)	4	23
14	N	184/187 (98%)	156 (85%)	23 (12%)	5 (3%)	4	22
15	O	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
16	P	141/149 (95%)	125 (89%)	13 (9%)	3 (2%)	5	26
17	Q	93/96 (97%)	82 (88%)	7 (8%)	4 (4%)	2	14
18	R	148/155 (96%)	132 (89%)	15 (10%)	1 (1%)	18	49
19	S	79/85 (93%)	67 (85%)	11 (14%)	1 (1%)	9	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	117/120 (98%)	95 (81%)	18 (15%)	4 (3%)	3	18
21	U	51/67 (76%)	46 (90%)	3 (6%)	2 (4%)	2	16
22	V	63/71 (89%)	57 (90%)	5 (8%)	1 (2%)	7	31
23	W	152/154 (99%)	129 (85%)	21 (14%)	2 (1%)	9	35
24	X	80/92 (87%)	68 (85%)	8 (10%)	4 (5%)	1	11
25	Y	140/241 (58%)	131 (94%)	8 (6%)	1 (1%)	18	49
26	Z	71/116 (61%)	52 (73%)	13 (18%)	6 (8%)	0	4
27	1	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	28
28	2	42/50 (84%)	37 (88%)	4 (10%)	1 (2%)	4	24
29	3	90/92 (98%)	73 (81%)	14 (16%)	3 (3%)	3	19
All	All	3705/4472 (83%)	3193 (86%)	426 (12%)	86 (2%)	5	25

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	123	GLY
4	D	65	GLU
4	D	137	PRO
6	F	61	MET
6	F	101	ALA

### 5.3.2 Protein sidechains [i](#)

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%)	172 (96%)	7 (4%)	28	56
2	B	282/283 (100%)	260 (92%)	22 (8%)	11	36
3	C	193/193 (100%)	177 (92%)	16 (8%)	10	34
4	D	117/148 (79%)	111 (95%)	6 (5%)	21	50
5	E	152/156 (97%)	143 (94%)	9 (6%)	18	46
6	F	93/94 (99%)	88 (95%)	5 (5%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	27/282 (10%)	25 (93%)	2 (7%)	13	38
8	H	134/145 (92%)	125 (93%)	9 (7%)	15	42
9	I	58/130 (45%)	55 (95%)	3 (5%)	21	49
10	J	118/121 (98%)	112 (95%)	6 (5%)	21	50
11	K	106/106 (100%)	97 (92%)	9 (8%)	10	33
12	L	113/127 (89%)	105 (93%)	8 (7%)	13	40
13	M	158/160 (99%)	151 (96%)	7 (4%)	25	54
14	N	149/150 (99%)	142 (95%)	7 (5%)	23	52
15	O	93/94 (99%)	90 (97%)	3 (3%)	34	60
16	P	113/117 (97%)	111 (98%)	2 (2%)	51	70
17	Q	79/80 (99%)	75 (95%)	4 (5%)	21	50
18	R	117/122 (96%)	112 (96%)	5 (4%)	26	54
19	S	71/74 (96%)	68 (96%)	3 (4%)	26	55
20	T	105/106 (99%)	98 (93%)	7 (7%)	15	42
21	U	44/53 (83%)	42 (96%)	2 (4%)	24	53
22	V	51/57 (90%)	47 (92%)	4 (8%)	11	36
23	W	130/130 (100%)	127 (98%)	3 (2%)	44	66
24	X	66/74 (89%)	60 (91%)	6 (9%)	9	31
25	Y	120/196 (61%)	117 (98%)	3 (2%)	42	64
26	Z	60/94 (64%)	56 (93%)	4 (7%)	15	42
27	1	46/47 (98%)	45 (98%)	1 (2%)	45	66
28	2	42/46 (91%)	41 (98%)	1 (2%)	43	65
29	3	79/79 (100%)	76 (96%)	3 (4%)	29	57
All	All	3095/3646 (85%)	2928 (95%)	167 (5%)	20	49

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N	177	GLU
22	V	13	PRO
16	P	91	LYS
19	S	44	GLN
24	X	51	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 94 such sidechains are listed below:

Mol	Chain	Res	Type
17	Q	16	ASN
21	U	39	ASN
17	Q	40	HIS
19	S	9	HIS
23	W	28	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	268 (9%)	14 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	286 (9%)	15 (0%)

5 of 286 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	11	A
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	2718	C
30	0	1377	C
31	9	65	A
30	0	2466	G

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
30	UR3	0	2619	30	19,22,23	0.53	0	26,32,35	0.68	1 (3%)
30	1MA	0	628	35,30	21,25,26	0.73	1 (4%)	30,37,40	0.80	1 (3%)
30	PSU	0	2621	30	18,21,22	1.46	3 (16%)	21,30,33	1.43	3 (14%)
30	OMU	0	2587	30	19,22,23	0.44	0	25,31,34	0.40	0
30	OMG	0	2588	30	23,26,27	0.37	0	32,38,41	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	UR3	0	2619	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	35,30	-	0/7/25/26	0/3/3/3
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	OMU	0	2587	30	-	0/9/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/9/27/28	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C2-N1	4.49	1.42	1.36
30	0	2621	PSU	C6-C5	2.75	1.38	1.35
30	0	628	1MA	C6-N6	2.41	1.33	1.28
30	0	2621	PSU	C4-C5	-2.19	1.38	1.44

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	C6-C5-C4	3.74	120.70	118.17
30	0	2621	PSU	C6-N1-C2	-3.27	119.66	122.69
30	0	2619	UR3	C4-N3-C2	2.86	126.88	124.58
30	0	2621	PSU	O2-C2-N1	2.80	125.67	122.79
30	0	628	1MA	N1-C2-N3	2.78	129.29	126.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2619	UR3	1	0
30	0	2621	PSU	2	0
30	0	2587	OMU	5	0
30	0	2588	OMG	3	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.02	1 (0%) 88 79	36, 78, 117, 135	0
2	B	337/338 (99%)	0.06	7 (2%) 63 44	36, 72, 106, 116	0
3	C	246/246 (100%)	-0.14	4 (1%) 70 52	31, 60, 87, 97	0
4	D	140/177 (79%)	0.63	9 (6%) 25 17	91, 126, 152, 162	0
5	E	172/178 (96%)	0.06	5 (2%) 53 35	62, 89, 116, 123	0
6	F	119/120 (99%)	0.30	4 (3%) 48 32	68, 96, 130, 142	0
7	G	29/348 (8%)	0.39	0 100 100	104, 117, 126, 127	0
8	H	160/177 (90%)	0.01	5 (3%) 51 35	57, 81, 125, 130	0
9	I	70/162 (43%)	1.30	18 (25%) 1 1	149, 172, 188, 190	0
10	J	142/145 (97%)	0.08	3 (2%) 63 44	48, 67, 90, 114	0
11	K	132/132 (100%)	-0.09	2 (1%) 72 53	38, 69, 98, 107	0
12	L	145/165 (87%)	0.44	9 (6%) 26 18	50, 96, 141, 147	0
13	M	194/196 (98%)	0.38	20 (10%) 12 10	41, 61, 109, 119	0
14	N	186/187 (99%)	0.34	7 (3%) 44 30	72, 94, 145, 152	0
15	O	115/116 (99%)	0.11	2 (1%) 69 50	57, 72, 93, 98	0
16	P	143/149 (95%)	0.05	1 (0%) 84 70	52, 74, 92, 103	0
17	Q	95/96 (98%)	0.07	2 (2%) 63 44	55, 71, 88, 103	0
18	R	150/155 (96%)	-0.25	1 (0%) 84 70	45, 61, 87, 109	0
19	S	81/85 (95%)	0.02	2 (2%) 58 39	61, 80, 103, 113	0
20	T	119/120 (99%)	0.04	2 (1%) 69 50	51, 74, 105, 132	0
21	U	53/67 (79%)	1.46	13 (24%) 2 1	119, 128, 137, 138	0
22	V	65/71 (91%)	0.30	2 (3%) 51 35	68, 97, 141, 146	0
23	W	154/154 (100%)	0.09	8 (5%) 33 22	49, 66, 88, 103	0
24	X	82/92 (89%)	0.30	5 (6%) 27 18	57, 81, 104, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.15	1 (0%) 84 70	39, 59, 87, 116	0
26	Z	73/116 (62%)	1.75	22 (30%) 1 1	109, 128, 137, 141	0
27	1	56/57 (98%)	-0.44	0 100 100	34, 47, 56, 60	0
28	2	46/50 (92%)	0.36	3 (6%) 25 17	43, 84, 116, 122	0
29	3	92/92 (100%)	1.83	31 (33%) 1 1	112, 132, 141, 144	0
30	0	2749/2923 (94%)	-0.64	6 (0%) 91 86	31, 64, 118, 195	0
31	9	122/122 (100%)	-0.52	0 100 100	53, 94, 121, 167	0
All	All	6646/7517 (88%)	-0.15	195 (2%) 53 35	31, 72, 133, 195	0

The worst 5 of 195 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	80	GLY	11.3
13	M	89	THR	7.8
29	3	35	TRP	7.2
29	3	39	GLN	7.0
13	M	78	LYS	6.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
30	1MA	0	628	23/24	0.97	0.07	37,44,45,46	0
30	OMG	0	2588	24/25	0.97	0.07	48,51,54,55	0
30	UR3	0	2619	21/22	0.97	0.08	56,57,60,60	0
30	PSU	0	2621	20/21	0.97	0.07	49,51,60,60	0
30	OMU	0	2587	21/22	0.98	0.06	51,52,54,56	0

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
35	NA	0	8574	1/1	0.49	0.47	92,92,92,92	0
34	SR	0	8977	1/1	0.65	0.10	200,200,200,200	0
37	CD	U	8701	1/1	0.71	0.35	180,180,180,180	0
37	CD	3	8704	1/1	0.71	0.47	183,183,183,183	0
35	NA	0	8518	1/1	0.72	0.40	91,91,91,91	0
35	NA	9	8572	1/1	0.72	0.19	71,71,71,71	0
35	NA	0	8522	1/1	0.74	0.73	130,130,130,130	0
33	CL	3	8804	1/1	0.75	0.12	98,98,98,98	0
34	SR	3	8999	1/1	0.76	0.22	200,200,200,200	0
35	NA	0	8558	1/1	0.76	0.37	82,82,82,82	0
37	CD	Z	8703	1/1	0.76	0.36	188,188,188,188	0
34	SR	0	8957	1/1	0.76	0.29	200,200,200,200	0
34	SR	0	8955	1/1	0.78	0.23	200,200,200,200	0
32	MG	0	8030	1/1	0.79	0.34	75,75,75,75	0
33	CL	A	8809	1/1	0.80	0.35	116,116,116,116	0
34	SR	0	8983	1/1	0.80	0.11	200,200,200,200	0
33	CL	0	8815	1/1	0.81	0.20	130,130,130,130	0
35	NA	0	8559	1/1	0.81	0.32	96,96,96,96	0
35	NA	0	8573	1/1	0.81	0.24	89,89,89,89	0
34	SR	0	8993	1/1	0.81	0.10	200,200,200,200	0
33	CL	N	8807	1/1	0.82	0.37	99,99,99,99	0
35	NA	0	8506	1/1	0.82	0.13	91,91,91,91	0
32	MG	9	8074	1/1	0.82	0.14	97,97,97,97	0
34	SR	B	8987	1/1	0.83	0.37	200,200,200,200	0
34	SR	0	8982	1/1	0.83	0.33	200,200,200,200	0
34	SR	0	8938	1/1	0.83	0.08	200,200,200,200	0
34	SR	0	8976	1/1	0.84	0.20	195,195,195,195	0
34	SR	0	9006	1/1	0.84	0.39	200,200,200,200	0
34	SR	0	8919	1/1	0.84	0.24	185,185,185,185	0
35	NA	0	8571	1/1	0.84	0.17	99,99,99,99	0
34	SR	0	8988	1/1	0.84	0.08	200,200,200,200	0
32	MG	0	8066	1/1	0.85	0.24	71,71,71,71	0
34	SR	0	8953	1/1	0.85	0.11	179,179,179,179	0
35	NA	0	8544	1/1	0.85	0.24	76,76,76,76	0
34	SR	9	9003	1/1	0.86	0.07	200,200,200,200	0
35	NA	0	8560	1/1	0.86	0.16	80,80,80,80	0
32	MG	0	8029	1/1	0.86	0.18	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	2	8947	1/1	0.86	0.12	195,195,195,195	0
35	NA	0	8520	1/1	0.86	0.12	44,44,44,44	0
34	SR	0	8979	1/1	0.86	0.15	200,200,200,200	0
35	NA	0	8528	1/1	0.86	0.32	113,113,113,113	0
34	SR	0	8997	1/1	0.86	0.51	200,200,200,200	0
34	SR	0	8959	1/1	0.86	0.10	190,190,190,190	0
34	SR	0	8969	1/1	0.87	0.39	200,200,200,200	0
34	SR	0	8975	1/1	0.87	0.09	189,189,189,189	0
35	NA	0	8537	1/1	0.87	0.06	46,46,46,46	0
32	MG	A	8051	1/1	0.87	0.10	95,95,95,95	0
35	NA	0	8557	1/1	0.87	0.16	70,70,70,70	0
35	NA	J	8538	1/1	0.88	0.18	84,84,84,84	0
35	NA	0	8554	1/1	0.88	0.41	124,124,124,124	0
35	NA	L	8568	1/1	0.88	0.09	59,59,59,59	0
35	NA	R	8575	1/1	0.88	0.27	97,97,97,97	0
34	SR	0	8956	1/1	0.88	0.12	200,200,200,200	0
35	NA	0	8509	1/1	0.88	0.20	84,84,84,84	0
34	SR	0	9000	1/1	0.88	0.19	200,200,200,200	0
34	SR	0	9001	1/1	0.88	0.11	200,200,200,200	0
34	SR	0	9004	1/1	0.88	0.25	200,200,200,200	0
35	NA	0	8524	1/1	0.88	0.08	53,53,53,53	0
35	NA	0	8525	1/1	0.88	0.18	113,113,113,113	0
32	MG	0	8038	1/1	0.88	0.06	94,94,94,94	0
32	MG	0	8036	1/1	0.88	0.13	62,62,62,62	0
35	NA	0	8529	1/1	0.89	0.10	61,61,61,61	0
32	MG	0	8091	1/1	0.89	0.13	67,67,67,67	0
34	SR	0	8967	1/1	0.89	0.07	163,163,163,163	0
32	MG	0	8042	1/1	0.89	0.21	75,75,75,75	0
33	CL	0	8822	1/1	0.89	0.32	140,140,140,140	0
32	MG	9	8040	1/1	0.90	0.19	101,101,101,101	0
35	NA	0	8511	1/1	0.90	0.07	53,53,53,53	0
32	MG	T	8057	1/1	0.90	0.22	80,80,80,80	0
34	SR	0	9002	1/1	0.90	0.13	200,200,200,200	0
34	SR	0	8971	1/1	0.90	0.12	200,200,200,200	0
34	SR	0	8922	1/1	0.90	0.14	181,181,181,181	0
34	SR	0	8991	1/1	0.90	0.08	188,188,188,188	0
35	NA	0	8527	1/1	0.90	0.16	92,92,92,92	0
32	MG	0	8047	1/1	0.90	0.48	90,90,90,90	0
34	SR	0	8994	1/1	0.90	0.42	200,200,200,200	0
34	SR	0	8939	1/1	0.90	0.24	155,155,155,155	0
34	SR	0	8998	1/1	0.90	0.32	200,200,200,200	0
34	SR	9	8980	1/1	0.91	0.06	191,191,191,191	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8556	1/1	0.91	0.29	94,94,94,94	0
35	NA	0	8562	1/1	0.91	0.35	83,83,83,83	0
33	CL	0	8805	1/1	0.91	0.12	105,105,105,105	0
34	SR	0	9007	1/1	0.91	0.32	200,200,200,200	0
34	SR	0	8951	1/1	0.92	0.07	183,183,183,183	0
33	CL	J	8821	1/1	0.92	0.14	99,99,99,99	0
32	MG	0	8056	1/1	0.92	0.09	47,47,47,47	0
34	SR	0	8927	1/1	0.92	0.16	171,171,171,171	0
35	NA	0	8523	1/1	0.92	0.10	51,51,51,51	0
34	SR	0	8933	1/1	0.92	0.16	126,126,126,126	0
34	SR	3	8932	1/1	0.92	0.20	148,148,148,148	0
35	NA	Q	8540	1/1	0.92	0.09	74,74,74,74	0
35	NA	R	8533	1/1	0.92	0.08	94,94,94,94	0
32	MG	0	8037	1/1	0.92	0.33	92,92,92,92	0
35	NA	9	8543	1/1	0.92	0.26	51,51,51,51	0
34	SR	0	8985	1/1	0.92	0.12	168,168,168,168	0
36	K	0	8401	1/1	0.92	0.18	145,145,145,145	0
34	SR	0	8941	1/1	0.92	0.09	141,141,141,141	0
35	NA	0	8545	1/1	0.92	0.19	74,74,74,74	0
35	NA	0	8553	1/1	0.92	0.22	81,81,81,81	0
35	NA	0	8507	1/1	0.93	0.08	38,38,38,38	0
34	SR	0	8984	1/1	0.93	0.05	124,124,124,124	0
33	CL	J	8816	1/1	0.93	0.53	99,99,99,99	0
35	NA	0	8514	1/1	0.93	0.36	74,74,74,74	0
32	MG	0	8039	1/1	0.93	0.34	94,94,94,94	0
34	SR	0	8974	1/1	0.93	0.12	196,196,196,196	0
34	SR	0	8992	1/1	0.93	0.24	141,141,141,141	0
34	SR	A	8930	1/1	0.93	0.16	131,131,131,131	0
33	CL	M	8818	1/1	0.93	0.16	58,58,58,58	0
34	SR	0	8996	1/1	0.93	0.22	200,200,200,200	0
32	MG	0	8043	1/1	0.93	0.16	62,62,62,62	0
35	NA	R	8532	1/1	0.93	0.13	68,68,68,68	0
32	MG	0	8093	1/1	0.93	0.14	48,48,48,48	0
34	SR	0	8964	1/1	0.93	0.08	176,176,176,176	0
35	NA	0	8542	1/1	0.93	0.30	79,79,79,79	0
35	NA	S	8510	1/1	0.93	0.05	41,41,41,41	0
33	CL	J	8802	1/1	0.93	0.08	86,86,86,86	0
35	NA	0	8516	1/1	0.94	0.11	27,27,27,27	0
35	NA	B	8552	1/1	0.94	0.20	70,70,70,70	0
34	SR	0	8915	1/1	0.94	0.11	123,123,123,123	0
32	MG	0	8082	1/1	0.94	0.09	62,62,62,62	0
34	SR	0	8920	1/1	0.94	0.11	145,145,145,145	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8089	1/1	0.94	0.13	56,56,56,56	0
32	MG	0	8061	1/1	0.94	0.09	47,47,47,47	0
35	NA	0	8567	1/1	0.94	0.43	83,83,83,83	0
35	NA	0	8570	1/1	0.94	0.07	57,57,57,57	0
32	MG	0	8092	1/1	0.94	0.07	53,53,53,53	0
33	CL	L	8810	1/1	0.94	0.14	91,91,91,91	0
35	NA	0	8502	1/1	0.94	0.10	66,66,66,66	0
35	NA	0	8536	1/1	0.94	0.05	64,64,64,64	0
32	MG	0	8065	1/1	0.94	0.09	66,66,66,66	0
36	K	M	8402	1/1	0.94	0.12	96,96,96,96	0
34	SR	0	8970	1/1	0.94	0.08	158,158,158,158	0
32	MG	0	8031	1/1	0.94	0.04	68,68,68,68	0
34	SR	0	8973	1/1	0.94	0.06	142,142,142,142	0
32	MG	0	8075	1/1	0.94	0.07	50,50,50,50	0
34	SR	0	8935	1/1	0.95	0.06	101,101,101,101	0
34	SR	0	8995	1/1	0.95	0.06	123,123,123,123	0
32	MG	0	8046	1/1	0.95	0.06	44,44,44,44	0
35	NA	0	8546	1/1	0.95	0.12	108,108,108,108	0
35	NA	0	8548	1/1	0.95	0.14	44,44,44,44	0
35	NA	0	8551	1/1	0.95	0.20	75,75,75,75	0
34	SR	0	8972	1/1	0.95	0.11	138,138,138,138	0
34	SR	F	9005	1/1	0.95	0.11	170,170,170,170	0
35	NA	0	8508	1/1	0.95	0.49	118,118,118,118	0
34	SR	J	8986	1/1	0.95	0.08	200,200,200,200	0
34	SR	0	8944	1/1	0.95	0.07	168,168,168,168	0
35	NA	0	8512	1/1	0.95	0.14	40,40,40,40	0
34	SR	0	8946	1/1	0.95	0.07	144,144,144,144	0
32	MG	0	8020	1/1	0.95	0.09	50,50,50,50	0
32	MG	0	8090	1/1	0.95	0.14	57,57,57,57	0
35	NA	0	8569	1/1	0.95	0.12	71,71,71,71	0
33	CL	O	8808	1/1	0.95	0.13	114,114,114,114	0
33	CL	Q	8811	1/1	0.95	0.12	124,124,124,124	0
33	CL	B	8819	1/1	0.95	0.35	83,83,83,83	0
33	CL	J	8801	1/1	0.95	0.11	85,85,85,85	0
35	NA	C	8503	1/1	0.95	0.05	36,36,36,36	0
32	MG	0	8049	1/1	0.95	0.12	82,82,82,82	0
34	SR	0	8989	1/1	0.95	0.09	174,174,174,174	0
34	SR	0	8965	1/1	0.95	0.08	160,160,160,160	0
35	NA	0	8535	1/1	0.95	0.06	58,58,58,58	0
32	MG	0	8071	1/1	0.95	0.23	78,78,78,78	0
32	MG	0	8034	1/1	0.95	0.06	50,50,50,50	0
34	SR	0	8963	1/1	0.96	0.04	117,117,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8541	1/1	0.96	0.10	60,60,60,60	0
33	CL	0	8814	1/1	0.96	0.20	51,51,51,51	0
32	MG	0	8014	1/1	0.96	0.06	25,25,25,25	0
35	NA	0	8501	1/1	0.96	0.08	53,53,53,53	0
34	SR	0	8928	1/1	0.96	0.06	156,156,156,156	0
34	SR	0	8968	1/1	0.96	0.08	175,175,175,175	0
35	NA	0	8550	1/1	0.96	0.24	129,129,129,129	0
32	MG	0	8017	1/1	0.96	0.04	28,28,28,28	0
34	SR	A	8929	1/1	0.96	0.19	139,139,139,139	0
34	SR	0	8937	1/1	0.96	0.07	126,126,126,126	0
32	MG	Y	8086	1/1	0.96	0.18	52,52,52,52	0
32	MG	0	8073	1/1	0.96	0.23	89,89,89,89	0
35	NA	0	8513	1/1	0.96	0.24	67,67,67,67	0
32	MG	0	8059	1/1	0.96	0.05	55,55,55,55	0
34	SR	0	8942	1/1	0.96	0.07	123,123,123,123	0
35	NA	0	8517	1/1	0.96	0.13	69,69,69,69	0
35	NA	0	8563	1/1	0.96	0.10	66,66,66,66	0
35	NA	0	8564	1/1	0.96	0.10	87,87,87,87	0
35	NA	0	8565	1/1	0.96	0.11	85,85,85,85	0
32	MG	0	8076	1/1	0.96	0.06	76,76,76,76	0
34	SR	R	8912	1/1	0.96	0.06	107,107,107,107	0
35	NA	0	8521	1/1	0.96	0.14	40,40,40,40	0
34	SR	0	8978	1/1	0.96	0.07	132,132,132,132	0
32	MG	0	8078	1/1	0.96	0.21	72,72,72,72	0
32	MG	0	8081	1/1	0.96	0.18	116,116,116,116	0
32	MG	0	8032	1/1	0.96	0.03	47,47,47,47	0
33	CL	0	8803	1/1	0.96	0.13	82,82,82,82	0
32	MG	0	8083	1/1	0.96	0.11	58,58,58,58	0
35	NA	M	8539	1/1	0.96	0.06	38,38,38,38	0
35	NA	0	8531	1/1	0.96	0.22	54,54,54,54	0
33	CL	0	8813	1/1	0.96	0.11	64,64,64,64	0
34	SR	0	8960	1/1	0.96	0.05	156,156,156,156	0
32	MG	0	8068	1/1	0.97	0.06	44,44,44,44	0
32	MG	0	8053	1/1	0.97	0.07	88,88,88,88	0
35	NA	0	8555	1/1	0.97	0.10	80,80,80,80	0
32	MG	0	8055	1/1	0.97	0.06	60,60,60,60	0
34	SR	0	8908	1/1	0.97	0.04	99,99,99,99	0
32	MG	0	8044	1/1	0.97	0.12	59,59,59,59	0
34	SR	0	8916	1/1	0.97	0.06	110,110,110,110	0
34	SR	0	8917	1/1	0.97	0.05	111,111,111,111	0
35	NA	0	8561	1/1	0.97	0.17	53,53,53,53	0
32	MG	0	8015	1/1	0.97	0.04	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8504	1/1	0.97	0.10	41,41,41,41	0
35	NA	0	8530	1/1	0.97	0.07	53,53,53,53	0
32	MG	A	8050	1/1	0.97	0.06	69,69,69,69	0
35	NA	0	8566	1/1	0.97	0.13	86,86,86,86	0
35	NA	0	8534	1/1	0.97	0.16	53,53,53,53	0
32	MG	0	8079	1/1	0.97	0.08	57,57,57,57	0
34	SR	0	8926	1/1	0.97	0.09	131,131,131,131	0
34	SR	0	8981	1/1	0.97	0.07	198,198,198,198	0
34	SR	B	8950	1/1	0.97	0.06	123,123,123,123	0
32	MG	0	8062	1/1	0.97	0.09	66,66,66,66	0
33	CL	Y	8820	1/1	0.97	0.10	58,58,58,58	0
34	SR	0	8934	1/1	0.97	0.13	138,138,138,138	0
32	MG	0	8035	1/1	0.97	0.11	76,76,76,76	0
35	NA	0	8547	1/1	0.97	0.30	115,115,115,115	0
34	SR	0	8936	1/1	0.97	0.04	114,114,114,114	0
32	MG	0	8052	1/1	0.97	0.10	63,63,63,63	0
35	NA	0	8519	1/1	0.97	0.06	51,51,51,51	0
34	SR	0	8924	1/1	0.98	0.10	131,131,131,131	0
34	SR	0	8925	1/1	0.98	0.06	98,98,98,98	0
32	MG	0	8027	1/1	0.98	0.05	44,44,44,44	0
32	MG	0	8063	1/1	0.98	0.09	60,60,60,60	0
32	MG	0	8064	1/1	0.98	0.05	51,51,51,51	0
34	SR	0	8931	1/1	0.98	0.03	120,120,120,120	0
32	MG	0	8048	1/1	0.98	0.09	26,26,26,26	0
32	MG	0	8085	1/1	0.98	0.07	67,67,67,67	0
32	MG	Y	8077	1/1	0.98	0.11	58,58,58,58	0
32	MG	0	8067	1/1	0.98	0.07	47,47,47,47	0
32	MG	0	8001	1/1	0.98	0.05	42,42,42,42	0
35	NA	0	8505	1/1	0.98	0.14	37,37,37,37	0
34	SR	S	8961	1/1	0.98	0.05	130,130,130,130	0
34	SR	1	8952	1/1	0.98	0.04	92,92,92,92	0
33	CL	R	8806	1/1	0.98	0.05	66,66,66,66	0
32	MG	0	8070	1/1	0.98	0.12	39,39,39,39	0
34	SR	0	8943	1/1	0.98	0.09	89,89,89,89	0
32	MG	0	8008	1/1	0.98	0.07	26,26,26,26	0
32	MG	0	8072	1/1	0.98	0.05	45,45,45,45	0
34	SR	0	8948	1/1	0.98	0.04	110,110,110,110	0
34	SR	0	8949	1/1	0.98	0.03	128,128,128,128	0
34	SR	0	8910	1/1	0.98	0.05	118,118,118,118	0
34	SR	0	8911	1/1	0.98	0.04	100,100,100,100	0
34	SR	0	8954	1/1	0.98	0.04	115,115,115,115	0
34	SR	0	8914	1/1	0.98	0.04	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8018	1/1	0.98	0.03	34,34,34,34	0
33	CL	0	8812	1/1	0.98	0.07	70,70,70,70	0
34	SR	0	8958	1/1	0.98	0.04	126,126,126,126	0
32	MG	0	8033	1/1	0.98	0.05	69,69,69,69	0
34	SR	0	8918	1/1	0.98	0.03	88,88,88,88	0
35	NA	0	8526	1/1	0.98	0.03	67,67,67,67	0
34	SR	0	8962	1/1	0.98	0.07	168,168,168,168	0
32	MG	0	8010	1/1	0.98	0.04	46,46,46,46	0
32	MG	0	8022	1/1	0.98	0.07	25,25,25,25	0
34	SR	0	8921	1/1	0.98	0.03	88,88,88,88	0
37	CD	O	8705	1/1	0.98	0.10	105,105,105,105	0
34	SR	0	8966	1/1	0.98	0.03	101,101,101,101	0
33	CL	0	8817	1/1	0.98	0.05	84,84,84,84	0
34	SR	0	8923	1/1	0.98	0.04	108,108,108,108	0
32	MG	0	8006	1/1	0.99	0.03	44,44,44,44	0
35	NA	0	8515	1/1	0.99	0.04	35,35,35,35	0
32	MG	0	8016	1/1	0.99	0.03	41,41,41,41	0
32	MG	0	8045	1/1	0.99	0.02	28,28,28,28	0
32	MG	0	8080	1/1	0.99	0.04	65,65,65,65	0
34	SR	0	9008	1/1	0.99	0.03	94,94,94,94	0
34	SR	0	8945	1/1	0.99	0.03	119,119,119,119	0
32	MG	0	8007	1/1	0.99	0.03	21,21,21,21	0
32	MG	K	8054	1/1	0.99	0.05	42,42,42,42	0
32	MG	0	8009	1/1	0.99	0.10	24,24,24,24	0
32	MG	0	8084	1/1	0.99	0.06	37,37,37,37	0
32	MG	0	8003	1/1	0.99	0.06	27,27,27,27	0
32	MG	0	8087	1/1	0.99	0.03	22,22,22,22	0
32	MG	0	8088	1/1	0.99	0.11	53,53,53,53	0
32	MG	0	8023	1/1	0.99	0.06	38,38,38,38	0
34	SR	1	8913	1/1	0.99	0.03	108,108,108,108	0
32	MG	0	8069	1/1	0.99	0.07	73,73,73,73	0
32	MG	0	8024	1/1	0.99	0.07	39,39,39,39	0
34	SR	0	8990	1/1	0.99	0.10	113,113,113,113	0
32	MG	0	8026	1/1	0.99	0.02	37,37,37,37	0
32	MG	0	8011	1/1	0.99	0.06	33,33,33,33	0
34	SR	0	8901	1/1	0.99	0.03	73,73,73,73	0
34	SR	0	8903	1/1	0.99	0.10	63,63,63,63	0
34	SR	0	8904	1/1	0.99	0.10	73,73,73,73	0
34	SR	0	8905	1/1	0.99	0.10	68,68,68,68	0
32	MG	0	8005	1/1	0.99	0.08	24,24,24,24	0
34	SR	0	8909	1/1	0.99	0.03	100,100,100,100	0
32	MG	0	8060	1/1	0.99	0.02	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8940	1/1	0.99	0.03	93,93,93,93	0
35	NA	0	8549	1/1	0.99	0.15	96,96,96,96	0
32	MG	0	8012	1/1	1.00	0.06	26,26,26,26	0
32	MG	0	8013	1/1	1.00	0.04	19,19,19,19	0
32	MG	0	8041	1/1	1.00	0.02	25,25,25,25	0
32	MG	0	8004	1/1	1.00	0.02	19,19,19,19	0
32	MG	0	8025	1/1	1.00	0.04	23,23,23,23	0
32	MG	0	8019	1/1	1.00	0.03	19,19,19,19	0
32	MG	0	8058	1/1	1.00	0.02	7,7,7,7	0
34	SR	0	8902	1/1	1.00	0.02	72,72,72,72	0
32	MG	0	8002	1/1	1.00	0.02	31,31,31,31	0
32	MG	0	8028	1/1	1.00	0.01	13,13,13,13	0
32	MG	0	8021	1/1	1.00	0.03	31,31,31,31	0
34	SR	0	8906	1/1	1.00	0.02	66,66,66,66	0
37	CD	1	8702	1/1	1.00	0.05	78,78,78,78	0
34	SR	0	8907	1/1	1.00	0.04	60,60,60,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.