



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2018 – 08:29 am GMT

PDB ID : 3CC4  
Title : Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-24  
Resolution : 2.70 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : trunk30967  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk30967

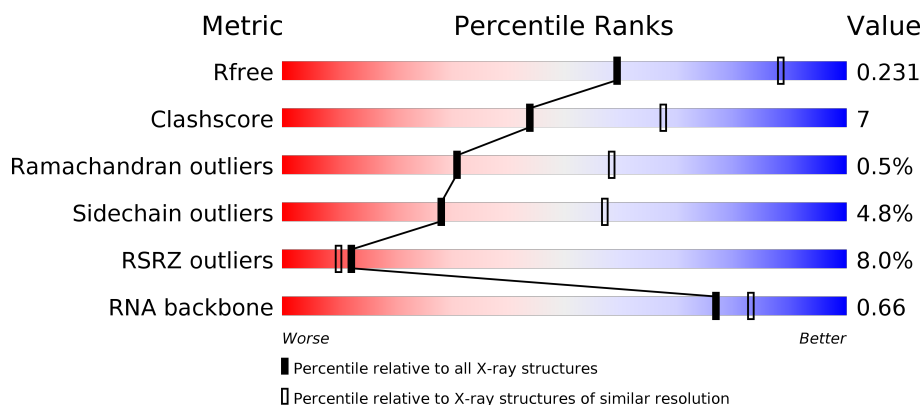
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	111664	2449 (2.70-2.70)
Clashscore	122126	2756 (2.70-2.70)
Ramachandran outliers	120053	2716 (2.70-2.70)
Sidechain outliers	120020	2716 (2.70-2.70)
RSRZ outliers	108989	2376 (2.70-2.70)
RNA backbone	2636	1009 (3.00-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>9%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>0%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>40%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>21%</div> </div> </div>

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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8069	-	-	-	X
32	MG	A	8051	-	-	-	X
34	SR	0	8933	-	-	-	X
34	SR	0	8947	-	-	-	X
34	SR	0	8957	-	-	-	X
34	SR	0	8976	-	-	-	X
34	SR	0	8982	-	-	-	X
34	SR	0	8986	-	-	-	X
34	SR	0	8994	-	-	-	X
34	SR	0	8996	-	-	-	X
34	SR	0	9006	-	-	-	X
34	SR	B	8987	-	-	-	X
35	NA	0	8512	-	-	-	X
35	NA	0	8522	-	-	-	X
35	NA	0	8546	-	-	-	X
35	NA	0	8549	-	-	-	X
35	NA	0	8553	-	-	-	X
35	NA	0	8554	-	-	-	X
35	NA	0	8555	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8561	-	-	-	X
35	NA	0	8562	-	-	-	X
35	NA	0	8573	-	-	-	X
35	NA	9	8572	-	-	-	X
35	NA	S	8510	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99135 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	U	53	Total	C	N	O	S	0	0	0
			410	244	75	86	5			

- Molecule 22 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	65	Total	C	N	O	S	0	0	0
			499	304	94	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L30P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	154	Total	C	N	O	S	0	0	0
			1196	737	209	244	6			

- Molecule 24 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	82	Total	C	N	O	S	0	0	0
			654	402	129	122	1			

- Molecule 25 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	142	Total	C	N	O		0	0	0
			1130	686	228	216				

- Molecule 26 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	Z	73	Total	C	N	O	S	0	0	0
			573	343	113	112	5			

- Molecule 27 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 28 is a protein called 50S ribosomal protein L39e.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 29 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 30 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	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	87	Total	Mg	0	0
			87	87		
32	9	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

- Molecule 33 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	10	Total 10	Cl 10	0	0
33	J	3	Total 3	Cl 3	0	0
33	B	1	Total 1	Cl 1	0	0
33	A	1	Total 1	Cl 1	0	0
33	N	1	Total 1	Cl 1	0	0
33	O	1	Total 1	Cl 1	0	0
33	R	1	Total 1	Cl 1	0	0
33	Y	1	Total 1	Cl 1	0	0
33	L	1	Total 1	Cl 1	0	0
33	3	1	Total 1	Cl 1	0	0
33	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	92	Total 92	Sr 92	0	0
34	1	2	Total 2	Sr 2	0	0
34	H	1	Total 1	Sr 1	0	0
34	B	2	Total 2	Sr 2	0	0
34	3	2	Total 2	Sr 2	0	0
34	A	3	Total 3	Sr 3	0	0
34	R	1	Total 1	Sr 1	0	0
34	9	3	Total 3	Sr 3	0	0
34	S	1	Total 1	Sr 1	0	0

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	66	Total 66	Na 66	0	0
35	J	1	Total 1	Na 1	0	0
35	Q	1	Total 1	Na 1	0	0
35	B	1	Total 1	Na 1	0	0
35	C	1	Total 1	Na 1	0	0
35	R	1	Total 1	Na 1	0	0
35	9	2	Total 2	Na 2	0	0
35	S	1	Total 1	Na 1	0	0
35	M	1	Total 1	Na 1	0	0

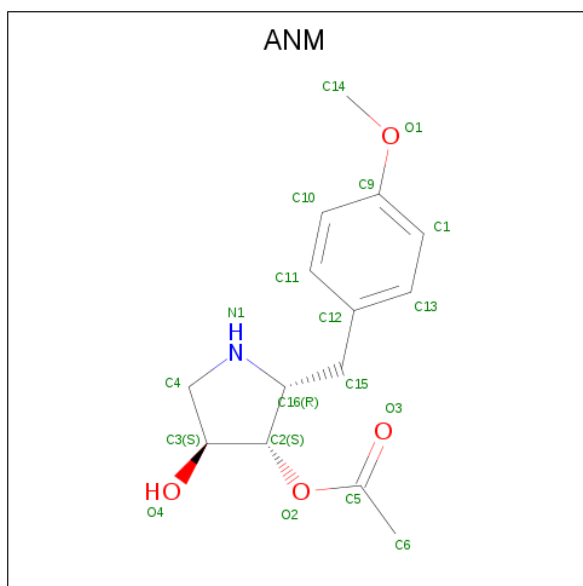
- Molecule 36 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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

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

- Molecule 38 is ANISOMYCIN (three-letter code: ANM) (formula: C<sub>14</sub>H<sub>19</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	0	1	Total C N O 19 14 1 4	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	A	110	Total O 110 110	0	0
39	B	140	Total O 140 140	0	0
39	C	163	Total O 163 163	0	0
39	D	46	Total O 46 46	0	0
39	E	44	Total O 44 44	0	0
39	F	26	Total O 26 26	0	0
39	G	17	Total O 17 17	0	0
39	H	67	Total O 67 67	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	I	6	Total 6	O 6	0	0
39	J	49	Total 49	O 49	0	0
39	K	56	Total 56	O 56	0	0
39	L	85	Total 85	O 85	0	0
39	M	121	Total 121	O 121	0	0
39	N	61	Total 61	O 61	0	0
39	O	44	Total 44	O 44	0	0
39	P	62	Total 62	O 62	0	0
39	Q	48	Total 48	O 48	0	0
39	R	78	Total 78	O 78	0	0
39	S	32	Total 32	O 32	0	0
39	T	39	Total 39	O 39	0	0
39	U	27	Total 27	O 27	0	0
39	V	13	Total 13	O 13	0	0
39	W	65	Total 65	O 65	0	0
39	X	23	Total 23	O 23	0	0
39	Y	92	Total 92	O 92	0	0
39	Z	31	Total 31	O 31	0	0
39	1	48	Total 48	O 48	0	0
39	2	38	Total 38	O 38	0	0
39	3	66	Total 66	O 66	0	0

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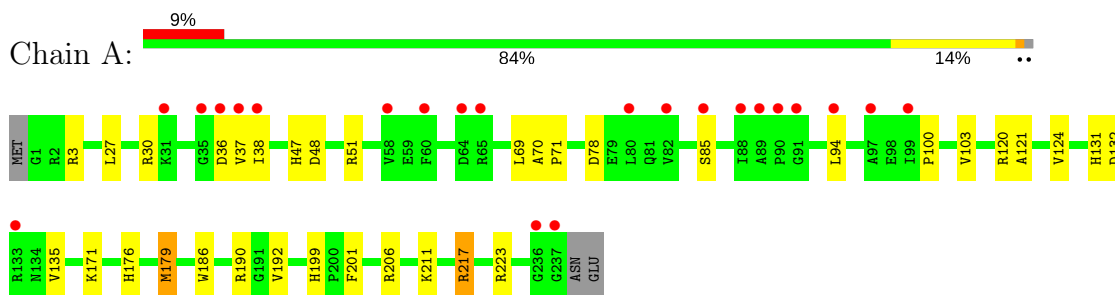
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5972	Total 5972	O 5972	0	0
39	9	147	Total 147	O 147	0	0

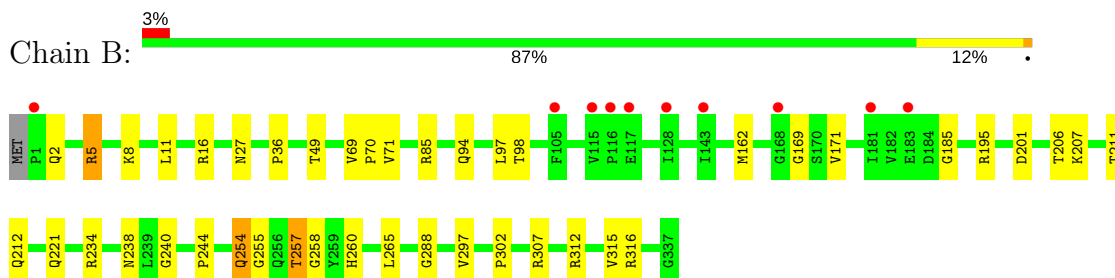
### 3 Residue-property plots [i](#)

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

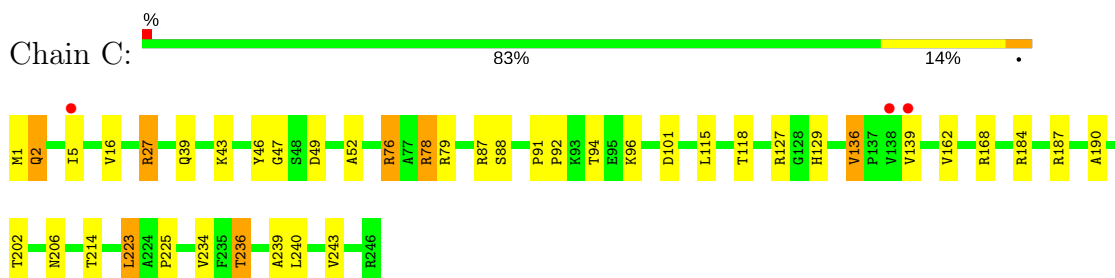
- Molecule 1: 50S ribosomal protein L2P



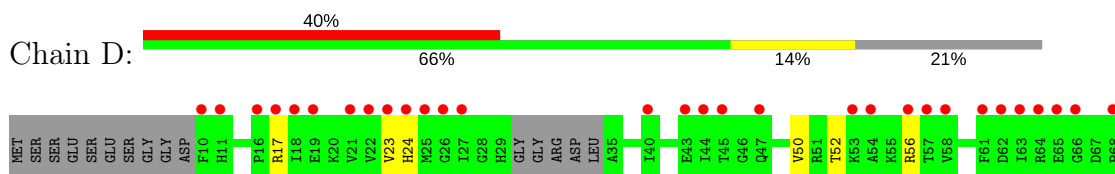
- Molecule 2: 50S ribosomal protein L3P



- Molecule 3: 50S ribosomal protein L4P

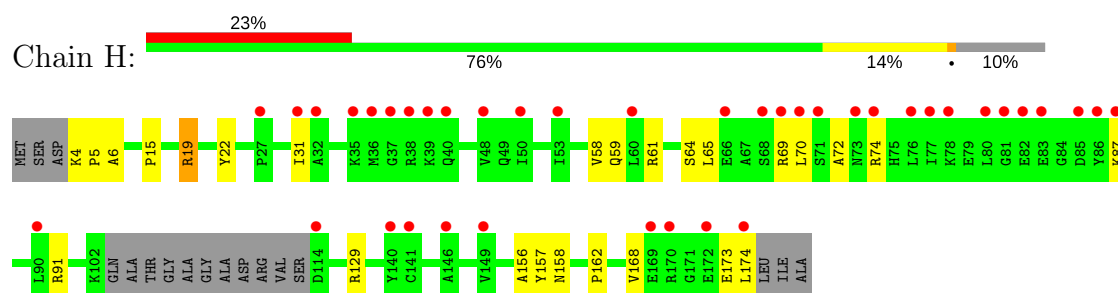


- Molecule 4: 50S ribosomal protein L5P

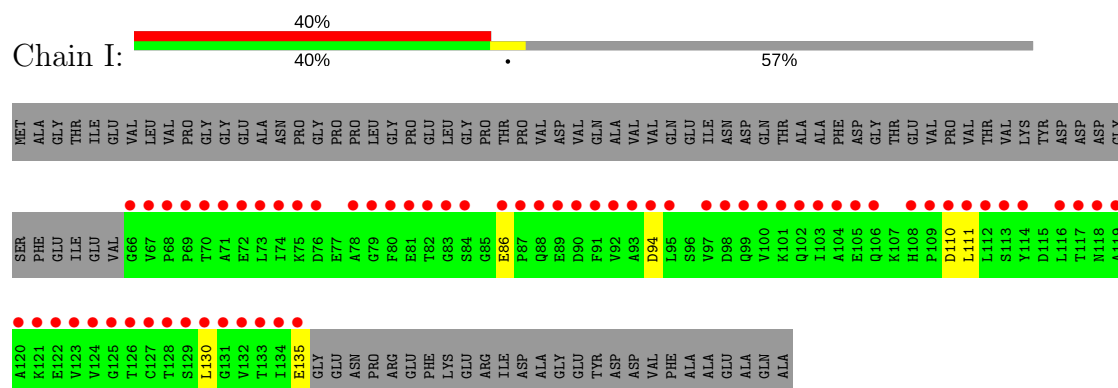




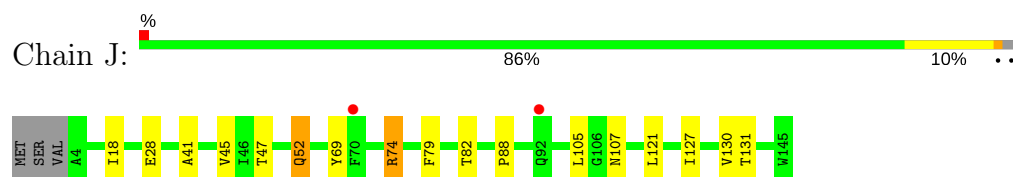




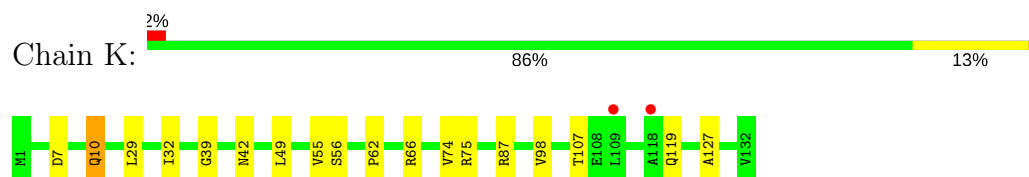
- Molecule 9: 50S ribosomal protein L11P



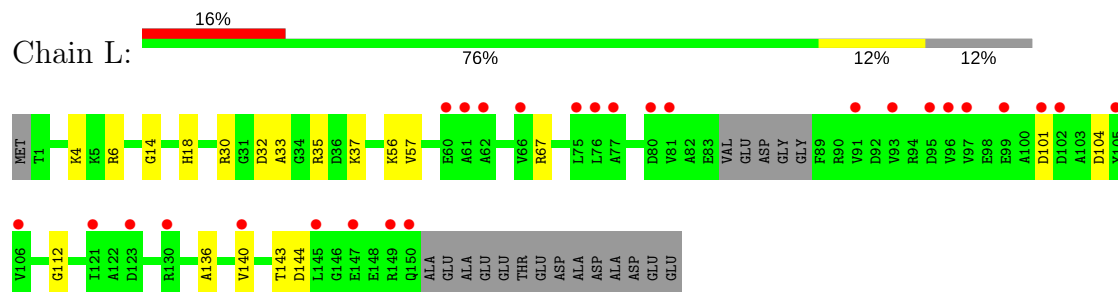
- Molecule 10: 50S ribosomal protein L13P



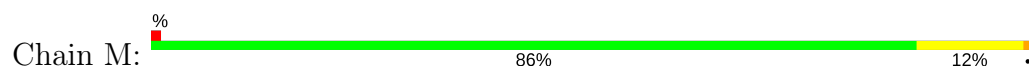
- Molecule 11: 50S ribosomal protein L14P

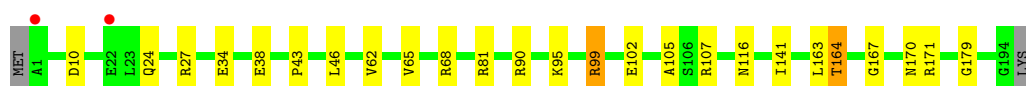


- Molecule 12: 50S ribosomal protein L15P

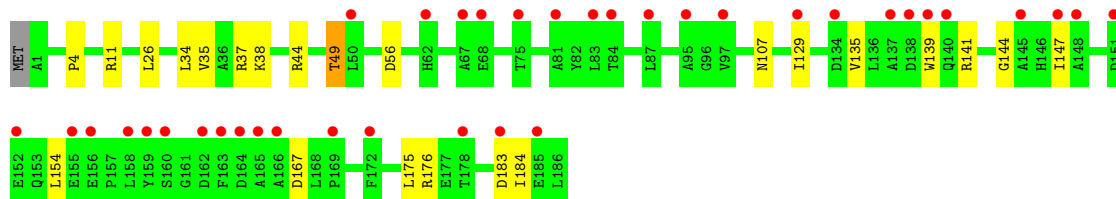
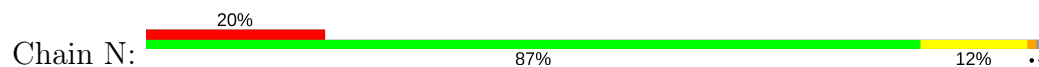


- Molecule 13: 50S ribosomal protein L15e

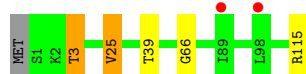




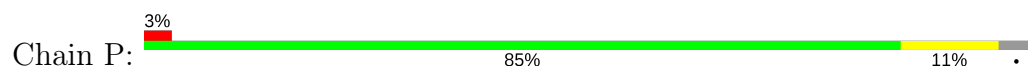
- Molecule 14: 50S ribosomal protein L18P



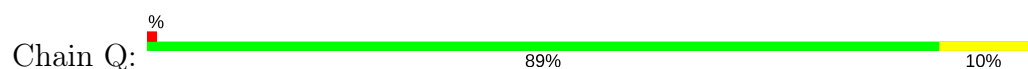
- Molecule 15: 50S ribosomal protein L18e



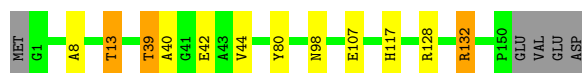
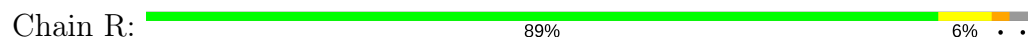
- Molecule 16: 50S ribosomal protein L19e



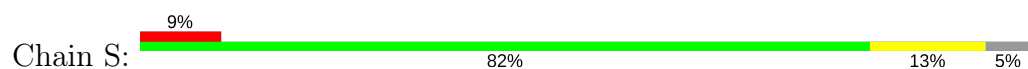
- Molecule 17: 50S ribosomal protein L21e



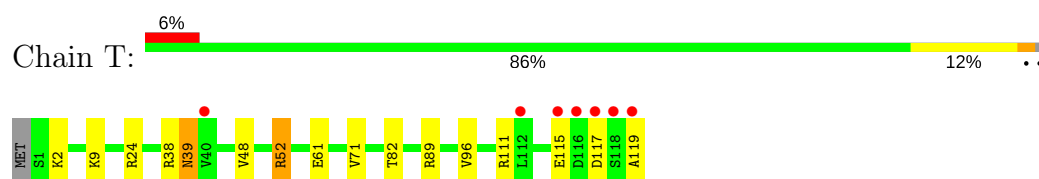
- Molecule 18: 50S ribosomal protein L22P



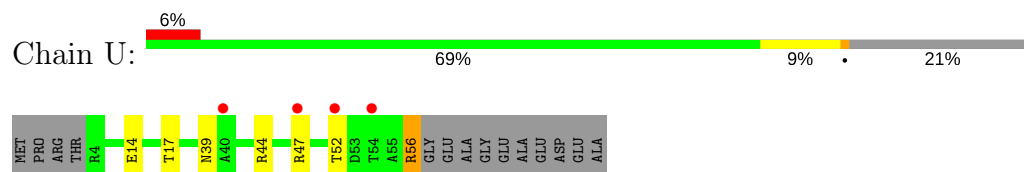
- Molecule 19: 50S ribosomal protein L23P



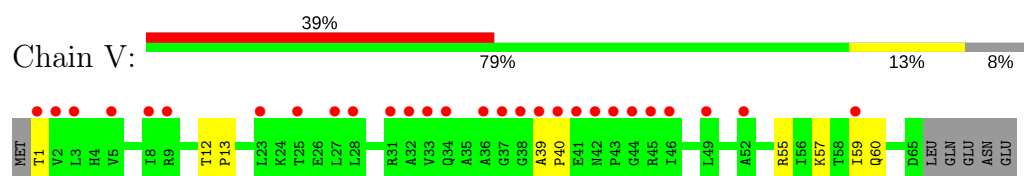
- Molecule 20: 50S ribosomal protein L24P



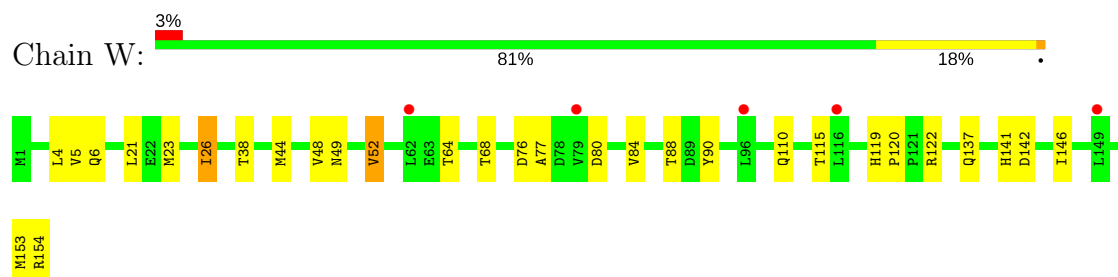
- Molecule 21: 50S ribosomal protein L24e



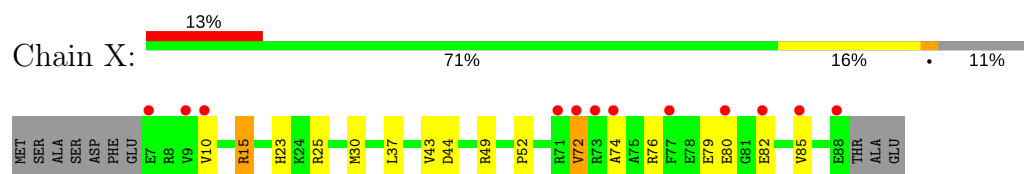
- Molecule 22: 50S ribosomal protein L29P



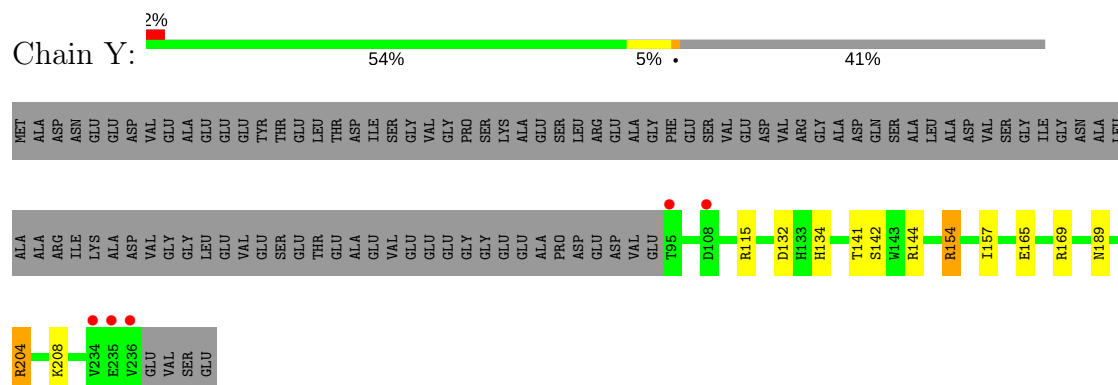
- Molecule 23: 50S ribosomal protein L30P



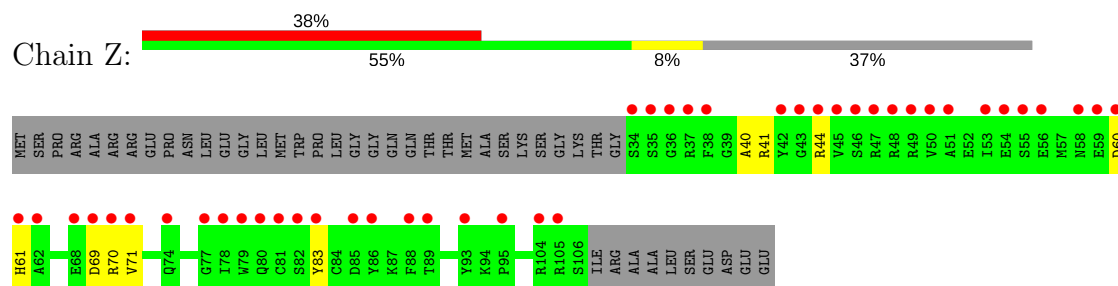
- Molecule 24: 50S ribosomal protein L31e



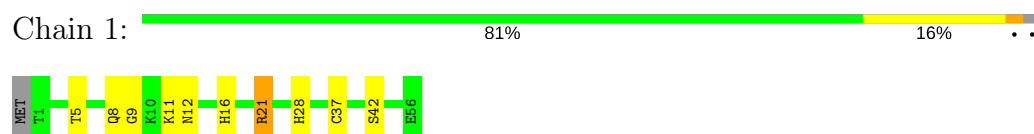
- Molecule 25: 50S ribosomal protein L32e



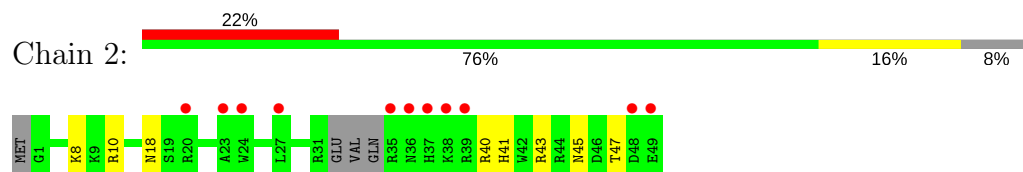
• Molecule 26: 50S ribosomal protein L37Ae



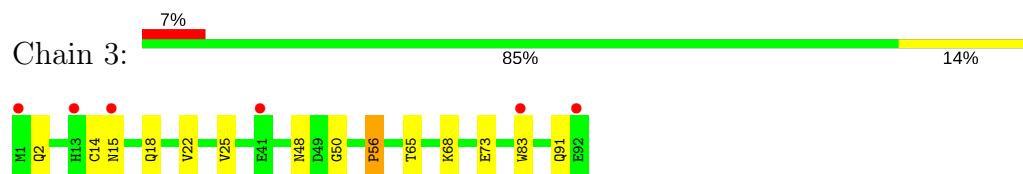
• Molecule 27: 50S ribosomal protein L37e



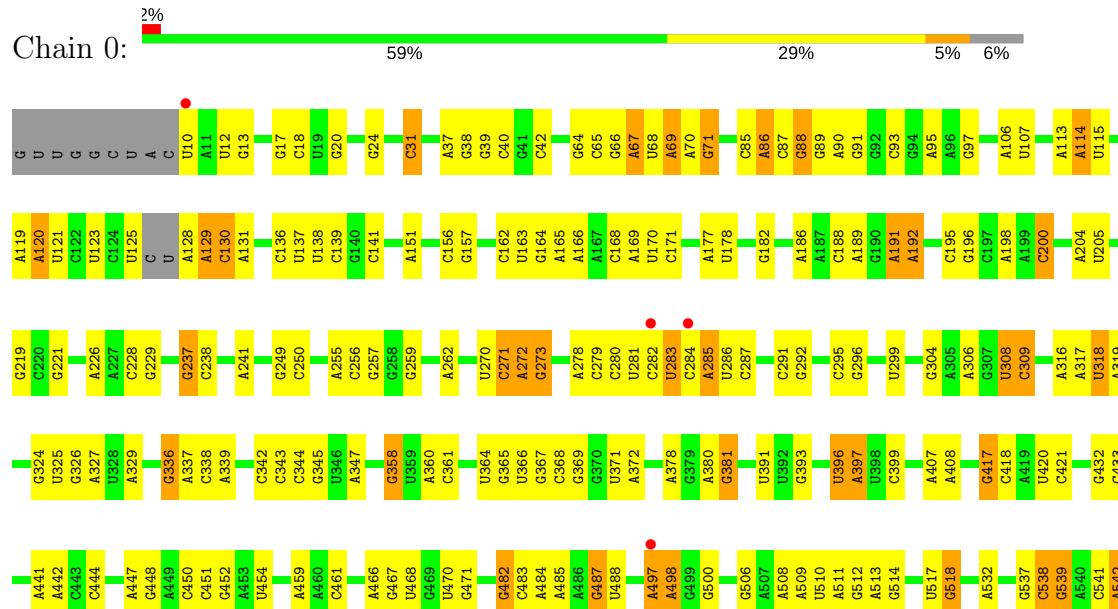
• Molecule 28: 50S ribosomal protein L39e



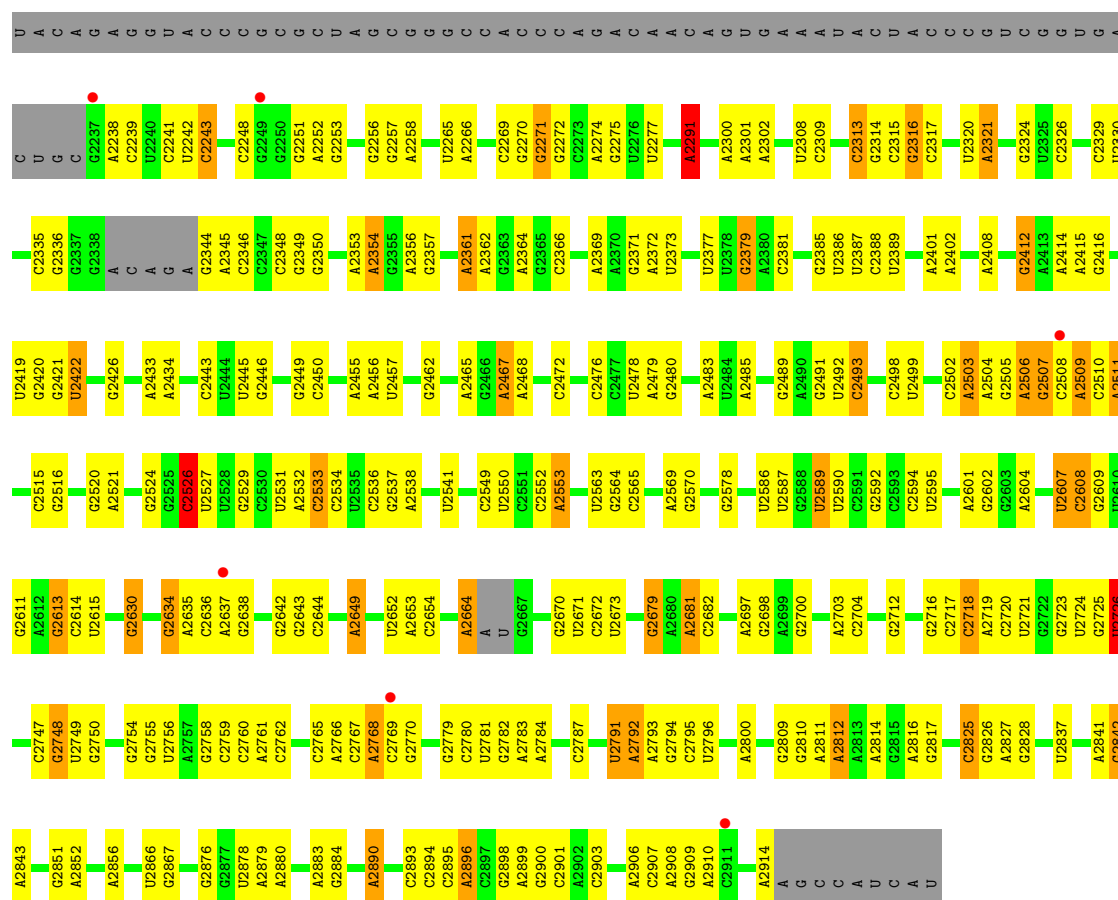
• Molecule 29: 50S ribosomal protein L44E



• Molecule 30: 23S ribosomal RNA



A2089	G1971	G1863	A1755	G1634	U1506	G1391	U1266	U1186	G1087	G	G902	A791	A660	G543
G2090	U1972	G1863	G1756	U1635	A1516	A1392	C1267	C1186	A1088	A	G902	G792	A661	G544
G2091	A1973	G1867	C1762	G1636	U1516	C1396	G1268	A1187	U1088	G	C905	A793	A666	G545
G2092	G1974	G1868	C1763	A1637	U1516	C1397	G1269	A1188	U1094	U	A907	U794	C667	G553
A2096	G1975	G1868	U1766	A1641	U1524	G1398	A1278	A1189	A1097	C	A907	A807	C668	G558
A2100	U1977	G1878	U1766	A1642	G1525	A1399	U1279	A1191	A1098	G	A908	A808	C669	G568
A2101	A1978	G1879	U1771	U1654	A1527	A1406	C1289	A1192	G1099	C	A912	G809	C670	U560
G2102	G1979	G1880	G1772	G1655	A1528	A1407	U1290	A1193	C1104	A	U919	A812	C672	G561
A2103	U1980	A1881	G1773	A1656	G1529	G1409	A1294	G1195	U1109	C	U919	A813	C677	G564
C1993	G1983	C1882	A1778	A1657	U1533	A1413	G1295	G1196	G1110	A	G921	G814	C678	U567
A1994	U1883	U1882	A1779	A1658	C1534	A1414	G1299	A1199	U1116	A1005	A922	G815	G681	G567
G1995	G1884	G1885	A1779	U1662	G1535	A1415	G1300	A1200	A1117	A1006	A923	U816	A682	G581
U1996	A1886	A1887	U1783	G1663	C1536	G1416	U1304	G1197	A1118	A1007	U932	U815	A683	G582
A1997	A1886	A1887	U1784	G1663	C1537	G1417	C1305	U1198	G1119	C1008	U933	G820	U582	U582
G2000	C1894	C1895	U1787	G1666	U1544	U1418	C1305	U1198	U1121	C1010	G938	U821	C686	G588
G2001	A1895	A1896	C1787	A1667	C1545	U1419	A1313	A1205	G1135	A1014	G941	C522	A688	U595
G2002	U1897	U1897	U1788	U1668	G1546	C1420	G1314	U1206	U1136	C1015	U942	U827	C689	C596
U2003	U1906	U1906	U1790	U1677	A1559	C1421	G1315	U1207	G1137	U1016	U943	U832	C694	A602
G2005	A1919	A1920	U1791	A1678	U	C1422	G1316	C1208	G1138	U1016	U944	U833	C695	G604
U2008	C1921	C1921	C1798	C1679	U1561	C1423	A1321	C1209	G1151	C1023	G944	U834	C699	C605
G2009	A1922	A1922	G1799	G1681	C1562	A1427	G1322	G1210	U1135	G1024	U947	U835	C699	U612
A2010	G1925	G1925	A1804	A1682	A1573	G1430	G1328	G1211	U1136	C1025	U948	U836	C699	C613
G2011	U1926	U1926	G1805	G1683	A1573	G1430	G1329	G1212	U1137	U1029	U949	U840	U701	U614
G2012	A1927	A1927	G1809	A1685	U1587	U1440	A1330	G1213	G1138	G1039	U950	U841	G702	U619
U2013	U1927	U1927	G1809	A1686	G1588	G1441	G1331	G1214	G1151	U1040	U951	C847	G703	A620
U2016	U1939	U1939	A1815	C1687	G1589	A1442	C1332	G1215	C1157	U1041	C952	C848	C704	C621
G2033	C1940	C1940	C1816	G1688	G1592	C1451	C1333	G1216	G1158	U1042	G953	C849	C705	G622
U2034	A1941	A1941	G1816	C1692	C1593	C1451	C1334	U1218	G1159	C1043	G958	U850	G709	U623
G	C1943	C1943	G1820	A1693	C1594	C1456	C1334	U1219	G1160	C1044	C959	U851	G710	U624
U2039	U1946	U1946	A1701	U1702	U1596	U1457	G1339	U1220	A1161	G1045	G960	C853	G711	U625
G2040	G1947	G1947	U1702	U1702	A1597	U1473	A1341	C1229	G1162	C1046	C962	C856	U714	A629
U2044	G1948	G1948	A1710	A1598	C1598	C1474	C1342	A1230	G1163	C1051	C963	A857	U	A630
G2050	G1949	G1949	G1714	A1603	U1598	C1477	C1343	A1231	U1164	C1052	U970	U858	G716	A632
A2054	U1951	U1951	C1715	G1604	A1605	U1478	G1350	A1232	G1165	C1053	G969	G868	G722	A631
C2055	U	U	A1836	G1605	G1606	U1478	G1351	A1233	C1166	U1056	G	G869	G722	A632
U2064	A	A	G1837	A1607	A1607	G1481	A1352	U1237	U1169	A1057	U	G870	C735	A635
A	C	C	U1838	A1607	A1607	A1482	C1363	C1238	U1170	A1058	G	C871	A736	G636
U2067	U	U	A1839	C1613	C1613	A1485	C1360	G1239	A1171	C1059	U	U872	G737	C637
G2068	U	U	A1840	G1614	G1614	A1485	C1360	U1234	G1172	C1060	C	A875	G738	C638
G2072	U	U	G1848	A1615	A1615	G1490	G1363	A1242	A1173	U1066	C	A876	C741	A639
A2074	G	G	G1849	U1622	U1622	C1495	A1372	C1243	A1174	A1067	C	G877	C741	G644
U2078	A	A	C1851	C1623	C1623	C1496	A1372	U1244	G1175	C	C	G878	C759	U645
A2081	C	C	A1852	A1624	A1624	G1497	C1377	C1245	C1176	G1071	C	C884	G760	G653
G2088	U	U	C1853	U1625	U1625	U1500	C1377	A1246	G1177	C	C	G885	A761	U653
U2088	U	U	C1854	A1626	A1626	U1500	C1384	U1249	A1178	A1078	C	C885	A761	U653
U2088	U	U	C1855	G1627	G1627	U1500	G1384	C1250	C1179	A1079	C	U888	A776	G655
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U2088	U	U	C1857	G1627	G1627	U1500	G1384	C1251	A1181	A1079	C	U888	A776	G655
U2088	U	U	C1858	G1627	G1627	U1500	G1384	C1251	A1182	C1080	A	U888	A776	G655
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U2088	U	U	C1860	G1627	G1627	U1500	G1384	C1251	C1183	A1081	A	U888	A776	G655
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U2088	U	U	C1866	G1627	G1627	U1500	G1384	C1251	C1183	A1081	A	U888	A776	G655
U2088	U	U	C1867	G1627	G1627	U1500	G1384	C1251	C1183	A1081	A	U888	A776	G655
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U2088	U	U	C1901	G1627	G1627	U1500	G1384	C1251	C1183	A1081	A	U888	A776	G655
U2088	U	U	C1902	G1627	G1627	U1500	G1384	C1251	C1183	A1081	A	U888	A776	G655



• 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, $\alpha$ , $\beta$ , $\gamma$	211.78Å 299.08Å 573.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.85 – 2.70 85.45 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (49.85-2.70) 96.9 (85.45-2.40)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.202 , 0.244 0.191 , 0.231	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.7	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 63.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99135	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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

### 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, ANM, 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	0.51	0/1786	0.78	0/2408
2	B	0.53	0/2690	0.78	0/3652
3	C	0.54	0/1885	0.77	0/2552
4	D	0.65	0/1111	0.71	1/1498 (0.1%)
5	E	0.60	0/1382	0.68	0/1880
6	F	0.54	0/901	0.71	0/1224
7	G	0.51	0/241	0.67	0/324
8	H	0.60	0/1302	0.79	0/1743
9	I	0.59	0/526	0.62	0/716
10	J	0.61	0/1136	0.72	0/1530
11	K	0.51	0/1004	0.80	0/1351
12	L	0.49	0/1130	0.76	0/1509
13	M	0.51	0/1582	0.77	0/2116
14	N	0.55	0/1474	0.77	0/1999
15	O	0.47	0/874	0.73	1/1181 (0.1%)
16	P	0.52	0/1147	0.67	0/1528
17	Q	0.49	0/749	0.77	0/1005
18	R	0.54	0/1172	0.74	0/1578
19	S	0.54	0/648	0.67	0/875
20	T	0.46	0/958	0.76	1/1289 (0.1%)
21	U	0.57	0/417	0.71	0/562
22	V	0.44	0/502	0.67	0/675
23	W	0.52	0/1219	0.78	1/1655 (0.1%)
24	X	0.52	0/664	0.72	0/895
25	Y	0.52	0/1146	0.74	0/1536
26	Z	0.69	0/584	0.74	0/781
27	1	0.55	0/438	0.75	0/578
28	2	0.45	0/401	0.70	0/529
29	3	0.59	0/771	0.70	0/1024
30	0	0.37	0/65958	0.68	15/102869 (0.0%)
31	9	0.32	0/2904	0.69	1/4526 (0.0%)
All	All	0.43	0/98702	0.70	20/147588 (0.0%)



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

Mol	Chain	#Chirality outliers	#Planarity outliers
23	W	0	1
30	0	0	42
31	9	0	2
All	All	0	45

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	4	LEU	CA-CB-CG	7.59	132.77	115.30
30	0	1942	A	C5'-C4'-C3'	6.82	126.92	116.00
30	0	871	G	C5'-C4'-O4'	-6.64	101.13	109.10
30	0	1504	A	N9-C1'-C2'	5.91	121.68	114.00
30	0	2726	U	N1-C1'-C2'	5.85	121.60	114.00

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	221	G	Sidechain
30	0	270	U	Sidechain
30	0	391	U	Sidechain
30	0	396	U	Sidechain
23	W	90	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1753	0	1766	21	0
2	B	2625	0	2533	29	0
3	C	1860	0	1813	22	0
4	D	1094	0	1085	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1357	0	1266	10	0
6	F	890	0	843	8	0
7	G	240	0	231	0	0
8	H	1282	0	1292	18	0
9	I	519	0	500	4	0
10	J	1120	0	1098	14	0
11	K	994	0	1027	11	0
12	L	1118	0	1076	12	0
13	M	1558	0	1573	19	0
14	N	1445	0	1401	16	0
15	O	865	0	873	4	0
16	P	1136	0	1123	11	0
17	Q	735	0	729	6	0
18	R	1149	0	1122	11	0
19	S	641	0	605	5	0
20	T	950	0	924	8	0
21	U	410	0	364	3	0
22	V	499	0	511	4	0
23	W	1196	0	1137	22	0
24	X	654	0	653	11	0
25	Y	1130	0	1133	13	0
26	Z	573	0	532	6	0
27	1	431	0	426	10	0
28	2	396	0	413	5	0
29	3	755	0	729	7	0
30	0	59021	0	29812	846	0
31	9	2599	0	1325	64	0
32	0	87	0	0	0	0
32	9	1	0	0	0	0
32	A	1	0	0	0	0
32	B	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	10	0	0	0	0
33	3	1	0	0	0	0
33	A	1	0	0	0	0
33	B	1	0	0	0	0
33	J	3	0	0	1	0
33	L	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	O	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	92	0	0	0	0
34	1	2	0	0	0	0
34	3	2	0	0	0	0
34	9	3	0	0	0	0
34	A	3	0	0	0	0
34	B	2	0	0	0	0
34	F	1	0	0	0	0
34	H	1	0	0	0	0
34	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	66	0	0	0	0
35	9	2	0	0	0	0
35	B	1	0	0	0	0
35	C	1	0	0	0	0
35	J	1	0	0	0	0
35	M	1	0	0	0	0
35	Q	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	3	1	0	0	0	0
36	O	1	0	0	0	0
36	U	1	0	0	0	0
36	Z	1	0	0	0	0
37	0	2	0	0	0	0
38	0	19	0	19	5	0
39	0	5972	0	0	121	0
39	1	48	0	0	0	0
39	2	38	0	0	0	0
39	3	66	0	0	1	0
39	9	147	0	0	5	0
39	A	110	0	0	4	0
39	B	140	0	0	5	0
39	C	163	0	0	2	0
39	D	46	0	0	0	0
39	E	44	0	0	0	0
39	F	26	0	0	0	0
39	G	17	0	0	0	0
39	H	67	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	I	6	0	0	1	0
39	J	49	0	0	1	0
39	K	56	0	0	0	0
39	L	85	0	0	2	0
39	M	121	0	0	1	0
39	N	61	0	0	1	0
39	O	44	0	0	0	0
39	P	62	0	0	0	0
39	Q	48	0	0	0	0
39	R	78	0	0	0	0
39	S	32	0	0	0	0
39	T	39	0	0	0	0
39	U	27	0	0	0	0
39	V	13	0	0	0	0
39	W	65	0	0	2	0
39	X	23	0	0	1	0
39	Y	92	0	0	3	0
39	Z	31	0	0	1	0
All	All	99135	0	59934	1085	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 7.

The worst 5 of 1085 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:0:1160:G:H5'	30:0:1161:A:H5'	1.22	1.16
31:9:76:G:H3'	31:9:77:A:H5''	1.34	1.02
15:O:3:THR:HG22	30:0:656:G:H5'	1.43	1.00
30:0:871:G:H8	30:0:871:G:H5'	1.27	0.98
30:0:871:G:C8	30:0:871:G:H5'	1.98	0.97

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%)	220 (94%)	13 (6%)	2 (1%)	19	44
2	B	335/338 (99%)	314 (94%)	19 (6%)	2 (1%)	27	54
3	C	244/246 (99%)	229 (94%)	15 (6%)	0	100	100
4	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	11	29
5	E	170/178 (96%)	159 (94%)	11 (6%)	0	100	100
6	F	117/120 (98%)	110 (94%)	4 (3%)	3 (3%)	6	15
7	G	25/348 (7%)	25 (100%)	0	0	100	100
8	H	156/177 (88%)	148 (95%)	7 (4%)	1 (1%)	27	54
9	I	68/162 (42%)	60 (88%)	8 (12%)	0	100	100
10	J	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
11	K	130/132 (98%)	123 (95%)	6 (5%)	1 (1%)	21	47
12	L	141/165 (86%)	134 (95%)	7 (5%)	0	100	100
13	M	192/196 (98%)	188 (98%)	4 (2%)	0	100	100
14	N	184/187 (98%)	174 (95%)	5 (3%)	5 (3%)	5	14
15	O	113/116 (97%)	112 (99%)	1 (1%)	0	100	100
16	P	141/149 (95%)	139 (99%)	2 (1%)	0	100	100
17	Q	93/96 (97%)	88 (95%)	5 (5%)	0	100	100
18	R	148/155 (96%)	143 (97%)	5 (3%)	0	100	100
19	S	79/85 (93%)	76 (96%)	3 (4%)	0	100	100
20	T	117/120 (98%)	111 (95%)	6 (5%)	0	100	100
21	U	51/67 (76%)	50 (98%)	1 (2%)	0	100	100
22	V	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
23	W	152/154 (99%)	148 (97%)	2 (1%)	2 (1%)	13	33
24	X	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
25	Y	140/241 (58%)	139 (99%)	1 (1%)	0	100	100
26	Z	71/116 (61%)	64 (90%)	6 (8%)	1 (1%)	12	31
27	1	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
28	2	42/50 (84%)	42 (100%)	0	0	100	100
29	3	90/92 (98%)	87 (97%)	2 (2%)	1 (1%)	16	38
All	All	3705/4472 (83%)	3524 (95%)	161 (4%)	20 (0%)	31	58

5 of 20 Ramachandran outliers are listed below:

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

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	179/182 (98%)	170 (95%)	9 (5%)	27	55
2	B	282/283 (100%)	269 (95%)	13 (5%)	29	59
3	C	193/193 (100%)	177 (92%)	16 (8%)	12	28
4	D	117/148 (79%)	107 (92%)	10 (8%)	12	27
5	E	152/156 (97%)	148 (97%)	4 (3%)	49	79
6	F	93/94 (99%)	91 (98%)	2 (2%)	55	83
7	G	27/282 (10%)	27 (100%)	0	100	100
8	H	134/145 (92%)	127 (95%)	7 (5%)	25	53
9	I	58/130 (45%)	56 (97%)	2 (3%)	40	71
10	J	118/121 (98%)	110 (93%)	8 (7%)	17	40
11	K	106/106 (100%)	99 (93%)	7 (7%)	18	41
12	L	113/127 (89%)	107 (95%)	6 (5%)	25	52
13	M	158/160 (99%)	150 (95%)	8 (5%)	26	54
14	N	149/150 (99%)	144 (97%)	5 (3%)	40	71
15	O	93/94 (99%)	91 (98%)	2 (2%)	55	83
16	P	113/117 (97%)	109 (96%)	4 (4%)	39	69
17	Q	79/80 (99%)	76 (96%)	3 (4%)	36	66
18	R	117/122 (96%)	114 (97%)	3 (3%)	49	79
19	S	71/74 (96%)	69 (97%)	2 (3%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	T	105/106 (99%)	96 (91%)	9 (9%)	11	26
21	U	44/53 (83%)	41 (93%)	3 (7%)	17	40
22	V	51/57 (90%)	49 (96%)	2 (4%)	35	65
23	W	130/130 (100%)	123 (95%)	7 (5%)	24	51
24	X	66/74 (89%)	59 (89%)	7 (11%)	7	17
25	Y	120/196 (61%)	116 (97%)	4 (3%)	41	71
26	Z	60/94 (64%)	60 (100%)	0	100	100
27	1	46/47 (98%)	45 (98%)	1 (2%)	55	83
28	2	42/46 (91%)	41 (98%)	1 (2%)	52	81
29	3	79/79 (100%)	75 (95%)	4 (5%)	26	54
All	All	3095/3646 (85%)	2946 (95%)	149 (5%)	28	57

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	79	PHE
12	L	140	VAL
24	X	80	GLU
10	J	130	VAL
11	K	98	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	140	GLN
18	R	22	GLN
27	1	28	HIS
16	P	50	GLN
16	P	118	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	232 (8%)	28 (1%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	249 (8%)	29 (1%)

5 of 249 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
30	0	31	C
30	0	67	A
30	0	69	A
30	0	70	A
30	0	71	G

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1352	A
30	0	1692	C
30	0	2761	A
30	0	1377	C
30	0	1856	C

## 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	OMU	0	2587	30	14,22,23	0.96	1 (7%)	18,31,34	3.74	2 (11%)
30	OMG	0	2588	30	19,26,27	1.04	2 (10%)	22,38,41	2.46	5 (22%)
30	UR3	0	2619	30	13,22,23	0.77	0	15,32,35	0.72	0
30	PSU	0	2621	30	16,21,22	1.57	3 (18%)	20,30,33	5.42	4 (20%)
30	1MA	0	628	30,35	16,25,26	1.06	1 (6%)	12,37,40	1.25	1 (8%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	OMU	0	2587	30	-	0/5/27/28	0/2/2/2
30	OMG	0	2588	30	-	0/5/27/28	0/3/3/3
30	UR3	0	2619	30	-	0/3/25/26	0/2/2/2
30	PSU	0	2621	30	-	0/7/25/26	0/2/2/2
30	1MA	0	628	30,35	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.86	1.48	1.52
30	0	2588	OMG	C8-N7	-2.16	1.30	1.34
30	0	2621	PSU	C2-N1	2.22	1.42	1.38
30	0	2587	OMU	C4-N3	2.45	1.37	1.33
30	0	2621	PSU	C4-N3	2.69	1.37	1.33

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.13	114.64	128.41
30	0	2588	OMG	C5-C6-N1	-8.34	111.60	123.47
30	0	2621	PSU	C5-C4-N3	-8.23	114.76	125.36
30	0	628	1MA	C2-N3-C4	-3.68	110.89	116.51
30	0	2587	OMU	C5-C4-N3	-3.65	114.70	123.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
38	ANM	0	2924	37	19,20,20	0.48	0	22,27,27	1.93	6 (27%)

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
38	ANM	0	2924	37	-	0/10/23/23	0/2/2/2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	0	2924	ANM	C4-C3-C2	-3.74	98.31	103.22
38	0	2924	ANM	C2-O2-C5	-3.72	111.92	117.72
38	0	2924	ANM	C3-C2-C16	-2.94	99.95	104.21
38	0	2924	ANM	C14-O1-C9	-2.79	111.46	117.51
38	0	2924	ANM	O2-C5-O3	-2.03	118.84	122.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	0	2924	ANM	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	237/240 (98%)	0.63	22 (9%) 8 6	24, 49, 88, 107	0
2	B	337/338 (99%)	0.37	10 (2%) 50 50	27, 53, 82, 95	0
3	C	246/246 (100%)	0.29	3 (1%) 79 80	21, 42, 65, 78	0
4	D	140/177 (79%)	2.48	71 (50%) 0 0	61, 99, 124, 134	0
5	E	172/178 (96%)	0.70	15 (8%) 10 8	44, 69, 88, 94	0
6	F	119/120 (99%)	1.32	31 (26%) 0 0	43, 69, 99, 114	0
7	G	29/348 (8%)	1.76	10 (34%) 0 0	77, 95, 103, 106	0
8	H	160/177 (90%)	1.29	40 (25%) 0 0	44, 61, 96, 101	0
9	I	70/162 (43%)	5.14	65 (92%) 0 0	131, 146, 163, 164	0
10	J	142/145 (97%)	0.31	2 (1%) 75 76	35, 50, 71, 91	0
11	K	132/132 (100%)	0.15	2 (1%) 73 75	32, 49, 72, 77	0
12	L	145/165 (87%)	0.94	27 (18%) 1 1	25, 63, 109, 125	0
13	M	194/196 (98%)	0.12	2 (1%) 82 83	28, 40, 56, 63	0
14	N	186/187 (99%)	1.13	37 (19%) 1 0	42, 64, 112, 121	0
15	O	115/116 (99%)	0.50	2 (1%) 70 71	33, 53, 69, 80	0
16	P	143/149 (95%)	0.42	4 (2%) 53 53	38, 53, 67, 74	0
17	Q	95/96 (98%)	0.28	1 (1%) 80 81	34, 45, 62, 73	0
18	R	150/155 (96%)	0.14	0 100 100	30, 43, 63, 71	0
19	S	81/85 (95%)	0.91	8 (9%) 7 5	42, 56, 79, 90	0
20	T	119/120 (99%)	0.65	7 (5%) 22 21	35, 54, 84, 109	0
21	U	53/67 (79%)	0.62	4 (7%) 14 12	40, 56, 78, 84	0
22	V	65/71 (91%)	2.56	28 (43%) 0 0	52, 73, 117, 123	0
23	W	154/154 (100%)	0.54	5 (3%) 47 47	33, 49, 65, 75	0
24	X	82/92 (89%)	0.86	12 (14%) 2 1	43, 60, 85, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	0.18	5 (3%) 44 43	22, 41, 64, 89	0
26	Z	73/116 (62%)	2.49	44 (60%) 0 0	58, 76, 89, 100	0
27	1	56/57 (98%)	0.04	0 100 100	24, 30, 36, 43	0
28	2	46/50 (92%)	1.02	11 (23%) 0 0	34, 60, 91, 101	0
29	3	92/92 (100%)	0.70	6 (6%) 19 17	36, 59, 72, 86	0
30	0	2749/2923 (94%)	-0.32	56 (2%) 65 66	18, 43, 87, 165	0
31	9	122/122 (100%)	-0.29	4 (3%) 46 46	34, 65, 86, 145	0
All	All	6646/7517 (88%)	0.31	534 (8%) 12 10	18, 50, 99, 165	0

The worst 5 of 534 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	V	39	ALA	14.6
22	V	1	THR	12.8
22	V	40	PRO	12.0
9	I	74	ILE	11.8
14	N	166	ALA	10.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	OMU	0	2587	21/22	0.98	0.15	31,33,35,37	0
30	UR3	0	2619	21/22	0.98	0.17	30,34,36,39	0
30	PSU	0	2621	20/21	0.98	0.16	22,26,34,34	0
30	1MA	0	628	23/24	0.98	0.18	25,28,29,31	0
30	OMG	0	2588	24/25	0.98	0.15	27,30,33,35	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
34	SR	9	8978	1/1	0.09	0.14	144,144,144,144	0
34	SR	0	9006	1/1	0.15	1.95	200,200,200,200	0
34	SR	0	8955	1/1	0.16	0.35	200,200,200,200	0
34	SR	0	8957	1/1	0.29	0.75	200,200,200,200	0
35	NA	S	8510	1/1	0.35	0.43	79,79,79,79	0
35	NA	9	8572	1/1	0.38	0.43	76,76,76,76	0
34	SR	0	8976	1/1	0.40	0.45	186,186,186,186	0
32	MG	0	8089	1/1	0.43	0.17	48,48,48,48	0
34	SR	0	8919	1/1	0.47	0.24	178,178,178,178	0
34	SR	0	8922	1/1	0.48	0.37	159,159,159,159	0
34	SR	0	8996	1/1	0.50	0.82	200,200,200,200	0
34	SR	0	8986	1/1	0.51	1.96	200,200,200,200	0
34	SR	0	8959	1/1	0.54	0.26	169,169,169,169	0
34	SR	0	8947	1/1	0.54	0.47	200,200,200,200	0
34	SR	A	8977	1/1	0.54	0.17	172,172,172,172	0
34	SR	0	8979	1/1	0.56	0.29	194,194,194,194	0
35	NA	0	8546	1/1	0.57	1.03	95,95,95,95	0
34	SR	0	8994	1/1	0.60	0.60	190,190,190,190	0
34	SR	9	9003	1/1	0.61	0.10	162,162,162,162	0
34	SR	0	8983	1/1	0.64	0.23	164,164,164,164	0
34	SR	0	8934	1/1	0.64	0.13	90,90,90,90	0
34	SR	0	8984	1/1	0.65	0.10	128,128,128,128	0
34	SR	0	8924	1/1	0.65	0.13	145,145,145,145	0
35	NA	0	8573	1/1	0.67	0.63	69,69,69,69	0
34	SR	B	8987	1/1	0.67	0.69	200,200,200,200	0
34	SR	S	8961	1/1	0.67	0.10	114,114,114,114	0
35	NA	0	8522	1/1	0.67	0.52	78,78,78,78	0
34	SR	0	8989	1/1	0.67	0.39	187,187,187,187	0
35	NA	0	8561	1/1	0.69	0.83	74,74,74,74	0
32	MG	0	8069	1/1	0.69	0.57	47,47,47,47	0
34	SR	0	8944	1/1	0.70	0.26	185,185,185,185	0
34	SR	0	8971	1/1	0.70	0.17	170,170,170,170	0
34	SR	0	8993	1/1	0.70	0.17	168,168,168,168	0
34	SR	0	8916	1/1	0.71	0.15	118,118,118,118	0
35	NA	0	8557	1/1	0.72	0.15	67,67,67,67	0
32	MG	0	8092	1/1	0.72	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8969	1/1	0.72	0.39	150,150,150,150	0
35	NA	0	8571	1/1	0.72	0.32	83,83,83,83	0
35	NA	0	8512	1/1	0.72	0.51	43,43,43,43	0
35	NA	0	8553	1/1	0.73	0.41	79,79,79,79	0
32	MG	0	8050	1/1	0.73	0.18	37,37,37,37	0
35	NA	M	8539	1/1	0.74	0.25	41,41,41,41	0
35	NA	0	8554	1/1	0.74	0.76	65,65,65,65	0
35	NA	0	8549	1/1	0.74	0.42	81,81,81,81	0
34	SR	0	8960	1/1	0.75	0.11	145,145,145,145	0
32	MG	0	8040	1/1	0.75	0.34	83,83,83,83	0
34	SR	0	8956	1/1	0.75	0.14	142,142,142,142	0
34	SR	0	8949	1/1	0.76	0.20	110,110,110,110	0
34	SR	0	8982	1/1	0.76	0.85	180,180,180,180	0
34	SR	0	8933	1/1	0.76	0.52	138,138,138,138	0
35	NA	0	8533	1/1	0.77	0.25	63,63,63,63	0
35	NA	0	8555	1/1	0.77	0.74	54,54,54,54	0
34	SR	0	8990	1/1	0.77	0.22	118,118,118,118	0
34	SR	0	8953	1/1	0.77	0.24	160,160,160,160	0
34	SR	0	8963	1/1	0.77	0.12	133,133,133,133	0
32	MG	A	8051	1/1	0.77	0.50	81,81,81,81	0
34	SR	0	9002	1/1	0.78	0.15	184,184,184,184	0
34	SR	0	8981	1/1	0.78	0.23	167,167,167,167	0
35	NA	0	8562	1/1	0.78	0.85	69,69,69,69	0
35	NA	0	8531	1/1	0.78	0.16	40,40,40,40	0
35	NA	0	8511	1/1	0.78	0.33	59,59,59,59	0
34	SR	9	8980	1/1	0.78	0.27	182,182,182,182	0
35	NA	0	8568	1/1	0.78	0.39	47,47,47,47	0
32	MG	0	8062	1/1	0.78	0.23	34,34,34,34	0
35	NA	0	8560	1/1	0.78	0.46	69,69,69,69	0
34	SR	0	8917	1/1	0.79	0.18	119,119,119,119	0
34	SR	0	8914	1/1	0.79	0.34	118,118,118,118	0
32	MG	0	8079	1/1	0.80	0.24	47,47,47,47	0
34	SR	0	8988	1/1	0.80	0.08	163,163,163,163	0
34	SR	0	8974	1/1	0.80	0.29	166,166,166,166	0
35	NA	9	8543	1/1	0.80	0.08	70,70,70,70	0
34	SR	0	8938	1/1	0.80	0.08	159,159,159,159	0
34	SR	0	8958	1/1	0.81	0.11	108,108,108,108	0
32	MG	0	8063	1/1	0.81	0.28	72,72,72,72	0
32	MG	0	8031	1/1	0.81	0.20	61,61,61,61	0
34	SR	0	8951	1/1	0.81	0.07	146,146,146,146	0
34	SR	0	8997	1/1	0.81	0.64	184,184,184,184	0
32	MG	0	8024	1/1	0.82	0.57	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8998	1/1	0.82	0.41	173,173,173,173	0
34	SR	0	8991	1/1	0.82	0.23	191,191,191,191	0
35	NA	0	8575	1/1	0.82	0.34	94,94,94,94	0
34	SR	0	8948	1/1	0.82	0.17	102,102,102,102	0
34	SR	0	8939	1/1	0.82	0.18	152,152,152,152	0
32	MG	0	8088	1/1	0.82	0.16	37,37,37,37	0
35	NA	0	8565	1/1	0.82	0.54	62,62,62,62	0
34	SR	0	8973	1/1	0.83	0.10	137,137,137,137	0
34	SR	0	8966	1/1	0.83	0.08	110,110,110,110	0
34	SR	0	9000	1/1	0.83	0.17	159,159,159,159	0
37	K	0	8401	1/1	0.83	0.41	81,81,81,81	0
34	SR	0	8995	1/1	0.83	0.19	136,136,136,136	0
34	SR	0	8975	1/1	0.83	0.11	134,134,134,134	0
35	NA	0	8506	1/1	0.83	0.25	47,47,47,47	0
34	SR	0	8928	1/1	0.83	0.20	138,138,138,138	0
34	SR	0	9007	1/1	0.83	0.39	200,200,200,200	0
34	SR	0	9001	1/1	0.84	0.24	169,169,169,169	0
35	NA	0	8505	1/1	0.84	0.57	39,39,39,39	0
32	MG	0	8080	1/1	0.84	0.28	57,57,57,57	0
32	MG	0	8072	1/1	0.84	0.28	52,52,52,52	0
32	MG	0	8006	1/1	0.85	0.21	30,30,30,30	0
34	SR	0	8910	1/1	0.85	0.12	97,97,97,97	0
34	SR	0	8941	1/1	0.85	0.19	115,115,115,115	0
35	NA	Q	8540	1/1	0.85	0.22	60,60,60,60	0
35	NA	0	8567	1/1	0.85	0.43	78,78,78,78	0
32	MG	0	8043	1/1	0.85	0.15	49,49,49,49	0
32	MG	0	8030	1/1	0.85	0.37	55,55,55,55	0
32	MG	0	8016	1/1	0.85	0.33	49,49,49,49	0
32	MG	0	8038	1/1	0.86	0.12	58,58,58,58	0
34	SR	0	9004	1/1	0.86	0.42	200,200,200,200	0
34	SR	0	8926	1/1	0.86	0.12	115,115,115,115	0
34	SR	0	8945	1/1	0.86	0.11	99,99,99,99	0
32	MG	B	8042	1/1	0.86	0.12	50,50,50,50	0
35	NA	0	8501	1/1	0.86	0.20	39,39,39,39	0
35	NA	0	8518	1/1	0.86	0.41	79,79,79,79	0
32	MG	0	8055	1/1	0.86	0.27	38,38,38,38	0
32	MG	0	8071	1/1	0.86	0.27	55,55,55,55	0
35	NA	0	8504	1/1	0.87	0.28	26,26,26,26	0
35	NA	0	8502	1/1	0.87	0.34	67,67,67,67	0
34	SR	0	8970	1/1	0.87	0.07	131,131,131,131	0
34	SR	A	8930	1/1	0.87	0.08	116,116,116,116	0
35	NA	0	8574	1/1	0.87	0.43	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8525	1/1	0.87	0.12	69,69,69,69	0
35	NA	0	8548	1/1	0.87	0.37	57,57,57,57	0
35	NA	0	8556	1/1	0.87	0.50	44,44,44,44	0
35	NA	0	8542	1/1	0.87	0.41	42,42,42,42	0
34	SR	0	8942	1/1	0.87	0.15	121,121,121,121	0
32	MG	0	8044	1/1	0.88	0.12	33,33,33,33	0
35	NA	0	8523	1/1	0.88	0.26	48,48,48,48	0
34	SR	B	8950	1/1	0.88	0.19	108,108,108,108	0
32	MG	0	8081	1/1	0.88	0.24	54,54,54,54	0
32	MG	0	8085	1/1	0.88	0.28	80,80,80,80	0
35	NA	0	8509	1/1	0.88	0.34	64,64,64,64	0
32	MG	0	8066	1/1	0.88	0.22	52,52,52,52	0
34	SR	0	8920	1/1	0.88	0.12	124,124,124,124	0
34	SR	0	8964	1/1	0.88	0.08	126,126,126,126	0
32	MG	0	8075	1/1	0.89	0.08	45,45,45,45	0
34	SR	0	8968	1/1	0.89	0.10	143,143,143,143	0
35	NA	J	8538	1/1	0.89	0.20	56,56,56,56	0
34	SR	0	8908	1/1	0.89	0.18	107,107,107,107	0
35	NA	0	8544	1/1	0.89	0.30	64,64,64,64	0
35	NA	0	8508	1/1	0.89	0.23	37,37,37,37	0
34	SR	0	8967	1/1	0.89	0.11	133,133,133,133	0
35	NA	0	8530	1/1	0.89	0.27	42,42,42,42	0
34	SR	0	8909	1/1	0.89	0.14	94,94,94,94	0
35	NA	0	8521	1/1	0.89	0.29	61,61,61,61	0
35	NA	R	8532	1/1	0.89	0.18	53,53,53,53	0
35	NA	0	8520	1/1	0.89	0.18	54,54,54,54	0
32	MG	0	8039	1/1	0.89	0.33	69,69,69,69	0
35	NA	0	8519	1/1	0.89	0.42	39,39,39,39	0
35	NA	0	8514	1/1	0.90	0.28	42,42,42,42	0
34	SR	0	8992	1/1	0.90	0.24	123,123,123,123	0
36	CD	O	8705	1/1	0.90	0.06	124,124,124,124	0
35	NA	0	8545	1/1	0.90	0.30	37,37,37,37	0
32	MG	0	8037	1/1	0.90	0.22	83,83,83,83	0
32	MG	0	8083	1/1	0.90	0.15	56,56,56,56	0
34	SR	0	9008	1/1	0.90	0.14	90,90,90,90	0
32	MG	T	8057	1/1	0.90	0.15	57,57,57,57	0
32	MG	0	8073	1/1	0.90	0.14	76,76,76,76	0
34	SR	0	8911	1/1	0.90	0.08	78,78,78,78	0
34	SR	0	8965	1/1	0.91	0.12	120,120,120,120	0
32	MG	0	8059	1/1	0.91	0.09	36,36,36,36	0
32	MG	0	8077	1/1	0.91	0.16	32,32,32,32	0
35	NA	0	8559	1/1	0.91	0.23	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8008	1/1	0.91	0.19	25,25,25,25	0
35	NA	B	8552	1/1	0.92	0.34	56,56,56,56	0
32	MG	0	8076	1/1	0.92	0.22	35,35,35,35	0
35	NA	0	8563	1/1	0.92	0.37	60,60,60,60	0
32	MG	0	8020	1/1	0.92	0.20	54,54,54,54	0
33	CL	0	8817	1/1	0.92	0.12	53,53,53,53	0
34	SR	0	8923	1/1	0.92	0.19	101,101,101,101	0
35	NA	C	8503	1/1	0.92	0.28	37,37,37,37	0
35	NA	0	8564	1/1	0.92	0.19	65,65,65,65	0
34	SR	A	8929	1/1	0.92	0.27	131,131,131,131	0
34	SR	H	8972	1/1	0.92	0.20	130,130,130,130	0
35	NA	0	8529	1/1	0.93	0.09	37,37,37,37	0
32	MG	0	8017	1/1	0.93	0.19	56,56,56,56	0
32	MG	0	8056	1/1	0.93	0.20	42,42,42,42	0
32	MG	0	8010	1/1	0.93	0.17	26,26,26,26	0
37	K	0	8402	1/1	0.93	0.17	64,64,64,64	0
34	SR	0	8921	1/1	0.93	0.12	92,92,92,92	0
32	MG	0	8047	1/1	0.93	0.44	49,49,49,49	0
36	CD	Z	8703	1/1	0.93	0.06	81,81,81,81	0
34	SR	0	8985	1/1	0.93	0.12	110,110,110,110	0
32	MG	0	8068	1/1	0.93	0.09	47,47,47,47	0
34	SR	0	8943	1/1	0.93	0.08	95,95,95,95	0
32	MG	0	8078	1/1	0.93	0.37	51,51,51,51	0
34	SR	0	8936	1/1	0.93	0.13	89,89,89,89	0
33	CL	0	8805	1/1	0.93	0.15	59,59,59,59	0
32	MG	0	8049	1/1	0.93	0.37	55,55,55,55	0
32	MG	0	8036	1/1	0.93	0.12	49,49,49,49	0
32	MG	0	8033	1/1	0.93	0.11	45,45,45,45	0
32	MG	0	8034	1/1	0.93	0.11	32,32,32,32	0
32	MG	0	8091	1/1	0.94	0.07	42,42,42,42	0
35	NA	0	8516	1/1	0.94	0.23	30,30,30,30	0
32	MG	0	8007	1/1	0.94	0.30	26,26,26,26	0
35	NA	0	8570	1/1	0.94	0.17	49,49,49,49	0
35	NA	0	8547	1/1	0.94	0.42	54,54,54,54	0
32	MG	0	8053	1/1	0.94	0.16	61,61,61,61	0
32	MG	0	8070	1/1	0.94	0.17	45,45,45,45	0
32	MG	0	8012	1/1	0.94	0.23	21,21,21,21	0
34	SR	0	8962	1/1	0.94	0.26	167,167,167,167	0
32	MG	0	8029	1/1	0.94	0.18	39,39,39,39	0
34	SR	0	8918	1/1	0.94	0.14	79,79,79,79	0
33	CL	A	8809	1/1	0.94	0.15	57,57,57,57	0
32	MG	0	8064	1/1	0.94	0.27	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8569	1/1	0.94	0.26	53,53,53,53	0
35	NA	0	8517	1/1	0.94	0.32	30,30,30,30	0
34	SR	F	9005	1/1	0.94	0.06	136,136,136,136	0
34	SR	3	8999	1/1	0.94	0.08	95,95,95,95	0
32	MG	0	8061	1/1	0.94	0.39	37,37,37,37	0
35	NA	0	8550	1/1	0.94	0.25	54,54,54,54	0
33	CL	O	8808	1/1	0.94	0.17	61,61,61,61	0
35	NA	0	8541	1/1	0.94	0.34	53,53,53,53	0
32	MG	0	8018	1/1	0.95	0.24	38,38,38,38	0
33	CL	0	8822	1/1	0.95	0.25	68,68,68,68	0
32	MG	0	8032	1/1	0.95	0.09	40,40,40,40	0
32	MG	0	8045	1/1	0.95	0.17	32,32,32,32	0
33	CL	L	8810	1/1	0.95	0.09	49,49,49,49	0
33	CL	Y	8820	1/1	0.95	0.11	38,38,38,38	0
34	SR	0	8946	1/1	0.95	0.16	108,108,108,108	0
38	ANM	0	2924	19/19	0.95	0.22	31,37,40,40	0
32	MG	9	8074	1/1	0.95	0.13	67,67,67,67	0
35	NA	0	8515	1/1	0.95	0.23	33,33,33,33	0
34	SR	0	8954	1/1	0.95	0.08	105,105,105,105	0
32	MG	0	8035	1/1	0.95	0.10	44,44,44,44	0
34	SR	0	8927	1/1	0.95	0.15	167,167,167,167	0
32	MG	0	8084	1/1	0.95	0.18	31,31,31,31	0
32	MG	0	8093	1/1	0.95	0.11	29,29,29,29	0
32	MG	0	8041	1/1	0.95	0.33	24,24,24,24	0
35	NA	0	8507	1/1	0.95	0.30	45,45,45,45	0
35	NA	0	8535	1/1	0.95	0.25	52,52,52,52	0
33	CL	J	8821	1/1	0.95	0.15	56,56,56,56	0
35	NA	0	8537	1/1	0.95	0.12	34,34,34,34	0
32	MG	K	8054	1/1	0.95	0.16	39,39,39,39	0
34	SR	0	8931	1/1	0.95	0.11	108,108,108,108	0
32	MG	0	8067	1/1	0.95	0.28	34,34,34,34	0
32	MG	0	8048	1/1	0.95	0.28	28,28,28,28	0
33	CL	J	8801	1/1	0.95	0.13	62,62,62,62	0
35	NA	0	8528	1/1	0.95	0.20	45,45,45,45	0
32	MG	0	8023	1/1	0.96	0.18	22,22,22,22	0
32	MG	0	8014	1/1	0.96	0.22	30,30,30,30	0
33	CL	0	8814	1/1	0.96	0.17	47,47,47,47	0
34	SR	1	8913	1/1	0.96	0.09	85,85,85,85	0
33	CL	0	8811	1/1	0.96	0.11	53,53,53,53	0
32	MG	0	8001	1/1	0.96	0.20	25,25,25,25	0
35	NA	0	8566	1/1	0.96	0.29	37,37,37,37	0
35	NA	0	8527	1/1	0.96	0.26	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8090	1/1	0.96	0.13	54,54,54,54	0
34	SR	3	8932	1/1	0.96	0.13	73,73,73,73	0
33	CL	N	8807	1/1	0.96	0.14	61,61,61,61	0
34	SR	0	8902	1/1	0.96	0.15	69,69,69,69	0
35	NA	0	8534	1/1	0.96	0.28	32,32,32,32	0
33	CL	0	8816	1/1	0.96	0.19	60,60,60,60	0
32	MG	0	8011	1/1	0.96	0.29	23,23,23,23	0
32	MG	0	8019	1/1	0.96	0.30	24,24,24,24	0
33	CL	0	8815	1/1	0.96	0.11	57,57,57,57	0
35	NA	0	8526	1/1	0.96	0.09	32,32,32,32	0
34	SR	0	8937	1/1	0.96	0.21	100,100,100,100	0
35	NA	0	8524	1/1	0.96	0.26	45,45,45,45	0
32	MG	0	8046	1/1	0.96	0.16	28,28,28,28	0
32	MG	0	8087	1/1	0.96	0.20	42,42,42,42	0
32	MG	0	8022	1/1	0.96	0.21	29,29,29,29	0
34	SR	0	8901	1/1	0.96	0.16	58,58,58,58	0
32	MG	0	8058	1/1	0.96	0.12	23,23,23,23	0
35	NA	0	8558	1/1	0.96	0.26	44,44,44,44	0
32	MG	0	8060	1/1	0.96	0.10	42,42,42,42	0
35	NA	0	8536	1/1	0.96	0.12	50,50,50,50	0
34	SR	0	8935	1/1	0.97	0.11	79,79,79,79	0
32	MG	0	8004	1/1	0.97	0.24	25,25,25,25	0
32	MG	Y	8086	1/1	0.97	0.11	39,39,39,39	0
32	MG	0	8065	1/1	0.97	0.13	33,33,33,33	0
33	CL	M	8818	1/1	0.97	0.15	37,37,37,37	0
35	NA	0	8513	1/1	0.97	0.27	44,44,44,44	0
33	CL	0	8813	1/1	0.97	0.07	48,48,48,48	0
33	CL	J	8802	1/1	0.97	0.15	60,60,60,60	0
32	MG	0	8003	1/1	0.97	0.19	30,30,30,30	0
35	NA	0	8551	1/1	0.97	0.23	46,46,46,46	0
32	MG	0	8027	1/1	0.97	0.14	34,34,34,34	0
32	MG	0	8013	1/1	0.97	0.08	26,26,26,26	0
34	SR	0	8940	1/1	0.97	0.10	85,85,85,85	0
32	MG	0	8025	1/1	0.97	0.13	24,24,24,24	0
32	MG	0	8009	1/1	0.97	0.26	21,21,21,21	0
34	SR	1	8952	1/1	0.97	0.12	79,79,79,79	0
34	SR	R	8912	1/1	0.97	0.16	84,84,84,84	0
32	MG	0	8082	1/1	0.97	0.33	48,48,48,48	0
33	CL	0	8803	1/1	0.98	0.07	46,46,46,46	0
32	MG	0	8021	1/1	0.98	0.13	32,32,32,32	0
34	SR	0	8903	1/1	0.98	0.20	53,53,53,53	0
32	MG	0	8002	1/1	0.98	0.17	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8015	1/1	0.98	0.19	27,27,27,27	0
32	MG	0	8005	1/1	0.98	0.30	26,26,26,26	0
34	SR	0	8925	1/1	0.98	0.12	90,90,90,90	0
33	CL	3	8804	1/1	0.98	0.05	54,54,54,54	0
33	CL	0	8812	1/1	0.98	0.11	48,48,48,48	0
32	MG	0	8026	1/1	0.98	0.14	31,31,31,31	0
32	MG	0	8052	1/1	0.98	0.11	40,40,40,40	0
36	CD	U	8701	1/1	0.99	0.12	58,58,58,58	0
34	SR	0	8906	1/1	0.99	0.21	56,56,56,56	0
34	SR	0	8904	1/1	0.99	0.20	52,52,52,52	0
33	CL	B	8819	1/1	0.99	0.12	46,46,46,46	0
32	MG	0	8028	1/1	0.99	0.26	22,22,22,22	0
33	CL	R	8806	1/1	0.99	0.17	43,43,43,43	0
36	CD	1	8702	1/1	0.99	0.08	57,57,57,57	0
34	SR	0	8907	1/1	0.99	0.32	76,76,76,76	0
36	CD	3	8704	1/1	0.99	0.09	66,66,66,66	0
34	SR	0	8905	1/1	0.99	0.26	57,57,57,57	0
34	SR	0	8915	1/1	0.99	0.06	117,117,117,117	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.