



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:55 AM GMT

PDB ID : 3G4S  
Title : Co-crystal structure of Tiamulin bound to the large ribosomal subunit  
Authors : Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2009-02-04  
Resolution : 3.20 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  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

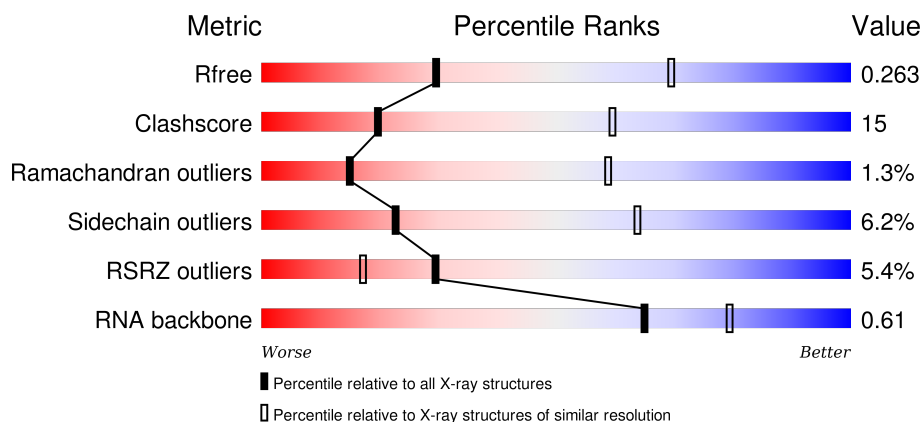
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)
RNA backbone	2183	1079 (3.70-2.70)

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	0	2923	<div> <div></div> <div>34%53%7%6%</div> </div>
2	A	237	<div> <div>4%</div> <div>83%16%</div> </div>
3	B	337	<div> <div></div> <div>81%17%.</div> </div>
4	C	246	<div> <div>%</div> <div>82%15%.</div> </div>


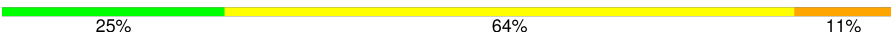
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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z	73	
28	1	56	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	0	8009	-	-	-	X
32	MG	0	8034	-	-	-	X
32	MG	0	8047	-	-	-	X
32	MG	0	8062	-	-	-	X
32	MG	0	8067	-	-	-	X
32	MG	0	8070	-	-	-	X
32	MG	0	8073	-	-	-	X
32	MG	0	8090	-	-	-	X
32	MG	C	8012	-	-	-	X
34	NA	0	8502	-	-	-	X
34	NA	0	8512	-	-	-	X
34	NA	0	8524	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8530	-	-	-	X
34	NA	0	8535	-	-	-	X
34	NA	0	8542	-	-	-	X
34	NA	0	8546	-	-	-	X
34	NA	0	8547	-	-	-	X
34	NA	0	8555	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8558	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8562	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8565	-	-	-	X
34	NA	0	8568	-	-	-	X
34	NA	0	8571	-	-	-	X
34	NA	9	8572	-	-	-	X
34	NA	R	8575	-	-	-	X
35	CL	B	8819	-	-	-	X
35	CL	O	8808	-	-	-	X
36	SR	0	8943	-	-	-	X
36	SR	B	8987	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
36	SR	L	8969	-	-	-	X
37	MUL	0	9101	-	-	-	X
38	CD	3	8704	-	-	-	X

## 2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99167 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 RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	0	2754	Total	C	N	O	P	0	0	0
			59021	26349	10873	19054	2745			

- Molecule 2 is a protein called 50S ribosomal protein L2P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	237	Total	C	N	O	S	0	0	0
			1754	1072	352	325	5			

- Molecule 3 is a protein called 50S ribosomal protein L3P.

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

- Molecule 4 is a protein called 50S ribosomal protein L4P.

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

- Molecule 5 is a protein called 50S ribosomal protein L5P.

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

- Molecule 6 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 8 is a protein called 50S ribosomal protein L10.

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

- Molecule 9 is a protein called 50S ribosomal protein L10e.

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

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	70	Total	C	N	O	S	0	0	0
			520	323	81	115	1			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1137	683	229	225				

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	150	Total	C	N	O	S	0	0	0
			1150	713	209	224	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	81	Total	C	N	O	S	0	0	0
			642	389	111	139	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.



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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	53	Total	C	N	O	S			
			411	244	75	87	5	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S			
			500	304	94	101	1	0	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	82	Total	C	N	O	S			
			655	402	129	123	1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O			
			1131	686	228	217	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S			
			574	343	113	113	5	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	84	Total	Mg	0	0
			84	84		
32	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	C	1	Total	Mg	0	0
			1	1		
32	A	2	Total	Mg	0	0
			2	2		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	0	1	Total K 1 1	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0

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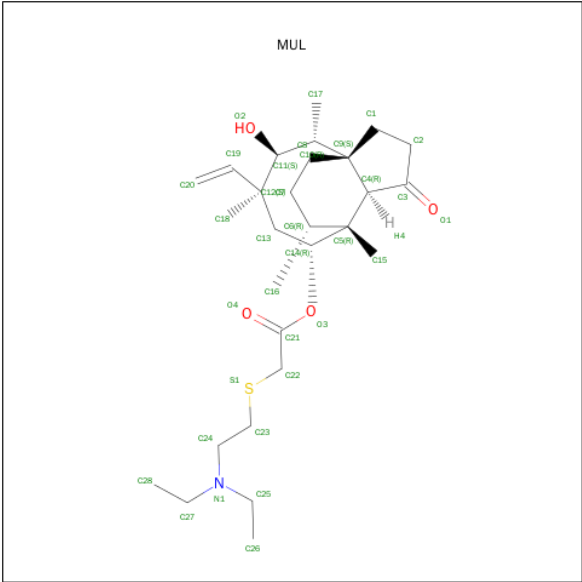
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	L	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	91	Total 91	Sr 91	0	0
36	J	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	H	1	Total 1	Sr 1	0	0
36	B	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	A	3	Total 3	Sr 3	0	0
36	R	1	Total 1	Sr 1	0	0
36	9	2	Total 2	Sr 2	0	0
36	L	1	Total 1	Sr 1	0	0
36	S	1	Total 1	Sr 1	0	0
36	F	1	Total 1	Sr 1	0	0

- Molecule 37 is TIAMULIN (three-letter code: MUL) (formula: C<sub>28</sub>H<sub>47</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	0	1	Total	C	N	O	S	0	0
			34	28	1	4	1		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	O	1	Total	Cd	0	0
			1	1		
38	Z	1	Total	Cd	0	0
			1	1		
38	1	1	Total	Cd	0	0
			1	1		
38	3	1	Total	Cd	0	0
			1	1		
38	U	1	Total	Cd	0	0
			1	1		

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5940	Total	O	0	0
			5940	5940		
39	A	125	Total	O	0	0
			125	125		
39	B	140	Total	O	0	0
			140	140		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	158	Total 158	O 158	0	0
39	D	45	Total 45	O 45	0	0
39	E	42	Total 42	O 42	0	0
39	F	26	Total 26	O 26	0	0
39	G	18	Total 18	O 18	0	0
39	H	70	Total 70	O 70	0	0
39	I	4	Total 4	O 4	0	0
39	J	47	Total 47	O 47	0	0
39	K	58	Total 58	O 58	0	0
39	L	94	Total 94	O 94	0	0
39	M	132	Total 132	O 132	0	0
39	N	55	Total 55	O 55	0	0
39	O	43	Total 43	O 43	0	0
39	P	59	Total 59	O 59	0	0
39	Q	52	Total 52	O 52	0	0
39	R	80	Total 80	O 80	0	0
39	S	30	Total 30	O 30	0	0
39	T	30	Total 30	O 30	0	0
39	U	30	Total 30	O 30	0	0
39	V	11	Total 11	O 11	0	0
39	W	59	Total 59	O 59	0	0

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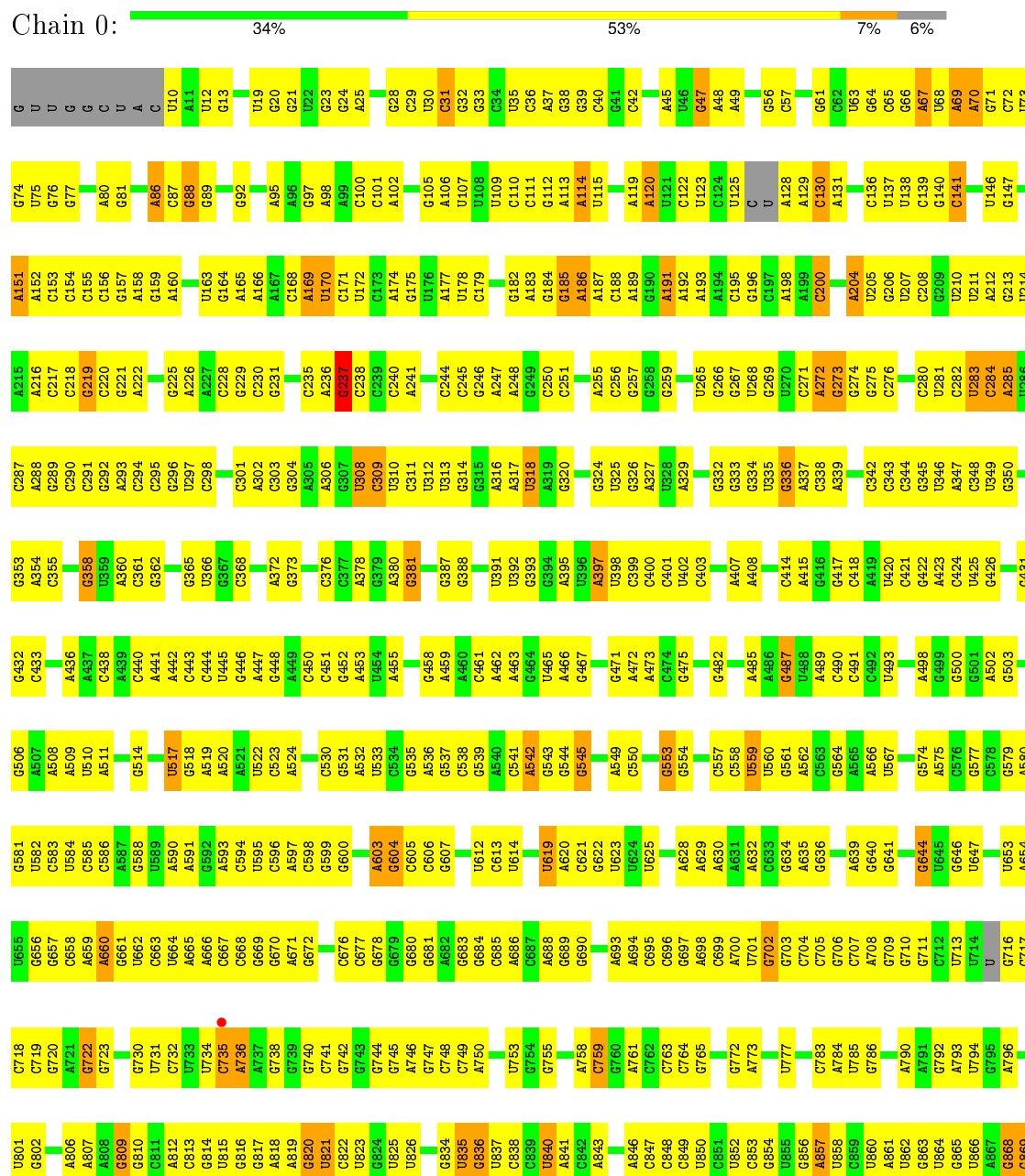
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	22	Total 22	O 22	0	0
39	Y	105	Total 105	O 105	0	0
39	Z	30	Total 30	O 30	0	0
39	1	55	Total 55	O 55	0	0
39	2	48	Total 48	O 48	0	0
39	3	62	Total 62	O 62	0	0
39	9	152	Total 152	O 152	0	0

### 3 Residue-property plots

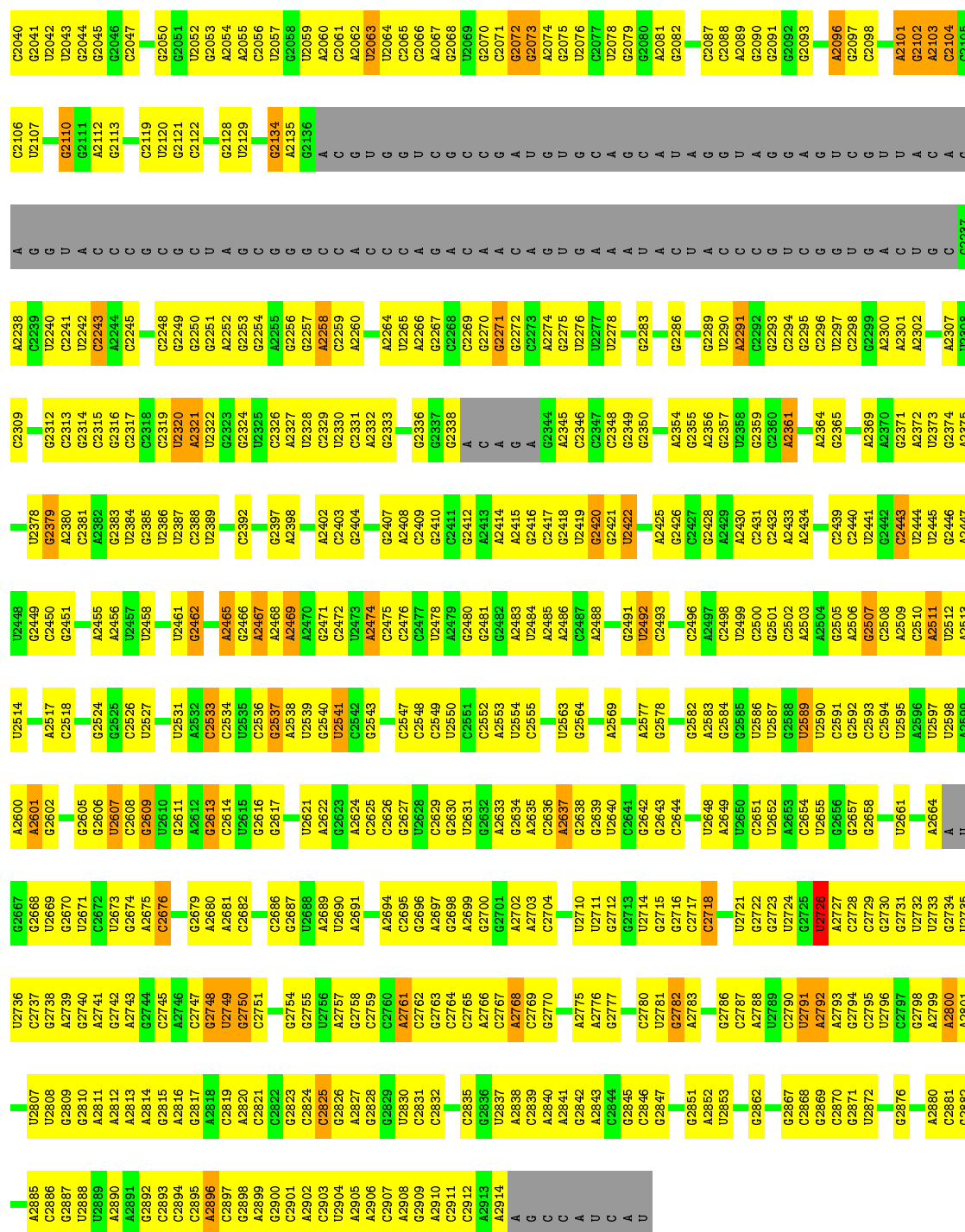
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $\text{RSRZ} > 2$ ). 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: 23S ribosomal RNA

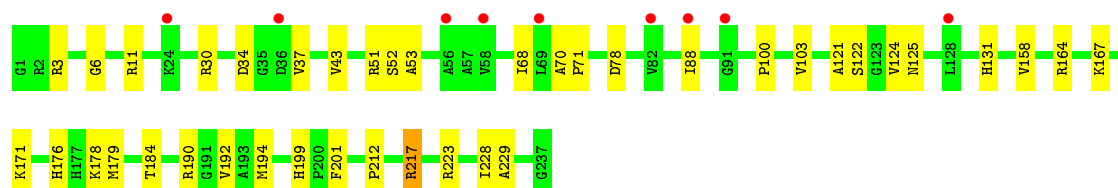





C1965	C1889	C1818	G1752	C1680	G1608	U1524	C1450	G1376	C1305	G1159	C1085	A1006	G943	6870
U1966	U1890	G1819	C1753	G1681	C1609	G1525	C1451	C1377	U1306	G1160	A1086	A1007	G944	6871
A1969	C1892	G1820	A1754	A1682	G1610	A1526	G1452	G1378	A1307	A1161	A1087	C1008	U945	6872
G1970	C1893	A1821	G1756	G1683	G1611	A1527	G1453	A1379	A1308	G1162	A1088	U1009	C946	
G1971	C1894	G1822	A1757	A1684	C1612	A1528	G1454	U1383	U1309	G1163	U1086	G1010	U947	6875
U1972	C1894	G1823	U1758	G1685	C1613	U1531	C1455	C1384	U1310	U1164	U1097	G1011	A876	
A1973	G1902	U1825	A1759	C1686	G1614	U1531	C1456	U1384	G1311	G1165	A1097	A1012	6877	
G1974	U1903	G1826	G1760	G1688	A1616	G1535	A1458	G1387	G1312	A1166	A1098	A1013	6878	
C1975	G1904	G1827	U1761	A1689	G1617	C1536	A1459	U1388	A1313	G1167	G1099	A1014	6879	
U1976	U1905	G1828	C1762	U1698	C1618	U1536	G1460	G1389	G1314	C1168	U1100	C1015	6880	
U1977	C1894	G1834	G1768	U1698	A1624	C1549	A1465	C1396	G1316	U1170	G1102	U1016	6882	
A1978	A1909	A1829	C1763	C1692	G1619	U1544	A1461	A1390	G1323	A1171	C1103	G1023	6883	
G1979	A1910	U1830	C1764		C1620	C1545	C1462	A1391	G1324	A1172	G1104	G1024	6885	
U1980	C1916	G1832	G1766	G1695	G1621	G1546	U1463	A1392	G1325	G1173	C1105	G1025	6886	
A1981	G1917	U1833	A1767	G1697	C1622	U1547	A1464	U1389	G1326	A1174	G1106	U1026	6887	
C1988	U1918	U1834	C1768	U1698	A1624	C1549	A1465	C1396	G1326	A1175	U1109	U1029	6888	
G1989	G1919	U1835	U1770	U1701	U1625	C1549	U1473	C1397	G1327	G1176	U1110	U1030	6889	
U1992	C1920	U1838	U1771	U1702	A1626	C1554	C1474	A1399	A1328		U1111	G1031	6890	
C1993	A1921	A1839	G1772	G1703	G1627	G1555	G1475	C1400	G1331	C1179	U1112	G1032	6893	
A1994	G1922	A1840	G1773	G1704	A1630	G1557	U1476	A1401	U1332	A1181	G1113	A1041	6895	
G1995	G1923	C1841	G1774	C1705	A1631	C1558	U1477	A1407	U1333	C1182	G1114		6896	
U1996	A1924	A1775	G1775	G1706	A1632	A1559	U1478	U1408	C1334	C1183	U1115		6897	
C1999	G1925	A1776	A1776	G1707	C1633	U	C1483	G1409	C1335	C1184	U1116	G1044	6898	
G2000	G1926	U1844	G1777	U1698	G1634	U1561	G1484	U1412	G1338	U1185	A1117	G1045	6899	
C2001	A1927	U1846	A1778	U1698	U1635	C1566	A1485	U1415	U1339	C1186	G1118	U1046		
G2002	C1928	A1847	A1779	G1714	G1636	G1567	A1486	G1416	G1342	A1187	G1119	U1047		
U2003	G1930	G1849	C1715	C1714	U1639	C1570	U1488	G1416	C1343	A1189	G1120	G1051		
U2004	A1931	A1850	A1716	A1716	C1640	G1571	A1482	U1419	G1344	G1190	G1121	G1052		
C2006	G1933	A1852	G1785	A1642	A1641	A1572	A1493	C1420	U1347	A1191	A1124	G1053		
A2007	C1934	C1854	C1787	C1643	C1643	A1573	A1496	U1422	U1348	A1192	U1125	G1054		
U2008	G1935	G1854	U1724	U1645	G1646	C1575	G1497	C1423	C1273	A1193	C1126	G1055		
G2009	U1937	G1855	C1725	G1646	G1646	C1575	G1498	A1424	A1275	A1194	C1127	U1056		
A2010	U1938	A1857	G1725	G1647	G1647	C1585	G1498	U1424	G1350	G1195	U1128	A1057		
U2011	C1939	A1858	G1728	G1648	G1648	G1586	U1501	A1427	G1351	C1196	U1129	G1058		
U2012	G1942	C1861	A1729	G1649	G1649	U1587	A1502	C1428	A1352	A1200	G1131	G1059		
C2013	C1943	C1862	G1730	A1656	A1656	G1587	A1503	U1429	C1353	C1201	A1132	C1060		
U2016	G1947	A1866	A1732	A1657	A1657	A1590	U1505	G1430	A1355	A1202	G1134	U1066		
A2018	G1950	G1867	C1734	A1661	A1661	A1591	U1506	G1433	A1356	G1203	G1135	A1067		
A2022	U	G1873	C1735	C1662	C1662	G1592	C1507	A1434	G1283	U1205	U1136	G1068		
C2026	A	G1877	G1739	G1665	G1665	C1593	C1508	U1435	A1287	U1206	G1137	C1069		
U2027	C	G1878	U1740	G1666	G1666	C1594	U1509	C1436	U1288	C1207	G1138	A1070		
U2028	U	U1879	U1741	A1667	A1667	G1595	G1510	A1437	C1289	C1209	U1139	G1071		
G2032	A	A1880	G1743	A1668	A1668	U1597	G1511	U1438	G1361	G1210	C1140	A1072		
U2033	U	A1881	G1744	U1673	U1673	A1597	G1512	C1439	U1362	G1211	U1141	A1073		
U2034	G	G1882	G1745	C1674	C1674	G1600	U1516	U1441	G1365	C1212	U1149	G1075		
C2035	A	U1883	A1746	C1675	C1675	G1601	U1516	A1442	C1366	G1213	A1150	G1076		
C2036	C	G1884	A1747	G1676	G1676	A1602	C1517	G1444	A1367	A1215	G1151	A1077		
C2037	C	A1885	U1748	G1677	G1677	G1604	U1518	U1446	U1368	G1216	A1152	C1079		
A2038	C	A1886	U1749	A1678	A1678	G1605	C1521	U1447	G1299	U1218	C1153	A1081		
A2039	U1964		U1817	C1679	C1679	A1607	G1523	U1449	G1300	U1219	G1156	U1001		
									C1303	C1157	C1083	G1002		
									A1375	G1221	G1158	A1005		

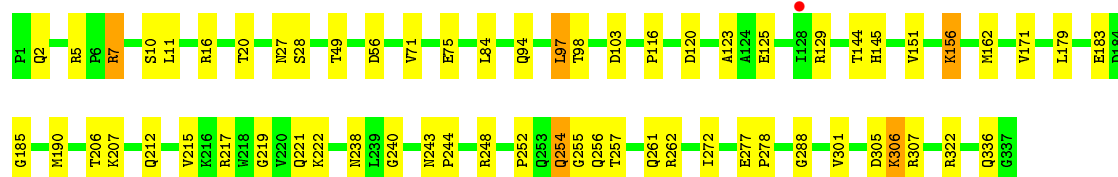


Chain A: 




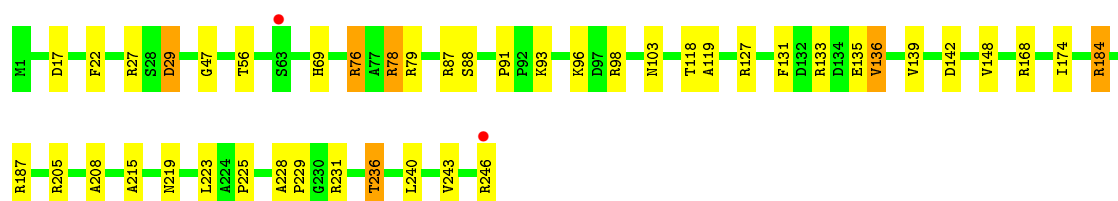
- Molecule 3: 50S ribosomal protein L3P

Chain B:  81% 17%



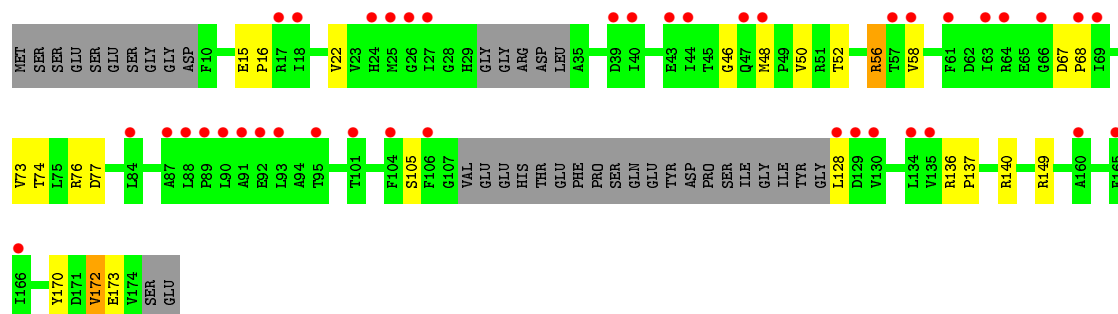
- Molecule 4: 50S ribosomal protein L4P

Chain C:  82% 15%




- Molecule 5: 50S ribosomal protein L5P

Chain D:  23% 66% 12% 21%




- Molecule 6: 50S ribosomal protein L6P

Chain E:  2% 83% 16%

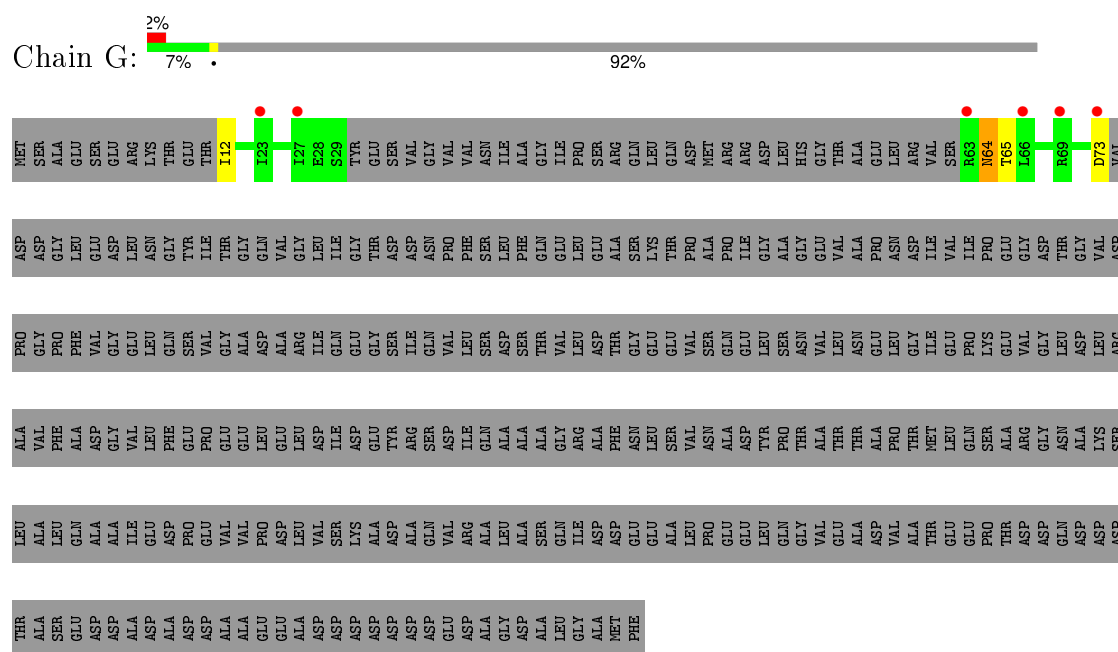


- Molecule 7: 50S ribosomal protein L7Ae

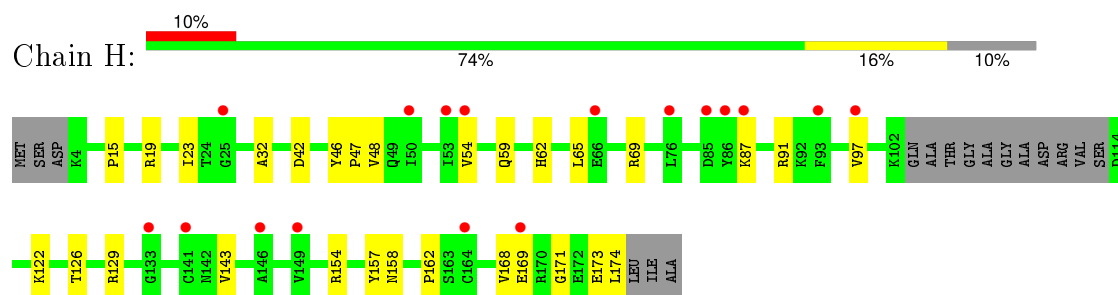
Chain F:  8% 85% 15%



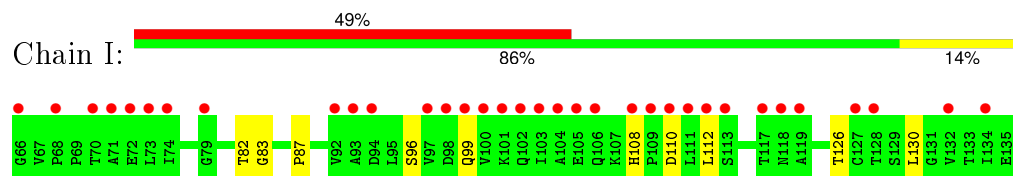
- Molecule 8: 50S ribosomal protein L10



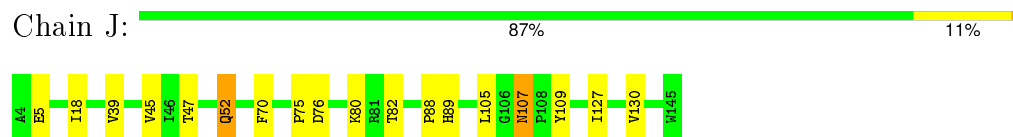
- Molecule 9: 50S ribosomal protein L10e



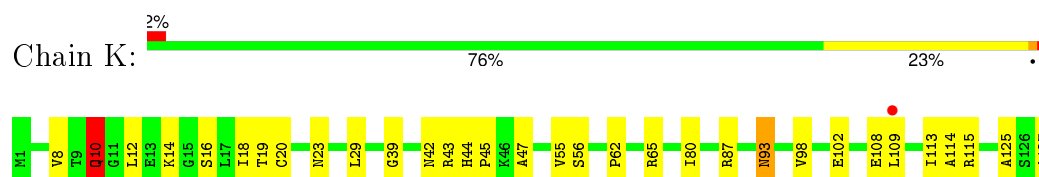
- Molecule 10: 50S ribosomal protein L11P



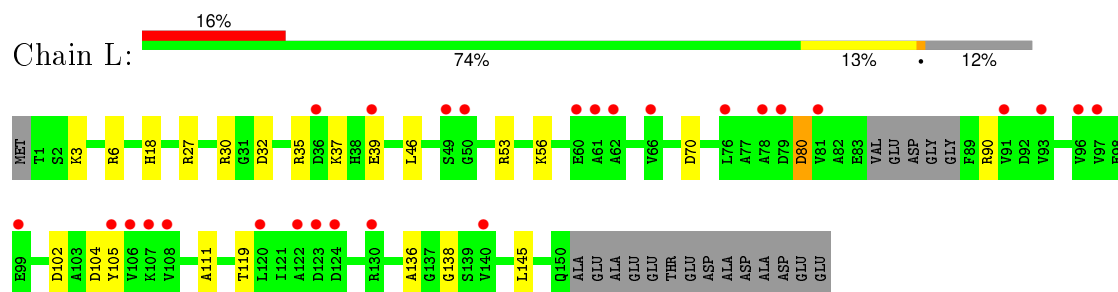
- Molecule 11: 50S ribosomal protein L13P



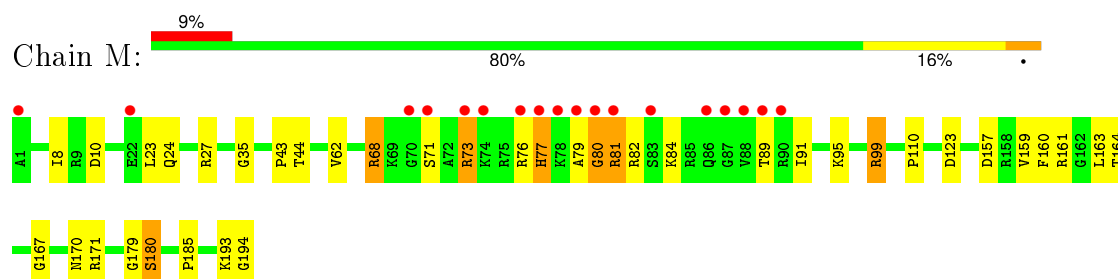
- Molecule 12: 50S ribosomal protein L14P



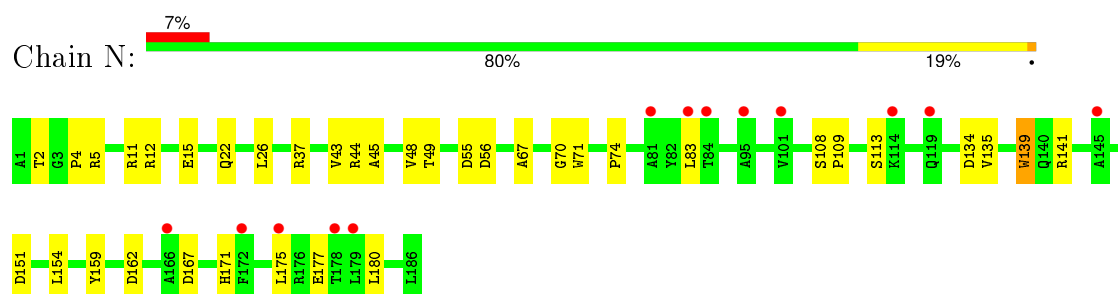
- Molecule 13: 50S ribosomal protein L15P



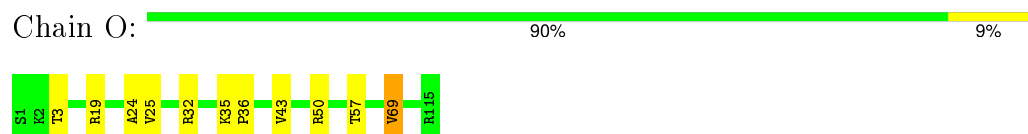
- Molecule 14: 50S ribosomal protein L15e



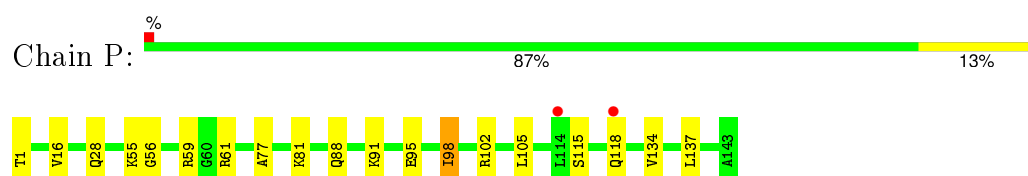
- Molecule 15: 50S ribosomal protein L18P



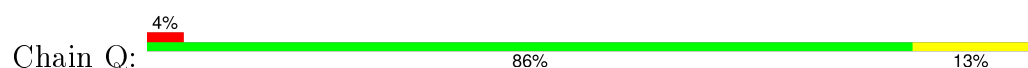
- Molecule 16: 50S ribosomal protein L18e



- Molecule 17: 50S ribosomal protein L19e

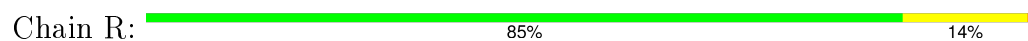


- Molecule 18: 50S ribosomal protein L21e

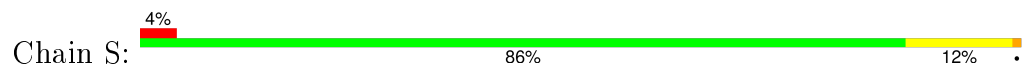




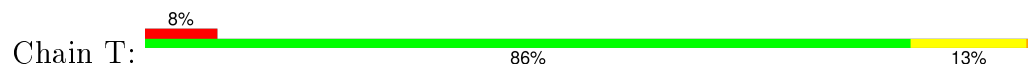
- Molecule 19: 50S ribosomal protein L22P



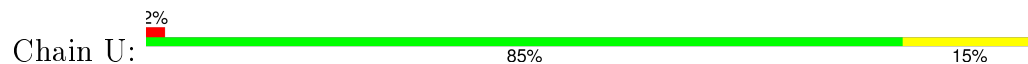
- Molecule 20: 50S ribosomal protein L23P



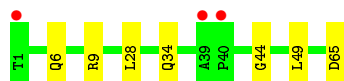
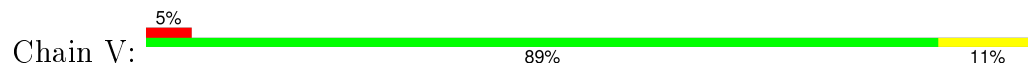
- Molecule 21: 50S ribosomal protein L24P



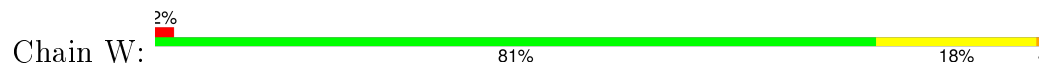
- Molecule 22: 50S ribosomal protein L24e



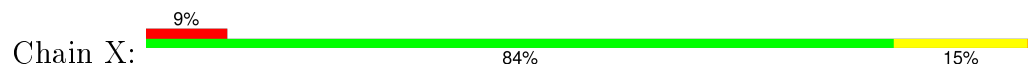
- Molecule 23: 50S ribosomal protein L29P

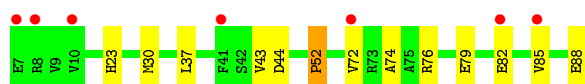


- Molecule 24: 50S ribosomal protein L30P

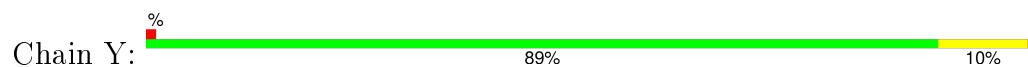


- Molecule 25: 50S ribosomal protein L31e

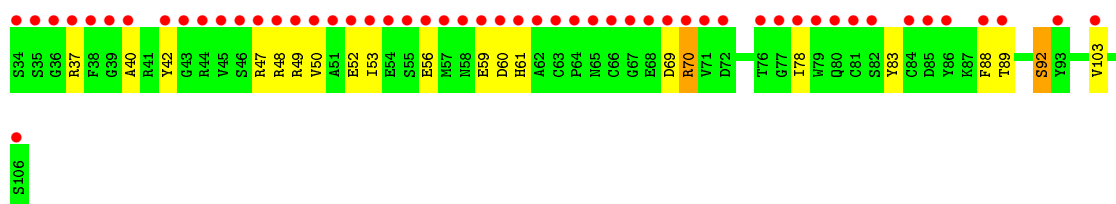




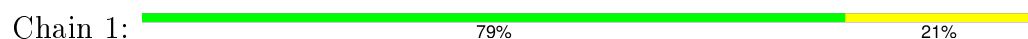
- Molecule 26: 50S ribosomal protein L32e



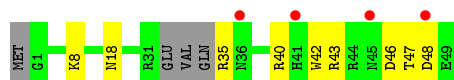
- Molecule 27: 50S ribosomal protein L37Ae



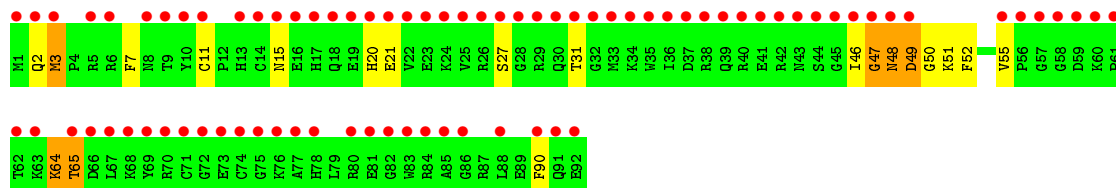
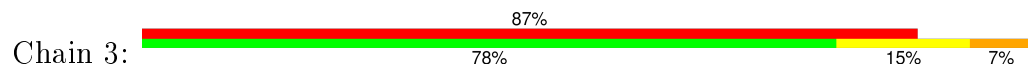
- Molecule 28: 50S ribosomal protein L37e



- Molecule 29: 50S ribosomal protein L39e

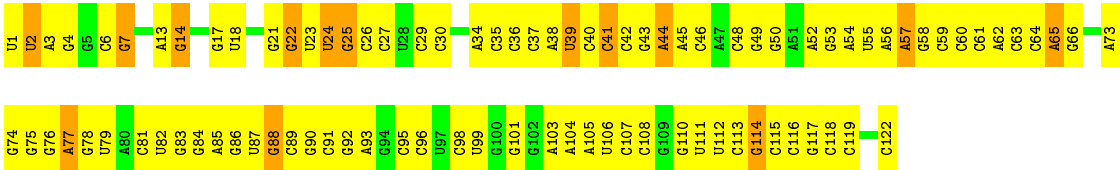


- Molecule 30: 50S ribosomal protein L44E



- 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, $\alpha$ , $\beta$ , $\gamma$	212.27Å 299.84Å 574.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.20 85.66 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.7 (49.84-3.20) 82.8 (85.66-2.41)	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)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.215 , 0.290 0.200 , 0.263	Depositor DCC
$R_{free}$ test set	2920 reflections (1.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 119.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 667047 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	99167	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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, MUL, 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	0	0.47	0/65958	0.69	6/102869 (0.0%)
2	A	0.53	0/1787	0.77	0/2408
3	B	0.54	0/2690	0.77	1/3652 (0.0%)
4	C	0.56	0/1885	0.80	0/2552
5	D	0.70	0/1111	0.74	1/1498 (0.1%)
6	E	0.62	0/1383	0.71	0/1880
7	F	0.56	0/901	0.73	1/1224 (0.1%)
8	G	0.55	0/241	0.66	0/324
9	H	0.61	0/1302	0.78	0/1743
10	I	0.63	0/527	0.66	0/716
11	J	0.63	0/1136	0.75	0/1530
12	K	0.51	0/1004	0.78	0/1351
13	L	0.56	0/1130	0.77	0/1509
14	M	0.55	0/1583	0.79	1/2116 (0.0%)
15	N	0.60	0/1474	0.79	0/1999
16	O	0.52	0/874	0.77	0/1181
17	P	0.56	0/1148	0.69	0/1528
18	Q	0.53	0/749	0.74	0/1005
19	R	0.58	0/1173	0.74	0/1578
20	S	0.56	0/649	0.70	0/875
21	T	0.50	0/958	0.76	1/1289 (0.1%)
22	U	0.65	0/418	0.72	0/562
23	V	0.49	0/503	0.70	0/675
24	W	0.54	0/1219	0.78	0/1655
25	X	0.53	0/665	0.74	0/895
26	Y	0.55	0/1147	0.76	0/1536
27	Z	0.74	0/585	0.84	0/781
28	1	0.62	0/438	0.77	0/578
29	2	0.46	0/401	0.74	0/529
30	3	0.78	0/771	0.81	0/1024
31	9	0.38	0/2904	0.68	0/4526
All	All	0.50	0/98714	0.71	11/147588 (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
1	0	0	25
24	W	0	1
All	All	0	26

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	6.64	122.64	114.00
1	0	237	G	N9-C1'-C2'	-6.25	105.12	112.00
3	B	84	LEU	CA-CB-CG	5.84	128.74	115.30
1	0	871	G	C5'-C4'-O4'	-5.68	102.28	109.10
1	0	820	G	N9-C1'-C2'	5.65	121.34	114.00

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	436	A	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	49	A	Sidechain
1	0	493	U	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	0	59021	0	29812	1915	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	37	0
4	C	1860	0	1813	32	0
5	D	1094	0	1085	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1358	0	1266	12	0
7	F	890	0	843	7	0
8	G	240	0	231	1	0
9	H	1282	0	1292	12	0
10	I	520	0	500	6	0
11	J	1120	0	1098	16	0
12	K	994	0	1027	20	0
13	L	1118	0	1076	13	0
14	M	1559	0	1573	32	0
15	N	1445	0	1401	20	0
16	O	865	0	873	9	0
17	P	1137	0	1123	17	0
18	Q	735	0	729	9	0
19	R	1150	0	1122	15	0
20	S	642	0	605	6	0
21	T	950	0	924	13	0
22	U	411	0	368	3	0
23	V	500	0	511	3	0
24	W	1196	0	1137	25	0
25	X	655	0	653	6	0
26	Y	1131	0	1133	10	0
27	Z	574	0	535	15	0
28	1	431	0	426	8	0
29	2	396	0	413	6	0
30	3	755	0	732	16	0
31	9	2599	0	1325	113	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	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	1	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	91	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	34	0	47	17	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5940	0	0	278	0
39	1	55	0	0	0	0
39	2	48	0	0	1	0
39	3	62	0	0	1	0
39	9	152	0	0	12	0
39	A	125	0	0	3	0
39	B	140	0	0	2	0
39	C	158	0	0	3	0
39	D	45	0	0	1	0
39	E	42	0	0	0	0
39	F	26	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	G	18	0	0	0	0
39	H	70	0	0	1	0
39	I	4	0	0	0	0
39	J	47	0	0	1	0
39	K	58	0	0	0	0
39	L	94	0	0	4	0
39	M	132	0	0	1	0
39	N	55	0	0	1	0
39	O	43	0	0	1	0
39	P	59	0	0	0	0
39	Q	52	0	0	0	0
39	R	80	0	0	0	0
39	S	30	0	0	1	0
39	T	30	0	0	0	0
39	U	30	0	0	1	0
39	V	11	0	0	0	0
39	W	59	0	0	0	0
39	X	22	0	0	0	0
39	Y	105	0	0	1	0
39	Z	30	0	0	2	0
All	All	99167	0	59972	2229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 2229 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)
1:0:871:G:H8	1:0:871:G:H5'	1.00	1.13
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.13
1:0:2121:G:H4'	30:3:47:GLY:HA2	1.29	1.12
1:0:2717:C:H2'	1:0:2718:C:H5''	1.27	1.12
1:0:871:G:C8	1:0:871:G:H5'	1.88	1.08

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	
2	A	235/237 (99%)	210 (89%)	20 (8%)	5 (2%)	9	46
3	B	335/337 (99%)	305 (91%)	27 (8%)	3 (1%)	21	67
4	C	244/246 (99%)	223 (91%)	18 (7%)	3 (1%)	16	60
5	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	8	45
6	E	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	30	75
7	F	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	5	31
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	145 (93%)	10 (6%)	1 (1%)	30	75
10	I	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	13	55
11	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	14	57
12	K	130/132 (98%)	116 (89%)	13 (10%)	1 (1%)	24	69
13	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	26	72
14	M	192/194 (99%)	180 (94%)	7 (4%)	5 (3%)	7	40
15	N	184/186 (99%)	165 (90%)	15 (8%)	4 (2%)	8	45
16	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
17	P	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	26	72
18	Q	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	8	45
19	R	148/150 (99%)	141 (95%)	6 (4%)	1 (1%)	26	72
20	S	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
21	T	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
22	U	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
23	V	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	139 (91%)	13 (9%)	0	100	100
25	X	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	15	59
26	Y	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	26	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	6	37
28	1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	10	50
29	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
30	3	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	3	24
All	All	3705/4172 (89%)	3381 (91%)	277 (8%)	47 (1%)	15	59

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	52	SER
3	B	306	LYS
7	F	61	MET
11	J	5	GLU
14	M	80	GLY

### 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	
2	A	179/179 (100%)	169 (94%)	10 (6%)	26	68
3	B	282/282 (100%)	263 (93%)	19 (7%)	20	60
4	C	193/193 (100%)	179 (93%)	14 (7%)	17	57
5	D	117/148 (79%)	109 (93%)	8 (7%)	20	59
6	E	152/152 (100%)	139 (91%)	13 (9%)	13	46
7	F	93/93 (100%)	91 (98%)	2 (2%)	60	87
8	G	27/282 (10%)	23 (85%)	4 (15%)	4	18
9	H	134/145 (92%)	121 (90%)	13 (10%)	10	39
10	I	58/58 (100%)	56 (97%)	2 (3%)	44	80
11	J	118/118 (100%)	112 (95%)	6 (5%)	29	70
12	K	106/106 (100%)	99 (93%)	7 (7%)	21	61
13	L	113/127 (89%)	105 (93%)	8 (7%)	18	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	158/158 (100%)	146 (92%)	12 (8%)	16	55
15	N	149/149 (100%)	135 (91%)	14 (9%)	11	41
16	O	93/93 (100%)	88 (95%)	5 (5%)	27	68
17	P	113/113 (100%)	110 (97%)	3 (3%)	52	85
18	Q	79/79 (100%)	77 (98%)	2 (2%)	55	86
19	R	117/117 (100%)	111 (95%)	6 (5%)	29	70
20	S	71/71 (100%)	68 (96%)	3 (4%)	36	75
21	T	105/105 (100%)	99 (94%)	6 (6%)	25	67
22	U	44/44 (100%)	40 (91%)	4 (9%)	12	42
23	V	51/51 (100%)	47 (92%)	4 (8%)	16	53
24	W	130/130 (100%)	127 (98%)	3 (2%)	58	87
25	X	66/66 (100%)	60 (91%)	6 (9%)	12	42
26	Y	120/120 (100%)	114 (95%)	6 (5%)	30	71
27	Z	60/60 (100%)	57 (95%)	3 (5%)	30	71
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	42/46 (91%)	39 (93%)	3 (7%)	18	57
30	3	79/79 (100%)	73 (92%)	6 (8%)	16	55
All	All	3095/3410 (91%)	2903 (94%)	192 (6%)	23	64

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	45	VAL
14	M	23	LEU
26	Y	200	THR
11	J	107	ASN
12	K	115	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	170	ASN
17	P	88	GLN
29	2	16	ASN
15	N	40	ASN

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Mol	Chain	Res	Type
16	O	100	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	263 (9%)	19 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	280 (9%)	20 (0%)

5 of 280 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	47	G
1	0	67	A
1	0	69	A
1	0	70	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1667	A
1	0	1730	G
1	0	2718	C
1	0	1352	A
1	0	1377	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMU	0	2587	1	12,22,23	1.00	2 (16%)	19,31,34	3.18	2 (10%)
1	OMG	0	2588	1	17,26,27	1.07	2 (11%)	21,38,41	2.53	3 (14%)
1	UR3	0	2619	1	12,22,23	0.81	0	16,32,35	0.80	0
1	PSU	0	2621	1	13,21,22	1.62	2 (15%)	18,30,33	6.11	4 (22%)
1	1MA	0	628	1,34	14,25,26	1.02	1 (7%)	15,37,40	1.15	1 (6%)

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
1	OMU	0	2587	1	-	0/5/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/3/25/26	0/2/2/2
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	1,34	-	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)
1	0	2621	PSU	C5-C1'	-4.98	1.47	1.52
1	0	2587	OMU	C6-C5	-2.02	1.33	1.38
1	0	2588	OMG	C8-N7	-2.01	1.30	1.34
1	0	2587	OMU	C4-N3	2.23	1.37	1.33
1	0	2621	PSU	C4-N3	2.51	1.37	1.33

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-21.43	114.66	128.33
1	0	2588	OMG	C5-C6-N1	-8.68	111.72	123.59
1	0	628	1MA	C2-N3-C4	-3.68	110.70	116.40
1	0	2587	OMU	C5-C4-N3	-3.32	114.61	123.12
1	0	2588	OMG	N3-C2-N1	-2.37	123.83	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	2621	PSU	1	0
1	0	628	1MA	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 304 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	$\# Z  > 2$
37	MUL	0	9101	-	31,36,36	1.05	1 (3%)	28,55,55	1.38	5 (17%)

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
37	MUL	0	9101	-	-	0/16/79/79	0/1/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	MUL	C12-C19	-3.70	1.39	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C14-O3-C21	-3.39	110.79	118.03
37	0	9101	MUL	C1-C2-C3	-2.89	101.70	105.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C8-C7-C6	-2.45	109.12	112.34
37	0	9101	MUL	C23-S1-C22	-2.30	98.06	101.89
37	0	9101	MUL	O3-C21-C22	3.23	119.56	111.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	MUL	17	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	0	2749/2923 (94%)	-0.66	3 (0%) 95 95	29, 74, 140, 200	0
2	A	237/237 (100%)	0.06	9 (3%) 44 29	43, 97, 143, 167	0
3	B	337/337 (100%)	-0.38	1 (0%) 94 93	40, 86, 129, 148	0
4	C	246/246 (100%)	-0.37	2 (0%) 87 80	41, 72, 103, 112	0
5	D	140/177 (79%)	1.15	40 (28%) 1 0	118, 160, 184, 191	0
6	E	172/172 (100%)	-0.11	3 (1%) 73 60	76, 104, 134, 146	0
7	F	119/119 (100%)	0.33	9 (7%) 17 9	74, 113, 153, 166	0
8	G	29/348 (8%)	1.05	6 (20%) 1 1	118, 140, 146, 150	0
9	H	160/177 (90%)	0.58	17 (10%) 8 4	77, 104, 146, 162	0
10	I	70/70 (100%)	1.92	34 (48%) 0 0	173, 199, 200, 200	0
11	J	142/142 (100%)	-0.27	0 100 100	55, 80, 104, 123	0
12	K	132/132 (100%)	-0.18	2 (1%) 76 63	54, 79, 112, 118	0
13	L	145/165 (87%)	0.70	27 (18%) 2 1	62, 121, 171, 175	0
14	M	194/194 (100%)	0.12	18 (9%) 11 6	49, 70, 145, 160	0
15	N	186/186 (100%)	0.52	13 (6%) 19 11	82, 118, 178, 187	0
16	O	115/115 (100%)	-0.42	0 100 100	66, 87, 105, 111	0
17	P	143/143 (100%)	-0.20	2 (1%) 78 65	65, 88, 117, 124	0
18	Q	95/95 (100%)	0.05	4 (4%) 40 26	67, 87, 110, 117	0
19	R	150/150 (100%)	-0.46	0 100 100	47, 72, 103, 112	0
20	S	81/81 (100%)	-0.03	3 (3%) 45 30	68, 93, 114, 130	0
21	T	119/119 (100%)	0.26	10 (8%) 14 7	69, 92, 136, 155	0
22	U	53/53 (100%)	0.12	1 (1%) 70 55	94, 114, 136, 145	0
23	V	65/65 (100%)	0.26	3 (4%) 36 23	79, 113, 164, 170	0
24	W	154/154 (100%)	-0.20	3 (1%) 70 55	56, 78, 110, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	82/82 (100%)	0.14	7 (8%) 13 7	63, 92, 125, 135	0
26	Y	142/142 (100%)	-0.31	2 (1%) 78 65	45, 73, 109, 134	0
27	Z	73/73 (100%)	5.47	53 (72%) 0 0	149, 179, 191, 194	0
28	1	56/56 (100%)	-0.29	0 100 100	42, 53, 66, 76	0
29	2	46/50 (92%)	0.29	4 (8%) 13 7	48, 95, 145, 146	0
30	3	92/92 (100%)	6.26	80 (86%) 0 0	163, 185, 199, 200	0
31	9	122/122 (100%)	-0.83	0 100 100	66, 114, 143, 191	0
All	All	6646/7217 (92%)	-0.11	356 (5%) 29 17	29, 85, 168, 200	0

The worst 5 of 356 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	30.5
30	3	82	GLY	27.0
27	Z	35	SER	25.3
30	3	37	ASP	18.5
30	3	41	GLU	17.2

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	1MA	0	628	23/24	0.97	0.15	-	49,56,63,64	0
1	OMU	0	2587	21/22	0.98	0.12	-	60,63,64,64	0
1	UR3	0	2619	21/22	0.98	0.15	-	61,65,71,72	0
1	PSU	0	2621	20/21	0.97	0.20	-	59,63,65,66	0
1	OMG	0	2588	24/25	0.97	0.14	-	50,54,58,60	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
34	NA	0	8565	1/1	0.87	1.17	66.60	106,106,106,106	0
34	NA	0	8562	1/1	0.84	1.23	55.58	85,85,85,85	0
34	NA	0	8535	1/1	0.96	0.55	41.17	45,45,45,45	0
34	NA	0	8564	1/1	0.70	0.57	39.91	95,95,95,95	0
34	NA	0	8547	1/1	0.88	0.90	26.34	81,81,81,81	0
34	NA	0	8555	1/1	0.97	0.55	18.70	50,50,50,50	0
34	NA	0	8546	1/1	0.97	1.30	18.14	69,69,69,69	0
34	NA	0	8556	1/1	0.65	0.81	18.02	95,95,95,95	0
34	NA	0	8558	1/1	0.89	0.60	17.10	50,50,50,50	0
34	NA	0	8559	1/1	0.90	0.32	16.87	94,94,94,94	0
34	NA	0	8542	1/1	0.96	0.52	16.84	51,51,51,51	0
34	NA	R	8575	1/1	0.80	0.50	16.63	96,96,96,96	0
34	NA	0	8528	1/1	0.71	0.48	16.39	80,80,80,80	0
34	NA	9	8572	1/1	0.62	0.32	13.62	88,88,88,88	0
32	MG	0	8070	1/1	0.98	0.39	13.15	54,54,54,54	0
34	NA	0	8524	1/1	0.54	0.38	11.61	47,47,47,47	0
32	MG	0	8073	1/1	0.80	0.68	11.10	110,110,110,110	0
35	CL	B	8819	1/1	0.97	0.77	10.93	68,68,68,68	0
32	MG	0	8090	1/1	0.68	0.93	10.61	81,81,81,81	0
32	MG	0	8034	1/1	0.96	0.30	9.67	43,43,43,43	0
36	SR	L	8969	1/1	0.92	0.92	8.88	198,198,198,198	0
34	NA	0	8571	1/1	0.85	0.26	8.59	89,89,89,89	0
34	NA	0	8568	1/1	0.77	0.58	8.57	51,51,51,51	0
36	SR	B	8987	1/1	0.55	0.83	8.45	200,200,200,200	0
32	MG	0	8067	1/1	0.94	0.42	7.28	42,42,42,42	0
32	MG	0	8047	1/1	0.86	0.36	5.26	70,70,70,70	0
34	NA	0	8530	1/1	0.97	0.31	4.93	49,49,49,49	0
36	SR	0	8943	1/1	0.96	0.17	4.35	99,99,99,99	0
34	NA	0	8512	1/1	0.98	0.29	3.41	49,49,49,49	0
34	NA	0	8502	1/1	0.80	0.19	3.41	51,51,51,51	0
32	MG	0	8062	1/1	0.99	0.28	2.84	47,47,47,47	0
32	MG	C	8012	1/1	0.98	0.22	2.44	19,19,19,19	0
32	MG	0	8009	1/1	0.97	0.21	2.43	28,28,28,28	0
37	MUL	0	9101	34/34	0.94	0.26	2.16	85,87,104,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
35	CL	O	8808	1/1	0.98	0.30	2.10	98,98,98,98	0
34	NA	Q	8540	1/1	0.74	0.30	1.84	92,92,92,92	0
34	NA	0	8517	1/1	0.98	0.20	1.83	30,30,30,30	0
34	NA	0	8522	1/1	0.21	0.14	1.75	87,87,87,87	0
34	NA	0	8569	1/1	0.98	0.17	1.06	72,72,72,72	0
34	NA	0	8533	1/1	0.83	0.21	1.05	68,68,68,68	0
34	NA	0	8534	1/1	0.97	0.22	0.99	45,45,45,45	0
32	MG	0	8011	1/1	0.98	0.21	0.99	18,18,18,18	0
32	MG	0	8084	1/1	0.99	0.16	0.95	50,50,50,50	0
34	NA	0	8553	1/1	0.62	0.20	0.86	81,81,81,81	0
32	MG	0	8010	1/1	0.93	0.18	0.59	35,35,35,35	0
34	NA	0	8563	1/1	0.97	0.18	0.51	74,74,74,74	0
32	MG	A	8050	1/1	0.98	0.20	0.49	52,52,52,52	0
34	NA	0	8551	1/1	0.94	0.16	0.44	81,81,81,81	0
32	MG	0	8065	1/1	0.97	0.14	0.33	41,41,41,41	0
34	NA	0	8537	1/1	0.88	0.15	0.26	43,43,43,43	0
34	NA	0	8550	1/1	0.81	0.19	0.21	98,98,98,98	0
32	MG	0	8003	1/1	0.96	0.16	0.16	31,31,31,31	0
32	MG	0	8002	1/1	0.98	0.17	0.08	26,26,26,26	0
36	SR	A	8929	1/1	0.95	0.17	0.07	157,157,157,157	0
33	K	0	8402	1/1	0.95	0.21	0.00	67,67,67,67	0
32	MG	0	8007	1/1	0.97	0.17	-0.09	10,10,10,10	0
32	MG	A	8051	1/1	0.99	0.27	-0.09	90,90,90,90	0
34	NA	0	8523	1/1	0.93	0.14	-0.17	58,58,58,58	0
32	MG	0	8016	1/1	0.98	0.16	-0.20	38,38,38,38	0
34	NA	0	8560	1/1	0.82	0.28	-0.23	64,64,64,64	0
36	SR	H	8972	1/1	0.88	0.15	-0.26	157,157,157,157	0
32	MG	0	8045	1/1	1.00	0.12	-0.26	44,44,44,44	0
36	SR	0	8904	1/1	0.99	0.16	-0.27	64,64,64,64	0
36	SR	A	8930	1/1	0.69	0.24	-0.27	133,133,133,133	0
36	SR	1	8913	1/1	0.95	0.18	-0.31	97,97,97,97	0
32	MG	0	8043	1/1	0.89	0.13	-0.33	55,55,55,55	0
32	MG	0	8004	1/1	0.92	0.15	-0.45	32,32,32,32	0
32	MG	0	8044	1/1	0.77	0.11	-0.53	49,49,49,49	0
35	CL	J	8821	1/1	0.97	0.17	-0.63	70,70,70,70	0
34	NA	0	8515	1/1	0.90	0.21	-0.68	45,45,45,45	0
32	MG	0	8029	1/1	0.96	0.12	-0.77	54,54,54,54	0
32	MG	0	8021	1/1	0.95	0.10	-0.82	28,28,28,28	0
32	MG	0	8006	1/1	0.98	0.12	-0.83	62,62,62,62	0
34	NA	0	8519	1/1	0.99	0.18	-0.86	44,44,44,44	0
38	CD	1	8702	1/1	0.99	0.13	-0.94	68,68,68,68	0
32	MG	0	8014	1/1	0.96	0.12	-0.97	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	R	8532	1/1	0.84	0.11	-0.97	57,57,57,57	0
34	NA	J	8538	1/1	0.91	0.14	-1.06	45,45,45,45	0
32	MG	0	8058	1/1	0.93	0.07	-1.06	25,25,25,25	0
36	SR	3	8932	1/1	0.94	0.29	-1.15	149,149,149,149	0
35	CL	0	8812	1/1	0.90	0.09	-1.38	58,58,58,58	0
36	SR	0	8992	1/1	0.88	0.09	-1.64	149,149,149,149	0
34	NA	0	8521	1/1	0.96	0.11	-1.91	34,34,34,34	0
34	NA	0	8557	1/1	0.98	0.07	-1.98	71,71,71,71	0
36	SR	0	8910	1/1	0.89	0.12	-2.00	113,113,113,113	0
32	MG	0	8001	1/1	0.93	0.10	-2.08	28,28,28,28	0
34	NA	M	8539	1/1	0.89	0.12	-2.09	34,34,34,34	0
38	CD	U	8701	1/1	0.98	0.04	-2.17	104,104,104,104	0
32	MG	0	8041	1/1	0.97	0.14	-2.20	27,27,27,27	0
32	MG	T	8057	1/1	0.93	0.03	-2.30	67,67,67,67	0
36	SR	0	8935	1/1	0.98	0.05	-2.47	106,106,106,106	0
38	CD	3	8704	1/1	0.97	0.41	-2.51	176,176,176,176	0
32	MG	0	8025	1/1	0.97	0.07	-2.61	44,44,44,44	0
35	CL	M	8818	1/1	0.93	0.09	-3.14	73,73,73,73	0
32	MG	0	8052	1/1	0.97	0.04	-3.17	40,40,40,40	0
38	CD	Z	8703	1/1	0.97	0.14	-3.17	155,155,155,155	0
36	SR	0	8985	1/1	0.82	0.04	-3.30	173,173,173,173	0
36	SR	0	8902	1/1	0.98	0.13	-3.34	63,63,63,63	0
36	SR	0	8936	1/1	0.78	0.06	-3.47	109,109,109,109	0
36	SR	0	8975	1/1	0.87	0.04	-3.60	158,158,158,158	0
32	MG	Y	8086	1/1	0.96	0.04	-3.63	55,55,55,55	0
34	NA	0	8504	1/1	1.00	0.09	-3.85	22,22,22,22	0
36	SR	0	8949	1/1	0.96	0.10	-4.11	120,120,120,120	0
32	MG	0	8088	1/1	0.95	0.05	-4.74	39,39,39,39	0
32	MG	0	8013	1/1	0.98	0.04	-5.62	21,21,21,21	0
36	SR	0	8984	1/1	0.88	0.06	-6.86	139,139,139,139	0
32	MG	0	8075	1/1	0.97	0.06	-8.19	40,40,40,40	0
35	CL	0	8813	1/1	0.96	0.15	-	68,68,68,68	0
36	SR	0	8964	1/1	0.96	0.10	-	149,149,149,149	0
32	MG	0	8036	1/1	0.61	0.21	-	82,82,82,82	0
36	SR	0	8942	1/1	0.96	0.07	-	129,129,129,129	0
34	NA	0	8536	1/1	0.90	0.12	-	72,72,72,72	0
36	SR	0	8918	1/1	0.99	0.13	-	84,84,84,84	0
36	SR	0	8915	1/1	0.93	0.07	-	125,125,125,125	0
32	MG	0	8040	1/1	0.94	0.32	-	100,100,100,100	0
36	SR	0	8997	1/1	-0.12	5.66	-	200,200,200,200	0
36	SR	0	8959	1/1	0.87	0.15	-	194,194,194,194	0
35	CL	0	8814	1/1	0.96	0.41	-	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8028	1/1	0.99	0.13	-	14,14,14,14	0
34	NA	0	8549	1/1	0.64	0.17	-	83,83,83,83	0
36	SR	0	8957	1/1	0.74	0.23	-	200,200,200,200	0
36	SR	0	9001	1/1	0.90	0.09	-	189,189,189,189	0
34	NA	0	8513	1/1	0.98	0.23	-	63,63,63,63	0
38	CD	O	8705	1/1	0.96	0.03	-	115,115,115,115	0
32	MG	0	8030	1/1	1.00	0.48	-	60,60,60,60	0
36	SR	S	8961	1/1	0.99	0.10	-	127,127,127,127	0
32	MG	0	8023	1/1	0.98	0.16	-	21,21,21,21	0
34	NA	9	8543	1/1	0.77	0.17	-	57,57,57,57	0
32	MG	0	8027	1/1	0.97	0.05	-	30,30,30,30	0
32	MG	0	8082	1/1	0.94	0.40	-	86,86,86,86	0
34	NA	0	8507	1/1	0.98	0.27	-	39,39,39,39	0
32	MG	0	8068	1/1	0.64	0.08	-	49,49,49,49	0
32	MG	0	8083	1/1	0.99	0.08	-	59,59,59,59	0
34	NA	0	8548	1/1	0.96	0.25	-	52,52,52,52	0
36	SR	0	8962	1/1	0.69	0.15	-	155,155,155,155	0
32	MG	B	8042	1/1	0.96	0.08	-	67,67,67,67	0
32	MG	0	8080	1/1	0.98	0.51	-	98,98,98,98	0
34	NA	0	8574	1/1	0.94	0.81	-	67,67,67,67	0
36	SR	0	8976	1/1	0.88	0.22	-	185,185,185,185	0
36	SR	0	8923	1/1	0.98	0.17	-	120,120,120,120	0
36	SR	0	8998	1/1	0.62	0.62	-	169,169,169,169	0
36	SR	0	8922	1/1	0.76	0.47	-	190,190,190,190	0
36	SR	0	9008	1/1	0.98	0.16	-	99,99,99,99	0
32	MG	0	8022	1/1	0.98	0.13	-	29,29,29,29	0
34	NA	0	8541	1/1	0.94	0.15	-	46,46,46,46	0
36	SR	0	8948	1/1	0.99	0.08	-	104,104,104,104	0
36	SR	0	8906	1/1	0.98	0.19	-	65,65,65,65	0
36	SR	0	8978	1/1	0.97	0.04	-	130,130,130,130	0
36	SR	0	8945	1/1	0.93	0.04	-	111,111,111,111	0
34	NA	0	8561	1/1	0.96	0.36	-	73,73,73,73	0
36	SR	0	8947	1/1	0.78	0.60	-	200,200,200,200	0
32	MG	0	8019	1/1	0.99	0.16	-	10,10,10,10	0
32	MG	0	8085	1/1	0.94	0.12	-	83,83,83,83	0
36	SR	0	8974	1/1	0.84	0.42	-	191,191,191,191	0
36	SR	0	8920	1/1	0.97	0.11	-	132,132,132,132	0
32	MG	0	8079	1/1	0.93	0.20	-	63,63,63,63	0
36	SR	0	8982	1/1	0.91	1.68	-	200,200,200,200	0
34	NA	0	8570	1/1	0.98	0.11	-	65,65,65,65	0
36	SR	F	9005	1/1	0.90	0.13	-	154,154,154,154	0
36	SR	0	8911	1/1	0.98	0.13	-	109,109,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8901	1/1	0.94	0.12	-	89,89,89,89	0
35	CL	R	8806	1/1	0.95	0.17	-	62,62,62,62	0
32	MG	0	8005	1/1	0.96	0.28	-	30,30,30,30	0
36	SR	A	8993	1/1	0.85	0.04	-	177,177,177,177	0
36	SR	0	8996	1/1	0.89	0.40	-	200,200,200,200	0
34	NA	S	8510	1/1	0.38	0.30	-	69,69,69,69	0
32	MG	0	8071	1/1	0.95	0.12	-	50,50,50,50	0
32	MG	0	8046	1/1	0.98	0.21	-	48,48,48,48	0
32	MG	0	8048	1/1	0.99	0.31	-	38,38,38,38	0
32	MG	0	8055	1/1	0.88	0.26	-	67,67,67,67	0
36	SR	0	8994	1/1	0.75	0.72	-	200,200,200,200	0
35	CL	3	8804	1/1	0.73	0.15	-	96,96,96,96	0
34	NA	0	8531	1/1	0.85	0.27	-	42,42,42,42	0
36	SR	0	8971	1/1	0.17	0.12	-	200,200,200,200	0
36	SR	0	8970	1/1	0.91	0.06	-	150,150,150,150	0
36	SR	0	8925	1/1	0.99	0.13	-	105,105,105,105	0
35	CL	Y	8820	1/1	0.86	0.06	-	59,59,59,59	0
36	SR	0	8967	1/1	0.94	0.08	-	157,157,157,157	0
34	NA	0	8518	1/1	0.90	0.39	-	82,82,82,82	0
32	MG	0	8063	1/1	0.97	0.15	-	67,67,67,67	0
36	SR	B	8950	1/1	0.96	0.28	-	151,151,151,151	0
36	SR	0	8905	1/1	0.99	0.27	-	70,70,70,70	0
36	SR	0	9007	1/1	0.85	0.78	-	180,180,180,180	0
36	SR	0	8919	1/1	0.97	0.18	-	194,194,194,194	0
32	MG	0	8026	1/1	0.99	0.04	-	32,32,32,32	0
32	MG	0	8008	1/1	0.97	0.14	-	15,15,15,15	0
36	SR	0	8951	1/1	0.94	0.19	-	177,177,177,177	0
32	MG	K	8054	1/1	0.98	0.11	-	32,32,32,32	0
36	SR	0	8989	1/1	0.85	0.26	-	196,196,196,196	0
36	SR	0	8946	1/1	0.94	0.27	-	138,138,138,138	0
32	MG	0	8081	1/1	0.78	0.44	-	104,104,104,104	0
32	MG	9	8074	1/1	0.77	0.12	-	127,127,127,127	0
34	NA	C	8503	1/1	0.96	0.32	-	39,39,39,39	0
32	MG	0	8091	1/1	0.97	0.18	-	42,42,42,42	0
36	SR	0	9006	1/1	0.81	0.49	-	200,200,200,200	0
36	SR	0	8960	1/1	0.88	0.10	-	174,174,174,174	0
32	MG	0	8089	1/1	0.94	0.29	-	72,72,72,72	0
36	SR	0	8968	1/1	0.90	0.12	-	181,181,181,181	0
34	NA	0	8527	1/1	0.75	0.24	-	60,60,60,60	0
36	SR	9	8980	1/1	0.89	0.05	-	192,192,192,192	0
35	CL	0	8811	1/1	0.89	0.60	-	99,99,99,99	0
34	NA	0	8526	1/1	0.95	0.27	-	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8056	1/1	0.98	0.07	-	47,47,47,47	0
36	SR	0	9004	1/1	0.86	0.46	-	200,200,200,200	0
32	MG	0	8069	1/1	0.87	0.55	-	68,68,68,68	0
34	NA	0	8520	1/1	0.99	0.19	-	57,57,57,57	0
36	SR	0	8983	1/1	0.96	0.21	-	185,185,185,185	0
35	CL	0	8805	1/1	0.83	0.39	-	97,97,97,97	0
34	NA	0	8505	1/1	0.61	0.44	-	56,56,56,56	0
35	CL	A	8809	1/1	0.98	0.67	-	96,96,96,96	0
36	SR	0	8955	1/1	0.94	0.17	-	199,199,199,199	0
34	NA	0	8511	1/1	0.86	0.22	-	64,64,64,64	0
32	MG	0	8015	1/1	0.95	0.10	-	25,25,25,25	0
36	SR	3	8999	1/1	0.92	0.18	-	160,160,160,160	0
32	MG	0	8053	1/1	0.92	0.05	-	57,57,57,57	0
35	CL	0	8817	1/1	0.99	0.11	-	63,63,63,63	0
34	NA	0	8567	1/1	0.96	0.20	-	58,58,58,58	0
32	MG	0	8020	1/1	0.99	0.11	-	52,52,52,52	0
32	MG	0	8018	1/1	0.99	0.18	-	42,42,42,42	0
34	NA	0	8573	1/1	0.86	0.19	-	92,92,92,92	0
34	NA	0	8525	1/1	0.52	0.33	-	92,92,92,92	0
36	SR	0	8941	1/1	0.96	0.31	-	143,143,143,143	0
32	MG	0	8076	1/1	0.97	0.06	-	36,36,36,36	0
36	SR	1	8952	1/1	0.96	0.19	-	81,81,81,81	0
36	SR	0	8939	1/1	0.98	0.05	-	145,145,145,145	0
35	CL	0	8816	1/1	0.98	0.71	-	86,86,86,86	0
36	SR	0	8965	1/1	0.99	0.16	-	135,135,135,135	0
36	SR	0	8907	1/1	0.99	0.16	-	63,63,63,63	0
32	MG	0	8039	1/1	0.90	0.27	-	76,76,76,76	0
35	CL	0	8803	1/1	0.94	0.08	-	66,66,66,66	0
32	MG	0	8017	1/1	0.99	0.07	-	29,29,29,29	0
36	SR	0	8954	1/1	0.95	0.12	-	122,122,122,122	0
36	SR	0	8909	1/1	0.98	0.07	-	89,89,89,89	0
36	SR	0	8903	1/1	0.98	0.19	-	62,62,62,62	0
36	SR	0	9002	1/1	0.98	0.09	-	188,188,188,188	0
36	SR	0	8940	1/1	0.95	0.03	-	117,117,117,117	0
34	NA	0	8554	1/1	0.61	0.38	-	71,71,71,71	0
36	SR	0	8937	1/1	0.98	0.17	-	108,108,108,108	0
35	CL	0	8815	1/1	0.95	0.24	-	90,90,90,90	0
36	SR	0	8917	1/1	0.97	0.13	-	121,121,121,121	0
35	CL	N	8807	1/1	0.79	0.38	-	134,134,134,134	0
36	SR	9	9003	1/1	0.78	0.06	-	200,200,200,200	0
35	CL	0	8822	1/1	0.88	1.37	-	94,94,94,94	0
36	SR	0	8990	1/1	0.98	0.19	-	111,111,111,111	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8516	1/1	0.94	0.26	-	26,26,26,26	0
36	SR	0	8933	1/1	0.97	0.04	-	122,122,122,122	0
32	MG	0	8066	1/1	0.84	0.92	-	70,70,70,70	0
34	NA	0	8509	1/1	0.78	0.49	-	66,66,66,66	0
32	MG	0	8077	1/1	0.77	0.16	-	47,47,47,47	0
36	SR	0	8958	1/1	0.69	0.08	-	150,150,150,150	0
34	NA	0	8529	1/1	0.77	0.11	-	49,49,49,49	0
34	NA	0	8544	1/1	0.90	0.17	-	68,68,68,68	0
36	SR	R	8912	1/1	0.99	0.23	-	106,106,106,106	0
32	MG	0	8093	1/1	0.97	0.11	-	40,40,40,40	0
34	NA	0	8514	1/1	0.83	0.26	-	61,61,61,61	0
36	SR	0	8914	1/1	0.91	0.32	-	130,130,130,130	0
32	MG	0	8033	1/1	0.89	0.26	-	56,56,56,56	0
36	SR	0	8931	1/1	0.99	0.10	-	123,123,123,123	0
36	SR	0	9000	1/1	0.96	0.23	-	200,200,200,200	0
34	NA	0	8566	1/1	0.79	0.86	-	51,51,51,51	0
35	CL	J	8802	1/1	0.98	0.08	-	100,100,100,100	0
32	MG	0	8038	1/1	0.95	0.12	-	81,81,81,81	0
32	MG	0	8061	1/1	0.82	0.30	-	42,42,42,42	0
36	SR	0	8928	1/1	0.92	0.05	-	164,164,164,164	0
36	SR	0	8988	1/1	0.88	0.11	-	181,181,181,181	0
36	SR	0	8926	1/1	0.99	0.16	-	145,145,145,145	0
36	SR	J	8986	1/1	0.66	1.53	-	200,200,200,200	0
32	MG	0	8049	1/1	0.70	0.20	-	61,61,61,61	0
36	SR	0	8916	1/1	0.74	0.08	-	129,129,129,129	0
32	MG	0	8032	1/1	0.94	0.08	-	64,64,64,64	0
34	NA	0	8506	1/1	0.47	0.60	-	105,105,105,105	0
32	MG	0	8078	1/1	0.97	0.23	-	64,64,64,64	0
32	MG	0	8024	1/1	0.97	0.14	-	58,58,58,58	0
34	NA	0	8552	1/1	0.85	0.31	-	68,68,68,68	0
32	MG	0	8031	1/1	0.94	0.35	-	71,71,71,71	0
36	SR	0	8995	1/1	0.84	0.25	-	128,128,128,128	0
32	MG	2	8060	1/1	0.95	0.09	-	56,56,56,56	0
32	MG	0	8035	1/1	0.94	0.12	-	47,47,47,47	0
34	NA	0	8545	1/1	0.83	0.30	-	40,40,40,40	0
35	CL	L	8810	1/1	0.96	0.24	-	86,86,86,86	0
36	SR	0	8938	1/1	0.89	0.07	-	200,200,200,200	0
34	NA	0	8508	1/1	0.77	0.98	-	70,70,70,70	0
32	MG	0	8072	1/1	0.89	0.08	-	37,37,37,37	0
36	SR	0	8991	1/1	0.68	0.10	-	190,190,190,190	0
34	NA	0	8501	1/1	0.73	0.22	-	41,41,41,41	0
32	MG	0	8092	1/1	0.65	0.12	-	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8037	1/1	0.95	0.29	-	84,84,84,84	0
32	MG	0	8064	1/1	0.97	0.20	-	48,48,48,48	0
32	MG	0	8087	1/1	0.92	0.18	-	20,20,20,20	0
36	SR	0	8924	1/1	0.94	0.17	-	138,138,138,138	0
36	SR	0	8908	1/1	0.95	0.06	-	109,109,109,109	0
35	CL	J	8801	1/1	0.97	0.20	-	90,90,90,90	0
36	SR	0	8981	1/1	0.95	0.11	-	151,151,151,151	0
36	SR	0	8934	1/1	0.96	0.09	-	114,114,114,114	0
36	SR	0	8944	1/1	0.93	0.17	-	171,171,171,171	0
36	SR	0	8966	1/1	0.95	0.10	-	110,110,110,110	0
36	SR	0	8921	1/1	0.97	0.09	-	90,90,90,90	0
36	SR	0	8963	1/1	0.94	0.15	-	135,135,135,135	0
36	SR	0	8953	1/1	0.91	0.24	-	185,185,185,185	0
32	MG	0	8059	1/1	0.97	0.12	-	40,40,40,40	0
36	SR	0	8927	1/1	0.87	0.16	-	172,172,172,172	0
36	SR	0	8973	1/1	0.87	0.16	-	134,134,134,134	0
36	SR	0	8977	1/1	0.83	0.14	-	197,197,197,197	0
36	SR	0	8956	1/1	0.98	0.23	-	178,178,178,178	0
36	SR	0	8979	1/1	0.82	0.10	-	200,200,200,200	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.