



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 03:33 am BST

PDB ID : 3CCQ  
Title : Structure of Anisomycin resistant 50S Ribosomal Subunit: 23S rRNA mutation A2488U  
Authors : Blaha, G.; Gurel, G.  
Deposited on : 2008-02-26  
Resolution : 2.90 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

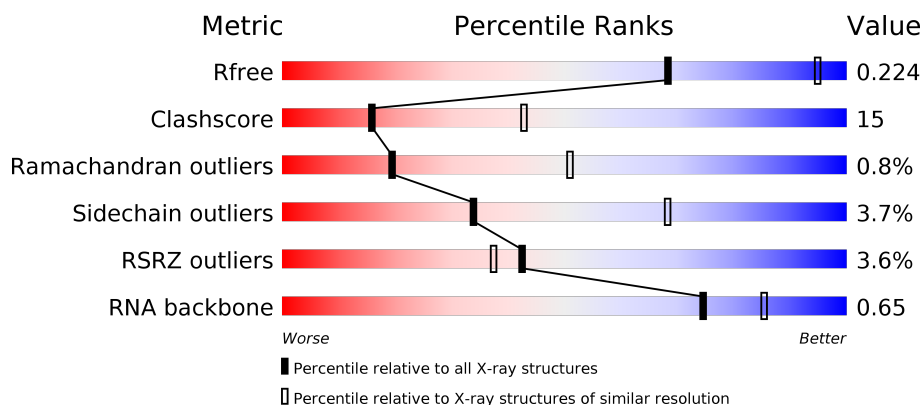
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)
RNA backbone	3102	1007 (3.16-2.64)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>25%</div> <div>..</div> </div> </div>
2	B	338	<div> <div>%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>.</div> </div> </div>
3	C	246	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>.</div> </div> </div>
4	D	177	<div> <div>29%</div> <div> <div></div> <div>40%</div> <div>37%</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
34	SR	0	8947	-	-	-	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
35	NA	0	8509	-	-	-	X
35	NA	0	8528	-	-	-	X
35	NA	0	8560	-	-	-	X
35	NA	0	8562	-	-	-	X
37	K	0	8401	-	-	-	X

## 2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 99120 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
			59018	26348	10870	19055	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	9	Total Cl 9 9	0	0
33	J	3	Total Cl 3 3	0	0
33	Q	1	Total Cl 1 1	0	0
33	B	1	Total Cl 1 1	0	0
33	A	1	Total Cl 1 1	0	0
33	N	1	Total Cl 1 1	0	0
33	O	1	Total Cl 1 1	0	0
33	R	1	Total Cl 1 1	0	0
33	Y	1	Total Cl 1 1	0	0
33	L	1	Total Cl 1 1	0	0
33	3	1	Total Cl 1 1	0	0
33	M	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	93	Total Sr 93 93	0	0
34	1	2	Total Sr 2 2	0	0
34	B	2	Total Sr 2 2	0	0
34	3	2	Total Sr 2 2	0	0
34	A	3	Total Sr 3 3	0	0
34	R	1	Total Sr 1 1	0	0
34	9	3	Total Sr 3 3	0	0
34	S	1	Total Sr 1 1	0	0

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	65	Total	Na	0	0
			65	65		
35	J	1	Total	Na	0	0
			1	1		
35	Q	1	Total	Na	0	0
			1	1		
35	B	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	R	2	Total	Na	0	0
			2	2		
35	9	2	Total	Na	0	0
			2	2		
35	S	1	Total	Na	0	0
			1	1		
35	M	1	Total	Na	0	0
			1	1		

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

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

- 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 water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	A	112	Total O 112 112	0	0
38	B	142	Total O 142 142	0	0
38	C	168	Total O 168 168	0	0
38	D	45	Total O 45 45	0	0
38	E	42	Total O 42 42	0	0
38	F	26	Total O 26 26	0	0
38	G	17	Total O 17 17	0	0
38	H	65	Total O 65 65	0	0
38	I	5	Total O 5 5	0	0
38	J	56	Total O 56 56	0	0
38	K	60	Total O 60 60	0	0
38	L	82	Total O 82 82	0	0
38	M	123	Total O 123 123	0	0
38	N	59	Total O 59 59	0	0
38	O	47	Total O 47 47	0	0
38	P	59	Total O 59 59	0	0
38	Q	47	Total O 47 47	0	0
38	R	76	Total O 76 76	0	0
38	S	33	Total O 33 33	0	0

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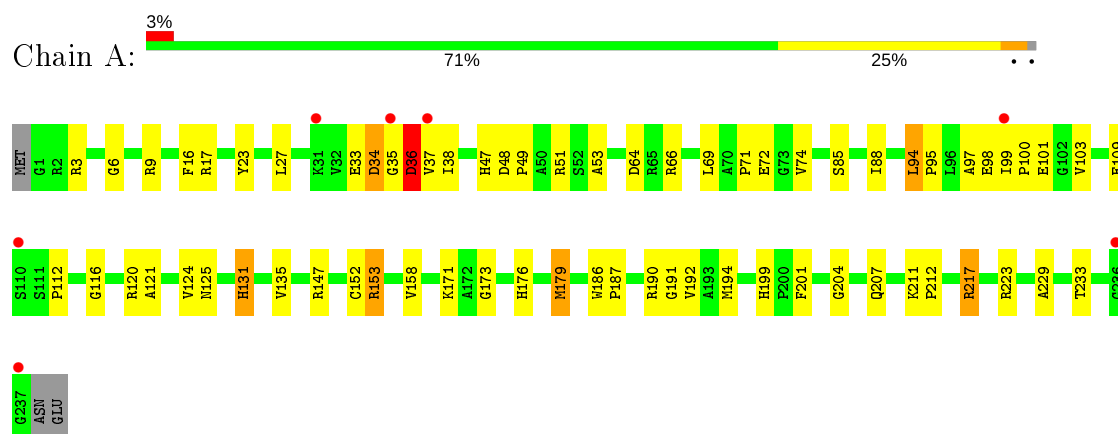
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	36	Total 36	O 36	0	0
38	U	26	Total 26	O 26	0	0
38	V	12	Total 12	O 12	0	0
38	W	66	Total 66	O 66	0	0
38	X	28	Total 28	O 28	0	0
38	Y	97	Total 97	O 97	0	0
38	Z	31	Total 31	O 31	0	0
38	1	54	Total 54	O 54	0	0
38	2	43	Total 43	O 43	0	0
38	3	68	Total 68	O 68	0	0
38	0	5950	Total 5950	O 5950	0	0
38	9	148	Total 148	O 148	0	0

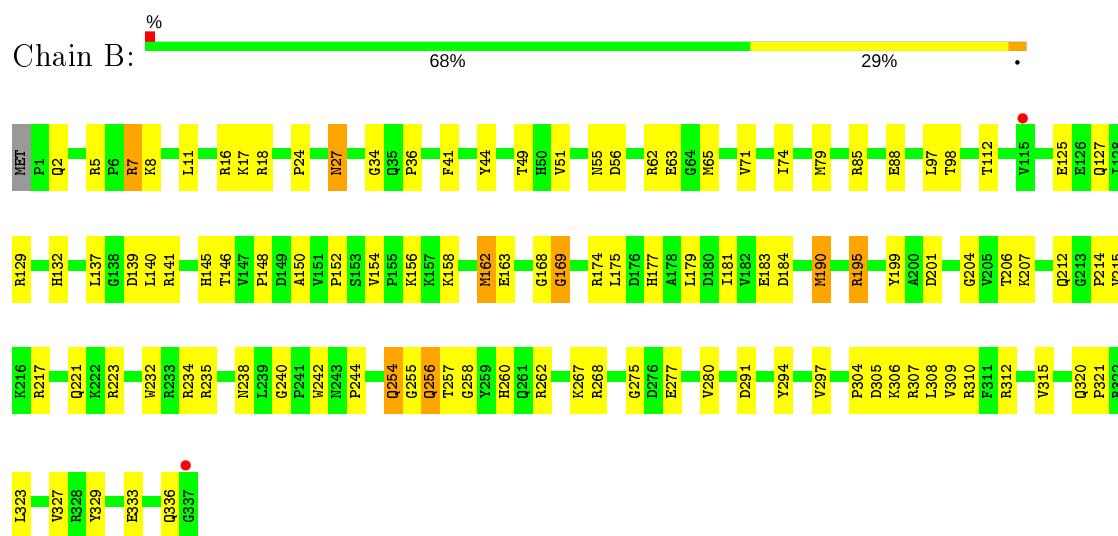
### 3 Residue-property plots [i](#)

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.

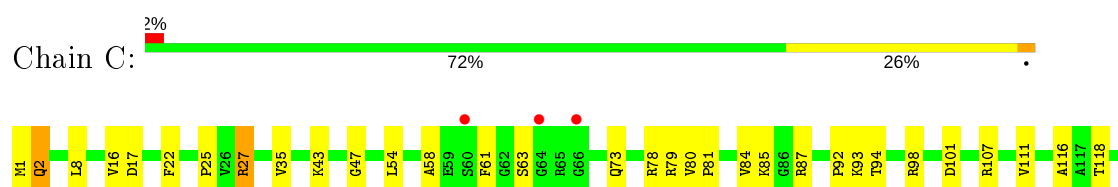
- Molecule 1: 50S ribosomal protein L2P

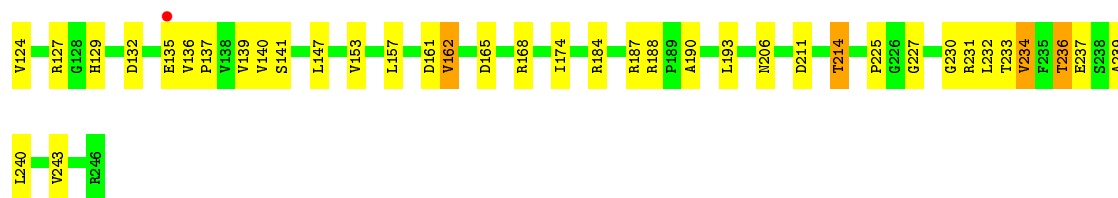


- Molecule 2: 50S ribosomal protein L3P

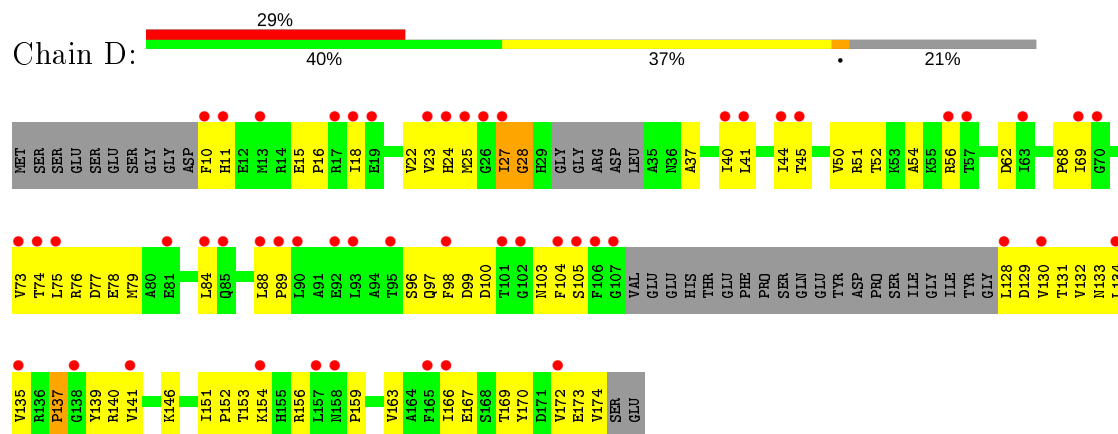


- Molecule 3: 50S ribosomal protein L4P

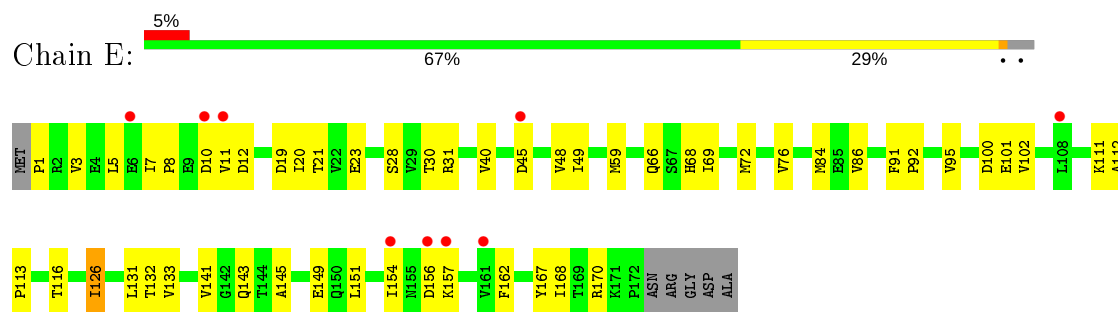




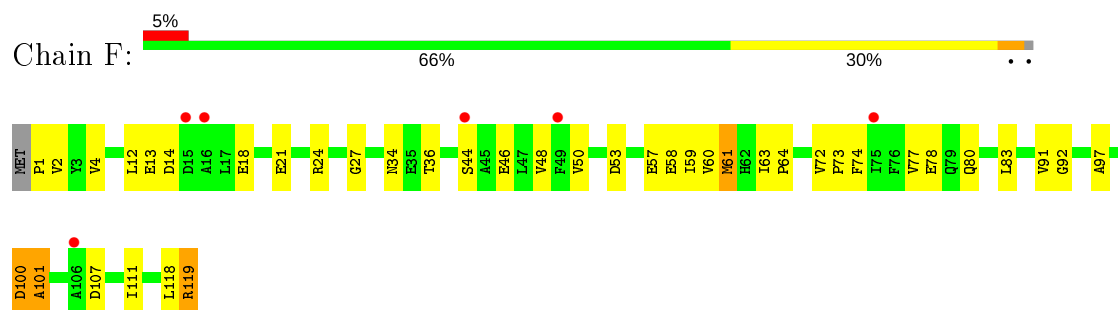
• Molecule 4: 50S ribosomal protein L5P



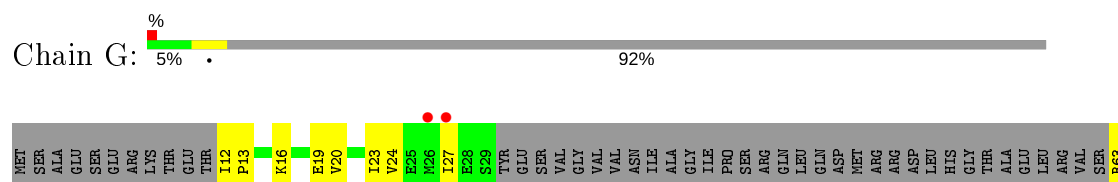
• Molecule 5: 50S ribosomal protein L6P



• Molecule 6: 50S ribosomal protein L7Ae

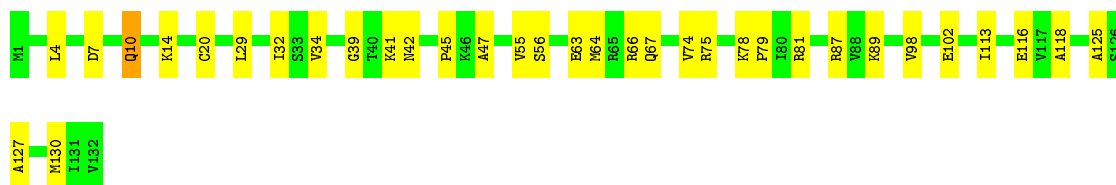


• Molecule 7: 50S ribosomal protein L10E

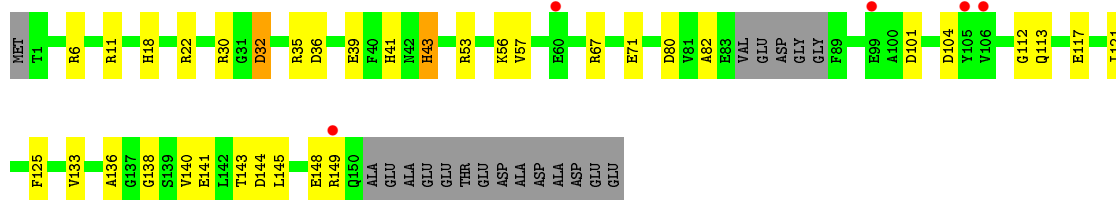




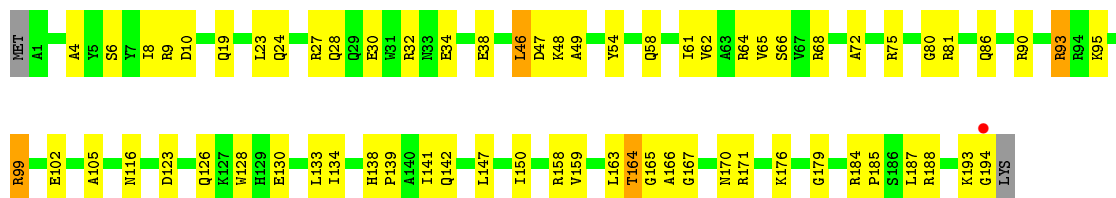




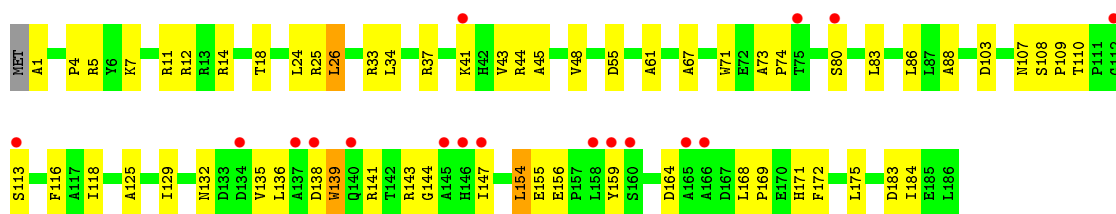
- Molecule 12: 50S ribosomal protein L15P



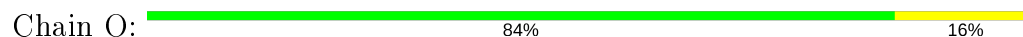
- Molecule 13: 50S ribosomal protein L15e



- Molecule 14: 50S ribosomal protein L18P

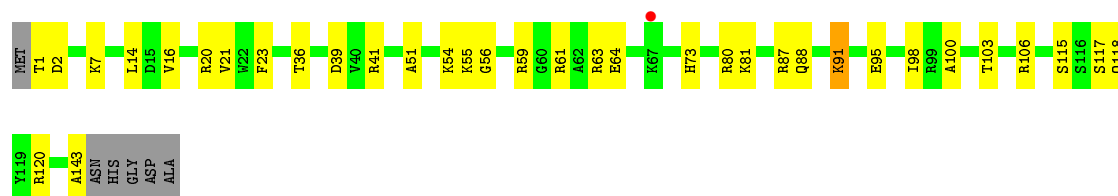


- Molecule 15: 50S ribosomal protein L18e



- Molecule 16: 50S ribosomal protein L19e

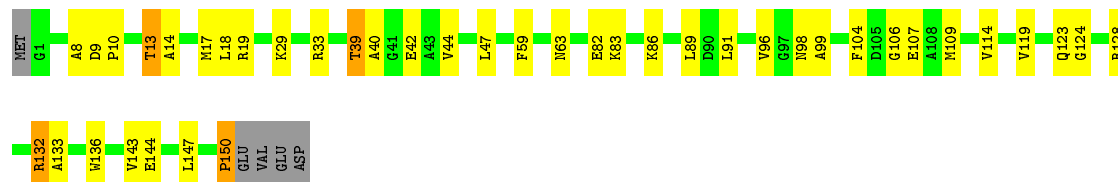




- Molecule 17: 50S ribosomal protein L21e



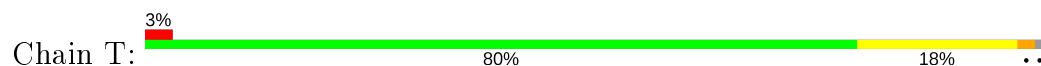
- Molecule 18: 50S ribosomal protein L22P



- Molecule 19: 50S ribosomal protein L23P



- Molecule 20: 50S ribosomal protein L24P



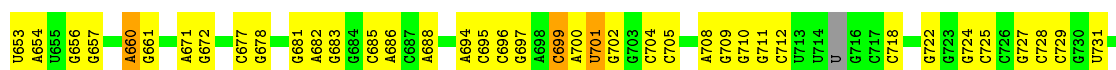
- Molecule 21: 50S ribosomal protein L24e



- Molecule 22: 50S ribosomal protein L29P







A1909	U1825	C1731	G1555	U1359	C1267	A1188	U1109	A	U932	C842	U734
U1915	C1826	A1732	A1559	C1360	C1268	A1189	G1110	C	A843	A843	C735
C1916	A1829	C1734	U	C1366	G1269	G1191	U1116	A	U845	A844	A736
A1919	C1834	C1735	U1561	A1372	C1273	A1192	U1116	C999	U846	A846	A737
C1920	U1835	A1736	C1562	G1377	A1278	A1193	U1117	C1000	C847	G738	
A1921	U1741	A1742	C1563	G1378	U1279	A1194	U1118	U1001		G743	
A1922	U1748	C1662	C1564	G1379	A1279	A1195	U1119	G1002		G744	
U1838	A1839	C1663	C1565	U1380	C1289	G1196	U1120	U1003	C851	G745	
A1840	U1749	A1664	C1566	G1381	G1289	G1197	U1121	C1004	U852	G746	
G1925	C1841	C1750	C1567	U1382	A1291	U1198	U1122	A1005	C853	G747	
C1842	A1842	G1751	C1568	G1383	A1294	U1199	U1123	A1006	U854		
A1927		G1752	C1569	U1384	G1295	A1200	U1124	A1007	U855	G748	
A1845	U1755	A1756	U1577	C1385	A1296	C1201	U1125	C1008	G856	C749	
A1930	A1667	C1668	G1578	U1386	G1297	A1202	U1126	A1013	U857	A750	
A1931	A1669	A1670	U1579	G1387	U1297	G1203	U1127	A1014	U858	A758	
G1849	A1670	C1675	U1581	U1388	U1298	C1204	U1128	C1015	U859	C759	
C1853	A1671	C1676	C1582	G1389	G1300	U1205	U1129	U1016	U860	G760	
C1854	U1759	G1677	C1583	U1390	U1304	U1206	U1130	C1023	U862	A761	
G1855	G1760	U1677	G1586	C1391	U1305	A1207	U1131	G1024	U863	C764	
C1856	C1762	A1678	U1587	C1392	C1306	C1208	U1132	U1028	U868	G765	
A1857	C1763	G1679	G1588	U1393	U1307	G1210	U1133	G1027	U869	G772	
A1858	C1680	C1681	G1589	C1395	A1308	C1213	U1134	U1029	G871	A773	
C1861	U1766	A1682	C1592	G1396	U1309	G1214	U1135	C1044	U872	C774	
C1862	A1767	C1683	C1593	G1397	U1310	A1215	U1136	G1045	U875	G775	
G1863	U1761	C1684	C1594	U1398	U1311	G1216	U1137	A1057	A876	A776	
C1864	C1769	A1884	G1595	A1399	U1312	G1217	U1138	G1052	G877	U777	
G1866	U1770	A1685	C1596	A1407	U1313	U1218	U1139	G1053	G878	A790	
C	U1771	C1686	A1597	U1408	G1315	U1219	U1140	G1054	A882	A791	
U	G1772	C1687	A1598	G1409	U1316	U1220	U1141	G1055	U885	U794	
C	G1773	C1688	U1599	A1413	A1317	G1221	U1142	U1056	G890	U801	
A	G1774	C1689	C1602	A1414	G1318	G1226	U1143	A1057	C891	U806	
G	A1778	G1697	G1604	G1415	G1319	U1227	U1144	A1058	A894	A807	
A	A1779	U1700	G1605	G1416	C1320	C1229	U1145	G1059	G898	A808	
C	C1787	A1701	A1607	G1417	G1322	A1230	U1146	C1060	C899	G809	
U1964	U1788	U1702	A1615	U1418	G1325	U1234	U1147	G1063	G902	A812	
C1965	G1789	C1705	C1615	U1419	C1326	U1237	U1148	C	U903	C813	
U1966	U1790	G1706	G1622	U1422	G1327	U1238	U1149	C	U904	U815	
C	C1792	G1707	C1623	C1423	A1328	G1239	U1150	C	G905	G816	
G1971	G1795	A1710	A1625	A1427	G1331	U1242	U1151	U1066	G906	G817	
U1972	A1796	A1711	A1626	C1428	C1339	A1243	U1152	A1067	A907	A818	
A1973	C1797	A1712	G1627	U1433	G1340	U1244	U1153	U1068	A908	A819	
G1974	C1798	G1713	G1630	A1434	C1342	G1245	U1154	G1072	G920	U821	
C1975	G1714	C1714	A1631	U1441	C1343	A1246	U1155	C	A912	C822	
U1977	G1715	C1715	A1632	A1442	G1344	A1247	U1156	A1086	G921	G834	
C1889	C1803	A1716	C1633	U1443	U1350	U1248	U1157	G1087	U922	U835	
U1890	G1805	A1717	G1634	G1444	G1351	C1250	U1158	A1088	A923	U840	
C1894	U1722	U1723	C1635	U1445	A1352	C1251	U1159	A1097	G926	A841	
A1895	A1815	G1723	U1635	U1446	C1353	C1252	U1160	A1098	C		
G1896	C1818	U1724	C1636	U1447	A1357	C1253	U1161	G1099	G		
U1897	C1725	G1730	A1641	C1450	A1358	G1265	U1162	C1104	C		
G1902	U1903		A1642	C1451		U1266	U1167				
A1994	U1904										
G1995											
U1996											
A1997											



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	212.33Å 299.62Å 575.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 85.65 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-2.90) 98.2 (85.65-2.41)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.186 , 0.233 0.177 , 0.224	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	61.2	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 82.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	99120	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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, PSU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.33	0/1786	0.64	0/2408
2	B	0.34	0/2690	0.65	0/3652
3	C	0.36	0/1885	0.62	0/2552
4	D	0.32	0/1111	0.56	1/1498 (0.1%)
5	E	0.33	0/1382	0.57	0/1880
6	F	0.35	0/901	0.57	0/1224
7	G	0.33	0/241	0.51	0/324
8	H	0.33	0/1302	0.63	0/1743
9	I	0.30	0/526	0.50	0/716
10	J	0.36	0/1136	0.61	0/1530
11	K	0.34	0/1004	0.66	0/1351
12	L	0.35	0/1130	0.64	0/1509
13	M	0.36	0/1582	0.61	0/2116
14	N	0.30	0/1474	0.61	0/1999
15	O	0.35	0/874	0.59	0/1181
16	P	0.33	0/1147	0.53	0/1528
17	Q	0.34	0/749	0.65	0/1005
18	R	1.26	7/1172 (0.6%)	1.09	6/1578 (0.4%)
19	S	0.33	0/648	0.54	0/875
20	T	0.32	0/958	0.64	0/1289
21	U	0.32	0/417	0.57	0/562
22	V	0.32	0/502	0.54	0/675
23	W	0.36	0/1219	0.63	0/1655
24	X	0.35	0/664	0.60	0/895
25	Y	0.37	0/1146	0.62	0/1536
26	Z	0.36	0/584	0.63	0/781
27	1	0.39	0/438	0.62	0/578
28	2	0.34	0/401	0.58	0/529
29	3	0.37	0/771	0.57	0/1024
30	0	0.39	0/65954	0.68	9/102862 (0.0%)
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.40	7/98698 (0.0%)	0.67	17/147581 (0.0%)



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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	R	1	0
23	W	0	1
30	0	0	32
31	9	0	3
All	All	1	36

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	150	PRO	CB-CG	27.45	2.87	1.50
18	R	150	PRO	CA-C	-18.11	1.16	1.52
18	R	150	PRO	CG-CD	13.90	1.96	1.50
18	R	150	PRO	C-O	11.92	1.47	1.23
18	R	150	PRO	N-CA	11.35	1.66	1.47

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	R	150	PRO	CB-CA-C	-22.47	55.81	112.00
18	R	150	PRO	N-CA-C	-19.38	61.71	112.10
18	R	150	PRO	CA-N-CD	12.28	128.89	111.70
18	R	150	PRO	N-CA-CB	10.98	116.47	103.30
18	R	150	PRO	CA-C-O	-8.52	99.75	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	R	150	PRO	CA

5 of 36 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	0	202	U	Sidechain
30	0	205	U	Sidechain
30	0	221	G	Sidechain
30	0	48	A	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	66	0
2	B	2625	0	2533	94	0
3	C	1860	0	1813	53	0
4	D	1094	0	1085	52	0
5	E	1357	0	1266	36	0
6	F	890	0	843	30	0
7	G	240	0	231	11	0
8	H	1282	0	1292	41	0
9	I	519	0	500	21	0
10	J	1120	0	1098	38	0
11	K	994	0	1027	39	0
12	L	1118	0	1076	33	0
13	M	1558	0	1573	59	0
14	N	1445	0	1401	54	0
15	O	865	0	873	18	0
16	P	1136	0	1123	30	0
17	Q	735	0	729	26	0
18	R	1149	0	1122	32	0
19	S	641	0	605	10	0
20	T	950	0	924	22	0
21	U	410	0	364	17	0
22	V	499	0	511	17	0
23	W	1196	0	1137	66	0
24	X	654	0	653	22	0
25	Y	1130	0	1133	33	0
26	Z	573	0	531	21	0
27	1	431	0	426	21	0
28	2	396	0	413	21	0
29	3	755	0	728	17	0
30	0	59018	0	29809	1329	0
31	9	2599	0	1325	97	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	Y	1	0	0	0	0
33	0	9	0	0	3	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	2	0
33	L	1	0	0	0	0
33	M	1	0	0	1	0
33	N	1	0	0	1	0
33	O	1	0	0	0	0
33	Q	1	0	0	0	0
33	R	1	0	0	0	0
33	Y	1	0	0	0	0
34	0	93	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	R	1	0	0	0	0
34	S	1	0	0	0	0
35	0	65	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	2	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	5950	0	0	203	0
38	1	54	0	0	3	0
38	2	43	0	0	1	0
38	3	68	0	0	6	0
38	9	148	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	A	112	0	0	5	0
38	B	142	0	0	14	0
38	C	168	0	0	13	0
38	D	45	0	0	4	0
38	E	42	0	0	4	0
38	F	26	0	0	1	0
38	G	17	0	0	1	0
38	H	65	0	0	5	0
38	I	5	0	0	0	0
38	J	56	0	0	2	0
38	K	60	0	0	5	0
38	L	82	0	0	8	0
38	M	123	0	0	2	0
38	N	59	0	0	3	0
38	O	47	0	0	4	0
38	P	59	0	0	2	0
38	Q	47	0	0	2	0
38	R	76	0	0	1	0
38	S	33	0	0	0	0
38	T	36	0	0	4	0
38	U	26	0	0	2	0
38	V	12	0	0	1	0
38	W	66	0	0	6	0
38	X	28	0	0	3	0
38	Y	97	0	0	7	0
38	Z	31	0	0	4	0
All	All	99120	0	59910	2191	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 2191 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:150:PRO:CG	18:R:150:PRO:CD	1.96	1.44
30:0:871:G:C8	30:0:871:G:H5'	1.75	1.21
14:N:37:ARG:NH1	31:9:6:C:H5''	1.62	1.12
31:9:56:A:H2'	31:9:57:A:H5''	1.21	1.11
30:0:1160:G:C5'	30:0:1161:A:H5'	1.79	1.11

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%)	213 (91%)	18 (8%)	4 (2%)	9	31
2	B	335/338 (99%)	309 (92%)	22 (7%)	4 (1%)	13	40
3	C	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
4	D	134/177 (76%)	107 (80%)	22 (16%)	5 (4%)	3	13
5	E	170/178 (96%)	156 (92%)	14 (8%)	0	100	100
6	F	117/120 (98%)	104 (89%)	9 (8%)	4 (3%)	3	15
7	G	25/348 (7%)	23 (92%)	2 (8%)	0	100	100
8	H	156/177 (88%)	145 (93%)	11 (7%)	0	100	100
9	I	68/162 (42%)	54 (79%)	13 (19%)	1 (2%)	10	34
10	J	140/145 (97%)	132 (94%)	8 (6%)	0	100	100
11	K	130/132 (98%)	124 (95%)	6 (5%)	0	100	100
12	L	141/165 (86%)	124 (88%)	14 (10%)	3 (2%)	7	26
13	M	192/196 (98%)	182 (95%)	10 (5%)	0	100	100
14	N	184/187 (98%)	169 (92%)	11 (6%)	4 (2%)	6	24
15	O	113/116 (97%)	108 (96%)	5 (4%)	0	100	100
16	P	141/149 (95%)	138 (98%)	3 (2%)	0	100	100
17	Q	93/96 (97%)	89 (96%)	4 (4%)	0	100	100
18	R	148/155 (96%)	137 (93%)	11 (7%)	0	100	100
19	S	79/85 (93%)	72 (91%)	7 (9%)	0	100	100
20	T	117/120 (98%)	107 (92%)	9 (8%)	1 (1%)	17	48
21	U	51/67 (76%)	48 (94%)	3 (6%)	0	100	100
22	V	63/71 (89%)	58 (92%)	3 (5%)	2 (3%)	4	16
23	W	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	54
24	X	80/92 (87%)	71 (89%)	8 (10%)	1 (1%)	12	37
25	Y	140/241 (58%)	140 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	71/116 (61%)	62 (87%)	8 (11%)	1 (1%)	11	36
27	1	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
28	2	42/50 (84%)	37 (88%)	5 (12%)	0	100	100
29	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4472 (83%)	3416 (92%)	258 (7%)	31 (1%)	19	51

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	36	ASP
1	A	37	VAL
6	F	101	ALA
14	N	154	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%)	171 (96%)	8 (4%)	27	61
2	B	282/283 (100%)	268 (95%)	14 (5%)	24	57
3	C	193/193 (100%)	180 (93%)	13 (7%)	16	43
4	D	117/148 (79%)	113 (97%)	4 (3%)	37	71
5	E	152/156 (97%)	148 (97%)	4 (3%)	46	77
6	F	93/94 (99%)	91 (98%)	2 (2%)	52	81
7	G	27/282 (10%)	26 (96%)	1 (4%)	34	68
8	H	134/145 (92%)	128 (96%)	6 (4%)	27	61
9	I	58/130 (45%)	56 (97%)	2 (3%)	37	71
10	J	118/121 (98%)	110 (93%)	8 (7%)	16	42
11	K	106/106 (100%)	103 (97%)	3 (3%)	43	76
12	L	113/127 (89%)	108 (96%)	5 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	M	158/160 (99%)	151 (96%)	7 (4%)	28	61
14	N	149/150 (99%)	147 (99%)	2 (1%)	69	90
15	O	93/94 (99%)	92 (99%)	1 (1%)	73	92
16	P	113/117 (97%)	111 (98%)	2 (2%)	59	85
17	Q	79/80 (99%)	75 (95%)	4 (5%)	24	56
18	R	117/122 (96%)	112 (96%)	5 (4%)	29	62
19	S	71/74 (96%)	71 (100%)	0	100	100
20	T	105/106 (99%)	101 (96%)	4 (4%)	33	67
21	U	44/53 (83%)	42 (96%)	2 (4%)	27	61
22	V	51/57 (90%)	48 (94%)	3 (6%)	19	49
23	W	130/130 (100%)	127 (98%)	3 (2%)	50	80
24	X	66/74 (89%)	63 (96%)	3 (4%)	27	61
25	Y	120/196 (61%)	116 (97%)	4 (3%)	38	72
26	Z	60/94 (64%)	59 (98%)	1 (2%)	60	86
27	1	46/47 (98%)	46 (100%)	0	100	100
28	2	42/46 (91%)	41 (98%)	1 (2%)	49	79
29	3	79/79 (100%)	78 (99%)	1 (1%)	69	90
All	All	3095/3646 (85%)	2982 (96%)	113 (4%)	34	68

5 of 113 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	H	173	GLU
11	K	10	GLN
24	X	46	ASP
9	I	110	ASP
10	J	74	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 77 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	88	GLN
27	1	28	HIS
13	M	137	ASN

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Mol	Chain	Res	Type
14	N	107	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	0	2745/2923 (93%)	242 (8%)	22 (0%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	260 (9%)	23 (0%)

5 of 260 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 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
30	0	1246	A
30	0	1377	C
30	0	2718	C
30	0	1352	A
30	0	1474	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
30	1MA	0	628	30,35	15,25,26	0.80	0	15,37,40	1.44	1 (6%)
30	OMG	0	2588	30	18,26,27	1.08	2 (11%)	20,38,41	2.58	5 (25%)
30	OMU	0	2587	30	14,22,23	1.02	1 (7%)	14,31,34	1.16	1 (7%)
30	PSU	0	2621	30	17,21,22	1.57	3 (17%)	20,30,33	5.47	4 (20%)
30	UR3	0	2619	30	14,22,23	0.73	0	15,32,35	0.65	0

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

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

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	0	2621	PSU	C5-C1'	-4.97	1.48	1.52
30	0	2588	OMG	C6-N1	3.46	1.39	1.33
30	0	2587	OMU	C4-N3	2.76	1.37	1.33
30	0	2621	PSU	C4-N3	2.72	1.37	1.33
30	0	2621	PSU	C2-N1	2.26	1.42	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	0	2621	PSU	N1-C2-N3	-17.33	114.66	128.43
30	0	2621	PSU	C4-N3-C2	14.41	127.31	115.14
30	0	2588	OMG	C5-C6-N1	-8.61	111.66	123.43
30	0	2621	PSU	C5-C4-N3	-8.24	114.74	125.36
30	0	2588	OMG	C6-N1-C2	5.84	125.21	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	0	628	1MA	1	0
30	0	2587	OMU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 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%)	-0.22	7 (2%) 50 45	34, 56, 94, 116	0
2	B	337/338 (99%)	-0.42	2 (0%) 89 89	34, 58, 89, 99	0
3	C	246/246 (100%)	-0.24	4 (1%) 72 71	32, 51, 75, 87	0
4	D	140/177 (79%)	1.64	51 (36%) 0 0	69, 106, 134, 144	0
5	E	172/178 (96%)	-0.10	9 (5%) 27 23	49, 73, 97, 102	0
6	F	119/120 (99%)	-0.01	6 (5%) 28 25	52, 76, 109, 124	0
7	G	29/348 (8%)	0.52	2 (6%) 16 13	79, 103, 110, 113	0
8	H	160/177 (90%)	-0.34	2 (1%) 77 77	53, 73, 107, 111	0
9	I	70/162 (43%)	3.80	49 (70%) 0 0	137, 155, 173, 175	0
10	J	142/145 (97%)	-0.65	0 100 100	43, 57, 77, 99	0
11	K	132/132 (100%)	-0.62	0 100 100	39, 54, 79, 83	0
12	L	145/165 (87%)	0.33	5 (3%) 45 40	32, 71, 123, 134	0
13	M	194/196 (98%)	-0.48	1 (0%) 91 91	35, 49, 64, 71	0
14	N	186/187 (99%)	0.24	17 (9%) 9 6	51, 74, 121, 131	0
15	O	115/116 (99%)	-0.49	0 100 100	44, 61, 78, 85	0
16	P	143/149 (95%)	-0.41	1 (0%) 87 87	47, 61, 74, 83	0
17	Q	95/96 (98%)	-0.49	0 100 100	44, 55, 72, 85	0
18	R	150/155 (96%)	-0.50	0 100 100	37, 51, 73, 84	0
19	S	81/85 (95%)	-0.06	2 (2%) 57 55	49, 64, 87, 97	0
20	T	119/120 (99%)	-0.17	3 (2%) 57 55	42, 62, 92, 121	0
21	U	53/67 (79%)	0.01	1 (1%) 66 65	51, 64, 83, 91	0
22	V	65/71 (91%)	1.07	15 (23%) 0 0	53, 76, 130, 134	0
23	W	154/154 (100%)	-0.69	0 100 100	41, 56, 74, 88	0
24	X	82/92 (89%)	-0.31	0 100 100	49, 66, 91, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	Y	142/241 (58%)	-0.51	1 (0%) 87 87	34, 48, 72, 94	0
26	Z	73/116 (62%)	0.19	6 (8%) 11 9	59, 77, 92, 101	0
27	1	56/57 (98%)	-0.25	0 100 100	33, 39, 48, 56	0
28	2	46/50 (92%)	-0.14	1 (2%) 62 59	41, 69, 102, 114	0
29	3	92/92 (100%)	-0.13	1 (1%) 80 80	43, 65, 78, 91	0
30	0	2749/2923 (94%)	-0.32	51 (1%) 66 65	28, 51, 95, 171	0
31	9	122/122 (100%)	-0.24	3 (2%) 57 55	45, 72, 95, 154	0
All	All	6646/7517 (88%)	-0.20	240 (3%) 42 37	28, 57, 106, 175	0

The worst 5 of 240 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
9	I	71	ALA	15.5
9	I	74	ILE	13.2
31	9	1	U	12.1
22	V	1	THR	11.8
9	I	72	GLU	11.1

## 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	1MA	0	628	23/24	0.98	0.18	33,37,38,39	0
30	OMG	0	2588	24/25	0.98	0.14	36,39,42,43	0
30	PSU	0	2621	20/21	0.98	0.18	34,35,47,48	0
30	UR3	0	2619	21/22	0.98	0.15	42,44,47,47	0
30	OMU	0	2587	21/22	0.99	0.13	38,40,44,45	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	0	9006	1/1	-0.21	2.27	200,200,200,200	0
35	NA	0	8560	1/1	0.19	0.88	101,101,101,101	0
35	NA	0	8525	1/1	0.30	0.25	92,92,92,92	0
34	SR	0	8924	1/1	0.32	0.09	154,154,154,154	0
37	K	0	8401	1/1	0.41	0.77	128,128,128,128	0
34	SR	0	8962	1/1	0.53	0.19	169,169,169,169	0
34	SR	0	8947	1/1	0.54	0.51	200,200,200,200	0
34	SR	0	8991	1/1	0.65	0.07	199,199,199,199	0
35	NA	0	8528	1/1	0.65	0.56	66,66,66,66	0
34	SR	0	8955	1/1	0.68	0.20	199,199,199,199	0
35	NA	0	8506	1/1	0.68	0.16	64,64,64,64	0
35	NA	0	8563	1/1	0.69	0.28	88,88,88,88	0
35	NA	0	8562	1/1	0.69	1.31	78,78,78,78	0
35	NA	0	8509	1/1	0.70	0.93	85,85,85,85	0
35	NA	0	8502	1/1	0.72	0.15	66,66,66,66	0
35	NA	0	8530	1/1	0.73	0.32	59,59,59,59	0
34	SR	0	8982	1/1	0.73	2.26	200,200,200,200	0
34	SR	0	8994	1/1	0.74	0.43	200,200,200,200	0
34	SR	0	8993	1/1	0.74	0.10	176,176,176,176	0
35	NA	0	8548	1/1	0.75	0.26	58,58,58,58	0
35	NA	0	8511	1/1	0.75	0.29	69,69,69,69	0
34	SR	0	8979	1/1	0.76	0.14	200,200,200,200	0
35	NA	9	8543	1/1	0.77	0.11	74,74,74,74	0
34	SR	0	8986	1/1	0.78	0.41	200,200,200,200	0
35	NA	Q	8540	1/1	0.78	0.11	64,64,64,64	0
34	SR	0	8944	1/1	0.79	0.14	169,169,169,169	0
35	NA	0	8568	1/1	0.79	0.20	52,52,52,52	0
34	SR	0	8996	1/1	0.79	1.20	200,200,200,200	0
34	SR	B	8987	1/1	0.80	0.56	200,200,200,200	0
32	MG	0	8072	1/1	0.81	0.19	63,63,63,63	0
35	NA	S	8510	1/1	0.81	0.48	64,64,64,64	0
35	NA	0	8527	1/1	0.81	0.27	71,71,71,71	0
34	SR	0	9001	1/1	0.81	0.08	173,173,173,173	0
35	NA	0	8571	1/1	0.82	0.17	76,76,76,76	0
35	NA	0	8557	1/1	0.82	0.06	53,53,53,53	0
34	SR	0	8998	1/1	0.82	0.19	173,173,173,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8067	1/1	0.83	0.16	40,40,40,40	0
35	NA	0	8546	1/1	0.83	0.38	65,65,65,65	0
35	NA	0	8535	1/1	0.83	0.53	61,61,61,61	0
35	NA	J	8538	1/1	0.83	0.18	56,56,56,56	0
34	SR	0	8960	1/1	0.83	0.10	141,141,141,141	0
34	SR	A	8977	1/1	0.83	0.06	160,160,160,160	0
34	SR	0	8997	1/1	0.84	0.84	200,200,200,200	0
32	MG	9	8074	1/1	0.84	0.09	86,86,86,86	0
35	NA	0	8518	1/1	0.85	0.58	88,88,88,88	0
35	NA	0	8544	1/1	0.86	0.17	67,67,67,67	0
35	NA	0	8550	1/1	0.86	0.95	57,57,57,57	0
35	NA	0	8501	1/1	0.87	0.08	40,40,40,40	0
35	NA	0	8565	1/1	0.87	1.24	79,79,79,79	0
34	SR	0	8974	1/1	0.87	0.24	165,165,165,165	0
35	NA	0	8504	1/1	0.88	0.18	44,44,44,44	0
35	NA	0	8545	1/1	0.88	0.26	47,47,47,47	0
32	MG	0	8049	1/1	0.88	0.29	69,69,69,69	0
35	NA	0	8567	1/1	0.88	0.36	76,76,76,76	0
34	SR	0	8976	1/1	0.88	0.28	194,194,194,194	0
34	SR	0	8922	1/1	0.88	0.47	161,161,161,161	0
35	NA	0	8573	1/1	0.88	0.34	73,73,73,73	0
35	NA	0	8574	1/1	0.89	0.26	59,59,59,59	0
34	SR	0	8992	1/1	0.89	0.15	136,136,136,136	0
32	MG	0	8092	1/1	0.89	0.18	53,53,53,53	0
35	NA	0	8570	1/1	0.90	0.09	52,52,52,52	0
35	NA	0	8547	1/1	0.90	0.70	80,80,80,80	0
34	SR	0	8951	1/1	0.90	0.04	148,148,148,148	0
35	NA	0	8554	1/1	0.90	1.00	65,65,65,65	0
32	MG	0	8038	1/1	0.90	0.15	70,70,70,70	0
34	SR	0	8985	1/1	0.90	0.14	134,134,134,134	0
32	MG	0	8081	1/1	0.90	0.22	73,73,73,73	0
34	SR	0	8927	1/1	0.90	0.09	153,153,153,153	0
35	NA	0	8522	1/1	0.90	1.12	79,79,79,79	0
34	SR	0	8972	1/1	0.90	0.13	146,146,146,146	0
32	MG	0	8062	1/1	0.91	0.15	59,59,59,59	0
32	MG	0	8031	1/1	0.91	0.11	62,62,62,62	0
34	SR	0	8936	1/1	0.91	0.11	94,94,94,94	0
34	SR	0	8975	1/1	0.91	0.14	130,130,130,130	0
35	NA	0	8549	1/1	0.91	0.52	52,52,52,52	0
33	CL	O	8808	1/1	0.91	0.08	70,70,70,70	0
33	CL	0	8815	1/1	0.91	0.12	77,77,77,77	0
34	SR	0	8959	1/1	0.91	0.38	163,163,163,163	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8083	1/1	0.91	0.10	60,60,60,60	0
33	CL	A	8809	1/1	0.91	0.11	80,80,80,80	0
35	NA	0	8521	1/1	0.91	0.40	61,61,61,61	0
34	SR	0	8946	1/1	0.91	0.22	123,123,123,123	0
35	NA	0	8536	1/1	0.91	0.23	61,61,61,61	0
35	NA	0	8529	1/1	0.92	0.15	39,39,39,39	0
32	MG	0	8045	1/1	0.92	0.09	44,44,44,44	0
32	MG	0	8039	1/1	0.92	0.27	76,76,76,76	0
35	NA	0	8559	1/1	0.92	0.29	91,91,91,91	0
32	MG	0	8044	1/1	0.92	0.16	50,50,50,50	0
34	SR	0	8915	1/1	0.92	0.08	121,121,121,121	0
32	MG	0	8087	1/1	0.92	0.12	51,51,51,51	0
34	SR	0	9002	1/1	0.92	0.29	177,177,177,177	0
32	MG	0	8066	1/1	0.92	0.18	70,70,70,70	0
34	SR	A	8929	1/1	0.92	0.23	144,144,144,144	0
34	SR	0	8989	1/1	0.92	0.16	168,168,168,168	0
32	MG	0	8011	1/1	0.92	0.23	25,25,25,25	0
32	MG	A	8051	1/1	0.93	0.66	70,70,70,70	0
32	MG	0	8056	1/1	0.93	0.10	47,47,47,47	0
32	MG	0	8089	1/1	0.93	0.17	72,72,72,72	0
34	SR	0	8988	1/1	0.93	0.05	158,158,158,158	0
33	CL	N	8807	1/1	0.93	0.17	69,69,69,69	0
35	NA	0	8564	1/1	0.93	0.39	68,68,68,68	0
35	NA	0	8505	1/1	0.93	0.87	48,48,48,48	0
33	CL	0	8813	1/1	0.93	0.09	66,66,66,66	0
33	CL	Q	8811	1/1	0.93	0.15	82,82,82,82	0
35	NA	0	8526	1/1	0.93	0.08	47,47,47,47	0
34	SR	0	8942	1/1	0.93	0.08	122,122,122,122	0
32	MG	0	8075	1/1	0.93	0.03	42,42,42,42	0
32	MG	0	8077	1/1	0.93	0.07	45,45,45,45	0
32	MG	0	8037	1/1	0.93	0.14	88,88,88,88	0
32	MG	0	8091	1/1	0.93	0.07	57,57,57,57	0
35	NA	R	8575	1/1	0.93	0.25	99,99,99,99	0
32	MG	0	8006	1/1	0.93	0.10	32,32,32,32	0
34	SR	0	8928	1/1	0.93	0.06	135,135,135,135	0
35	NA	0	8569	1/1	0.93	0.15	48,48,48,48	0
34	SR	0	8965	1/1	0.93	0.09	132,132,132,132	0
33	CL	0	8814	1/1	0.94	0.21	72,72,72,72	0
34	SR	9	8980	1/1	0.94	0.15	175,175,175,175	0
34	SR	0	8969	1/1	0.94	0.12	159,159,159,159	0
35	NA	0	8561	1/1	0.94	0.22	68,68,68,68	0
35	NA	0	8512	1/1	0.94	0.14	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8901	1/1	0.94	0.08	91,91,91,91	0
32	MG	0	8033	1/1	0.94	0.09	55,55,55,55	0
32	MG	T	8057	1/1	0.94	0.12	60,60,60,60	0
35	NA	0	8551	1/1	0.94	0.37	52,52,52,52	0
33	CL	L	8810	1/1	0.94	0.09	68,68,68,68	0
34	SR	S	8961	1/1	0.94	0.06	121,121,121,121	0
34	SR	9	9003	1/1	0.94	0.09	171,171,171,171	0
35	NA	0	8515	1/1	0.94	0.20	41,41,41,41	0
34	SR	0	9000	1/1	0.94	0.07	176,176,176,176	0
34	SR	0	8973	1/1	0.94	0.05	130,130,130,130	0
32	MG	0	8055	1/1	0.94	0.16	53,53,53,53	0
34	SR	0	8995	1/1	0.94	0.15	136,136,136,136	0
32	MG	0	8014	1/1	0.94	0.20	33,33,33,33	0
32	MG	0	8060	1/1	0.94	0.08	53,53,53,53	0
32	MG	0	8036	1/1	0.94	0.12	56,56,56,56	0
34	SR	0	8968	1/1	0.94	0.03	160,160,160,160	0
33	CL	J	8821	1/1	0.95	0.14	67,67,67,67	0
32	MG	0	8070	1/1	0.95	0.12	46,46,46,46	0
32	MG	0	8082	1/1	0.95	0.78	89,89,89,89	0
35	NA	0	8520	1/1	0.95	0.07	49,49,49,49	0
35	NA	0	8533	1/1	0.95	0.10	55,55,55,55	0
35	NA	0	8523	1/1	0.95	0.09	50,50,50,50	0
33	CL	0	8803	1/1	0.95	0.10	58,58,58,58	0
34	SR	0	9008	1/1	0.95	0.17	95,95,95,95	0
32	MG	0	8093	1/1	0.95	0.08	42,42,42,42	0
33	CL	J	8802	1/1	0.95	0.21	75,75,75,75	0
35	NA	0	8516	1/1	0.95	0.11	45,45,45,45	0
32	MG	0	8053	1/1	0.95	0.19	47,47,47,47	0
34	SR	0	8966	1/1	0.95	0.10	107,107,107,107	0
35	NA	0	8537	1/1	0.95	0.18	38,38,38,38	0
35	NA	R	8532	1/1	0.96	0.12	58,58,58,58	0
35	NA	0	8519	1/1	0.96	0.20	43,43,43,43	0
32	MG	0	8040	1/1	0.96	0.21	96,96,96,96	0
34	SR	0	8943	1/1	0.96	0.04	124,124,124,124	0
32	MG	0	8035	1/1	0.96	0.10	54,54,54,54	0
32	MG	0	8046	1/1	0.96	0.14	43,43,43,43	0
34	SR	0	8971	1/1	0.96	0.07	171,171,171,171	0
34	SR	0	9004	1/1	0.96	0.31	200,200,200,200	0
32	MG	0	8016	1/1	0.96	0.14	48,48,48,48	0
35	NA	0	8556	1/1	0.96	0.82	64,64,64,64	0
32	MG	0	8041	1/1	0.96	0.21	29,29,29,29	0
34	SR	0	8908	1/1	0.96	0.08	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
35	NA	0	8542	1/1	0.96	0.45	49,49,49,49	0
35	NA	9	8572	1/1	0.96	0.89	81,81,81,81	0
32	MG	0	8047	1/1	0.96	0.32	51,51,51,51	0
33	CL	M	8818	1/1	0.96	0.10	40,40,40,40	0
32	MG	0	8001	1/1	0.96	0.11	33,33,33,33	0
34	SR	0	8963	1/1	0.96	0.17	112,112,112,112	0
34	SR	0	8953	1/1	0.96	0.13	144,144,144,144	0
32	MG	0	8003	1/1	0.96	0.19	45,45,45,45	0
34	SR	0	8917	1/1	0.96	0.10	107,107,107,107	0
35	NA	0	8555	1/1	0.96	0.81	75,75,75,75	0
34	SR	0	8921	1/1	0.96	0.15	96,96,96,96	0
32	MG	0	8013	1/1	0.97	0.06	25,25,25,25	0
34	SR	1	8913	1/1	0.97	0.14	95,95,95,95	0
34	SR	0	8957	1/1	0.97	0.13	195,195,195,195	0
32	MG	0	8079	1/1	0.97	0.11	51,51,51,51	0
32	MG	0	8002	1/1	0.97	0.15	36,36,36,36	0
32	MG	0	8020	1/1	0.97	0.07	40,40,40,40	0
32	MG	0	8050	1/1	0.97	0.09	32,32,32,32	0
32	MG	0	8024	1/1	0.97	0.12	49,49,49,49	0
34	SR	0	8939	1/1	0.97	0.10	149,149,149,149	0
32	MG	0	8021	1/1	0.97	0.05	40,40,40,40	0
34	SR	0	8919	1/1	0.97	0.07	170,170,170,170	0
35	NA	0	8558	1/1	0.97	0.23	49,49,49,49	0
33	CL	Y	8820	1/1	0.97	0.04	48,48,48,48	0
35	NA	0	8524	1/1	0.97	0.25	58,58,58,58	0
32	MG	0	8071	1/1	0.97	0.09	72,72,72,72	0
35	NA	0	8534	1/1	0.97	0.14	44,44,44,44	0
32	MG	0	8026	1/1	0.97	0.08	35,35,35,35	0
34	SR	0	8945	1/1	0.97	0.07	106,106,106,106	0
34	SR	0	8958	1/1	0.97	0.06	122,122,122,122	0
33	CL	0	8822	1/1	0.97	0.45	81,81,81,81	0
34	SR	0	8954	1/1	0.97	0.10	109,109,109,109	0
35	NA	C	8503	1/1	0.97	0.21	36,36,36,36	0
35	NA	0	8531	1/1	0.97	0.06	40,40,40,40	0
34	SR	0	9007	1/1	0.97	0.66	200,200,200,200	0
34	SR	0	8920	1/1	0.97	0.08	135,135,135,135	0
32	MG	0	8022	1/1	0.97	0.22	44,44,44,44	0
32	MG	0	8017	1/1	0.98	0.19	52,52,52,52	0
35	NA	0	8566	1/1	0.98	0.12	64,64,64,64	0
34	SR	0	8949	1/1	0.98	0.17	122,122,122,122	0
32	MG	0	8065	1/1	0.98	0.06	57,57,57,57	0
35	NA	0	8513	1/1	0.98	0.21	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8012	1/1	0.98	0.14	18,18,18,18	0
34	SR	0	8938	1/1	0.98	0.02	147,147,147,147	0
34	SR	0	8981	1/1	0.98	0.33	178,178,178,178	0
33	CL	3	8804	1/1	0.98	0.06	63,63,63,63	0
33	CL	B	8819	1/1	0.98	0.09	58,58,58,58	0
34	SR	0	8941	1/1	0.98	0.14	108,108,108,108	0
34	SR	0	8914	1/1	0.98	0.32	120,120,120,120	0
34	SR	0	8940	1/1	0.98	0.07	97,97,97,97	0
32	MG	0	8069	1/1	0.98	0.30	73,73,73,73	0
35	NA	0	8508	1/1	0.98	0.20	35,35,35,35	0
34	SR	0	8923	1/1	0.98	0.10	101,101,101,101	0
32	MG	0	8025	1/1	0.98	0.12	37,37,37,37	0
34	SR	0	8933	1/1	0.98	0.16	139,139,139,139	0
35	NA	0	8507	1/1	0.98	0.11	37,37,37,37	0
32	MG	0	8023	1/1	0.98	0.10	37,37,37,37	0
32	MG	0	8088	1/1	0.98	0.20	52,52,52,52	0
35	NA	0	8541	1/1	0.98	0.18	75,75,75,75	0
34	SR	0	8983	1/1	0.98	0.24	170,170,170,170	0
32	MG	0	8030	1/1	0.98	0.30	68,68,68,68	0
32	MG	0	8063	1/1	0.98	0.14	80,80,80,80	0
32	MG	0	8068	1/1	0.98	0.08	51,51,51,51	0
32	MG	0	8052	1/1	0.98	0.07	56,56,56,56	0
32	MG	0	8028	1/1	0.98	0.16	26,26,26,26	0
34	SR	0	8984	1/1	0.98	0.03	121,121,121,121	0
33	CL	0	8805	1/1	0.98	0.06	67,67,67,67	0
32	MG	0	8078	1/1	0.98	0.27	69,69,69,69	0
34	SR	B	8950	1/1	0.98	0.14	116,116,116,116	0
32	MG	0	8085	1/1	0.98	0.53	97,97,97,97	0
34	SR	1	8952	1/1	0.98	0.15	89,89,89,89	0
32	MG	K	8054	1/1	0.98	0.16	46,46,46,46	0
35	NA	0	8553	1/1	0.98	0.47	65,65,65,65	0
32	MG	0	8034	1/1	0.98	0.16	46,46,46,46	0
33	CL	0	8812	1/1	0.98	0.06	58,58,58,58	0
34	SR	0	8910	1/1	0.98	0.04	100,100,100,100	0
34	SR	0	8964	1/1	0.98	0.09	131,131,131,131	0
34	SR	0	8937	1/1	0.98	0.27	112,112,112,112	0
35	NA	0	8514	1/1	0.98	0.50	56,56,56,56	0
34	SR	3	8999	1/1	0.98	0.10	110,110,110,110	0
34	SR	0	8934	1/1	0.98	0.24	134,134,134,134	0
35	NA	B	8552	1/1	0.98	0.10	83,83,83,83	0
34	SR	0	8926	1/1	0.98	0.17	108,108,108,108	0
37	K	0	8402	1/1	0.98	0.25	76,76,76,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
33	CL	R	8806	1/1	0.98	0.18	57,57,57,57	0
33	CL	J	8801	1/1	0.99	0.07	79,79,79,79	0
34	SR	0	8911	1/1	0.99	0.08	85,85,85,85	0
32	MG	0	8043	1/1	0.99	0.06	52,52,52,52	0
32	MG	0	8064	1/1	0.99	0.19	44,44,44,44	0
34	SR	0	8970	1/1	0.99	0.02	123,123,123,123	0
32	MG	Y	8086	1/1	0.99	0.08	44,44,44,44	0
34	SR	0	8990	1/1	0.99	0.10	139,139,139,139	0
32	MG	0	8009	1/1	0.99	0.25	36,36,36,36	0
34	SR	F	9005	1/1	0.99	0.08	133,133,133,133	0
32	MG	0	8059	1/1	0.99	0.07	57,57,57,57	0
34	SR	0	8902	1/1	0.99	0.17	66,66,66,66	0
33	CL	0	8817	1/1	0.99	0.15	67,67,67,67	0
32	MG	0	8076	1/1	0.99	0.08	40,40,40,40	0
36	CD	O	8705	1/1	0.99	0.06	118,118,118,118	0
32	MG	0	8061	1/1	0.99	0.23	37,37,37,37	0
35	NA	M	8539	1/1	0.99	0.18	34,34,34,34	0
32	MG	0	8048	1/1	0.99	0.24	33,33,33,33	0
32	MG	0	8010	1/1	0.99	0.22	45,45,45,45	0
34	SR	3	8932	1/1	0.99	0.14	76,76,76,76	0
32	MG	0	8027	1/1	0.99	0.11	51,51,51,51	0
36	CD	Z	8703	1/1	0.99	0.13	75,75,75,75	0
32	MG	0	8032	1/1	0.99	0.05	44,44,44,44	0
34	SR	0	8931	1/1	0.99	0.07	113,113,113,113	0
32	MG	0	8007	1/1	0.99	0.16	32,32,32,32	0
32	MG	0	8029	1/1	0.99	0.15	49,49,49,49	0
32	MG	0	8080	1/1	0.99	0.12	75,75,75,75	0
34	SR	0	8909	1/1	0.99	0.15	88,88,88,88	0
33	CL	0	8816	1/1	0.99	0.08	79,79,79,79	0
32	MG	0	8019	1/1	0.99	0.20	28,28,28,28	0
36	CD	1	8702	1/1	0.99	0.13	67,67,67,67	0
34	SR	R	8912	1/1	0.99	0.16	92,92,92,92	0
32	MG	0	8073	1/1	0.99	0.35	73,73,73,73	0
34	SR	9	8978	1/1	0.99	0.08	135,135,135,135	0
34	SR	0	8948	1/1	0.99	0.10	92,92,92,92	0
32	MG	0	8084	1/1	0.99	0.15	33,33,33,33	0
34	SR	0	8967	1/1	0.99	0.06	133,133,133,133	0
34	SR	0	8906	1/1	0.99	0.24	64,64,64,64	0
34	SR	0	8918	1/1	0.99	0.15	80,80,80,80	0
35	NA	0	8517	1/1	0.99	0.15	31,31,31,31	0
32	MG	0	8015	1/1	0.99	0.13	30,30,30,30	0
32	MG	0	8005	1/1	0.99	0.23	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	SR	0	8904	1/1	0.99	0.18	65,65,65,65	0
36	CD	U	8701	1/1	0.99	0.10	63,63,63,63	0
34	SR	0	8956	1/1	0.99	0.06	155,155,155,155	0
32	MG	B	8042	1/1	0.99	0.07	44,44,44,44	0
34	SR	0	8935	1/1	0.99	0.09	79,79,79,79	0
34	SR	A	8930	1/1	0.99	0.06	97,97,97,97	0
32	MG	0	8090	1/1	0.99	0.10	65,65,65,65	0
34	SR	0	8916	1/1	1.00	0.03	120,120,120,120	0
34	SR	0	8903	1/1	1.00	0.19	59,59,59,59	0
32	MG	0	8008	1/1	1.00	0.09	28,28,28,28	0
34	SR	0	8905	1/1	1.00	0.27	61,61,61,61	0
32	MG	0	8018	1/1	1.00	0.23	40,40,40,40	0
32	MG	0	8058	1/1	1.00	0.09	22,22,22,22	0
34	SR	0	8907	1/1	1.00	0.15	56,56,56,56	0
36	CD	3	8704	1/1	1.00	0.10	74,74,74,74	0
32	MG	0	8004	1/1	1.00	0.19	32,32,32,32	0
34	SR	0	8925	1/1	1.00	0.08	86,86,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.