



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 03:33 am BST

PDB ID : 1K73
Title : Co-crystal Structure of Anisomycin Bound to the 50S Ribosomal Subunit
Authors : Hansen, J.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on : 2001-10-18
Resolution : 3.01 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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
buster-report : 1.1.7 (2018)
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

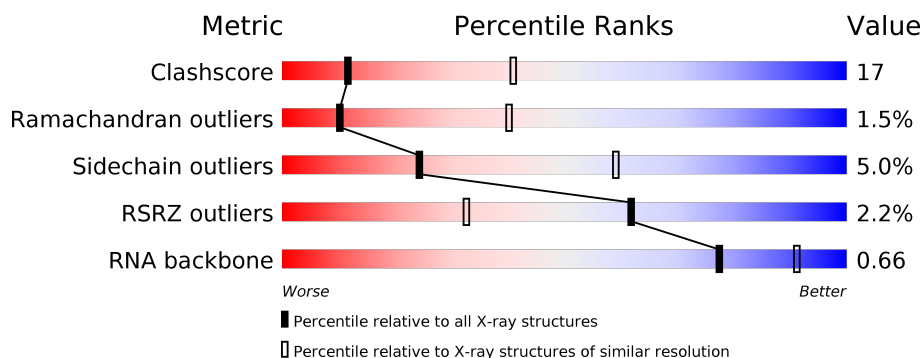
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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.



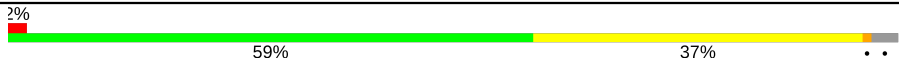

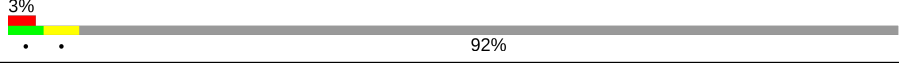
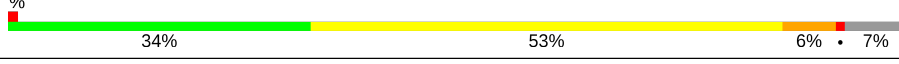

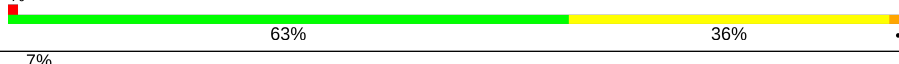
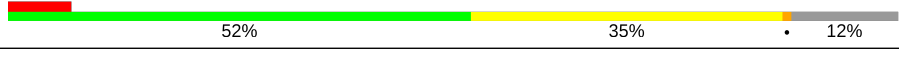
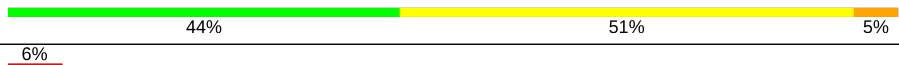



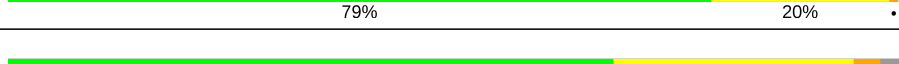


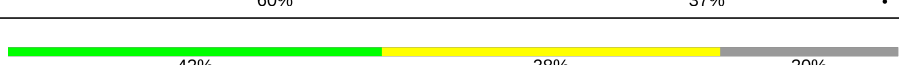

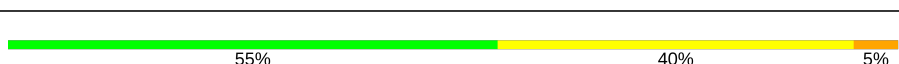

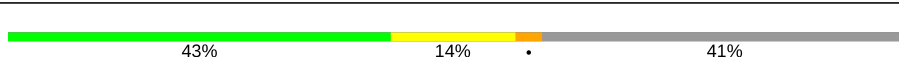


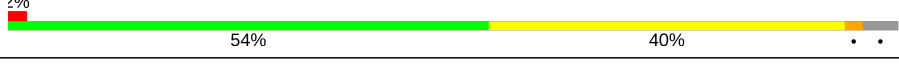
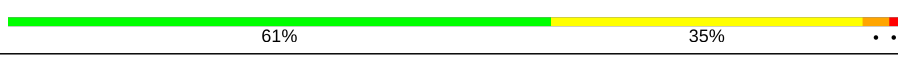

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)
RNA backbone	3102	1066 (3.30-2.74)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	2922	<div> <div>4%</div> <div>59%</div> <div>29%</div> <div>5%</div> <div>6%</div> </div>
2	B	122	<div> <div>4%</div> <div>54%</div> <div>32%</div> <div>8%</div> <div>6%</div> </div>
3	C	239	<div> <div>3%</div> <div>56%</div> <div>37%</div> <div>6%</div> </div>
4	D	337	<div> <div>53%</div> <div>42%</div> <div>5%</div> </div>
5	E	246	<div> <div>61%</div> <div>35%</div> <div>5%</div> </div>
6	F	176	<div> <div>16%</div> <div>26%</div> <div>45%</div> <div>7%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	177	
8	H	119	
9	I	348	
10	J	167	
11	K	145	
12	L	132	
13	M	164	
14	N	194	
15	O	186	
16	P	115	
17	Q	148	
18	R	95	
19	S	154	
20	T	84	
21	U	119	
22	V	66	
23	W	70	
24	X	154	
25	Y	91	
26	Z	240	
27	1	73	
28	2	56	
29	3	48	
30	4	92	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	A	8049	-	-	-	X
34	NA	A	8306	-	-	-	X
34	NA	A	8313	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8329	-	-	-	X
34	NA	A	8361	-	-	-	X
34	NA	A	8363	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	A	8385	-	-	-	X
34	NA	J	8322	-	-	-	X
34	NA	S	8386	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98548 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	CONFLICT	? 3377779

- Molecule 2 is a RNA chain called 5S RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	337	Total	C	N	O	S	0	0	0
			2624	1616	493	510	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	DELETION	UNP P20279
D	310	ARG	PHE	CONFLICT	UNP P20279

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	246	Total	C	N	O	S	0	0	0
			1858	1131	344	382	1			

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	119	Total	C	N	O	S	0	0	0
			885	552	141	191	1			

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	156	Total	C	N	O	S	0	0	0
			1215	766	233	212	4			

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	142	Total	C	N	O	S	0	0	0
			1119	696	199	221	3			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	132	Total	C	N	O	S	0	0	0
			993	609	189	191	4			

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	145	Total	C	N	O	S	0	0	0
			1114	668	222	224				

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	194	Total	C	N	O	S	0	0	0
			1605	988	346	266	5			

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	186	Total	C	N	O	S	0	0	0
			1444	895	262	285	2			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	115	Total	C	N	O	S	0	0	0
			864	529	161	174				

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	143	Total	C	N	O	S	0	0	0
			1133	680	230	223				

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	71	LYS	TYR	CONFLICT	UNP P14119

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	95	Total	C	N	O			
			734	450	141	143	0	0	0

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	119	Total	C	N	O			
			949	568	180	201		0	0

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	X	154	Total	C	N	O	S		
			1195	737	209	243	6	0	0

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

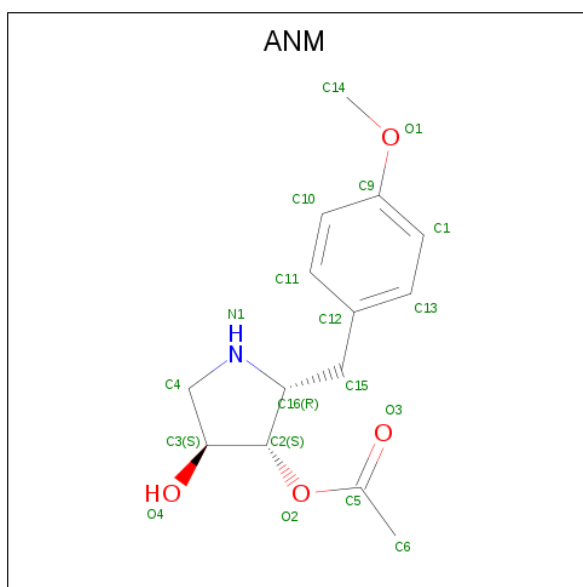
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	?	-	ARG	DELETION	UNP P22452

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is ANISOMYCIN (three-letter code: ANM) (formula: C₁₄H₁₉NO₄).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	D	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	C	2	Total	Mg	0	0
			2	2		
32	Z	1	Total	Mg	0	0
			1	1		
32	A	109	Total	Mg	0	0
			109	109		
32	4	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	L	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	A	2	Total K 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	2	Total Na 2 2	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	71	Total Na 71 71	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0
34	U	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	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	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	3	Total Cl 3 3	0	0
35	C	1	Total Cl 1 1	0	0
35	Z	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	9	Total 9	Cl 9	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cd 1	0	0
36	2	1	Total 1	Cd 1	0	0
36	1	1	Total 1	Cd 1	0	0
36	4	1	Total 1	Cd 1	0	0
36	V	1	Total 1	Cd 1	0	0

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5924	Total 5924	O 5924	0	0
37	B	143	Total 143	O 143	0	0
37	C	127	Total 127	O 127	0	0
37	D	146	Total 146	O 146	0	0
37	E	164	Total 164	O 164	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	F	54	Total 54	O 54	0	0
37	G	42	Total 42	O 42	0	0
37	H	28	Total 28	O 28	0	0
37	I	22	Total 22	O 22	0	0
37	J	79	Total 79	O 79	0	0
37	K	56	Total 56	O 56	0	0
37	L	62	Total 62	O 62	0	0
37	M	81	Total 81	O 81	0	0
37	N	126	Total 126	O 126	0	0
37	O	66	Total 66	O 66	0	0
37	P	44	Total 44	O 44	0	0
37	Q	65	Total 65	O 65	0	0
37	R	54	Total 54	O 54	0	0
37	S	86	Total 86	O 86	0	0
37	T	35	Total 35	O 35	0	0
37	U	41	Total 41	O 41	0	0
37	V	25	Total 25	O 25	0	0
37	W	15	Total 15	O 15	0	0
37	X	67	Total 67	O 67	0	0
37	Y	29	Total 29	O 29	0	0
37	Z	92	Total 92	O 92	0	0

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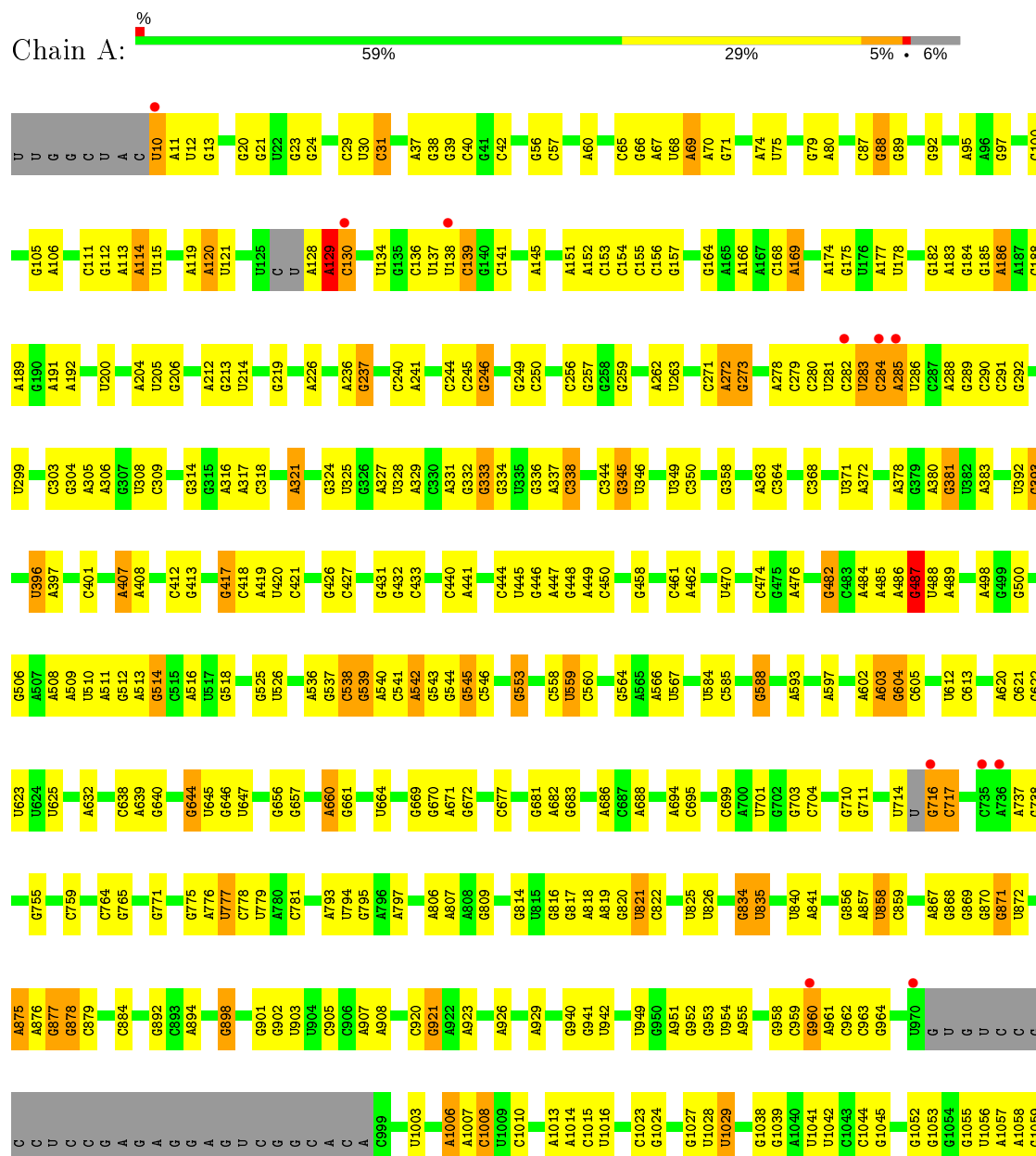
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	1	38	Total 38	O 38	0	0
37	2	56	Total 56	O 56	0	0
37	3	40	Total 40	O 40	0	0
37	4	72	Total 72	O 72	0	0

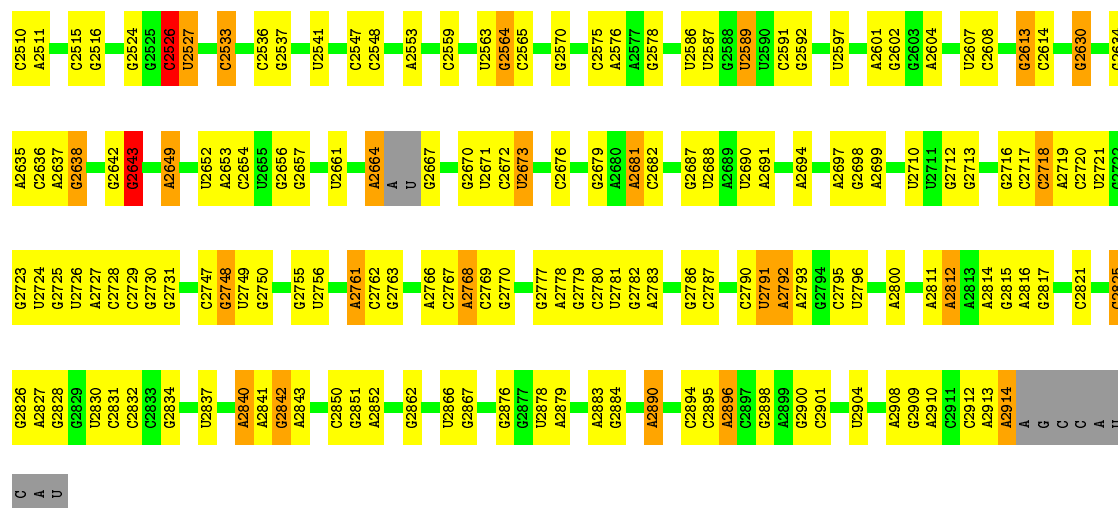
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

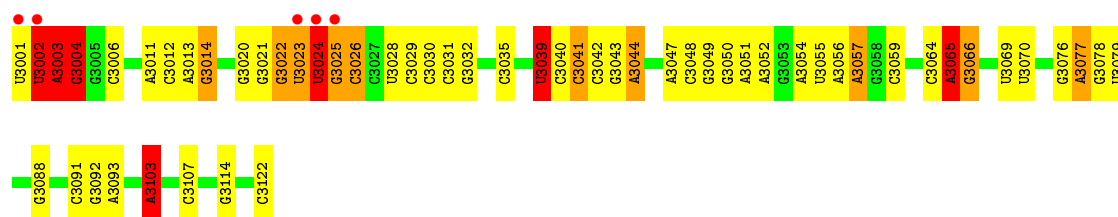
• Molecule 1: 23S rRNA



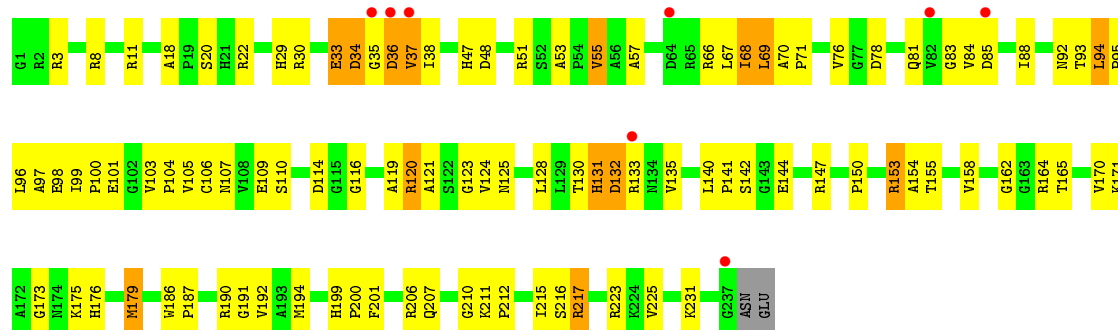
A2414	G2310	G1947	C1826	A1712	C1613	G1497	A1375	G1239	G1167	G1060
A2415	A2311	G1948	C1829	G1713	G1614	G1497	G1376	A1242	C1168	
G2416	G2312	G1951	A1829	G1714	A1615	U1500	C1377	A1243	U1169	G1072
G2417	C2313	U	C1830	C1715	A1616	A1501	U1380	G1244	U1170	
G2418	G2314	A	C1834	A1716	A1617	A1502	U1384	G1245	A1171	G1076
U2419	G2315	A	U1835	A1717	C1617	U1503	C1384	C1246	G1172	
G2420	G2316	C	A1840	U1722	U1625	A1504	U1384	A1246	A1173	A1079
G2421	C2317	U	A1845	U1723	U1626	A1506	A1393	U1249	A1174	C1080
U2422	U2318	A	U1847	C1725	G1627	U1517	C1394	C1251	G1175	A1081
A2425	U2320	U	A1848	G1730	A1630	A1515	G1398	U1266	A1176	C1082
A2426	A2321	G	U1849	G1731	C1633	U1517	A1399	C1267	G1178	G1085
G2427	G2322	A	G1849	A1732	U1634	G1523	A1407	C1268	U1180	A1086
G2428	G2323	C	U1850	A1733	G1636	G1524	U1408	C1269	A1181	G1087
G2429	G2324	C	G1851	C1734	A1637	U1525	G1409	U1270	C1182	A1088
A2434	U2325	U	A1852	G1735	A1641	A1526	G1415	C1273	C1183	U1096
U2435	G2326	U	C1853	A1736	A1642	A1527	G1416	U1279	C1184	A1097
C2443	C2327	A	U1854	A1737	A1643	A1528	G1417	C1289	U1185	A1098
U2445	U2328	C	G1855	C1738	A1644	A1529	G1418	G1290	A1187	A1099
G2446	G2329	C	A1857	U1741	A1653	G1535	U1422	U1298	A1188	U1109
A2456	U2330	U	C1862	A1742	U1654	C1536	G1423	G1299	G1190	G1110
U2457	G2338	C	G1868	G1751	G1655	G1543	U1424	U1304	A1191	A1114
G2462	A2344	U	U1874	G1752	A1656	U1544	G1430	U1305	A1192	U1115
A2463	G2345	U	U1877	A1766	A1657	U1545	G1437	U1306	U1197	U1116
G2464	C2346	A	G1878	U1767	A1666	G1546	U1437	C1305	U1198	A1117
A2465	U2347	C	U1879	C1768	A1667	G1555	A1437	U1309	A1119	G1119
G2466	A2348	C	A1982	U1770	U1668	U1559	G1441	U1310	U1200	U1120
A2467	G2349	C	U1986	G1771	A1669	U1561	G1442	G1311	G1121	G1121
G2468	U2350	C	A1987	C1772	G1670	C1562	G1443	G1312	A1202	A1122
A2469	G2351	C	U1989	G1773	C1679	U1563	G1444	A1313	G1203	U1123
C2472	C2352	C	G2001	A1778	G1680	C1564	G1445	U1314	U1205	G1127
G2476	U2353	C	U2002	A1779	G1681	U1564	U1446	G1325	U1206	U1128
G2482	A2361	C	U2003	U1788	A1682	C1574	U1447	U1326	A1207	C1129
A2483	G2362	C	U2004	C1787	A1683	C1574	C1450	A1328	C1208	U1130
U2484	A2363	U	U2008	U1789	A1684	A1580	C1451	A1329	G1131	A1132
A2485	G2364	C	A2010	G1789	A1685	U1586	A1458	U1333	A1133	G1134
G2486	U2365	C	A1910	C1798	G1688	U1587	A1458	C1334	G1137	
C2487	C2366	C	A1919	A1804	C1692	U1592	C1462	C1335	U1138	
A2488	G2367	C	A1921	G1805	A1693	C1593	A1463	G1216	G1139	
U2490	U2368	C	A1922	G1809	G1694	C1594	A1470	U1218	C1140	
G2493	U2369	C	A1923	U1809	C1699	C1595	C1474	C1342	G1151	
G2501	A2401	C	A1924	A1815	C1700	U1596	C1477	G1351	G1159	
C2502	U2402	A	A1927	C1816	A1701	A1597	U1478	A1352	U1160	
A2503	C2403	C	U1927	G1819	U1702	A1598	U1478	C1353	A1161	
G2504	U2404	C	C1940	U1820	G1706	A1603	A1482	U1234	G1162	
A2505	A2405	C	A1941	A1821	G1707	G1604	C1483	G1235	G1163	
G2506	U2406	C	C1942	A1822	A1710	A1605	G1484	U1237	U1164	
C2507	A2412	C	C1943	U1825	A1711	A1607	A1485	A1372	G1165	
A2509	G2413	C							C1238	A1166



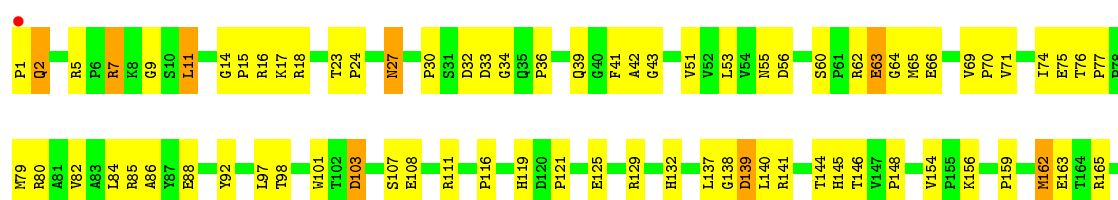
- Molecule 2: 5S rRNA

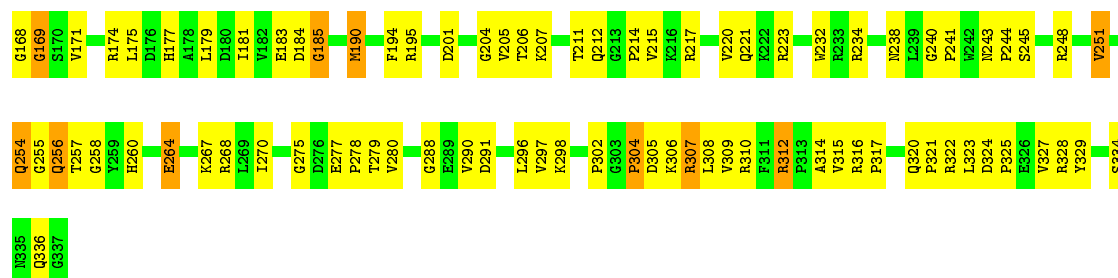


- Molecule 3: RIBOSOMAL PROTEIN L2



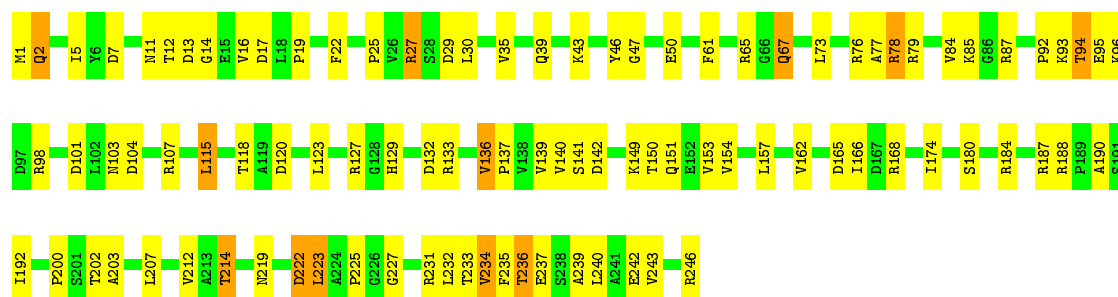
- Molecule 4: RIBOSOMAL PROTEIN L3





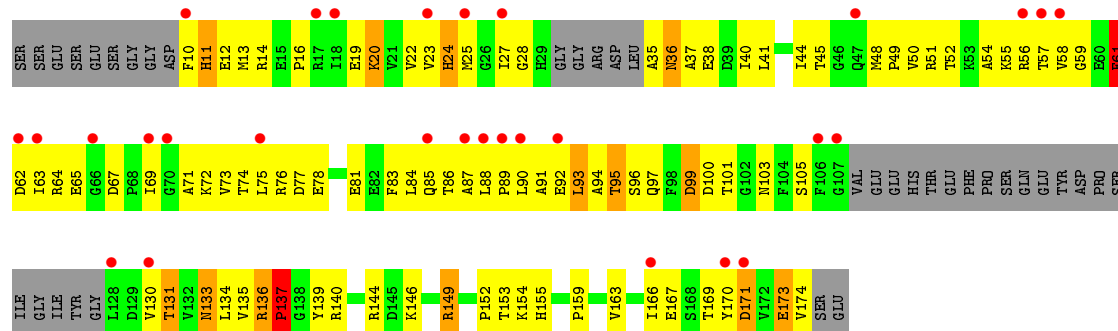
• Molecule 5: RIBOSOMAL PROTEIN L4

Chain E: 61% 35% 5%



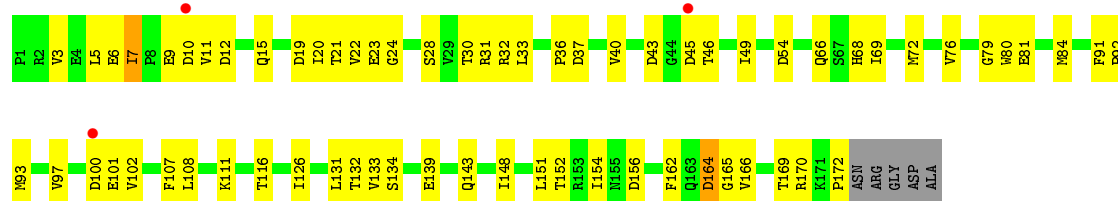
• Molecule 6: RIBOSOMAL PROTEIN L5

Chain F: 16% 26% 45% 7% 20%



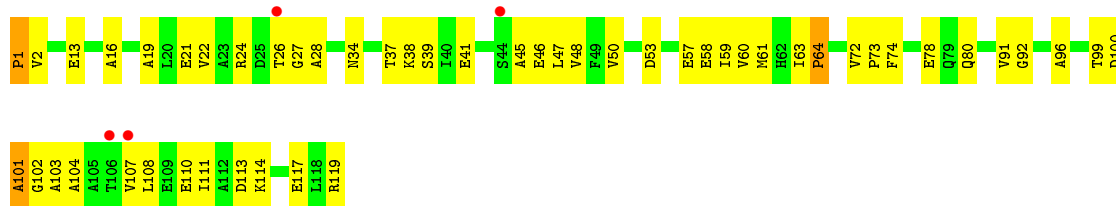
• Molecule 7: RIBOSOMAL PROTEIN L6

Chain G: 2% 59% 37%

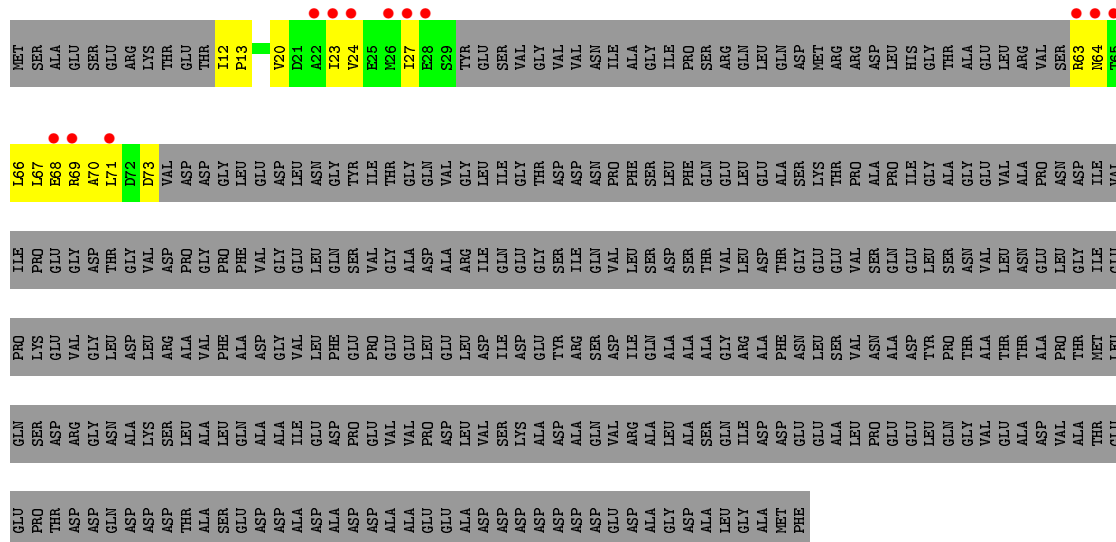


• Molecule 8: RIBOSOMAL PROTEIN L7AE

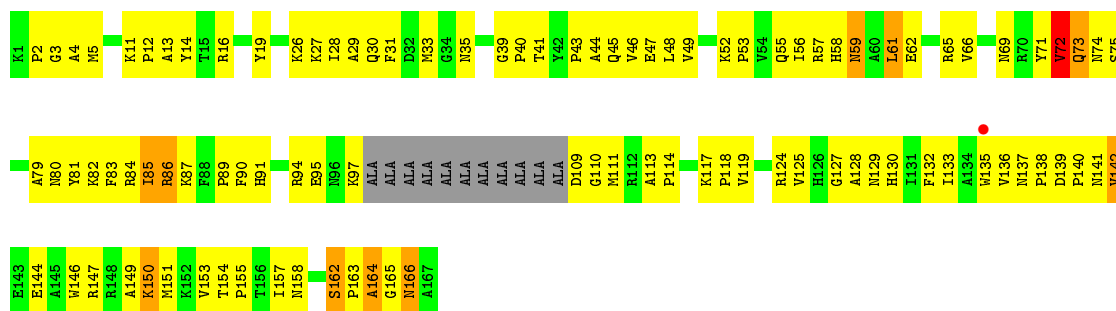
Chain H: 3% 57% 40%



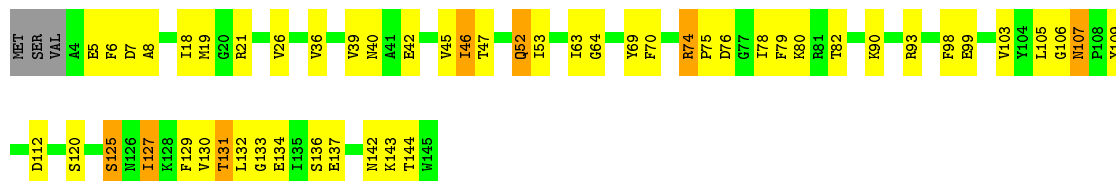
● Molecule 9: RIBOSOMAL PROTEIN L10



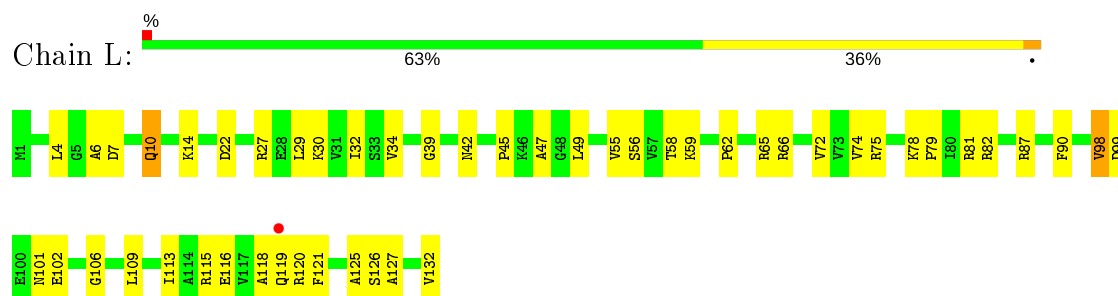
● Molecule 10: RIBOSOMAL PROTEIN L10E



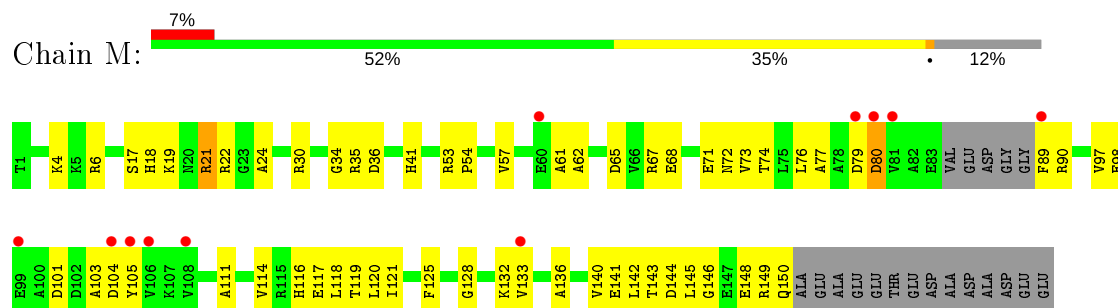
● Molecule 11: RIBOSOMAL PROTEIN L13



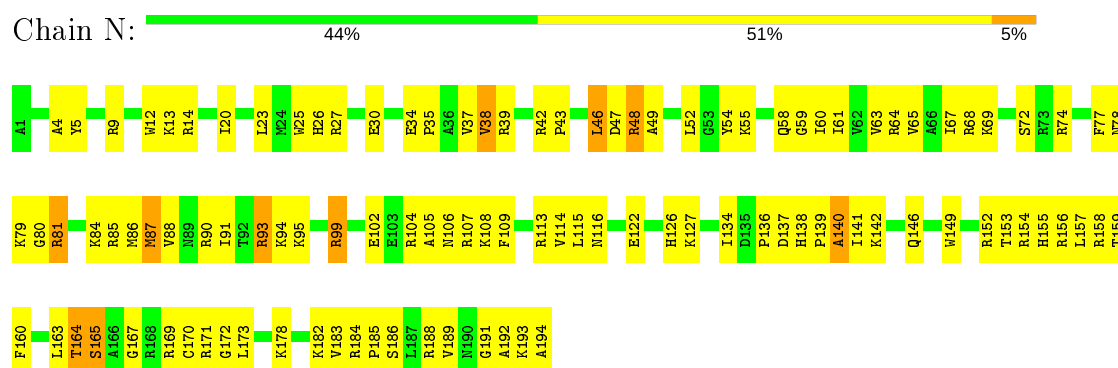
- Molecule 12: RIBOSOMAL PROTEIN L14



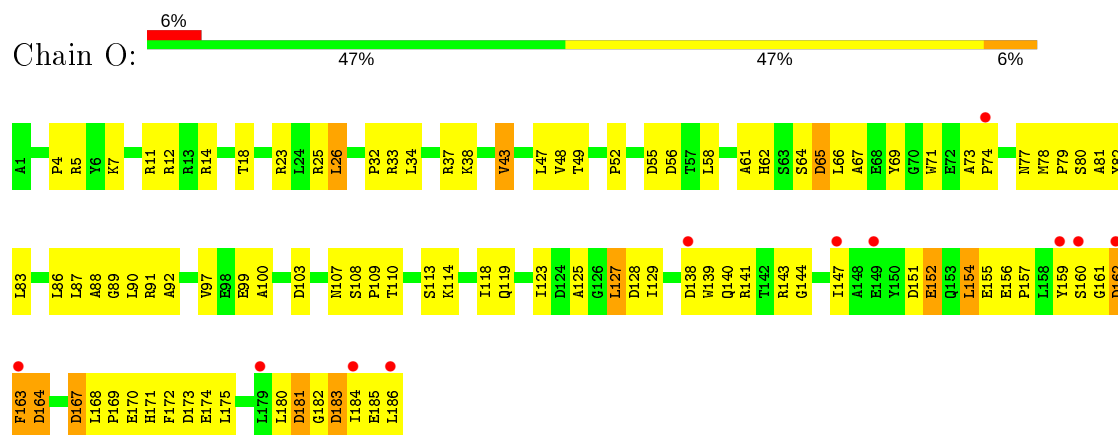
- Molecule 13: RIBOSOMAL PROTEIN L15



- Molecule 14: RIBOSOMAL PROTEIN L15E



- Molecule 15: RIBOSOMAL PROTEIN L18



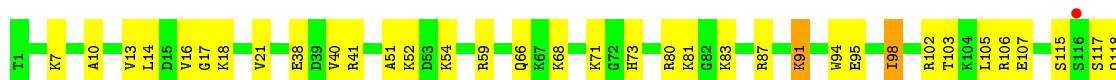
- Molecule 16: RIBOSOMAL PROTEIN L18E

Chain P:  75% 24%




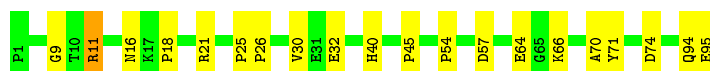
• Molecule 17: RIBOSOMAL PROTEIN L19E

Chain Q:  69% 26%



• Molecule 18: RIBOSOMAL PROTEIN L21E

Chain R:  79% 20%



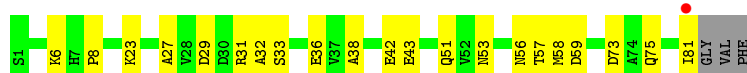
• Molecule 19: RIBOSOMAL PROTEIN L22

Chain S:  68% 27%



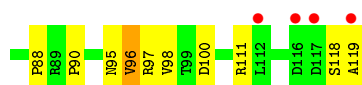
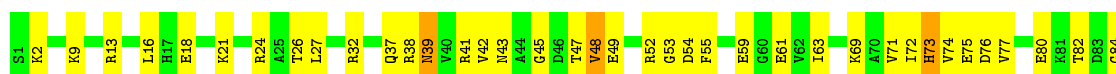
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain T:  71% 25%



• Molecule 21: RIBOSOMAL PROTEIN L24

Chain U:  3% 60% 37%



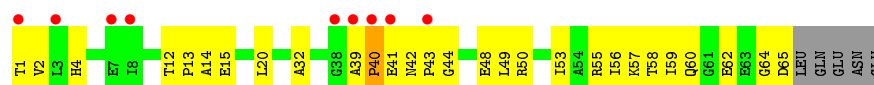
- Molecule 22: RIBOSOMAL PROTEIN L24E

Chain V: 



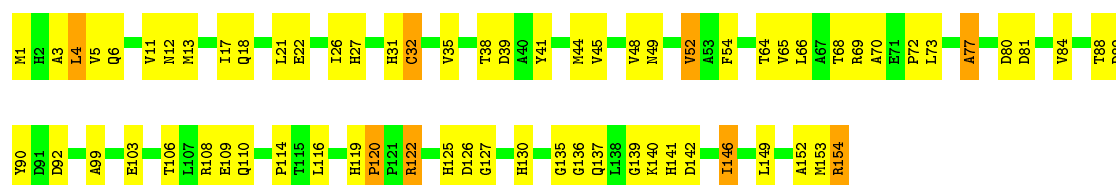
- Molecule 23: RIBOSOMAL PROTEIN L29

Chain W: 



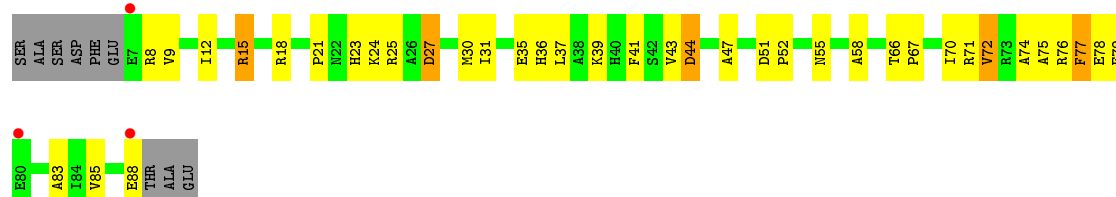
- Molecule 24: RIBOSOMAL PROTEIN L30

Chain X: 



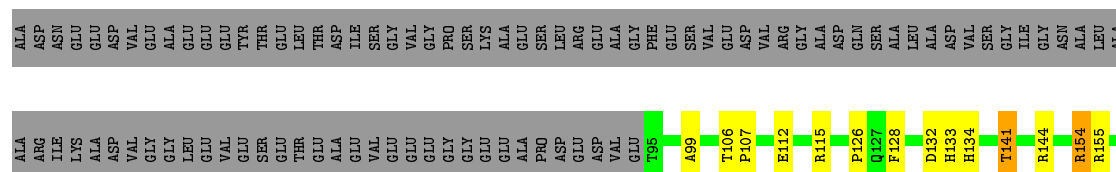
- Molecule 25: RIBOSOMAL PROTEIN L31E

Chain Y: 

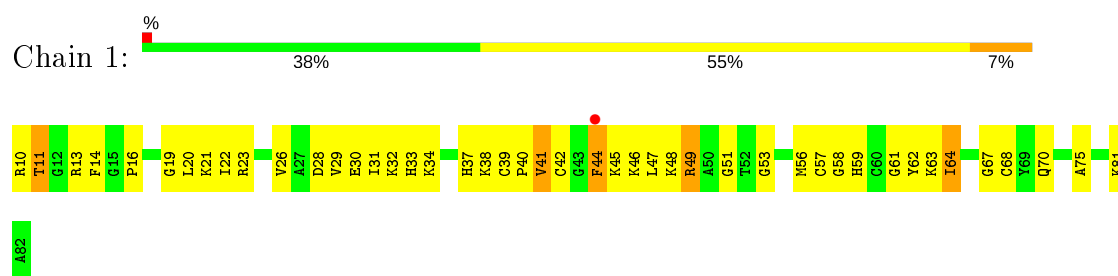


- Molecule 26: RIBOSOMAL PROTEIN L32E

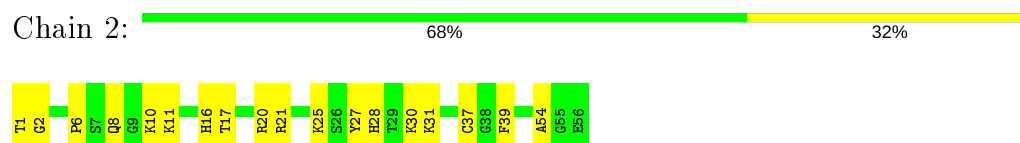
Chain Z: 



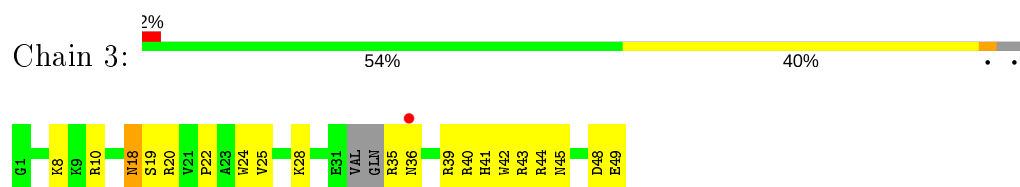
- Molecule 27: RIBOSOMAL PROTEIN L37Ae



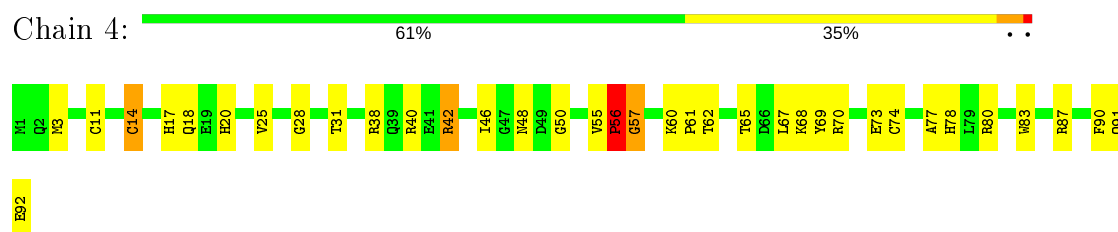
- Molecule 28: RIBOSOMAL PROTEIN L37E



- Molecule 29: RIBOSOMAL PROTEIN L39E



- Molecule 30: RIBOSOMAL PROTEIN L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.25Å 300.75Å 574.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.01 49.94 – 3.01	Depositor EDS
% Data completeness (in resolution range)	90.9 (20.00-3.01) 90.9 (49.94-3.01)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.246 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	98548	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, CL, ANM, K, CD, NA

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	0.76	25/66076 (0.0%)	0.79	41/103052 (0.0%)
2	B	0.69	3/2905 (0.1%)	0.85	7/4528 (0.2%)
3	C	0.51	0/1787	0.76	0/2409
4	D	0.53	0/2689	0.74	0/3652
5	E	0.59	0/1883	0.78	0/2551
6	F	0.44	0/1111	0.66	0/1498
7	G	0.49	0/1382	0.66	0/1880
8	H	0.53	0/896	0.65	0/1219
9	I	0.41	0/241	0.57	0/324
10	J	0.57	0/1246	0.83	1/1686 (0.1%)
11	K	0.56	0/1135	0.71	0/1530
12	L	0.53	0/1003	0.78	0/1351
13	M	0.51	0/1126	0.77	0/1504
14	N	0.59	0/1633	0.81	0/2180
15	O	0.50	0/1473	0.74	0/1999
16	P	0.57	0/873	0.77	0/1181
17	Q	0.49	0/1143	0.68	0/1521
18	R	0.57	0/748	0.79	0/1005
19	S	0.58	0/1172	0.78	0/1578
20	T	0.50	0/648	0.68	0/875
21	U	0.48	0/957	0.74	0/1289
22	V	0.52	0/417	0.68	0/562
23	W	0.45	0/502	0.60	0/675
24	X	0.59	1/1218 (0.1%)	0.76	0/1655
25	Y	0.51	0/664	0.70	0/895
26	Z	0.53	0/1146	0.75	0/1536
27	1	0.56	0/575	0.80	0/763
28	2	0.61	0/437	0.80	0/578
29	3	0.51	0/398	0.63	0/527
30	4	0.57	1/771 (0.1%)	0.77	0/1024
All	All	0.70	30/98255 (0.0%)	0.78	49/147027 (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	A	1	58
2	B	1	2
All	All	2	60

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2486	A	O3'-P	41.07	2.10	1.61
1	A	2487	C	P-OP2	9.93	1.65	1.49
1	A	2486	A	C4'-C3'	-8.66	1.43	1.53
1	A	2487	C	P-O5'	-8.62	1.51	1.59
1	A	2486	A	C3'-C2'	-6.98	1.45	1.52

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1165	G	O5'-P-OP1	-20.25	86.40	110.70
1	A	1164	U	OP1-P-O3'	-19.15	63.06	105.20
1	A	1164	U	OP2-P-O3'	-16.02	69.95	105.20
1	A	1165	G	O5'-P-OP2	-13.21	93.81	105.70
2	B	3003	A	O5'-P-OP1	-11.17	95.65	105.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	A	Sidechain
1	A	246	G	Sidechain
1	A	321	A	Sidechain
1	A	333	G	Sidechain
1	A	396	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	A	59017	0	29807	895	0
2	B	2600	0	1326	83	0
3	C	1754	0	1763	120	0
4	D	2624	0	2533	173	0
5	E	1858	0	1816	111	0
6	F	1094	0	1085	134	0
7	G	1357	0	1266	74	0
8	H	885	0	854	62	0
9	I	240	0	231	21	0
10	J	1215	0	1215	153	0
11	K	1119	0	1098	57	0
12	L	993	0	1027	53	0
13	M	1114	0	1072	59	0
14	N	1605	0	1676	148	0
15	O	1444	0	1401	121	0
16	P	864	0	873	30	0
17	Q	1133	0	1127	44	0
18	R	734	0	728	15	0
19	S	1149	0	1122	56	0
20	T	641	0	605	23	0
21	U	949	0	923	52	0
22	V	410	0	364	33	0
23	W	499	0	511	27	0
24	X	1195	0	1137	88	0
25	Y	654	0	653	45	0
26	Z	1130	0	1133	55	0
27	1	563	0	597	56	0
28	2	430	0	426	22	0
29	3	393	0	406	28	0
30	4	755	0	730	36	0
31	A	19	0	19	1	0
32	4	1	0	0	0	0
32	A	109	0	0	0	0
32	B	1	0	0	0	0
32	C	2	0	0	0	0
32	D	1	0	0	0	0
32	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	M	1	0	0	0	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	38	0	0	14	0
37	2	56	0	0	1	0
37	3	40	0	0	6	0
37	4	72	0	0	9	0
37	A	5924	0	0	183	0
37	B	143	0	0	15	0
37	C	127	0	0	22	0
37	D	146	0	0	24	0
37	E	164	0	0	28	0
37	F	54	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	42	0	0	11	0
37	H	28	0	0	9	0
37	I	22	0	0	6	0
37	J	79	0	0	23	0
37	K	56	0	0	5	0
37	L	62	0	0	10	0
37	M	81	0	0	18	0
37	N	126	0	0	21	0
37	O	66	0	0	17	0
37	P	44	0	0	5	0
37	Q	65	0	0	3	0
37	R	54	0	0	2	0
37	S	86	0	0	11	0
37	T	35	0	0	5	0
37	U	41	0	0	4	0
37	V	25	0	0	6	0
37	W	15	0	0	2	0
37	X	67	0	0	8	0
37	Y	29	0	0	4	0
37	Z	92	0	0	16	0
All	All	98548	0	59524	2621	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 17.

The worst 5 of 2621 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:A:1160:G:H5'	1:A:1161:A:H5'	1.24	1.18
5:E:236:THR:HG22	5:E:239:ALA:H	1.04	1.14
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.64	1.12
1:A:1134:G:H4'	10:J:151:MET:HE1	1.31	1.10
1:A:2486:A:O3'	1:A:2487:C:P	2.10	1.09

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	
3	C	235/239 (98%)	212 (90%)	19 (8%)	4 (2%)	9	37
4	D	335/337 (99%)	310 (92%)	18 (5%)	7 (2%)	7	31
5	E	244/246 (99%)	222 (91%)	22 (9%)	0	100	100
6	F	134/176 (76%)	99 (74%)	24 (18%)	11 (8%)	1	3
7	G	170/177 (96%)	162 (95%)	8 (5%)	0	100	100
8	H	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	9	37
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	132 (87%)	15 (10%)	5 (3%)	4	20
11	K	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	7	31
12	L	130/132 (98%)	121 (93%)	7 (5%)	2 (2%)	10	40
13	M	141/164 (86%)	122 (86%)	17 (12%)	2 (1%)	11	41
14	N	192/194 (99%)	177 (92%)	12 (6%)	3 (2%)	9	38
15	O	184/186 (99%)	167 (91%)	10 (5%)	7 (4%)	3	17
16	P	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
17	Q	141/148 (95%)	137 (97%)	4 (3%)	0	100	100
18	R	93/95 (98%)	87 (94%)	6 (6%)	0	100	100
19	S	148/154 (96%)	142 (96%)	6 (4%)	0	100	100
20	T	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
21	U	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
22	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
23	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	4	21
24	X	152/154 (99%)	146 (96%)	4 (3%)	2 (1%)	12	43
25	Y	80/91 (88%)	70 (88%)	9 (11%)	1 (1%)	12	43
26	Z	140/240 (58%)	140 (100%)	0	0	100	100
27	1	71/73 (97%)	64 (90%)	5 (7%)	2 (3%)	5	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	87 (97%)	1 (1%)	2 (2%)	6	30
All	All	3633/4235 (86%)	3351 (92%)	227 (6%)	55 (2%)	10	40

5 of 55 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	137	PRO
6	F	173	GLU

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	
3	C	179/181 (99%)	166 (93%)	13 (7%)	14	43
4	D	282/282 (100%)	263 (93%)	19 (7%)	16	47
5	E	193/193 (100%)	178 (92%)	15 (8%)	12	40
6	F	117/147 (80%)	108 (92%)	9 (8%)	13	41
7	G	152/155 (98%)	148 (97%)	4 (3%)	46	77
8	H	92/92 (100%)	91 (99%)	1 (1%)	73	90
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	112 (92%)	10 (8%)	11	38
11	K	118/121 (98%)	108 (92%)	10 (8%)	10	36
12	L	106/106 (100%)	103 (97%)	3 (3%)	43	76
13	M	112/126 (89%)	109 (97%)	3 (3%)	44	76
14	N	166/166 (100%)	157 (95%)	9 (5%)	22	56
15	O	149/149 (100%)	143 (96%)	6 (4%)	31	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	91 (98%)	2 (2%)	52	80
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44	76
18	R	79/79 (100%)	74 (94%)	5 (6%)	18	49
19	S	117/121 (97%)	113 (97%)	4 (3%)	37	72
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	101 (96%)	4 (4%)	33	68
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	51 (100%)	0	100	100
24	X	130/130 (100%)	121 (93%)	9 (7%)	15	46
25	Y	66/73 (90%)	62 (94%)	4 (6%)	18	51
26	Z	120/195 (62%)	111 (92%)	9 (8%)	13	42
27	1	56/56 (100%)	52 (93%)	4 (7%)	14	44
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	49	79
30	4	79/79 (100%)	76 (96%)	3 (4%)	33	68
All	All	3027/3441 (88%)	2877 (95%)	150 (5%)	24	59

5 of 150 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	86	ARG
12	L	98	VAL
26	Z	189	ASN
10	J	150	LYS
11	K	112	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 93 such sidechains are listed below:

Mol	Chain	Res	Type
14	N	26	HIS
17	Q	50	GLN
28	2	28	HIS
14	N	58	GLN
15	O	21	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	237 (8%)	35 (1%)
2	B	121/122 (99%)	19 (15%)	7 (5%)
All	All	2868/3044 (94%)	256 (8%)	42 (1%)

5 of 256 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	11	A
1	A	31	C
1	A	60	A
1	A	67	A
1	A	69	A

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1450	C
1	A	1942	A
2	B	3024	U
1	A	1506	U
1	A	1685	A

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 233 ligands modelled in this entry, 232 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	$\# Z > 2$
31	ANM	A	9000	33	20,20,20	1.68	4 (20%)	22,27,27	1.72	6 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	ANM	A	9000	33	-	2/10/23/23	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	9000	ANM	C1-C9	5.23	1.49	1.38
31	A	9000	ANM	C10-C9	2.78	1.44	1.38
31	A	9000	ANM	C11-C12	2.60	1.44	1.38
31	A	9000	ANM	O1-C9	2.46	1.42	1.37

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	9000	ANM	C2-O2-C5	3.51	123.15	117.72
31	A	9000	ANM	C10-C9-C1	-3.12	115.37	120.18
31	A	9000	ANM	C13-C1-C9	2.59	122.91	119.73
31	A	9000	ANM	C12-C15-C16	-2.45	109.08	113.33
31	A	9000	ANM	C14-O1-C9	2.09	122.04	117.51

There are no chirality outliers.

All (2) torsion outliers are listed below:

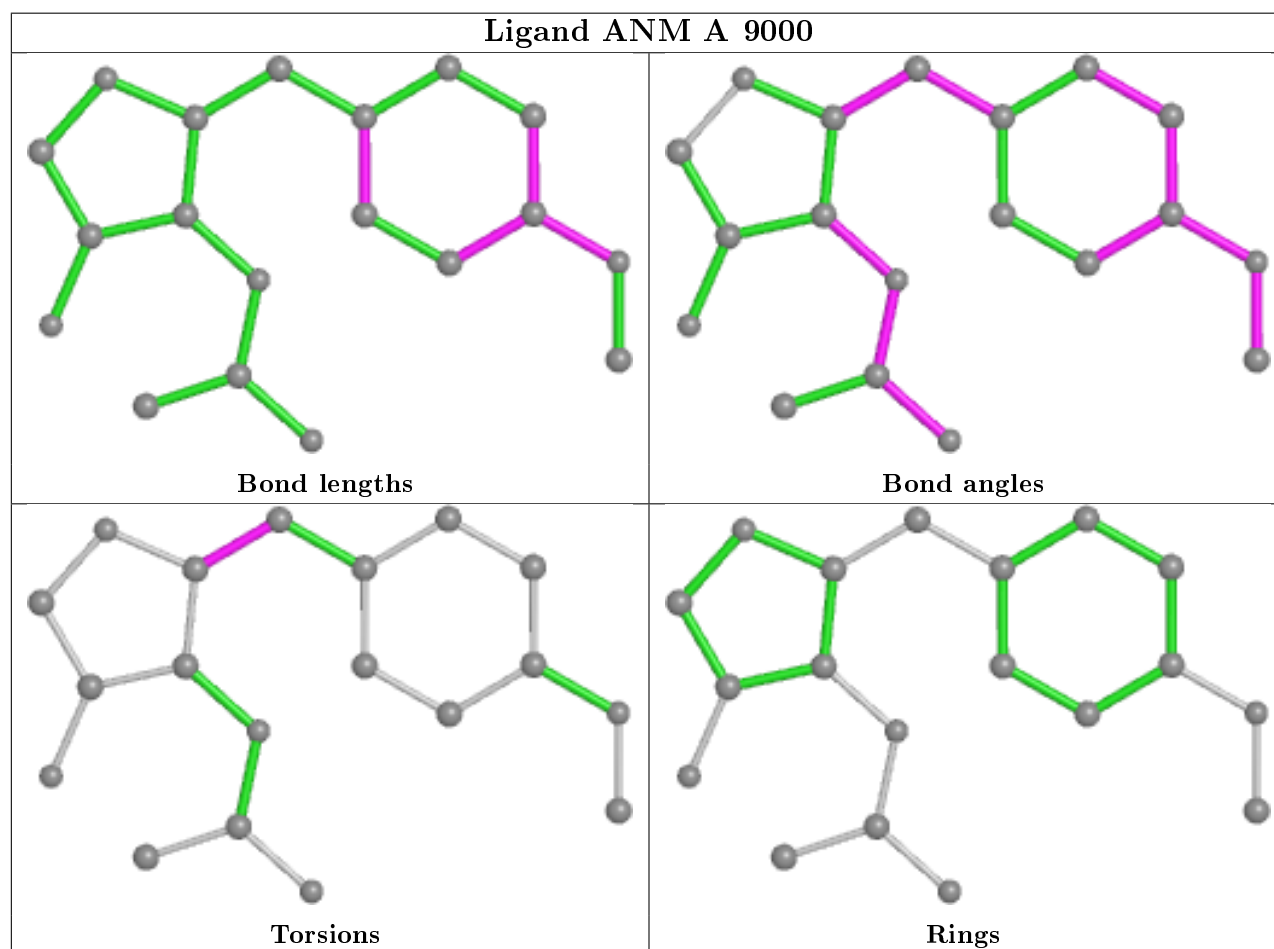
Mol	Chain	Res	Type	Atoms
31	A	9000	ANM	C12-C15-C16-C2
31	A	9000	ANM	C12-C15-C16-N1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	9000	ANM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2486:A	O3'	2487:C	P	2.10

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2754/2922 (94%)	-0.17	38 (1%) 75 48	20, 45, 89, 137	0
2	B	122/122 (100%)	0.15	5 (4%) 37 15	33, 61, 88, 146	0
3	C	237/239 (99%)	-0.02	8 (3%) 45 19	27, 49, 83, 104	0
4	D	337/337 (100%)	-0.18	1 (0%) 94 83	25, 54, 79, 88	0
5	E	246/246 (100%)	-0.24	0 100 100	18, 44, 68, 79	0
6	F	140/176 (79%)	1.15	29 (20%) 1 0	51, 96, 114, 118	0
7	G	172/177 (97%)	0.42	3 (1%) 70 41	44, 66, 85, 91	0
8	H	119/119 (100%)	0.36	4 (3%) 45 19	50, 68, 93, 100	0
9	I	29/348 (8%)	1.74	12 (41%) 0 0	73, 88, 96, 100	0
10	J	156/167 (93%)	-0.04	1 (0%) 89 72	34, 55, 84, 88	0
11	K	142/145 (97%)	-0.23	0 100 100	34, 49, 70, 90	0
12	L	132/132 (100%)	-0.13	1 (0%) 86 65	30, 50, 71, 78	0
13	M	145/164 (88%)	0.35	11 (7%) 13 4	23, 64, 101, 112	0
14	N	194/194 (100%)	-0.30	0 100 100	29, 43, 60, 72	0
15	O	186/186 (100%)	0.34	11 (5%) 22 7	40, 61, 101, 114	0
16	P	115/115 (100%)	-0.11	0 100 100	38, 53, 69, 75	0
17	Q	143/148 (96%)	0.01	1 (0%) 87 68	35, 54, 68, 75	0
18	R	95/95 (100%)	-0.25	0 100 100	33, 43, 58, 71	0
19	S	150/154 (97%)	-0.30	0 100 100	24, 43, 65, 71	0
20	T	81/84 (96%)	-0.06	1 (1%) 79 53	41, 58, 78, 81	0
21	U	119/119 (100%)	0.25	4 (3%) 45 19	37, 56, 79, 92	0
22	V	53/66 (80%)	0.09	0 100 100	40, 55, 72, 79	0
23	W	65/70 (92%)	0.93	9 (13%) 2 1	49, 71, 105, 112	0
24	X	154/154 (100%)	-0.37	0 100 100	34, 46, 65, 75	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.15	3 (3%) 41 17	42, 57, 82, 99	0
26	Z	142/240 (59%)	-0.10	1 (0%) 87 68	26, 44, 65, 83	0
27	1	73/73 (100%)	-0.01	1 (1%) 75 48	45, 59, 75, 84	0
28	2	56/56 (100%)	-0.47	0 100 100	21, 34, 39, 41	0
29	3	46/48 (95%)	0.20	1 (2%) 62 32	35, 60, 85, 96	0
30	4	92/92 (100%)	0.13	0 100 100	35, 55, 69, 80	0
All	All	6577/7279 (90%)	-0.05	145 (2%) 62 32	18, 50, 90, 146	0

The worst 5 of 145 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	W	1	THR	8.4
2	B	3001	U	6.8
2	B	3025	G	5.8
6	F	63	ILE	4.8
1	A	1172	G	4.4

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

There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	A	8384	1/1	0.48	1.27	79,79,79,79	0
34	NA	S	8386	1/1	0.53	0.53	83,83,83,83	0
34	NA	A	8363	1/1	0.53	0.87	54,54,54,54	0
34	NA	A	8371	1/1	0.54	0.37	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8385	1/1	0.62	0.44	50,50,50,50	0
34	NA	J	8322	1/1	0.67	0.40	59,59,59,59	0
34	NA	A	8306	1/1	0.69	0.63	39,39,39,39	0
32	MG	A	8049	1/1	0.69	0.47	68,68,68,68	0
34	NA	A	8326	1/1	0.71	0.56	61,61,61,61	0
34	NA	A	8370	1/1	0.75	0.32	58,58,58,58	0
34	NA	A	8377	1/1	0.76	0.33	61,61,61,61	0
34	NA	A	8361	1/1	0.76	0.49	60,60,60,60	0
34	NA	A	8329	1/1	0.76	0.47	60,60,60,60	0
32	MG	A	8102	1/1	0.78	0.17	48,48,48,48	0
34	NA	A	8368	1/1	0.79	0.20	57,57,57,57	0
35	CL	M	8510	1/1	0.79	0.23	74,74,74,74	0
34	NA	A	8341	1/1	0.80	0.21	36,36,36,36	0
34	NA	A	8340	1/1	0.80	0.26	47,47,47,47	0
34	NA	A	8313	1/1	0.80	0.42	64,64,64,64	0
32	MG	U	8073	1/1	0.81	0.18	52,52,52,52	0
34	NA	A	8358	1/1	0.82	0.55	86,86,86,86	0
32	MG	A	8111	1/1	0.82	0.11	49,49,49,49	0
34	NA	A	8382	1/1	0.82	0.35	71,71,71,71	0
34	NA	A	8373	1/1	0.83	0.66	49,49,49,49	0
34	NA	B	8351	1/1	0.83	0.14	30,30,30,30	0
34	NA	A	8374	1/1	0.83	0.72	65,65,65,65	0
32	MG	A	8087	1/1	0.83	0.14	67,67,67,67	0
34	NA	E	8304	1/1	0.84	0.25	35,35,35,35	0
34	NA	A	8333	1/1	0.84	0.12	38,38,38,38	0
34	NA	A	8364	1/1	0.84	0.27	43,43,43,43	0
34	NA	A	8372	1/1	0.84	0.53	60,60,60,60	0
34	NA	A	8369	1/1	0.84	0.50	49,49,49,49	0
34	NA	A	8355	1/1	0.85	0.36	58,58,58,58	0
34	NA	S	8337	1/1	0.85	0.20	41,41,41,41	0
34	NA	R	8348	1/1	0.85	0.11	34,34,34,34	0
32	MG	A	8099	1/1	0.86	0.19	47,47,47,47	0
34	NA	A	8328	1/1	0.86	0.48	41,41,41,41	0
34	NA	A	8365	1/1	0.86	0.45	36,36,36,36	0
34	NA	A	8330	1/1	0.86	0.35	41,41,41,41	0
34	NA	T	8312	1/1	0.86	0.16	39,39,39,39	0
34	NA	B	8383	1/1	0.87	0.71	52,52,52,52	0
32	MG	A	8106	1/1	0.87	0.35	50,50,50,50	0
32	MG	A	8076	1/1	0.87	0.17	68,68,68,68	0
32	MG	A	8112	1/1	0.87	0.13	45,45,45,45	0
32	MG	A	8108	1/1	0.87	0.19	79,79,79,79	0
32	MG	A	8068	1/1	0.87	0.10	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8075	1/1	0.87	0.13	51,51,51,51	0
35	CL	Z	8520	1/1	0.88	0.17	39,39,39,39	0
34	NA	A	8381	1/1	0.88	0.31	44,44,44,44	0
32	MG	A	8024	1/1	0.88	0.20	29,29,29,29	0
34	NA	A	8357	1/1	0.88	0.09	50,50,50,50	0
34	NA	A	8310	1/1	0.88	0.37	32,32,32,32	0
34	NA	A	8375	1/1	0.88	0.24	47,47,47,47	0
32	MG	A	8115	1/1	0.88	0.09	41,41,41,41	0
35	CL	A	8522	1/1	0.88	0.37	85,85,85,85	0
32	MG	A	8016	1/1	0.88	0.15	46,46,46,46	0
34	NA	A	8359	1/1	0.88	0.45	53,53,53,53	0
32	MG	A	8050	1/1	0.88	0.15	57,57,57,57	0
32	MG	Z	8109	1/1	0.89	0.18	41,41,41,41	0
34	NA	A	8307	1/1	0.89	0.38	45,45,45,45	0
32	MG	A	8041	1/1	0.89	0.15	43,43,43,43	0
35	CL	A	8505	1/1	0.89	0.23	85,85,85,85	0
32	MG	A	8082	1/1	0.89	0.23	60,60,60,60	0
35	CL	4	8504	1/1	0.89	0.25	54,54,54,54	0
32	MG	A	8090	1/1	0.89	0.30	55,55,55,55	0
34	NA	A	8311	1/1	0.90	0.12	55,55,55,55	0
32	MG	A	8093	1/1	0.90	0.09	37,37,37,37	0
32	MG	A	8091	1/1	0.90	0.09	52,52,52,52	0
34	NA	A	8301	1/1	0.90	0.17	16,16,16,16	0
32	MG	C	8105	1/1	0.90	0.15	6,6,6,6	0
32	MG	A	8046	1/1	0.90	0.08	53,53,53,53	0
32	MG	A	8008	1/1	0.90	0.07	37,37,37,37	0
35	CL	A	8517	1/1	0.90	0.12	52,52,52,52	0
32	MG	A	8045	1/1	0.91	0.12	49,49,49,49	0
34	NA	A	8316	1/1	0.91	0.33	52,52,52,52	0
32	MG	A	8081	1/1	0.91	0.17	60,60,60,60	0
34	NA	S	8338	1/1	0.91	0.07	38,38,38,38	0
34	NA	A	8332	1/1	0.91	0.35	42,42,42,42	0
34	NA	A	8302	1/1	0.91	0.14	44,44,44,44	0
35	CL	K	8502	1/1	0.91	0.10	62,62,62,62	0
32	MG	A	8085	1/1	0.91	0.13	63,63,63,63	0
34	NA	M	8380	1/1	0.92	0.55	48,48,48,48	0
34	NA	A	8331	1/1	0.92	0.25	51,51,51,51	0
35	CL	O	8507	1/1	0.92	0.28	65,65,65,65	0
34	NA	A	8352	1/1	0.92	0.25	49,49,49,49	0
32	MG	A	8089	1/1	0.92	0.24	63,63,63,63	0
34	NA	K	8346	1/1	0.92	0.17	35,35,35,35	0
32	MG	A	8113	1/1	0.92	0.18	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8308	1/1	0.92	0.13	53,53,53,53	0
35	CL	C	8509	1/1	0.92	0.19	64,64,64,64	0
34	NA	A	8317	1/1	0.92	0.06	29,29,29,29	0
32	MG	A	8053	1/1	0.92	0.10	34,34,34,34	0
34	NA	A	8378	1/1	0.92	0.41	41,41,41,41	0
34	NA	A	8324	1/1	0.92	0.14	43,43,43,43	0
35	CL	N	8518	1/1	0.92	0.20	53,53,53,53	0
34	NA	A	8318	1/1	0.93	0.14	40,40,40,40	0
35	CL	A	8514	1/1	0.93	0.12	67,67,67,67	0
32	MG	A	8104	1/1	0.93	0.14	42,42,42,42	0
32	MG	A	8066	1/1	0.93	0.20	94,94,94,94	0
34	NA	A	8367	1/1	0.93	0.17	41,41,41,41	0
35	CL	A	8516	1/1	0.93	0.15	45,45,45,45	0
35	CL	A	8503	1/1	0.93	0.21	60,60,60,60	0
32	MG	A	8088	1/1	0.93	0.16	24,24,24,24	0
34	NA	A	8321	1/1	0.93	0.40	39,39,39,39	0
34	NA	A	8362	1/1	0.93	0.38	66,66,66,66	0
34	NA	A	8315	1/1	0.93	0.24	36,36,36,36	0
32	MG	A	8035	1/1	0.93	0.09	38,38,38,38	0
32	MG	A	8052	1/1	0.93	0.17	63,63,63,63	0
34	NA	U	8343	1/1	0.93	0.14	24,24,24,24	0
32	MG	A	8114	1/1	0.94	0.30	54,54,54,54	0
34	NA	A	8314	1/1	0.94	0.11	13,13,13,13	0
35	CL	R	8511	1/1	0.94	0.19	63,63,63,63	0
32	MG	A	8064	1/1	0.94	0.32	20,20,20,20	0
32	MG	L	8069	1/1	0.94	0.10	55,55,55,55	0
34	NA	A	8319	1/1	0.94	0.12	23,23,23,23	0
32	MG	B	8095	1/1	0.94	0.17	75,75,75,75	0
34	NA	A	8376	1/1	0.94	0.30	38,38,38,38	0
34	NA	A	8325	1/1	0.94	0.21	51,51,51,51	0
34	NA	A	8335	1/1	0.94	0.27	52,52,52,52	0
32	MG	A	8101	1/1	0.94	0.12	55,55,55,55	0
32	MG	A	8042	1/1	0.94	0.18	41,41,41,41	0
34	NA	A	8336	1/1	0.94	0.11	45,45,45,45	0
34	NA	A	8327	1/1	0.94	0.13	18,18,18,18	0
34	NA	A	8349	1/1	0.94	0.28	49,49,49,49	0
32	MG	A	8018	1/1	0.95	0.10	49,49,49,49	0
33	K	A	8200	1/1	0.95	0.21	66,66,66,66	0
32	MG	A	8079	1/1	0.95	0.08	39,39,39,39	0
34	NA	A	8323	1/1	0.95	0.17	33,33,33,33	0
35	CL	K	8521	1/1	0.95	0.13	44,44,44,44	0
36	CD	P	8405	1/1	0.95	0.07	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8051	1/1	0.95	0.18	70,70,70,70	0
34	NA	A	8305	1/1	0.95	0.14	34,34,34,34	0
34	NA	A	8354	1/1	0.95	0.45	39,39,39,39	0
32	MG	A	8070	1/1	0.95	0.12	33,33,33,33	0
31	ANM	A	9000	19/19	0.95	0.21	27,35,41,42	0
35	CL	A	8512	1/1	0.95	0.15	22,22,22,22	0
32	MG	A	8003	1/1	0.95	0.13	17,17,17,17	0
34	NA	A	8356	1/1	0.95	0.53	53,53,53,53	0
32	MG	A	8094	1/1	0.95	0.15	65,65,65,65	0
32	MG	A	8096	1/1	0.95	0.13	52,52,52,52	0
35	CL	A	8513	1/1	0.95	0.10	44,44,44,44	0
34	NA	A	8334	1/1	0.95	0.08	30,30,30,30	0
32	MG	A	8116	1/1	0.95	0.14	46,46,46,46	0
32	MG	A	8097	1/1	0.95	0.21	30,30,30,30	0
32	MG	A	8039	1/1	0.95	0.04	47,47,47,47	0
35	CL	D	8519	1/1	0.95	0.29	57,57,57,57	0
34	NA	A	8339	1/1	0.96	0.14	15,15,15,15	0
32	MG	A	8100	1/1	0.96	0.10	72,72,72,72	0
35	CL	A	8515	1/1	0.96	0.32	68,68,68,68	0
32	MG	A	8103	1/1	0.96	0.29	49,49,49,49	0
32	MG	A	8059	1/1	0.96	0.08	32,32,32,32	0
32	MG	A	8043	1/1	0.96	0.07	23,23,23,23	0
32	MG	A	8092	1/1	0.96	0.18	75,75,75,75	0
32	MG	D	8055	1/1	0.96	0.08	34,34,34,34	0
32	MG	A	8048	1/1	0.96	0.06	39,39,39,39	0
32	MG	A	8061	1/1	0.96	0.04	22,22,22,22	0
32	MG	A	8117	1/1	0.96	0.11	40,40,40,40	0
32	MG	A	8083	1/1	0.96	0.08	35,35,35,35	0
34	NA	A	8342	1/1	0.96	0.17	28,28,28,28	0
34	NA	A	8360	1/1	0.96	0.83	53,53,53,53	0
32	MG	A	8001	1/1	0.96	0.06	16,16,16,16	0
34	NA	A	8366	1/1	0.96	0.25	60,60,60,60	0
32	MG	A	8023	1/1	0.96	0.05	33,33,33,33	0
32	MG	A	8056	1/1	0.96	0.08	37,37,37,37	0
34	NA	A	8350	1/1	0.96	0.23	45,45,45,45	0
32	MG	A	8044	1/1	0.97	0.30	51,51,51,51	0
32	MG	A	8028	1/1	0.97	0.04	41,41,41,41	0
34	NA	N	8347	1/1	0.97	0.05	12,12,12,12	0
32	MG	A	8072	1/1	0.97	0.11	60,60,60,60	0
32	MG	A	8071	1/1	0.97	0.04	75,75,75,75	0
33	K	A	8201	1/1	0.97	0.28	69,69,69,69	0
32	MG	A	8057	1/1	0.97	0.12	31,31,31,31	0

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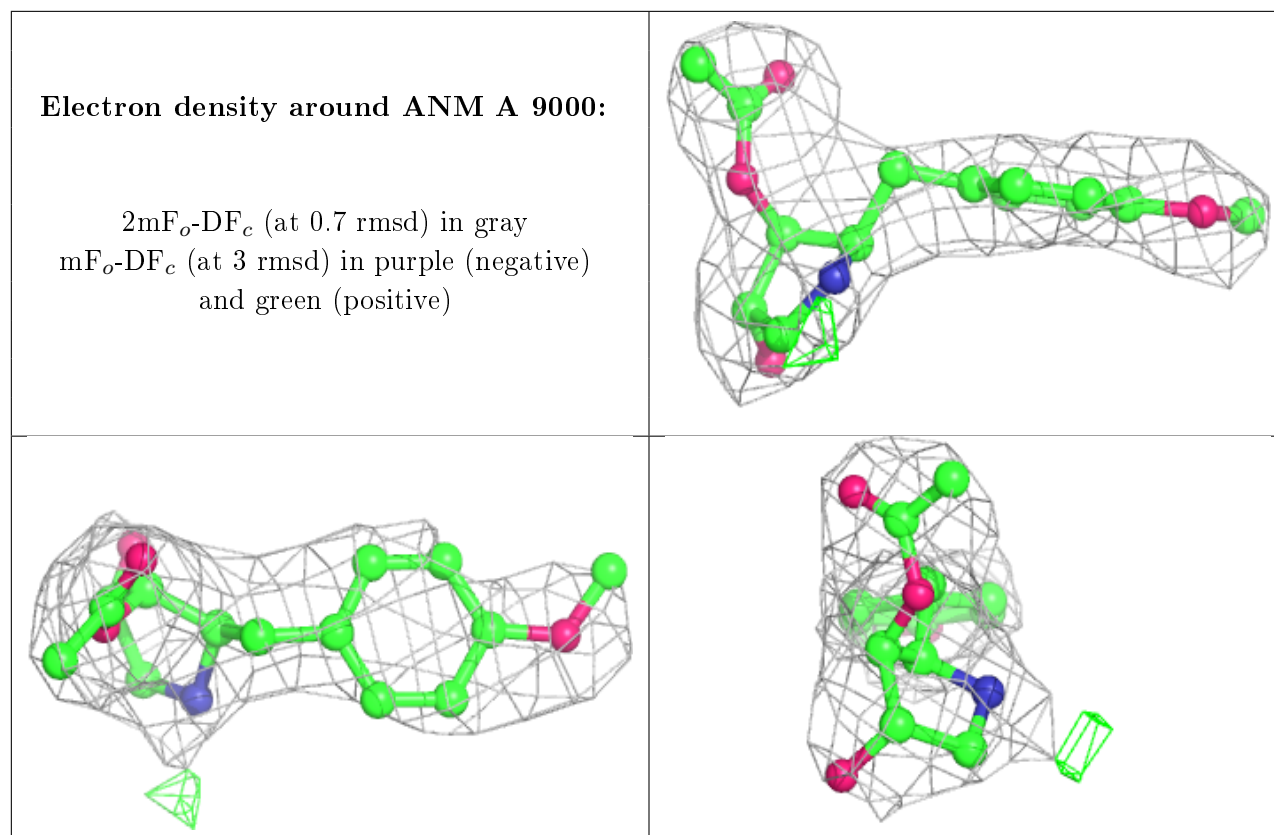
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CL	P	8508	1/1	0.97	0.39	85,85,85,85	0
35	CL	S	8506	1/1	0.97	0.12	44,44,44,44	0
32	MG	A	8086	1/1	0.97	0.16	47,47,47,47	0
36	CD	4	8404	1/1	0.97	0.07	62,62,62,62	0
34	NA	A	8344	1/1	0.97	0.10	29,29,29,29	0
32	MG	A	8077	1/1	0.97	0.04	20,20,20,20	0
32	MG	A	8007	1/1	0.97	0.06	14,14,14,14	0
32	MG	A	8054	1/1	0.97	0.07	40,40,40,40	0
32	MG	A	8047	1/1	0.97	0.12	55,55,55,55	0
34	NA	A	8353	1/1	0.97	0.08	27,27,27,27	0
32	MG	A	8062	1/1	0.97	0.08	64,64,64,64	0
34	NA	A	8379	1/1	0.97	0.16	44,44,44,44	0
32	MG	A	8014	1/1	0.97	0.09	18,18,18,18	0
32	MG	A	8032	1/1	0.97	0.05	30,30,30,30	0
32	MG	A	8110	1/1	0.97	0.06	20,20,20,20	0
32	MG	A	8098	1/1	0.97	0.12	18,18,18,18	0
32	MG	A	8004	1/1	0.98	0.05	24,24,24,24	0
32	MG	C	8065	1/1	0.98	0.07	35,35,35,35	0
32	MG	A	8010	1/1	0.98	0.07	26,26,26,26	0
32	MG	A	8027	1/1	0.98	0.07	45,45,45,45	0
32	MG	A	8019	1/1	0.98	0.05	27,27,27,27	0
32	MG	A	8015	1/1	0.98	0.08	47,47,47,47	0
34	NA	A	8303	1/1	0.98	0.32	62,62,62,62	0
32	MG	A	8013	1/1	0.98	0.16	39,39,39,39	0
32	MG	A	8058	1/1	0.98	0.09	42,42,42,42	0
32	MG	A	8029	1/1	0.98	0.09	49,49,49,49	0
32	MG	4	8078	1/1	0.98	0.05	45,45,45,45	0
32	MG	A	8021	1/1	0.98	0.05	22,22,22,22	0
32	MG	A	8107	1/1	0.98	0.04	41,41,41,41	0
32	MG	A	8084	1/1	0.98	0.06	49,49,49,49	0
32	MG	A	8074	1/1	0.98	0.05	16,16,16,16	0
32	MG	A	8030	1/1	0.98	0.08	19,19,19,19	0
32	MG	A	8033	1/1	0.98	0.06	27,27,27,27	0
32	MG	A	8034	1/1	0.98	0.03	10,10,10,10	0
32	MG	A	8040	1/1	0.98	0.06	49,49,49,49	0
34	NA	C	8345	1/1	0.98	0.14	52,52,52,52	0
32	MG	A	8005	1/1	0.98	0.10	49,49,49,49	0
32	MG	A	8063	1/1	0.98	0.08	78,78,78,78	0
32	MG	A	8011	1/1	0.98	0.06	20,20,20,20	0
32	MG	A	8031	1/1	0.98	0.04	22,22,22,22	0
32	MG	A	8080	1/1	0.98	0.06	55,55,55,55	0
32	MG	A	8060	1/1	0.98	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8020	1/1	0.98	0.07	38,38,38,38	0
32	MG	A	8002	1/1	0.98	0.06	32,32,32,32	0
32	MG	A	8038	1/1	0.99	0.05	16,16,16,16	0
34	NA	J	8309	1/1	0.99	0.09	18,18,18,18	0
32	MG	A	8012	1/1	0.99	0.07	29,29,29,29	0
32	MG	A	8006	1/1	0.99	0.05	46,46,46,46	0
32	MG	A	8067	1/1	0.99	0.14	48,48,48,48	0
32	MG	A	8026	1/1	0.99	0.03	12,12,12,12	0
32	MG	A	8009	1/1	0.99	0.04	37,37,37,37	0
32	MG	A	8036	1/1	0.99	0.06	25,25,25,25	0
34	NA	A	8320	1/1	0.99	0.14	31,31,31,31	0
32	MG	A	8025	1/1	0.99	0.04	37,37,37,37	0
35	CL	K	8501	1/1	0.99	0.14	58,58,58,58	0
32	MG	A	8017	1/1	0.99	0.03	20,20,20,20	0
36	CD	1	8403	1/1	0.99	0.09	60,60,60,60	0
32	MG	A	8022	1/1	0.99	0.09	53,53,53,53	0
32	MG	A	8037	1/1	0.99	0.05	34,34,34,34	0
36	CD	2	8402	1/1	0.99	0.06	59,59,59,59	0
36	CD	V	8401	1/1	1.00	0.05	59,59,59,59	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.