



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 09:30 PM UTC

PDB ID : 3CXC / pdb_00003cxc
Title : The structure of an enhanced oxazolidinone inhibitor bound to the 50S ribosomal subunit of *H. marismortui*
Authors : Ippolito, J.A.; Wang, D.; Kanyo, Z.F.; Duffy, E.M.
Deposited on : 2008-04-24
Resolution : 3.00 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

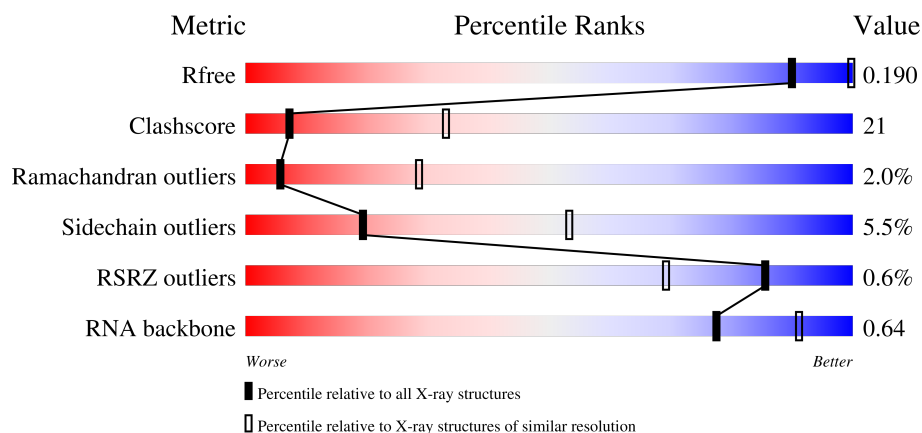
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	0	2922	47% 41% 6% 6%
2	9	122	4% 38% 49% 11% .
3	4	3	33% 33% 33%
4	A	239	50% 40% 8% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	B	337	
6	C	246	
7	D	176	
8	E	177	
9	F	119	
10	G	348	
11	H	167	
12	I	145	
13	J	132	
14	K	164	
15	L	194	
16	M	186	
17	N	115	
18	O	148	
19	P	95	
20	Q	154	
21	R	84	
22	S	119	
23	T	66	
24	U	70	
25	V	154	
26	W	91	
27	X	240	
28	Y	73	
29	Z	56	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
30	1	48	
31	2	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	K	0	8201	-	-	-	X
37	CD	2	8404	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S RIBOSOMAL RNA.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	560	C	U	conflict	GB 3377779

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	9	122	Total	C	N	O	P	0	0	0
			2600	1160	472	847	121			

- Molecule 3 is a RNA chain called 5'-R(*CP*CP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L3.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	310	ARG	PRO	conflict	UNP P20279

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	C	246	Total	C	N	O	S	0	0	0
			1859	1131	344	383	1			

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L7AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	F	119	Total	C	N	O	S	0	0	0
			886	552	141	192	1			

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L10E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	H	156	Total	C	N	O	S	0	0	0
			1216	766	233	213	4			

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	K	145	Total	C	N	O	S	0	0	0
			1118	670	222	226				

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L15E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	L	194	Total	C	N	O	S	0	0	0
			1606	988	346	267	5			

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L19E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	O	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
O	71	LYS	TYR	conflict	UNP P14119

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L32E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	X	142	Total	C	N	O	S	0	0	0
			1130	686	228	216				

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37AE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Y	73	Total	C	N	O	S	0	0	0
			564	359	111	87	7			

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L39E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	1	46	Total	C	N	O	S	0	0	0
			394	238	86	69	1			

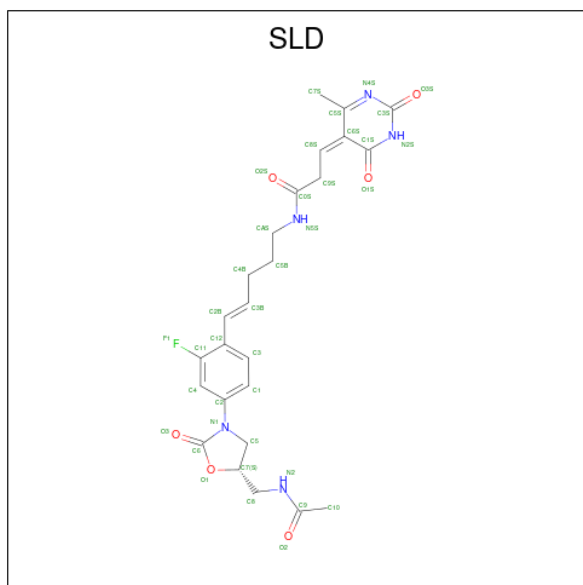
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	?	-	ARG	deletion	UNP P22452

- Molecule 31 is a protein called RIBOSOMAL PROTEIN L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	2	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 32 is (3Z)-N-[(4E)-5-(4-{(5S)-5-[(acetylamino)methyl]-2-oxo-1,3-oxazolidin-3-yl}-2-fluorophenyl)pent-4-en-1-yl]-3-(4-methyl-2,6-dioxo-1,6-dihydropyrimidin-5(2H)-ylidene)propanamide (CCD ID: SLD) (formula: C₂₅H₂₈FN₅O₆).



Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	X	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	0	2	Total	K	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	0	73	Total	Na	0	0
			73	73		
35	9	2	Total	Na	0	0
			2	2		
35	A	1	Total	Na	0	0
			1	1		
35	C	1	Total	Na	0	0
			1	1		
35	H	2	Total	Na	0	0
			2	2		
35	I	1	Total	Na	0	0
			1	1		
35	K	1	Total	Na	0	0
			1	1		
35	L	1	Total	Na	0	0
			1	1		
35	P	1	Total	Na	0	0
			1	1		
35	Q	2	Total	Na	0	0
			2	2		
35	R	1	Total	Na	0	0
			1	1		

- Molecule 36 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	8	Total	Cl	0	0
			8	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	A	1	Total 1	Cl 1	0	0
36	B	1	Total 1	Cl 1	0	0
36	I	3	Total 3	Cl 3	0	0
36	J	1	Total 1	Cl 1	0	0
36	K	1	Total 1	Cl 1	0	0
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0
36	N	1	Total 1	Cl 1	0	0
36	P	1	Total 1	Cl 1	0	0
36	Q	1	Total 1	Cl 1	0	0
36	X	1	Total 1	Cl 1	0	0
36	2	1	Total 1	Cl 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	N	1	Total 1	Cd 1	0	0
37	T	1	Total 1	Cd 1	0	0
37	Y	1	Total 1	Cd 1	0	0
37	Z	1	Total 1	Cd 1	0	0
37	2	1	Total 1	Cd 1	0	0

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	0	5806	Total 5806	O 5806	0	0
38	9	147	Total 147	O 147	0	0
38	4	1	Total 1	O 1	0	0
38	A	136	Total 136	O 136	0	0
38	B	160	Total 160	O 160	0	0
38	C	180	Total 180	O 180	0	0
38	D	49	Total 49	O 49	0	0
38	E	47	Total 47	O 47	0	0
38	F	26	Total 26	O 26	0	0
38	G	21	Total 21	O 21	0	0
38	H	82	Total 82	O 82	0	0
38	I	61	Total 61	O 61	0	0
38	J	63	Total 63	O 63	0	0
38	K	85	Total 85	O 85	0	0
38	L	130	Total 130	O 130	0	0
38	M	69	Total 69	O 69	0	0
38	N	45	Total 45	O 45	0	0
38	O	70	Total 70	O 70	0	0
38	P	56	Total 56	O 56	0	0
38	Q	92	Total 92	O 92	0	0
38	R	40	Total 40	O 40	0	0
38	S	37	Total 37	O 37	0	0

Continued on next page...

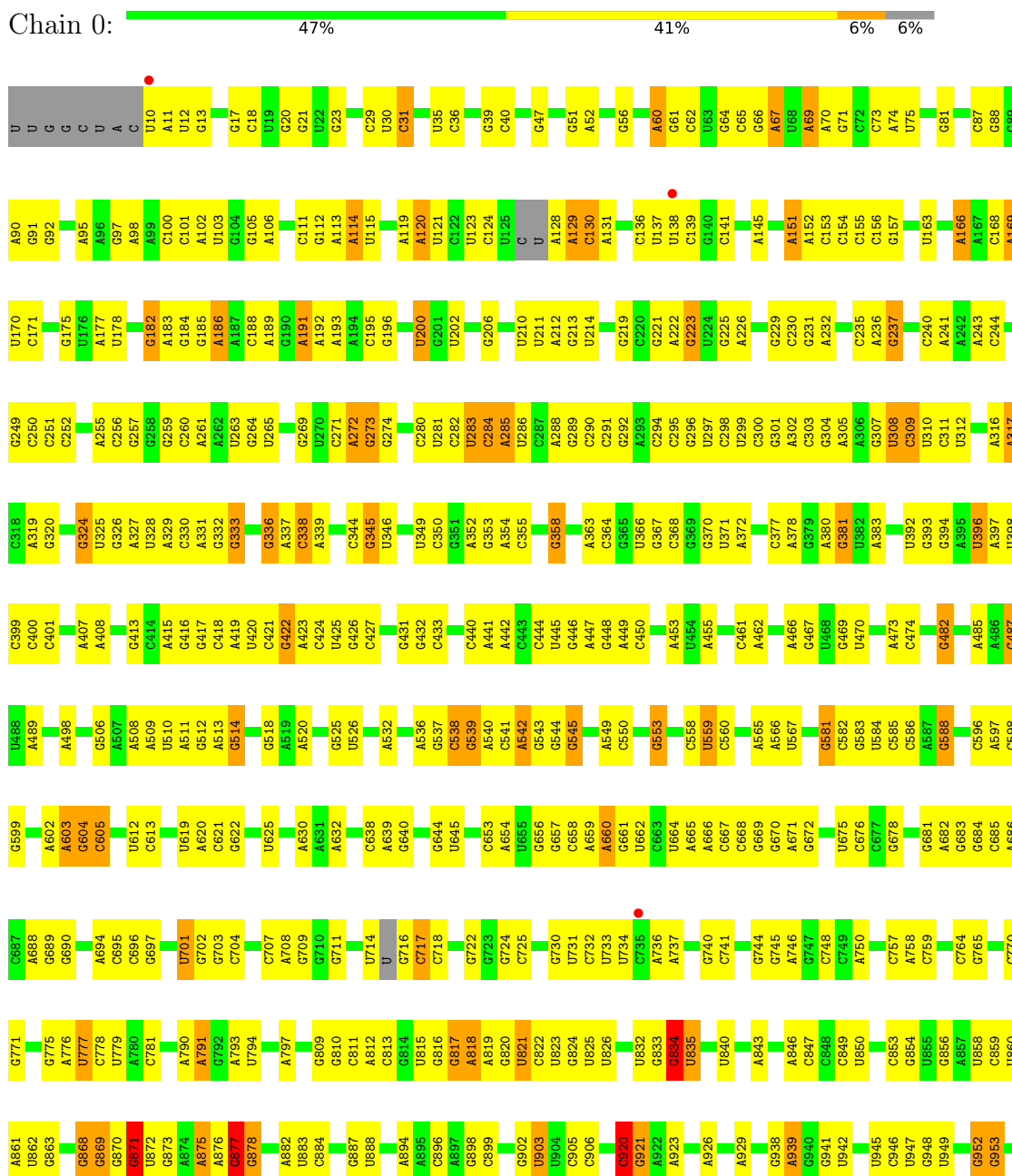
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	T	27	Total 27	O 27	0	0
38	U	13	Total 13	O 13	0	0
38	V	74	Total 74	O 74	0	0
38	W	29	Total 29	O 29	0	0
38	X	105	Total 105	O 105	0	0
38	Y	41	Total 41	O 41	0	0
38	Z	57	Total 57	O 57	0	0
38	1	45	Total 45	O 45	0	0
38	2	76	Total 76	O 76	0	0

3 Residue-property plots

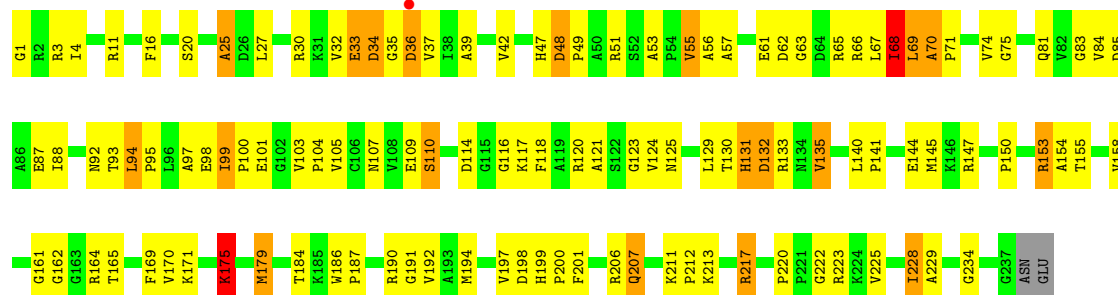
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 23S RIBOSOMAL RNA



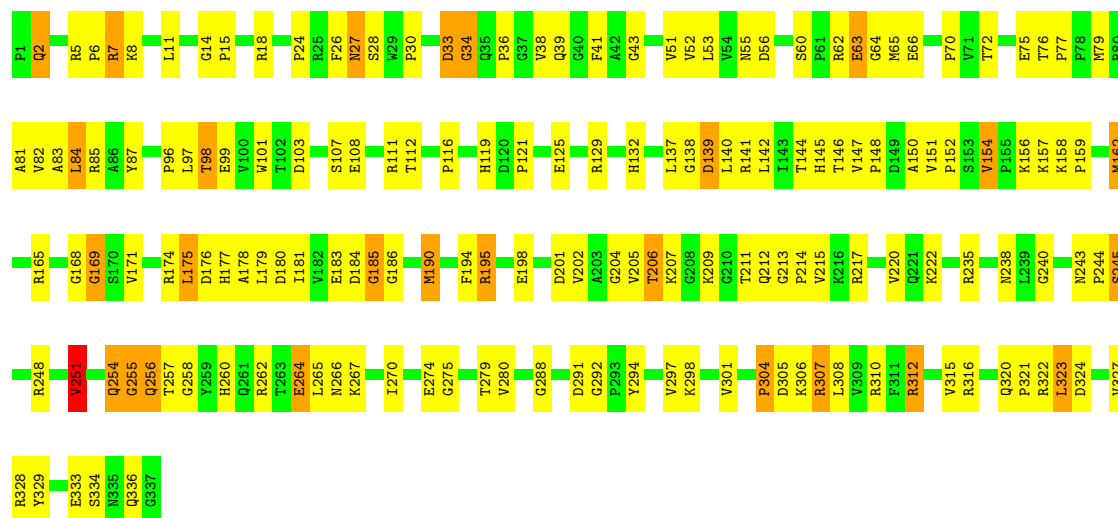
C	G2072	C1988	A1909	G1819	A1746	U1654	A1572	G1497	U1418	G1312	U1219	G1151	U1028	G958	
A	G2073	C1989	A1910	G1820	A1747	G1655	A1573	G1498	U1419	A1313	G1223	A1154	U1029	C959	
G	A2074	C1990	A1911	A1821	U1748	A1656	C1574	U1499	C1421	U1314	G1224	A1155	U1030	A960	
C	G2075	U1992	G1917	A1822	G1751	A1657	C1575	U1500	C1422	U1320	G1225	C1156	G1031	A961	
A	G2082	C1993	U1918	G1823	G1752	A1658	A1580	A1501	U1423	A1321	G1226	C1157	G1044	C962	
U	A2083	G1994	A1919	C1824	G1753	C1686	C1584	U1502	A1424	G1322	C1229	G1158	G1045	C963	
A	G2089	G1995	C1920	U1825	A1755	A1687	C1585	A1503	G1425	G1323	C1230	G1159	G1046	G964	
G	G2090	U1996	A1921	C1826	G1756	A1688	C1586	U1504	G1426	U1324	U1234	G1160	G1052	G968	
G	G2091	G2000	A1922	G1827	U1757	A1689	U1587	A1505	A1427	G1325	U1235	A1161	G1055	G969	
A	G2092	G2001	U1758	A1828	U1758	C1670	U1587	U1506			G1236	G1162	G1056	U970	
G	G2093	A1829	C1830	G1830	G1759	C1671	G1592				G1237	G1163	A1057	G	
C	G2094	G1925	U1926	C1831	G1760	C1672	C1593	U1511	G1430	A1328	A1236	G1164	A1058	U	
A	A2095	G1926	A1927	C1834	U1761	G1675	C1594	C1512	U1431	A1329	A1237	G1165	A1059	G	
G	A2096	U1928	C1929	U1835	C1762	G1676	G1595	C1513	G1432	A1330	C1238	G1166	C1060	C	
A	G2101	G1929	U1930	A1840	C1763	A1678	U1596	C1514	G1433	A1331	G1239			U	
C	A2102	G1930	A1931	A1841	U1766	C1679	A1597	U1515	U1434	C1332				C	
U	G2103	U1931	G1932	A1842	U1767	A1682	U1598	A1518	C1435	G1333	A1242	U1170	U1064	C	
C	G2104	A1845	G1933	U1846	A1768	G1683	U1599	U1519	U1440	A1181	C1243	U1171	U1065	G	
U	U2012	U1847	G1934	G1847	C1768	G1684	G1600	G1520	G1441	C1182	U1244	G1172	G1065	C	
A	G2105	G1848	C1935	G1848	C1769	A1685	G1601	A1527	A1442	G1183	A1245	A1173	C1069	C	
C	U2107	G1849	U1936	G1849	U1770	C1686	A1602	A1528	G1443	C1184	A1246	A1174	A1070	C	
A	G2110	U1850	U1937	G1851	U1771	C1687	A1603	G1529	G1444	U1185	A1247	G1175	G1071	C	
C	G2111	G1851	G1938	A1852	G1772	C1687	G1604	U1534	G1445	C1186	U1249		G1072	G	
G	A2112	U1852	U1939	A1853	G1773		G1605	U1524		U1187	C1250	U1180	A1078	A	
G	G2023	A1853	U1940	C1854	G1774	C1689		G1525		A1188	C1251	A1181	A1079	G	
U	U2028	U1854	A1941	C1855	A1778	G1697	G1609	A1526	C1450	G1352	C1246	U1177	A1080	A	
A	G2113	G1855	C1942	G1856	A1779	U1698	G1610	A1527	C1451	C1189	A1247	A1174	A1081	G	
C	U2115	G1856	A1943	C1857	G1780	C1688	A1612	A1528	G1452	C1190	A1248	G1176	A1082	A	
C	U2116	A1857	G1944	A1857	G1781	U1701	A1613	G1529	U1454	C1360	U1266	U1187	A1086	G	
C	G2119	G1858	G1945	C1858	G1782	U1702	G1614	G1536	G1455	U1362	C1267	A1188	G1087	U	
G	U2120	U1859	G1946	C1859	A1783		A1615	U1536	C1456	A1189	G1268	A1189	A1088	C	
C	G2121	G1860	U1947	G1861	U1784	U1711	C1616	C1537	U1457	C1365	U1270	A1191	U1109	G	
C	U2122	A1861	G1948	C1862	U1785	G1712	C1617	U1538	G1460	C1366	C1273	A1192	G1110	C	
U	G2124	G1862	A1949	C1863	C1787	A1713	G1618	U1539	U1461	A1372		A1193		A	
C	U2125	C1864	G1950	C1864	U1788	G1714			C1462	C1196	U1276	C1196	A1114	C	
A	G2126	A1865	G1951	C1865	G1789	C1715	U1624	C1545	C1463	C1197	G1277	C1197	U1115	A	
G	G2127	U1866	U1952	C1866	U1790	G1716	U1625	G1546	U1464	A1375	A1278		U1116	G	
A	U2128	G1867	G1953	C1867	U1791	A1717	U1626	A1547		C1377	U1279		A1117	C	
C	G2134	U1868	U1954	C1868	C1792	A1717	G1627	U1548	A1470	G1381	G1283	A1200	A1118	G	
G	A2135	U1869	G1955	C1869	C1793		G1628	C1549	U1471	G1382	G1284	A1201	G1119	C	
C	G2136	G1870	U1956	C1870	U1794	U1722	C1633	U1550	U1472	U1383		A1202	U1120	G	
C	A	U1871	G1957	C1871	G1795	G1723	G1634	G1552	U1473	G1384	G1289	C1204	G1123	A	
C	C	A1872	U1958	C1872	U1796	U1724	U1635	C1553	C1474	G1385	G1290	U1205	A1123	C	
C	G	U1873	G1959	C1873	A1801	C1725	A1637	G1557		G1386		U1206	C1129	A	
C	A	G1874	U1960	C1874	G1802	G1730	U1638	C1558	U1477	A1393	U1298	A1207	U1130	C	
C	U	U1875	G1961	C1875	C1803	A1731	U1639	U1559	C1478	C1394	G1299	C1208	G1131	G	
A	G	G1876	U1962	C1876	A1804	A1732	G1640	U			G1300	C1209	A1132	A	
G	C	U1877	G1963	C1877	G1805	U1733	A1641	U1561	C1483	G1398		G1210	A1133	C	
U	U	G1878	U1964	C1878	G1806	C1734	A1642	G1562	G1484	A1399	U1304	G1211	G1134	G	
C	G	U1879	G1965	C1879	U1807	A1736	C1643	C1563	A1485	A1407	C1305	C1212	G1135	C	
C	G	U1880	U1966	C1880	U1808	U1737	C1644	C1564	A1486	U1408	U1306	C1213	G1136	A	
C	A	G1881	G1967	C1881	G1809	A1738	G1649	C1565	A1487	U1409	A1308	G1214	G1137	C	
C	U	U1882	U1968	C1882	C1810	U1741	G1650	C1566	U1488			A1215	A1019	G	
A	G	G1883	G1969	C1883	U1813	A1742	C1651	A1567	U1489	G1416	U1309	G1216	G1021	A	
A	U	U1884	U1970	C1884	C1818	G1743	C1652	U1568	C1494	G1417	G1311	G1217	A1022	C	
C	C	G1885	G1971	C1885		G1745	A1653		G1496				A1150	G	
C	A	U1886	U1972	C1886											
C	G	G1887	U1973	C1887											
C	U	U1888	G1974	C1888											
C	C	G1889	U1975	C1889											
C	A	A1890	G1976	C1890											
C	G	U1891	U1977	C1891											
C	C	G1892	G1978	C1892											
C	U	U1893	U1979	C1893											
C	A	A1894	G1980	C1894											
C	G	G1895	U1981	C1895											
C	C	U1896	G1982	C1896											
C	A	G1897	U1983	C1897											
C	G	U1898	G1984	C1898											
C	U	A1899	U1985	C1899											
C	C	U1900	G1986	C1900											
C	A	G1901	U1987	C1901											
C	G	U1902	G1988	C1902											
C	A	A1903	U1989	C1903											
C	U	U1904	G1990	C1904											
C	G	G1905	U1991	C1905											
C	U	A1906	G1992	C1906											
C	G	U1907	U1993	C1907											
C	A	G1908	G1994	C1908											
C	G	U1909	U1995	C1909											
C	U	A1910	G1996	C1910											
C	G	G1911	U1997	C1911											
C	A	U1912	G1998	C1912											
C	U	A1913	U1999	C1913											
C	G	G1914	G2000	C1914											
C	A	U1915	U2001	C1915											
C	G	G1916	G2002	C1916											
C	U	A1917	U2003	C1917											
C	A	U1918	G2004	C1918											
C	G	G1919	U2005	C1919											
C	U	A1920	G2006	C1920											
C	A	U1921	U2007	C1921											
C	G	G1922	G2008	C1922											
C	U	A1923	A2011	C1923											
C	A	U1924	U2012	C1924											
C	G	G1925	G2013	C1925											
C	U	A1926	U2014	C1926											
C	A	U1927	G2015	C1927											
C	G	G1928	U2016	C1928											
C	U	A1929	G2017	C1929											
C	A	U1930	U2018	C1930											
C	G	G1931	A2019	C1931											
C	U	U1932	G2020	C1932											
C	A	A1933	U2021	C1933											
C	G	G1934	G2022	C1934											
C	U	U1935	U2023	C1935											
C	A	A1936	A2024	C1936											
C	G	G1937	G2025	C1937											
C	U	U1938	U2026	C1938											
C	A	A1939	G2027	C1939											
C	G	G1940	U2028	C1940											
C	U	U1941	G2029	C1941											
C	A	A1942	U2030	C1942											
C	G	G1943	G2031	C1943											

Chain A:  50% 40% 8% ..



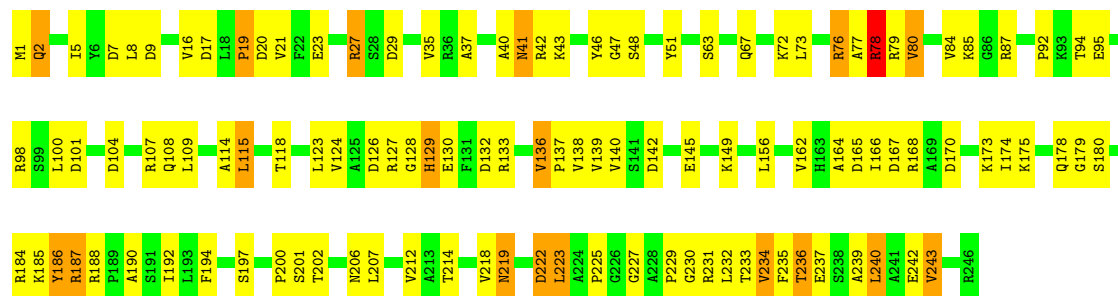
• Molecule 5: RIBOSOMAL PROTEIN L3

Chain B:  51% 41% 8%

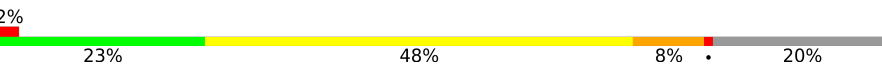


• Molecule 6: RIBOSOMAL PROTEIN L4

Chain C:  53% 39% 7%

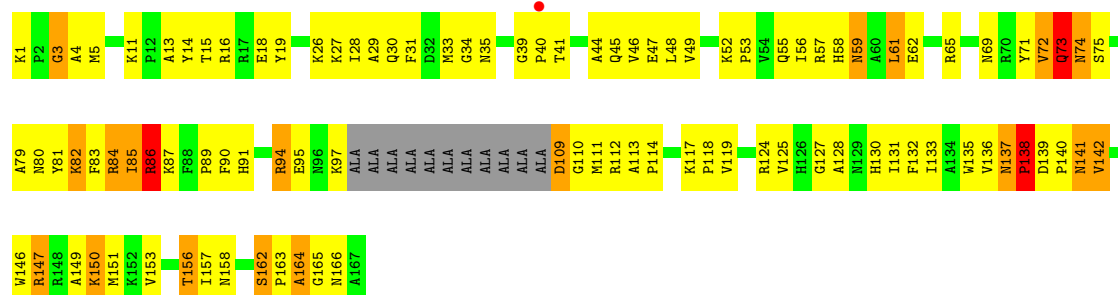


• Molecule 7: RIBOSOMAL PROTEIN L5

Chain D:  2% 23% 48% 8% 20%

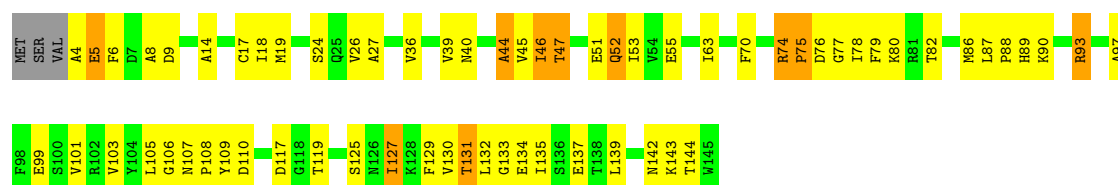
● Molecule 11: RIBOSOMAL PROTEIN L10E

Chain H: 



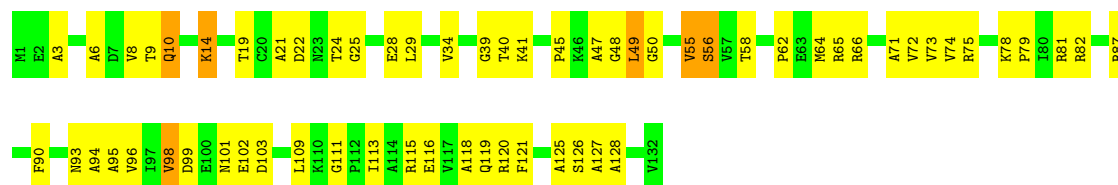
● Molecule 12: RIBOSOMAL PROTEIN L13

Chain I: 



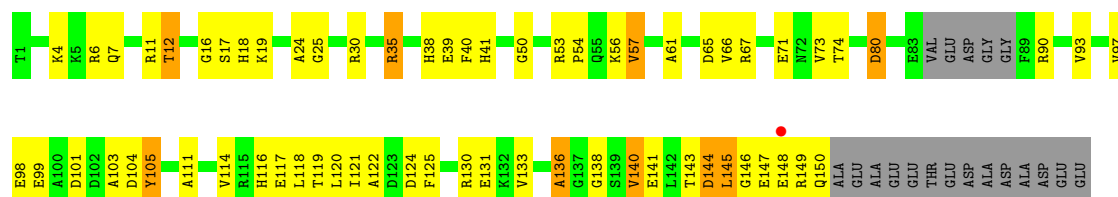
● Molecule 13: RIBOSOMAL PROTEIN L14

Chain J: 



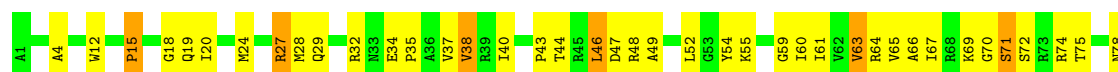
● Molecule 14: RIBOSOMAL PROTEIN L15

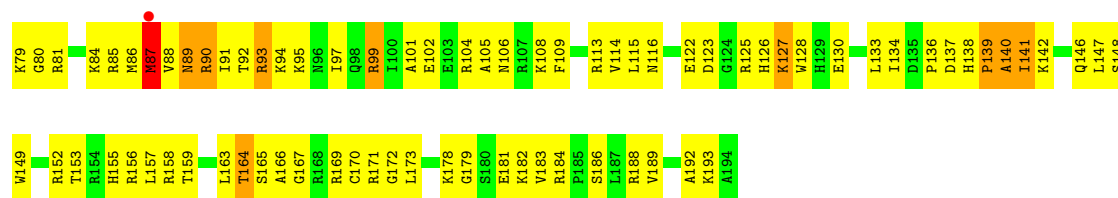
Chain K: 



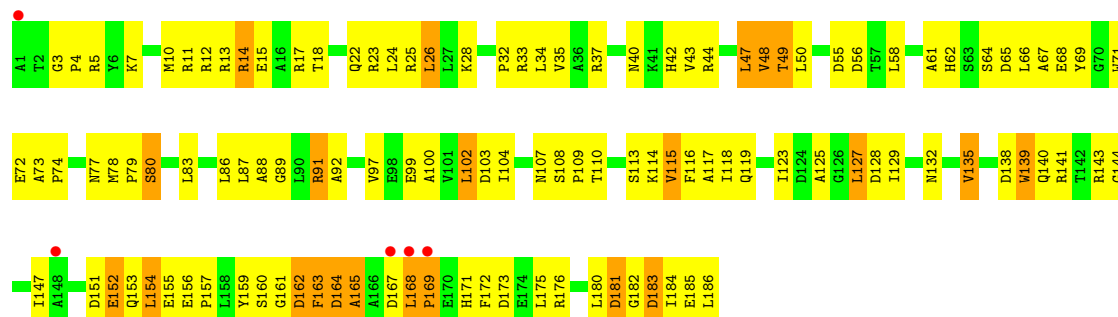
● Molecule 15: RIBOSOMAL PROTEIN L15E

Chain L: 

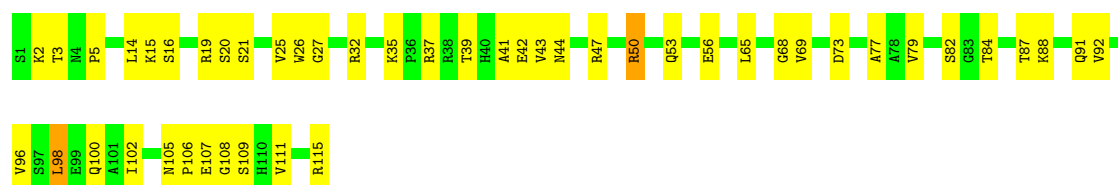




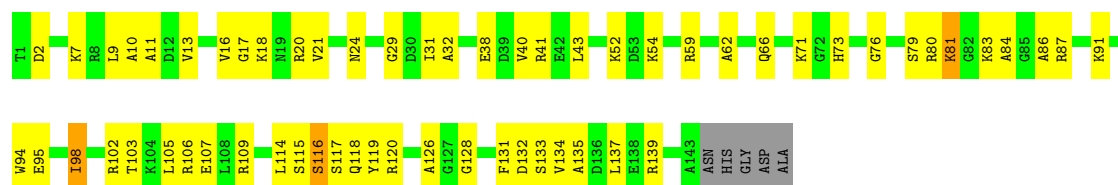
• Molecule 16: RIBOSOMAL PROTEIN L18



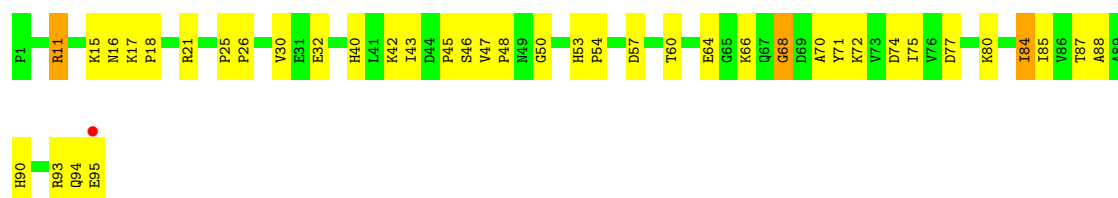
• Molecule 17: RIBOSOMAL PROTEIN L18E



• Molecule 18: RIBOSOMAL PROTEIN L19E

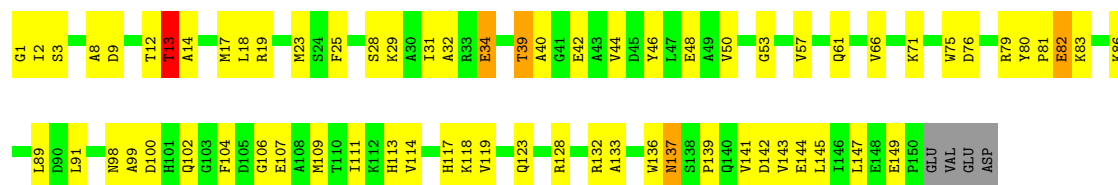


• Molecule 19: RIBOSOMAL PROTEIN L21E



- Molecule 20: RIBOSOMAL PROTEIN L22

Chain Q:  53% 41% . . .



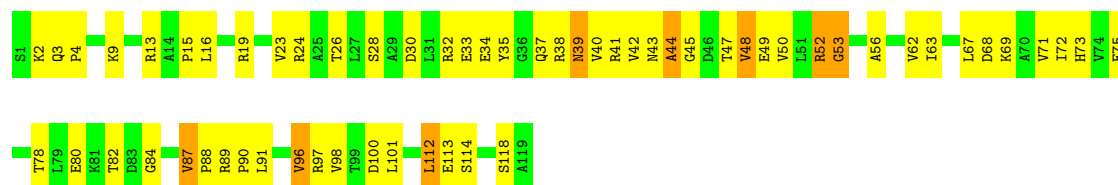
- Molecule 21: RIBOSOMAL PROTEIN L23

Chain R:  60% 35% . .

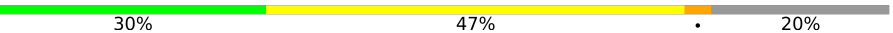


- Molecule 22: RIBOSOMAL PROTEIN L24

Chain S:  50% 44% 7%



- Molecule 23: RIBOSOMAL PROTEIN L24E

Chain T:  30% 47% . 20%



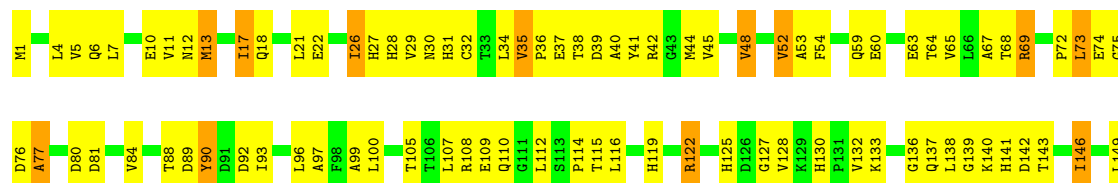
- Molecule 24: RIBOSOMAL PROTEIN L29

Chain U:  3% 39% 49% 6% 7%



- Molecule 25: RIBOSOMAL PROTEIN L30

Chain V:  40% 52% 8%



L150
E151
A152
M153
R154

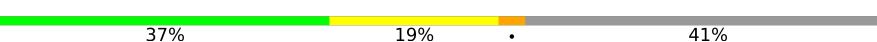
• Molecule 26: RIBOSOMAL PROTEIN L31E

Chain W:  3% 42% 36% 12% 10%

SER ALA ASP ASP PHE GLU E7 R8 V9 L14 R15 R18 A19 E20 P21 N22 H23 K24 R25 A26 D27 M30 I31 E35 H36 L37 F41 S42 V43 D44 A47 V48 R49 L50 D51 P52 N55 A58 A64 N65 T66 P67 I70 R71 R72 R73 A74 A75 R76 F77

E78 E79 A83 I84 V85 E86 A87 E88 THR ALA GLU

• Molecule 27: RIBOSOMAL PROTEIN L32E

Chain X:  37% 19% 41%

ALA ASP ASN GLU ASP VAL GLU ALA GLU TYR THR LEU THR ASP ILE SER GLY VAL GLY PRO SER LYS ALA GLU SER LEU ARG GLU ALA PHE GLU SER VAL ASP VAL ARG GLY ASP GLN ALA LEU ASP VAL SER GLY ILE GLY ASN ALA LEU ALA

ALA ARG ILE LYS ALA ASP VAL GLY GLY LEU VAL GLU SER THR THR GLU ALA GLU VAL ASP GLU ASP VAL T95 A99 R100 T103 E104 K105 T106 P107 D108 E112 R115 L116 L117 P126 Q127 F128 N129 R130 Q131 D132

T141 S142 W143 R144 R147 G148 Q149 S151 L150 S151 R154 K158 T163 R169 T172 A173 V174 H178 P179 F182 E183 A184 V185 R186 V187 H188 M189 D192 D197 G198 D199 T200 E201 A202 V203 R204 I205 A206 S207 R212 E219 E220 V228 Y233 V234 E235 V236

GLU VAL SER GLU

• Molecule 28: RIBOSOMAL PROTEIN L37AE

Chain Y:  33% 58% 10%

R10 T11 G12 R13 F14 G19 L20 K21 I22 R23 V26 A27 D28 V29 E30 I31 K32 K33 K34 H37 K38 C39 P40 V41 C42 G43 F44 K45 K46 L47 K48 R49 A50 G53 I54 W55 M56 C57 G58 H59 Y62 K63 I64 G67 C68 Y69 T73 V74 K77 M80 K81

A82

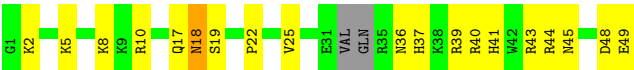
• Molecule 29: RIBOSOMAL PROTEIN L37E

Chain Z:  64% 32%

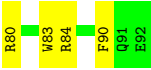
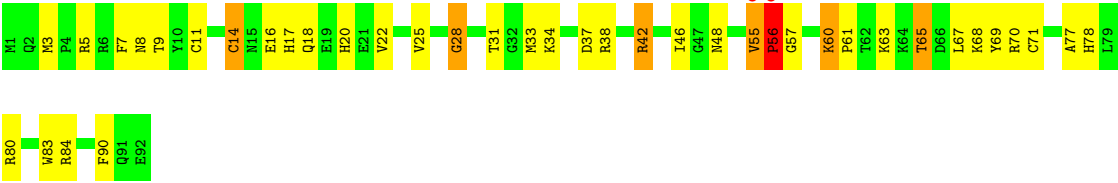
T1 T5 P6 S7 Q8 G9 K10 K11 T14 T15 H16 R20 R21 K25 H28 I29 K30 K31 K32 S36 F39 A43 Q51 S52 K53 E56

• Molecule 30: RIBOSOMAL PROTEIN L39E

Chain 1:  56% 38%



● Molecule 31: 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	213.66Å 300.71Å 575.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-3.00) 90.9 (20.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.98Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.186 , 0.229 0.186 , 0.190	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	66.9	Xtriage
Anisotropy	0.417	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98635	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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: NA, MG, K, CD, SLD, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	0	0.43	0/66076	0.64	26/103052 (0.0%)
2	9	0.40	0/2905	0.69	4/4528 (0.1%)
3	4	0.65	0/65	1.05	1/99 (1.0%)
4	A	0.49	0/1787	1.09	13/2409 (0.5%)
5	B	0.51	0/2690	1.07	16/3652 (0.4%)
6	C	0.55	0/1884	1.07	7/2551 (0.3%)
7	D	0.43	0/1111	0.94	4/1498 (0.3%)
8	E	0.48	0/1382	0.93	3/1880 (0.2%)
9	F	0.45	0/897	0.94	2/1219 (0.2%)
10	G	0.52	0/241	0.86	1/324 (0.3%)
11	H	0.56	0/1247	1.28	14/1686 (0.8%)
12	I	0.53	0/1136	1.00	5/1530 (0.3%)
13	J	0.52	0/1004	1.07	6/1351 (0.4%)
14	K	0.45	0/1130	1.07	7/1509 (0.5%)
15	L	0.56	0/1634	1.07	10/2180 (0.5%)
16	M	0.48	1/1474 (0.1%)	1.12	12/1999 (0.6%)
17	N	0.50	0/874	1.02	8/1181 (0.7%)
18	O	0.51	0/1143	0.96	2/1521 (0.1%)
19	P	0.53	0/749	1.17	5/1005 (0.5%)
20	Q	0.59	0/1172	1.03	6/1578 (0.4%)
21	R	0.44	0/648	0.91	2/875 (0.2%)
22	S	0.47	0/958	0.99	4/1289 (0.3%)
23	T	0.56	0/417	1.08	4/562 (0.7%)
24	U	0.45	0/502	1.04	3/675 (0.4%)
25	V	0.60	1/1219 (0.1%)	1.01	4/1655 (0.2%)
26	W	0.55	0/664	1.06	4/895 (0.4%)
27	X	0.54	0/1146	1.01	3/1536 (0.2%)
28	Y	0.59	0/576	1.10	2/763 (0.3%)
29	Z	0.55	0/438	1.06	3/578 (0.5%)
30	1	0.48	0/399	0.82	0/527
31	2	0.65	1/771 (0.1%)	1.07	4/1024 (0.4%)
All	All	0.46	3/98339 (0.0%)	0.77	185/147131 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	70
2	9	0	2
25	V	0	1
All	All	0	73

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	V	13	MET	SD-CE	-6.45	1.63	1.79
31	2	14	CYS	CB-SG	-6.16	1.60	1.81
16	M	115	VAL	CA-CB	5.63	1.60	1.54

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	74	ASN	N-CA-C	-15.10	92.50	114.39
11	H	141	ASN	N-CA-C	-14.65	95.47	113.50
2	9	3024	U	C2'-C3'-O3'	12.44	128.16	109.50
1	0	1979	G	C2'-C3'-O3'	10.16	124.75	109.50
1	0	1563	G	C2'-C3'-O3'	9.96	124.45	109.50

There are no chirality outliers.

5 of 73 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	182	G	Sidechain
1	0	202	U	Sidechain
1	0	223	G	Sidechain
1	0	261	A	Sidechain
1	0	324	G	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59017	0	29800	1230	0
2	9	2600	0	1326	88	0
3	4	59	0	35	2	0
4	A	1754	0	1763	135	0
5	B	2625	0	2533	174	0
6	C	1859	0	1816	116	0
7	D	1094	0	1085	132	0
8	E	1357	0	1266	74	0
9	F	886	0	854	71	0
10	G	240	0	231	24	0
11	H	1216	0	1215	160	0
12	I	1120	0	1098	69	0
13	J	994	0	1027	62	0
14	K	1118	0	1076	67	0
15	L	1606	0	1676	148	0
16	M	1445	0	1401	143	0
17	N	865	0	873	37	0
18	O	1133	0	1127	60	0
19	P	735	0	729	30	0
20	Q	1149	0	1122	67	0
21	R	641	0	605	25	0
22	S	950	0	923	54	0
23	T	410	0	364	35	0
24	U	499	0	511	38	0
25	V	1196	0	1137	101	0
26	W	654	0	653	49	0
27	X	1130	0	1133	55	0
28	Y	564	0	598	58	0
29	Z	431	0	426	24	0
30	1	394	0	406	31	0
31	2	755	0	729	54	0
32	0	37	0	28	4	0
33	0	107	0	0	0	0
33	2	1	0	0	0	0
33	4	1	0	0	0	0
33	9	2	0	0	0	0
33	A	2	0	0	0	0
33	B	1	0	0	0	0
33	J	1	0	0	0	0
33	S	1	0	0	0	0
33	X	1	0	0	0	0
34	0	2	0	0	0	0
35	0	73	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	9	2	0	0	0	0
35	A	1	0	0	0	0
35	C	1	0	0	0	0
35	H	2	0	0	0	0
35	I	1	0	0	0	0
35	K	1	0	0	0	0
35	L	1	0	0	0	0
35	P	1	0	0	0	0
35	Q	2	0	0	0	0
35	R	1	0	0	0	0
36	0	8	0	0	1	0
36	2	1	0	0	0	0
36	A	1	0	0	0	0
36	B	1	0	0	0	0
36	I	3	0	0	1	0
36	J	1	0	0	0	0
36	K	1	0	0	0	0
36	L	1	0	0	1	0
36	M	1	0	0	1	0
36	N	1	0	0	0	0
36	P	1	0	0	0	0
36	Q	1	0	0	0	0
36	X	1	0	0	0	0
37	2	1	0	0	2	0
37	N	1	0	0	0	0
37	T	1	0	0	0	0
37	Y	1	0	0	0	0
37	Z	1	0	0	0	0
38	0	5806	0	0	71	0
38	1	45	0	0	1	0
38	2	76	0	0	4	0
38	4	1	0	0	0	0
38	9	147	0	0	5	0
38	A	136	0	0	12	0
38	B	160	0	0	16	0
38	C	180	0	0	11	0
38	D	49	0	0	8	0
38	E	47	0	0	1	0
38	F	26	0	0	6	0
38	G	21	0	0	2	0
38	H	82	0	0	9	0
38	I	61	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	J	63	0	0	4	0
38	K	85	0	0	9	0
38	L	130	0	0	4	0
38	M	69	0	0	8	0
38	N	45	0	0	5	0
38	O	70	0	0	0	0
38	P	56	0	0	1	0
38	Q	92	0	0	4	0
38	R	40	0	0	1	0
38	S	37	0	0	3	0
38	T	27	0	0	2	0
38	U	13	0	0	1	0
38	V	74	0	0	6	0
38	W	29	0	0	3	0
38	X	105	0	0	4	0
38	Y	41	0	0	5	0
38	Z	57	0	0	1	0
All	All	98635	0	59566	3095	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 21.

The worst 5 of 3095 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)
24:U:12:THR:HG22	24:U:15:GLU:HG3	1.24	1.14
13:J:10:GLN:NE2	13:J:10:GLN:H	1.47	1.13
20:Q:99:ALA:HB1	20:Q:109:MET:HE1	1.29	1.12
7:D:25:MET:HE2	7:D:41:LEU:HG	1.31	1.10
1:O:871:G:H5'	1:O:871:G:H8	1.13	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	A	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	7	32
5	B	335/337 (99%)	300 (90%)	28 (8%)	7 (2%)	5	27
6	C	244/246 (99%)	213 (87%)	28 (12%)	3 (1%)	10	40
7	D	134/176 (76%)	96 (72%)	26 (19%)	12 (9%)	0	3
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	21	56
9	F	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	4	23
10	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	2	14
11	H	152/167 (91%)	132 (87%)	16 (10%)	4 (3%)	4	23
12	I	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	5	27
13	J	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	8	35
14	K	141/164 (86%)	116 (82%)	23 (16%)	2 (1%)	9	36
15	L	192/194 (99%)	167 (87%)	20 (10%)	5 (3%)	4	23
16	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	2	15
17	N	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	14	48
18	O	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	18	53
19	P	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	5	26
20	Q	148/154 (96%)	134 (90%)	14 (10%)	0	100	100
21	R	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
22	S	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	7	32
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	6	28
24	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	3	18
25	V	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	18	53
26	W	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	4	23
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100	100
28	Y	71/73 (97%)	58 (82%)	10 (14%)	3 (4%)	2	13
29	Z	54/56 (96%)	50 (93%)	4 (7%)	0	100	100
30	1	42/48 (88%)	40 (95%)	2 (5%)	0	100	100
31	2	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	5	26
All	All	3633/4235 (86%)	3224 (89%)	338 (9%)	71 (2%)	6	28

5 of 71 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	B	139	ASP
7	D	93	LEU
7	D	95	THR
7	D	137	PRO
7	D	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	
4	A	179/181 (99%)	167 (93%)	12 (7%)	15	46
5	B	282/282 (100%)	262 (93%)	20 (7%)	13	43
6	C	193/193 (100%)	176 (91%)	17 (9%)	9	35
7	D	117/147 (80%)	110 (94%)	7 (6%)	17	50
8	E	152/155 (98%)	147 (97%)	5 (3%)	33	67
9	F	92/92 (100%)	91 (99%)	1 (1%)	65	83
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	108 (88%)	14 (12%)	5	24
12	I	118/121 (98%)	111 (94%)	7 (6%)	18	50
13	J	106/106 (100%)	101 (95%)	5 (5%)	23	58
14	K	113/126 (90%)	110 (97%)	3 (3%)	39	71
15	L	166/166 (100%)	157 (95%)	9 (5%)	20	53
16	M	149/149 (100%)	139 (93%)	10 (7%)	15	46
17	N	93/93 (100%)	90 (97%)	3 (3%)	34	67
18	O	113/116 (97%)	109 (96%)	4 (4%)	32	65
19	P	79/79 (100%)	75 (95%)	4 (5%)	21	55
20	Q	117/121 (97%)	114 (97%)	3 (3%)	40	72
21	R	71/73 (97%)	69 (97%)	2 (3%)	38	70
22	S	105/105 (100%)	99 (94%)	6 (6%)	18	52
23	T	44/52 (85%)	44 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	U	51/56 (91%)	50 (98%)	1 (2%)	48 76
25	V	130/130 (100%)	119 (92%)	11 (8%)	10 36
26	W	66/73 (90%)	59 (89%)	7 (11%)	6 27
27	X	120/195 (62%)	113 (94%)	7 (6%)	18 51
28	Y	56/56 (100%)	52 (93%)	4 (7%)	13 43
29	Z	46/46 (100%)	44 (96%)	2 (4%)	26 60
30	1	42/44 (96%)	41 (98%)	1 (2%)	43 73
31	2	79/79 (100%)	76 (96%)	3 (4%)	29 63
All	All	3028/3441 (88%)	2860 (94%)	168 (6%)	19 53

5 of 168 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
18	O	91	LYS
25	V	154	ARG
19	P	57	ASP
22	S	96	VAL
26	W	85	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
16	M	132	ASN
20	Q	140	GLN
30	1	17	GLN
18	O	50	GLN
19	P	94	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	245 (8%)	25 (0%)
2	9	121/122 (99%)	18 (14%)	3 (2%)
3	4	2/3 (66%)	1 (50%)	0
All	All	2868/3047 (94%)	264 (9%)	28 (0%)

5 of 264 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	60	A
1	0	67	A
1	0	69	A
1	0	70	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1667	A
2	9	3103	A
1	0	2011	A
1	0	2791	U
1	0	1979	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
32	SLD	0	9500	-	38,39,39	4.86	18 (47%)	47,53,53	2.60	19 (40%)

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
32	SLD	0	9500	-	-	4/23/51/51	0/3/3/3

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	SLD	C8S-C6S	17.00	1.58	1.34
32	0	9500	SLD	C9S-C8S	-9.48	1.35	1.50
32	0	9500	SLD	C5S-N4S	9.45	1.45	1.32
32	0	9500	SLD	C12-C11	8.09	1.53	1.39
32	0	9500	SLD	C6-N1	8.07	1.45	1.36

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	0	9500	SLD	O3-C6-N1	-7.30	122.04	128.80
32	0	9500	SLD	O1-C6-O3	6.28	129.77	122.40
32	0	9500	SLD	C3S-N4S-C5S	5.16	123.64	118.86
32	0	9500	SLD	C2-N1-C6	5.13	131.36	125.98
32	0	9500	SLD	C5-N1-C6	-4.06	108.17	111.17

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	0	9500	SLD	C5-C7-C8-N2
32	0	9500	SLD	C4B-C5B-CAS-N5S
32	0	9500	SLD	O1-C7-C8-N2
32	0	9500	SLD	C6S-C8S-C9S-C0S

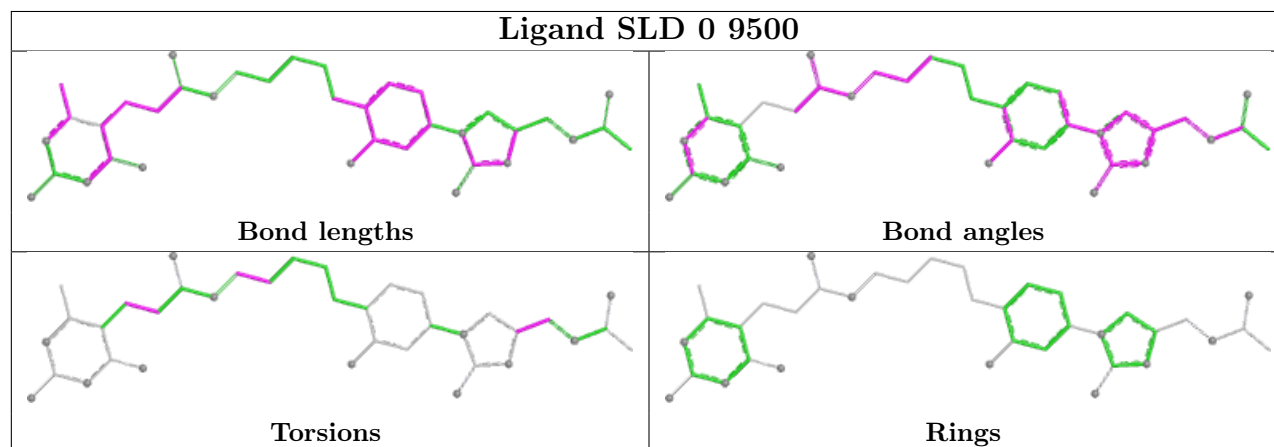
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	0	9500	SLD	4	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 [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, 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	0	2754/2922 (94%)	-0.66	12 (0%) 88 76	35, 63, 107, 150	0
2	9	122/122 (100%)	-0.31	5 (4%) 41 23	52, 80, 106, 150	0
3	4	3/3 (100%)	-0.71	0 100 100	49, 49, 51, 51	0
4	A	237/239 (99%)	-0.44	1 (0%) 88 76	44, 69, 101, 121	0
5	B	337/337 (100%)	-0.36	0 100 100	42, 72, 98, 108	0
6	C	246/246 (100%)	-0.47	0 100 100	36, 63, 87, 99	0
7	D	140/176 (79%)	0.43	4 (2%) 53 31	70, 115, 131, 136	0
8	E	172/177 (97%)	-0.19	1 (0%) 85 69	61, 84, 102, 107	0
9	F	119/119 (100%)	-0.13	0 100 100	70, 88, 112, 118	0
10	G	29/348 (8%)	0.39	1 (3%) 48 27	85, 105, 113, 117	0
11	H	156/167 (93%)	-0.20	1 (0%) 85 69	51, 72, 100, 108	0
12	I	142/145 (97%)	-0.44	0 100 100	50, 66, 85, 102	0
13	J	132/132 (100%)	-0.32	0 100 100	53, 71, 89, 96	0
14	K	145/164 (88%)	-0.24	1 (0%) 84 66	39, 83, 117, 129	0
15	L	194/194 (100%)	-0.40	1 (0%) 87 72	47, 62, 79, 90	0
16	M	186/186 (100%)	0.01	5 (2%) 56 33	58, 81, 120, 133	0
17	N	115/115 (100%)	-0.29	0 100 100	56, 72, 90, 94	0
18	O	143/148 (96%)	-0.42	0 100 100	50, 72, 87, 94	0
19	P	95/95 (100%)	-0.49	1 (1%) 78 57	51, 62, 75, 88	0
20	Q	150/154 (97%)	-0.59	0 100 100	46, 61, 81, 88	0
21	R	81/84 (96%)	-0.47	0 100 100	59, 76, 95, 103	0
22	S	119/119 (100%)	-0.32	0 100 100	55, 74, 97, 113	0
23	T	53/66 (80%)	-0.24	0 100 100	57, 73, 92, 99	0
24	U	65/70 (92%)	-0.01	2 (3%) 51 30	68, 90, 123, 129	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	V	154/154 (100%)	-0.51	0 100 100	51, 64, 82, 94	0
26	W	82/91 (90%)	-0.18	3 (3%) 45 25	58, 75, 99, 117	0
27	X	142/240 (59%)	-0.53	1 (0%) 84 66	43, 61, 82, 101	0
28	Y	73/73 (100%)	0.07	0 100 100	62, 76, 95, 104	0
29	Z	56/56 (100%)	-0.73	0 100 100	42, 52, 58, 68	0
30	1	46/48 (95%)	-0.21	0 100 100	49, 77, 105, 117	0
31	2	92/92 (100%)	-0.15	2 (2%) 62 39	53, 73, 87, 98	0
All	All	6580/7282 (90%)	-0.45	41 (0%) 85 69	35, 69, 108, 150	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	U	1	THR	4.0
2	9	3025	G	3.9
31	2	55	VAL	3.4
7	D	10	PHE	3.3
2	9	3001	U	3.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
35	NA	9	8351	1/1	0.42	0.17	94,94,94,94	0
35	NA	R	8312	1/1	0.51	0.18	84,84,84,84	0
35	NA	0	8341	1/1	0.54	0.10	60,60,60,60	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8329	1/1	0.62	0.17	98,98,98,98	0
35	NA	0	8366	1/1	0.66	0.15	82,82,82,82	0
35	NA	0	8368	1/1	0.66	0.24	69,69,69,69	0
35	NA	Q	8386	1/1	0.68	0.36	107,107,107,107	0
35	NA	0	8324	1/1	0.68	0.21	58,58,58,58	0
35	NA	0	8340	1/1	0.71	0.28	69,69,69,69	0
35	NA	0	8384	1/1	0.72	0.10	85,85,85,85	0
35	NA	0	8382	1/1	0.73	0.30	89,89,89,89	0
34	K	0	8201	1/1	0.77	0.48	141,141,141,141	0
35	NA	0	8385	1/1	0.80	0.29	73,73,73,73	0
33	MG	9	8095	1/1	0.82	0.26	106,106,106,106	0
33	MG	0	8092	1/1	0.82	0.40	111,111,111,111	0
36	CL	0	8505	1/1	0.82	0.18	99,99,99,99	0
33	MG	0	8046	1/1	0.83	0.08	86,86,86,86	0
35	NA	0	8375	1/1	0.84	0.24	81,81,81,81	0
35	NA	0	8352	1/1	0.84	0.10	61,61,61,61	0
33	MG	0	8102	1/1	0.84	0.12	91,91,91,91	0
33	MG	0	8114	1/1	0.84	0.21	95,95,95,95	0
36	CL	B	8519	1/1	0.84	0.11	95,95,95,95	0
36	CL	N	8508	1/1	0.84	0.15	116,116,116,116	0
33	MG	0	8049	1/1	0.85	0.12	90,90,90,90	0
35	NA	0	8325	1/1	0.85	0.12	64,64,64,64	0
35	NA	9	8383	1/1	0.85	0.09	67,67,67,67	0
35	NA	0	8374	1/1	0.85	0.29	77,77,77,77	0
34	K	0	8202	1/1	0.86	0.29	92,92,92,92	0
35	NA	0	8307	1/1	0.86	0.12	71,71,71,71	0
35	NA	0	8369	1/1	0.86	0.38	96,96,96,96	0
35	NA	0	8308	1/1	0.86	0.20	77,77,77,77	0
35	NA	0	8362	1/1	0.86	0.27	79,79,79,79	0
35	NA	0	8302	1/1	0.87	0.11	55,55,55,55	0
35	NA	0	8360	1/1	0.87	0.62	69,69,69,69	0
35	NA	0	8311	1/1	0.88	0.18	73,73,73,73	0
35	NA	0	8313	1/1	0.88	0.11	89,89,89,89	0
35	NA	0	8326	1/1	0.88	0.18	73,73,73,73	0
35	NA	0	8350	1/1	0.88	0.13	57,57,57,57	0
36	CL	I	8502	1/1	0.88	0.12	93,93,93,93	0
36	CL	K	8510	1/1	0.88	0.11	104,104,104,104	0
35	NA	0	8378	1/1	0.88	0.16	65,65,65,65	0
35	NA	H	8322	1/1	0.89	0.21	78,78,78,78	0
35	NA	0	8377	1/1	0.89	0.26	75,75,75,75	0
35	NA	0	8365	1/1	0.89	0.18	47,47,47,47	0
33	MG	0	8101	1/1	0.89	0.13	94,94,94,94	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	NA	0	8330	1/1	0.89	0.08	61,61,61,61	0
33	MG	A	8105	1/1	0.89	0.14	52,52,52,52	0
35	NA	0	8328	1/1	0.89	0.11	55,55,55,55	0
35	NA	0	8363	1/1	0.89	0.22	83,83,83,83	0
33	MG	0	8103	1/1	0.90	0.16	97,97,97,97	0
33	MG	0	8045	1/1	0.90	0.19	91,91,91,91	0
33	MG	0	8022	1/1	0.90	0.14	83,83,83,83	0
35	NA	0	8314	1/1	0.90	0.26	53,53,53,53	0
35	NA	0	8361	1/1	0.90	0.15	77,77,77,77	0
35	NA	0	8321	1/1	0.90	0.19	67,67,67,67	0
35	NA	0	8379	1/1	0.90	0.09	48,48,48,48	0
36	CL	I	8501	1/1	0.90	0.11	99,99,99,99	0
35	NA	0	8333	1/1	0.90	0.16	40,40,40,40	0
35	NA	0	8339	1/1	0.90	0.09	33,33,33,33	0
33	MG	0	8024	1/1	0.90	0.23	98,98,98,98	0
35	NA	0	8334	1/1	0.91	0.22	48,48,48,48	0
36	CL	0	8515	1/1	0.91	0.20	100,100,100,100	0
35	NA	0	8335	1/1	0.91	0.22	83,83,83,83	0
35	NA	0	8357	1/1	0.91	0.24	61,61,61,61	0
35	NA	0	8306	1/1	0.91	0.20	59,59,59,59	0
35	NA	0	8323	1/1	0.91	0.14	66,66,66,66	0
35	NA	0	8316	1/1	0.91	0.09	52,52,52,52	0
33	MG	0	8047	1/1	0.92	0.12	90,90,90,90	0
35	NA	0	8370	1/1	0.92	0.33	76,76,76,76	0
33	MG	0	8104	1/1	0.92	0.08	66,66,66,66	0
36	CL	A	8509	1/1	0.92	0.23	89,89,89,89	0
33	MG	0	8050	1/1	0.92	0.04	68,68,68,68	0
33	MG	0	8115	1/1	0.92	0.07	73,73,73,73	0
35	NA	0	8367	1/1	0.92	0.11	85,85,85,85	0
35	NA	Q	8337	1/1	0.92	0.05	64,64,64,64	0
33	MG	0	8067	1/1	0.92	0.09	81,81,81,81	0
37	CD	N	8405	1/1	0.92	0.25	150,150,150,150	0
33	MG	0	8072	1/1	0.93	0.09	78,78,78,78	0
33	MG	0	8111	1/1	0.93	0.05	75,75,75,75	0
35	NA	0	8332	1/1	0.93	0.09	50,50,50,50	0
36	CL	0	8522	1/1	0.93	0.24	92,92,92,92	0
35	NA	0	8371	1/1	0.93	0.35	69,69,69,69	0
35	NA	0	8373	1/1	0.93	0.08	57,57,57,57	0
35	NA	0	8343	1/1	0.93	0.06	48,48,48,48	0
35	NA	A	8345	1/1	0.93	0.06	48,48,48,48	0
35	NA	0	8301	1/1	0.93	0.09	59,59,59,59	0
35	NA	0	8318	1/1	0.93	0.09	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	S	8073	1/1	0.93	0.05	71,71,71,71	0
33	MG	O	8097	1/1	0.94	0.11	53,53,53,53	0
33	MG	O	8100	1/1	0.94	0.16	97,97,97,97	0
35	NA	O	8359	1/1	0.94	0.18	81,81,81,81	0
33	MG	O	8044	1/1	0.94	0.13	59,59,59,59	0
32	SLD	O	9500	37/37	0.94	0.09	46,50,53,59	0
33	MG	O	8087	1/1	0.94	0.11	82,82,82,82	0
33	MG	O	8042	1/1	0.94	0.08	61,61,61,61	0
35	NA	O	8364	1/1	0.94	0.15	66,66,66,66	0
35	NA	P	8348	1/1	0.94	0.05	68,68,68,68	0
36	CL	L	8518	1/1	0.94	0.07	69,69,69,69	0
36	CL	M	8507	1/1	0.94	0.06	86,86,86,86	0
35	NA	O	8349	1/1	0.94	0.11	69,69,69,69	0
36	CL	P	8511	1/1	0.94	0.10	84,84,84,84	0
33	MG	O	8106	1/1	0.94	0.08	78,78,78,78	0
35	NA	O	8303	1/1	0.95	0.08	55,55,55,55	0
33	MG	O	8071	1/1	0.95	0.08	104,104,104,104	0
35	NA	O	8338	1/1	0.95	0.06	66,66,66,66	0
35	NA	O	8376	1/1	0.95	0.34	79,79,79,79	0
33	MG	O	8064	1/1	0.95	0.08	39,39,39,39	0
33	MG	O	8085	1/1	0.95	0.06	92,92,92,92	0
35	NA	O	8310	1/1	0.95	0.07	46,46,46,46	0
35	NA	O	8381	1/1	0.95	0.05	69,69,69,69	0
33	MG	O	8066	1/1	0.95	0.09	105,105,105,105	0
33	MG	O	8088	1/1	0.95	0.13	40,40,40,40	0
33	MG	O	8090	1/1	0.95	0.20	81,81,81,81	0
36	CL	J	8512	1/1	0.95	0.07	67,67,67,67	0
33	MG	O	8013	1/1	0.95	0.07	60,60,60,60	0
35	NA	O	8353	1/1	0.95	0.06	43,43,43,43	0
35	NA	O	8356	1/1	0.95	0.15	73,73,73,73	0
35	NA	H	8309	1/1	0.95	0.09	49,49,49,49	0
33	MG	O	8070	1/1	0.95	0.06	63,63,63,63	0
36	CL	X	8520	1/1	0.95	0.10	57,57,57,57	0
35	NA	L	8347	1/1	0.95	0.04	55,55,55,55	0
36	CL	O	8514	1/1	0.96	0.07	75,75,75,75	0
33	MG	O	8112	1/1	0.96	0.09	64,64,64,64	0
36	CL	O	8516	1/1	0.96	0.21	64,64,64,64	0
36	CL	O	8517	1/1	0.96	0.08	82,82,82,82	0
33	MG	O	8076	1/1	0.96	0.05	102,102,102,102	0
33	MG	O	8041	1/1	0.96	0.08	68,68,68,68	0
33	MG	O	8094	1/1	0.96	0.28	97,97,97,97	0
35	NA	O	8317	1/1	0.96	0.04	57,57,57,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8096	1/1	0.96	0.07	70,70,70,70	0
36	CL	I	8521	1/1	0.96	0.08	69,69,69,69	0
35	NA	K	8380	1/1	0.96	0.12	85,85,85,85	0
33	MG	B	8055	1/1	0.96	0.06	71,71,71,71	0
33	MG	0	8003	1/1	0.96	0.05	51,51,51,51	0
33	MG	0	8060	1/1	0.96	0.15	63,63,63,63	0
35	NA	0	8354	1/1	0.96	0.17	58,58,58,58	0
35	NA	0	8355	1/1	0.96	0.12	77,77,77,77	0
36	CL	0	8503	1/1	0.96	0.10	82,82,82,82	0
35	NA	0	8336	1/1	0.96	0.08	63,63,63,63	0
36	CL	0	8513	1/1	0.97	0.06	74,74,74,74	0
33	MG	0	8108	1/1	0.97	0.10	102,102,102,102	0
33	MG	0	8110	1/1	0.97	0.04	56,56,56,56	0
33	MG	0	8043	1/1	0.97	0.05	64,64,64,64	0
35	NA	0	8344	1/1	0.97	0.03	48,48,48,48	0
33	MG	0	8082	1/1	0.97	0.11	79,79,79,79	0
33	MG	0	8098	1/1	0.97	0.07	50,50,50,50	0
33	MG	0	8053	1/1	0.97	0.07	63,63,63,63	0
35	NA	C	8304	1/1	0.97	0.03	51,51,51,51	0
33	MG	9	8052	1/1	0.97	0.04	60,60,60,60	0
33	MG	0	8068	1/1	0.97	0.04	64,64,64,64	0
35	NA	0	8372	1/1	0.97	0.13	72,72,72,72	0
33	MG	4	8063	1/1	0.97	0.08	62,62,62,62	0
33	MG	0	8011	1/1	0.97	0.08	50,50,50,50	0
33	MG	0	8062	1/1	0.97	0.09	90,90,90,90	0
33	MG	J	8069	1/1	0.97	0.04	87,87,87,87	0
33	MG	0	8028	1/1	0.97	0.04	57,57,57,57	0
33	MG	0	8075	1/1	0.97	0.09	77,77,77,77	0
36	CL	2	8504	1/1	0.97	0.11	100,100,100,100	0
35	NA	0	8320	1/1	0.97	0.07	40,40,40,40	0
33	MG	0	8057	1/1	0.98	0.05	53,53,53,53	0
33	MG	0	8006	1/1	0.98	0.10	60,60,60,60	0
33	MG	0	8093	1/1	0.98	0.03	63,63,63,63	0
35	NA	0	8327	1/1	0.98	0.05	46,46,46,46	0
33	MG	0	8008	1/1	0.98	0.06	52,52,52,52	0
35	NA	0	8305	1/1	0.98	0.04	42,42,42,42	0
35	NA	0	8358	1/1	0.98	0.16	109,109,109,109	0
33	MG	0	8113	1/1	0.98	0.04	60,60,60,60	0
35	NA	0	8331	1/1	0.98	0.06	60,60,60,60	0
33	MG	0	8048	1/1	0.98	0.04	66,66,66,66	0
33	MG	0	8077	1/1	0.98	0.04	54,54,54,54	0
33	MG	0	8116	1/1	0.98	0.04	84,84,84,84	0

Continued on next page...

Continued from previous page...

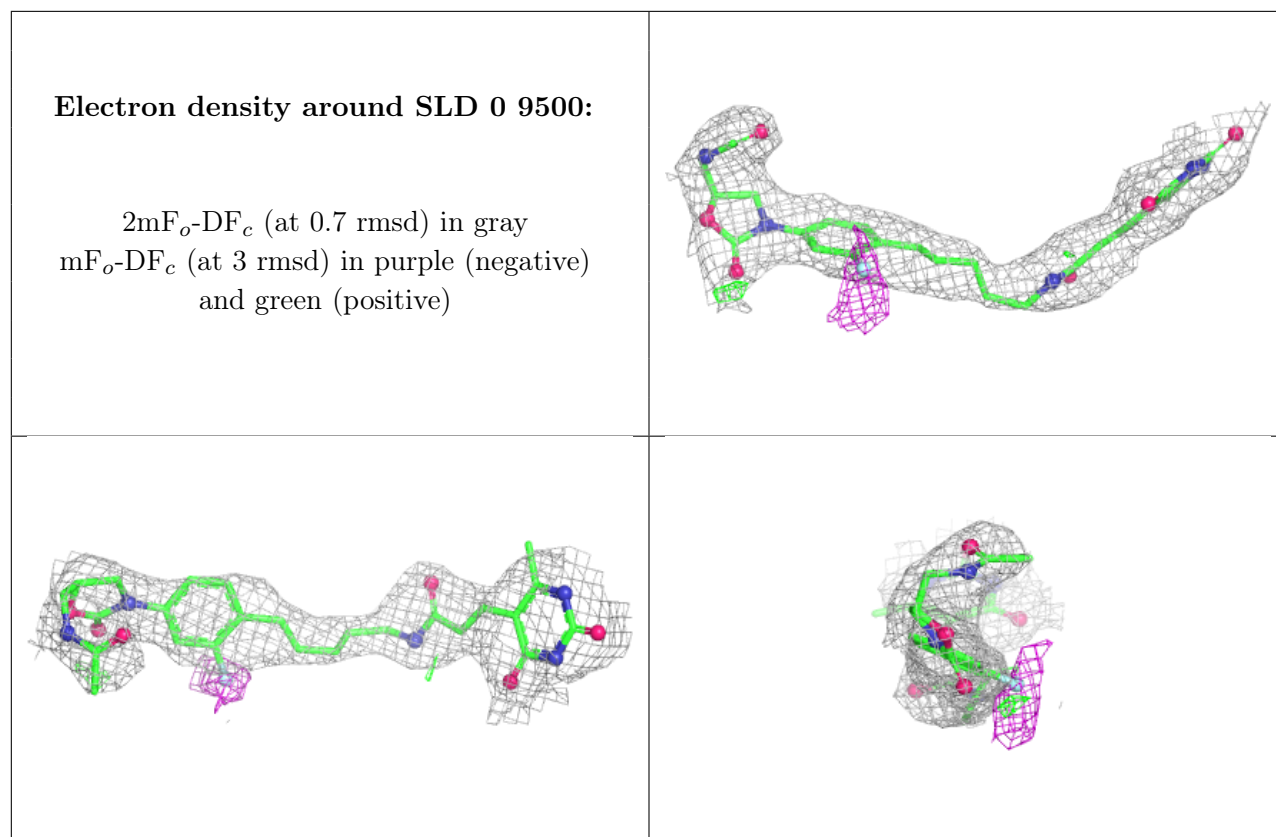
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8081	1/1	0.98	0.04	67,67,67,67	0
33	MG	0	8099	1/1	0.98	0.07	80,80,80,80	0
33	MG	0	8009	1/1	0.98	0.04	44,44,44,44	0
35	NA	0	8315	1/1	0.98	0.07	70,70,70,70	0
33	MG	0	8025	1/1	0.98	0.06	59,59,59,59	0
33	MG	0	8086	1/1	0.98	0.04	62,62,62,62	0
33	MG	0	8051	1/1	0.98	0.05	97,97,97,97	0
33	MG	0	8004	1/1	0.98	0.05	50,50,50,50	0
33	MG	X	8109	1/1	0.98	0.05	66,66,66,66	0
33	MG	0	8089	1/1	0.98	0.04	82,82,82,82	0
33	MG	0	8074	1/1	0.99	0.04	51,51,51,51	0
33	MG	0	8107	1/1	0.99	0.06	55,55,55,55	0
33	MG	0	8019	1/1	0.99	0.04	43,43,43,43	0
33	MG	0	8020	1/1	0.99	0.08	53,53,53,53	0
33	MG	0	8005	1/1	0.99	0.06	58,58,58,58	0
35	NA	I	8346	1/1	0.99	0.04	45,45,45,45	0
33	MG	0	8079	1/1	0.99	0.04	53,53,53,53	0
33	MG	0	8023	1/1	0.99	0.02	46,46,46,46	0
35	NA	0	8319	1/1	0.99	0.02	41,41,41,41	0
33	MG	0	8001	1/1	0.99	0.06	46,46,46,46	0
33	MG	0	8083	1/1	0.99	0.03	65,65,65,65	0
33	MG	0	8012	1/1	0.99	0.04	42,42,42,42	0
33	MG	0	8117	1/1	0.99	0.03	45,45,45,45	0
33	MG	0	8026	1/1	0.99	0.05	39,39,39,39	0
33	MG	0	8027	1/1	0.99	0.09	65,65,65,65	0
33	MG	0	8002	1/1	0.99	0.03	51,51,51,51	0
33	MG	A	8065	1/1	0.99	0.04	55,55,55,55	0
33	MG	0	8054	1/1	0.99	0.07	45,45,45,45	0
33	MG	0	8056	1/1	0.99	0.03	60,60,60,60	0
33	MG	0	8091	1/1	0.99	0.03	65,65,65,65	0
33	MG	0	8029	1/1	0.99	0.05	60,60,60,60	0
33	MG	0	8059	1/1	0.99	0.03	60,60,60,60	0
33	MG	2	8078	1/1	0.99	0.02	65,65,65,65	0
33	MG	0	8031	1/1	0.99	0.04	54,54,54,54	0
33	MG	0	8061	1/1	0.99	0.05	45,45,45,45	0
33	MG	0	8034	1/1	0.99	0.04	46,46,46,46	0
33	MG	0	8035	1/1	0.99	0.05	69,69,69,69	0
33	MG	0	8036	1/1	0.99	0.04	52,52,52,52	0
33	MG	0	8037	1/1	0.99	0.03	54,54,54,54	0
35	NA	0	8342	1/1	0.99	0.06	42,42,42,42	0
33	MG	0	8039	1/1	0.99	0.06	53,53,53,53	0
36	CL	Q	8506	1/1	0.99	0.07	80,80,80,80	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	MG	0	8014	1/1	0.99	0.02	46,46,46,46	0
33	MG	0	8016	1/1	0.99	0.10	71,71,71,71	0
33	MG	0	8018	1/1	0.99	0.04	57,57,57,57	0
37	CD	Y	8403	1/1	0.99	0.02	84,84,84,84	0
37	CD	Z	8402	1/1	0.99	0.04	89,89,89,89	0
37	CD	2	8404	1/1	0.99	0.03	90,90,90,90	0
33	MG	0	8033	1/1	1.00	0.03	48,48,48,48	0
33	MG	0	8084	1/1	1.00	0.05	70,70,70,70	0
33	MG	0	8021	1/1	1.00	0.06	54,54,54,54	0
33	MG	0	8017	1/1	1.00	0.03	43,43,43,43	0
33	MG	0	8058	1/1	1.00	0.05	61,61,61,61	0
33	MG	0	8010	1/1	1.00	0.03	47,47,47,47	0
33	MG	0	8015	1/1	1.00	0.04	60,60,60,60	0
33	MG	0	8038	1/1	1.00	0.02	56,56,56,56	0
33	MG	0	8030	1/1	1.00	0.07	48,48,48,48	0
33	MG	0	8040	1/1	1.00	0.03	88,88,88,88	0
37	CD	T	8401	1/1	1.00	0.02	83,83,83,83	0
33	MG	0	8080	1/1	1.00	0.02	52,52,52,52	0
33	MG	0	8007	1/1	1.00	0.03	47,47,47,47	0
33	MG	0	8032	1/1	1.00	0.02	52,52,52,52	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.