



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2020 – 12:00 PM BST

PDB ID : 3CXC
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 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 : 2.13
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) : 2.13

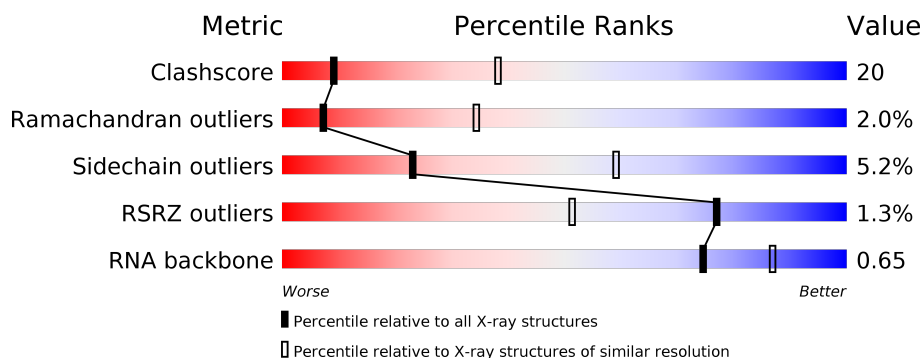
1 Overall quality at a glance

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))
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>%</div> <div> <div></div> <div>47%</div> <div>40%</div> <div>6%</div> <div>6%</div> </div> </div>
2	9	122	<div> <div>4%</div> <div> <div></div> <div>38%</div> <div>49%</div> <div>11%</div> </div> </div>
3	4	3	<div> <div> <div></div> <div>33%</div> <div>33%</div> <div>33%</div> </div> </div>
4	A	239	<div> <div>%</div> <div> <div></div> <div>54%</div> <div>41%</div> <div>5%</div> </div> </div>
5	B	337	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>42%</div> <div>6%</div> </div> </div>
6	C	246	<div> <div> <div></div> <div>55%</div> <div>39%</div> <div>5%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
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
33	MG	0	8024	-	-	-	X
33	MG	0	8114	-	-	-	X
35	NA	0	8329	-	-	-	X
35	NA	0	8363	-	-	-	X
35	NA	0	8371	-	-	-	X
35	NA	0	8384	-	-	-	X
35	NA	H	8322	-	-	-	X
35	NA	Q	8386	-	-	-	X
35	NA	R	8312	-	-	-	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			

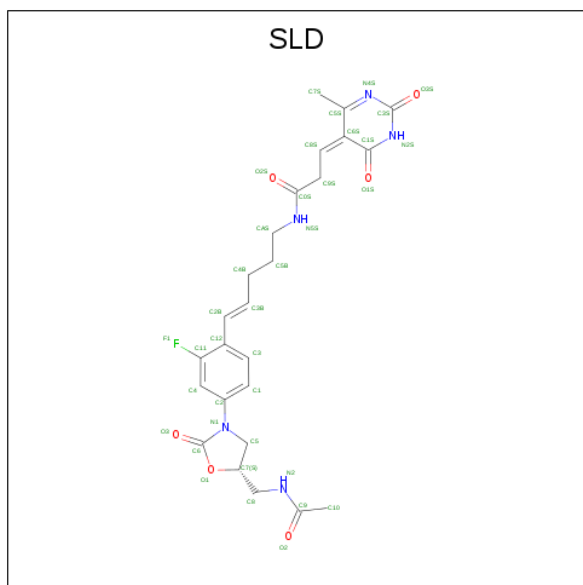
There is a discrepancy between the modelled and reference sequences:

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 (three-letter code: SLD) (formula: C₂₅H₂₈FN₅O₆).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	0	1	Total	C	F	N	O	0	0
			37	25	1	5	6		

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	0	107	Total	Mg	0	0
			107	107		
33	J	1	Total	Mg	0	0
			1	1		
33	B	1	Total	Mg	0	0
			1	1		
33	A	2	Total	Mg	0	0
			2	2		
33	4	1	Total	Mg	0	0
			1	1		
33	X	1	Total	Mg	0	0
			1	1		
33	2	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	9	2	Total 2	Mg 2	0	0
33	S	1	Total 1	Mg 1	0	0

- Molecule 34 is POTASSIUM ION (three-letter code: K) (formula: K).

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

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

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

- Molecule 36 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	P	1	Total 1	Cl 1	0	0
36	J	1	Total 1	Cl 1	0	0
36	Q	1	Total 1	Cl 1	0	0
36	K	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	A	1	Total 1	Cl 1	0	0
36	N	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
36	L	1	Total 1	Cl 1	0	0
36	M	1	Total 1	Cl 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

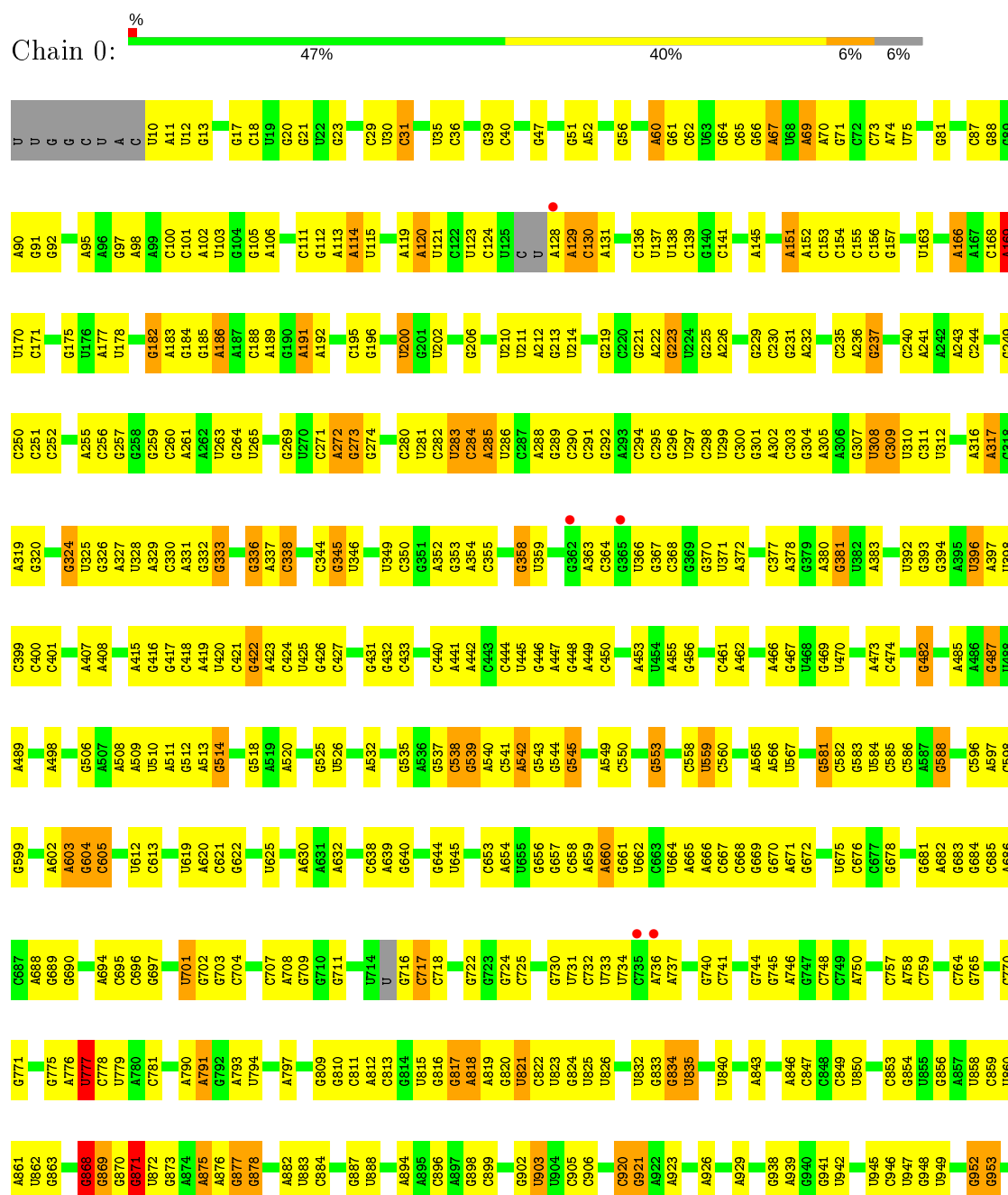
Continued from previous page...

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

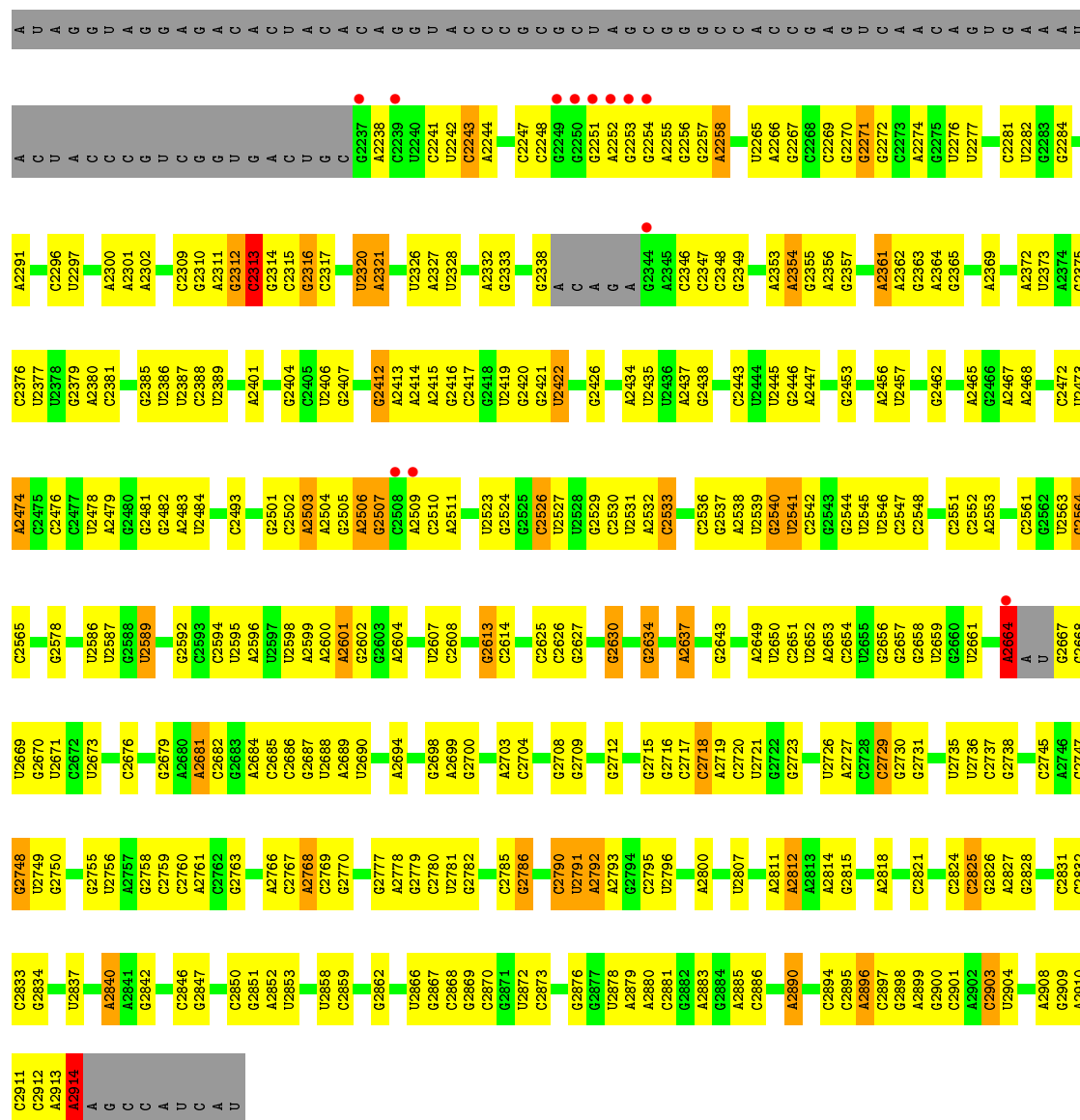
3 Residue-property plots

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.

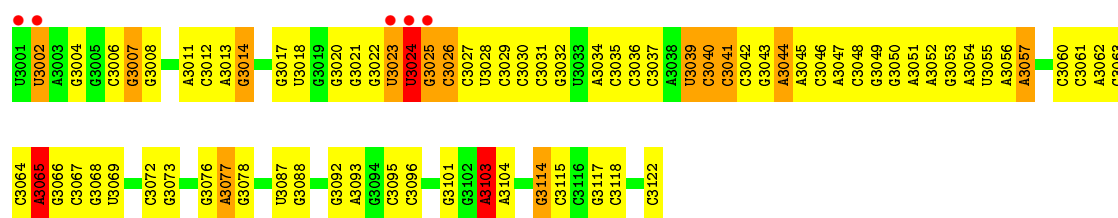
• Molecule 1: 23S RIBOSOMAL RNA



G2082	G2083	C1988	A1910	U1748	A1656	C1574	G1498	U1419	A1313	G1223	A1154	U1029	G958
A2089	A2090	C1992	G1917	G1751	A1657	C1575	U1499	C1420	U1314	G1224	G1155	U1030	C959
G2090	G2091	C1993	U1918	G1752	A1658	A1580	U1500	C1421	U1320	G1225	C1156	G1031	G960
G2094	A2095	C1994	A1919	A1755	A1666	C1584	U1503	C1423	G1322	G1226	G1158	C1044	C961
A2096	A2097	C1995	C1920	G1756	U1668	C1585	U1505	C1424	G1323	G1229	G1159	C1045	C962
A2101	G2102	U1996	A1921	U1757	A1669	G1586	U1506	C1425	G1324	G1230	G1160	G1046	C963
G2105	A2095	G2000	A1922	U1758	A1670	U1587	U1511	C1426	G1325	U1234	A1161	G1052	G964
C2106	A2096	G2001	C1830	A1759	C1675	G1592	G1512	A1427	U1235	U1234	G1162	G1053	G968
U2107	U2003	C2002	G1834	G1760	C1676	C1593	G1513	G1430	A1328	A1235	G1163	G1055	G969
G2110	U2012	U2004	U1835	C1762	U1677	C1594	C1514	C1431	A1329	A1236	U1164	A1058	G970
A2112	G2014	G2005	U1836	C1763	A1678	G1595	A1515	C1432	A1330	U1237	G1165	A1059	G
G2113	A2015	U2016	G1772	U1771	C1687	A1603	C1516	C1433	A1331	C1238	G1166	G1060	U
U2115	U1938	A1852	G1773	G1774	C1692	G1605	U1517	A1434	U1332	G1239	A1170	U1064	C
U2116	U1939	C1853	G1774	U1775	C1693	G1606	U1518	C1436	U1333	U1242	A1171	U1065	C
C2119	A1941	G1854	A1776	U1776	G1694	G1607	U1519	U1440	C1342	U1244	A1172	G1069	C
U2120	A1942	C1855	A1777	G1777	U1698	G1608	U1520	G1441	C1343	A1246	A1173	A1070	C
A2030	C1856	A1857	G1778	U1778	U1699	G1609	U1521	G1442	C1344	U1247	A1174	C1069	C
G2033	G1857	A1858	G1779	U1779	U1700	G1610	U1522	G1443	C1345	A1248	G1175	A1071	C
U2034	C1858	C1859	G1780	U1780	U1701	G1611	U1523	G1444	C1346	U1249	A1180	G1072	C
C2036	C1860	C1861	G1781	U1781	U1702	G1612	U1524	G1445	U1345	A1250	A1181	G1073	C
A2039	C1862	C1863	G1782	U1782	U1703	G1613	U1525	G1446	U1346	C1251	A1182	A1078	G
G2040	C1864	C1865	G1783	U1783	U1704	G1614	U1526	G1447	U1347	C1252	A1183	A1079	A
G2041	C1866	C1867	G1784	U1784	U1705	G1615	U1527	G1448	U1348	A1253	A1184	G1080	G
U2042	C1868	C1869	G1785	U1785	U1706	G1616	U1528	G1449	U1349	C1254	A1185	G1081	A
U2043	C1870	C1871	G1786	U1786	U1707	G1617	U1529	G1450	U1350	U1266	A1186	A1086	G
G2044	C1872	C1873	G1787	U1787	U1708	G1618	U1530	G1451	U1351	C1267	A1187	G1087	A
U2050	C1874	C1875	G1788	U1788	U1709	G1619	U1531	G1452	U1352	U1268	A1188	A1088	G
G2053	C1876	C1877	G1789	U1789	U1710	G1620	U1532	G1453	U1353	C1269	A1189	A1089	G
A2054	C1878	C1879	G1790	U1790	U1711	G1621	U1533	G1454	U1354	U1270	A1190	U1109	U
C2055	C1880	C1881	G1791	U1791	U1712	G1622	U1534	G1455	U1355	C1271	A1191	G1110	C
A2060	C1882	C1883	G1792	U1792	U1713	G1623	U1535	G1456	U1356	C1272	A1192	G1111	G
C2061	C1884	C1885	G1793	U1793	U1714	G1624	U1536	G1457	U1357	U1273	A1193	A1114	C
G2062	C1886	C1887	G1794	U1794	U1715	G1625	U1537	G1458	U1358	U1274	G1196	A1115	A
A2063	C1888	C1889	G1795	U1795	U1716	G1626	U1538	G1459	U1359	C1275	G1197	U1116	C
U2064	C1890	C1891	G1796	U1796	U1717	G1627	U1539	G1460	U1360	U1276	U1198	A1117	A
C2065	C1892	C1893	G1797	U1797	U1718	G1628	U1540	G1461	U1361	C1277	A1199	A1118	C
U2070	C1894	C1895	G1798	U1798	U1719	G1629	U1541	G1462	U1362	U1278	A1200	G1119	A1006
G2071	C1896	C1897	G1799	U1799	U1720	G1630	U1542	G1463	U1363	U1279	A1201	U1120	A1007
C2072	C1898	C1899	G1800	U1800	U1721	G1631	U1543	G1464	U1364	U1280	A1202	G1121	C1008
G2073	C1900	C1901	G1801	U1801	U1722	G1632	U1544	G1465	U1365	U1281	A1203	A1123	U1009
U2074	C1902	C1903	G1802	U1802	U1723	G1633	U1545	G1466	U1366	U1282	A1204	A1124	A1014
	C1904	C1905	G1803	U1803	U1724	G1634	U1546	G1467	U1367	U1283	A1205	C1129	A1015
	C1906	C1907	G1804	U1804	U1725	G1635	U1547	G1468	U1368	G1284	A1206	U1130	C1016
	C1908	C1909	G1805	U1805	U1726	G1636	U1548	G1469	U1369	U1285	A1207	G1131	U1017
	C1910	C1911	G1806	U1806	U1727	G1637	U1549	G1470	U1370	U1286	A1208	A1132	G1019
	C1912	C1913	G1807	U1807	U1728	G1638	U1550	G1471	U1371	U1287	A1209	A1133	A1020
	C1914	C1915	G1808	U1808	U1729	G1639	U1551	G1472	U1372	U1288	A1210	G1134	A1021
	C1916	C1917	G1809	U1809	U1730	G1640	U1552	G1473	U1373	U1289	A1211	G1135	G1022
	C1918	C1919	G1810	U1810	U1731	G1641	U1553	G1474	U1374	U1290	A1212	G1136	A1023
	C1920	C1921	G1811	U1811	U1732	G1642	U1554	G1475	U1375	U1291	A1213	G1137	U1018
	C1922	C1923	G1812	U1812	U1733	G1643	U1555	G1476	U1376	U1292	A1214	G1138	G1019
	C1924	C1925	G1813	U1813	U1734	G1644	U1556	G1477	U1377	U1293	A1215	G1139	A1020
	C1926	C1927	G1814	U1814	U1735	G1645	U1557	G1478	U1378	U1294	A1216	C1140	G1021
	C1928	C1929	G1815	U1815	U1736	G1646	U1558	G1479	U1379	U1295	A1217	A1150	A1022
	C1930	C1931	G1816	U1816	U1737	G1647	U1559	G1480	U1380	U1296	A1218	G1151	U1028
	C1932	C1933	G1817	U1817	U1738	G1648	U1560	G1481	U1381	U1297	A1219		
	C1934	C1935	G1818	U1818	U1739	G1649	U1561	G1482	U1382	U1298			
	C1936	C1937	G1819	U1819	U1740	G1650	U1562	G1483	U1383	U1299			
	C1938	C1939	G1820	U1820	U1741	G1651	U1563	G1484	U1384	U1300			
	C1940	C1941	G1821	U1821	U1742	G1652	U1564	G1485	U1385	U1301			
	C1942	C1943	G1822	U1822	U1743	G1653	U1565	G1486	U1386	U1302			
	C1944	C1945	G1823	U1823	U1744	G1654	U1566	G1487	U1387	U1303			
	C1946	C1947	G1824	U1824	U1745	G1655	U1567	G1488	U1388	U1304			
	C1948	C1949	G1825	U1825	U1746	G1656	U1568	G1489	U1389	U1305			
	C1950	C1951	G1826	U1826	U1747	G1657	U1569	G1490	U1390	U1306			
	C1952	C1953	G1827	U1827	U1748	G1658	U1570	G1491	U1391	U1307			
	C1954	C1955	G1828	U1828	U1749	G1659	U1571	G1492	U1392	U1308			
	C1956	C1957	G1829	U1829	U1750	G1660	U1572	G1493	U1393	U1309			
	C1958	C1959	G1830	U1830	U1751	G1661	U1573	G1494	U1394	U1310			
	C1960	C1961	G1831	U1831	U1752	G1662	U1574	G1495	U1395	U1311			
	C1962	C1963	G1832	U1832	U1753	G1663	U1575	G1496	U1396	U1312			
	C1964	C1965	G1833	U1833	U1754	G1664	U1576	G1497	U1397	U1313			
	C1966	C1967	G1834	U1834	U1755	G1665	U1577	G1498	U1398	U1314			
	C1968	C1969	G1835	U1835	U1756	G1666	U1578	G1499	U1399	U1315			
	C1970	C1971	G1836	U1836	U1757	G1667	U1579	G1500	U1400	U1316			
	C1972	C1973	G1837	U1837	U1758	G1668	U1580	G1501	U1401	U1317			
	C1974	C1975	G1838	U1838	U1759	G1669	U1581	G1502	U1402	U1318			
	C1976	C1977	G1839	U1839	U1760	G1670	U1582	G1503	U1403	U1319			
	C1978	C1979	G1840	U1840	U1761	G1671	U1583	G1504	U1404	U1320			
	C1980	C1981	G1841	U1841	U1762	G1672	U1584	G1505	U1405	U1321			
	C1982	C1983	G1842	U1842	U1763	G1673	U1585	G1506	U1406	U1322			
	C1984	C1985	G1843	U1843	U1764	G1674	U1586	G1507	U1407	U1323			
	C1986	C1987	G1844	U1844	U1765	G1675	U1587	G1508	U1408	U1324			
	C1988	C1989	G1845	U1845	U1766	G1676	U1588	G1509	U1409	U1325			
	C1990	C1991	G1846	U1846	U1767	G1677	U1589	G1510	U1410	U1326			
	C1992	C1993	G1847	U1847	U1768	G1678	U1590	G1511	U1411	U1327			
	C1994	C1995	G1848	U1848	U1769	G1679	U1591	G1512	U1412	U1328			
	C1996	C1997	G1849	U1849	U1770	G1680	U1592	G1513	U1413	U1329			
	C1998	C1999	G1850	U1850	U1771	G1681	U1593	G1514	U1414	U1330			
	C2000	C2001	G1851	U1851	U1772	G1682	U1594	G1515	U1415	U1331			
	C2002	C2003	G1852	U1852	U1773	G1683	U1595	G1516	U1416	U1332			
	C2004	C2005	G1853	U1853	U1774	G1684	U1596	G1517	U1417	U1333			
	C2006	C2007	G1854	U1854	U1775	G1685	U1597	G1518	U1418	U1334			
	C2008	C2009	G1855	U1855	U1776	G1686	U1598	G1519	U1419	U1335			
	C2010	C2011	G1856	U1856	U1777	G1687	U1599	G1520	U1420	U1336			
	C2012	C2013	G1857	U1857	U1778	G1688	U1600	G1521	U1421	U1337			
	C2014	C2015	G1858	U1858	U1779	G1689	G1601	G1522	U1422	U1338			
	C2016	C2017	G1859	U1859	U1780	G1690	G1602	G1523	U1423	U1339			
	C2018	C2019	G1860	U1860	U1781	G1691	G1603	G1524	U1424	U1			



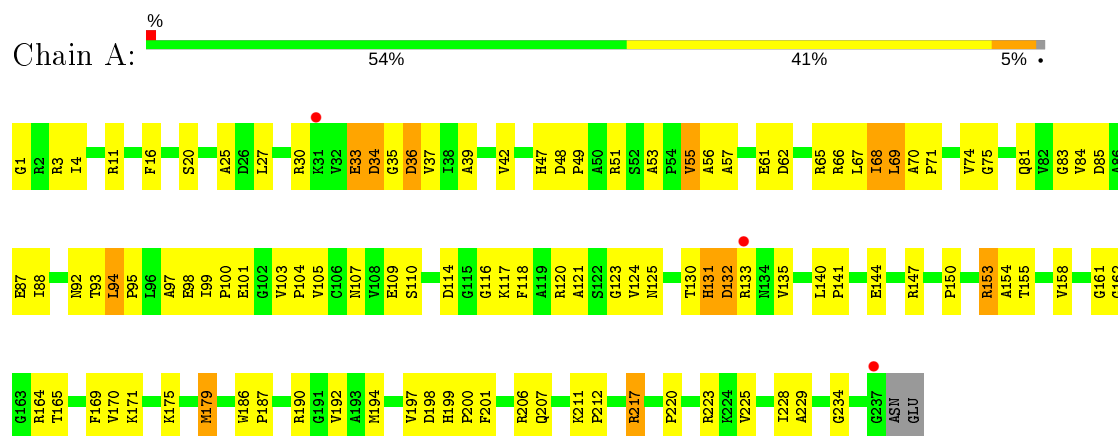
• Molecule 2: 5S RIBOSOMAL RNA



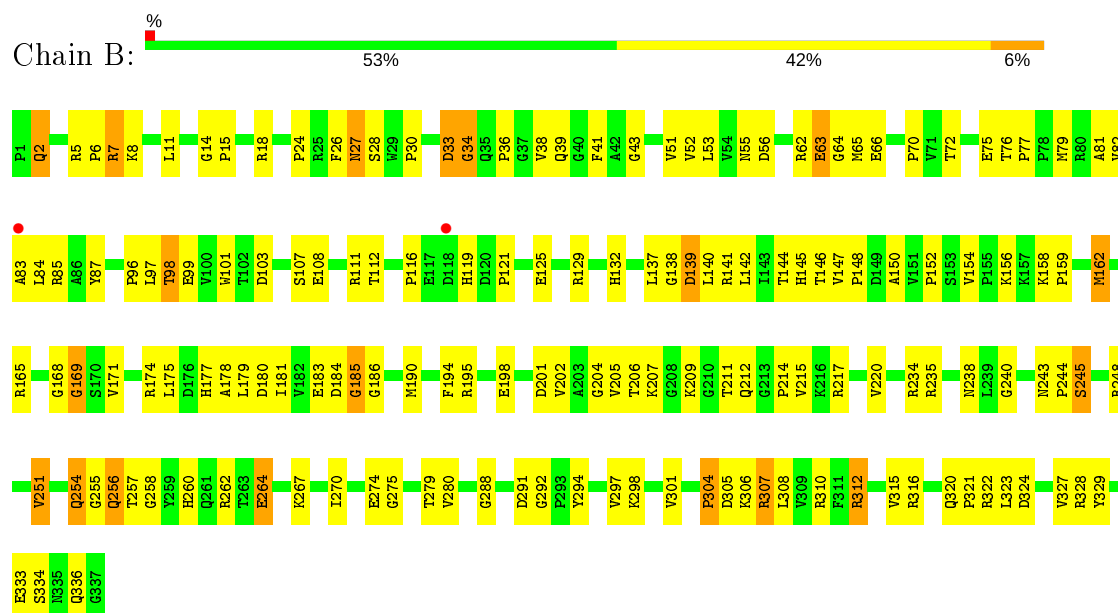
• Molecule 3: 5'-R(*CP*CP*A)-3'



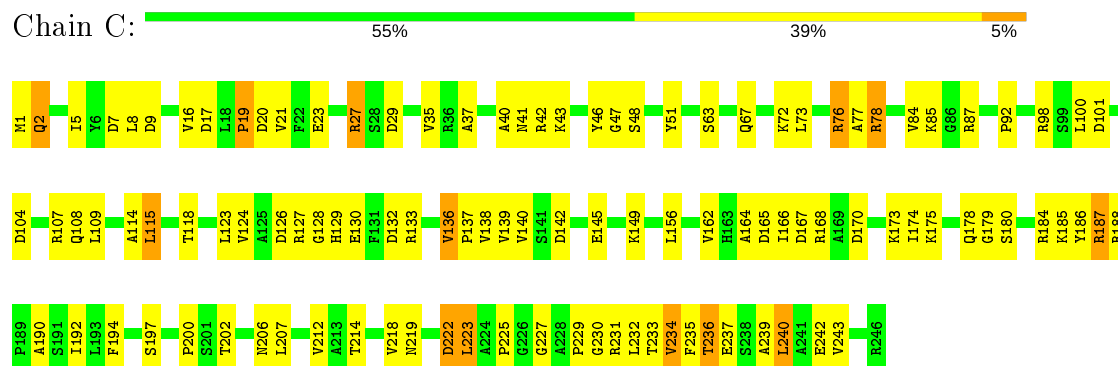
• Molecule 4: RIBOSOMAL PROTEIN L2



• Molecule 5: RIBOSOMAL PROTEIN L3

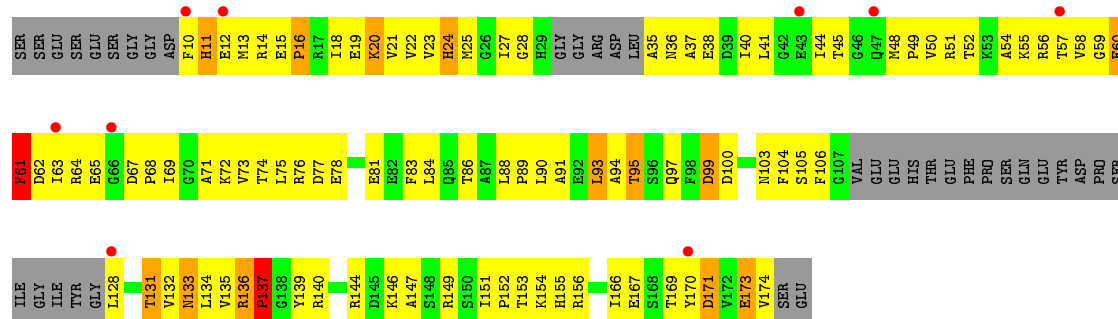


• Molecule 6: RIBOSOMAL PROTEIN L4

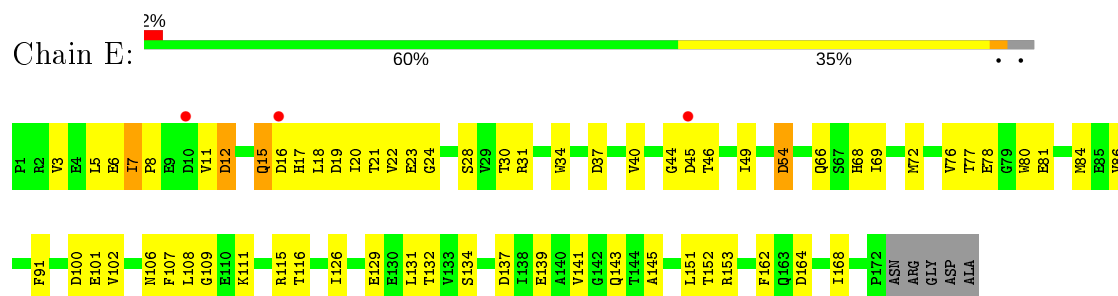


• Molecule 7: RIBOSOMAL PROTEIN L5

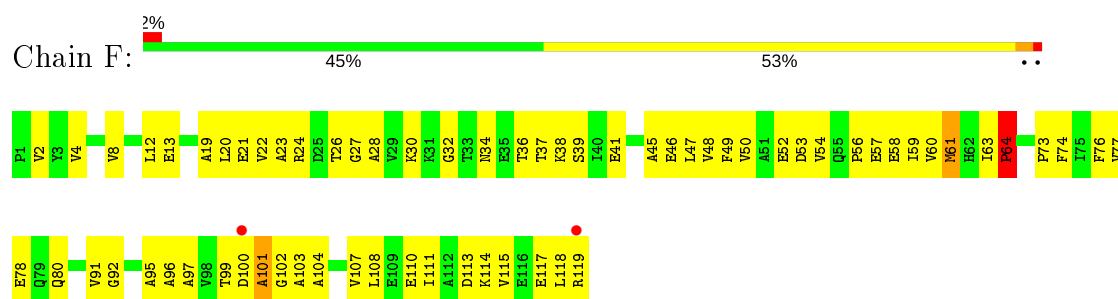




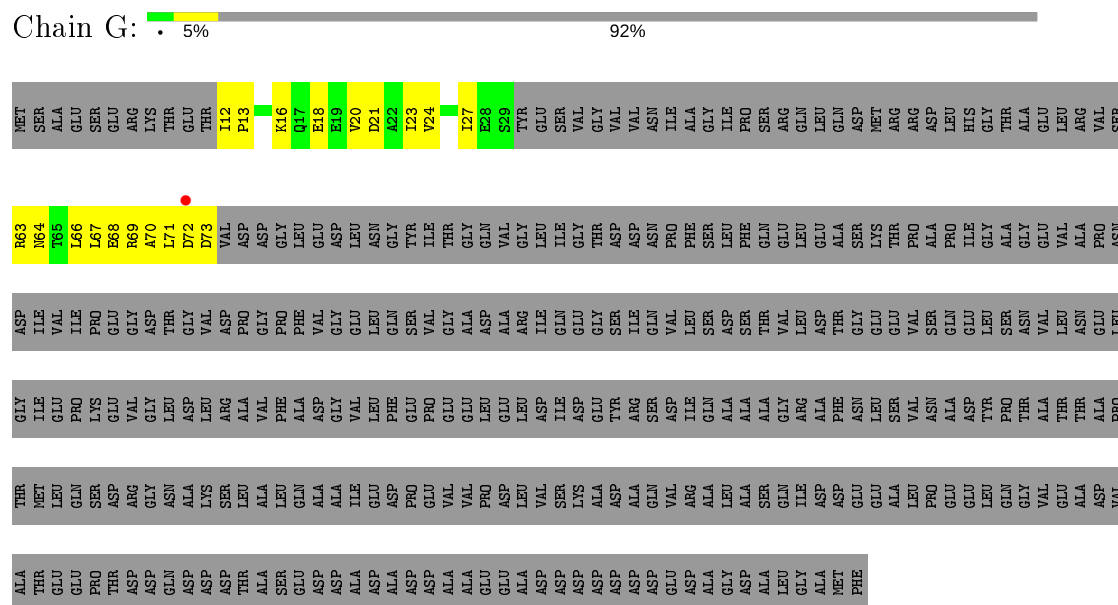
• Molecule 8: RIBOSOMAL PROTEIN L6



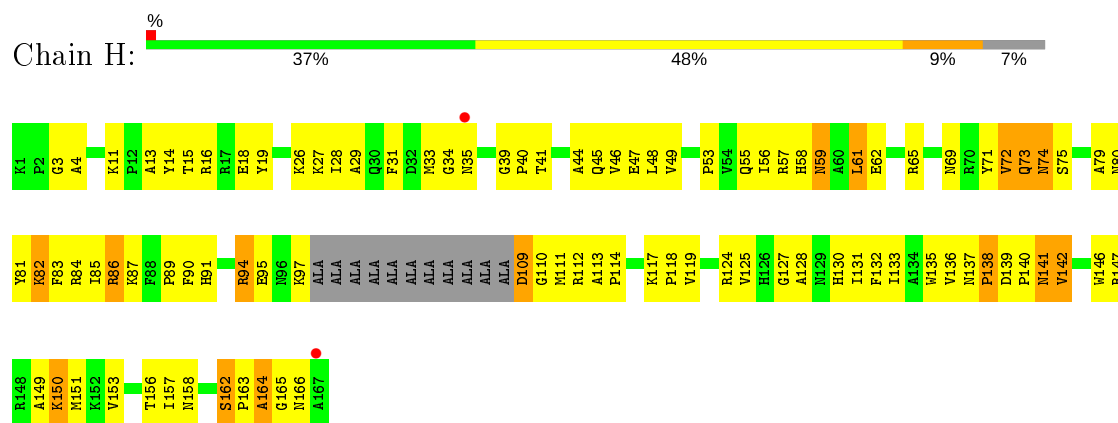
• Molecule 9: RIBOSOMAL PROTEIN L7AE



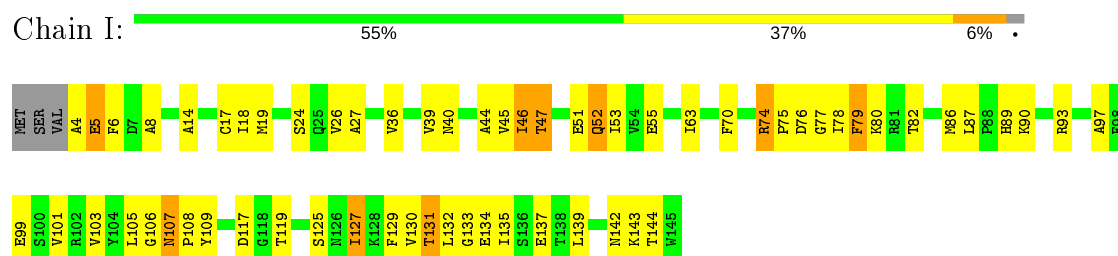
• Molecule 10: RIBOSOMAL PROTEIN L10



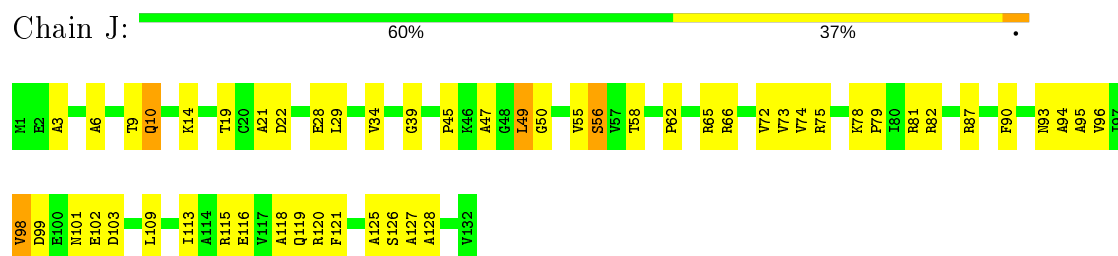
- Molecule 11: RIBOSOMAL PROTEIN L10E



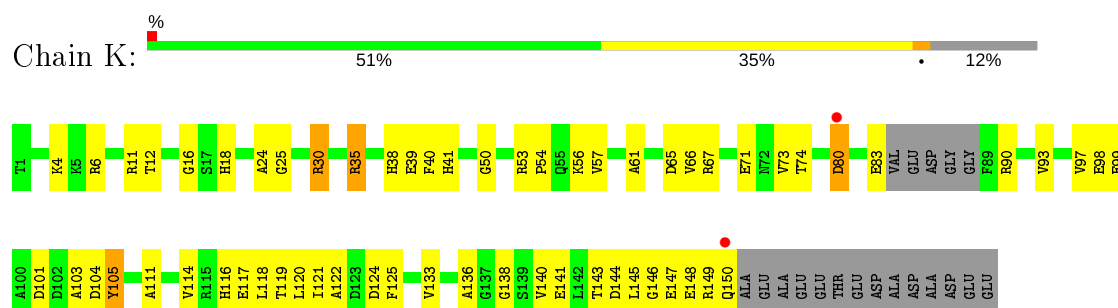
- Molecule 12: RIBOSOMAL PROTEIN L13



- Molecule 13: RIBOSOMAL PROTEIN L14

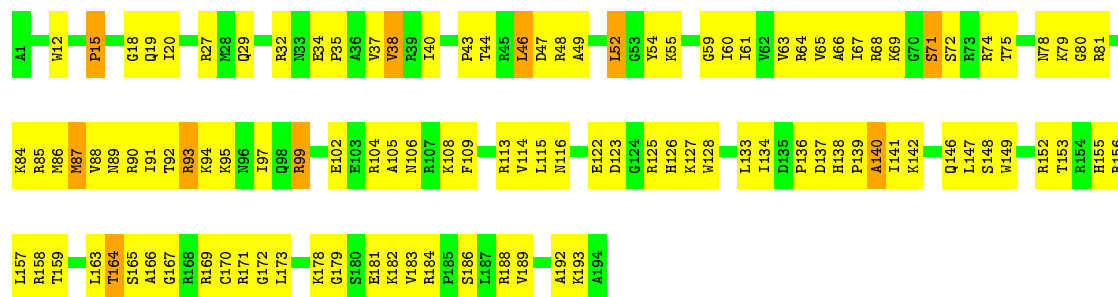


- Molecule 14: RIBOSOMAL PROTEIN L15

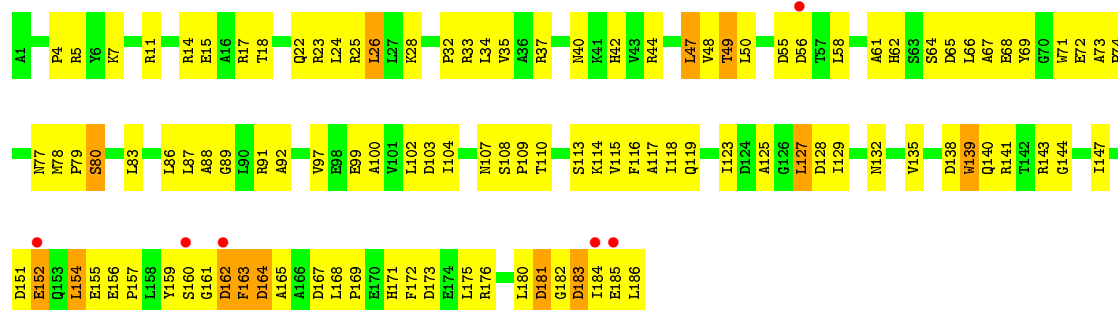
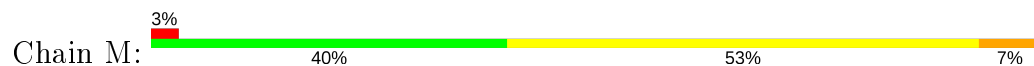


- Molecule 15: RIBOSOMAL PROTEIN L15E

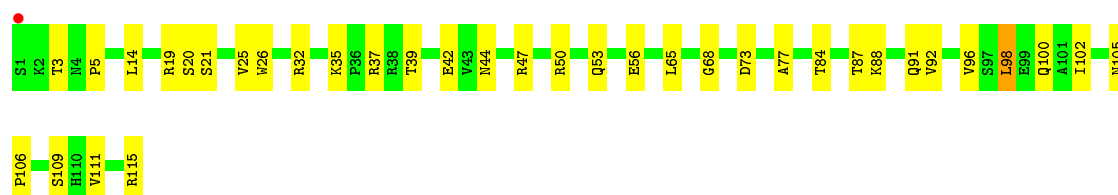




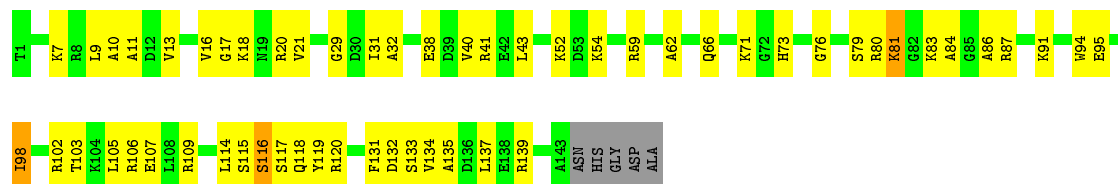
• Molecule 16: RIBOSOMAL PROTEIN L18



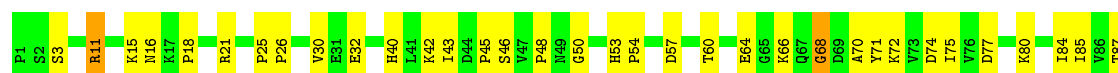
• Molecule 17: RIBOSOMAL PROTEIN L18E



• Molecule 18: RIBOSOMAL PROTEIN L19E



• Molecule 19: RIBOSOMAL PROTEIN L21E





• Molecule 20: RIBOSOMAL PROTEIN L22

Chain Q: 60% 36%



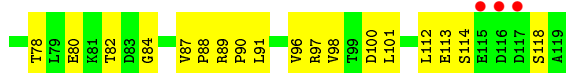
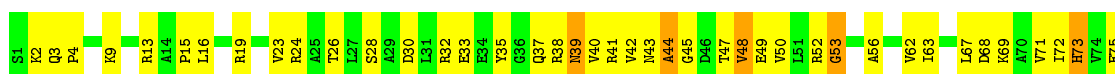
• Molecule 21: RIBOSOMAL PROTEIN L23

Chain R: 60% 37%



• Molecule 22: RIBOSOMAL PROTEIN L24

Chain S: 3% 50% 45%



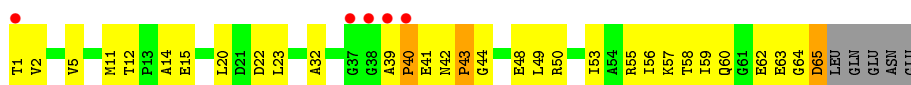
• Molecule 23: RIBOSOMAL PROTEIN L24E

Chain T: 38% 39% 20%



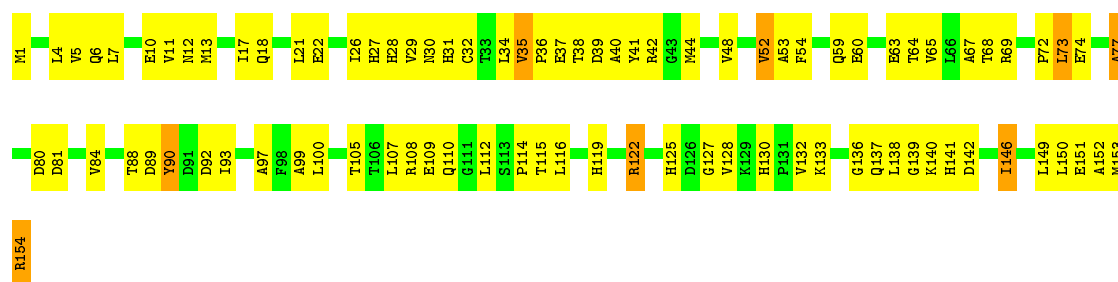
• Molecule 24: RIBOSOMAL PROTEIN L29

Chain U: 7% 49% 40% 7%

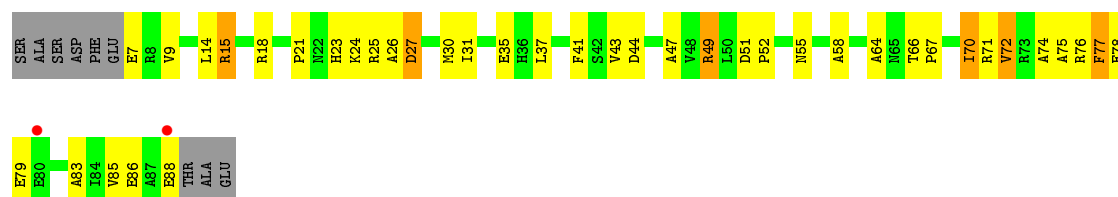


• Molecule 25: RIBOSOMAL PROTEIN L30

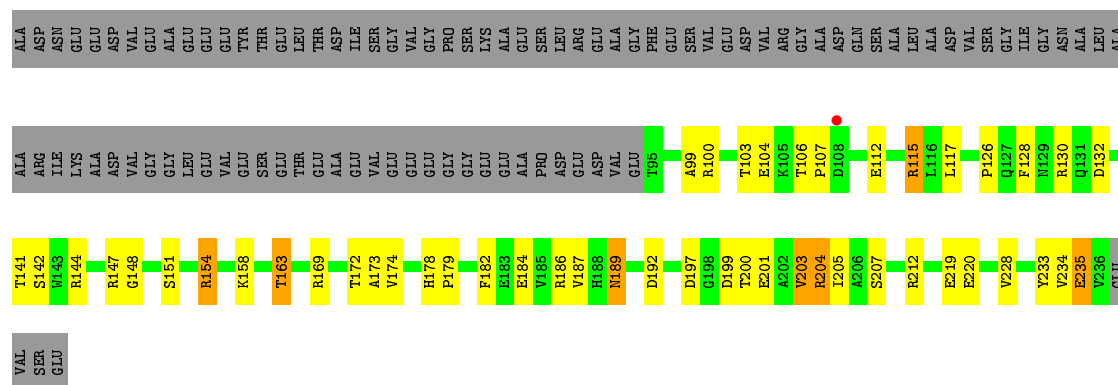
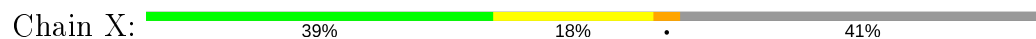
Chain V: 43% 52% 5%



- Molecule 26: RIBOSOMAL PROTEIN L31E



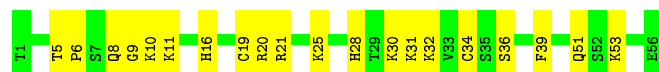
- Molecule 27: RIBOSOMAL PROTEIN L32E



- Molecule 28: RIBOSOMAL PROTEIN L37AE



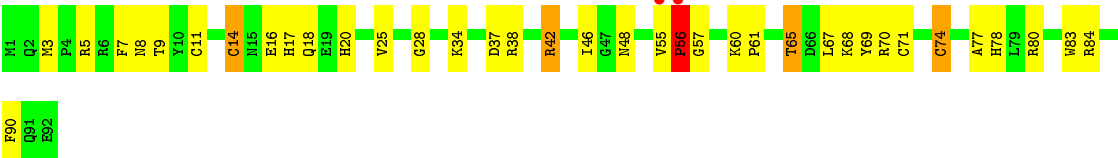
- Molecule 29: RIBOSOMAL PROTEIN L37E



- Molecule 30: RIBOSOMAL PROTEIN L39E



● 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 – 2.99	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-3.00) 90.8 (20.00-2.99)	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 , (Not available)	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 , 63.5	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: MG, CL, NA, K, CD, SLD

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	0.52	4/66076 (0.0%)	0.71	23/103052 (0.0%)
2	9	0.46	0/2905	0.76	3/4528 (0.1%)
3	4	0.89	0/65	1.01	0/99
4	A	0.39	0/1787	0.70	0/2409
5	B	0.40	0/2690	0.68	0/3652
6	C	0.45	0/1884	0.71	0/2551
7	D	0.37	0/1111	0.62	0/1498
8	E	0.38	0/1382	0.61	0/1880
9	F	0.38	0/897	0.60	0/1219
10	G	0.38	0/241	0.58	0/324
11	H	0.44	0/1247	0.79	3/1686 (0.2%)
12	I	0.43	0/1136	0.65	0/1530
13	J	0.41	0/1004	0.72	0/1351
14	K	0.41	0/1130	0.71	0/1509
15	L	0.49	0/1634	0.75	1/2180 (0.0%)
16	M	0.39	0/1474	0.68	0/1999
17	N	0.41	0/874	0.67	0/1181
18	O	0.41	0/1143	0.60	0/1521
19	P	0.44	0/749	0.74	1/1005 (0.1%)
20	Q	0.44	0/1172	0.69	0/1578
21	R	0.38	0/648	0.62	0/875
22	S	0.40	0/958	0.69	0/1289
23	T	0.61	2/417 (0.5%)	0.68	0/562
24	U	0.36	0/502	0.60	0/675
25	V	0.43	0/1219	0.67	0/1655
26	W	0.41	0/664	0.65	0/895
27	X	0.43	0/1146	0.68	0/1536
28	Y	0.54	1/576 (0.2%)	0.80	0/763
29	Z	0.54	0/438	0.78	2/578 (0.3%)
30	1	0.43	0/399	0.58	0/527
31	2	0.73	2/771 (0.3%)	0.72	0/1024
All	All	0.49	9/98339 (0.0%)	0.70	33/147131 (0.0%)

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

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

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	2	14	CYS	CB-SG	-12.55	1.60	1.82
1	0	2102	G	C6-O6	-6.72	1.18	1.24
28	Y	60	CYS	CB-SG	-6.10	1.71	1.82
1	0	2474	A	N1-C2	5.85	1.39	1.34
23	T	9	CYS	CB-SG	-5.75	1.72	1.81

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	3024	U	C2'-C3'-O3'	8.48	128.16	109.50
1	0	1979	G	C2'-C3'-O3'	6.90	124.75	113.70
11	H	74	ASN	N-CA-C	-6.85	92.50	111.00
2	9	3103	A	C5'-C4'-O4'	6.75	117.20	109.10
1	0	1563	G	C2'-C3'-O3'	6.72	124.45	113.70

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	1222	0
2	9	2600	0	1326	88	0
3	4	59	0	35	2	0
4	A	1754	0	1763	127	0
5	B	2625	0	2533	170	0
6	C	1859	0	1816	112	0
7	D	1094	0	1085	125	0
8	E	1357	0	1266	65	0
9	F	886	0	854	67	0
10	G	240	0	231	22	0
11	H	1216	0	1215	155	0
12	I	1120	0	1098	69	0
13	J	994	0	1027	57	0
14	K	1118	0	1076	64	0
15	L	1606	0	1676	142	0
16	M	1445	0	1401	139	0
17	N	865	0	873	35	0
18	O	1133	0	1127	57	0
19	P	735	0	729	29	0
20	Q	1149	0	1122	61	0
21	R	641	0	605	24	0
22	S	950	0	923	53	0
23	T	410	0	364	33	0
24	U	499	0	511	32	0
25	V	1196	0	1137	97	0
26	W	654	0	653	46	0
27	X	1130	0	1133	51	0
28	Y	564	0	598	54	0
29	Z	431	0	426	24	0
30	1	394	0	406	32	0
31	2	755	0	729	51	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	0	2	0	0	0	0
35	0	73	0	0	0	0
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	72	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	11	0
38	B	160	0	0	17	0
38	C	180	0	0	10	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	82	0	0	9	0
38	I	61	0	0	3	0
38	J	63	0	0	4	0
38	K	85	0	0	9	0
38	L	130	0	0	5	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	2990	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 20.

The worst 5 of 2990 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
1:O:871:G:H8	1:O:871:G:H5'	1.13	1.10
11:H:86:ARG:NH1	11:H:133:ILE:HG13	1.66	1.08
15:L:87:MET:HB3	31:2:46:ILE:HD13	1.31	1.07

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	
4	A	235/239 (98%)	207 (88%)	24 (10%)	4 (2%)	9	39
5	B	335/337 (99%)	300 (90%)	28 (8%)	7 (2%)	7	33
6	C	244/246 (99%)	213 (87%)	28 (12%)	3 (1%)	13	48
7	D	134/176 (76%)	96 (72%)	26 (19%)	12 (9%)	1	3
8	E	170/177 (96%)	157 (92%)	12 (7%)	1 (1%)	25	64
9	F	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5	27
10	G	25/348 (7%)	22 (88%)	2 (8%)	1 (4%)	3	17
11	H	152/167 (91%)	132 (87%)	16 (10%)	4 (3%)	5	27
12	I	140/145 (97%)	127 (91%)	10 (7%)	3 (2%)	7	33
13	J	130/132 (98%)	117 (90%)	11 (8%)	2 (2%)	10	42
14	K	141/164 (86%)	116 (82%)	23 (16%)	2 (1%)	11	43
15	L	192/194 (99%)	167 (87%)	20 (10%)	5 (3%)	5	27
16	M	184/186 (99%)	153 (83%)	24 (13%)	7 (4%)	3	18
17	N	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	17	55
18	O	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	22	60
19	P	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	6	31
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%)	9	39
23	T	51/66 (77%)	47 (92%)	3 (6%)	1 (2%)	7	34
24	U	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	22
25	V	152/154 (99%)	140 (92%)	11 (7%)	1 (1%)	22	60
26	W	80/91 (88%)	71 (89%)	7 (9%)	2 (2%)	5	28
27	X	140/240 (58%)	134 (96%)	6 (4%)	0	100	100
28	Y	71/73 (97%)	58 (82%)	10 (14%)	3 (4%)	3	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	6	31
All	All	3633/4235 (86%)	3224 (89%)	338 (9%)	71 (2%)	7	34

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%)	168 (94%)	11 (6%)	18	53
5	B	282/282 (100%)	264 (94%)	18 (6%)	17	51
6	C	193/193 (100%)	178 (92%)	15 (8%)	12	42
7	D	117/147 (80%)	108 (92%)	9 (8%)	13	42
8	E	152/155 (98%)	146 (96%)	6 (4%)	32	69
9	F	92/92 (100%)	91 (99%)	1 (1%)	73	90
10	G	27/283 (10%)	27 (100%)	0	100	100
11	H	122/122 (100%)	111 (91%)	11 (9%)	9	35
12	I	118/121 (98%)	110 (93%)	8 (7%)	16	48
13	J	106/106 (100%)	102 (96%)	4 (4%)	33	69
14	K	113/126 (90%)	108 (96%)	5 (4%)	28	65
15	L	166/166 (100%)	157 (95%)	9 (5%)	22	57
16	M	149/149 (100%)	141 (95%)	8 (5%)	22	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	N	93/93 (100%)	90 (97%)	3 (3%)	39	74
18	O	113/116 (97%)	109 (96%)	4 (4%)	36	71
19	P	79/79 (100%)	75 (95%)	4 (5%)	24	60
20	Q	117/121 (97%)	114 (97%)	3 (3%)	46	78
21	R	71/73 (97%)	69 (97%)	2 (3%)	43	77
22	S	105/105 (100%)	100 (95%)	5 (5%)	25	62
23	T	44/52 (85%)	44 (100%)	0	100	100
24	U	51/56 (91%)	49 (96%)	2 (4%)	32	69
25	V	130/130 (100%)	122 (94%)	8 (6%)	18	52
26	W	66/73 (90%)	62 (94%)	4 (6%)	18	53
27	X	120/195 (62%)	113 (94%)	7 (6%)	20	55
28	Y	56/56 (100%)	52 (93%)	4 (7%)	14	46
29	Z	46/46 (100%)	45 (98%)	1 (2%)	52	81
30	1	42/44 (96%)	41 (98%)	1 (2%)	49	79
31	2	79/79 (100%)	75 (95%)	4 (5%)	24	60
All	All	3028/3441 (88%)	2871 (95%)	157 (5%)	23	59

5 of 157 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	I	46	ILE
14	K	117	GLU
27	X	204	ARG
12	I	52	GLN
13	J	10	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 91 such sidechains are listed below:

Mol	Chain	Res	Type
14	K	41	HIS
17	N	53	GLN
30	1	16	ASN
15	L	26	HIS
16	M	107	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2922 (93%)	241 (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%)	260 (9%)	28 (0%)

5 of 260 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	1450	C
1	0	1856	C
2	9	3024	U
1	0	1563	G
1	0	1667	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 monosaccharides 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	$\# Z > 2$
32	SLD	0	9500	-	37,39,39	4.15	17 (45%)	47,53,53	2.75	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	-	-	5/23/51/51	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	0	9500	SLD	C9S-C8S	-10.37	1.35	1.50
32	0	9500	SLD	C5S-N4S	9.66	1.45	1.32
32	0	9500	SLD	C6-N1	8.90	1.45	1.36
32	0	9500	SLD	C12-C11	8.08	1.53	1.39
32	0	9500	SLD	C6S-C1S	7.18	1.58	1.45

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	-8.66	122.04	128.91
32	0	9500	SLD	O1-C6-O3	6.68	129.77	122.37
32	0	9500	SLD	C5-N1-C6	-5.37	108.17	111.28
32	0	9500	SLD	C2-N1-C6	5.09	131.36	125.91
32	0	9500	SLD	C3S-N4S-C5S	5.04	123.64	118.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

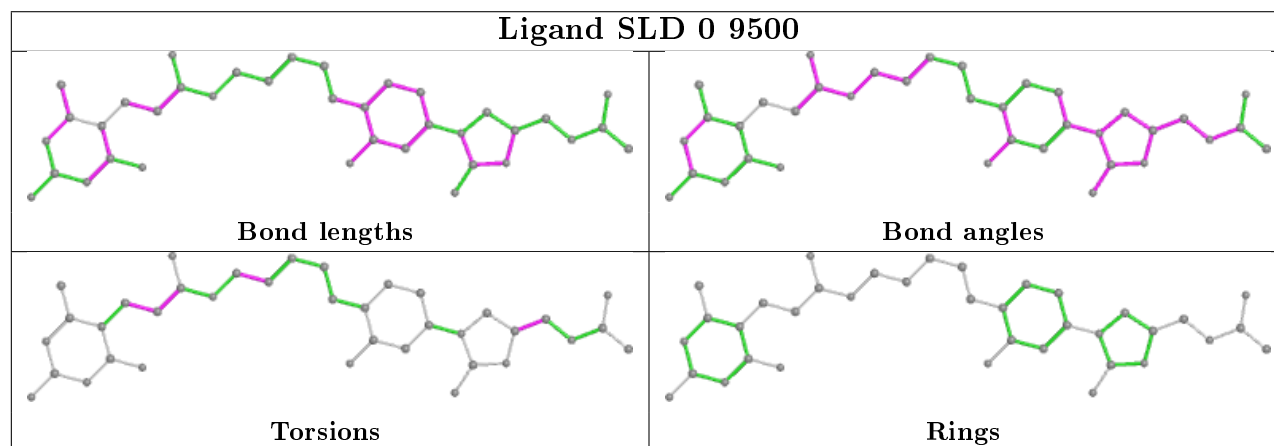
Mol	Chain	Res	Type	Atoms
32	0	9500	SLD	C5-C7-C8-N2
32	0	9500	SLD	N5S-C0S-C9S-C8S
32	0	9500	SLD	C4B-C5B-CAS-N5S
32	0	9500	SLD	C6S-C8S-C9S-C0S
32	0	9500	SLD	O1-C7-C8-N2

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 [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	0	2754/2922 (94%)	-0.44	32 (1%) 79 54	35, 63, 107, 150	0
2	9	122/122 (100%)	-0.02	5 (4%) 37 14	52, 80, 106, 150	0
3	4	3/3 (100%)	-0.43	0 100 100	49, 49, 51, 51	0
4	A	237/239 (99%)	-0.48	3 (1%) 77 51	44, 69, 101, 121	0
5	B	337/337 (100%)	-0.38	2 (0%) 89 72	42, 72, 98, 108	0
6	C	246/246 (100%)	-0.54	0 100 100	36, 63, 87, 99	0
7	D	140/176 (79%)	0.32	9 (6%) 19 6	70, 115, 131, 137	0
8	E	172/177 (97%)	-0.28	3 (1%) 70 41	61, 84, 102, 107	0
9	F	119/119 (100%)	-0.07	2 (1%) 70 41	70, 88, 112, 118	0
10	G	29/348 (8%)	0.09	1 (3%) 45 19	85, 105, 113, 117	0
11	H	156/167 (93%)	-0.30	2 (1%) 77 51	51, 72, 100, 108	0
12	I	142/145 (97%)	-0.51	0 100 100	50, 66, 85, 102	0
13	J	132/132 (100%)	-0.38	0 100 100	53, 71, 89, 96	0
14	K	145/164 (88%)	-0.29	2 (1%) 75 49	39, 83, 117, 129	0
15	L	194/194 (100%)	-0.63	0 100 100	47, 62, 79, 90	0
16	M	186/186 (100%)	-0.04	6 (3%) 47 20	58, 81, 120, 133	0
17	N	115/115 (100%)	-0.35	1 (0%) 84 63	56, 72, 90, 94	0
18	O	143/148 (96%)	-0.49	0 100 100	50, 72, 87, 94	0
19	P	95/95 (100%)	-0.48	1 (1%) 80 56	51, 62, 75, 88	0
20	Q	150/154 (97%)	-0.53	0 100 100	46, 61, 81, 88	0
21	R	81/84 (96%)	-0.35	1 (1%) 79 54	59, 76, 95, 103	0
22	S	119/119 (100%)	-0.34	3 (2%) 57 29	55, 74, 97, 113	0
23	T	53/66 (80%)	-0.31	0 100 100	57, 73, 92, 99	0
24	U	65/70 (92%)	0.11	5 (7%) 13 4	68, 91, 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%)	-0.54	0 100 100	51, 64, 82, 94	0
26	W	82/91 (90%)	-0.25	2 (2%) 59 30	58, 75, 99, 117	0
27	X	142/240 (59%)	-0.60	1 (0%) 87 69	43, 61, 82, 101	0
28	Y	73/73 (100%)	-0.28	0 100 100	62, 76, 95, 104	0
29	Z	56/56 (100%)	-0.71	0 100 100	42, 52, 58, 68	0
30	1	46/48 (95%)	-0.15	2 (4%) 35 13	49, 77, 105, 117	0
31	2	92/92 (100%)	-0.19	2 (2%) 62 33	53, 73, 87, 98	0
All	All	6580/7282 (90%)	-0.38	85 (1%) 77 51	35, 69, 108, 150	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	9	3001	U	6.1
1	0	2250	G	5.8
22	S	116	ASP	4.8
2	9	3025	G	4.7
24	U	1	THR	4.5

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 monosaccharides 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	0.33	0.25	94,94,94,94	0
35	NA	Q	8386	1/1	0.43	0.64	107,107,107,107	0
35	NA	0	8384	1/1	0.48	0.62	85,85,85,85	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8363	1/1	0.49	0.62	83,83,83,83	0
35	NA	R	8312	1/1	0.53	0.92	84,84,84,84	0
35	NA	0	8329	1/1	0.56	1.24	98,98,98,98	0
35	NA	0	8371	1/1	0.65	0.72	69,69,69,69	0
33	MG	0	8049	1/1	0.66	0.33	90,90,90,90	0
35	NA	H	8322	1/1	0.70	0.41	78,78,78,78	0
35	NA	0	8324	1/1	0.71	0.39	58,58,58,58	0
35	NA	0	8361	1/1	0.73	0.36	77,77,77,77	0
34	K	0	8201	1/1	0.75	0.12	141,141,141,141	0
33	MG	0	8024	1/1	0.76	0.62	98,98,98,98	0
35	NA	0	8368	1/1	0.77	0.36	69,69,69,69	0
35	NA	0	8340	1/1	0.77	0.37	69,69,69,69	0
35	NA	0	8385	1/1	0.78	0.36	73,73,73,73	0
35	NA	0	8341	1/1	0.78	0.34	60,60,60,60	0
35	NA	9	8383	1/1	0.78	0.38	67,67,67,67	0
33	MG	0	8114	1/1	0.79	0.69	95,95,95,95	0
35	NA	0	8352	1/1	0.80	0.33	61,61,61,61	0
35	NA	0	8382	1/1	0.80	0.17	89,89,89,89	0
37	CD	N	8405	1/1	0.80	0.23	150,150,150,150	0
35	NA	0	8332	1/1	0.80	0.37	50,50,50,50	0
35	NA	0	8362	1/1	0.81	0.25	79,79,79,79	0
35	NA	0	8323	1/1	0.81	0.44	66,66,66,66	0
35	NA	0	8326	1/1	0.81	0.30	73,73,73,73	0
34	K	0	8202	1/1	0.81	0.77	92,92,92,92	0
35	NA	0	8307	1/1	0.82	0.32	71,71,71,71	0
36	CL	0	8505	1/1	0.82	0.44	99,99,99,99	0
33	MG	A	8105	1/1	0.82	0.30	52,52,52,52	0
35	NA	0	8366	1/1	0.82	0.36	82,82,82,82	0
33	MG	0	8113	1/1	0.83	0.10	60,60,60,60	0
35	NA	0	8365	1/1	0.83	0.43	47,47,47,47	0
36	CL	K	8510	1/1	0.83	0.25	104,104,104,104	0
35	NA	0	8378	1/1	0.84	0.75	65,65,65,65	0
33	MG	0	8102	1/1	0.84	0.38	91,91,91,91	0
35	NA	0	8316	1/1	0.84	0.21	52,52,52,52	0
35	NA	0	8369	1/1	0.84	0.35	96,96,96,96	0
35	NA	0	8360	1/1	0.84	0.41	69,69,69,69	0
36	CL	0	8515	1/1	0.85	0.30	100,100,100,100	0
33	MG	0	8071	1/1	0.85	0.07	104,104,104,104	0
33	MG	0	8013	1/1	0.85	0.17	60,60,60,60	0
33	MG	0	8092	1/1	0.86	0.37	111,111,111,111	0
35	NA	0	8350	1/1	0.86	0.28	57,57,57,57	0
33	MG	0	8066	1/1	0.86	0.17	105,105,105,105	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8313	1/1	0.86	0.21	89,89,89,89	0
33	MG	0	8046	1/1	0.87	0.15	86,86,86,86	0
35	NA	0	8381	1/1	0.87	0.31	69,69,69,69	0
35	NA	0	8325	1/1	0.87	0.28	64,64,64,64	0
36	CL	P	8511	1/1	0.87	0.37	84,84,84,84	0
35	NA	0	8364	1/1	0.88	0.24	66,66,66,66	0
33	MG	0	8085	1/1	0.88	0.22	92,92,92,92	0
36	CL	B	8519	1/1	0.88	0.38	95,95,95,95	0
35	NA	0	8374	1/1	0.88	0.14	77,77,77,77	0
35	NA	0	8328	1/1	0.88	0.22	55,55,55,55	0
33	MG	0	8011	1/1	0.88	0.19	50,50,50,50	0
33	MG	0	8022	1/1	0.88	0.58	83,83,83,83	0
33	MG	0	8045	1/1	0.89	0.25	91,91,91,91	0
36	CL	N	8508	1/1	0.89	0.22	116,116,116,116	0
35	NA	0	8333	1/1	0.89	0.26	40,40,40,40	0
33	MG	S	8073	1/1	0.89	0.14	71,71,71,71	0
33	MG	0	8003	1/1	0.89	0.15	51,51,51,51	0
33	MG	0	8076	1/1	0.89	0.16	102,102,102,102	0
35	NA	0	8370	1/1	0.90	0.40	76,76,76,76	0
36	CL	I	8502	1/1	0.90	0.11	93,93,93,93	0
36	CL	A	8509	1/1	0.90	0.72	89,89,89,89	0
35	NA	0	8311	1/1	0.90	0.26	73,73,73,73	0
35	NA	P	8348	1/1	0.90	0.09	68,68,68,68	0
33	MG	0	8028	1/1	0.90	0.17	57,57,57,57	0
36	CL	2	8504	1/1	0.90	0.49	100,100,100,100	0
35	NA	0	8375	1/1	0.91	0.69	81,81,81,81	0
35	NA	Q	8337	1/1	0.91	0.26	64,64,64,64	0
35	NA	0	8357	1/1	0.91	0.26	61,61,61,61	0
33	MG	0	8097	1/1	0.91	0.30	53,53,53,53	0
36	CL	I	8501	1/1	0.91	0.18	99,99,99,99	0
33	MG	0	8104	1/1	0.92	0.14	66,66,66,66	0
33	MG	0	8111	1/1	0.92	0.12	75,75,75,75	0
35	NA	0	8310	1/1	0.92	0.20	46,46,46,46	0
33	MG	0	8107	1/1	0.92	0.09	55,55,55,55	0
33	MG	0	8100	1/1	0.92	0.19	97,97,97,97	0
36	CL	Q	8506	1/1	0.92	0.23	80,80,80,80	0
33	MG	0	8081	1/1	0.92	0.08	67,67,67,67	0
36	CL	0	8513	1/1	0.92	0.24	74,74,74,74	0
33	MG	0	8103	1/1	0.92	0.42	97,97,97,97	0
35	NA	0	8377	1/1	0.92	0.58	75,75,75,75	0
33	MG	0	8054	1/1	0.93	0.19	45,45,45,45	0
35	NA	0	8336	1/1	0.93	0.13	63,63,63,63	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8330	1/1	0.93	0.11	61,61,61,61	0
35	NA	C	8304	1/1	0.93	0.38	51,51,51,51	0
36	CL	0	8503	1/1	0.93	0.30	82,82,82,82	0
33	MG	0	8115	1/1	0.93	0.12	73,73,73,73	0
35	NA	0	8308	1/1	0.93	0.25	77,77,77,77	0
35	NA	0	8372	1/1	0.93	0.74	72,72,72,72	0
33	MG	0	8112	1/1	0.93	0.15	64,64,64,64	0
33	MG	9	8095	1/1	0.93	0.36	106,106,106,106	0
35	NA	0	8353	1/1	0.93	0.14	43,43,43,43	0
32	SLD	0	9500	37/37	0.93	0.21	46,50,53,59	0
33	MG	0	8082	1/1	0.93	0.16	79,79,79,79	0
35	NA	0	8354	1/1	0.93	0.41	58,58,58,58	0
33	MG	0	8108	1/1	0.93	0.27	102,102,102,102	0
33	MG	0	8099	1/1	0.93	0.23	80,80,80,80	0
33	MG	0	8116	1/1	0.94	0.17	84,84,84,84	0
35	NA	0	8321	1/1	0.94	0.42	67,67,67,67	0
33	MG	J	8069	1/1	0.94	0.05	87,87,87,87	0
36	CL	0	8514	1/1	0.94	0.13	75,75,75,75	0
33	MG	0	8035	1/1	0.94	0.06	69,69,69,69	0
33	MG	0	8062	1/1	0.94	0.09	90,90,90,90	0
35	NA	0	8317	1/1	0.94	0.11	57,57,57,57	0
35	NA	0	8373	1/1	0.94	0.24	57,57,57,57	0
33	MG	0	8067	1/1	0.94	0.12	81,81,81,81	0
36	CL	M	8507	1/1	0.94	0.24	86,86,86,86	0
33	MG	0	8020	1/1	0.94	0.19	53,53,53,53	0
35	NA	0	8356	1/1	0.94	0.96	73,73,73,73	0
35	NA	0	8359	1/1	0.94	0.15	81,81,81,81	0
35	NA	0	8338	1/1	0.94	0.08	66,66,66,66	0
33	MG	0	8064	1/1	0.94	0.37	39,39,39,39	0
33	MG	0	8029	1/1	0.95	0.07	60,60,60,60	0
35	NA	0	8335	1/1	0.95	0.17	83,83,83,83	0
35	NA	0	8334	1/1	0.95	0.20	48,48,48,48	0
33	MG	0	8053	1/1	0.95	0.29	63,63,63,63	0
33	MG	0	8072	1/1	0.95	0.33	78,78,78,78	0
36	CL	I	8521	1/1	0.95	0.25	69,69,69,69	0
33	MG	0	8034	1/1	0.95	0.10	46,46,46,46	0
36	CL	0	8517	1/1	0.95	0.33	82,82,82,82	0
33	MG	0	8051	1/1	0.95	0.19	97,97,97,97	0
35	NA	0	8303	1/1	0.95	0.49	55,55,55,55	0
33	MG	0	8018	1/1	0.95	0.09	57,57,57,57	0
33	MG	0	8101	1/1	0.95	0.14	94,94,94,94	0
33	MG	0	8087	1/1	0.95	0.07	82,82,82,82	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	0	8339	1/1	0.95	0.13	33,33,33,33	0
33	MG	B	8055	1/1	0.95	0.06	71,71,71,71	0
33	MG	0	8090	1/1	0.95	0.33	81,81,81,81	0
35	NA	0	8376	1/1	0.95	0.46	79,79,79,79	0
33	MG	0	8016	1/1	0.96	0.07	71,71,71,71	0
33	MG	0	8026	1/1	0.96	0.08	39,39,39,39	0
33	MG	0	8001	1/1	0.96	0.17	46,46,46,46	0
35	NA	0	8367	1/1	0.96	0.25	85,85,85,85	0
33	MG	0	8042	1/1	0.96	0.15	61,61,61,61	0
33	MG	0	8008	1/1	0.96	0.16	52,52,52,52	0
35	NA	L	8347	1/1	0.96	0.13	55,55,55,55	0
33	MG	0	8075	1/1	0.96	0.09	77,77,77,77	0
33	MG	0	8031	1/1	0.96	0.12	54,54,54,54	0
33	MG	0	8060	1/1	0.96	0.15	63,63,63,63	0
36	CL	J	8512	1/1	0.96	0.21	67,67,67,67	0
33	MG	0	8044	1/1	0.96	0.27	59,59,59,59	0
36	CL	L	8518	1/1	0.96	0.10	69,69,69,69	0
35	NA	A	8345	1/1	0.96	0.10	48,48,48,48	0
33	MG	0	8096	1/1	0.96	0.09	70,70,70,70	0
33	MG	9	8052	1/1	0.96	0.10	60,60,60,60	0
33	MG	0	8110	1/1	0.96	0.12	56,56,56,56	0
33	MG	X	8109	1/1	0.96	0.17	66,66,66,66	0
35	NA	0	8301	1/1	0.96	0.12	59,59,59,59	0
35	NA	0	8306	1/1	0.96	0.38	59,59,59,59	0
33	MG	0	8009	1/1	0.96	0.18	44,44,44,44	0
33	MG	0	8057	1/1	0.96	0.08	53,53,53,53	0
35	NA	0	8302	1/1	0.96	0.16	55,55,55,55	0
35	NA	0	8343	1/1	0.96	0.14	48,48,48,48	0
35	NA	0	8358	1/1	0.96	0.28	109,109,109,109	0
33	MG	0	8040	1/1	0.96	0.08	88,88,88,88	0
33	MG	0	8088	1/1	0.96	0.22	40,40,40,40	0
36	CL	0	8516	1/1	0.96	0.26	64,64,64,64	0
33	MG	0	8079	1/1	0.96	0.12	53,53,53,53	0
33	MG	0	8043	1/1	0.97	0.07	64,64,64,64	0
33	MG	0	8019	1/1	0.97	0.15	43,43,43,43	0
35	NA	0	8305	1/1	0.97	0.08	42,42,42,42	0
33	MG	0	8086	1/1	0.97	0.06	62,62,62,62	0
33	MG	2	8078	1/1	0.97	0.04	65,65,65,65	0
36	CL	0	8522	1/1	0.97	0.63	92,92,92,92	0
35	NA	0	8355	1/1	0.97	0.40	77,77,77,77	0
33	MG	0	8050	1/1	0.97	0.14	68,68,68,68	0
35	NA	0	8318	1/1	0.97	0.23	48,48,48,48	0

Continued on next page...

Continued from previous page...

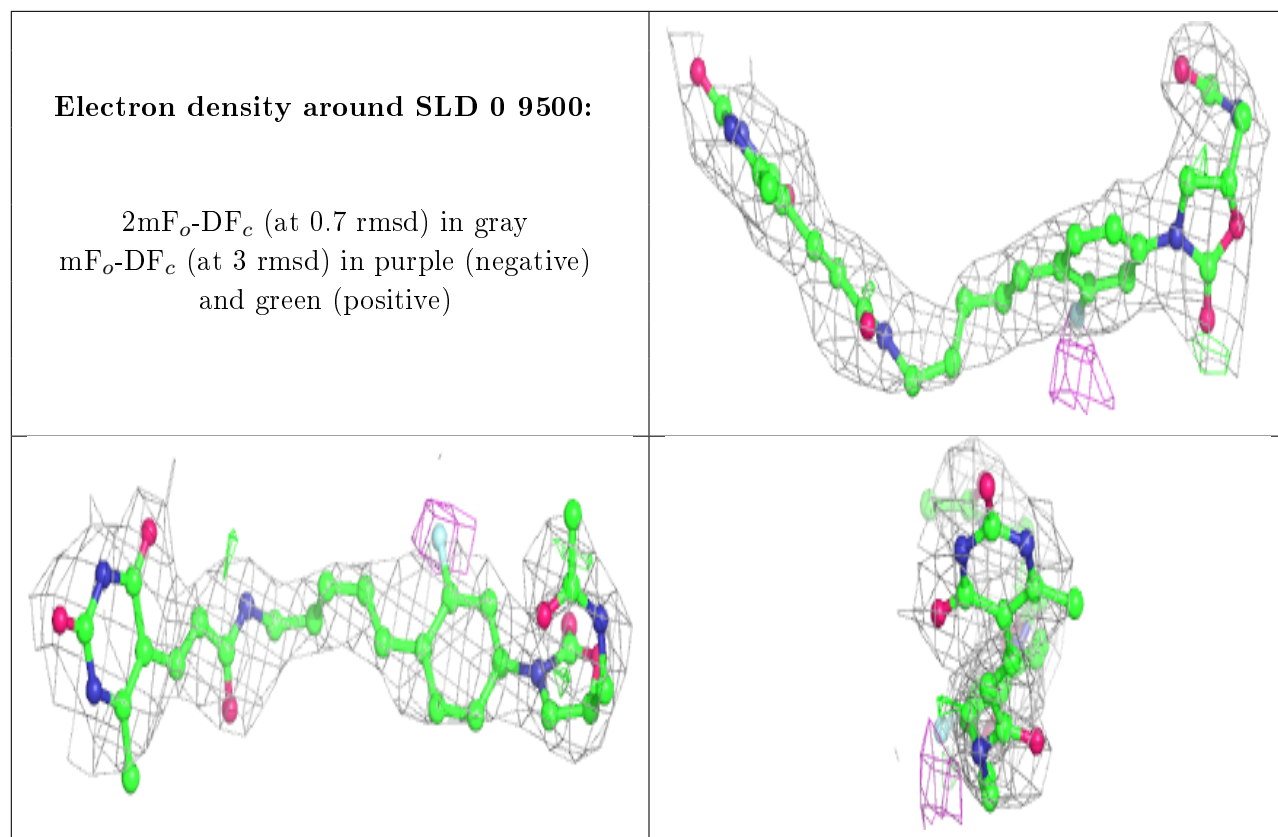
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CL	X	8520	1/1	0.97	0.28	57,57,57,57	0
33	MG	0	8070	1/1	0.97	0.07	63,63,63,63	0
33	MG	0	8002	1/1	0.97	0.09	51,51,51,51	0
33	MG	0	8025	1/1	0.97	0.06	59,59,59,59	0
35	NA	K	8380	1/1	0.97	0.36	85,85,85,85	0
35	NA	0	8327	1/1	0.97	0.10	46,46,46,46	0
33	MG	0	8089	1/1	0.97	0.07	82,82,82,82	0
35	NA	0	8314	1/1	0.97	0.23	53,53,53,53	0
33	MG	0	8004	1/1	0.97	0.19	50,50,50,50	0
33	MG	4	8063	1/1	0.97	0.11	62,62,62,62	0
33	MG	0	8106	1/1	0.97	0.26	78,78,78,78	0
35	NA	0	8344	1/1	0.97	0.12	48,48,48,48	0
35	NA	0	8379	1/1	0.97	0.24	48,48,48,48	0
33	MG	0	8036	1/1	0.97	0.06	52,52,52,52	0
33	MG	0	8117	1/1	0.98	0.07	45,45,45,45	0
33	MG	0	8007	1/1	0.98	0.12	47,47,47,47	0
33	MG	0	8027	1/1	0.98	0.08	65,65,65,65	0
33	MG	0	8037	1/1	0.98	0.07	54,54,54,54	0
33	MG	0	8083	1/1	0.98	0.07	65,65,65,65	0
33	MG	0	8048	1/1	0.98	0.06	66,66,66,66	0
33	MG	0	8077	1/1	0.98	0.13	54,54,54,54	0
35	NA	0	8349	1/1	0.98	0.44	69,69,69,69	0
35	NA	0	8331	1/1	0.98	0.12	60,60,60,60	0
33	MG	0	8041	1/1	0.98	0.24	68,68,68,68	0
33	MG	0	8059	1/1	0.98	0.06	60,60,60,60	0
33	MG	0	8039	1/1	0.98	0.10	53,53,53,53	0
33	MG	0	8006	1/1	0.98	0.28	60,60,60,60	0
33	MG	0	8084	1/1	0.98	0.05	70,70,70,70	0
33	MG	0	8032	1/1	0.98	0.08	52,52,52,52	0
33	MG	0	8014	1/1	0.98	0.18	46,46,46,46	0
33	MG	0	8098	1/1	0.98	0.06	50,50,50,50	0
35	NA	0	8315	1/1	0.98	0.19	70,70,70,70	0
33	MG	0	8047	1/1	0.98	0.10	90,90,90,90	0
33	MG	0	8058	1/1	0.98	0.11	61,61,61,61	0
37	CD	Y	8403	1/1	0.98	0.07	84,84,84,84	0
35	NA	0	8319	1/1	0.98	0.18	41,41,41,41	0
35	NA	H	8309	1/1	0.98	0.25	49,49,49,49	0
33	MG	0	8033	1/1	0.98	0.11	48,48,48,48	0
35	NA	0	8320	1/1	0.98	0.20	40,40,40,40	0
33	MG	0	8074	1/1	0.98	0.07	51,51,51,51	0
33	MG	0	8093	1/1	0.98	0.10	63,63,63,63	0
35	NA	0	8342	1/1	0.98	0.14	42,42,42,42	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	NA	I	8346	1/1	0.99	0.08	45,45,45,45	0
37	CD	Z	8402	1/1	0.99	0.07	89,89,89,89	0
37	CD	T	8401	1/1	0.99	0.07	83,83,83,83	0
33	MG	0	8038	1/1	0.99	0.19	56,56,56,56	0
33	MG	0	8094	1/1	0.99	0.07	97,97,97,97	0
33	MG	0	8056	1/1	0.99	0.09	60,60,60,60	0
33	MG	0	8061	1/1	0.99	0.05	45,45,45,45	0
33	MG	0	8023	1/1	0.99	0.06	46,46,46,46	0
33	MG	0	8030	1/1	0.99	0.16	48,48,48,48	0
33	MG	A	8065	1/1	0.99	0.15	55,55,55,55	0
33	MG	0	8068	1/1	0.99	0.06	64,64,64,64	0
37	CD	2	8404	1/1	0.99	0.09	90,90,90,90	0
33	MG	0	8012	1/1	0.99	0.06	42,42,42,42	0
33	MG	0	8080	1/1	0.99	0.08	52,52,52,52	0
33	MG	0	8017	1/1	0.99	0.15	43,43,43,43	0
33	MG	0	8010	1/1	0.99	0.10	47,47,47,47	0
33	MG	0	8015	1/1	0.99	0.11	60,60,60,60	0
33	MG	0	8005	1/1	0.99	0.10	58,58,58,58	0
33	MG	0	8021	1/1	0.99	0.18	54,54,54,54	0
33	MG	0	8091	1/1	0.99	0.06	65,65,65,65	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.