



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 02:53 am BST

PDB ID : 1M1K
Title : Co-crystal structure of azithromycin bound to the 50S ribosomal subunit of *Haloarcula marismortui*
Authors : Hansen, J.L.; Ippolito, J.A.; Ban, N.; Nissen, P.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-06-19
Resolution : 3.20 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

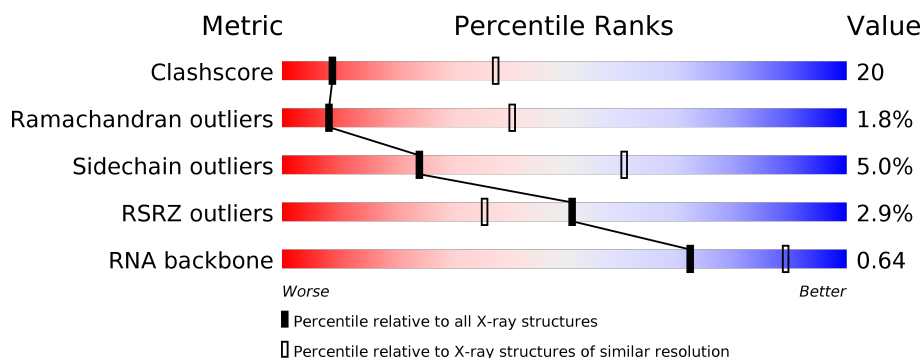
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)
RNA backbone	3102	1010 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2922	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 51% 36% 7% 6% </div> </div>
2	B	122	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 5% 43% 42% 9% 6% </div> </div>
3	C	239	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 4% 52% 42% 5% . </div> </div>
4	D	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 51% 43% 6% </div> </div>
5	E	246	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 61% 34% 6% </div> </div>
6	F	176	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> 24% 20% 49% 9% . 20% </div> </div>

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

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	A	8024	-	-	-	X
32	MG	A	8066	-	-	-	X
34	NA	A	8303	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8329	-	-	-	X
34	NA	A	8340	-	-	-	X
34	NA	A	8354	-	-	-	X
34	NA	A	8363	-	-	-	X
34	NA	A	8374	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	A	8385	-	-	-	X
34	NA	J	8322	-	-	-	X
34	NA	S	8386	-	-	-	X
35	CL	A	8513	-	-	X	-
35	CL	A	8515	-	-	-	X
35	CL	K	8502	-	-	X	-
35	CL	N	8518	-	-	X	-
35	CL	O	8507	-	-	X	X
35	CL	R	8511	-	-	-	X

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 98587 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 3 is a protein called RIBOSOMAL PROTEIN L2.

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

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L3.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 5 is a protein called RIBOSOMAL PROTEIN L4.

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

- Molecule 6 is a protein called RIBOSOMAL PROTEIN L5.

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

- Molecule 7 is a protein called RIBOSOMAL PROTEIN L6.

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

- Molecule 8 is a protein called RIBOSOMAL PROTEIN L7AE.

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

- Molecule 9 is a protein called RIBOSOMAL PROTEIN L10.

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

- Molecule 10 is a protein called RIBOSOMAL PROTEIN L10E.

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

- Molecule 11 is a protein called RIBOSOMAL PROTEIN L13.

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

- Molecule 12 is a protein called RIBOSOMAL PROTEIN L14.

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

- Molecule 13 is a protein called RIBOSOMAL PROTEIN L15.

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

- Molecule 14 is a protein called RIBOSOMAL PROTEIN L15E.

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

- Molecule 15 is a protein called RIBOSOMAL PROTEIN L18.

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

- Molecule 16 is a protein called RIBOSOMAL PROTEIN L18E.

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

- Molecule 17 is a protein called RIBOSOMAL PROTEIN L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 18 is a protein called RIBOSOMAL PROTEIN L21E.

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

- Molecule 19 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L31E.

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

- Molecule 26 is a protein called RIBOSOMAL PROTEIN L32E.

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

- Molecule 27 is a protein called RIBOSOMAL PROTEIN L37Ae.

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

- Molecule 28 is a protein called RIBOSOMAL PROTEIN L37E.

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

- Molecule 29 is a protein called RIBOSOMAL PROTEIN L39E.

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

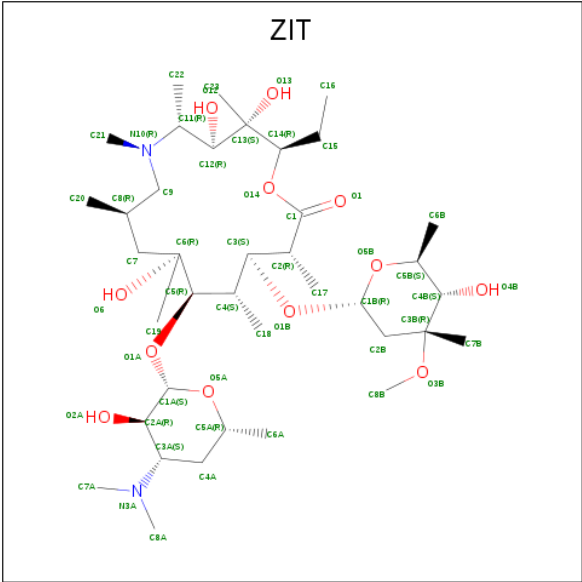
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 30 is a protein called RIBOSOMAL PROTEIN L44E.

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

- Molecule 31 is AZITHROMYCIN (three-letter code: ZIT) (formula: C₃₈H₇₂N₂O₁₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
31	A	1	Total	C	N	O	0	0
			52	38	2	12		

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	A	2	Total K 2 2	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	4	Total Cl 4 4	0	0
35	C	1	Total Cl 1 1	0	0
35	A	9	Total Cl 9 9	0	0

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

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

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

- Molecule 37 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	A	5898	Total 5898	O 5898	0	0
37	B	140	Total 140	O 140	0	0
37	C	129	Total 129	O 129	0	0
37	D	152	Total 152	O 152	0	0
37	E	169	Total 169	O 169	0	0
37	F	52	Total 52	O 52	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	G	42	Total 42	O 42	0	0
37	H	28	Total 28	O 28	0	0
37	I	21	Total 21	O 21	0	0
37	J	81	Total 81	O 81	0	0
37	K	56	Total 56	O 56	0	0
37	L	61	Total 61	O 61	0	0
37	M	81	Total 81	O 81	0	0
37	N	129	Total 129	O 129	0	0
37	O	68	Total 68	O 68	0	0
37	P	45	Total 45	O 45	0	0
37	Q	69	Total 69	O 69	0	0
37	R	56	Total 56	O 56	0	0
37	S	89	Total 89	O 89	0	0
37	T	36	Total 36	O 36	0	0
37	U	39	Total 39	O 39	0	0
37	V	27	Total 27	O 27	0	0
37	W	15	Total 15	O 15	0	0
37	X	73	Total 73	O 73	0	0
37	Y	30	Total 30	O 30	0	0
37	Z	93	Total 93	O 93	0	0
37	1	38	Total 38	O 38	0	0

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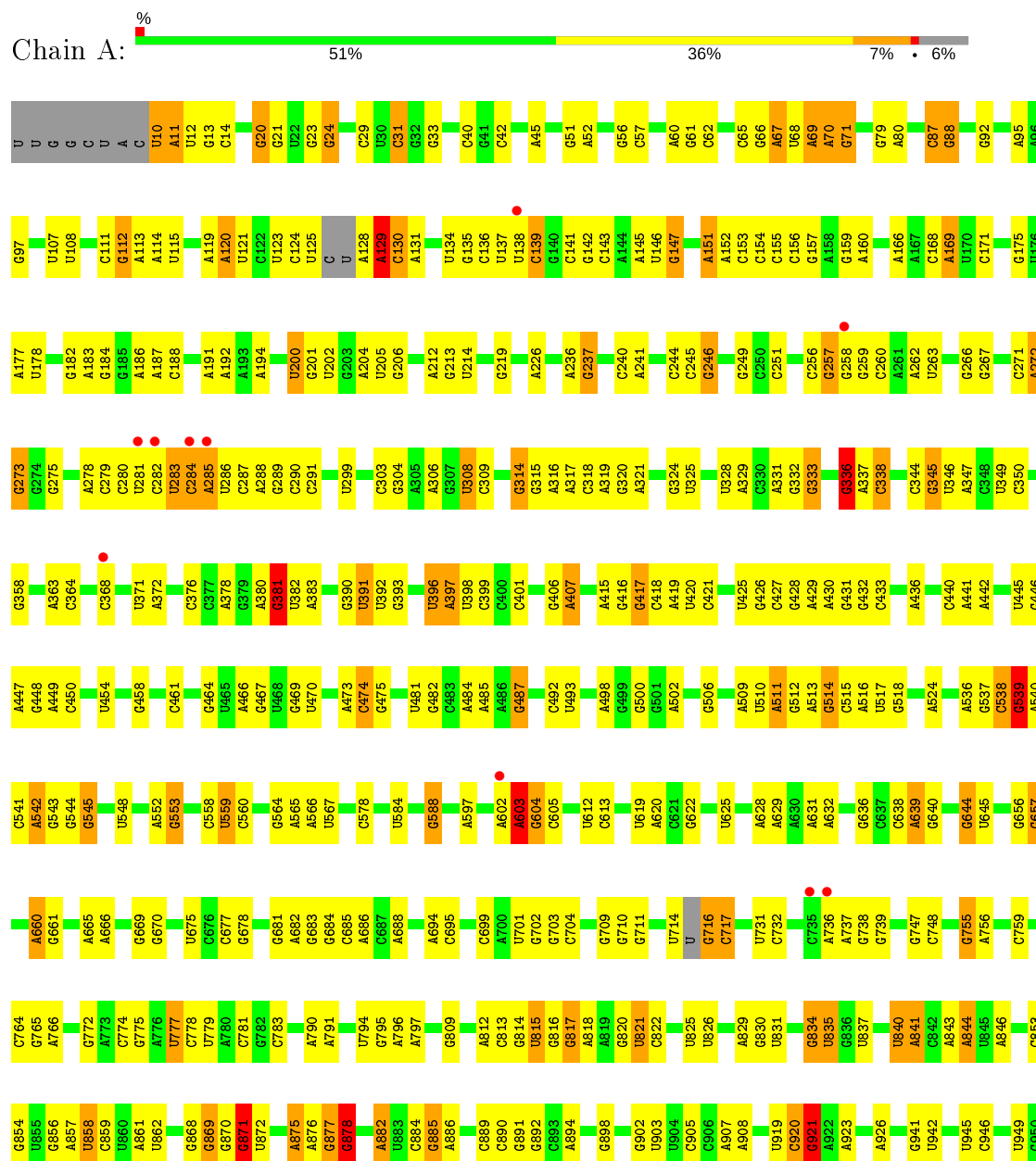
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	2	57	Total 57	O 57	0	0
37	3	39	Total 39	O 39	0	0
37	4	72	Total 72	O 72	0	0

3 Residue-property plots

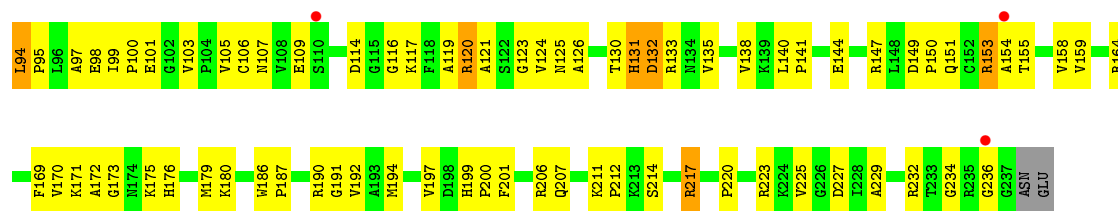
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: 23S rRNA

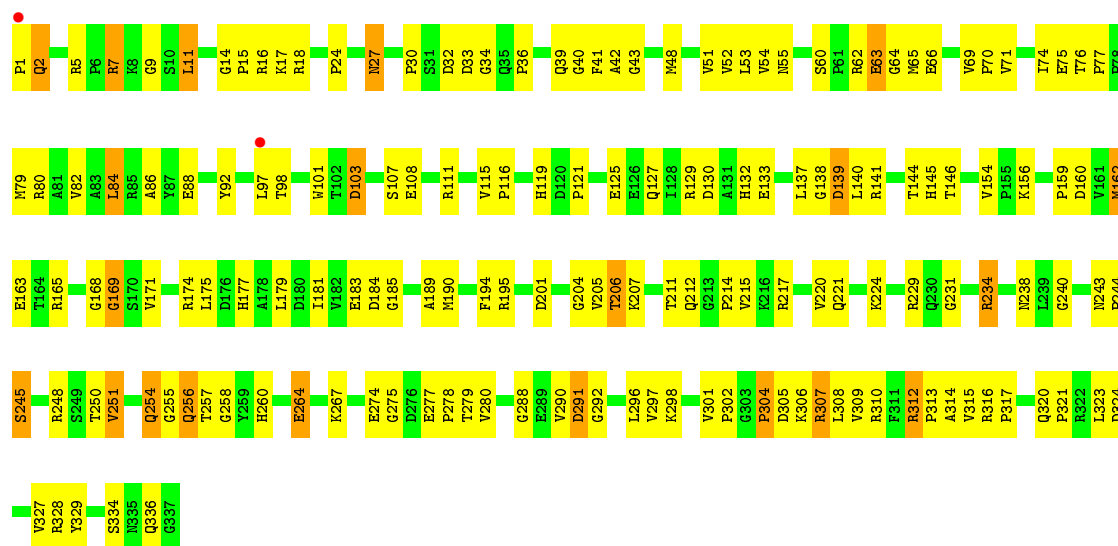


A2039	C1841	U1749	G1670	C1456	C1360	G1265	U1187	G1113	G1024	A951
C2040	A1942	C1750	C1675	U1457	C1361	U1266	A1198	A1114	C1025	G952
G2041	A1843	G1751	G1676	G1571	U1362	C1267	A1199	U1115	U1026	G953
U2042	G1752	G1752	U1677	U1461	U1368	C1268	G1190	U1116	U1028	U954
U2043	U1846	C1753	U1678	U1462	U1369	U1269	A1191	A1117	U1029	G958
G2044	A1847	U1758	C1679	A1463	A1678	G1270	A1192	A1118	G1036	C959
C2045	A1847	A1759	G1680	A1463	G1370	A1271	A1193	G1119	G1036	G960
G2046	C1854	U1766	G1681	A1470	U1371	C1272	G1197	U1120	G1037	A961
U2047	G1855	A1767	G1682	C1474	A1372	C1273	A1198	U1121	G1038	C962
G2050	C1856	U1768	C1593	C1477	A1376	U1279	A1199	U1122	G1044	C963
A2054	A1857	G1768	C1594	U1478	C1377	C1289	A1200	A1123	G1045	G964
A2055	A1858	C1769	G1595	U1478	G1378	G1292	A1201	C1127	G1046	U970
C2056	U1860	U1770	U1596	U1478	G1378	U1293	C1204	U1128	U1047	G
U2063	C1861	U1771	A1597	A1486	U1380	U1299	U1206	U1129	G1048	U
U2064	C1862	G1773	A1598	U1488	A1381	G1300	A1207	U1130	U1051	G
A2070	A1865	A1778	G1601	U1488	C1384	C1301	C1208	G1131	G1052	U
C2071	G1868	A1779	C1602	A1494	G1385	C1302	C1209	A1132	G1051	C
G2072	A1869	U1788	A1603	C1495	G1389	U1309	G1210	A1133	G1055	C
C2073	C1870	A1783	G1604	U1496	A1390	U1310	G1211	G1137	U1056	G
A2074	U1874	U1784	G1605	G1497	A1391	C1305	G1212	A1057	A1057	C
G2079	G1873	G1785	C1613	U1500	A1392	U1306	G1213	U1139	G1059	U
G2080	U1874	C1787	G1614	U1500	A1393	U1309	G1214	U1140	C1060	C
A2081	G1877	U1788	A1615	U1503	C1394	U1310	A1215	U1141	C1061	C
G2082	A1878	U1789	A1616	U1504	A1407	G1311	G1216	C1142	G1062	G
A2083	U1879	C1790	C1617	U1505	A1408	G1312	U1218	G1151	U1063	A
C2088	G1902	U1791	U1625	C1507	G1409	A1313	U1219	A1067	A1067	G
A2089	U1903	C1792	A1626	C1507	G1416	G1314	G1224	C1068	C1068	G
G2090	A1904	C1798	G1627	U1523	G1417	G1315	G1225	G1072	G1072	A
G2091	G1908	A1804	A1630	G1524	U1418	G1323	C1229	G1076	G1076	G
G2092	A1909	G1805	A1630	G1525	U1419	G1324	U1237	C1080	C1080	C
G2093	A1910	U1809	C1633	A1526	C1420	G1325	U1237	A1081	A1081	G
A2095	A1919	C1810	G1634	A1527	G1421	U1266	G1235	G1162	G1162	C
A2096	C1920	G1814	U1635	A1528	U1422	G1327	G1235	G1163	G1163	G
G2099	A1921	U1815	G1636	G1529	C1423	A1328	U1237	U1164	U1164	C
A2100	A1922	C1816	A1637	U1532	A1424	C1329	G1238	G1165	G1165	A
G2101	G1925	G1816	U1641	U1533	G1425	A1330	G1239	C1084	C1084	C
G2102	G1926	C1819	A1642	C1534	A1427	C1331	U1242	G1167	G1167	A
C2106	A1927	G1820	C1643	C1535	A1434	U1332	A1243	C1168	C1168	C999
U2107	G1930	G1823	U1654	C1536	U1435	U1333	G1243	U1169	G1087	A
G2110	A1931	U1827	G1655	U1549	C1436	C1334	U1244	U1170	A1088	U1003
G2113	A1934	G1828	A1656	C1549	U1440	C1335	C1245	A1171	G1094	C1004
C2114	C1935	A1829	A1657	G1555	G1441	U1336	A1247	G1172	U1095	A1005
U2115	C1936	C1830	A1658	G1556	A1442	U1337	U1248	A1173	A1006	A1007
U2116	C1940	U1834	A1659	U1559	U1445	C1342	U1249	U1174	U1096	C1008
U2117	A1941	U1835	A1661	U1561	G1446	C1342	C1250	G1175	A1097	A
G2123	C1943	A1836	C1662	C1562	U1447	C1342	A1251	C1176	A1098	A
C2121	A1947	U1839	C1666	U1562	G1451	A1348	C1252	U1177	G1099	A
A2123	G1947	U1840	U1667	C1563	G1452	G1349	C1253	U1180	C1102	A1014
			U1748	C1565	C1452	U1350	C1253	A1181	C1103	C1015
						A1352	A1261	C1182	G1019	G1019
						C1353	C1262	C1183	A1020	A1020
						A1357	C1263	C1184	G1021	G1021
							C1263	U1185	G1111	A1022
								C1196	G1112	C1023

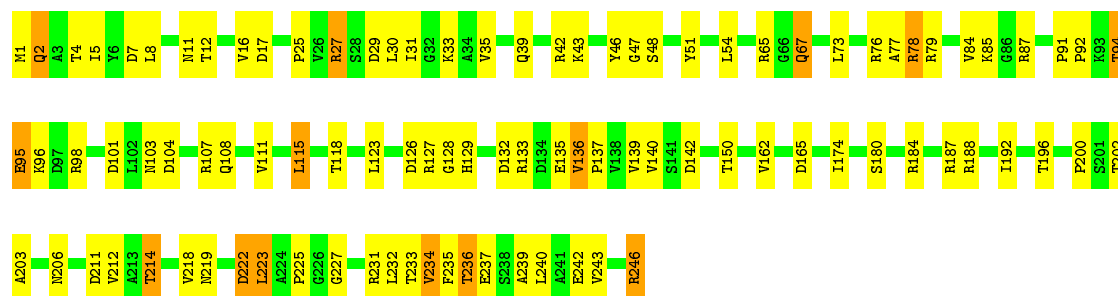




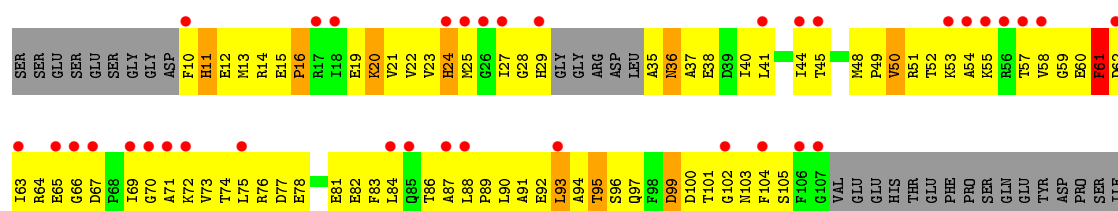
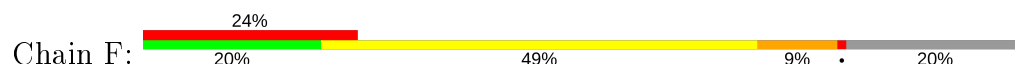
• Molecule 4: RIBOSOMAL PROTEIN L3



• Molecule 5: RIBOSOMAL PROTEIN L4

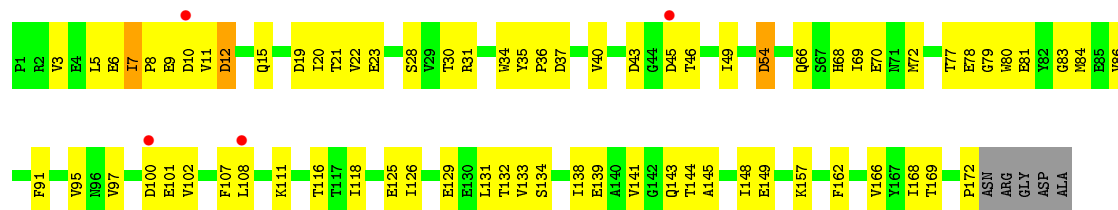


• Molecule 6: RIBOSOMAL PROTEIN L5

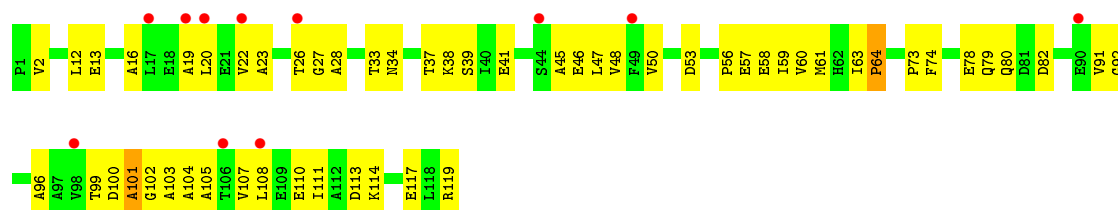




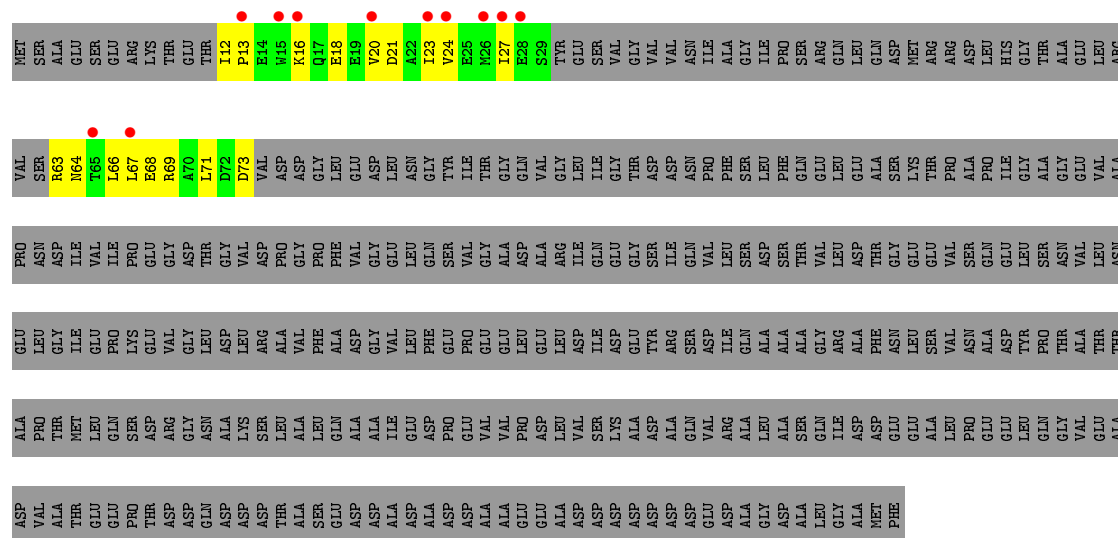
• Molecule 7: RIBOSOMAL PROTEIN L6



• Molecule 8: RIBOSOMAL PROTEIN L7AE

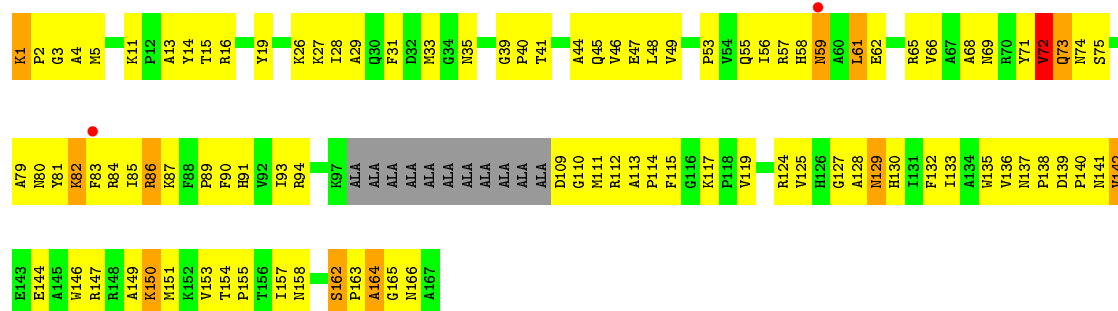


• Molecule 9: RIBOSOMAL PROTEIN L10



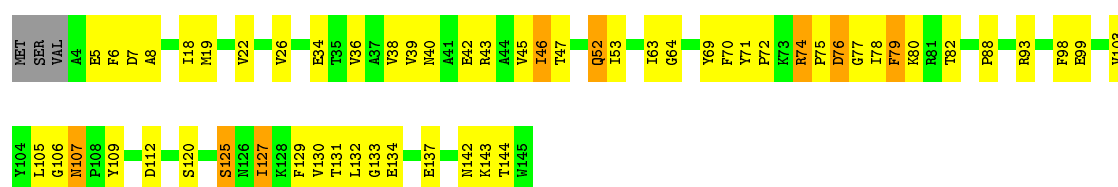
• Molecule 10: RIBOSOMAL PROTEIN L10E





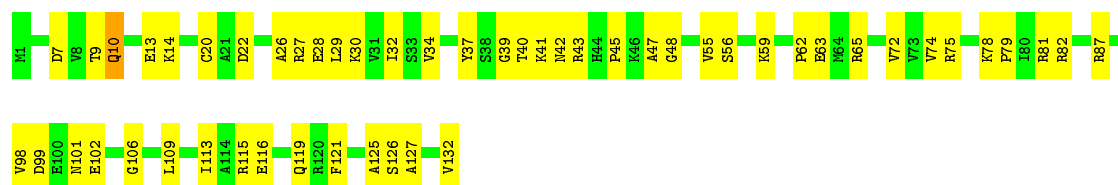
• Molecule 11: RIBOSOMAL PROTEIN L13

Chain K: 59% 34% 6%



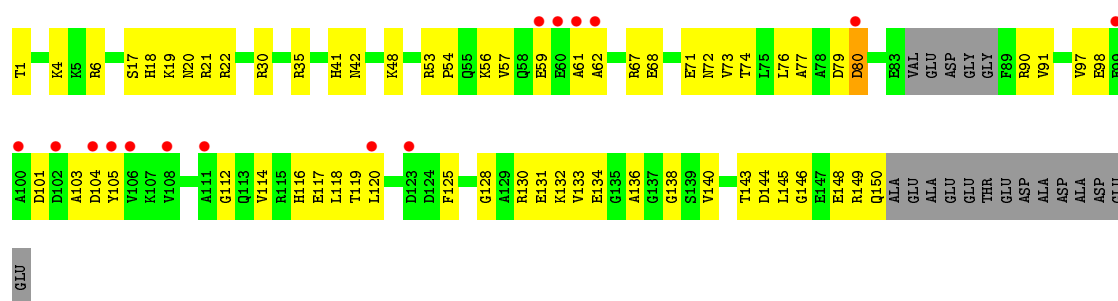
• Molecule 12: RIBOSOMAL PROTEIN L14

Chain L: 61% 39%



• Molecule 13: RIBOSOMAL PROTEIN L15

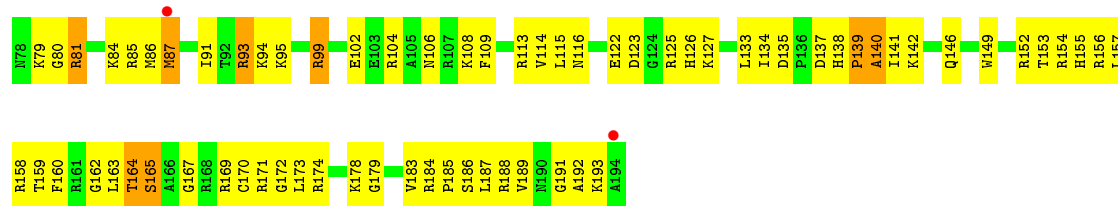
Chain M: 9% 50% 38% 12%



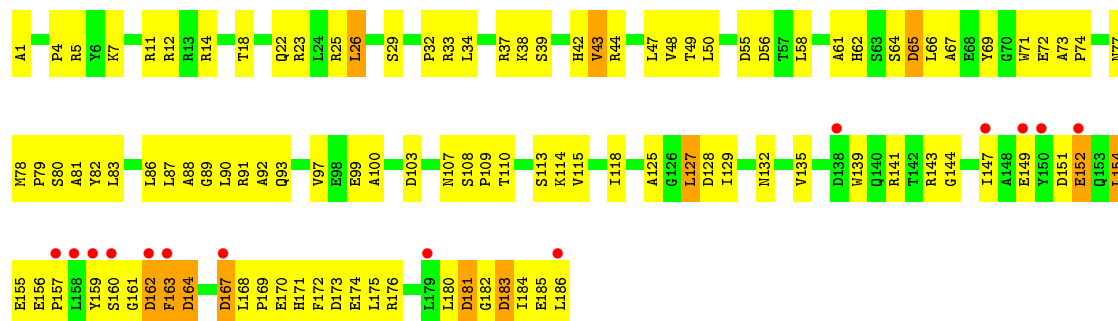
• Molecule 14: RIBOSOMAL PROTEIN L15E

Chain N: 43% 51% 6%





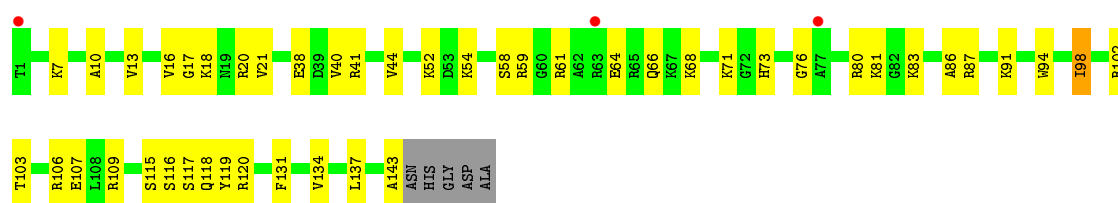
• Molecule 15: RIBOSOMAL PROTEIN L18



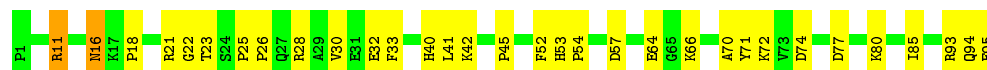
• Molecule 16: RIBOSOMAL PROTEIN L18E



• Molecule 17: RIBOSOMAL PROTEIN L19E

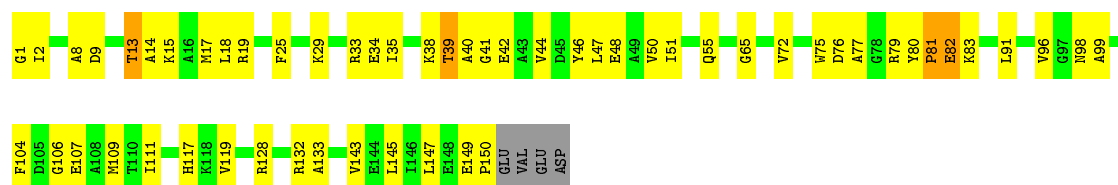


• Molecule 18: RIBOSOMAL PROTEIN L21E




• Molecule 19: RIBOSOMAL PROTEIN L22

Chain S: 



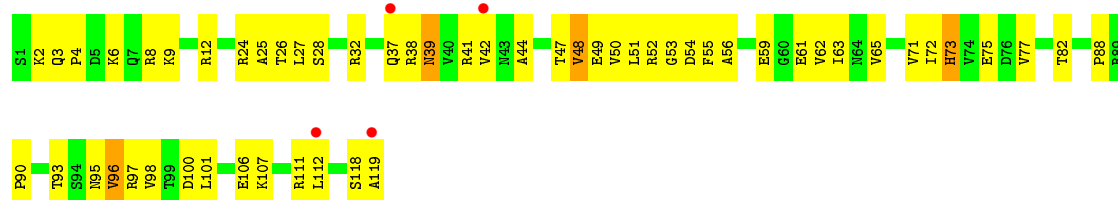
• Molecule 20: RIBOSOMAL PROTEIN L23

Chain T: 



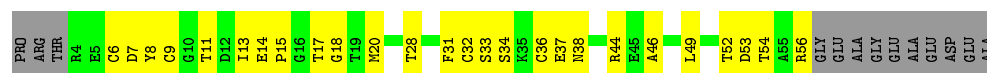
• Molecule 21: RIBOSOMAL PROTEIN L24

Chain U: 



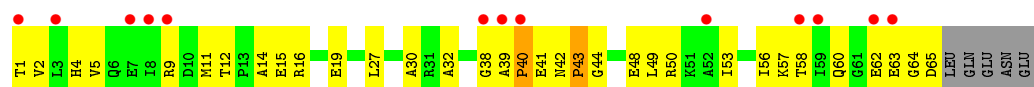
• Molecule 22: RIBOSOMAL PROTEIN L24E

Chain V: 



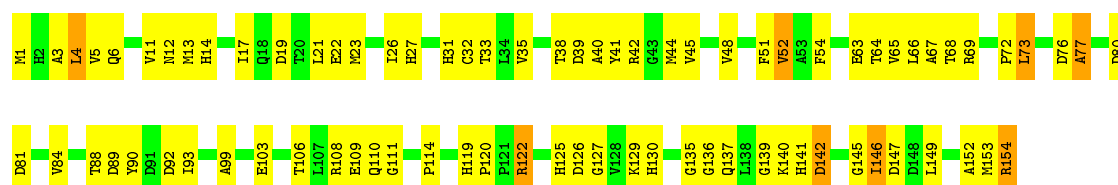
• Molecule 23: RIBOSOMAL PROTEIN L29

Chain W: 

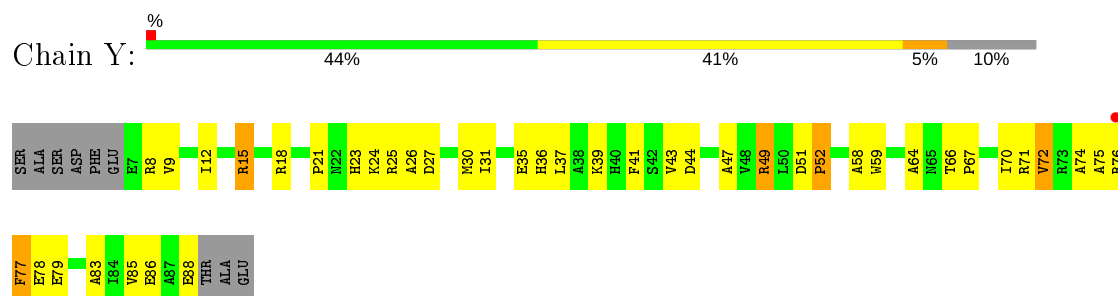


• Molecule 24: RIBOSOMAL PROTEIN L30

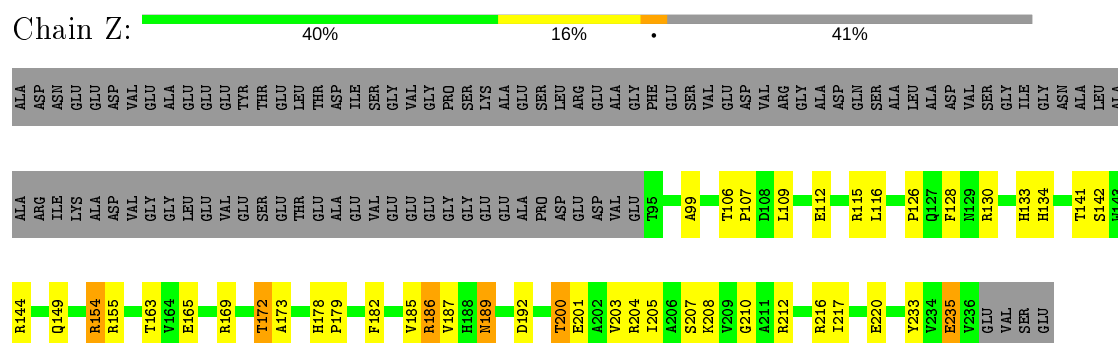
Chain X: 



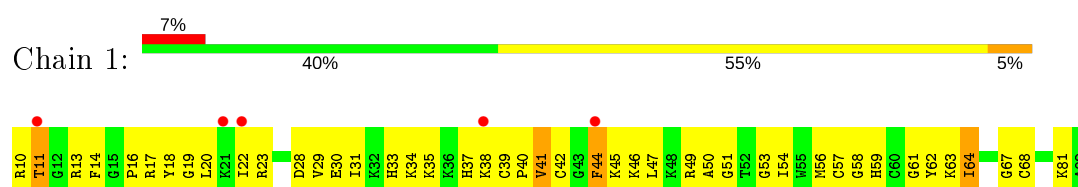
• Molecule 25: RIBOSOMAL PROTEIN L31E



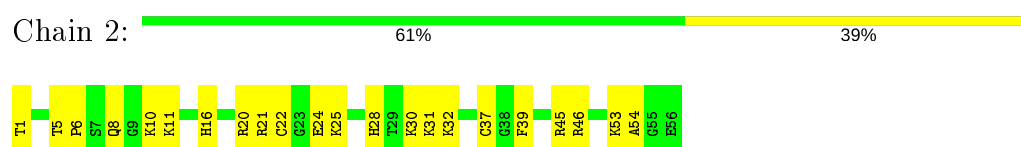
• Molecule 26: RIBOSOMAL PROTEIN L32E



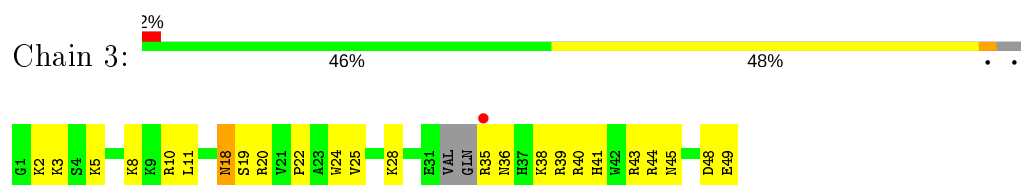
• Molecule 27: RIBOSOMAL PROTEIN L37Ae



• Molecule 28: RIBOSOMAL PROTEIN L37E

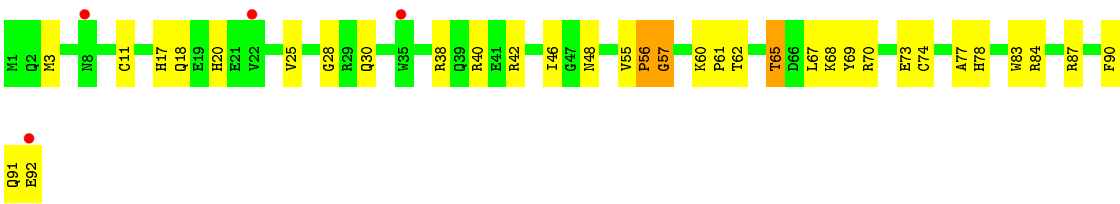


• Molecule 29: RIBOSOMAL PROTEIN L39E



• Molecule 30: RIBOSOMAL PROTEIN L44E





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.75Å 301.57Å 574.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.20 49.69 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (20.00-3.20) 87.9 (49.69-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.214 , 0.250 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	60.7	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 74.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	98587	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% 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, ZIT, CD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.59	1/66076 (0.0%)	0.76	33/103052 (0.0%)
2	B	0.92	16/2905 (0.6%)	0.98	20/4528 (0.4%)
3	C	0.47	0/1787	0.75	0/2409
4	D	0.52	0/2689	0.74	0/3652
5	E	0.49	0/1883	0.73	0/2551
6	F	0.43	0/1111	0.68	0/1498
7	G	0.48	0/1382	0.67	0/1880
8	H	0.44	0/896	0.64	0/1219
9	I	0.51	0/241	0.63	0/324
10	J	0.50	0/1246	0.82	2/1686 (0.1%)
11	K	0.53	0/1135	0.69	0/1530
12	L	0.57	1/1003 (0.1%)	0.78	0/1351
13	M	0.47	0/1126	0.76	0/1504
14	N	0.56	0/1633	0.81	1/2180 (0.0%)
15	O	0.44	0/1473	0.74	0/1999
16	P	0.49	0/873	0.69	0/1181
17	Q	0.49	0/1143	0.66	0/1521
18	R	0.52	0/748	0.78	0/1005
19	S	0.52	0/1172	0.77	0/1578
20	T	0.48	0/648	0.69	0/875
21	U	0.46	0/957	0.73	0/1289
22	V	0.47	0/417	0.67	0/562
23	W	0.43	0/502	0.63	0/675
24	X	0.52	0/1218	0.72	0/1655
25	Y	0.49	0/664	0.71	0/895
26	Z	0.50	0/1146	0.73	0/1536
27	1	0.52	0/575	0.75	0/763
28	2	0.57	0/437	0.78	0/578
29	3	0.45	0/398	0.63	0/527
30	4	0.57	0/771	0.73	0/1024
All	All	0.57	18/98255 (0.0%)	0.76	56/147027 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	141
2	B	0	5
All	All	1	146

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3025	G	O3'-P	10.69	1.74	1.61
2	B	3025	G	C4'-O4'	9.77	1.58	1.45
2	B	3023	U	C2'-O2'	9.46	1.53	1.41
2	B	3026	C	P-O5'	-8.76	1.50	1.59
2	B	3003	A	C5'-C4'	8.50	1.61	1.51

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-19.12	63.13	105.20
1	A	1164	U	OP2-P-O3'	-17.65	66.37	105.20
1	A	1165	G	O5'-P-OP1	-12.66	94.31	105.70
2	B	3024	U	O5'-P-OP2	11.59	124.60	110.70
2	B	3026	C	O5'-P-OP2	-11.13	95.68	105.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	112	G	Sidechain
1	A	146	U	Sidechain
1	A	20	G	Sidechain
1	A	24	G	Sidechain
1	A	33	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	A	59017	0	29803	1165	0
2	B	2600	0	1326	84	0
3	C	1754	0	1763	129	0
4	D	2624	0	2533	180	0
5	E	1858	0	1816	125	0
6	F	1094	0	1085	143	0
7	G	1357	0	1266	84	0
8	H	885	0	854	66	0
9	I	240	0	231	25	0
10	J	1215	0	1215	152	0
11	K	1119	0	1098	68	0
12	L	993	0	1027	56	0
13	M	1114	0	1072	67	0
14	N	1605	0	1676	159	0
15	O	1444	0	1401	142	0
16	P	864	0	873	46	0
17	Q	1133	0	1127	51	0
18	R	734	0	728	28	0
19	S	1149	0	1122	64	0
20	T	641	0	605	22	0
21	U	949	0	923	55	0
22	V	410	0	364	36	0
23	W	499	0	511	33	0
24	X	1195	0	1137	99	0
25	Y	654	0	653	50	0
26	Z	1130	0	1133	59	0
27	1	563	0	597	51	0
28	2	430	0	426	28	0
29	3	393	0	406	30	0
30	4	755	0	728	41	0
31	A	52	0	72	2	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	1	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	0	0	3	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	4	0
35	L	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	2	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
36	1	1	0	0	0	0
36	2	1	0	0	0	0
36	4	1	0	0	0	0
36	P	1	0	0	0	0
36	V	1	0	0	0	0
37	1	38	0	0	8	0
37	2	57	0	0	4	0
37	3	39	0	0	4	0
37	4	72	0	0	12	0
37	A	5898	0	0	232	0
37	B	140	0	0	15	0
37	C	129	0	0	24	0
37	D	152	0	0	27	0
37	E	169	0	0	34	0
37	F	52	0	0	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	G	42	0	0	13	0
37	H	28	0	0	10	0
37	I	21	0	0	5	0
37	J	81	0	0	17	0
37	K	56	0	0	6	0
37	L	61	0	0	13	0
37	M	81	0	0	19	0
37	N	129	0	0	22	0
37	O	68	0	0	20	0
37	P	45	0	0	13	0
37	Q	69	0	0	6	0
37	R	56	0	0	3	0
37	S	89	0	0	8	0
37	T	36	0	0	4	0
37	U	39	0	0	5	0
37	V	27	0	0	5	0
37	W	15	0	0	3	0
37	X	73	0	0	7	0
37	Y	30	0	0	8	0
37	Z	93	0	0	14	0
All	All	98587	0	59571	3047	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 3047 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1160:G:H5'	1:A:1161:A:H5'	1.22	1.15
25:Y:37:LEU:HD13	25:Y:85:VAL:HG21	1.26	1.13
21:U:71:VAL:HG11	21:U:90:PRO:HB3	1.33	1.11
10:J:86:ARG:NH1	10:J:133:ILE:HG13	1.67	1.10
1:A:871:G:H8	1:A:871:G:H5'	1.14	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	
3	C	235/239 (98%)	204 (87%)	26 (11%)	5 (2%)	7	37
4	D	335/337 (99%)	303 (90%)	23 (7%)	9 (3%)	5	30
5	E	244/246 (99%)	220 (90%)	23 (9%)	1 (0%)	34	69
6	F	134/176 (76%)	94 (70%)	26 (19%)	14 (10%)	0	3
7	G	170/177 (96%)	160 (94%)	10 (6%)	0	100	100
8	H	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	9	42
9	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
10	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	4	25
11	K	140/145 (97%)	130 (93%)	7 (5%)	3 (2%)	7	37
12	L	130/132 (98%)	116 (89%)	12 (9%)	2 (2%)	10	44
13	M	141/164 (86%)	119 (84%)	20 (14%)	2 (1%)	11	46
14	N	192/194 (99%)	174 (91%)	15 (8%)	3 (2%)	9	43
15	O	184/186 (99%)	164 (89%)	13 (7%)	7 (4%)	3	22
16	P	113/115 (98%)	108 (96%)	4 (4%)	1 (1%)	17	56
17	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	22	61
18	R	93/95 (98%)	86 (92%)	6 (6%)	1 (1%)	14	51
19	S	148/154 (96%)	139 (94%)	8 (5%)	1 (1%)	22	61
20	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
21	U	117/119 (98%)	107 (92%)	9 (8%)	1 (1%)	17	56
22	V	51/66 (77%)	46 (90%)	4 (8%)	1 (2%)	7	38
23	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	26
24	X	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22	61
25	Y	80/91 (88%)	71 (89%)	8 (10%)	1 (1%)	12	47
26	Z	140/240 (58%)	137 (98%)	3 (2%)	0	100	100
27	1	71/73 (97%)	61 (86%)	8 (11%)	2 (3%)	5	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	3	42/48 (88%)	42 (100%)	0	0	100	100
30	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	6	35
All	All	3633/4235 (86%)	3285 (90%)	281 (8%)	67 (2%)	8	41

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	139	ASP
6	F	93	LEU
6	F	95	THR
6	F	173	GLU
8	H	101	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	179/181 (99%)	166 (93%)	13 (7%)	14	46
4	D	282/282 (100%)	263 (93%)	19 (7%)	16	50
5	E	193/193 (100%)	175 (91%)	18 (9%)	9	33
6	F	117/147 (80%)	107 (92%)	10 (8%)	10	38
7	G	152/155 (98%)	148 (97%)	4 (3%)	46	76
8	H	92/92 (100%)	91 (99%)	1 (1%)	73	88
9	I	27/283 (10%)	27 (100%)	0	100	100
10	J	122/122 (100%)	111 (91%)	11 (9%)	9	34
11	K	118/121 (98%)	108 (92%)	10 (8%)	10	38
12	L	106/106 (100%)	103 (97%)	3 (3%)	43	74
13	M	112/126 (89%)	108 (96%)	4 (4%)	35	69
14	N	166/166 (100%)	158 (95%)	8 (5%)	25	61
15	O	149/149 (100%)	143 (96%)	6 (4%)	31	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	93/93 (100%)	90 (97%)	3 (3%)	39	71
17	Q	113/116 (97%)	110 (97%)	3 (3%)	44	75
18	R	79/79 (100%)	75 (95%)	4 (5%)	24	60
19	S	117/121 (97%)	114 (97%)	3 (3%)	46	76
20	T	71/73 (97%)	71 (100%)	0	100	100
21	U	105/105 (100%)	101 (96%)	4 (4%)	33	67
22	V	44/52 (85%)	44 (100%)	0	100	100
23	W	51/56 (91%)	50 (98%)	1 (2%)	55	80
24	X	130/130 (100%)	122 (94%)	8 (6%)	18	53
25	Y	66/73 (90%)	61 (92%)	5 (8%)	13	45
26	Z	120/195 (62%)	112 (93%)	8 (7%)	16	50
27	1	56/56 (100%)	53 (95%)	3 (5%)	22	58
28	2	46/46 (100%)	46 (100%)	0	100	100
29	3	42/44 (96%)	41 (98%)	1 (2%)	49	77
30	4	79/79 (100%)	78 (99%)	1 (1%)	69	87
All	All	3027/3441 (88%)	2876 (95%)	151 (5%)	24	60

5 of 151 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	72	VAL
11	K	125	SER
26	Z	163	THR
10	J	82	LYS
11	K	46	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 92 such sidechains are listed below:

Mol	Chain	Res	Type
13	M	58	GLN
16	P	100	GLN
29	3	16	ASN
13	M	116	HIS
14	N	176	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	245 (8%)	36 (1%)
2	B	121/122 (99%)	14 (11%)	6 (4%)
All	All	2868/3044 (94%)	259 (9%)	42 (1%)

5 of 259 RNA backbone outliers are listed below:

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

5 of 42 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1450	C
1	A	1856	C
2	B	3025	G
1	A	1563	G
1	A	1692	C

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 233 ligands modelled in this entry, 232 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
31	ZIT	A	8600	-	54,54,54	1.75	11 (20%)	82,83,83	1.27	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	ZIT	A	8600	-	-	1/72/107/107	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	A	8600	ZIT	C2-C3	4.53	1.65	1.55
31	A	8600	ZIT	C7-C6	4.33	1.61	1.54
31	A	8600	ZIT	C3A-N3A	4.23	1.57	1.48
31	A	8600	ZIT	C11-N10	3.47	1.54	1.49
31	A	8600	ZIT	C2B-C3B	3.18	1.60	1.52

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	A	8600	ZIT	C6-C5-C4	-4.02	108.35	114.05
31	A	8600	ZIT	O1A-C5-C6	3.07	110.17	106.39
31	A	8600	ZIT	C17-C2-C3	2.57	118.73	112.92
31	A	8600	ZIT	O1B-C3-C4	2.37	111.08	108.22
31	A	8600	ZIT	C21-N10-C9	2.34	113.83	110.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

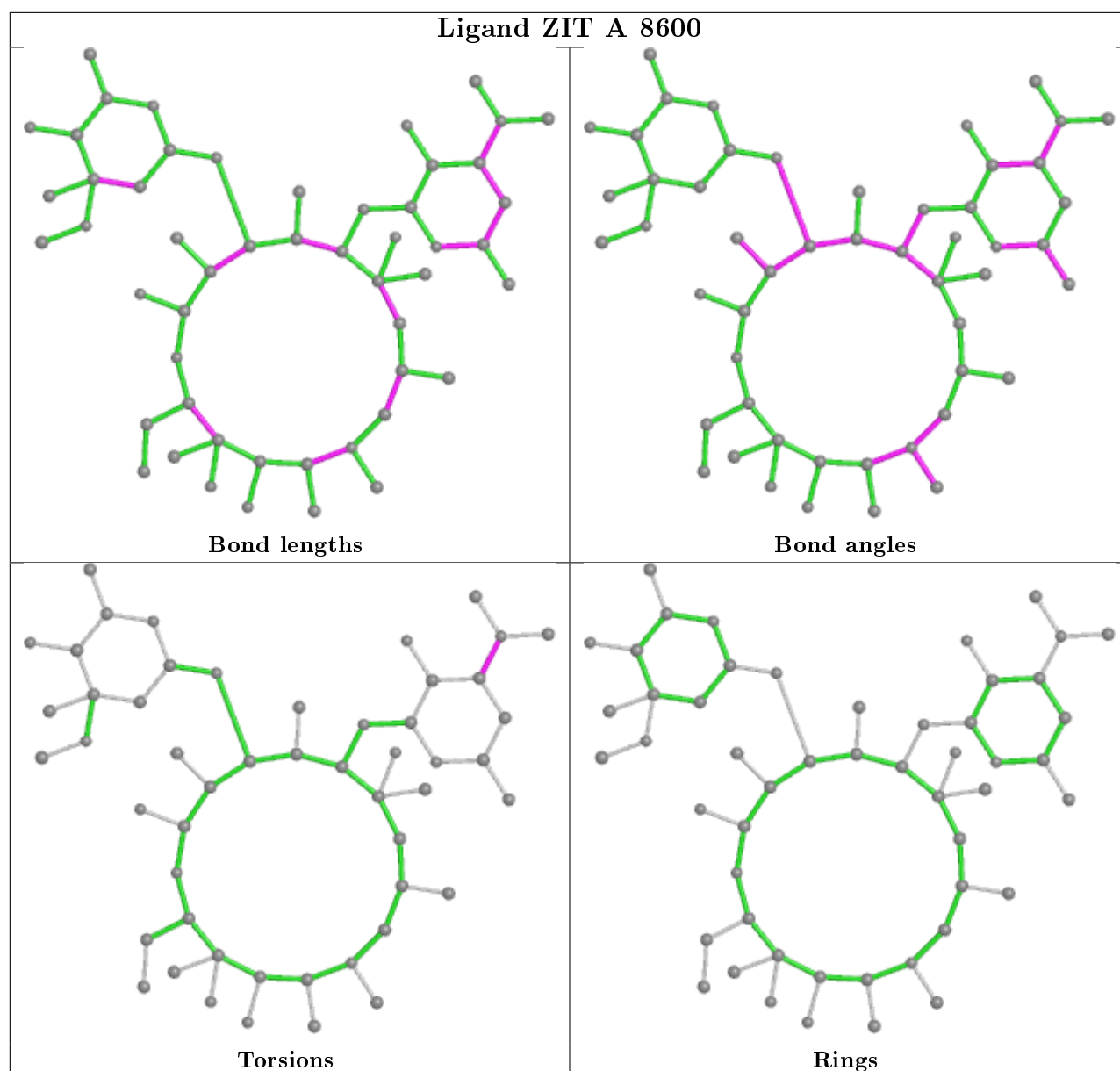
Mol	Chain	Res	Type	Atoms
31	A	8600	ZIT	C4A-C3A-N3A-C8A

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	A	8600	ZIT	2	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	A	2754/2922 (94%)	-0.10	37 (1%) 77 65	27, 56, 101, 149	0
2	B	122/122 (100%)	0.07	6 (4%) 29 17	43, 71, 98, 158	0
3	C	237/239 (99%)	0.05	10 (4%) 36 23	38, 62, 93, 114	0
4	D	337/337 (100%)	-0.12	2 (0%) 89 83	29, 64, 90, 99	0
5	E	246/246 (100%)	-0.14	0 100 100	30, 58, 81, 92	0
6	F	140/176 (79%)	1.34	43 (30%) 0 0	61, 108, 124, 131	0
7	G	172/177 (97%)	0.33	4 (2%) 60 47	50, 76, 97, 102	0
8	H	119/119 (100%)	0.46	11 (9%) 9 5	62, 82, 106, 110	0
9	I	29/348 (8%)	1.64	11 (37%) 0 0	80, 100, 109, 109	0
10	J	156/167 (93%)	0.04	2 (1%) 77 65	43, 65, 94, 101	0
11	K	142/145 (97%)	-0.12	0 100 100	45, 57, 80, 97	0
12	L	132/132 (100%)	-0.15	0 100 100	38, 58, 80, 87	0
13	M	145/164 (88%)	0.46	15 (10%) 6 4	33, 77, 113, 123	0
14	N	194/194 (100%)	-0.16	2 (1%) 82 72	42, 56, 73, 84	0
15	O	186/186 (100%)	0.36	14 (7%) 14 8	52, 74, 114, 124	0
16	P	115/115 (100%)	0.05	0 100 100	52, 66, 84, 88	0
17	Q	143/148 (96%)	0.22	3 (2%) 63 49	45, 65, 80, 89	0
18	R	95/95 (100%)	-0.11	0 100 100	38, 54, 70, 82	0
19	S	150/154 (97%)	-0.21	0 100 100	40, 54, 74, 82	0
20	T	81/84 (96%)	-0.02	1 (1%) 79 67	55, 71, 90, 97	0
21	U	119/119 (100%)	0.42	4 (3%) 45 29	52, 69, 92, 103	0
22	V	53/66 (80%)	-0.02	0 100 100	51, 64, 82, 89	0
23	W	65/70 (92%)	1.11	13 (20%) 1 1	62, 83, 118, 124	0
24	X	154/154 (100%)	-0.36	0 100 100	38, 56, 76, 85	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	82/91 (90%)	0.12	1 (1%) 79 67	53, 67, 91, 107	0
26	Z	142/240 (59%)	-0.11	0 100 100	33, 56, 77, 94	0
27	1	73/73 (100%)	0.04	5 (6%) 17 10	59, 71, 87, 94	0
28	2	56/56 (100%)	-0.31	0 100 100	35, 46, 51, 52	0
29	3	46/48 (95%)	0.10	1 (2%) 62 48	44, 72, 96, 106	0
30	4	92/92 (100%)	0.35	4 (4%) 35 22	44, 66, 79, 90	0
All	All	6577/7279 (90%)	0.03	189 (2%) 51 36	27, 62, 101, 158	0

The worst 5 of 189 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	3001	U	8.2
23	W	1	THR	7.5
9	I	27	ILE	5.8
6	F	57	THR	5.7
15	O	186	LEU	5.5

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	A	8329	1/1	0.28	0.45	70,70,70,70	0
34	NA	A	8374	1/1	0.32	1.54	89,89,89,89	0
34	NA	A	8384	1/1	0.40	1.14	90,90,90,90	0
34	NA	S	8386	1/1	0.51	0.45	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8363	1/1	0.55	0.91	79,79,79,79	0
34	NA	A	8341	1/1	0.57	0.31	63,63,63,63	0
35	CL	R	8511	1/1	0.61	0.59	102,102,102,102	0
34	NA	A	8326	1/1	0.63	1.00	92,92,92,92	0
34	NA	A	8364	1/1	0.64	0.23	52,52,52,52	0
35	CL	A	8515	1/1	0.65	0.88	110,110,110,110	0
34	NA	A	8303	1/1	0.66	0.40	54,54,54,54	0
34	NA	A	8375	1/1	0.67	0.28	86,86,86,86	0
34	NA	A	8328	1/1	0.69	0.28	61,61,61,61	0
35	CL	O	8507	1/1	0.71	0.52	84,84,84,84	0
34	NA	J	8322	1/1	0.71	0.43	62,62,62,62	0
32	MG	A	8066	1/1	0.72	0.69	48,48,48,48	0
34	NA	A	8371	1/1	0.74	0.33	48,48,48,48	0
32	MG	A	8041	1/1	0.75	0.26	69,69,69,69	0
34	NA	A	8377	1/1	0.75	0.34	68,68,68,68	0
34	NA	A	8385	1/1	0.75	0.67	73,73,73,73	0
34	NA	A	8305	1/1	0.76	0.25	46,46,46,46	0
34	NA	A	8340	1/1	0.76	0.61	56,56,56,56	0
34	NA	A	8332	1/1	0.76	0.16	50,50,50,50	0
35	CL	A	8510	1/1	0.77	0.34	97,97,97,97	0
34	NA	A	8354	1/1	0.78	0.61	54,54,54,54	0
32	MG	A	8053	1/1	0.78	0.15	40,40,40,40	0
32	MG	A	8024	1/1	0.79	0.48	79,79,79,79	0
32	MG	A	8096	1/1	0.79	0.10	64,64,64,64	0
34	NA	A	8357	1/1	0.79	0.07	64,64,64,64	0
34	NA	T	8312	1/1	0.79	0.25	51,51,51,51	0
35	CL	A	8522	1/1	0.80	0.70	83,83,83,83	0
32	MG	U	8073	1/1	0.80	0.08	62,62,62,62	0
34	NA	B	8351	1/1	0.80	0.15	54,54,54,54	0
35	CL	A	8503	1/1	0.80	0.50	74,74,74,74	0
34	NA	A	8368	1/1	0.81	0.25	65,65,65,65	0
34	NA	A	8366	1/1	0.81	0.40	79,79,79,79	0
34	NA	S	8337	1/1	0.81	0.22	58,58,58,58	0
34	NA	A	8381	1/1	0.81	0.15	61,61,61,61	0
34	NA	B	8383	1/1	0.81	0.52	40,40,40,40	0
32	MG	A	8011	1/1	0.81	0.08	44,44,44,44	0
34	NA	A	8323	1/1	0.81	0.45	57,57,57,57	0
34	NA	A	8373	1/1	0.81	0.52	67,67,67,67	0
34	NA	A	8310	1/1	0.81	0.21	29,29,29,29	0
35	CL	A	8513	1/1	0.82	0.15	67,67,67,67	0
35	CL	A	8505	1/1	0.82	0.43	92,92,92,92	0
35	CL	P	8508	1/1	0.82	0.35	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8367	1/1	0.83	0.24	38,38,38,38	0
32	MG	A	8116	1/1	0.83	0.10	54,54,54,54	0
34	NA	A	8330	1/1	0.84	0.29	57,57,57,57	0
35	CL	A	8520	1/1	0.84	0.19	65,65,65,65	0
32	MG	A	8088	1/1	0.84	0.13	64,64,64,64	0
34	NA	A	8316	1/1	0.84	0.41	61,61,61,61	0
31	ZIT	A	8600	52/52	0.84	0.30	81,91,95,96	0
32	MG	A	8092	1/1	0.84	0.32	95,95,95,95	0
32	MG	A	8087	1/1	0.85	0.10	75,75,75,75	0
32	MG	1	8105	1/1	0.85	0.43	38,38,38,38	0
32	MG	A	8071	1/1	0.86	0.13	85,85,85,85	0
32	MG	A	8099	1/1	0.86	0.17	55,55,55,55	0
35	CL	4	8504	1/1	0.86	0.54	93,93,93,93	0
34	NA	A	8342	1/1	0.86	0.38	51,51,51,51	0
34	NA	A	8308	1/1	0.86	0.23	53,53,53,53	0
34	NA	A	8365	1/1	0.87	0.58	76,76,76,76	0
32	MG	A	8001	1/1	0.87	0.10	41,41,41,41	0
34	NA	A	8325	1/1	0.87	0.25	62,62,62,62	0
34	NA	A	8352	1/1	0.87	0.32	56,56,56,56	0
32	MG	A	8067	1/1	0.87	0.21	51,51,51,51	0
34	NA	A	8372	1/1	0.87	0.48	87,87,87,87	0
32	MG	A	8114	1/1	0.88	0.26	47,47,47,47	0
32	MG	A	8112	1/1	0.88	0.22	50,50,50,50	0
32	MG	A	8050	1/1	0.88	0.25	67,67,67,67	0
34	NA	A	8313	1/1	0.88	0.23	66,66,66,66	0
34	NA	A	8355	1/1	0.88	0.49	60,60,60,60	0
34	NA	A	8307	1/1	0.88	0.40	48,48,48,48	0
34	NA	U	8343	1/1	0.89	0.26	38,38,38,38	0
32	MG	A	8106	1/1	0.89	0.14	71,71,71,71	0
34	NA	A	8333	1/1	0.89	0.13	51,51,51,51	0
32	MG	A	8082	1/1	0.89	0.22	83,83,83,83	0
32	MG	A	8049	1/1	0.89	0.18	74,74,74,74	0
35	CL	A	8517	1/1	0.89	0.16	52,52,52,52	0
32	MG	A	8113	1/1	0.90	0.15	53,53,53,53	0
35	CL	L	8512	1/1	0.90	0.13	55,55,55,55	0
32	MG	A	8017	1/1	0.90	0.06	42,42,42,42	0
32	MG	A	8089	1/1	0.90	0.11	70,70,70,70	0
32	MG	A	8111	1/1	0.90	0.08	62,62,62,62	0
34	NA	A	8349	1/1	0.90	0.32	57,57,57,57	0
34	NA	A	8356	1/1	0.90	0.70	78,78,78,78	0
34	NA	M	8380	1/1	0.90	0.67	75,75,75,75	0
34	NA	A	8318	1/1	0.90	0.67	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8100	1/1	0.90	0.15	88,88,88,88	0
34	NA	A	8378	1/1	0.90	1.11	48,48,48,48	0
36	CD	P	8405	1/1	0.91	0.09	152,152,152,152	0
32	MG	A	8040	1/1	0.91	0.10	63,63,63,63	0
34	NA	E	8304	1/1	0.91	0.20	32,32,32,32	0
35	CL	A	8514	1/1	0.91	0.18	57,57,57,57	0
32	MG	4	8078	1/1	0.91	0.06	54,54,54,54	0
34	NA	A	8302	1/1	0.91	0.24	52,52,52,52	0
34	NA	A	8336	1/1	0.91	0.15	85,85,85,85	0
35	CL	C	8509	1/1	0.91	0.27	69,69,69,69	0
34	NA	A	8360	1/1	0.91	0.86	59,59,59,59	0
34	NA	A	8321	1/1	0.91	0.47	42,42,42,42	0
34	NA	A	8382	1/1	0.91	0.29	74,74,74,74	0
32	MG	L	8069	1/1	0.91	0.16	79,79,79,79	0
35	CL	S	8506	1/1	0.91	0.27	69,69,69,69	0
32	MG	A	8057	1/1	0.91	0.18	54,54,54,54	0
32	MG	A	8093	1/1	0.91	0.09	59,59,59,59	0
32	MG	A	8097	1/1	0.92	0.31	45,45,45,45	0
32	MG	A	8064	1/1	0.92	0.45	36,36,36,36	0
32	MG	A	8101	1/1	0.92	0.15	60,60,60,60	0
32	MG	A	8052	1/1	0.92	0.13	58,58,58,58	0
34	NA	A	8311	1/1	0.92	0.15	63,63,63,63	0
34	NA	A	8331	1/1	0.93	0.19	55,55,55,55	0
34	NA	A	8369	1/1	0.93	0.33	55,55,55,55	0
32	MG	A	8021	1/1	0.93	0.09	32,32,32,32	0
35	CL	K	8521	1/1	0.93	0.17	64,64,64,64	0
34	NA	C	8345	1/1	0.93	0.20	57,57,57,57	0
32	MG	A	8090	1/1	0.93	0.16	47,47,47,47	0
32	MG	A	8042	1/1	0.93	0.23	52,52,52,52	0
34	NA	A	8314	1/1	0.93	0.17	48,48,48,48	0
35	CL	D	8519	1/1	0.93	0.43	65,65,65,65	0
32	MG	A	8108	1/1	0.93	0.13	85,85,85,85	0
32	MG	A	8059	1/1	0.94	0.15	56,56,56,56	0
34	NA	A	8362	1/1	0.94	0.68	62,62,62,62	0
32	MG	A	8033	1/1	0.94	0.11	36,36,36,36	0
32	MG	A	8063	1/1	0.94	0.10	92,92,92,92	0
32	MG	A	8075	1/1	0.94	0.11	56,56,56,56	0
34	NA	A	8376	1/1	0.94	0.28	49,49,49,49	0
32	MG	A	8091	1/1	0.94	0.07	58,58,58,58	0
32	MG	Z	8109	1/1	0.94	0.17	61,61,61,61	0
32	MG	A	8008	1/1	0.94	0.13	61,61,61,61	0
34	NA	R	8348	1/1	0.94	0.07	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8086	1/1	0.94	0.12	56,56,56,56	0
34	NA	A	8359	1/1	0.94	0.51	75,75,75,75	0
32	MG	A	8043	1/1	0.94	0.14	56,56,56,56	0
35	CL	N	8518	1/1	0.94	0.20	65,65,65,65	0
32	MG	A	8056	1/1	0.94	0.10	61,61,61,61	0
32	MG	A	8039	1/1	0.94	0.06	67,67,67,67	0
32	MG	B	8095	1/1	0.95	0.08	98,98,98,98	0
34	NA	A	8361	1/1	0.95	0.51	46,46,46,46	0
34	NA	A	8324	1/1	0.95	0.09	48,48,48,48	0
32	MG	A	8070	1/1	0.95	0.19	46,46,46,46	0
35	CL	K	8502	1/1	0.95	0.15	87,87,87,87	0
32	MG	A	8076	1/1	0.95	0.09	75,75,75,75	0
32	MG	A	8010	1/1	0.95	0.09	43,43,43,43	0
32	MG	A	8102	1/1	0.95	0.28	75,75,75,75	0
32	MG	A	8009	1/1	0.95	0.05	46,46,46,46	0
32	MG	A	8054	1/1	0.95	0.06	52,52,52,52	0
32	MG	A	8083	1/1	0.95	0.08	51,51,51,51	0
32	MG	A	8110	1/1	0.95	0.08	35,35,35,35	0
34	NA	A	8306	1/1	0.95	0.52	41,41,41,41	0
34	NA	K	8346	1/1	0.95	0.15	33,33,33,33	0
32	MG	A	8074	1/1	0.95	0.04	52,52,52,52	0
32	MG	A	8012	1/1	0.95	0.10	35,35,35,35	0
34	NA	A	8334	1/1	0.95	0.19	45,45,45,45	0
32	MG	A	8037	1/1	0.95	0.12	61,61,61,61	0
32	MG	A	8020	1/1	0.95	0.07	36,36,36,36	0
34	NA	A	8370	1/1	0.95	0.20	42,42,42,42	0
34	NA	A	8301	1/1	0.95	0.17	42,42,42,42	0
32	MG	A	8103	1/1	0.95	0.19	76,76,76,76	0
34	NA	A	8353	1/1	0.95	0.12	46,46,46,46	0
34	NA	A	8379	1/1	0.95	0.17	52,52,52,52	0
34	NA	A	8327	1/1	0.95	0.09	44,44,44,44	0
32	MG	A	8068	1/1	0.95	0.05	56,56,56,56	0
32	MG	A	8060	1/1	0.95	0.20	51,51,51,51	0
34	NA	A	8335	1/1	0.96	0.27	61,61,61,61	0
33	K	A	8201	1/1	0.96	0.16	70,70,70,70	0
32	MG	A	8013	1/1	0.96	0.20	56,56,56,56	0
32	MG	A	8016	1/1	0.96	0.13	50,50,50,50	0
34	NA	A	8358	1/1	0.96	0.65	107,107,107,107	0
35	CL	K	8501	1/1	0.96	0.33	81,81,81,81	0
32	MG	A	8027	1/1	0.96	0.05	51,51,51,51	0
32	MG	A	8022	1/1	0.96	0.05	55,55,55,55	0
32	MG	A	8084	1/1	0.96	0.05	41,41,41,41	0

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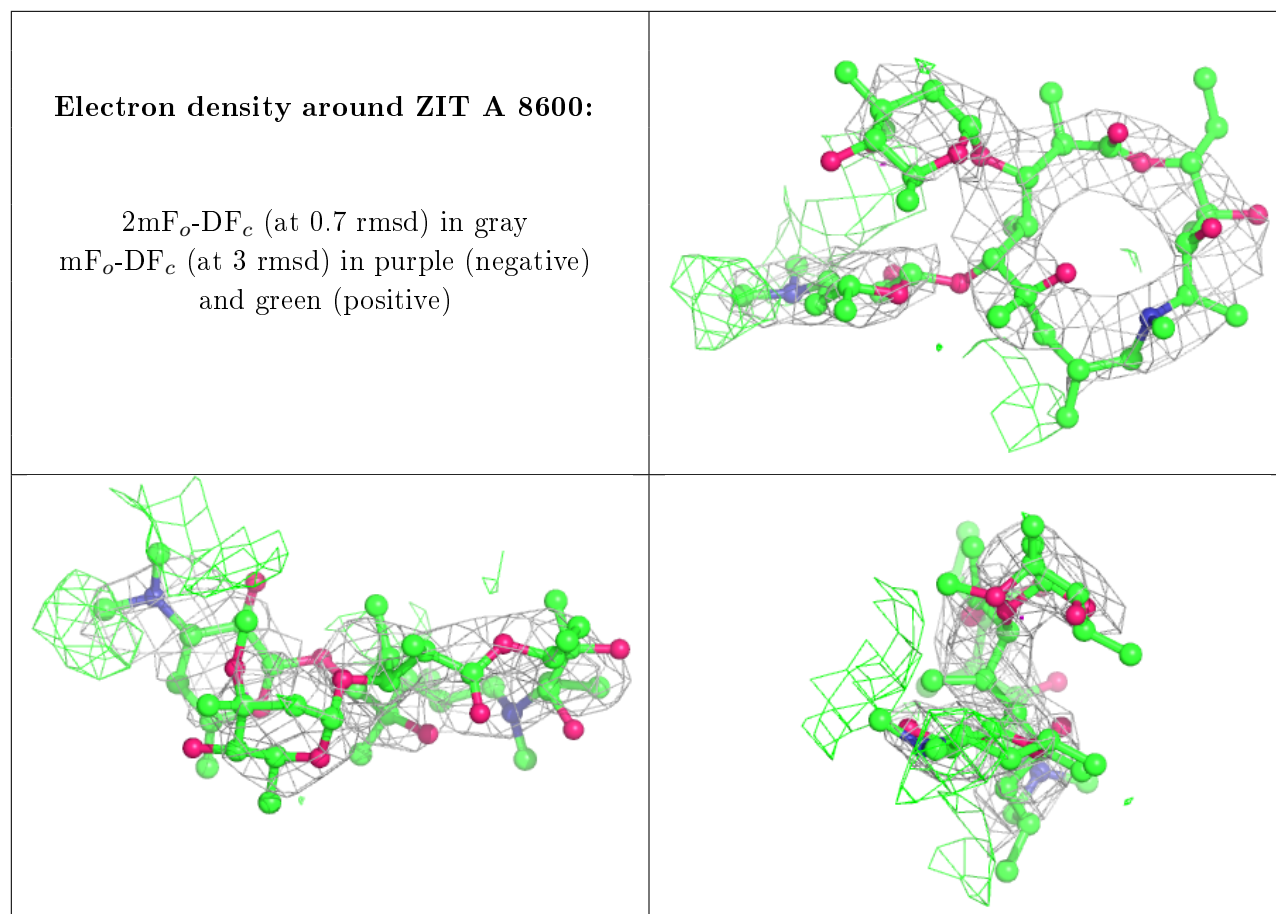
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	CD	4	8404	1/1	0.96	0.11	75,75,75,75	0
32	MG	A	8046	1/1	0.96	0.09	72,72,72,72	0
32	MG	A	8038	1/1	0.96	0.08	29,29,29,29	0
32	MG	A	8005	1/1	0.96	0.12	60,60,60,60	0
32	MG	A	8006	1/1	0.96	0.04	54,54,54,54	0
32	MG	A	8094	1/1	0.96	0.09	66,66,66,66	0
32	MG	A	8051	1/1	0.96	0.13	66,66,66,66	0
32	MG	A	8035	1/1	0.96	0.08	60,60,60,60	0
34	NA	A	8344	1/1	0.96	0.08	39,39,39,39	0
32	MG	A	8061	1/1	0.96	0.04	37,37,37,37	0
32	MG	A	8048	1/1	0.96	0.08	41,41,41,41	0
34	NA	J	8309	1/1	0.96	0.15	43,43,43,43	0
32	MG	A	8072	1/1	0.96	0.11	65,65,65,65	0
32	MG	A	8002	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8081	1/1	0.96	0.12	67,67,67,67	0
32	MG	A	8007	1/1	0.97	0.09	42,42,42,42	0
34	NA	A	8320	1/1	0.97	0.12	32,32,32,32	0
32	MG	A	8085	1/1	0.97	0.15	68,68,68,68	0
32	MG	A	8034	1/1	0.97	0.03	32,32,32,32	0
35	CL	K	8516	1/1	0.97	0.26	53,53,53,53	0
32	MG	A	8107	1/1	0.97	0.04	60,60,60,60	0
36	CD	1	8403	1/1	0.97	0.12	77,77,77,77	0
32	MG	A	8004	1/1	0.97	0.11	60,60,60,60	0
32	MG	A	8079	1/1	0.97	0.08	42,42,42,42	0
32	MG	A	8045	1/1	0.97	0.10	58,58,58,58	0
32	MG	A	8036	1/1	0.97	0.07	46,46,46,46	0
32	MG	A	8077	1/1	0.97	0.07	37,37,37,37	0
34	NA	A	8315	1/1	0.97	0.31	62,62,62,62	0
32	MG	A	8032	1/1	0.97	0.15	63,63,63,63	0
32	MG	A	8015	1/1	0.97	0.09	57,57,57,57	0
32	MG	A	8026	1/1	0.97	0.09	49,49,49,49	0
32	MG	A	8003	1/1	0.97	0.10	26,26,26,26	0
32	MG	A	8080	1/1	0.97	0.13	65,65,65,65	0
32	MG	A	8104	1/1	0.97	0.07	50,50,50,50	0
32	MG	A	8062	1/1	0.97	0.09	61,61,61,61	0
32	MG	A	8028	1/1	0.97	0.04	57,57,57,57	0
32	MG	A	8029	1/1	0.98	0.12	50,50,50,50	0
32	MG	A	8044	1/1	0.98	0.21	58,58,58,58	0
32	MG	A	8058	1/1	0.98	0.18	62,62,62,62	0
32	MG	A	8115	1/1	0.98	0.06	43,43,43,43	0
32	MG	D	8055	1/1	0.98	0.10	51,51,51,51	0
32	MG	A	8019	1/1	0.98	0.06	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8025	1/1	0.98	0.05	54,54,54,54	0
34	NA	S	8338	1/1	0.98	0.09	49,49,49,49	0
34	NA	A	8350	1/1	0.98	0.22	43,43,43,43	0
33	K	A	8202	1/1	0.98	0.14	61,61,61,61	0
34	NA	A	8339	1/1	0.98	0.06	33,33,33,33	0
34	NA	N	8347	1/1	0.98	0.12	23,23,23,23	0
32	MG	A	8047	1/1	0.98	0.17	81,81,81,81	0
32	MG	A	8023	1/1	0.98	0.03	33,33,33,33	0
34	NA	A	8317	1/1	0.98	0.04	43,43,43,43	0
32	MG	A	8018	1/1	0.98	0.11	54,54,54,54	0
32	MG	A	8030	1/1	0.99	0.10	40,40,40,40	0
32	MG	A	8117	1/1	0.99	0.10	33,33,33,33	0
32	MG	C	8065	1/1	0.99	0.05	40,40,40,40	0
32	MG	A	8098	1/1	0.99	0.25	52,52,52,52	0
36	CD	2	8402	1/1	0.99	0.08	70,70,70,70	0
34	NA	A	8319	1/1	0.99	0.14	57,57,57,57	0
32	MG	A	8014	1/1	0.99	0.07	24,24,24,24	0
36	CD	V	8401	1/1	1.00	0.11	75,75,75,75	0
32	MG	A	8031	1/1	1.00	0.03	44,44,44,44	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.