



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 24, 2021 – 10:32 AM EST

PDB ID : 3G4S
Title : Co-crystal structure of Tiamulin bound to the large ribosomal subunit
Authors : Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.
Deposited on : 2009-02-04
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 : 2.17.1
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) : 2.17.1

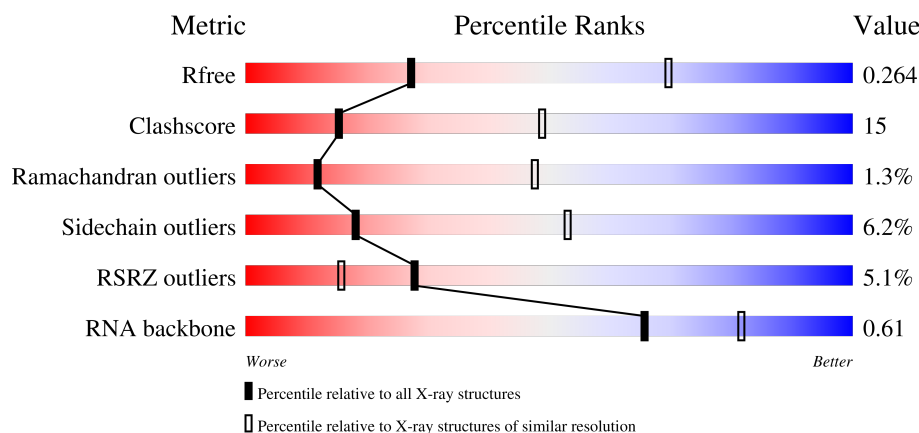
1 Overall quality at a glance

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))
R_{free}	130704	1133 (3.20-3.20)
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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	2923	<div> <div>4%</div> <div>34% 53% 7% 6%</div> </div>
2	A	237	<div> <div>4%</div> <div>83% 16%</div> </div>
3	B	337	<div> <div>81% 17%</div> </div>
4	C	246	<div> <div>%</div> <div>82% 15%</div> </div>

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z	73	
28	1	56	
29	2	50	

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Mol	Chain	Length	Quality of chain
30	3	92	<div> <div>86%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>
31	9	122	<div> <div>25%</div> <div>64%</div> <div>11%</div> </div>

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
32	MG	0	8081	-	-	-	X
32	MG	0	8090	-	-	-	X
34	NA	0	8505	-	-	-	X
34	NA	0	8506	-	-	-	X
34	NA	0	8508	-	-	-	X
34	NA	0	8509	-	-	-	X
34	NA	0	8528	-	-	-	X
34	NA	0	8556	-	-	-	X
34	NA	0	8564	-	-	-	X
34	NA	0	8566	-	-	-	X
34	NA	0	8568	-	-	-	X
36	SR	0	8922	-	-	-	X
36	SR	0	8947	-	-	-	X
36	SR	0	8994	-	-	-	X
36	SR	0	8997	-	-	-	X
36	SR	0	8998	-	-	-	X
36	SR	B	8987	-	-	-	X
36	SR	J	8986	-	-	-	X

2 Entry composition

There are 39 unique types of molecules in this entry. The entry contains 99167 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
			59021	26349	10873	19054	2745			

- Molecule 2 is a protein called 50S ribosomal protein L2P.

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

- Molecule 3 is a protein called 50S ribosomal protein L3P.

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

- Molecule 4 is a protein called 50S ribosomal protein L4P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	246	Total	C	N	O	S	0	0	0
			1860	1130	345	384	1			

- Molecule 5 is a protein called 50S ribosomal protein L5P.

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

- Molecule 6 is a protein called 50S ribosomal protein L6P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	E	172	Total	C	N	O	S	0	0	0
			1358	840	224	290	4			

- Molecule 7 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	F	119	Total	C	N	O	S	0	0	0
			890	551	141	197	1			

- Molecule 8 is a protein called 50S ribosomal protein L10.

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

- Molecule 9 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	160	Total	C	N	O	S	0	0	0
			1282	798	240	238	6			

- Molecule 10 is a protein called 50S ribosomal protein L11P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	70	Total	C	N	O	S	0	0	0
			520	323	81	115	1			

- Molecule 11 is a protein called 50S ribosomal protein L13P.

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

- Molecule 12 is a protein called 50S ribosomal protein L14P.

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

- Molecule 13 is a protein called 50S ribosomal protein L15P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	145	Total	C	N	O		0	0	0
			1118	670	222	226				

- Molecule 14 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	M	194	Total	C	N	O	S	0	0	0
			1559	943	333	282	1			

- Molecule 15 is a protein called 50S ribosomal protein L18P.

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

- Molecule 16 is a protein called 50S ribosomal protein L18e.

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

- Molecule 17 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	143	Total	C	N	O		0	0	0
			1137	683	229	225				

- Molecule 18 is a protein called 50S ribosomal protein L21e.

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

- Molecule 19 is a protein called 50S ribosomal protein L22P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	150	Total	C	N	O	S	0	0	0
			1150	713	209	224	4			

- Molecule 20 is a protein called 50S ribosomal protein L23P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	81	Total	C	N	O	S	0	0	0
			642	389	111	139	3			

- Molecule 21 is a protein called 50S ribosomal protein L24P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	53	Total	C	N	O	S	0	0	0
			411	244	75	87	5			

- Molecule 23 is a protein called 50S ribosomal protein L29P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	S	0	0	0
			500	304	94	101	1			

- Molecule 24 is a protein called 50S ribosomal protein L30P.

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

- Molecule 25 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	X	82	Total	C	N	O	S	0	0	0
			655	402	129	123	1			

- Molecule 26 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	Y	142	Total	C	N	O	0	0	0
			1131	686	228	217			

- Molecule 27 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Z	73	Total	C	N	O	S	0	0	0
			574	343	113	113	5			

- Molecule 28 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	56	Total	C	N	O	S	0	0	0
			431	258	86	83	4			

- Molecule 29 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	46	Total	C	N	O	S	0	0	0
			396	239	89	67	1			

- Molecule 30 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

- Molecule 31 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	122	Total	C	N	O	P	0	0	0
			2599	1160	471	847	121			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	84	Total	Mg	0	0
			84	84		
32	A	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	K	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	Y	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	9	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	0	1	Total K 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	0	66	Total Na 66 66	0	0
34	C	1	Total Na 1 1	0	0
34	J	1	Total Na 1 1	0	0
34	M	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	R	2	Total Na 2 2	0	0
34	S	1	Total Na 1 1	0	0
34	9	2	Total Na 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	0	10	Total Cl 10 10	0	0
35	A	1	Total Cl 1 1	0	0
35	B	1	Total Cl 1 1	0	0
35	J	3	Total Cl 3 3	0	0
35	L	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0

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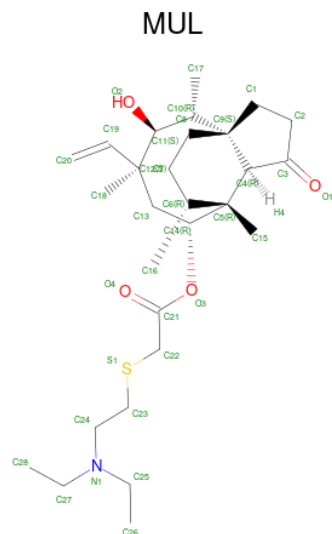
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	R	1	Total 1	Cl 1	0	0
35	Y	1	Total 1	Cl 1	0	0
35	3	1	Total 1	Cl 1	0	0

- Molecule 36 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	91	Total 91	Sr 91	0	0
36	A	3	Total 3	Sr 3	0	0
36	B	2	Total 2	Sr 2	0	0
36	F	1	Total 1	Sr 1	0	0
36	H	1	Total 1	Sr 1	0	0
36	J	1	Total 1	Sr 1	0	0
36	L	1	Total 1	Sr 1	0	0
36	R	1	Total 1	Sr 1	0	0
36	S	1	Total 1	Sr 1	0	0
36	1	2	Total 2	Sr 2	0	0
36	3	2	Total 2	Sr 2	0	0
36	9	2	Total 2	Sr 2	0	0

- Molecule 37 is TIAMULIN (three-letter code: MUL) (formula: C₂₈H₄₇NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
37	0	1	Total	C	N	O	S	0	0
			34	28	1	4	1		

- Molecule 38 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	O	1	Total Cd 1 1	0	0
38	U	1	Total Cd 1 1	0	0
38	Z	1	Total Cd 1 1	0	0
38	1	1	Total Cd 1 1	0	0
38	3	1	Total Cd 1 1	0	0

- Molecule 39 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
39	0	5940	Total O 5940 5940	0	0
39	A	125	Total O 125 125	0	0
39	B	140	Total O 140 140	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	158	Total 158	O 158	0	0
39	D	45	Total 45	O 45	0	0
39	E	42	Total 42	O 42	0	0
39	F	26	Total 26	O 26	0	0
39	G	18	Total 18	O 18	0	0
39	H	70	Total 70	O 70	0	0
39	I	4	Total 4	O 4	0	0
39	J	47	Total 47	O 47	0	0
39	K	58	Total 58	O 58	0	0
39	L	94	Total 94	O 94	0	0
39	M	132	Total 132	O 132	0	0
39	N	55	Total 55	O 55	0	0
39	O	43	Total 43	O 43	0	0
39	P	59	Total 59	O 59	0	0
39	Q	52	Total 52	O 52	0	0
39	R	80	Total 80	O 80	0	0
39	S	30	Total 30	O 30	0	0
39	T	30	Total 30	O 30	0	0
39	U	30	Total 30	O 30	0	0
39	V	11	Total 11	O 11	0	0
39	W	59	Total 59	O 59	0	0

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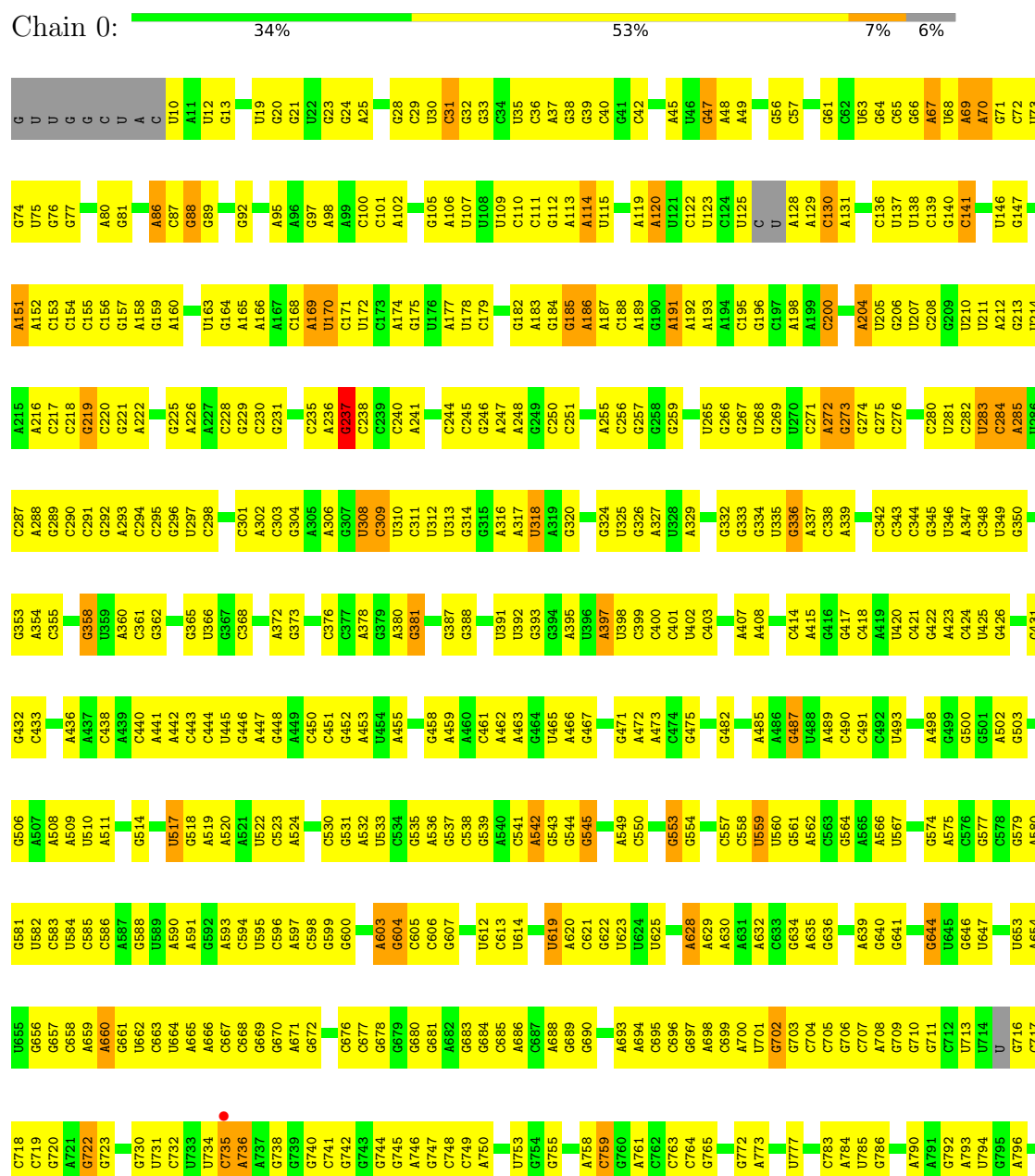
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	22	Total 22	O 22	0	0
39	Y	105	Total 105	O 105	0	0
39	Z	30	Total 30	O 30	0	0
39	1	55	Total 55	O 55	0	0
39	2	48	Total 48	O 48	0	0
39	3	62	Total 62	O 62	0	0
39	9	152	Total 152	O 152	0	0

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.

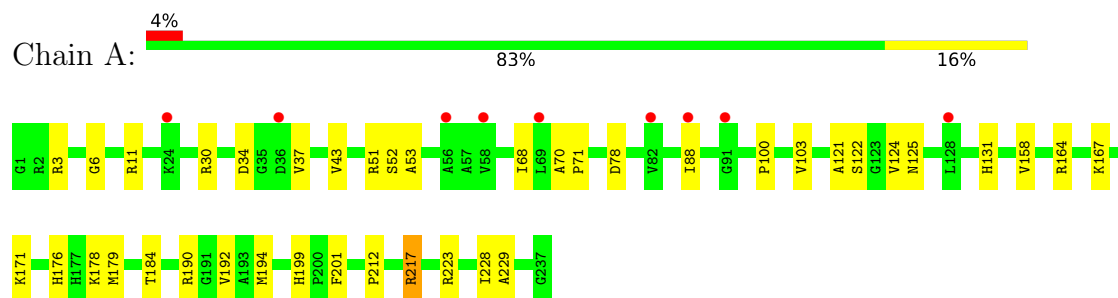
• Molecule 1: 23S ribosomal RNA



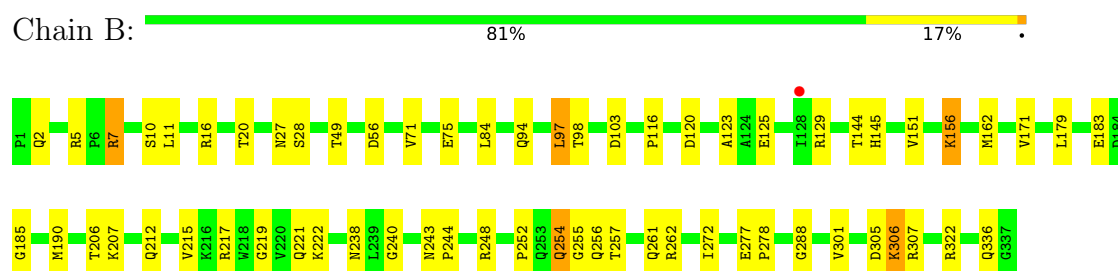
C1818	G1752	C1880	G1608	U1524	C1450	G1376	C1305	C1228	G1159	C1085	A1006	A943	G870	U801
G1819	C1783	G1681	C1609	G1525	C1451	C1377	U1306	C1228	G1160	A1086	A1007	G944	G871	G802
A1820	A1754	A1682	G1610	A1526	G1452	C1378	C1307	C1229	G1161	G1087	C1008	U945	U872	A806
A1821	A1755	G1683	G1611	A1527	G1453	A1379	A1308	A1230	G1162	A1088	U1009	C946	A875	A807
A1822	G1756	A1684	A1612	A1528	U1454	U1383	U1309	U1234	G1163	U1096	C1011	G948	A876	A808
G1823	C1613	A1685	C1613	U1531	C1455	C1384	G1311	U1234	G1164	A1097	A1012	G951	G877	G809
C1824	G1614	C1686	G1614	U1531	C1456	C1384	G1312	U1238	G1165	A1098	A1013	A951	G878	A810
U1825	A1615	C1687	A1615	G1535	U1457	C1387	A1313	C1238	G1166	G1099	A1014	G952	C811	C811
G1826	A1616	G1688	A1616	C1536	U1458	G1388	G1314	G1239	G1167	G1099	A1015	G953	C812	A812
G1827	C1617	A1689	G1617	C1536	U1459	G1389	G1315	A1242	U1169	U1101	U1016	U954	A882	C813
C1828	G1618	C1618	G1618	U1544	U1461	A1390	G1316	U1244	U1170	C1102	G1023	A955	U883	G814
A1829	G1619	U1544	C1619	U1544	U1461	G1391	G1316	U1244	U1171	C1103	G1024	G956	U884	U815
C1830	C1620	U1545	C1620	U1545	U1462	A1392	G1323	C1245	G1172	C1104	G1025	A957	G885	G816
U1831	G1621	G1546	G1621	U1546	U1463	C1392	G1324	C1246	G1173	C1105	U1026	G958	G887	G817
G1832	G1622	A1547	G1622	A1547	C1464	C1396	G1326	U1249	A1174	U1106	U1041	G959	U888	A818
U1833	C1623	U1548	C1623	U1548	U1465	C1397	G1326	U1250	G1175	U1109	U1029	A961	U889	A819
C1834	U1698	C1549	C1624	C1549	U1473	C1398	G1327	C1250	C1176	U1110	U1030	C962	C890	G820
U1835	U1625	C1554	U1625	C1554	U1474	A1399	A1328	C1251	U1111	U1111	U1031	C963	U821	U821
U1836	A1626	G1555	A1626	G1555	G1475	C1400	A1328	A1252	U1112	U1112	G1031	C964	U822	U822
U1837	G1627	G1556	G1627	G1556	U1476	G1401	G1331	C1253	U1113	U1113	A1032	A965	U823	U823
U1838	U1630	G1557	U1630	G1557	C1477	C1402	U1332	C1254	A1181	G1114	U1041	A965	U824	U824
A1839	A1631	C1558	A1631	C1558	U1478	A1407	U1333	C1255	C1182	U1115	U1042	A966	U825	U825
C1840	G1773	G1559	G1773	G1559	U1479	U1408	C1334	C1256	C1183	U1116	U1043	G968	A895	U826
C1841	U1706	U1559	C1632	U1559	U1480	G1409	C1335	C1257	C1184	U1117	G1044	G969	A896	U826
U1844	G1707	U1561	C1633	U1561	C1483	U1409	C1335	C1258	U1185	A1117	G1045	U970	A897	G834
A1845	U1634	U1561	G1634	U1561	G1484	U1412	U1338	C1259	U1186	U1118	G1046	G	U835	U835
U1846	U1635	C1566	U1635	C1566	U1485	U1415	G1339	C1260	U1187	G1119	U1047	U	U836	U836
A1847	U1636	G1567	U1636	G1567	U1486	G1416	U1342	C1261	A1188	U1120	U	G902	U837	U837
G1848	U1637	U1567	U1637	U1567	U1487	G1417	C1343	C1262	A1189	G1121	C1051	U	U838	U838
C1849	U1638	U1568	U1638	U1568	U1488	G1418	C1344	C1263	G1190	U1122	C1052	C	C905	C905
U1850	U1639	C1570	U1639	C1570	U1489	U1419	G1344	C1264	A1191	U1123	G1053	C	U840	U840
C1851	C1640	C1571	C1640	C1571	U1490	C1420	U1347	C1265	A1192	U1124	G1054	G	A841	A841
A1852	A1641	A1572	A1641	A1572	U1491	C1421	U1348	C1266	A1193	U1125	G1055	C	C942	C942
G1853	G1642	C1573	G1642	C1573	U1492	U1422	U1349	C1267	A1194	C1126	U1056	C	U909	U909
C1854	C1643	C1574	C1643	C1574	U1493	C1423	G1350	C1268	G1195	U1127	A1057	U	C910	C910
G1855	U1645	C1575	U1645	C1575	U1494	C1424	U1351	C1269	C1196	U1128	U1058	C	G911	G911
C1856	G1646	C1576	G1646	C1576	U1495	U1425	G1352	C1270	U1196	U1129	G1059	C	A846	A846
U1857	U1647	U1501	U1647	U1501	U1496	A1427	A1352	C1271	U1200	U1130	G1060	G	C847	C847
A1858	G1648	A1502	G1648	A1502	U1497	C1428	C1353	C1272	C1201	G1131	C1061	A	C848	C848
C1859	U1649	U1503	U1649	U1503	U1498	U1429	U1354	C1273	C1202	U1132	U1062	G	C849	C849
U1860	A1656	U1504	A1656	U1504	U1499	G1430	A1355	C1274	A1203	U1133	U1063	A	U850	U850
C1861	U1657	U1505	U1657	U1505	U1500	U1431	U1356	C1275	G1196	U1134	U1064	A	C851	C851
A1862	A1658	U1506	A1658	U1506	U1501	G1432	U1357	C1276	U1205	U1135	A1067	G	U852	U852
G1863	U1659	C1507	U1659	C1507	U1502	U1433	A1358	C1277	U1206	U1136	G1068	A	G921	G921
U1864	A1661	U1508	A1661	U1508	U1503	U1434	U1359	C1278	U1207	G1137	C1069	C	U853	U853
C1865	G1662	C1509	G1662	C1509	U1504	U1435	U1360	C1279	A1208	U1138	A1070	G	U854	U854
G1866	A1663	U1510	A1663	U1510	U1505	U1436	U1361	C1280	C1209	U1139	G1071	U	U855	U855
U1867	G1664	U1511	U1664	U1511	U1506	A1437	U1362	C1281	G1210	U1140	U1072	C	A926	A926
C1868	U1665	U1512	U1665	U1512	U1507	U1438	U1363	C1282	G1211	U1141	A1073	G	U857	U857
A1869	C1666	C1513	C1666	C1513	U1508	U1439	G1364	C1283	G1212	U1142	G1074	C	U858	U858
U1870	A1667	U1514	A1667	U1514	U1509	U1440	U1365	C1284	C1213	G1075	G1075	C	C859	C859
G1871	U1668	U1515	U1668	U1515	U1510	G1441	C1366	C1285	G1214	U1143	U1076	A	U860	U860
C1872	U1669	C1516	U1669	C1516	U1511	U1442	U1367	C1286	G1215	A1150	G1077	C	A861	A861
U1873	U1670	U1517	U1670	U1517	U1512	U1443	U1368	C1287	G1216	G1151	U1078	A	U862	U862
A1874	G1671	A1518	A1671	A1518	U1513	G1444	U1369	C1288	G1217	C1152	C1080	C	G935	G935
G1875	C1672	U1519	C1672	U1519	U1514	U1445	U1370	C1289	U1218	A1153	C1081	C	U863	U863
U1876	A1673	C1520	A1673	C1520	U1515	U1446	U1371	C1290	U1219	U1154	U1082	C	U864	U864
C1877	U1674	U1521	U1674	U1521	U1516	U1447	A1372	C1291	U1220	C1155	A1083	C	U865	U865
A1878	G1675	A1522	A1675	A1522	U1517	U1448	U1373	C1292	U1221	C1156	C1084	C	A867	A867
G1879	C1676	U1523	C1676	U1523	U1518	U1449	U1374	C1293	G1221	C1157	U1001	C	G940	G940
U1880	U1677	C1524	U1677	C1524	U1519	U1450	U1375	C1294	U1222	U1158	U1002	C	U868	U868
C1881	A1678	U1525	A1678	U1525	U1520	U1451	U1376	C1295	U1223	U1159	U1003	C	U869	U869
U1882	G1679	U1526	U1679	U1526	U1521	U1452	U1377	C1296	U1224	U1160	U1004	C	U870	U870
G1883	U1680	C1527	U1680	C1527	U1522	U1453	U1378	C1297	U1225	U1161	U1005	C	U871	U871
C1884	G1757	A1680	C1680	A1680	U1523	U1454	U1379	C1298	U1226	U1162	U1006	C	U872	U872
U1885	U1758	C1681	U1758	C1681	U1524	U1455	U1380	C1299	U1227	U1163	U1007	C	U873	U873
A1886	A1759	A1682	A1759	A1682	U1525	U1456	U1381	C1300	U1228	U1164	U1008	C	U874	U874
C1887	G1760	G1683	G1760	G1683	U1526	U1457	U1382	C1301	U1229	U1165	U1009	C	U875	U875
U1888	U1761	A1684	U1761	A1684	U1527	U1458	U1383	C1302	U1230	U1166	U1010	C	U876	U876
G1889	C1762	U1685	C1762	U1685	U1528	U1459	U1384	C1303	U1231	U1167	U1011	C	U877	U877
A1890	G1763	C1686	A1763	C1686	U1529	U1460	U1385	C1304	U1232	U1168	U1012	C	U878	U878
C1891	U1764	A1687	U1764	A1687	U1530	U1461	U1386	C1305	U1233	U1169	U1013	C	U879	U879
U1892	C1765	G1688	C1765	G1688	U1531	U1462	U1387	C1306	U1234	U1170	U1014	C	U880	U880
G1893	U1766	U1689	U1766	U1689	U1532	U1463	U1388	C1307	U1235	U1171	U1015	C	U881	U881
C1894	G1767	A1690	C1767	A1690	U1533	U1464	U1389	C1308	U1236	U1172	U1016	C	U882	U882
U1895	U1768	U1691	U1768	U1691	U1534	U1465	U1390	C1309	U1237	U1173	U1017	C	U883	U883
A1896	C1769	C1692	A1769	C1692	U1535	U1466	U1391	C1310	U1238	U1174	U1018	C	U884	U884
C1897	U1770	U1693	U1770	U1693	U1536	U1467	U1392	C1311	U1239	U1175	U1019	C	U885	U885
U1898	G1771	A1694	U1771	A1694	U1537	U1468	U1393	C1312	U1240	U1176	U1020	C	U886	U886
C1899	C1772	U1695	C1772	U1695	U1538	U1469	U1394	C1313	U1241	U1177	U1021	C	U887	U887
A1900	U1773	G1696	A1773	G1696	U1539	U1470	U1395	C1314	U1242	U1178	U1022	C	U888	U888
G1901	G1774	C1697	G1774	C1697	U1540	U1471	U1396	C1315	U1243	U1179	U1023	C	U889	U889
C1902	U1775	U1698	U1775	U1698	U1541	U1472	U1397	C1316	U1244	U1180	U1024	C	U890	U890
U1903	A1776	C1699	A1776	C1699	U1542	U1473	U1398	C1317	U1245	U1181	U1025	C	U891	U891
A1904	G1777	U1700	A1777	U1700	U1543	U1474	U1399	C1318	U1246	U1182	U1026	C	U892	U892
C1905	U1778	A1701	C1778	A1701	U1544	U1475	U1400	C1319	U1247	U1183	U1027	C	U893	U893
U1906	A1779	U1702	A1779	U1702	U1545	U1476	C1401	C1320	U1248	U1184	U1028	C	U894	U894



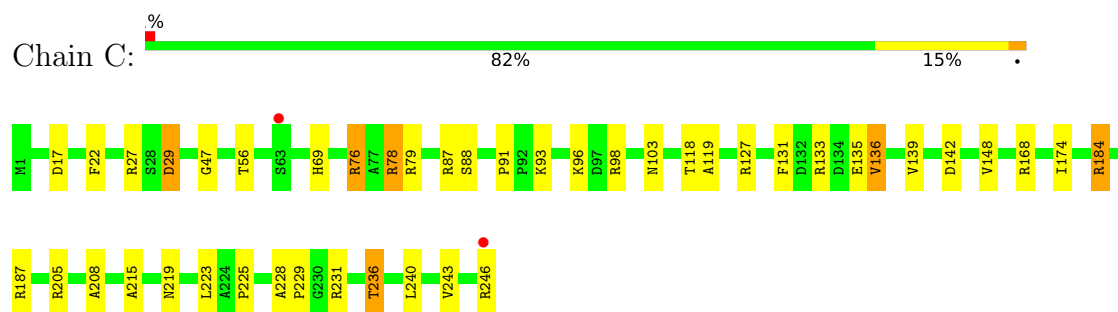
- Molecule 2: 50S ribosomal protein L2P



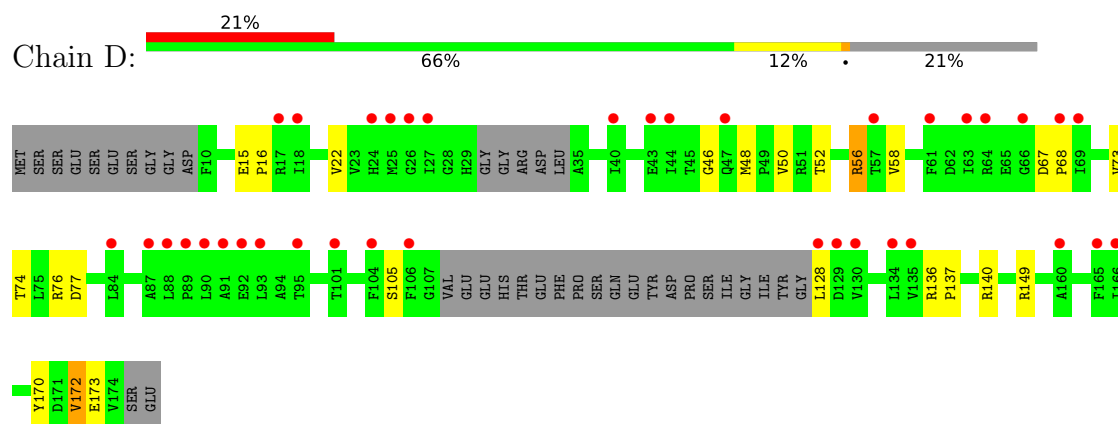
- Molecule 3: 50S ribosomal protein L3P



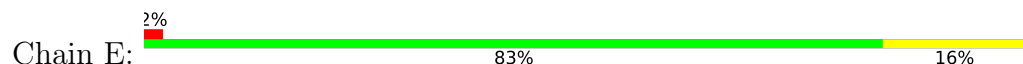
- Molecule 4: 50S ribosomal protein L4P



- Molecule 5: 50S ribosomal protein L5P

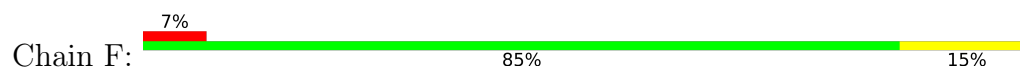


- Molecule 6: 50S ribosomal protein L6P

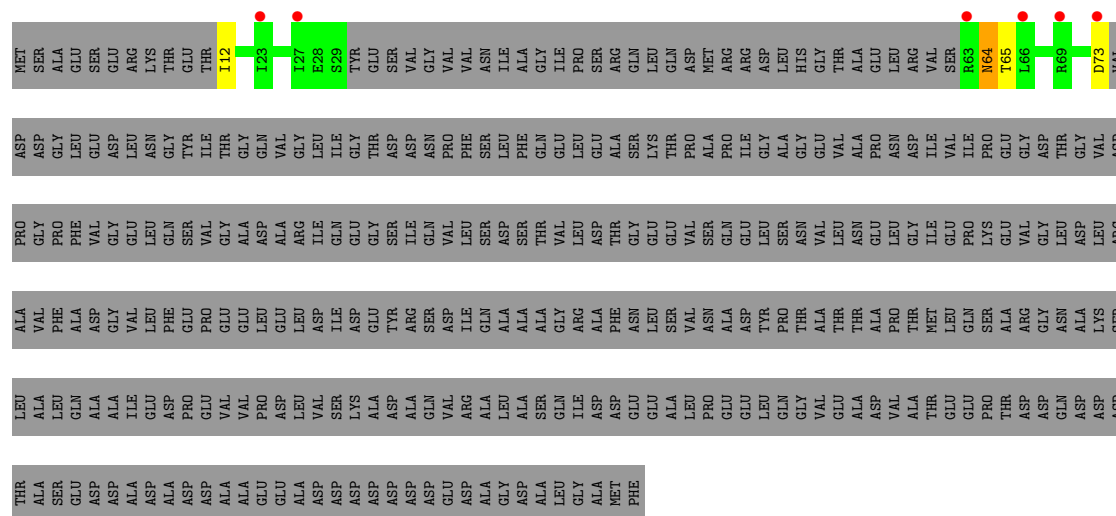




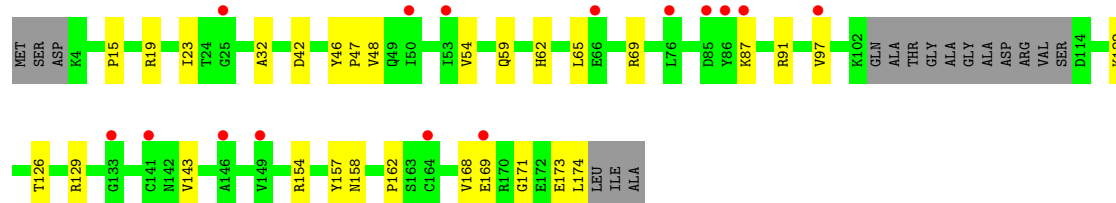
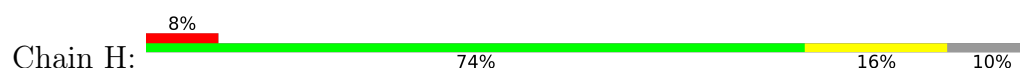
- Molecule 7: 50S ribosomal protein L7Ae



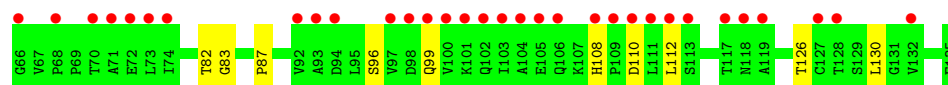
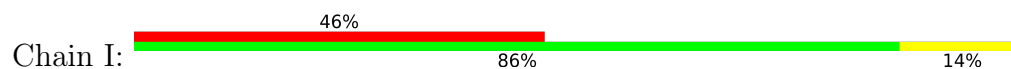
- Molecule 8: 50S ribosomal protein L10




- Molecule 9: 50S ribosomal protein L10e

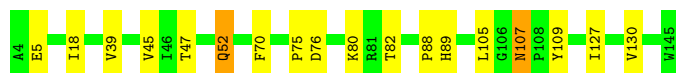


- Molecule 10: 50S ribosomal protein L11P




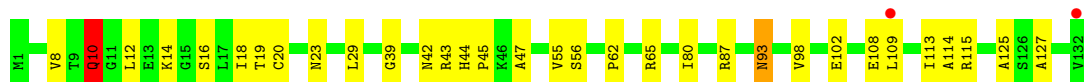
- Molecule 11: 50S ribosomal protein L13P

Chain J:  87% 11% .




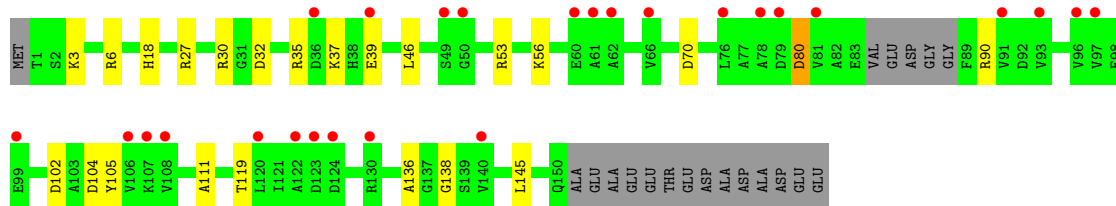
- Molecule 12: 50S ribosomal protein L14P

Chain K:  2% 76% 23% ..




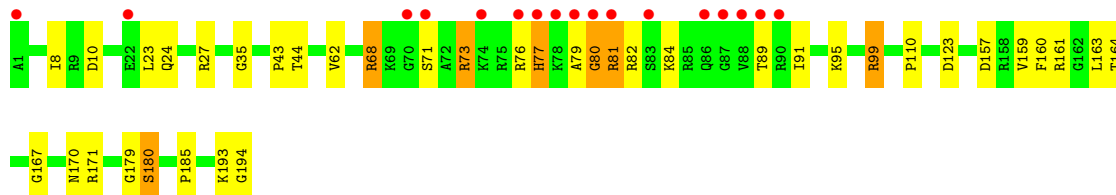
- Molecule 13: 50S ribosomal protein L15P

Chain L:  16% 74% 13% . 12%




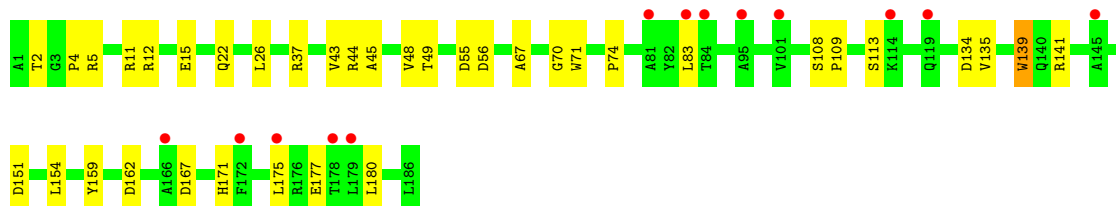
- Molecule 14: 50S ribosomal protein L15e

Chain M:  9% 80% 16% .



- Molecule 15: 50S ribosomal protein L18P

Chain N:  7% 80% 19% .

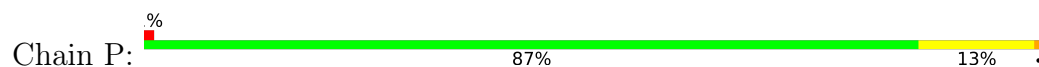


- Molecule 16: 50S ribosomal protein L18e

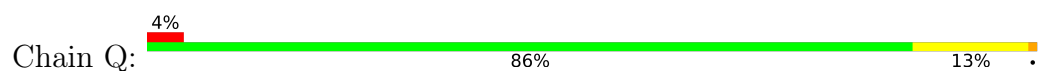
Chain O:  90% 9% .



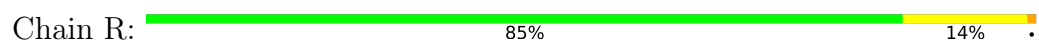
- Molecule 17: 50S ribosomal protein L19e



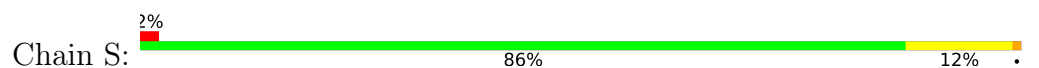
- Molecule 18: 50S ribosomal protein L21e



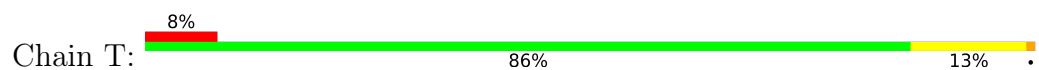
- Molecule 19: 50S ribosomal protein L22P



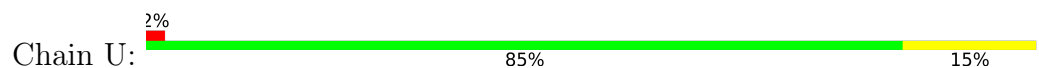
- Molecule 20: 50S ribosomal protein L23P



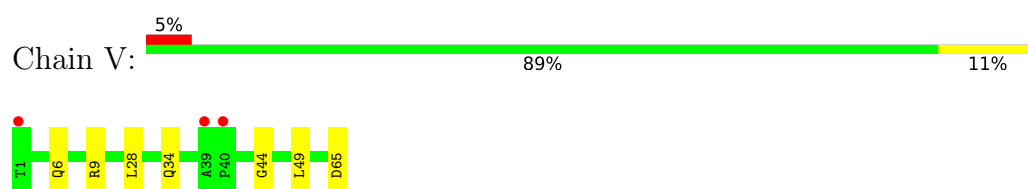
- Molecule 21: 50S ribosomal protein L24P



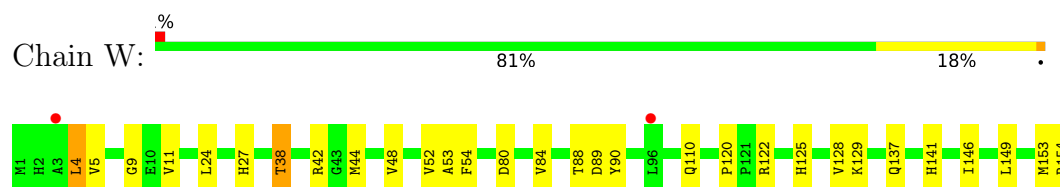
- Molecule 22: 50S ribosomal protein L24e



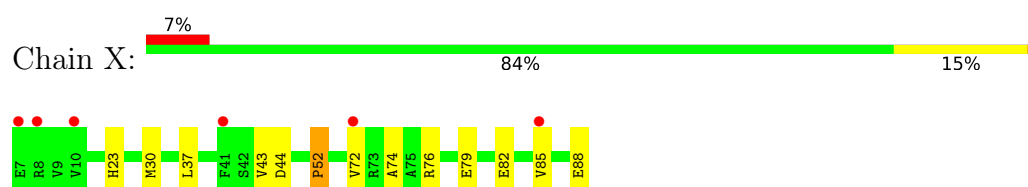
- Molecule 23: 50S ribosomal protein L29P



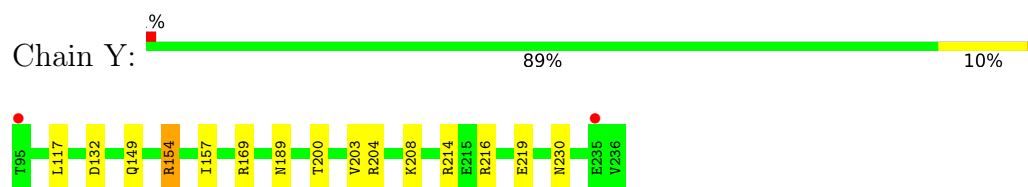
- Molecule 24: 50S ribosomal protein L30P



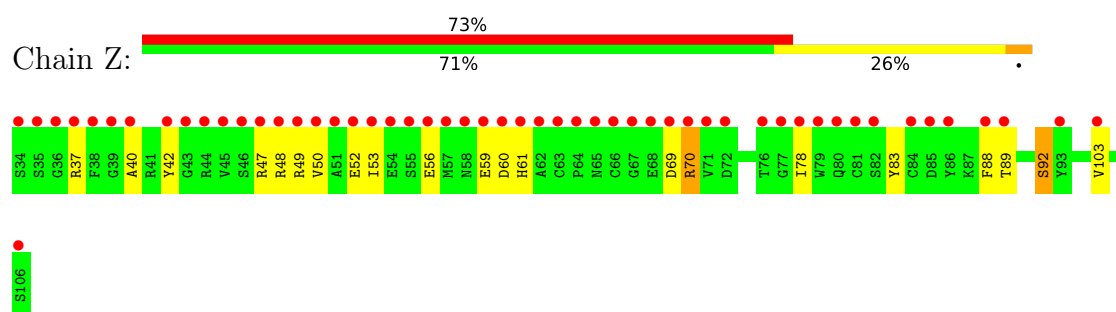
- Molecule 25: 50S ribosomal protein L31e



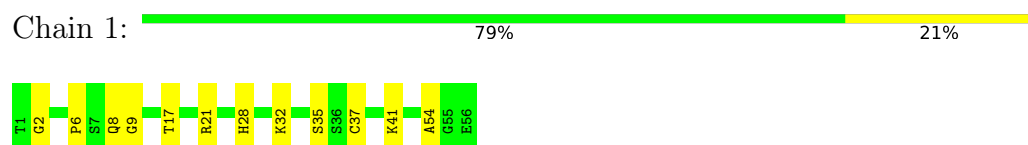
- Molecule 26: 50S ribosomal protein L32e



- Molecule 27: 50S ribosomal protein L37Ae

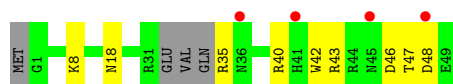


- Molecule 28: 50S ribosomal protein L37e

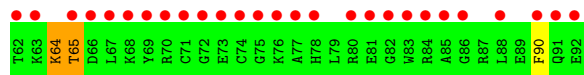
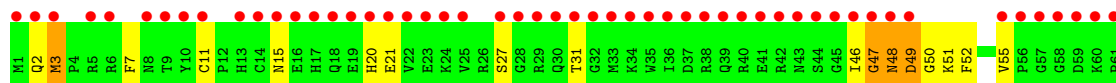
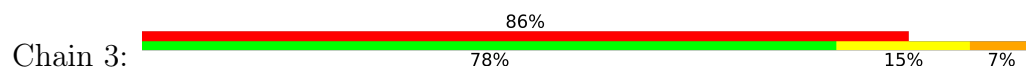


- Molecule 29: 50S ribosomal protein L39e

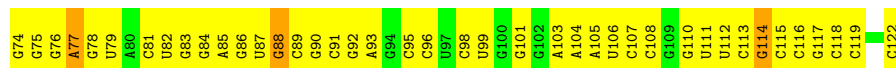




- Molecule 30: 50S ribosomal protein L44E



- Molecule 31: 5S ribosomal RNA



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	212.27Å 299.84Å 574.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 3.20 85.66 – 2.41	Depositor EDS
% Data completeness (in resolution range)	83.7 (49.84-3.20) 82.8 (85.66-2.41)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.215 , 0.290 0.199 , 0.264	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	78.3	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 119.7	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	0.93	EDS
Total number of atoms	99167	wwPDB-VP
Average B, all atoms (Å ²)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% 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: 1MA, PSU, CL, OMU, MG, K, MUL, SR, OMG, UR3, CD, NA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.47	0/65958	0.69	6/102869 (0.0%)
2	A	0.53	0/1787	0.77	0/2408
3	B	0.54	0/2690	0.77	1/3652 (0.0%)
4	C	0.56	0/1885	0.80	0/2552
5	D	0.70	0/1111	0.74	1/1498 (0.1%)
6	E	0.62	0/1383	0.71	0/1880
7	F	0.56	0/901	0.73	1/1224 (0.1%)
8	G	0.55	0/241	0.66	0/324
9	H	0.61	0/1302	0.78	0/1743
10	I	0.63	0/527	0.66	0/716
11	J	0.63	0/1136	0.75	0/1530
12	K	0.51	0/1004	0.78	0/1351
13	L	0.56	0/1130	0.77	0/1509
14	M	0.55	0/1583	0.79	1/2116 (0.0%)
15	N	0.60	0/1474	0.79	0/1999
16	O	0.52	0/874	0.77	0/1181
17	P	0.56	0/1148	0.69	0/1528
18	Q	0.53	0/749	0.74	0/1005
19	R	0.58	0/1173	0.74	0/1578
20	S	0.56	0/649	0.70	0/875
21	T	0.50	0/958	0.76	1/1289 (0.1%)
22	U	0.65	0/418	0.72	0/562
23	V	0.49	0/503	0.70	0/675
24	W	0.54	0/1219	0.78	0/1655
25	X	0.53	0/665	0.74	0/895
26	Y	0.55	0/1147	0.76	0/1536
27	Z	0.74	0/585	0.84	0/781
28	1	0.62	0/438	0.77	0/578
29	2	0.46	0/401	0.74	0/529
30	3	0.78	0/771	0.81	0/1024
31	9	0.38	0/2904	0.68	0/4526
All	All	0.50	0/98714	0.71	11/147588 (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	25
24	W	0	1
All	All	0	26

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	1504	A	N9-C1'-C2'	6.64	122.64	114.00
1	0	237	G	N9-C1'-C2'	-6.25	105.12	112.00
3	B	84	LEU	CA-CB-CG	5.84	128.74	115.30
1	0	871	G	C5'-C4'-O4'	-5.68	102.28	109.10
1	0	820	G	N9-C1'-C2'	5.65	121.34	114.00

There are no chirality outliers.

5 of 26 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	436	A	Sidechain
1	0	462	A	Sidechain
1	0	471	G	Sidechain
1	0	49	A	Sidechain
1	0	493	U	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	59021	0	29812	1915	0
2	A	1754	0	1766	26	0
3	B	2625	0	2533	37	0
4	C	1860	0	1813	32	0
5	D	1094	0	1085	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	1358	0	1266	12	0
7	F	890	0	843	7	0
8	G	240	0	231	1	0
9	H	1282	0	1292	12	0
10	I	520	0	500	6	0
11	J	1120	0	1098	16	0
12	K	994	0	1027	20	0
13	L	1118	0	1076	13	0
14	M	1559	0	1573	32	0
15	N	1445	0	1401	20	0
16	O	865	0	873	9	0
17	P	1137	0	1123	17	0
18	Q	735	0	729	9	0
19	R	1150	0	1122	15	0
20	S	642	0	605	6	0
21	T	950	0	924	13	0
22	U	411	0	368	3	0
23	V	500	0	511	3	0
24	W	1196	0	1137	25	0
25	X	655	0	653	6	0
26	Y	1131	0	1133	10	0
27	Z	574	0	535	15	0
28	1	431	0	426	8	0
29	2	396	0	413	6	0
30	3	755	0	732	16	0
31	9	2599	0	1325	113	0
32	0	84	0	0	0	0
32	2	1	0	0	0	0
32	9	1	0	0	0	0
32	A	2	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	K	1	0	0	0	0
32	T	1	0	0	0	0
32	Y	1	0	0	0	0
33	0	1	0	0	0	0
34	0	66	0	0	0	0
34	9	2	0	0	0	0
34	C	1	0	0	0	0
34	J	1	0	0	0	0
34	M	1	0	0	0	0
34	Q	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	R	2	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	2	0
35	3	1	0	0	0	0
35	A	1	0	0	0	0
35	B	1	0	0	0	0
35	J	3	0	0	1	0
35	L	1	0	0	0	0
35	M	1	0	0	1	0
35	N	1	0	0	0	0
35	O	1	0	0	0	0
35	R	1	0	0	0	0
35	Y	1	0	0	0	0
36	0	91	0	0	0	0
36	1	2	0	0	0	0
36	3	2	0	0	0	0
36	9	2	0	0	0	0
36	A	3	0	0	0	0
36	B	2	0	0	0	0
36	F	1	0	0	0	0
36	H	1	0	0	0	0
36	J	1	0	0	0	0
36	L	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	34	0	47	17	0
38	1	1	0	0	0	0
38	3	1	0	0	0	0
38	O	1	0	0	0	0
38	U	1	0	0	0	0
38	Z	1	0	0	0	0
39	0	5940	0	0	278	0
39	1	55	0	0	0	0
39	2	48	0	0	1	0
39	3	62	0	0	1	0
39	9	152	0	0	12	0
39	A	125	0	0	3	0
39	B	140	0	0	2	0
39	C	158	0	0	3	0
39	D	45	0	0	1	0
39	E	42	0	0	0	0
39	F	26	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	G	18	0	0	0	0
39	H	70	0	0	1	0
39	I	4	0	0	0	0
39	J	47	0	0	1	0
39	K	58	0	0	0	0
39	L	94	0	0	4	0
39	M	132	0	0	1	0
39	N	55	0	0	1	0
39	O	43	0	0	1	0
39	P	59	0	0	0	0
39	Q	52	0	0	0	0
39	R	80	0	0	0	0
39	S	30	0	0	1	0
39	T	30	0	0	0	0
39	U	30	0	0	1	0
39	V	11	0	0	0	0
39	W	59	0	0	0	0
39	X	22	0	0	0	0
39	Y	105	0	0	1	0
39	Z	30	0	0	2	0
All	All	99167	0	59972	2229	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

The worst 5 of 2229 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)
1:0:871:G:H8	1:0:871:G:H5'	1.00	1.13
1:0:1160:G:H5'	1:0:1161:A:H5'	1.28	1.13
1:0:2121:G:H4'	30:3:47:GLY:HA2	1.29	1.12
1:0:2717:C:H2'	1:0:2718:C:H5''	1.27	1.12
1:0:871:G:H5'	1:0:871:G:C8	1.88	1.08

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	
2	A	235/237 (99%)	210 (89%)	20 (8%)	5 (2%)	7	37
3	B	335/337 (99%)	305 (91%)	27 (8%)	3 (1%)	17	56
4	C	244/246 (99%)	223 (91%)	18 (7%)	3 (1%)	13	49
5	D	134/177 (76%)	112 (84%)	19 (14%)	3 (2%)	6	35
6	E	170/172 (99%)	157 (92%)	12 (7%)	1 (1%)	25	64
7	F	117/119 (98%)	108 (92%)	5 (4%)	4 (3%)	3	24
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	145 (93%)	10 (6%)	1 (1%)	25	64
10	I	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	10	44
11	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	11	46
12	K	130/132 (98%)	116 (89%)	13 (10%)	1 (1%)	19	58
13	L	141/165 (86%)	128 (91%)	12 (8%)	1 (1%)	22	61
14	M	192/194 (99%)	180 (94%)	7 (4%)	5 (3%)	5	31
15	N	184/186 (99%)	165 (90%)	15 (8%)	4 (2%)	6	35
16	O	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
17	P	141/143 (99%)	131 (93%)	9 (6%)	1 (1%)	22	61
18	Q	93/95 (98%)	85 (91%)	6 (6%)	2 (2%)	6	35
19	R	148/150 (99%)	141 (95%)	6 (4%)	1 (1%)	22	61
20	S	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
21	T	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
22	U	51/53 (96%)	49 (96%)	2 (4%)	0	100	100
23	V	63/65 (97%)	59 (94%)	4 (6%)	0	100	100
24	W	152/154 (99%)	139 (91%)	13 (9%)	0	100	100
25	X	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	12	47
26	Y	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	22	61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	5	29
28	1	54/56 (96%)	47 (87%)	6 (11%)	1 (2%)	8	39
29	2	42/50 (84%)	40 (95%)	2 (5%)	0	100	100
30	3	90/92 (98%)	75 (83%)	11 (12%)	4 (4%)	2	19
All	All	3705/4172 (89%)	3381 (91%)	277 (8%)	47 (1%)	12	47

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	52	SER
3	B	306	LYS
7	F	61	MET
11	J	5	GLU
14	M	80	GLY

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	
2	A	179/179 (100%)	169 (94%)	10 (6%)	21	57
3	B	282/282 (100%)	263 (93%)	19 (7%)	16	50
4	C	193/193 (100%)	179 (93%)	14 (7%)	14	46
5	D	117/148 (79%)	109 (93%)	8 (7%)	16	49
6	E	152/152 (100%)	139 (91%)	13 (9%)	10	38
7	F	93/93 (100%)	91 (98%)	2 (2%)	52	79
8	G	27/282 (10%)	23 (85%)	4 (15%)	3	14
9	H	134/145 (92%)	121 (90%)	13 (10%)	8	31
10	I	58/58 (100%)	56 (97%)	2 (3%)	37	70
11	J	118/118 (100%)	112 (95%)	6 (5%)	24	60
12	K	106/106 (100%)	99 (93%)	7 (7%)	16	51
13	L	113/127 (89%)	105 (93%)	8 (7%)	14	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	158/158 (100%)	146 (92%)	12 (8%)	13	45
15	N	149/149 (100%)	135 (91%)	14 (9%)	8	33
16	O	93/93 (100%)	88 (95%)	5 (5%)	22	58
17	P	113/113 (100%)	110 (97%)	3 (3%)	44	75
18	Q	79/79 (100%)	77 (98%)	2 (2%)	47	77
19	R	117/117 (100%)	111 (95%)	6 (5%)	24	60
20	S	71/71 (100%)	68 (96%)	3 (4%)	30	65
21	T	105/105 (100%)	99 (94%)	6 (6%)	20	56
22	U	44/44 (100%)	40 (91%)	4 (9%)	9	34
23	V	51/51 (100%)	47 (92%)	4 (8%)	12	43
24	W	130/130 (100%)	127 (98%)	3 (2%)	50	78
25	X	66/66 (100%)	60 (91%)	6 (9%)	9	34
26	Y	120/120 (100%)	114 (95%)	6 (5%)	24	60
27	Z	60/60 (100%)	57 (95%)	3 (5%)	24	60
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	42/46 (91%)	39 (93%)	3 (7%)	14	47
30	3	79/79 (100%)	73 (92%)	6 (8%)	13	45
All	All	3095/3410 (91%)	2903 (94%)	192 (6%)	18	53

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	M	123	ASP
19	R	52	GLU
15	N	22	GLN
15	N	177	GLU
20	S	44	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
26	Y	134	HIS
26	Y	189	ASN
29	2	45	ASN
12	K	93	ASN

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Mol	Chain	Res	Type
12	K	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	263 (9%)	19 (0%)
31	9	121/122 (99%)	17 (14%)	1 (0%)
All	All	2866/3045 (94%)	280 (9%)	20 (0%)

5 of 280 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	47	G
1	0	67	A
1	0	69	A
1	0	70	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	2467	A
1	0	2761	A
31	9	65	A
1	0	2791	U
1	0	1080	C

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	0	2587	1	14,22,23	1.00	1 (7%)	14,31,34	1.17	1 (7%)
1	UR3	0	2619	1	14,22,23	0.77	0	15,32,35	0.62	0
1	OMG	0	2588	1	18,26,27	1.11	2 (11%)	20,38,41	2.59	4 (20%)
1	1MA	0	628	1,34	15,25,26	0.77	0	15,37,40	1.40	1 (6%)
1	PSU	0	2621	1	17,21,22	1.59	3 (17%)	20,30,33	5.45	4 (20%)

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
1	OMU	0	2587	1	-	0/7/27/28	0/2/2/2
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	1MA	0	628	1,34	-	0/3/25/26	0/3/3/3
1	PSU	0	2621	1	-	0/7/25/26	0/2/2/2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C5-C1'	-5.09	1.47	1.52
1	0	2588	OMG	C6-N1	3.65	1.39	1.33
1	0	2621	PSU	C4-N3	2.71	1.37	1.33
1	0	2587	OMU	C4-N3	2.41	1.37	1.33
1	0	2588	OMG	C8-N7	-2.22	1.30	1.34

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.32	114.66	128.43
1	0	2621	PSU	C4-N3-C2	14.41	127.31	115.14
1	0	2588	OMG	C5-C6-N1	-8.57	111.72	123.43
1	0	2621	PSU	C5-C4-N3	-8.26	114.71	125.36
1	0	2588	OMG	C6-N1-C2	5.76	125.08	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0
1	0	628	1MA	1	0
1	0	2621	PSU	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 304 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	$\# Z > 2$
37	MUL	0	9101	-	36,36,36	1.47	5 (13%)	54,55,55	2.14	17 (31%)

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
37	MUL	0	9101	-	-	3/18/79/79	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	0	9101	MUL	C12-C19	-5.30	1.39	1.52
37	0	9101	MUL	C5-C14	-2.91	1.53	1.56
37	0	9101	MUL	C12-C11	-2.86	1.53	1.55
37	0	9101	MUL	C10-C11	-2.81	1.53	1.56
37	0	9101	MUL	C9-C10	-2.07	1.53	1.56

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	MUL	C13-C14-C5	-6.20	109.94	116.31
37	0	9101	MUL	O3-C21-C22	5.49	119.56	110.32
37	0	9101	MUL	C18-C12-C13	5.00	109.33	105.60
37	0	9101	MUL	C14-O3-C21	-3.79	110.79	117.92
37	0	9101	MUL	C8-C9-C4	3.49	111.41	106.56

There are no chirality outliers.

All (3) torsion outliers are listed below:

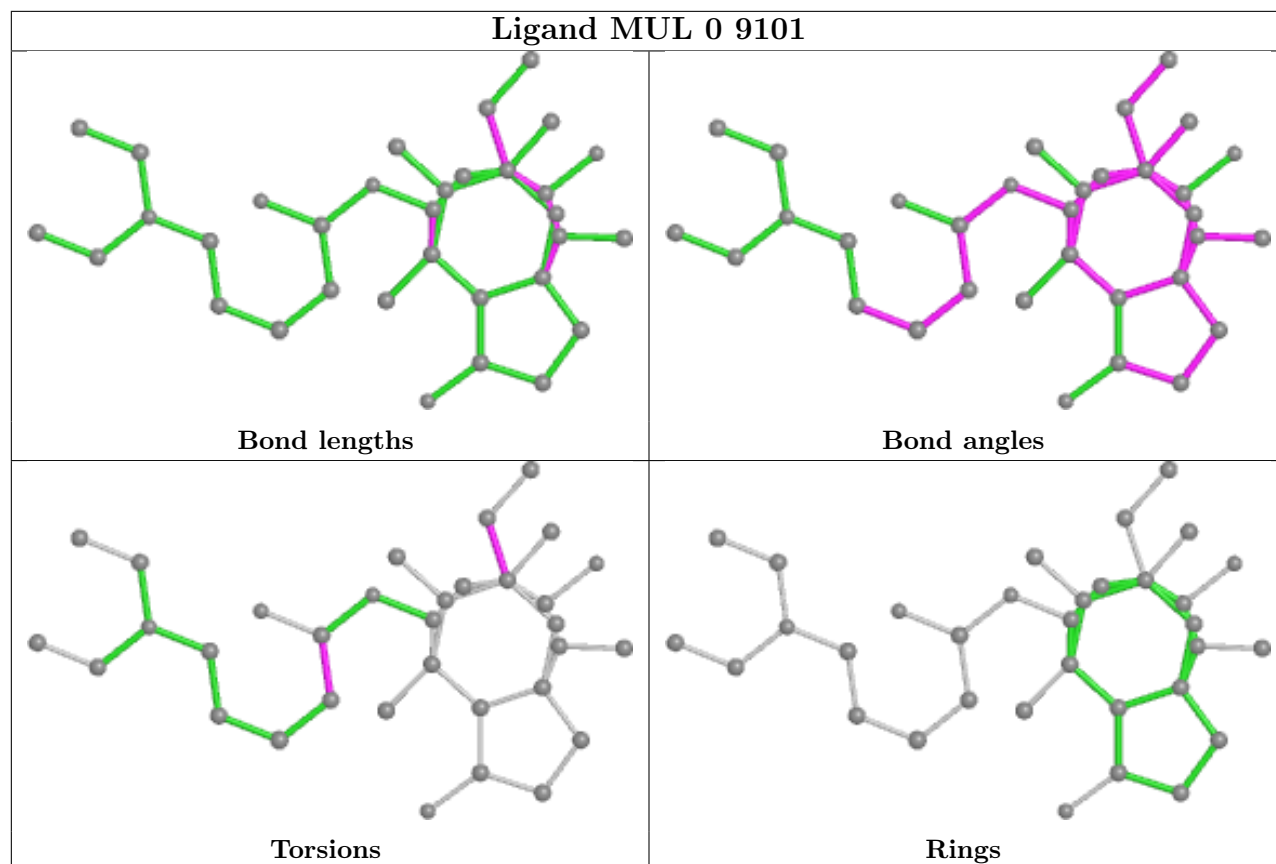
Mol	Chain	Res	Type	Atoms
37	0	9101	MUL	C13-C12-C19-C20
37	0	9101	MUL	O4-C21-C22-S1
37	0	9101	MUL	O3-C21-C22-S1

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	MUL	17	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	0	2749/2923 (94%)	-0.66	3 (0%) 95 95	29, 74, 140, 200	0
2	A	237/237 (100%)	0.04	9 (3%) 40 26	43, 97, 143, 167	0
3	B	337/337 (100%)	-0.40	1 (0%) 94 92	40, 86, 129, 148	0
4	C	246/246 (100%)	-0.39	2 (0%) 86 78	41, 72, 103, 112	0
5	D	140/177 (79%)	1.10	37 (26%) 0 0	118, 160, 184, 191	0
6	E	172/172 (100%)	-0.13	3 (1%) 70 57	76, 104, 134, 146	0
7	F	119/119 (100%)	0.30	8 (6%) 17 10	74, 113, 153, 166	0
8	G	29/348 (8%)	1.00	6 (20%) 1 1	118, 140, 146, 150	0
9	H	160/177 (90%)	0.54	15 (9%) 8 4	77, 104, 146, 162	0
10	I	70/70 (100%)	1.85	32 (45%) 0 0	173, 199, 200, 200	0
11	J	142/142 (100%)	-0.28	0 100 100	55, 80, 104, 123	0
12	K	132/132 (100%)	-0.20	2 (1%) 73 61	54, 79, 112, 118	0
13	L	145/165 (87%)	0.66	26 (17%) 1 1	62, 121, 171, 175	0
14	M	194/194 (100%)	0.09	17 (8%) 10 5	49, 70, 145, 160	0
15	N	186/186 (100%)	0.48	13 (6%) 16 9	82, 118, 178, 187	0
16	O	115/115 (100%)	-0.44	0 100 100	66, 87, 105, 111	0
17	P	143/143 (100%)	-0.22	2 (1%) 75 63	65, 88, 117, 124	0
18	Q	95/95 (100%)	0.02	4 (4%) 36 23	67, 87, 110, 117	0
19	R	150/150 (100%)	-0.48	0 100 100	47, 72, 103, 112	0
20	S	81/81 (100%)	-0.05	2 (2%) 57 43	68, 93, 114, 130	0
21	T	119/119 (100%)	0.23	10 (8%) 11 6	69, 92, 136, 155	0
22	U	53/53 (100%)	0.09	1 (1%) 66 53	94, 114, 136, 145	0
23	V	65/65 (100%)	0.23	3 (4%) 32 20	79, 112, 164, 170	0
24	W	154/154 (100%)	-0.22	2 (1%) 77 65	56, 78, 110, 120	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/82 (100%)	0.11	6 (7%) 15 9	63, 92, 125, 135	0
26	Y	142/142 (100%)	-0.33	2 (1%) 75 63	45, 73, 109, 134	0
27	Z	73/73 (100%)	5.32	53 (72%) 0 0	149, 179, 191, 194	0
28	1	56/56 (100%)	-0.31	0 100 100	42, 53, 66, 76	0
29	2	46/50 (92%)	0.26	4 (8%) 10 5	48, 95, 145, 146	0
30	3	92/92 (100%)	6.09	79 (85%) 0 0	163, 185, 199, 200	0
31	9	122/122 (100%)	-0.83	0 100 100	66, 114, 143, 191	0
All	All	6646/7217 (92%)	-0.13	342 (5%) 28 16	29, 85, 168, 200	0

The worst 5 of 342 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
27	Z	34	SER	29.8
30	3	82	GLY	26.5
27	Z	35	SER	24.8
30	3	37	ASP	18.0
30	3	41	GLU	16.7

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	1MA	0	628	23/24	0.97	0.15	49,56,63,64	0
1	OMG	0	2588	24/25	0.97	0.14	50,54,58,60	0
1	PSU	0	2621	20/21	0.97	0.20	59,63,65,66	0
1	UR3	0	2619	21/22	0.98	0.15	61,65,71,72	0
1	OMU	0	2587	21/22	0.98	0.12	60,63,64,64	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
36	SR	0	8997	1/1	-0.10	5.65	200,200,200,200	0
36	SR	0	8971	1/1	0.15	0.12	200,200,200,200	0
34	NA	0	8522	1/1	0.21	0.13	87,87,87,87	0
34	NA	S	8510	1/1	0.40	0.30	69,69,69,69	0
34	NA	0	8506	1/1	0.47	0.60	105,105,105,105	0
34	NA	0	8525	1/1	0.53	0.33	92,92,92,92	0
34	NA	0	8524	1/1	0.54	0.38	47,47,47,47	0
36	SR	B	8987	1/1	0.55	0.82	200,200,200,200	0
32	MG	0	8036	1/1	0.58	0.21	82,82,82,82	0
34	NA	0	8505	1/1	0.59	0.45	56,56,56,56	0
34	NA	0	8553	1/1	0.61	0.20	81,81,81,81	0
34	NA	0	8554	1/1	0.61	0.38	71,71,71,71	0
36	SR	0	8998	1/1	0.62	0.63	169,169,169,169	0
34	NA	9	8572	1/1	0.62	0.32	88,88,88,88	0
32	MG	0	8068	1/1	0.64	0.08	49,49,49,49	0
34	NA	0	8549	1/1	0.64	0.17	83,83,83,83	0
34	NA	0	8556	1/1	0.64	0.80	95,95,95,95	0
32	MG	0	8092	1/1	0.66	0.12	53,53,53,53	0
36	SR	J	8986	1/1	0.66	1.51	200,200,200,200	0
32	MG	0	8090	1/1	0.67	0.93	81,81,81,81	0
36	SR	A	8930	1/1	0.67	0.24	133,133,133,133	0
36	SR	0	8991	1/1	0.68	0.09	190,190,190,190	0
36	SR	0	8958	1/1	0.69	0.07	150,150,150,150	0
36	SR	0	8962	1/1	0.69	0.15	155,155,155,155	0
32	MG	0	8049	1/1	0.69	0.20	61,61,61,61	0
34	NA	0	8564	1/1	0.70	0.57	95,95,95,95	0
34	NA	0	8528	1/1	0.71	0.49	80,80,80,80	0
35	CL	3	8804	1/1	0.73	0.15	96,96,96,96	0
34	NA	0	8501	1/1	0.73	0.22	41,41,41,41	0
36	SR	0	8957	1/1	0.74	0.24	200,200,200,200	0
36	SR	0	8916	1/1	0.74	0.08	129,129,129,129	0
36	SR	0	8994	1/1	0.75	0.72	200,200,200,200	0
34	NA	Q	8540	1/1	0.75	0.29	92,92,92,92	0
32	MG	9	8074	1/1	0.76	0.13	127,127,127,127	0
34	NA	0	8527	1/1	0.76	0.24	60,60,60,60	0
36	SR	0	8922	1/1	0.77	0.47	190,190,190,190	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	0	8508	1/1	0.77	0.99	70,70,70,70	0
34	NA	9	8543	1/1	0.77	0.17	57,57,57,57	0
32	MG	0	8044	1/1	0.77	0.11	49,49,49,49	0
32	MG	0	8077	1/1	0.77	0.16	47,47,47,47	0
32	MG	0	8081	1/1	0.77	0.45	104,104,104,104	0
36	SR	9	9003	1/1	0.77	0.06	200,200,200,200	0
34	NA	0	8509	1/1	0.78	0.49	66,66,66,66	0
34	NA	0	8568	1/1	0.78	0.57	51,51,51,51	0
34	NA	0	8529	1/1	0.78	0.11	49,49,49,49	0
36	SR	0	8936	1/1	0.78	0.07	109,109,109,109	0
35	CL	N	8807	1/1	0.79	0.38	134,134,134,134	0
36	SR	0	8947	1/1	0.79	0.60	200,200,200,200	0
34	NA	0	8502	1/1	0.80	0.19	51,51,51,51	0
34	NA	0	8566	1/1	0.80	0.89	51,51,51,51	0
34	NA	R	8575	1/1	0.80	0.50	96,96,96,96	0
36	SR	0	9006	1/1	0.81	0.49	200,200,200,200	0
32	MG	0	8061	1/1	0.81	0.30	42,42,42,42	0
32	MG	0	8073	1/1	0.81	0.69	110,110,110,110	0
34	NA	0	8550	1/1	0.81	0.19	98,98,98,98	0
36	SR	0	8985	1/1	0.81	0.04	173,173,173,173	0
34	NA	0	8560	1/1	0.82	0.29	64,64,64,64	0
36	SR	0	8979	1/1	0.82	0.10	200,200,200,200	0
34	NA	0	8533	1/1	0.82	0.21	68,68,68,68	0
36	SR	0	8974	1/1	0.83	0.42	191,191,191,191	0
36	SR	0	8977	1/1	0.83	0.14	197,197,197,197	0
36	SR	0	8995	1/1	0.83	0.25	128,128,128,128	0
34	NA	0	8514	1/1	0.83	0.27	61,61,61,61	0
34	NA	0	8545	1/1	0.83	0.31	40,40,40,40	0
32	MG	0	8066	1/1	0.84	0.93	70,70,70,70	0
34	NA	0	8562	1/1	0.84	1.23	85,85,85,85	0
35	CL	0	8805	1/1	0.84	0.39	97,97,97,97	0
34	NA	R	8532	1/1	0.85	0.10	57,57,57,57	0
36	SR	0	9007	1/1	0.85	0.78	180,180,180,180	0
34	NA	0	8552	1/1	0.85	0.31	68,68,68,68	0
36	SR	A	8993	1/1	0.85	0.04	177,177,177,177	0
34	NA	0	8571	1/1	0.85	0.26	89,89,89,89	0
34	NA	0	8531	1/1	0.85	0.27	42,42,42,42	0
36	SR	0	8989	1/1	0.85	0.26	196,196,196,196	0
32	MG	0	8069	1/1	0.86	0.55	68,68,68,68	0
34	NA	0	8511	1/1	0.86	0.21	64,64,64,64	0
36	SR	0	9004	1/1	0.86	0.46	200,200,200,200	0
35	CL	Y	8820	1/1	0.86	0.06	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8047	1/1	0.86	0.37	70,70,70,70	0
34	NA	0	8573	1/1	0.87	0.19	92,92,92,92	0
36	SR	0	8992	1/1	0.87	0.10	149,149,149,149	0
36	SR	0	8975	1/1	0.87	0.04	158,158,158,158	0
36	SR	0	8927	1/1	0.87	0.16	172,172,172,172	0
34	NA	0	8565	1/1	0.87	1.16	106,106,106,106	0
32	MG	0	8055	1/1	0.87	0.28	67,67,67,67	0
36	SR	0	8973	1/1	0.87	0.17	134,134,134,134	0
36	SR	0	8960	1/1	0.88	0.11	174,174,174,174	0
36	SR	0	8984	1/1	0.88	0.06	139,139,139,139	0
34	NA	0	8547	1/1	0.88	0.91	81,81,81,81	0
34	NA	M	8539	1/1	0.88	0.12	34,34,34,34	0
34	NA	0	8537	1/1	0.88	0.16	43,43,43,43	0
35	CL	0	8811	1/1	0.88	0.61	99,99,99,99	0
35	CL	0	8822	1/1	0.88	1.36	94,94,94,94	0
36	SR	H	8972	1/1	0.88	0.15	157,157,157,157	0
36	SR	0	8976	1/1	0.88	0.22	185,185,185,185	0
36	SR	9	8980	1/1	0.88	0.05	192,192,192,192	0
36	SR	0	8959	1/1	0.88	0.15	194,194,194,194	0
36	SR	0	8910	1/1	0.89	0.12	113,113,113,113	0
32	MG	0	8039	1/1	0.89	0.27	76,76,76,76	0
34	NA	0	8536	1/1	0.89	0.13	72,72,72,72	0
32	MG	0	8043	1/1	0.89	0.13	55,55,55,55	0
34	NA	0	8558	1/1	0.89	0.60	50,50,50,50	0
36	SR	0	8996	1/1	0.89	0.40	200,200,200,200	0
36	SR	0	8938	1/1	0.89	0.07	200,200,200,200	0
32	MG	0	8072	1/1	0.89	0.08	37,37,37,37	0
36	SR	0	8988	1/1	0.89	0.11	181,181,181,181	0
34	NA	0	8559	1/1	0.90	0.32	94,94,94,94	0
34	NA	0	8518	1/1	0.90	0.40	82,82,82,82	0
36	SR	0	8968	1/1	0.90	0.11	181,181,181,181	0
36	SR	0	8982	1/1	0.90	1.70	200,200,200,200	0
32	MG	0	8033	1/1	0.90	0.26	56,56,56,56	0
36	SR	F	9005	1/1	0.90	0.13	154,154,154,154	0
35	CL	0	8812	1/1	0.90	0.09	58,58,58,58	0
34	NA	0	8544	1/1	0.90	0.17	68,68,68,68	0
36	SR	0	9001	1/1	0.90	0.09	189,189,189,189	0
34	NA	0	8515	1/1	0.90	0.22	45,45,45,45	0
36	SR	0	8970	1/1	0.91	0.06	150,150,150,150	0
34	NA	J	8538	1/1	0.91	0.14	45,45,45,45	0
36	SR	L	8969	1/1	0.91	0.93	198,198,198,198	0
36	SR	0	8914	1/1	0.91	0.32	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	0	8953	1/1	0.91	0.25	185,185,185,185	0
32	MG	0	8087	1/1	0.92	0.18	20,20,20,20	0
36	SR	3	8999	1/1	0.92	0.18	160,160,160,160	0
36	SR	0	8928	1/1	0.92	0.05	164,164,164,164	0
32	MG	0	8004	1/1	0.92	0.15	32,32,32,32	0
32	MG	0	8079	1/1	0.93	0.20	63,63,63,63	0
35	CL	M	8818	1/1	0.93	0.09	73,73,73,73	0
32	MG	0	8058	1/1	0.93	0.06	25,25,25,25	0
34	NA	0	8523	1/1	0.93	0.15	58,58,58,58	0
32	MG	0	8001	1/1	0.93	0.11	28,28,28,28	0
32	MG	0	8053	1/1	0.93	0.05	57,57,57,57	0
36	SR	0	8944	1/1	0.93	0.17	171,171,171,171	0
36	SR	0	8945	1/1	0.93	0.04	111,111,111,111	0
32	MG	0	8010	1/1	0.93	0.18	35,35,35,35	0
36	SR	0	8915	1/1	0.93	0.07	125,125,125,125	0
34	NA	0	8541	1/1	0.94	0.14	46,46,46,46	0
36	SR	0	8946	1/1	0.94	0.26	138,138,138,138	0
34	NA	0	8516	1/1	0.94	0.26	26,26,26,26	0
36	SR	0	8951	1/1	0.94	0.19	177,177,177,177	0
32	MG	2	8060	1/1	0.94	0.09	56,56,56,56	0
36	SR	0	8955	1/1	0.94	0.17	199,199,199,199	0
32	MG	0	8067	1/1	0.94	0.43	42,42,42,42	0
33	K	0	8402	1/1	0.94	0.21	67,67,67,67	0
32	MG	0	8032	1/1	0.94	0.08	64,64,64,64	0
34	NA	0	8574	1/1	0.94	0.80	67,67,67,67	0
36	SR	0	8901	1/1	0.94	0.12	89,89,89,89	0
36	SR	0	8963	1/1	0.94	0.15	135,135,135,135	0
36	SR	0	8967	1/1	0.94	0.07	157,157,157,157	0
34	NA	0	8551	1/1	0.94	0.16	81,81,81,81	0
32	MG	0	8031	1/1	0.94	0.34	71,71,71,71	0
32	MG	0	8082	1/1	0.94	0.41	86,86,86,86	0
32	MG	0	8085	1/1	0.94	0.13	83,83,83,83	0
32	MG	0	8071	1/1	0.94	0.12	50,50,50,50	0
36	SR	0	8924	1/1	0.94	0.17	138,138,138,138	0
32	MG	0	8089	1/1	0.94	0.29	72,72,72,72	0
32	MG	0	8040	1/1	0.94	0.32	100,100,100,100	0
36	SR	3	8932	1/1	0.94	0.29	149,149,149,149	0
32	MG	0	8035	1/1	0.94	0.12	47,47,47,47	0
35	CL	0	8803	1/1	0.94	0.08	66,66,66,66	0
32	MG	T	8057	1/1	0.94	0.03	67,67,67,67	0
37	MUL	0	9101	34/34	0.94	0.26	85,87,104,104	0
35	CL	R	8806	1/1	0.95	0.17	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	A	8929	1/1	0.95	0.17	157,157,157,157	0
32	MG	0	8088	1/1	0.95	0.05	39,39,39,39	0
32	MG	0	8038	1/1	0.95	0.12	81,81,81,81	0
36	SR	0	8954	1/1	0.95	0.12	122,122,122,122	0
32	MG	0	8021	1/1	0.95	0.10	28,28,28,28	0
36	SR	0	8908	1/1	0.95	0.06	109,109,109,109	0
35	CL	0	8815	1/1	0.95	0.24	90,90,90,90	0
36	SR	0	8940	1/1	0.95	0.03	117,117,117,117	0
36	SR	1	8913	1/1	0.95	0.17	97,97,97,97	0
34	NA	0	8526	1/1	0.95	0.27	52,52,52,52	0
32	MG	0	8015	1/1	0.95	0.10	25,25,25,25	0
36	SR	0	8981	1/1	0.95	0.10	151,151,151,151	0
32	MG	0	8037	1/1	0.95	0.29	84,84,84,84	0
36	SR	0	8966	1/1	0.95	0.10	110,110,110,110	0
34	NA	0	8542	1/1	0.96	0.52	51,51,51,51	0
32	MG	0	8005	1/1	0.96	0.27	30,30,30,30	0
34	NA	0	8561	1/1	0.96	0.36	73,73,73,73	0
32	MG	0	8003	1/1	0.96	0.16	31,31,31,31	0
32	MG	0	8029	1/1	0.96	0.12	54,54,54,54	0
34	NA	0	8548	1/1	0.96	0.25	52,52,52,52	0
32	MG	B	8042	1/1	0.96	0.08	67,67,67,67	0
34	NA	0	8567	1/1	0.96	0.21	58,58,58,58	0
36	SR	0	8964	1/1	0.96	0.09	149,149,149,149	0
34	NA	0	8530	1/1	0.96	0.31	49,49,49,49	0
35	CL	0	8813	1/1	0.96	0.15	68,68,68,68	0
36	SR	0	8934	1/1	0.96	0.09	114,114,114,114	0
35	CL	0	8814	1/1	0.96	0.41	67,67,67,67	0
34	NA	0	8521	1/1	0.96	0.11	34,34,34,34	0
32	MG	0	8065	1/1	0.96	0.14	41,41,41,41	0
36	SR	B	8950	1/1	0.96	0.28	151,151,151,151	0
36	SR	0	8941	1/1	0.96	0.31	143,143,143,143	0
36	SR	0	8942	1/1	0.96	0.08	129,129,129,129	0
36	SR	0	8943	1/1	0.96	0.17	99,99,99,99	0
35	CL	L	8810	1/1	0.96	0.24	86,86,86,86	0
34	NA	0	8535	1/1	0.96	0.54	45,45,45,45	0
34	NA	C	8503	1/1	0.96	0.32	39,39,39,39	0
36	SR	1	8952	1/1	0.96	0.19	81,81,81,81	0
32	MG	Y	8086	1/1	0.96	0.04	55,55,55,55	0
36	SR	0	8983	1/1	0.96	0.21	185,185,185,185	0
36	SR	0	8949	1/1	0.96	0.10	120,120,120,120	0
32	MG	0	8014	1/1	0.96	0.12	30,30,30,30	0
32	MG	0	8041	1/1	0.96	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
38	CD	O	8705	1/1	0.96	0.03	115,115,115,115	0
32	MG	0	8063	1/1	0.97	0.15	67,67,67,67	0
32	MG	0	8064	1/1	0.97	0.20	48,48,48,48	0
34	NA	0	8563	1/1	0.97	0.18	74,74,74,74	0
32	MG	0	8027	1/1	0.97	0.05	30,30,30,30	0
36	SR	0	8917	1/1	0.97	0.14	121,121,121,121	0
36	SR	0	8919	1/1	0.97	0.17	194,194,194,194	0
36	SR	0	8920	1/1	0.97	0.11	132,132,132,132	0
36	SR	0	9000	1/1	0.97	0.23	200,200,200,200	0
36	SR	0	8921	1/1	0.97	0.09	90,90,90,90	0
34	NA	0	8546	1/1	0.97	1.32	69,69,69,69	0
32	MG	0	8008	1/1	0.97	0.14	15,15,15,15	0
32	MG	0	8009	1/1	0.97	0.21	28,28,28,28	0
32	MG	0	8052	1/1	0.97	0.04	40,40,40,40	0
36	SR	0	8933	1/1	0.97	0.04	122,122,122,122	0
32	MG	0	8007	1/1	0.97	0.17	10,10,10,10	0
32	MG	0	8024	1/1	0.97	0.14	58,58,58,58	0
35	CL	A	8809	1/1	0.97	0.67	96,96,96,96	0
35	CL	B	8819	1/1	0.97	0.76	68,68,68,68	0
35	CL	J	8801	1/1	0.97	0.21	90,90,90,90	0
35	CL	J	8821	1/1	0.97	0.16	70,70,70,70	0
36	SR	0	8978	1/1	0.97	0.04	130,130,130,130	0
32	MG	0	8034	1/1	0.97	0.30	43,43,43,43	0
32	MG	0	8059	1/1	0.97	0.12	40,40,40,40	0
34	NA	0	8534	1/1	0.97	0.22	45,45,45,45	0
34	NA	0	8555	1/1	0.97	0.55	50,50,50,50	0
32	MG	0	8075	1/1	0.97	0.06	40,40,40,40	0
32	MG	0	8076	1/1	0.97	0.06	36,36,36,36	0
32	MG	0	8025	1/1	0.97	0.07	44,44,44,44	0
32	MG	0	8078	1/1	0.97	0.23	64,64,64,64	0
38	CD	Z	8703	1/1	0.97	0.14	155,155,155,155	0
38	CD	3	8704	1/1	0.97	0.41	176,176,176,176	0
36	SR	0	8939	1/1	0.98	0.05	145,145,145,145	0
34	NA	0	8517	1/1	0.98	0.20	30,30,30,30	0
35	CL	J	8802	1/1	0.98	0.08	100,100,100,100	0
34	NA	0	8569	1/1	0.98	0.17	72,72,72,72	0
34	NA	0	8570	1/1	0.98	0.11	65,65,65,65	0
36	SR	0	8990	1/1	0.98	0.19	111,111,111,111	0
32	MG	C	8012	1/1	0.98	0.21	19,19,19,19	0
34	NA	0	8520	1/1	0.98	0.19	57,57,57,57	0
35	CL	O	8808	1/1	0.98	0.30	98,98,98,98	0
32	MG	K	8054	1/1	0.98	0.12	32,32,32,32	0

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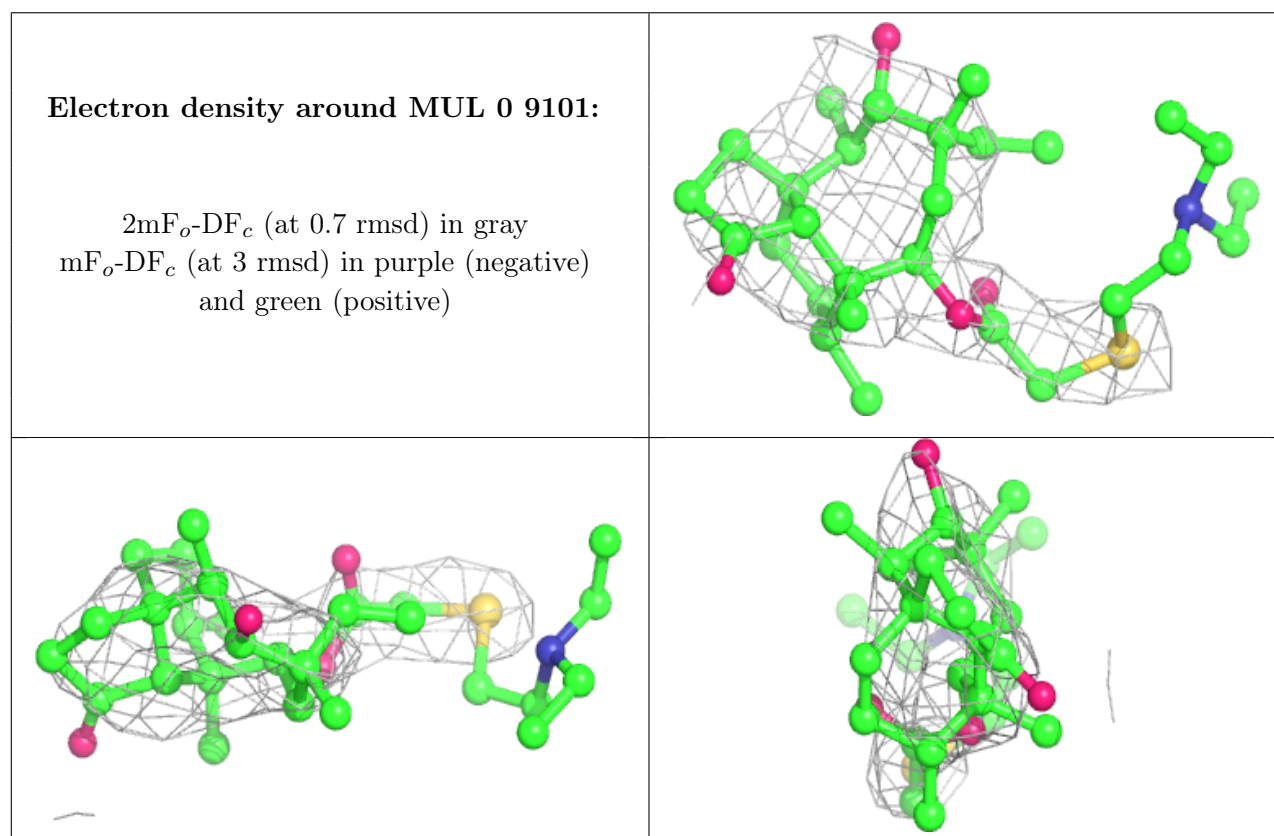
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	0	8056	1/1	0.98	0.07	47,47,47,47	0
32	MG	0	8080	1/1	0.98	0.52	98,98,98,98	0
32	MG	0	8002	1/1	0.98	0.17	26,26,26,26	0
36	SR	0	8902	1/1	0.98	0.13	63,63,63,63	0
36	SR	0	8903	1/1	0.98	0.19	62,62,62,62	0
36	SR	0	9002	1/1	0.98	0.09	188,188,188,188	0
36	SR	0	8956	1/1	0.98	0.23	178,178,178,178	0
32	MG	0	8070	1/1	0.98	0.39	54,54,54,54	0
36	SR	0	8909	1/1	0.98	0.07	89,89,89,89	0
36	SR	0	9008	1/1	0.98	0.16	99,99,99,99	0
32	MG	0	8006	1/1	0.98	0.12	62,62,62,62	0
36	SR	0	8911	1/1	0.98	0.13	109,109,109,109	0
32	MG	0	8046	1/1	0.98	0.21	48,48,48,48	0
32	MG	0	8016	1/1	0.98	0.16	38,38,38,38	0
32	MG	0	8011	1/1	0.98	0.21	18,18,18,18	0
34	NA	0	8557	1/1	0.98	0.07	71,71,71,71	0
32	MG	0	8022	1/1	0.98	0.13	29,29,29,29	0
34	NA	0	8507	1/1	0.98	0.27	39,39,39,39	0
32	MG	0	8091	1/1	0.98	0.18	42,42,42,42	0
32	MG	0	8023	1/1	0.98	0.15	21,21,21,21	0
36	SR	0	8923	1/1	0.98	0.17	120,120,120,120	0
32	MG	0	8093	1/1	0.98	0.10	40,40,40,40	0
34	NA	0	8512	1/1	0.98	0.30	49,49,49,49	0
34	NA	0	8513	1/1	0.98	0.23	63,63,63,63	0
35	CL	0	8816	1/1	0.98	0.71	86,86,86,86	0
32	MG	A	8050	1/1	0.98	0.19	52,52,52,52	0
36	SR	0	8935	1/1	0.98	0.05	106,106,106,106	0
38	CD	U	8701	1/1	0.98	0.04	104,104,104,104	0
32	MG	A	8051	1/1	0.98	0.28	90,90,90,90	0
32	MG	0	8013	1/1	0.98	0.04	21,21,21,21	0
36	SR	0	8948	1/1	0.99	0.08	104,104,104,104	0
36	SR	0	8905	1/1	0.99	0.27	70,70,70,70	0
36	SR	0	8925	1/1	0.99	0.13	105,105,105,105	0
36	SR	0	8926	1/1	0.99	0.16	145,145,145,145	0
36	SR	0	8906	1/1	0.99	0.19	65,65,65,65	0
36	SR	0	8907	1/1	0.99	0.16	63,63,63,63	0
36	SR	0	8931	1/1	0.99	0.10	123,123,123,123	0
32	MG	0	8020	1/1	0.99	0.11	52,52,52,52	0
32	MG	0	8083	1/1	0.99	0.08	59,59,59,59	0
32	MG	0	8084	1/1	0.99	0.16	50,50,50,50	0
32	MG	0	8017	1/1	0.99	0.07	29,29,29,29	0
36	SR	0	8937	1/1	0.99	0.17	108,108,108,108	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
36	SR	R	8912	1/1	0.99	0.23	106,106,106,106	0
36	SR	S	8961	1/1	0.99	0.10	127,127,127,127	0
32	MG	0	8026	1/1	0.99	0.04	32,32,32,32	0
32	MG	0	8048	1/1	0.99	0.31	38,38,38,38	0
36	SR	0	8965	1/1	0.99	0.17	135,135,135,135	0
34	NA	0	8519	1/1	0.99	0.18	44,44,44,44	0
35	CL	0	8817	1/1	0.99	0.11	63,63,63,63	0
36	SR	0	8918	1/1	0.99	0.13	84,84,84,84	0
32	MG	0	8018	1/1	0.99	0.18	42,42,42,42	0
32	MG	0	8062	1/1	0.99	0.28	47,47,47,47	0
32	MG	0	8028	1/1	0.99	0.13	14,14,14,14	0
32	MG	0	8019	1/1	0.99	0.16	10,10,10,10	0
38	CD	1	8702	1/1	0.99	0.13	68,68,68,68	0
36	SR	0	8904	1/1	0.99	0.16	64,64,64,64	0
32	MG	0	8030	1/1	1.00	0.48	60,60,60,60	0
34	NA	0	8504	1/1	1.00	0.09	22,22,22,22	0
32	MG	0	8045	1/1	1.00	0.12	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.