



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 04:57 pm BST

PDB ID : 3G6E  
Title : Co-crystal structure of Homoharringtonine bound to the large ribosomal subunit  
Authors : Gurel, G.; Blaha, G.; Moore, P.B.; Steitz, T.A.  
Deposited on : 2009-02-06  
Resolution : 2.70 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](mailto: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.

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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

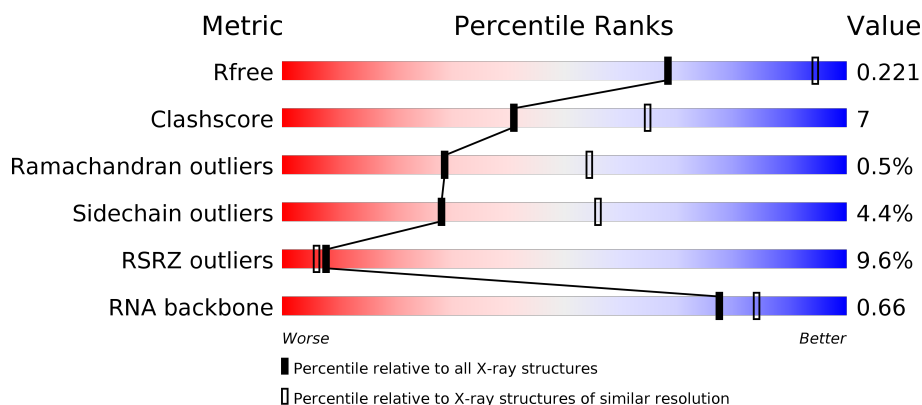
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)
RNA backbone	3102	1159 (3.00-2.40)

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  $\geq 3$ , 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>2%</div> <div> <div></div> <div>59%</div> <div>30%</div> <div>5%</div> <div>6%</div> </div> </div>
2	A	237	<div> <div>16%</div> <div> <div></div> <div>86%</div> <div>12%</div> <div>.</div> </div> </div>
3	B	337	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>12%</div> <div>.</div> </div> </div>
4	C	246	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>.</div> </div> </div>

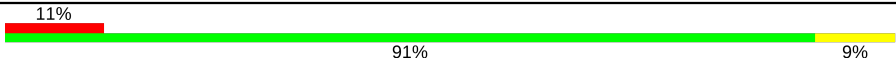

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Mol	Chain	Length	Quality of chain
5	D	177	
6	E	172	
7	F	119	
8	G	348	
9	H	177	
10	I	70	
11	J	142	
12	K	132	
13	L	165	
14	M	194	
15	N	186	
16	O	115	
17	P	143	
18	Q	95	
19	R	150	
20	S	81	
21	T	119	
22	U	53	
23	V	65	
24	W	154	
25	X	82	
26	Y	142	
27	Z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

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Mol	Chain	Length	Quality of chain
30	3	92	
31	9	122	

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	8030	-	-	-	X
34	NA	0	8522	-	-	-	X
34	NA	0	8546	-	-	-	X
34	NA	0	8561	-	-	-	X
34	NA	0	8562	-	-	-	X
36	SR	0	8913	-	-	-	X
36	SR	0	8923	-	-	-	X
36	SR	0	8933	-	-	-	X
36	SR	0	8934	-	-	-	X
36	SR	0	8957	-	-	-	X
36	SR	0	8974	-	-	-	X
36	SR	0	8976	-	-	-	X
36	SR	0	8982	-	-	-	X
36	SR	0	8994	-	-	-	X
36	SR	0	9004	-	-	-	X
36	SR	0	9006	-	-	-	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 99174 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 L10E.

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			
			950	568	180	202	0	0	0

- 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			
			411	244	75	87	5	0	0	0

- 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			
			500	304	94	101	1	0	0	0

- 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			
			1196	737	209	244	6	0	0	0

- 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			
			655	402	129	123	1	0	0	0

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

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

- 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			
			574	343	113	113	5	0	0	0

- 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	85	Total	Mg	0	0
			85	85		
32	9	2	Total	Mg	0	0
			2	2		
32	K	1	Total	Mg	0	0
			1	1		
32	B	1	Total	Mg	0	0
			1	1		
32	A	1	Total	Mg	0	0
			1	1		
32	T	1	Total	Mg	0	0
			1	1		
32	2	1	Total	Mg	0	0
			1	1		
32	Y	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	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	0	66	Total Na 66 66	0	0
34	J	1	Total Na 1 1	0	0
34	Q	1	Total Na 1 1	0	0
34	C	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	9	3	Total Na 3 3	0	0
34	S	1	Total Na 1 1	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	0	10	Total Cl 10 10	0	0
35	J	3	Total Cl 3 3	0	0
35	B	1	Total Cl 1 1	0	0
35	A	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
35	R	1	Total Cl 1 1	0	0
35	Y	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

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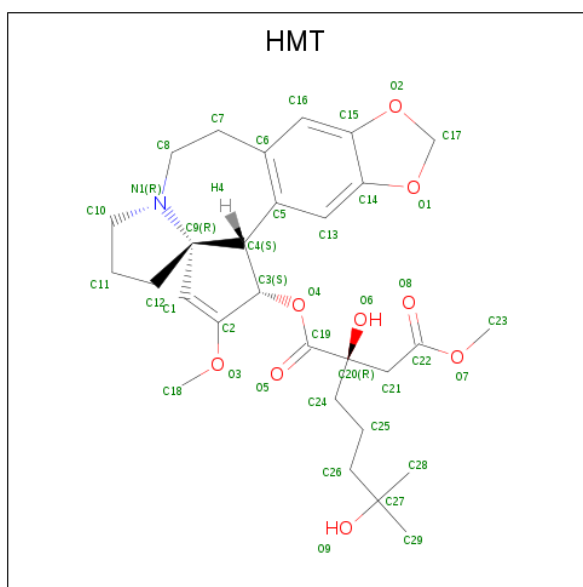
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	3	1	Total	Cl	0	0
			1	1		
35	M	1	Total	Cl	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
36	0	93	Total	Sr	0	0
			93	93		
36	J	1	Total	Sr	0	0
			1	1		
36	1	1	Total	Sr	0	0
			1	1		
36	B	2	Total	Sr	0	0
			2	2		
36	3	2	Total	Sr	0	0
			2	2		
36	A	3	Total	Sr	0	0
			3	3		
36	R	1	Total	Sr	0	0
			1	1		
36	9	3	Total	Sr	0	0
			3	3		
36	S	1	Total	Sr	0	0
			1	1		
36	F	1	Total	Sr	0	0
			1	1		

- Molecule 37 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano  
yl]cephalotaxine (three-letter code: HMT) (formula: C<sub>29</sub>H<sub>39</sub>NO<sub>9</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	0	1	Total	C	N	O	0	0
			39	29	1	9		

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

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

- Molecule 39 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	0	5969	Total	O	0	0
			5969	5969		
39	A	111	Total	O	0	0
			111	111		
39	B	138	Total	O	0	0
			138	138		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	C	169	Total 169	O 169	0	0
39	D	44	Total 44	O 44	0	0
39	E	45	Total 45	O 45	0	0
39	F	26	Total 26	O 26	0	0
39	G	17	Total 17	O 17	0	0
39	H	65	Total 65	O 65	0	0
39	I	6	Total 6	O 6	0	0
39	J	51	Total 51	O 51	0	0
39	K	59	Total 59	O 59	0	0
39	L	84	Total 84	O 84	0	0
39	M	119	Total 119	O 119	0	0
39	N	60	Total 60	O 60	0	0
39	O	37	Total 37	O 37	0	0
39	P	67	Total 67	O 67	0	0
39	Q	42	Total 42	O 42	0	0
39	R	81	Total 81	O 81	0	0
39	S	30	Total 30	O 30	0	0
39	T	34	Total 34	O 34	0	0
39	U	26	Total 26	O 26	0	0
39	V	10	Total 10	O 10	0	0
39	W	67	Total 67	O 67	0	0

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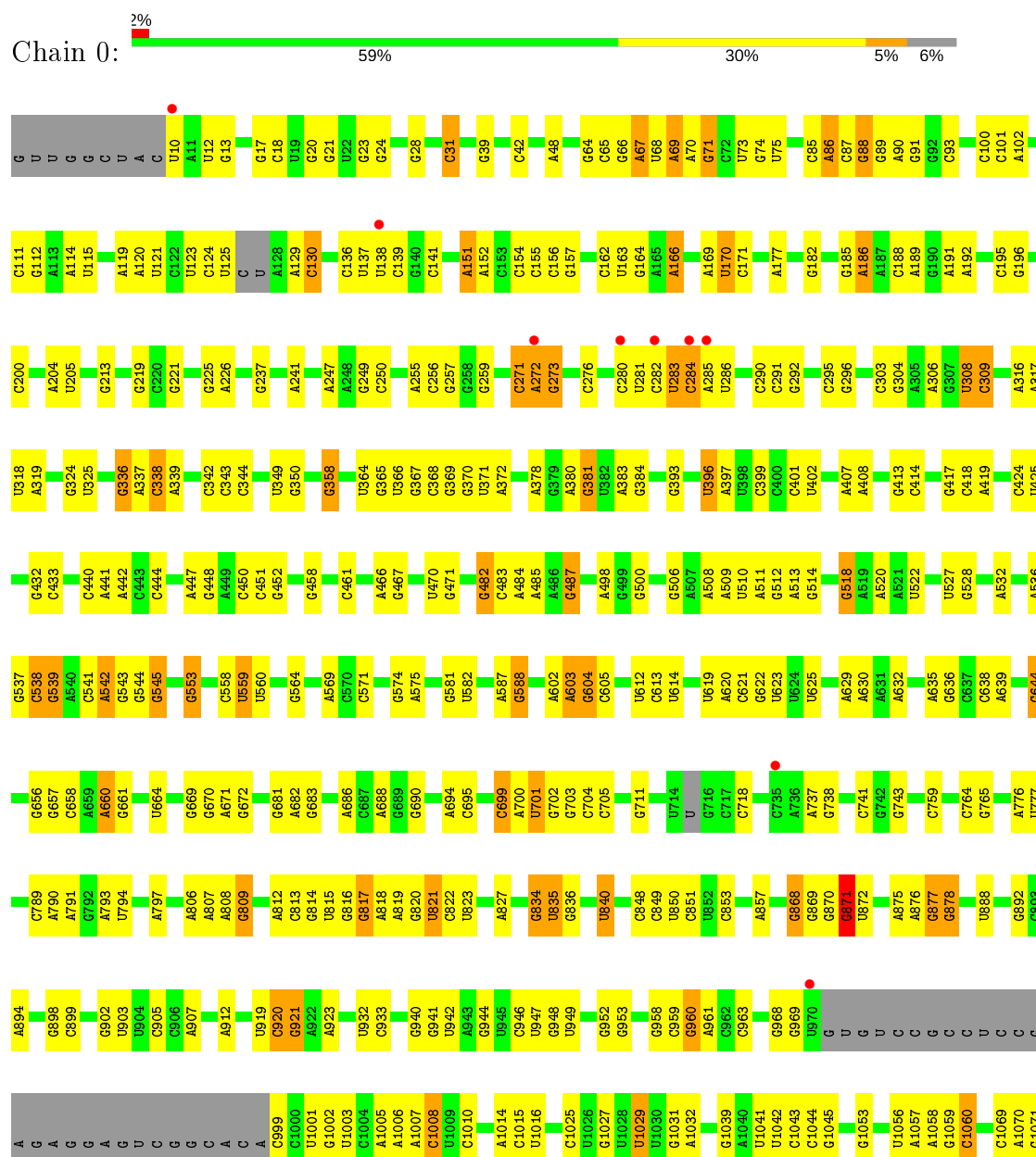
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	25	Total 25	O 25	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	32	Total 32	O 32	0	0
39	1	52	Total 52	O 52	0	0
39	2	44	Total 44	O 44	0	0
39	3	66	Total 66	O 66	0	0
39	9	151	Total 151	O 151	0	0

### 3 Residue-property plots [i](#)

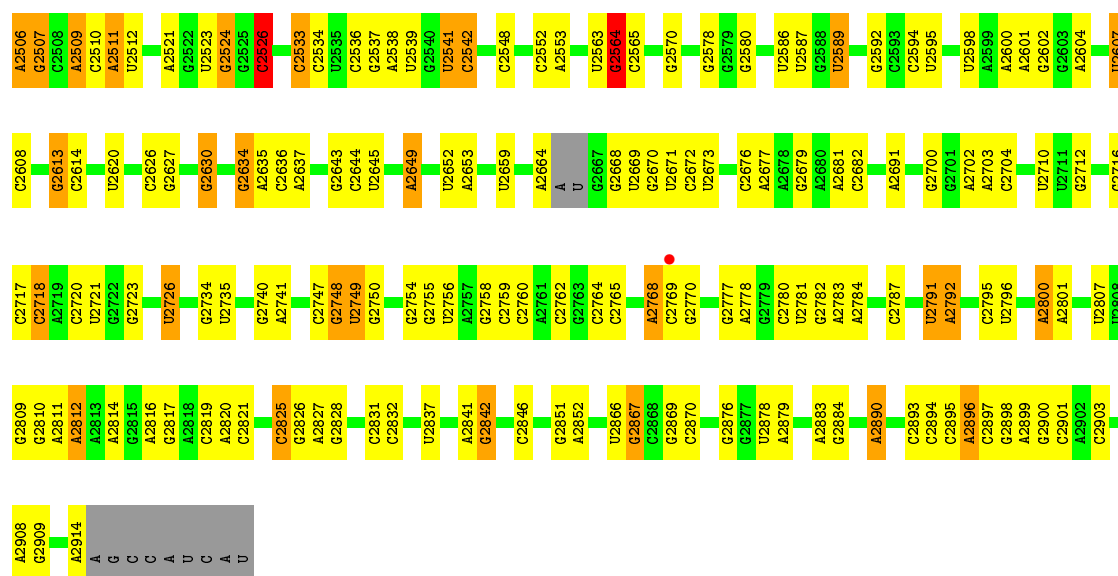
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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

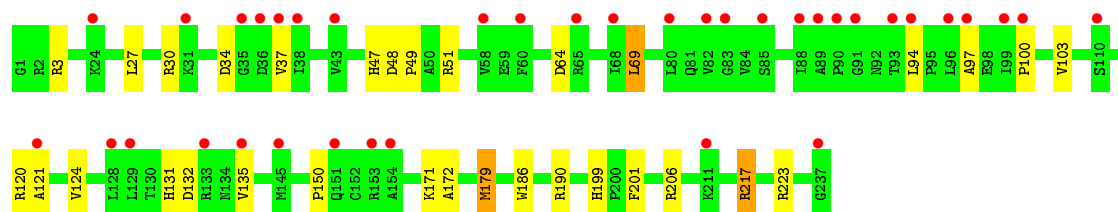
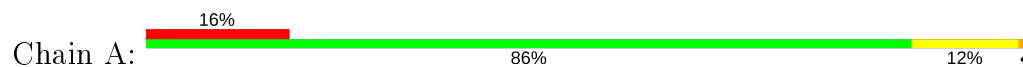


A2408	U2297	A	A1941	A1815	C1714	C1613	U1503	G1386	U1249	G1176	G1072
G2412	A2300	C	A1942	C1816	C1715	G1614	A1504	G1387	U1250	A1177	A1073
A2413	A2301	G	C1946	G1819	A1716	A1615	U1505	G1391	C1251	G1178	A1078
A2414	A2302	U	G1947	G1820	A1717	A1617	U1506	A1392		U1180	A1081
A2415	U2308	U	G1948	A1823	U1722	G1618	U1524	G1398	G1268	U1181	
G2416	C2309	C	G1949	C1830	G1723	G1619	G1525	A1399	G1269	C1182	A1088
		A	G1951	C1831	U1724	G1620	A1526	A1406		C1183	
U2419	C2313	A	U	C1834	C1725	G1621	A1527	A1407		C1184	
G2420	G2314	C	A	U1835	G1730	G1622	A1528	A1408	U1278	U1185	U1096
G2421	C2315	U	A	A1836	C1731	G1623	U1529	U1409		U1186	A1097
C2316	G2316	C	C	G1837	A1732	A1624	G1535	G1409	U1279	U1187	A1098
U2422	C2317	A	U	U1838	A1733	U1625	G1536	G1410		U1188	G1099
		G	A	A1839	A1734	G1626	C1537	A1413	C1289	A1189	
G2426	U2320	C	U	A1840	U1741	A1627	U1544	A1414	G1290	G1190	C1102
A2433	A2321	C	G	A1845	U1742	A1630	C1545	A1415	A1294	C1103	C1104
A2434		G	C	U1846	A1743	A1631		G1415	G1295	A1192	
U2435	G2338	U	C	A1847	C1750	A1632	U1548		G1299	U1198	U1109
	A	C	C	G1848	G1751	A1633		U1419	G1300	U1199	G1110
C2443	C	G	C	G1849	G1752	A1634	U1549	C1420		A1200	U1116
U2444	A	G	U1964	G1852	C1753	U1635	G1552	C1421	U1306	C1201	A1117
U2445	G	U	C1965	G1853	G1754	A1636	C1553	C1422	A1307	A1202	A1118
G2446	A	G	U1966	C1854	A1755	A1637	C1554	C1423	A1308	G1203	A1119
		A	U1967	G1855	G1756		G1555	G1424	U1309	U1120	
A2456	G2344	C		G1856		A1641	G1556	G1425	U1310	G1121	
U2457	A2345	U	G1971	A1857	C1762	A1642	U1569	C1426	U1205	U1222	
	C2346	G	U1972	C1858	C1763	A1643	U	A1427	A1328	A1207	A1123
G2462	C2348	A	A1973	A1858	U1766	A1644	G1569	G1439	G1329	G1208	
	G2338	U	G1974	G1863	U1767	A1645	U1561	U1440	U1330	C1209	G1129
A2465	A2353	A	C1975	G1867	A1768	A1654	C1562	G1441	U1331	G1210	U1130
G2466	A2354	G	G1976	G1868	U1769	A1655	U1563	G1442	C1332	G1211	
A2467	A2361	G	U1977	G1869	U1770	A1656	U1564	G1443	U1333	C1212	A1132
U2468	G2362	U	A1978	G1870	U1771		U1565	G1444	C1334	C1213	
A2469	G2363	C	U1979	G1871	G1772	C1666	A1573	U1445	G1340	G1214	G1137
G2470	A2364	C	U1980	G1872	G1773	A1667	C1574	U1446	A1341	A1215	
G2471	G2365	C	A1984	G1873	G1774	U1668	G1575		C1342	G1216	G1151
C2472		C	G1985	G1874	G1775	A1669	G1576	G1453	C1343	G1217	
U2473	A2369	C	U1986	G1875	G1776	A1670	U1577	U1454	G1344	U1218	A1154
A2474	G2370	C	U1987	G1876	A1778	U1671	U1578	C1455	G1351	U1219	G1155
C2475	A2371	G	A1988	G1877	A1779	C1672	U1579	U1456	A1352	U1220	
G2476	A2372	U	G2000	G1878	A1783	G1673	U1583	U1457	C1353	G1226	G1158
	U2373	A	G2001	G1879	U1784	A1681	C1584			G1159	
A2483		G	U2004	G1880	C1787	A1682	U1588	U1463	C1360	G1160	
U2484	G2379	C	G2005	G1881	C1788	A1683	G1589	C1464	C1229	A1161	
A2485	A2380	C	U2008	G1882	C1789	A1684	U1592	G1474	A1230	G1162	
A2486	C2381	G	G2009	G1883	U1791	C1686	C1593	C1365	U1234	U1163	
C2487	A2382	G	A2010	G1884	G1795	A1687	C1594	C1366	A1235	G1164	
A2490		C	A2011	G1885	A1796	C1688	G1595	U1477	A1236	G1165	
	G2385	C	U2012	G1886	A1797	G1689	U1596	U1478	U1237	A1166	
C2493	U2386	A	G2013	G1887	C1692	A1701	C1597	A1482	C1238	G1167	
U2494	U2387	C	G2014	G1888	G1693	U1702	A1598	C1375	U1169	U1170	
C2498	C2388	C	A2022	G1889	G1694	U1703		G1376	G1239	A1171	
U2499	U2389	C	U2023	G1890	G1695	G1800	C1602	G1377	A1242	G1172	
		A	U2024	G1891	G1696	G1801	U1603	G1378	G1243	G1173	
C2502	C2392	G	C2031	G1892	G1697	G1802	G1604	C1384	U1244	A1174	
A2503	A2401	C	U2032	G1893	G1698	G1803	G1605	G1385	A1245	G1175	
A2504	A2402	C	G2033	G1894	G1699	G1804					
G2505		A									

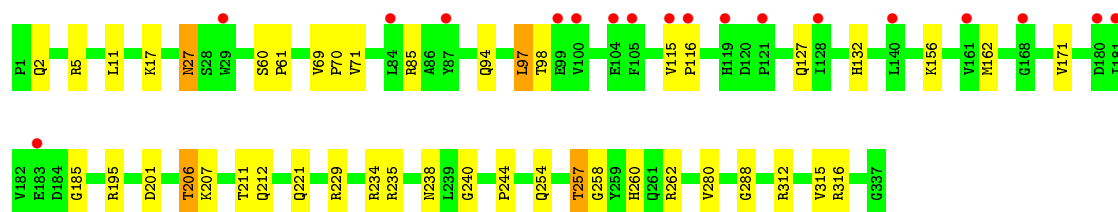
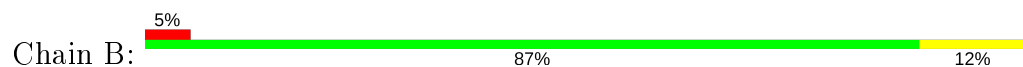




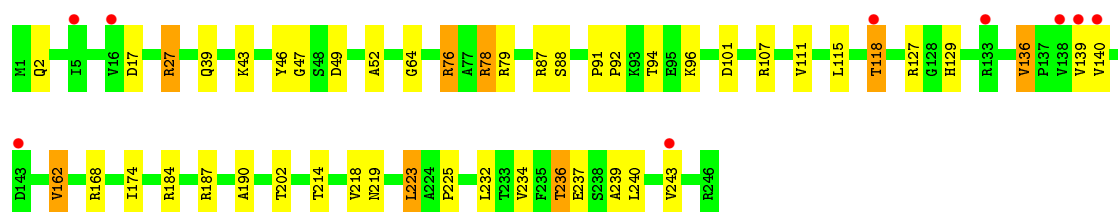
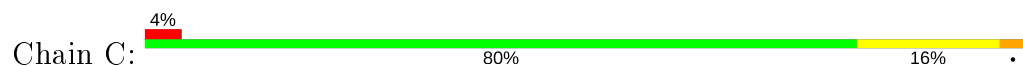
• Molecule 2: 50S ribosomal protein L2P



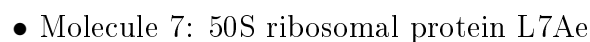
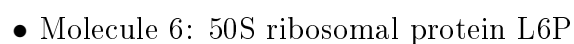
• Molecule 3: 50S ribosomal protein L3P



• Molecule 4: 50S ribosomal protein L4P

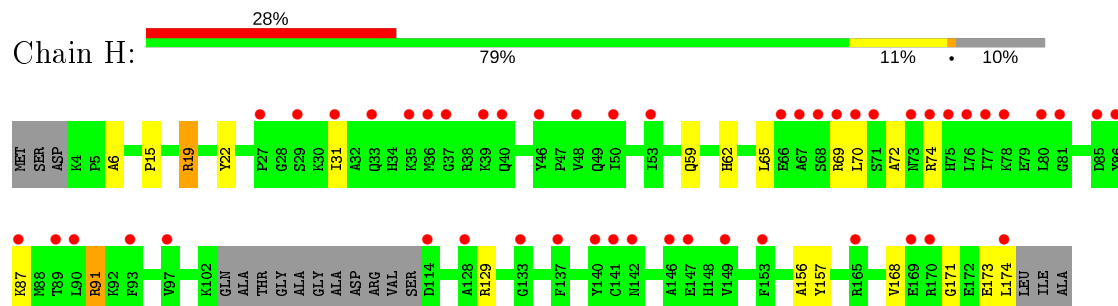


- Chain D:

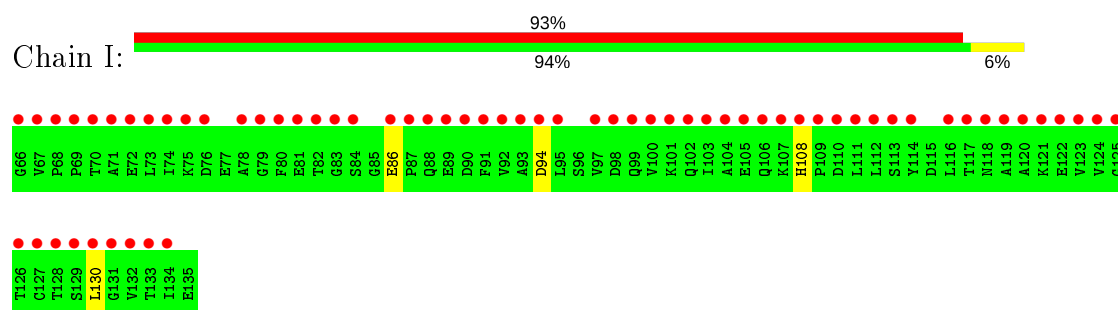


ALA	ANG	GLY	ASN	ASP	ALA	LYS	SER	LEU	GLN	ALA	ALA	ALA	ILE	GLU	ASP	PRO	GLU	VAL	VAL	PRO	LEU	ASP	ALA	GLN	GLY	ASP	ASP	GLU	ALA	THR	GLU	PRO
THR	ASP	ASP	GLN	ASP	ASP	ASP	THR	ALA	SER	GLU	ASP	ASP	ALA	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	ASP	GLN	GLY	ALA	ASP	ASP	ASP	THR	GLU	PRO

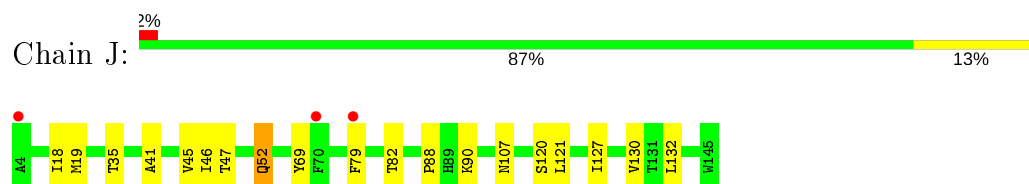
• Molecule 9: 50S ribosomal protein L10e



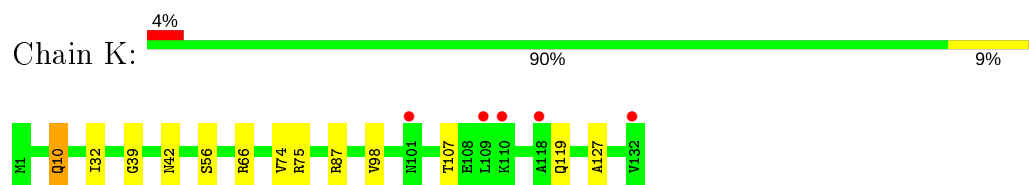
• Molecule 10: 50S ribosomal protein L11P



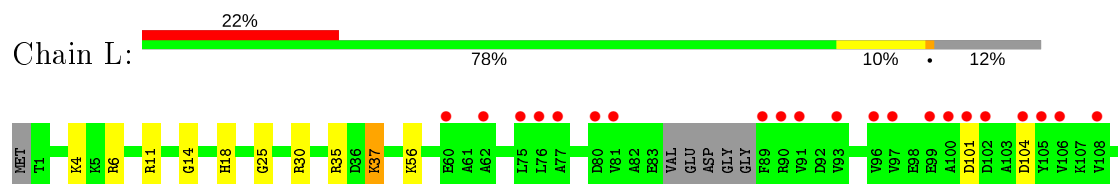
• Molecule 11: 50S ribosomal protein L13P

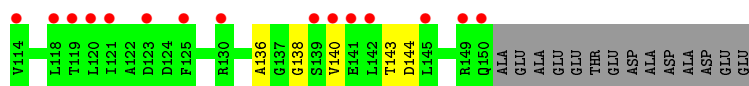


• Molecule 12: 50S ribosomal protein L14P

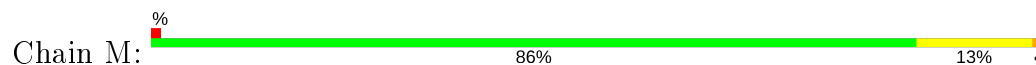


• Molecule 13: 50S ribosomal protein L15P

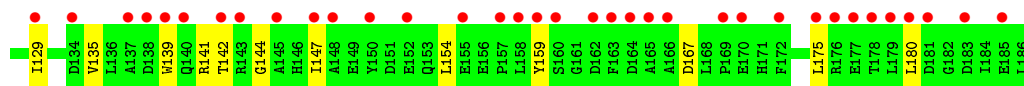
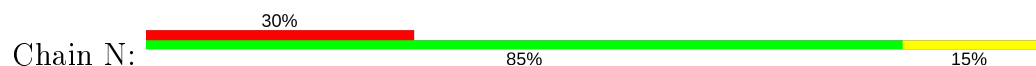




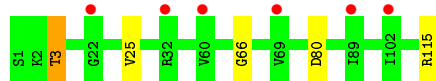
- Molecule 14: 50S ribosomal protein L15e



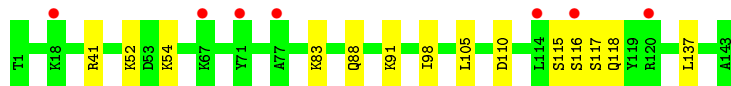
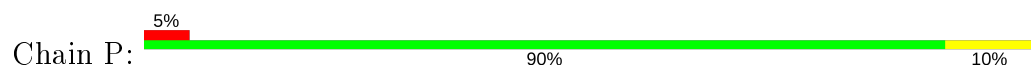
- Molecule 15: 50S ribosomal protein L18P



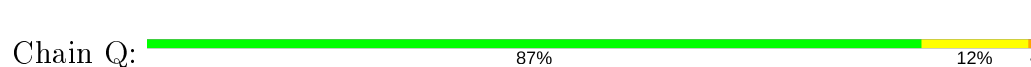
- Molecule 16: 50S ribosomal protein L18e



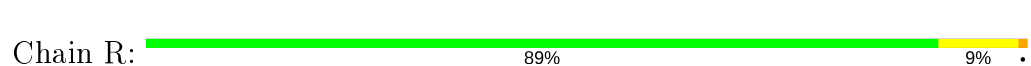
- Molecule 17: 50S ribosomal protein L19e



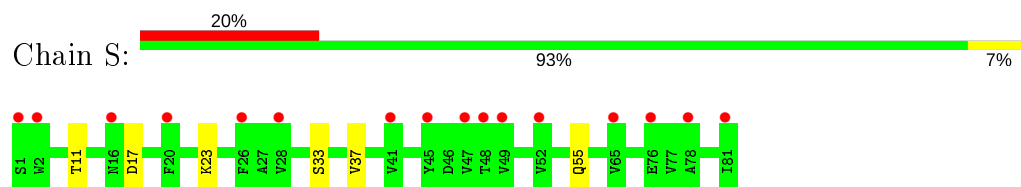
- Molecule 18: 50S ribosomal protein L21e



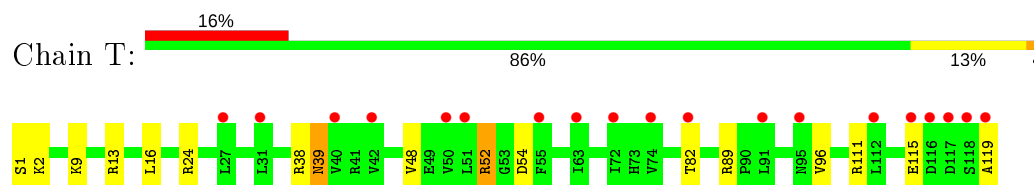
- Molecule 19: 50S ribosomal protein L22P



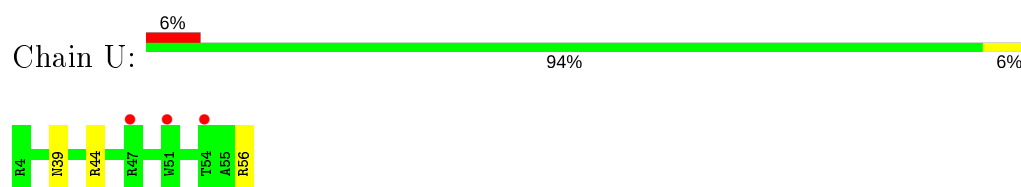
- Molecule 20: 50S ribosomal protein L23P



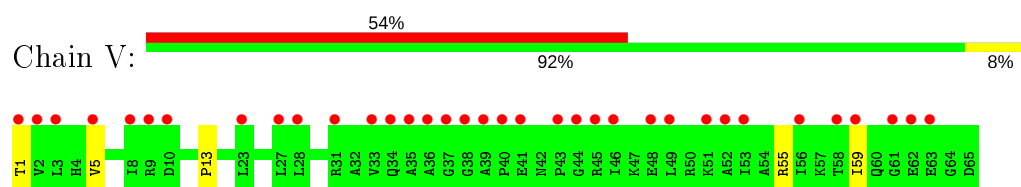
- Molecule 21: 50S ribosomal protein L24P



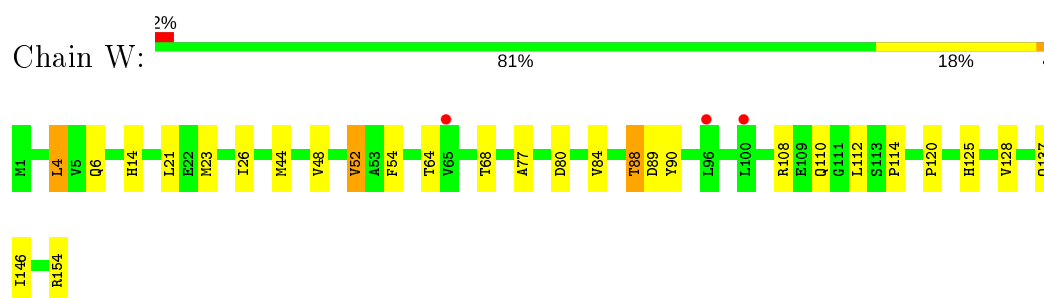
- Molecule 22: 50S ribosomal protein L24e



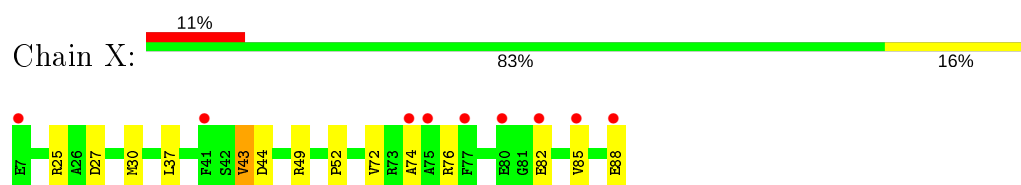
- Molecule 23: 50S ribosomal protein L29P



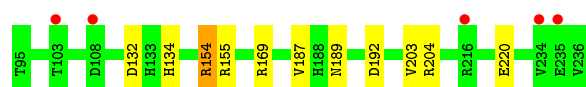
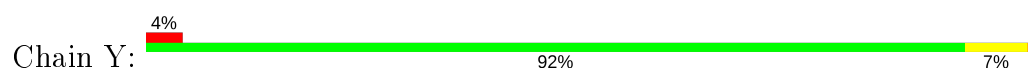
- Molecule 24: 50S ribosomal protein L30P



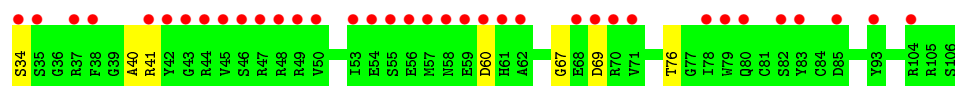
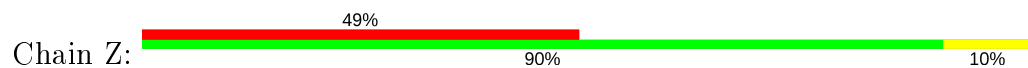
- Molecule 25: 50S ribosomal protein L31e



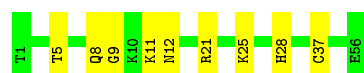
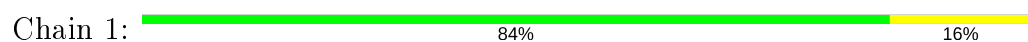
- Molecule 26: 50S ribosomal protein L32e



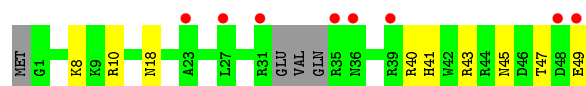
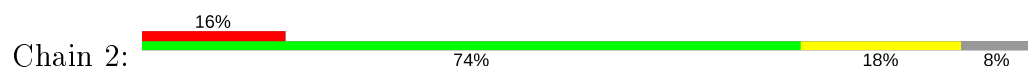
- Molecule 27: 50S ribosomal protein L37Ae



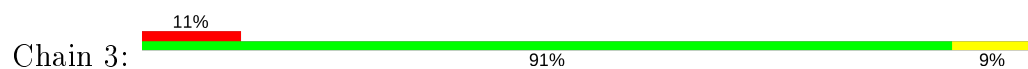
- Molecule 28: 50S ribosomal protein L37e



- 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, $\alpha$ , $\beta$ , $\gamma$	211.86Å 299.42Å 574.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 2.70 85.51 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.90-2.70) 92.7 (85.51-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.190 , 0.229 0.183 , 0.221	Depositor DCC
$R_{free}$ test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.8	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 72.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	99174	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SR, MG, OMG, CL, HMT, NA, K, CD, OMU, UR3, 1MA, PSU

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	0.37	0/65958	0.68	11/102869 (0.0%)
2	A	0.51	0/1787	0.77	1/2408 (0.0%)
3	B	0.54	0/2690	0.78	0/3652
4	C	0.56	0/1885	0.79	0/2552
5	D	0.64	0/1111	0.70	1/1498 (0.1%)
6	E	0.60	0/1383	0.68	0/1880
7	F	0.54	0/901	0.69	0/1224
8	G	0.51	0/241	0.65	0/324
9	H	0.61	0/1302	0.77	0/1743
10	I	0.59	0/527	0.61	0/716
11	J	0.62	0/1136	0.72	0/1530
12	K	0.50	0/1004	0.80	0/1351
13	L	0.52	0/1130	0.75	0/1509
14	M	0.51	0/1583	0.77	0/2116
15	N	0.56	0/1474	0.76	0/1999
16	O	0.49	0/874	0.72	1/1181 (0.1%)
17	P	0.53	0/1148	0.66	0/1528
18	Q	0.51	0/749	0.77	0/1005
19	R	0.55	0/1173	0.75	0/1578
20	S	0.55	0/649	0.67	0/875
21	T	0.48	0/958	0.75	1/1289 (0.1%)
22	U	0.59	0/418	0.70	0/562
23	V	0.44	0/503	0.65	0/675
24	W	0.53	0/1219	0.77	1/1655 (0.1%)
25	X	0.53	0/665	0.73	0/895
26	Y	0.53	0/1147	0.73	0/1536
27	Z	0.67	0/585	0.72	0/781
28	1	0.57	0/438	0.73	0/578
29	2	0.46	0/401	0.69	0/529
30	3	0.57	0/771	0.68	0/1024
31	9	0.33	0/2904	0.68	1/4526 (0.0%)
All	All	0.43	0/98714	0.70	17/147588 (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	42
24	W	0	1
31	9	0	2
All	All	0	45

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	871	G	C5'-C4'-O4'	-7.15	100.52	109.10
1	0	1942	A	C5'-C4'-C3'	7.11	127.37	116.00
24	W	4	LEU	CA-CB-CG	5.76	128.54	115.30
1	0	1504	A	C1'-O4'-C4'	-5.73	105.32	109.90
1	0	2726	U	N1-C1'-C2'	5.64	121.34	114.00

There are no chirality outliers.

5 of 45 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	0	221	G	Sidechain
1	0	396	U	Sidechain
1	0	458	G	Sidechain
1	0	470	U	Sidechain
1	0	48	A	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	849	0
2	A	1754	0	1766	20	0
3	B	2625	0	2533	28	0
4	C	1860	0	1813	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	1094	0	1085	11	0
6	E	1358	0	1266	8	0
7	F	890	0	843	4	0
8	G	240	0	231	2	0
9	H	1282	0	1292	14	0
10	I	520	0	500	2	0
11	J	1120	0	1098	15	0
12	K	994	0	1027	9	0
13	L	1118	0	1076	11	0
14	M	1559	0	1573	21	0
15	N	1445	0	1401	21	0
16	O	865	0	873	2	0
17	P	1137	0	1123	10	0
18	Q	735	0	729	8	0
19	R	1150	0	1122	12	0
20	S	642	0	605	4	0
21	T	950	0	924	11	0
22	U	411	0	364	2	0
23	V	500	0	511	3	0
24	W	1196	0	1137	17	0
25	X	655	0	653	6	0
26	Y	1131	0	1133	10	0
27	Z	574	0	532	6	0
28	1	431	0	426	8	0
29	2	396	0	413	8	0
30	3	755	0	729	4	0
31	9	2599	0	1325	69	0
32	0	85	0	0	0	0
32	2	1	0	0	0	0
32	9	2	0	0	0	0
32	A	1	0	0	0	0
32	B	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	2	0	0	0	0
34	0	66	0	0	0	0
34	9	3	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	1	0	0	0	0
34	S	1	0	0	0	0
35	0	10	0	0	0	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	0	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	93	0	0	0	0
36	1	1	0	0	0	0
36	3	2	0	0	0	0
36	9	3	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	J	1	0	0	0	0
36	R	1	0	0	0	0
36	S	1	0	0	0	0
37	0	39	0	39	11	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	5969	0	0	110	0
39	1	52	0	0	0	0
39	2	44	0	0	0	0
39	3	66	0	0	0	0
39	9	151	0	0	4	0
39	A	111	0	0	2	0
39	B	138	0	0	0	0
39	C	169	0	0	4	0
39	D	44	0	0	0	0
39	E	45	0	0	1	0
39	F	26	0	0	0	0
39	G	17	0	0	0	0
39	H	65	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
39	I	6	0	0	0	0
39	J	51	0	0	1	0
39	K	59	0	0	0	0
39	L	84	0	0	2	0
39	M	119	0	0	0	0
39	N	60	0	0	1	0
39	O	37	0	0	0	0
39	P	67	0	0	0	0
39	Q	42	0	0	0	0
39	R	81	0	0	0	0
39	S	30	0	0	0	0
39	T	34	0	0	0	0
39	U	26	0	0	0	0
39	V	10	0	0	1	0
39	W	67	0	0	1	0
39	X	25	0	0	1	0
39	Y	96	0	0	0	0
39	Z	32	0	0	1	0
All	All	99174	0	59954	1065	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 7.

The worst 5 of 1065 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)
1:0:1160:G:H5'	1:0:1161:A:H5'	1.19	1.14
31:9:76:G:H3'	31:9:77:A:H5''	1.38	1.04
1:0:871:G:C8	1:0:871:G:H5'	1.96	0.98
1:0:1242:A:H5'	11:J:82:THR:HG23	1.46	0.98
31:9:56:A:H2'	31:9:57:A:H5''	1.47	0.96

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%)	219 (93%)	13 (6%)	3 (1%)	12	30
3	B	335/337 (99%)	314 (94%)	18 (5%)	3 (1%)	17	40
4	C	244/246 (99%)	227 (93%)	17 (7%)	0	100	100
5	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	10	26
6	E	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
7	F	117/119 (98%)	112 (96%)	3 (3%)	2 (2%)	9	23
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	149 (96%)	5 (3%)	2 (1%)	12	30
10	I	68/70 (97%)	56 (82%)	11 (16%)	1 (2%)	10	26
11	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
12	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	19	43
13	L	141/165 (86%)	132 (94%)	9 (6%)	0	100	100
14	M	192/194 (99%)	188 (98%)	4 (2%)	0	100	100
15	N	184/186 (99%)	173 (94%)	8 (4%)	3 (2%)	9	24
16	O	113/115 (98%)	111 (98%)	2 (2%)	0	100	100
17	P	141/143 (99%)	141 (100%)	0	0	100	100
18	Q	93/95 (98%)	89 (96%)	4 (4%)	0	100	100
19	R	148/150 (99%)	143 (97%)	5 (3%)	0	100	100
20	S	79/81 (98%)	77 (98%)	2 (2%)	0	100	100
21	T	117/119 (98%)	112 (96%)	5 (4%)	0	100	100
22	U	51/53 (96%)	48 (94%)	3 (6%)	0	100	100
23	V	63/65 (97%)	60 (95%)	3 (5%)	0	100	100
24	W	152/154 (99%)	148 (97%)	3 (2%)	1 (1%)	22	46
25	X	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
26	Y	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
27	Z	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	11	28
28	1	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
29	2	42/50 (84%)	42 (100%)	0	0	100	100
30	3	90/92 (98%)	89 (99%)	1 (1%)	0	100	100
All	All	3705/4172 (89%)	3527 (95%)	159 (4%)	19 (0%)	29	54

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	37	VAL
15	N	154	LEU
2	A	27	LEU
9	H	19	ARG
24	W	77	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	
2	A	179/179 (100%)	171 (96%)	8 (4%)	27	55
3	B	282/282 (100%)	270 (96%)	12 (4%)	29	57
4	C	193/193 (100%)	174 (90%)	19 (10%)	8	18
5	D	117/148 (79%)	110 (94%)	7 (6%)	19	42
6	E	152/152 (100%)	148 (97%)	4 (3%)	46	75
7	F	93/93 (100%)	91 (98%)	2 (2%)	52	79
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/145 (92%)	128 (96%)	6 (4%)	27	55
10	I	58/58 (100%)	57 (98%)	1 (2%)	60	84
11	J	118/118 (100%)	110 (93%)	8 (7%)	16	36
12	K	106/106 (100%)	102 (96%)	4 (4%)	33	62
13	L	113/127 (89%)	106 (94%)	7 (6%)	18	40
14	M	158/158 (100%)	152 (96%)	6 (4%)	33	62
15	N	149/149 (100%)	143 (96%)	6 (4%)	31	60
16	O	93/93 (100%)	89 (96%)	4 (4%)	29	57
17	P	113/113 (100%)	109 (96%)	4 (4%)	36	65
18	Q	79/79 (100%)	75 (95%)	4 (5%)	24	50
19	R	117/117 (100%)	113 (97%)	4 (3%)	37	66
20	S	71/71 (100%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	T	105/105 (100%)	99 (94%)	6 (6%)	20	44
22	U	44/44 (100%)	44 (100%)	0	100	100
23	V	51/51 (100%)	50 (98%)	1 (2%)	55	81
24	W	130/130 (100%)	123 (95%)	7 (5%)	22	47
25	X	66/66 (100%)	59 (89%)	7 (11%)	6	15
26	Y	120/120 (100%)	116 (97%)	4 (3%)	38	67
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/46 (100%)	46 (100%)	0	100	100
29	2	42/46 (91%)	41 (98%)	1 (2%)	49	77
30	3	79/79 (100%)	76 (96%)	3 (4%)	33	62
All	All	3095/3410 (91%)	2960 (96%)	135 (4%)	28	56

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	47	THR
13	L	101	ASP
25	X	72	VAL
11	J	52	GLN
12	K	98	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
14	M	137	ASN
17	P	118	GLN
28	1	28	HIS
14	M	170	ASN
17	P	66	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	224 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	242 (8%)	31 (1%)

5 of 242 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	0	31	C
1	0	67	A
1	0	69	A
1	0	70	A
1	0	71	G

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	0	1352	A
1	0	1685	A
1	0	2726	U
1	0	1377	C
1	0	1692	C

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

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	1MA	0	628	1,34	15,25,26	0.75	0	15,37,40	1.38	1 (6%)
1	OMU	0	2587	1,34	14,22,23	1.03	1 (7%)	14,31,34	1.16	1 (7%)
1	OMG	0	2588	1	18,26,27	1.08	2 (11%)	20,38,41	2.59	5 (25%)
1	UR3	0	2619	1	14,22,23	0.85	0	15,32,35	0.59	0
1	PSU	0	2621	1	17,21,22	1.55	3 (17%)	20,30,33	5.47	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	1MA	0	628	1,34	-	0/3/25/26	0/3/3/3
1	OMU	0	2587	1,34	-	0/7/27/28	0/2/2/2
1	OMG	0	2588	1	-	0/5/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/5/25/26	0/2/2/2
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'	-4.89	1.48	1.52
1	0	2588	OMG	C6-N1	3.42	1.39	1.33
1	0	2621	PSU	C4-N3	2.90	1.38	1.33
1	0	2587	OMU	C4-N3	2.62	1.37	1.33
1	0	2621	PSU	C2-N1	2.31	1.42	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	N1-C2-N3	-17.45	114.56	128.43
1	0	2621	PSU	C4-N3-C2	14.37	127.28	115.14
1	0	2588	OMG	C5-C6-N1	-8.60	111.67	123.43
1	0	2621	PSU	C5-C4-N3	-8.26	114.71	125.36
1	0	2588	OMG	C6-N1-C2	5.82	125.18	115.93

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	0	2587	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 306 ligands modelled in this entry, 305 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	HMT	0	9101	-	40,43,43	0.66	0	41,66,66	2.05	13 (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	HMT	0	9101	-	-	5/27/74/74	0/5/5/5

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	HMT	O7-C22-C21	4.55	119.71	111.19
37	0	9101	HMT	O4-C19-C20	4.22	119.11	111.27
37	0	9101	HMT	O1-C17-O2	-4.12	101.49	108.08
37	0	9101	HMT	C18-O3-C2	-3.54	110.58	116.52
37	0	9101	HMT	O1-C14-C13	3.18	132.10	127.85

There are no chirality outliers.

All (5) torsion outliers are listed below:

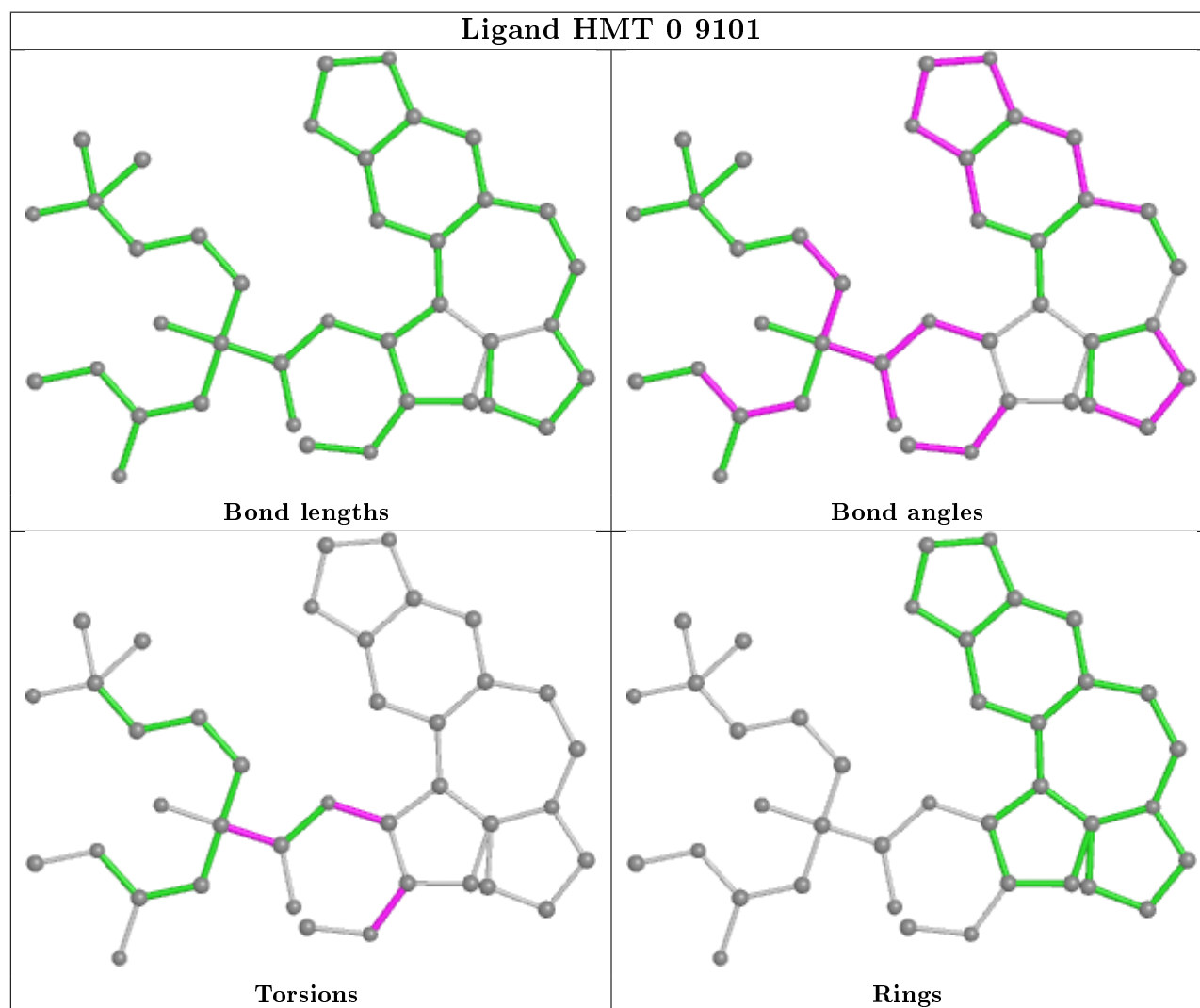
Mol	Chain	Res	Type	Atoms
37	0	9101	HMT	C1-C2-O3-C18
37	0	9101	HMT	C3-C2-O3-C18
37	0	9101	HMT	O5-C19-C20-C24
37	0	9101	HMT	O4-C19-C20-C24
37	0	9101	HMT	C2-C3-O4-C19

There are no ring outliers.

1 monomer is involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	0	9101	HMT	11	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	0	2749/2923 (94%)	-0.36	47 (1%) 70 72	22, 50, 99, 170	0
2	A	237/237 (100%)	0.86	37 (15%) 2 1	30, 62, 104, 124	0
3	B	337/337 (100%)	0.39	18 (5%) 26 25	30, 59, 88, 105	0
4	C	246/246 (100%)	0.46	9 (3%) 41 41	25, 51, 78, 88	0
5	D	140/177 (79%)	2.76	82 (58%) 0 0	70, 112, 138, 148	0
6	E	172/172 (100%)	0.74	18 (10%) 6 4	51, 76, 98, 104	0
7	F	119/119 (100%)	1.47	36 (30%) 0 0	58, 83, 116, 132	0
8	G	29/348 (8%)	2.03	12 (41%) 0 0	78, 102, 109, 111	0
9	H	160/177 (90%)	1.40	49 (30%) 0 0	49, 73, 112, 120	0
10	I	70/70 (100%)	5.45	65 (92%) 0 0	140, 157, 176, 177	0
11	J	142/142 (100%)	0.27	3 (2%) 63 65	39, 56, 79, 98	0
12	K	132/132 (100%)	0.28	5 (3%) 40 39	39, 56, 81, 85	0
13	L	145/165 (87%)	1.24	36 (24%) 0 0	30, 76, 128, 140	0
14	M	194/194 (100%)	0.22	2 (1%) 82 83	35, 49, 67, 73	0
15	N	186/186 (100%)	1.43	56 (30%) 0 0	48, 75, 130, 137	0
16	O	115/115 (100%)	0.58	6 (5%) 27 25	42, 61, 79, 88	0
17	P	143/143 (100%)	0.52	7 (4%) 29 28	43, 63, 80, 87	0
18	Q	95/95 (100%)	0.17	0 100 100	40, 53, 67, 79	0
19	R	150/150 (100%)	0.10	0 100 100	33, 51, 71, 82	0
20	S	81/81 (100%)	1.08	16 (19%) 1 0	49, 68, 90, 99	0
21	T	119/119 (100%)	1.06	19 (15%) 1 1	42, 66, 92, 119	0
22	U	53/53 (100%)	0.60	3 (5%) 23 22	46, 63, 84, 89	0
23	V	65/65 (100%)	2.96	35 (53%) 0 0	62, 87, 128, 136	0
24	W	154/154 (100%)	0.41	3 (1%) 66 69	38, 56, 73, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	X	82/82 (100%)	0.65	9 (10%) 5 4	50, 68, 93, 107	0
26	Y	142/142 (100%)	0.31	5 (3%) 44 44	26, 50, 75, 96	0
27	Z	73/73 (100%)	2.31	36 (49%) 0 0	69, 94, 110, 115	0
28	1	56/56 (100%)	0.12	0 100 100	30, 36, 44, 54	0
29	2	46/50 (92%)	0.74	8 (17%) 1 1	41, 70, 100, 111	0
30	3	92/92 (100%)	0.86	10 (10%) 5 4	42, 70, 83, 95	0
31	9	122/122 (100%)	-0.42	4 (3%) 46 46	42, 72, 98, 150	0
All	All	6646/7217 (92%)	0.36	636 (9%) 8 6	22, 58, 112, 177	0

The worst 5 of 636 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	18.1
23	V	39	ALA	16.9
10	I	74	ILE	13.1
5	D	63	ILE	12.3
10	I	128	THR	11.3

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1MA	0	628	23/24	0.98	0.18	31,34,35,38	0
1	OMG	0	2588	24/25	0.98	0.15	35,38,39,41	0
1	UR3	0	2619	21/22	0.98	0.16	40,43,45,50	0
1	PSU	0	2621	20/21	0.98	0.15	26,30,42,42	0
1	OMU	0	2587	21/22	0.99	0.14	35,38,41,42	0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
36	SR	0	8924	1/1	-0.05	0.23	166,166,166,166	0
36	SR	0	9006	1/1	-0.02	0.84	200,200,200,200	0
36	SR	0	8976	1/1	0.06	0.55	199,199,199,199	0
36	SR	J	8986	1/1	0.15	2.11	200,200,200,200	0
36	SR	0	8923	1/1	0.25	0.50	192,192,192,192	0
36	SR	0	8953	1/1	0.31	0.26	179,179,179,179	0
36	SR	0	8956	1/1	0.35	0.21	183,183,183,183	0
34	NA	0	8571	1/1	0.36	0.39	96,96,96,96	0
36	SR	A	8977	1/1	0.40	0.12	182,182,182,182	0
36	SR	B	8987	1/1	0.42	0.79	200,200,200,200	0
36	SR	0	8959	1/1	0.44	0.26	189,189,189,189	0
36	SR	0	8982	1/1	0.45	0.99	200,200,200,200	0
32	MG	A	8051	1/1	0.47	0.31	92,92,92,92	0
36	SR	9	9003	1/1	0.49	0.13	194,194,194,194	0
34	NA	0	8522	1/1	0.52	0.47	96,96,96,96	0
34	NA	0	8561	1/1	0.55	0.68	99,99,99,99	0
36	SR	0	8983	1/1	0.57	0.26	191,191,191,191	0
36	SR	0	8938	1/1	0.57	0.15	198,198,198,198	0
36	SR	0	8913	1/1	0.58	1.02	169,169,169,169	0
36	SR	0	8984	1/1	0.60	0.13	157,157,157,157	0
36	SR	0	8922	1/1	0.60	0.37	158,158,158,158	0
36	SR	0	8934	1/1	0.61	0.91	172,172,172,172	0
36	SR	0	8957	1/1	0.63	0.68	200,200,200,200	0
36	SR	0	8955	1/1	0.63	0.28	200,200,200,200	0
36	SR	9	8978	1/1	0.64	0.22	165,165,165,165	0
36	SR	B	8950	1/1	0.66	0.24	123,123,123,123	0
36	SR	0	8998	1/1	0.66	0.23	155,155,155,155	0
36	SR	0	8979	1/1	0.66	0.20	196,196,196,196	0
36	SR	0	8971	1/1	0.67	0.13	181,181,181,181	0
36	SR	0	8949	1/1	0.67	0.20	134,134,134,134	0
34	NA	0	8525	1/1	0.67	0.23	70,70,70,70	0
36	SR	0	8919	1/1	0.67	0.17	168,168,168,168	0
36	SR	0	8995	1/1	0.67	0.18	148,148,148,148	0
36	SR	0	9004	1/1	0.69	0.56	200,200,200,200	0
36	SR	9	8980	1/1	0.69	0.10	188,188,188,188	0
34	NA	0	8546	1/1	0.69	0.66	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	9	8572	1/1	0.69	0.29	82,82,82,82	0
34	NA	0	8523	1/1	0.70	0.27	54,54,54,54	0
36	SR	0	8994	1/1	0.70	0.76	200,200,200,200	0
36	SR	0	8933	1/1	0.70	0.47	159,159,159,159	0
36	SR	0	8916	1/1	0.73	0.15	118,118,118,118	0
36	SR	0	8993	1/1	0.74	0.12	186,186,186,186	0
36	SR	0	8974	1/1	0.74	0.42	183,183,183,183	0
34	NA	0	8533	1/1	0.74	0.23	73,73,73,73	0
36	SR	0	8988	1/1	0.74	0.12	182,182,182,182	0
34	NA	0	8573	1/1	0.75	0.30	92,92,92,92	0
36	SR	0	8990	1/1	0.75	0.30	161,161,161,161	0
36	SR	0	8968	1/1	0.76	0.13	168,168,168,168	0
36	SR	0	8981	1/1	0.76	0.21	159,159,159,159	0
36	SR	0	8992	1/1	0.76	0.17	132,132,132,132	0
32	MG	0	8010	1/1	0.77	0.29	52,52,52,52	0
34	NA	0	8562	1/1	0.77	0.56	63,63,63,63	0
32	MG	0	8030	1/1	0.77	0.53	91,91,91,91	0
36	SR	0	8948	1/1	0.78	0.16	107,107,107,107	0
32	MG	0	8083	1/1	0.78	0.15	68,68,68,68	0
36	SR	0	8917	1/1	0.79	0.15	117,117,117,117	0
36	SR	0	8965	1/1	0.79	0.19	145,145,145,145	0
36	SR	0	8944	1/1	0.80	0.18	187,187,187,187	0
34	NA	0	8506	1/1	0.80	0.17	65,65,65,65	0
32	MG	0	8063	1/1	0.80	0.29	79,79,79,79	0
36	SR	0	8989	1/1	0.80	0.34	191,191,191,191	0
32	MG	9	8074	1/1	0.80	0.18	71,71,71,71	0
36	SR	0	8942	1/1	0.80	0.18	138,138,138,138	0
32	MG	0	8075	1/1	0.80	0.13	58,58,58,58	0
34	NA	0	8511	1/1	0.80	0.56	91,91,91,91	0
34	NA	0	8549	1/1	0.81	0.45	64,64,64,64	0
34	NA	0	8509	1/1	0.81	0.33	71,71,71,71	0
34	NA	0	8554	1/1	0.82	0.78	72,72,72,72	0
32	MG	0	8069	1/1	0.82	0.62	82,82,82,82	0
32	MG	0	8071	1/1	0.82	0.27	72,72,72,72	0
36	SR	0	8969	1/1	0.82	0.14	149,149,149,149	0
36	SR	0	9001	1/1	0.83	0.17	187,187,187,187	0
34	NA	0	8559	1/1	0.83	0.42	98,98,98,98	0
36	SR	A	8930	1/1	0.83	0.15	147,147,147,147	0
36	SR	0	8958	1/1	0.83	0.14	105,105,105,105	0
36	SR	0	8920	1/1	0.83	0.56	200,200,200,200	0
32	MG	0	8049	1/1	0.83	0.92	95,95,95,95	0
34	NA	0	8570	1/1	0.84	0.18	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8947	1/1	0.84	0.49	199,199,199,199	0
34	NA	0	8530	1/1	0.84	0.43	56,56,56,56	0
34	NA	0	8564	1/1	0.84	0.36	74,74,74,74	0
32	MG	T	8057	1/1	0.84	0.09	70,70,70,70	0
37	HMT	0	9101	39/39	0.84	0.30	69,75,86,87	0
34	NA	0	8560	1/1	0.85	0.60	73,73,73,73	0
36	SR	0	8991	1/1	0.85	0.20	199,199,199,199	0
34	NA	0	8518	1/1	0.85	0.46	96,96,96,96	0
34	NA	0	8548	1/1	0.85	0.34	61,61,61,61	0
34	NA	0	8531	1/1	0.85	0.24	56,56,56,56	0
36	SR	0	8945	1/1	0.85	0.11	117,117,117,117	0
34	NA	0	8529	1/1	0.86	0.09	46,46,46,46	0
32	MG	0	8039	1/1	0.86	0.31	56,56,56,56	0
36	SR	0	8928	1/1	0.86	0.12	140,140,140,140	0
36	SR	0	9002	1/1	0.86	0.12	176,176,176,176	0
32	MG	0	8050	1/1	0.86	0.20	48,48,48,48	0
32	MG	0	8031	1/1	0.86	0.47	83,83,83,83	0
36	SR	0	8985	1/1	0.86	0.08	122,122,122,122	0
36	SR	S	8961	1/1	0.86	0.09	141,141,141,141	0
36	SR	0	9000	1/1	0.86	0.29	180,180,180,180	0
36	SR	0	8970	1/1	0.86	0.06	131,131,131,131	0
34	NA	0	8556	1/1	0.87	0.32	47,47,47,47	0
36	SR	0	8996	1/1	0.87	0.72	200,200,200,200	0
32	MG	0	8066	1/1	0.87	0.22	62,62,62,62	0
34	NA	0	8521	1/1	0.87	0.28	67,67,67,67	0
34	NA	R	8532	1/1	0.87	0.17	59,59,59,59	0
34	NA	0	8569	1/1	0.87	0.37	70,70,70,70	0
32	MG	0	8092	1/1	0.87	0.10	80,80,80,80	0
36	SR	0	8997	1/1	0.87	1.14	200,200,200,200	0
34	NA	0	8519	1/1	0.87	0.27	42,42,42,42	0
34	NA	0	8575	1/1	0.87	0.38	100,100,100,100	0
36	SR	0	8960	1/1	0.88	0.08	162,162,162,162	0
32	MG	9	8040	1/1	0.88	0.45	103,103,103,103	0
34	NA	0	8516	1/1	0.88	0.30	39,39,39,39	0
34	NA	J	8538	1/1	0.88	0.18	62,62,62,62	0
32	MG	K	8054	1/1	0.88	0.22	44,44,44,44	0
32	MG	0	8047	1/1	0.89	0.49	61,61,61,61	0
34	NA	0	8501	1/1	0.89	0.23	43,43,43,43	0
34	NA	Q	8540	1/1	0.89	0.18	67,67,67,67	0
36	SR	0	9007	1/1	0.89	0.44	200,200,200,200	0
36	SR	0	8926	1/1	0.89	0.12	132,132,132,132	0
36	SR	A	8929	1/1	0.89	0.22	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	F	9005	1/1	0.89	0.08	138,138,138,138	0
32	MG	0	8037	1/1	0.89	0.23	83,83,83,83	0
34	NA	0	8507	1/1	0.89	0.26	49,49,49,49	0
33	K	0	8401	1/1	0.89	0.45	130,130,130,130	0
32	MG	0	8056	1/1	0.90	0.17	67,67,67,67	0
36	SR	0	8918	1/1	0.90	0.17	87,87,87,87	0
32	MG	0	8034	1/1	0.90	0.15	48,48,48,48	0
34	NA	0	8553	1/1	0.90	0.40	75,75,75,75	0
32	MG	0	8081	1/1	0.90	0.19	63,63,63,63	0
34	NA	0	8524	1/1	0.91	0.37	57,57,57,57	0
34	NA	0	8542	1/1	0.91	0.47	52,52,52,52	0
35	CL	0	8822	1/1	0.91	0.36	74,74,74,74	0
32	MG	0	8001	1/1	0.91	0.22	32,32,32,32	0
34	NA	C	8503	1/1	0.91	0.27	40,40,40,40	0
36	SR	0	8975	1/1	0.91	0.17	150,150,150,150	0
32	MG	0	8020	1/1	0.91	0.12	66,66,66,66	0
32	MG	0	8087	1/1	0.91	0.17	38,38,38,38	0
34	NA	0	8567	1/1	0.91	0.48	81,81,81,81	0
32	MG	0	8065	1/1	0.91	0.18	45,45,45,45	0
34	NA	0	8574	1/1	0.91	0.64	75,75,75,75	0
34	NA	0	8514	1/1	0.92	0.27	47,47,47,47	0
32	MG	0	8045	1/1	0.92	0.13	36,36,36,36	0
36	SR	0	8901	1/1	0.92	0.14	93,93,93,93	0
34	NA	M	8539	1/1	0.92	0.16	42,42,42,42	0
36	SR	0	8951	1/1	0.92	0.05	144,144,144,144	0
36	SR	0	8911	1/1	0.92	0.09	92,92,92,92	0
34	NA	0	8528	1/1	0.92	0.21	50,50,50,50	0
32	MG	0	8055	1/1	0.92	0.27	44,44,44,44	0
32	MG	0	8073	1/1	0.92	0.28	96,96,96,96	0
36	SR	0	8936	1/1	0.92	0.15	106,106,106,106	0
34	NA	0	8565	1/1	0.92	0.67	73,73,73,73	0
34	NA	0	8536	1/1	0.92	0.09	56,56,56,56	0
34	NA	0	8504	1/1	0.92	0.26	34,34,34,34	0
32	MG	0	8067	1/1	0.92	0.31	35,35,35,35	0
34	NA	0	8515	1/1	0.92	0.23	43,43,43,43	0
34	NA	0	8552	1/1	0.92	0.35	73,73,73,73	0
34	NA	0	8534	1/1	0.92	0.35	44,44,44,44	0
36	SR	0	8963	1/1	0.92	0.15	132,132,132,132	0
36	SR	0	8943	1/1	0.92	0.11	97,97,97,97	0
32	MG	0	8085	1/1	0.92	0.14	89,89,89,89	0
36	SR	0	8914	1/1	0.92	0.29	113,113,113,113	0
34	NA	0	8557	1/1	0.92	0.15	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
32	MG	0	8032	1/1	0.92	0.08	41,41,41,41	0
32	MG	0	8090	1/1	0.93	0.25	96,96,96,96	0
34	NA	0	8547	1/1	0.93	0.55	49,49,49,49	0
34	NA	0	8558	1/1	0.93	0.48	50,50,50,50	0
36	SR	0	8972	1/1	0.93	0.15	135,135,135,135	0
32	MG	0	8041	1/1	0.93	0.34	26,26,26,26	0
36	SR	0	8927	1/1	0.93	0.19	172,172,172,172	0
36	SR	0	8941	1/1	0.93	0.17	113,113,113,113	0
32	MG	0	8088	1/1	0.93	0.17	42,42,42,42	0
32	MG	0	8025	1/1	0.93	0.14	28,28,28,28	0
36	SR	3	8999	1/1	0.93	0.11	110,110,110,110	0
34	NA	9	8544	1/1	0.93	0.23	68,68,68,68	0
32	MG	0	8059	1/1	0.93	0.11	50,50,50,50	0
32	MG	0	8070	1/1	0.93	0.21	58,58,58,58	0
34	NA	0	8568	1/1	0.93	0.32	60,60,60,60	0
32	MG	0	8016	1/1	0.93	0.32	50,50,50,50	0
32	MG	0	8079	1/1	0.93	0.32	60,60,60,60	0
35	CL	J	8802	1/1	0.93	0.12	72,72,72,72	0
32	MG	0	8018	1/1	0.93	0.27	39,39,39,39	0
34	NA	0	8502	1/1	0.93	0.27	69,69,69,69	0
36	SR	0	8915	1/1	0.93	0.09	128,128,128,128	0
32	MG	B	8042	1/1	0.93	0.16	60,60,60,60	0
36	SR	0	9008	1/1	0.93	0.15	96,96,96,96	0
32	MG	0	8036	1/1	0.93	0.10	50,50,50,50	0
32	MG	2	8060	1/1	0.93	0.12	56,56,56,56	0
32	MG	0	8072	1/1	0.93	0.24	62,62,62,62	0
32	MG	0	8044	1/1	0.93	0.13	55,55,55,55	0
34	NA	0	8520	1/1	0.93	0.24	60,60,60,60	0
35	CL	3	8804	1/1	0.93	0.07	65,65,65,65	0
35	CL	0	8805	1/1	0.93	0.10	70,70,70,70	0
34	NA	0	8541	1/1	0.93	0.31	59,59,59,59	0
32	MG	0	8078	1/1	0.94	0.30	49,49,49,49	0
32	MG	0	8062	1/1	0.94	0.32	55,55,55,55	0
35	CL	Y	8820	1/1	0.94	0.09	45,45,45,45	0
32	MG	0	8029	1/1	0.94	0.18	49,49,49,49	0
32	MG	0	8023	1/1	0.94	0.22	28,28,28,28	0
36	SR	0	8910	1/1	0.94	0.20	108,108,108,108	0
34	NA	0	8563	1/1	0.94	0.34	70,70,70,70	0
36	SR	0	8921	1/1	0.94	0.14	94,94,94,94	0
34	NA	S	8510	1/1	0.94	0.22	51,51,51,51	0
36	SR	0	8964	1/1	0.94	0.10	130,130,130,130	0
36	SR	0	8962	1/1	0.94	0.20	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
34	NA	0	8537	1/1	0.94	0.19	45,45,45,45	0
32	MG	0	8089	1/1	0.94	0.11	45,45,45,45	0
34	NA	0	8550	1/1	0.94	0.30	59,59,59,59	0
35	CL	J	8801	1/1	0.94	0.20	70,70,70,70	0
36	SR	0	8908	1/1	0.94	0.12	100,100,100,100	0
34	NA	0	8566	1/1	0.94	0.34	47,47,47,47	0
32	MG	0	8021	1/1	0.94	0.18	40,40,40,40	0
32	MG	0	8064	1/1	0.94	0.26	46,46,46,46	0
35	CL	0	8816	1/1	0.95	0.14	63,63,63,63	0
36	SR	0	8935	1/1	0.95	0.13	89,89,89,89	0
32	MG	0	8053	1/1	0.95	0.09	79,79,79,79	0
34	NA	0	8508	1/1	0.95	0.34	46,46,46,46	0
32	MG	0	8077	1/1	0.95	0.17	38,38,38,38	0
34	NA	9	8543	1/1	0.95	0.20	50,50,50,50	0
32	MG	0	8027	1/1	0.95	0.12	41,41,41,41	0
32	MG	0	8024	1/1	0.95	0.22	47,47,47,47	0
35	CL	L	8810	1/1	0.95	0.14	54,54,54,54	0
34	NA	0	8535	1/1	0.96	0.21	52,52,52,52	0
33	K	0	8402	1/1	0.96	0.11	65,65,65,65	0
34	NA	0	8512	1/1	0.96	0.35	48,48,48,48	0
32	MG	0	8043	1/1	0.96	0.13	45,45,45,45	0
32	MG	0	8061	1/1	0.96	0.30	30,30,30,30	0
36	SR	0	8967	1/1	0.96	0.06	132,132,132,132	0
36	SR	0	8966	1/1	0.96	0.08	113,113,113,113	0
32	MG	0	8013	1/1	0.96	0.08	35,35,35,35	0
36	SR	1	8952	1/1	0.96	0.16	85,85,85,85	0
34	NA	0	8505	1/1	0.96	0.48	42,42,42,42	0
35	CL	0	8811	1/1	0.96	0.14	65,65,65,65	0
35	CL	0	8815	1/1	0.96	0.16	66,66,66,66	0
32	MG	0	8019	1/1	0.96	0.35	28,28,28,28	0
32	MG	0	8068	1/1	0.96	0.09	57,57,57,57	0
32	MG	0	8082	1/1	0.96	0.31	70,70,70,70	0
36	SR	R	8912	1/1	0.96	0.21	90,90,90,90	0
36	SR	0	8939	1/1	0.96	0.14	147,147,147,147	0
34	NA	0	8551	1/1	0.96	0.30	49,49,49,49	0
32	MG	0	8008	1/1	0.96	0.20	29,29,29,29	0
34	NA	0	8555	1/1	0.96	0.52	59,59,59,59	0
32	MG	0	8093	1/1	0.96	0.10	42,42,42,42	0
32	MG	0	8035	1/1	0.96	0.22	63,63,63,63	0
32	MG	0	8009	1/1	0.96	0.29	31,31,31,31	0
34	NA	0	8513	1/1	0.96	0.20	53,53,53,53	0
32	MG	0	8080	1/1	0.96	0.35	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8973	1/1	0.96	0.16	139,139,139,139	0
35	CL	0	8817	1/1	0.97	0.11	64,64,64,64	0
32	MG	0	8017	1/1	0.97	0.23	39,39,39,39	0
32	MG	0	8084	1/1	0.97	0.18	40,40,40,40	0
32	MG	0	8004	1/1	0.97	0.23	29,29,29,29	0
32	MG	0	8011	1/1	0.97	0.35	31,31,31,31	0
35	CL	0	8813	1/1	0.97	0.08	53,53,53,53	0
36	SR	0	8909	1/1	0.97	0.16	100,100,100,100	0
36	SR	0	8946	1/1	0.97	0.19	117,117,117,117	0
32	MG	0	8052	1/1	0.97	0.10	54,54,54,54	0
36	SR	0	8931	1/1	0.97	0.10	114,114,114,114	0
36	SR	0	8940	1/1	0.97	0.11	84,84,84,84	0
32	MG	0	8038	1/1	0.97	0.07	63,63,63,63	0
32	MG	0	8002	1/1	0.97	0.19	25,25,25,25	0
32	MG	0	8046	1/1	0.97	0.17	39,39,39,39	0
36	SR	0	8902	1/1	0.97	0.18	59,59,59,59	0
32	MG	0	8033	1/1	0.97	0.16	54,54,54,54	0
32	MG	Y	8086	1/1	0.97	0.14	46,46,46,46	0
32	MG	0	8022	1/1	0.97	0.21	38,38,38,38	0
36	SR	0	8954	1/1	0.97	0.12	109,109,109,109	0
35	CL	0	8803	1/1	0.98	0.08	53,53,53,53	0
35	CL	B	8819	1/1	0.98	0.16	52,52,52,52	0
32	MG	0	8012	1/1	0.98	0.24	22,22,22,22	0
38	CD	Z	8703	1/1	0.98	0.07	98,98,98,98	0
34	NA	0	8526	1/1	0.98	0.07	47,47,47,47	0
32	MG	0	8006	1/1	0.98	0.19	30,30,30,30	0
35	CL	A	8809	1/1	0.98	0.35	72,72,72,72	0
36	SR	3	8932	1/1	0.98	0.15	84,84,84,84	0
34	NA	0	8527	1/1	0.98	0.22	55,55,55,55	0
35	CL	0	8812	1/1	0.98	0.09	46,46,46,46	0
34	NA	0	8545	1/1	0.98	0.14	35,35,35,35	0
35	CL	N	8807	1/1	0.98	0.17	68,68,68,68	0
36	SR	0	8937	1/1	0.98	0.27	104,104,104,104	0
32	MG	0	8028	1/1	0.98	0.28	33,33,33,33	0
32	MG	0	8048	1/1	0.98	0.29	28,28,28,28	0
34	NA	0	8517	1/1	0.98	0.20	38,38,38,38	0
35	CL	O	8808	1/1	0.98	0.27	69,69,69,69	0
35	CL	0	8814	1/1	0.98	0.11	49,49,49,49	0
35	CL	J	8821	1/1	0.98	0.12	57,57,57,57	0
32	MG	0	8058	1/1	0.99	0.12	30,30,30,30	0
35	CL	R	8806	1/1	0.99	0.16	47,47,47,47	0
36	SR	0	8903	1/1	0.99	0.21	58,58,58,58	0

*Continued on next page...*

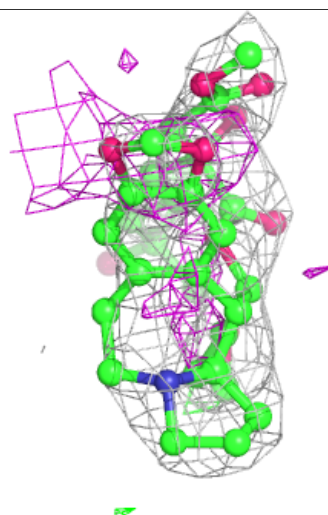
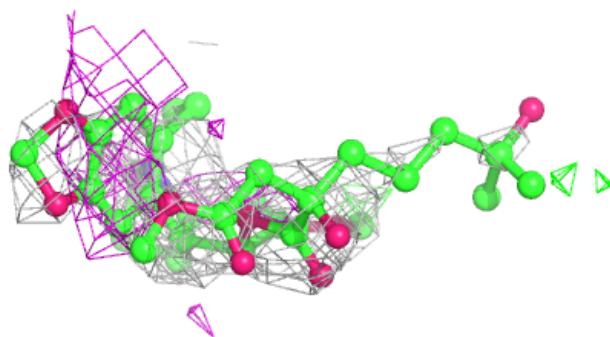
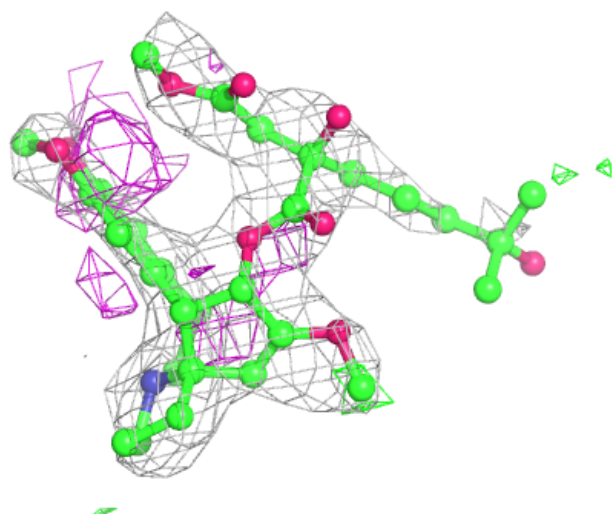
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
36	SR	0	8906	1/1	0.99	0.24	59,59,59,59	0
38	CD	U	8701	1/1	0.99	0.18	72,72,72,72	0
32	MG	0	8076	1/1	0.99	0.13	41,41,41,41	0
36	SR	0	8907	1/1	0.99	0.17	57,57,57,57	0
36	SR	0	8925	1/1	0.99	0.13	97,97,97,97	0
38	CD	O	8705	1/1	0.99	0.06	99,99,99,99	0
32	MG	0	8005	1/1	0.99	0.30	34,34,34,34	0
32	MG	0	8007	1/1	0.99	0.26	31,31,31,31	0
38	CD	3	8704	1/1	0.99	0.08	76,76,76,76	0
32	MG	0	8015	1/1	0.99	0.22	36,36,36,36	0
32	MG	0	8014	1/1	0.99	0.22	30,30,30,30	0
35	CL	M	8818	1/1	0.99	0.11	46,46,46,46	0
32	MG	0	8003	1/1	0.99	0.21	34,34,34,34	0
36	SR	0	8904	1/1	0.99	0.20	56,56,56,56	0
32	MG	0	8091	1/1	0.99	0.06	60,60,60,60	0
36	SR	0	8905	1/1	0.99	0.30	68,68,68,68	0
32	MG	0	8026	1/1	0.99	0.12	36,36,36,36	0
38	CD	1	8702	1/1	1.00	0.09	57,57,57,57	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.

**Electron density around HMT 0 9101:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.