



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 02:44 AM UTC

PDB ID : 3G6E / pdb_00003g6e
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

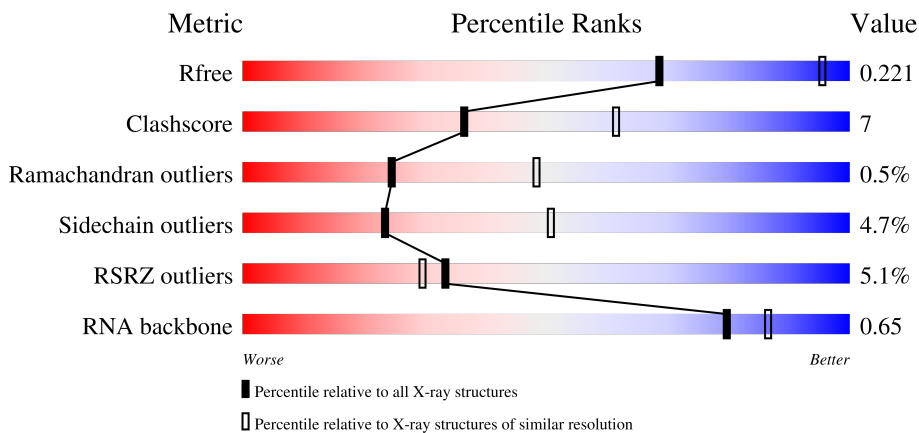
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



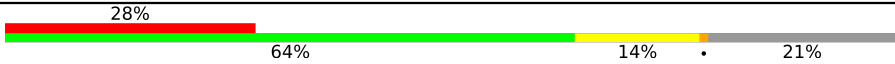
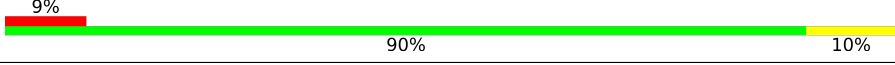
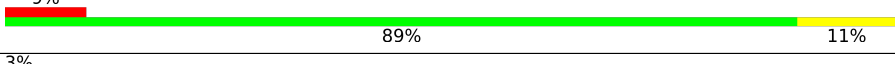
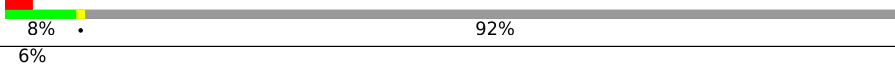
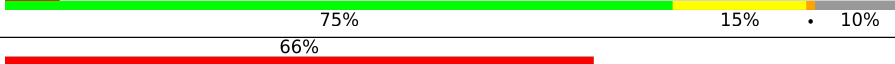
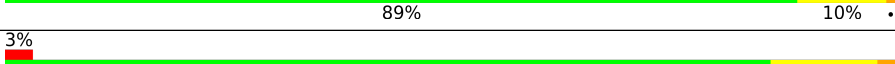
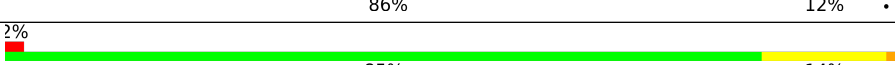
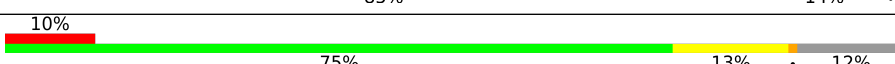
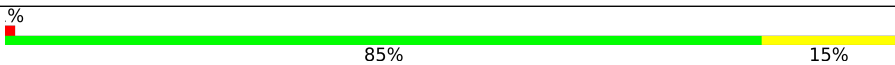
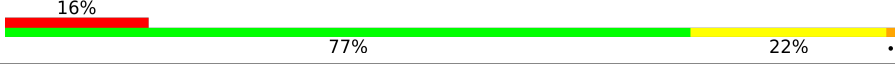
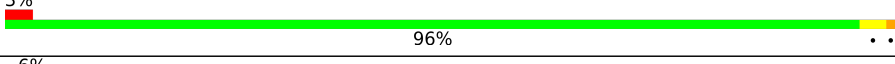
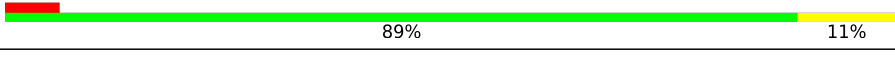
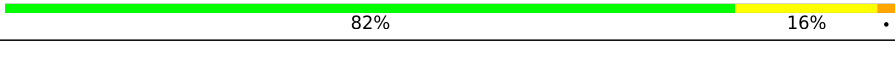
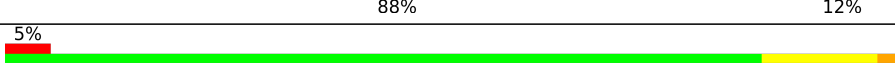
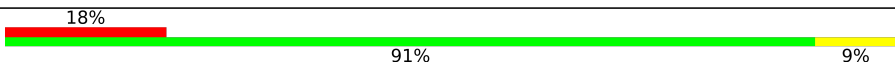
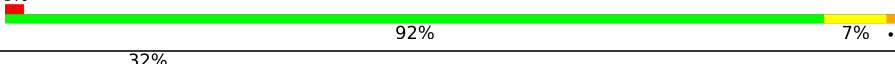
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)
RNA backbone	3983	1044 (2.90-2.50)

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	2% 59% 30% 5% 6%
2	A	237	5% 83% 16% .
3	B	337	2% 82% 16% .
4	C	246	2% 78% 18% .

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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
34	NA	0	8518	-	-	-	X
34	NA	0	8522	-	-	-	X
34	NA	0	8546	-	-	-	X
34	NA	0	8557	-	-	-	X
34	NA	0	8559	-	-	-	X
34	NA	0	8561	-	-	-	X
34	NA	0	8567	-	-	-	X
34	NA	0	8573	-	-	-	X
34	NA	0	8574	-	-	-	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	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 (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	0	85	Total	Mg	0	0
			85	85		
32	A	1	Total	Mg	0	0
			1	1		
32	B	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	2	Total	Mg	0	0
			2	2		

- Molecule 33 is POTASSIUM ION (CCD ID: K) (formula: K).

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

- Molecule 34 is SODIUM ION (CCD ID: 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	1	Total Na 1 1	0	0
34	S	1	Total Na 1 1	0	0
34	9	3	Total Na 3 3	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: 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
35	R	1	Total Cl 1 1	0	0

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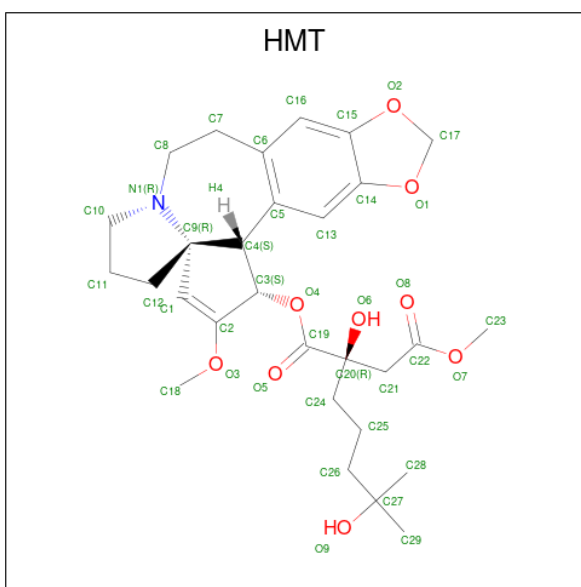
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Y	1	Total	Cl	0	0
			1	1		
35	3	1	Total	Cl	0	0
			1	1		

- Molecule 36 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

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

- Molecule 37 is (3beta)-O 3 -[(2R)-2,6-dihydroxy-2-(2-methoxy-2-oxoethyl)-6-methylheptano
yl]cephalotaxine (CCD ID: HMT) (formula: C₂₉H₃₉NO₉).



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

- Molecule 38 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

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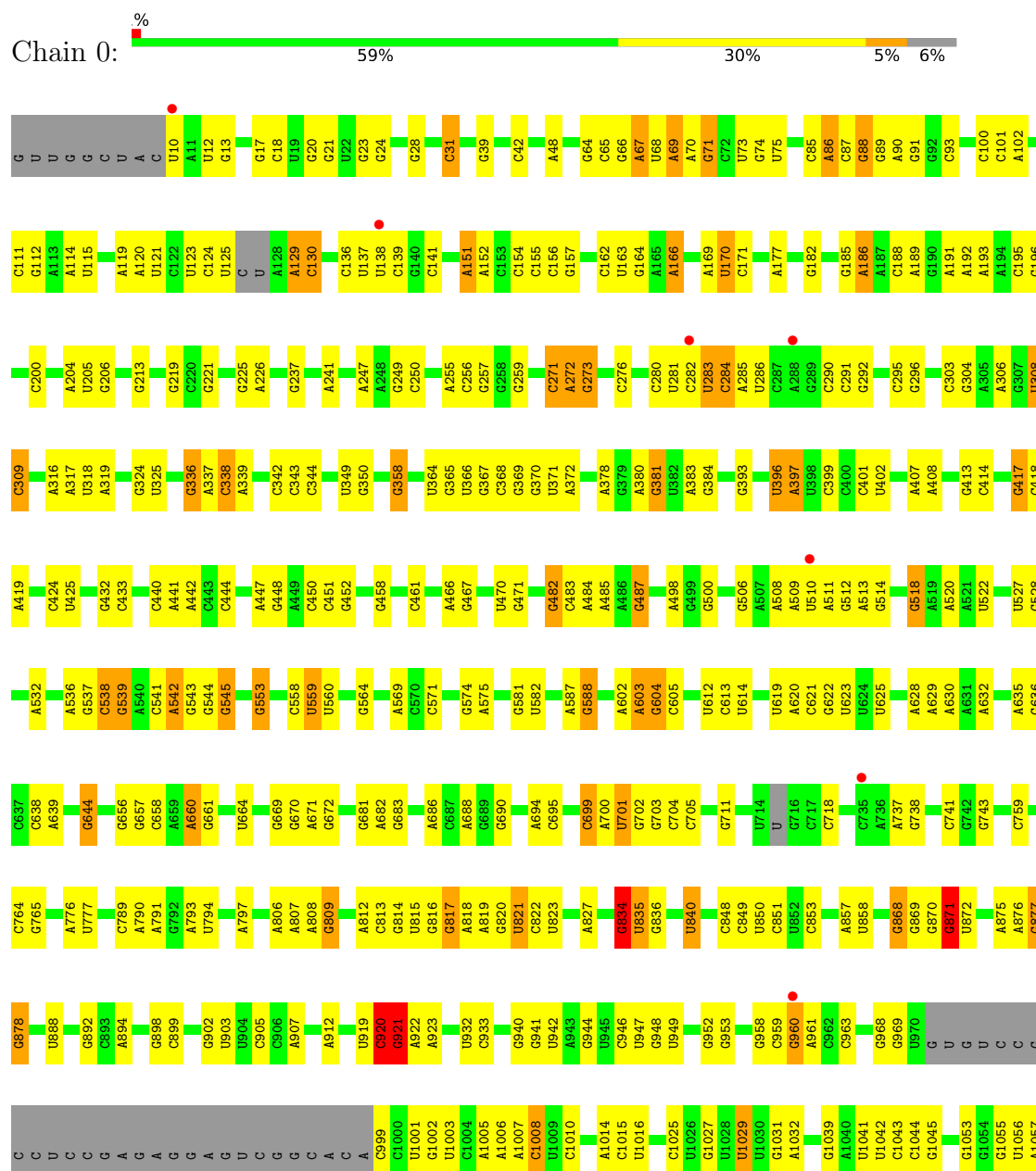
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	X	25	Total 25	O 25	0	0
39	Y	96	Total 96	O 96	0	0
39	Z	32	Total 32	O 32	0	0
39	1	52	Total 52	O 52	0	0
39	2	44	Total 44	O 44	0	0
39	3	66	Total 66	O 66	0	0
39	9	151	Total 151	O 151	0	0

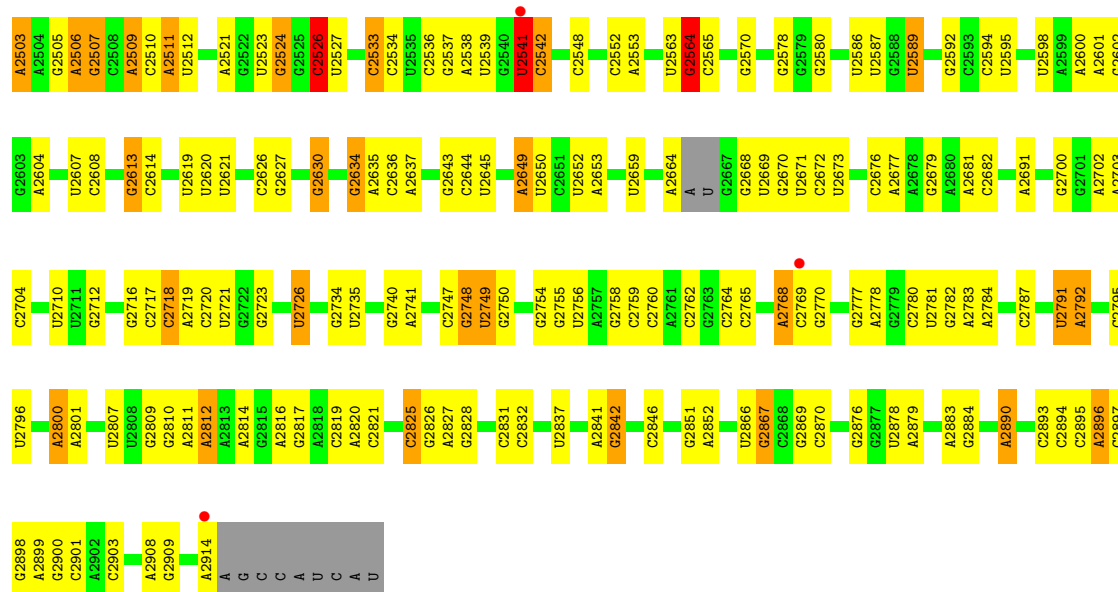
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

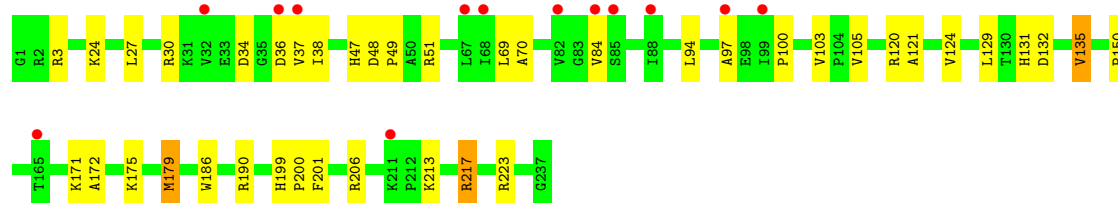
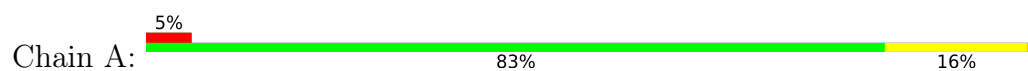
• Molecule 1: 23S ribosomal RNA



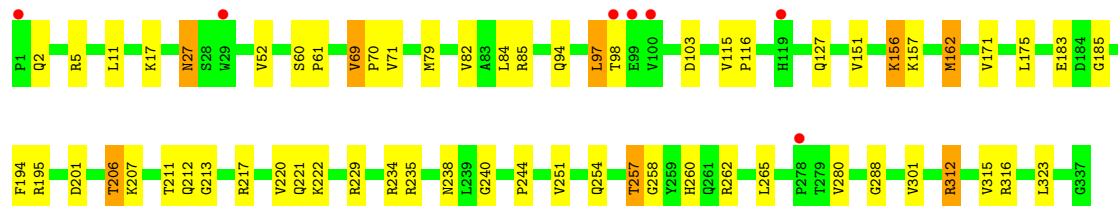
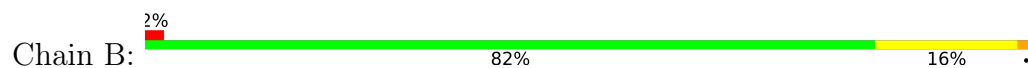
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A2291	U2297	A2300	A2301	A2302	A2414	U2308	C2309	C2313	G2314	G2315	G2316	C2317	U2320	A2321	G2338	A	C	A	G	G	G2344	G2345	G2346	C2347	C2348	C2241	U2242	C2243	A2361	A2362	G2363	A2364	G2365	A2369	G2370	G2371	A2372	U2373	G2379	A2380	G2381	A2382	G2385	U2386	U2387	C2388	U2389	C2502					
A	C	A	A	C	A	C	A	A	C	U	A	A	A	U	C	C	A	C	U	C	C	C	C	C	G2237	C2241	U2242	C2243	A2361	A2362	G2363	A2364	G2365	G2256	G2257	A2258	U2265	A2266	G2267	C2268	C2269	G2270	G2271	G2272	C2273	A2274	G2275	C2281	U2282				
C2031	U2032	G2033	U2034	A2039	C2040	G2050	A2054	U2064	C2065	C2066	G2072	G2073	A2074	A2081	C2087	C2088	A2089	C2090	G2091	G2092	A2096	A2100	A2101	G2102	C2103	C2104	G2110	G2111	C2114	U2115	G2121	C2122	G2128	U2133	G2134	A2135	G2136	A	C	A	G	U	C	G	C								
G1926	A1927	G1928	G1929	C1940	A1941	A1942	C1946	G1947	G1948	G1951	U	A	A	C	C	C	C	C	U	A	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U							
G1800	G1809	A1815	A1816	G1819	G1820	A1829	A1830	C1834	U1835	A1836	G1837	U1838	A1839	A1840	A1845	U1846	A1847	G1848	G1849	C1853	C1854	G1855	C1856	A1857	A1858	G1863	G1867	G1868	G1873	G1877	G1878	U1879	C1880	A1881	A1886	A1904	U1905	A1909	A2010	A2011	U2012	G2013	A1921	A1922	G1925								
U1702	C1705	G1706	C1714	C1715	A1716	A1717	U1722	G1723	U1724	C1725	G1730	C1731	A1732	A1733	U1741	A1742	C1750	G1751	G1752	C1753	A1754	A1755	G1756	C1762	C1763	U1766	A1767	C1768	C1769	U1770	U1771	C1772	G1773	G1774	A1778	A1779	A1783	U1784	C1787	C1790	U1791	G1795	A1796	A1797	C1798	G1799							
C1602	A1603	G1604	G1605	C1613	G1614	A1615	A1616	C1617	G1618	G1619	C1620	A1621	G1622	A1623	A1624	A1625	A1626	G1627	A1630	A1631	C1632	C1633	G1634	U1635	G1636	A1637	A1641	A1642	C1643	C1652	A1653	U1654	G1655	A1656	C1666	A1667	U1668	U1677	A1678	C1679	C1680	G1681	A1682	G1683	A1684	A1685	C1686	C1687	G1688	C1692	A1701		
G1497	U1500	U1503	A1504	U1505	U1506	U1524	G1525	A1526	A1527	G1529	G1535	C1536	C1537	U1544	C1545	U1548	G1552	C1553	A1554	G1555	G1556	A1559	U1561	C1562	G1568	U1569	A1573	C1574	G1575	G1576	U1577	U1583	C1584	U1588	G1589	G1592	C1594	G1595	U1596	A1597	A1598	U1599	A1482	C1483	G1484	A1485							
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A1058	G1059	C1060	C1069	A1070	G1071	G1072	U1169	A1078	A1081	A1088	U1096	A1097	A1098	G1099	C1102	C1103	C1104	U1109	G1110	U1116	A1117	G1118	G1119	U1120	G1121	A1123	C1129	U1130	G1131	A1132	G1137	G1151	A1154	G1155	G1158	G1159	A1161	G1162	G1163	U1164	G1165	A1166	G1167	C1168									



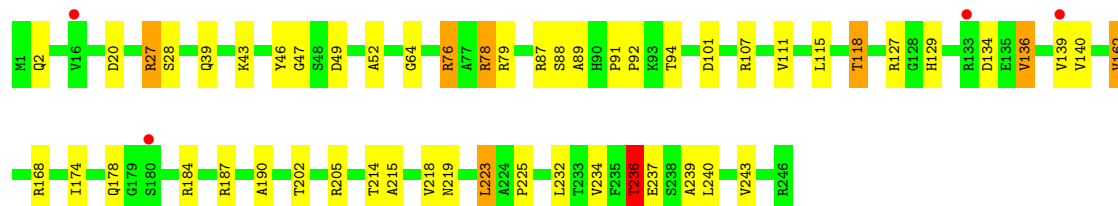
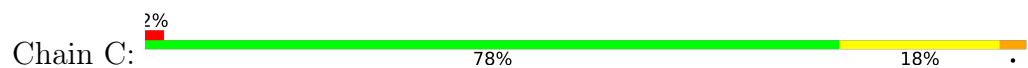
• Molecule 2: 50S ribosomal protein L2P



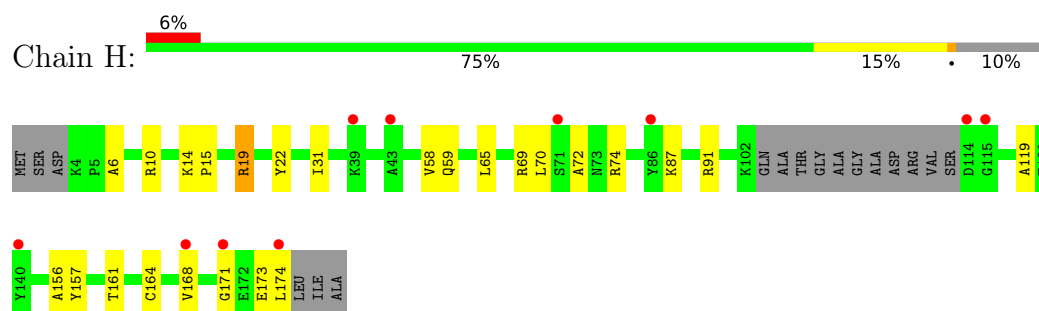
• Molecule 3: 50S ribosomal protein L3P



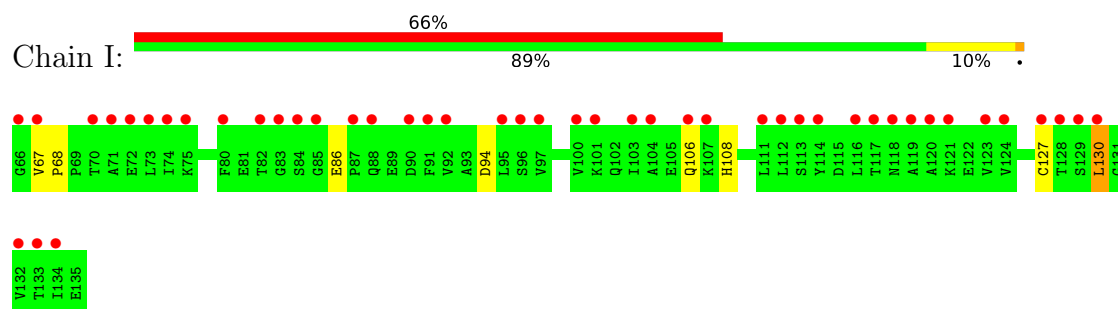
• Molecule 4: 50S ribosomal protein L4P



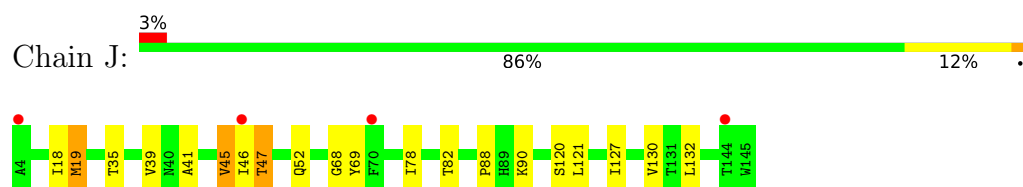
- Molecule 9: 50S ribosomal protein L10e



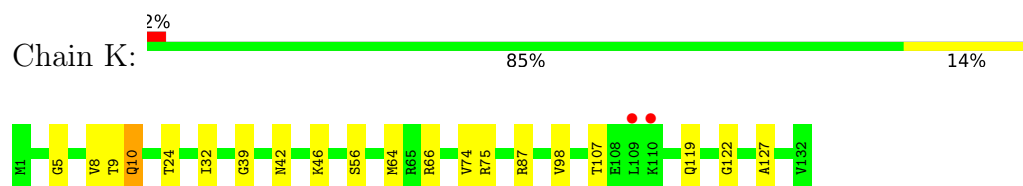
- Molecule 10: 50S ribosomal protein L11P



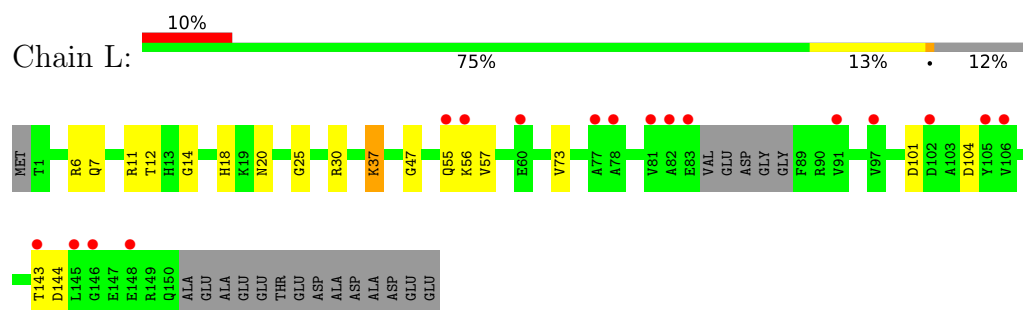
- Molecule 11: 50S ribosomal protein L13P



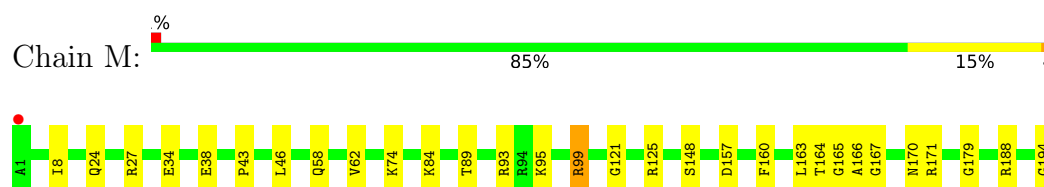
- Molecule 12: 50S ribosomal protein L14P



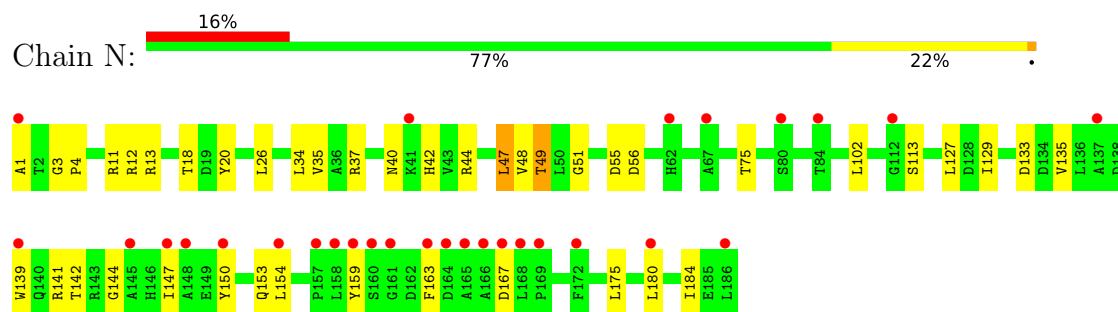
- Molecule 13: 50S ribosomal protein L15P



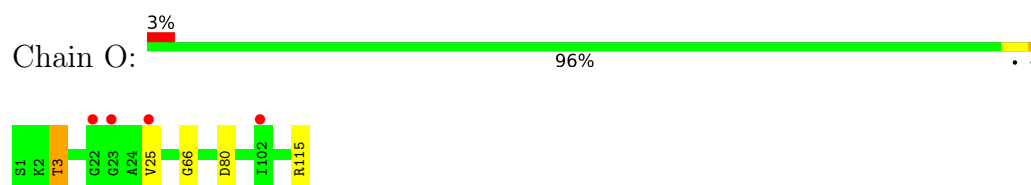
- Molecule 14: 50S ribosomal protein L15e



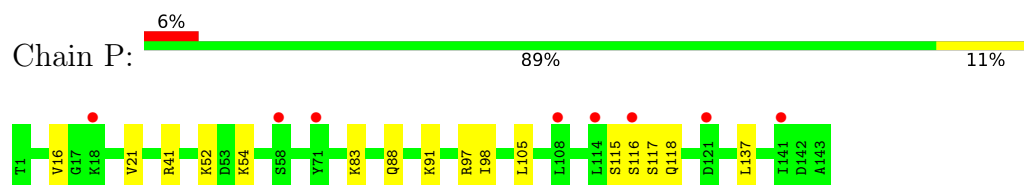
• Molecule 15: 50S ribosomal protein L18P



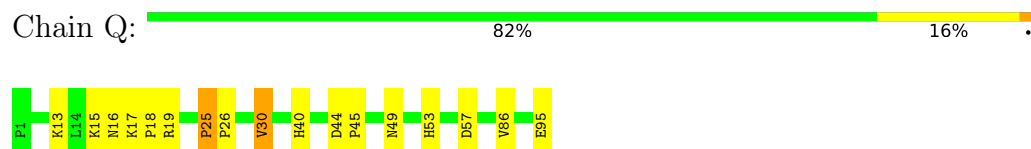
• Molecule 16: 50S ribosomal protein L18e



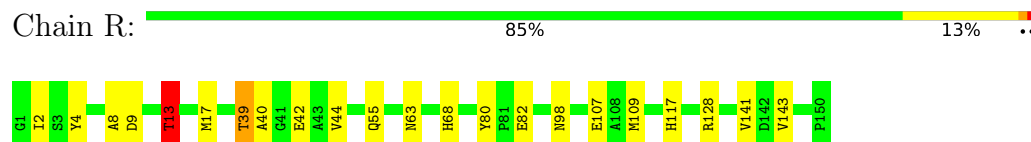
• Molecule 17: 50S ribosomal protein L19e



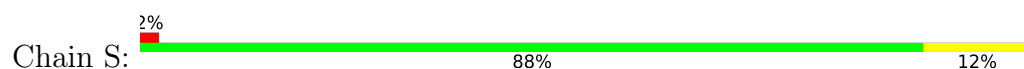
• Molecule 18: 50S ribosomal protein L21e

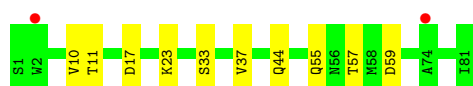


• Molecule 19: 50S ribosomal protein L22P

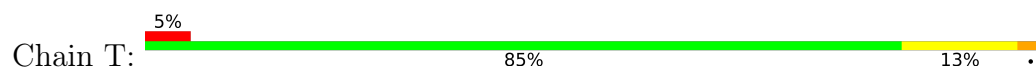


• Molecule 20: 50S ribosomal protein L23P

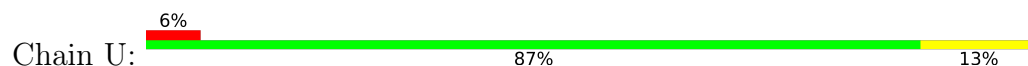




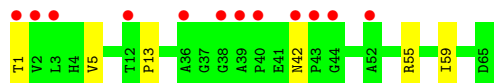
- Molecule 21: 50S ribosomal protein L24P



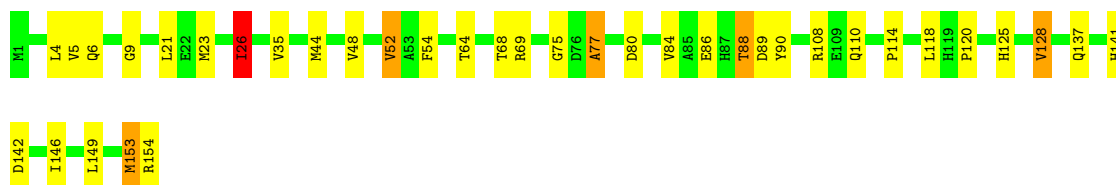
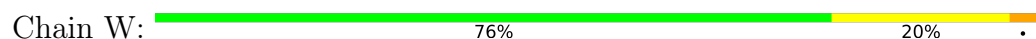
- Molecule 22: 50S ribosomal protein L24e



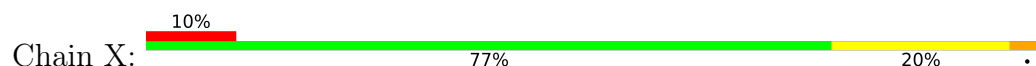
- Molecule 23: 50S ribosomal protein L29P



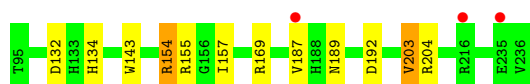
- Molecule 24: 50S ribosomal protein L30P



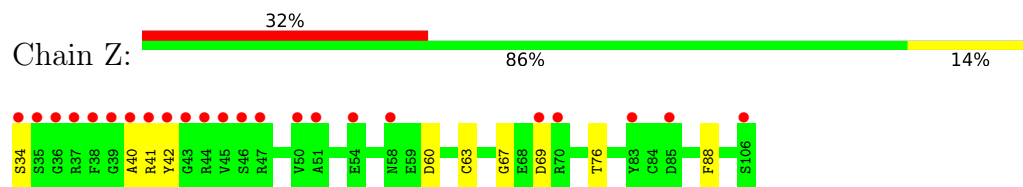
- Molecule 25: 50S ribosomal protein L31e



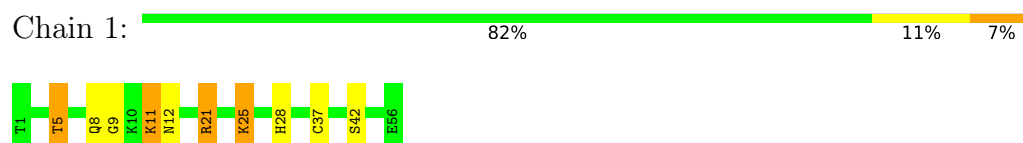
- Molecule 26: 50S ribosomal protein L32e



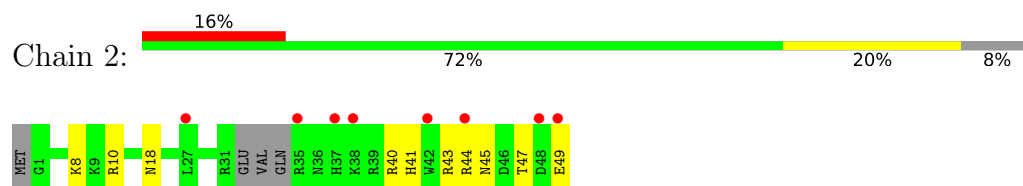
- Molecule 27: 50S ribosomal protein L37Ae



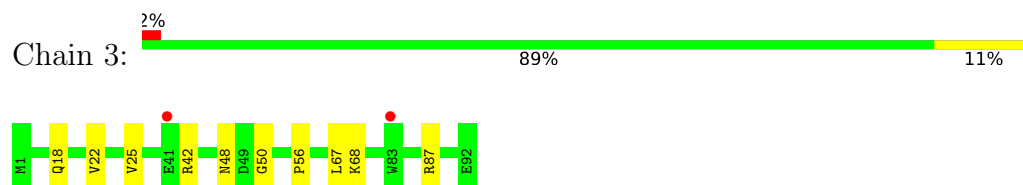
- Molecule 28: 50S ribosomal protein L37e



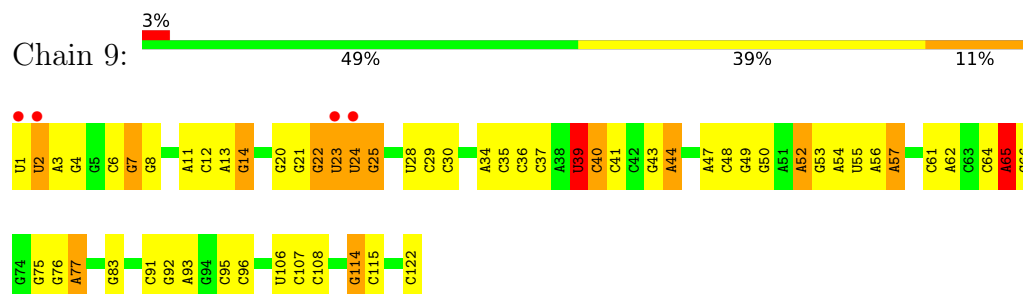
- Molecule 29: 50S ribosomal protein L39e



- 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, α , β , γ	211.86Å 299.42Å 574.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 2.70 49.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.90-2.70) 94.0 (49.90-2.70)	Depositor EDS
R_{merge}	0.07	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}	0.190 , 0.229 0.184 , 0.221	Depositor DCC
R_{free} test set	6547 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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, OMG, UR3, SR, CD, NA, K, OMU, HMT, PSU, CL, MG

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	0.60	19/102869 (0.0%)
2	A	0.64	0/1787	1.10	6/2408 (0.2%)
3	B	0.64	3/2690 (0.1%)	1.09	14/3652 (0.4%)
4	C	0.64	0/1885	1.12	8/2552 (0.3%)
5	D	0.71	0/1111	1.03	4/1498 (0.3%)
6	E	0.67	0/1383	0.99	3/1880 (0.2%)
7	F	0.71	1/901 (0.1%)	1.10	2/1224 (0.2%)
8	G	0.61	0/241	1.01	0/324
9	H	0.64	0/1302	1.05	6/1743 (0.3%)
10	I	0.78	1/527 (0.2%)	1.12	5/716 (0.7%)
11	J	0.64	1/1136 (0.1%)	1.11	3/1530 (0.2%)
12	K	0.62	0/1004	1.12	5/1351 (0.4%)
13	L	0.58	0/1130	1.08	7/1509 (0.5%)
14	M	0.56	0/1583	1.06	4/2116 (0.2%)
15	N	0.61	0/1474	1.19	15/1999 (0.8%)
16	O	0.60	0/874	1.08	1/1181 (0.1%)
17	P	0.55	0/1148	1.04	1/1528 (0.1%)
18	Q	0.59	0/749	1.13	7/1005 (0.7%)
19	R	0.65	1/1173 (0.1%)	1.08	4/1578 (0.3%)
20	S	0.60	0/649	0.96	0/875
21	T	0.57	0/958	1.10	4/1289 (0.3%)
22	U	0.60	0/418	1.09	3/562 (0.5%)
23	V	0.60	0/503	1.11	2/675 (0.3%)
24	W	0.68	1/1219 (0.1%)	1.17	9/1655 (0.5%)
25	X	0.67	0/665	1.18	6/895 (0.7%)
26	Y	0.61	0/1147	1.05	2/1536 (0.1%)
27	Z	0.66	0/585	1.11	3/781 (0.4%)
28	1	0.57	0/438	1.07	5/578 (0.9%)
29	2	0.53	0/401	0.98	1/529 (0.2%)
30	3	0.57	0/771	0.93	1/1024 (0.1%)
31	9	0.37	0/2904	0.58	1/4526 (0.0%)
All	All	0.47	8/98714 (0.0%)	0.76	151/147588 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	0	0	42
24	W	0	1
31	9	0	2
All	All	0	45

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	63	ILE	CA-CB	9.59	1.58	1.54
19	R	109	MET	SD-CE	-8.29	1.58	1.79
3	B	162	MET	SD-CE	-6.54	1.63	1.79
10	I	68	PRO	CA-C	5.95	1.55	1.51
24	W	153	MET	SD-CE	-5.88	1.64	1.79

The worst 5 of 151 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	170	TYR	N-CA-C	10.12	125.20	112.86
21	T	52	ARG	N-CA-C	9.29	125.14	113.43
15	N	163	PHE	N-CA-C	-8.86	100.25	112.12
18	Q	17	LYS	N-CA-C	-8.44	99.47	109.93
24	W	75	GLY	N-CA-C	8.08	120.28	112.04

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	852	0
2	A	1754	0	1766	21	0
3	B	2625	0	2533	28	0
4	C	1860	0	1813	26	0
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	15	0
10	I	520	0	500	2	0
11	J	1120	0	1098	16	0
12	K	994	0	1027	10	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	13	0
20	S	642	0	605	5	0
21	T	950	0	924	12	0
22	U	411	0	364	2	0
23	V	500	0	511	3	0
24	W	1196	0	1137	20	0
25	X	655	0	653	7	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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1077	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 1077 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:H5'	1:0:871:G:C8	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%)	9	25
3	B	335/337 (99%)	314 (94%)	18 (5%)	3 (1%)	14	35
4	C	244/246 (99%)	227 (93%)	17 (7%)	0	100	100
5	D	134/177 (76%)	121 (90%)	11 (8%)	2 (2%)	8	22
6	E	170/172 (99%)	161 (95%)	9 (5%)	0	100	100
7	F	117/119 (98%)	112 (96%)	3 (3%)	2 (2%)	7	19
8	G	25/348 (7%)	25 (100%)	0	0	100	100
9	H	156/177 (88%)	149 (96%)	5 (3%)	2 (1%)	9	25
10	I	68/70 (97%)	56 (82%)	11 (16%)	1 (2%)	8	22
11	J	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
12	K	130/132 (98%)	124 (95%)	5 (4%)	1 (1%)	16	37
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%)	7	20
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%)	18	41
25	X	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
26	Y	140/142 (99%)	137 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	Z	71/73 (97%)	65 (92%)	5 (7%)	1 (1%)	9	23
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%)	24	48

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%)	169 (94%)	10 (6%)	19	44
3	B	282/282 (100%)	265 (94%)	17 (6%)	17	41
4	C	193/193 (100%)	175 (91%)	18 (9%)	8	21
5	D	117/148 (79%)	108 (92%)	9 (8%)	12	30
6	E	152/152 (100%)	149 (98%)	3 (2%)	48	76
7	F	93/93 (100%)	90 (97%)	3 (3%)	34	64
8	G	27/282 (10%)	27 (100%)	0	100	100
9	H	134/145 (92%)	130 (97%)	4 (3%)	36	66
10	I	58/58 (100%)	56 (97%)	2 (3%)	32	62
11	J	118/118 (100%)	112 (95%)	6 (5%)	21	48
12	K	106/106 (100%)	102 (96%)	4 (4%)	29	58
13	L	113/127 (89%)	108 (96%)	5 (4%)	25	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	M	158/158 (100%)	153 (97%)	5 (3%)	34	64
15	N	149/149 (100%)	141 (95%)	8 (5%)	20	45
16	O	93/93 (100%)	89 (96%)	4 (4%)	26	54
17	P	113/113 (100%)	108 (96%)	5 (4%)	25	53
18	Q	79/79 (100%)	75 (95%)	4 (5%)	21	48
19	R	117/117 (100%)	113 (97%)	4 (3%)	32	62
20	S	71/71 (100%)	69 (97%)	2 (3%)	38	68
21	T	105/105 (100%)	99 (94%)	6 (6%)	18	43
22	U	44/44 (100%)	43 (98%)	1 (2%)	44	73
23	V	51/51 (100%)	50 (98%)	1 (2%)	48	76
24	W	130/130 (100%)	124 (95%)	6 (5%)	24	51
25	X	66/66 (100%)	59 (89%)	7 (11%)	6	17
26	Y	120/120 (100%)	116 (97%)	4 (3%)	33	63
27	Z	60/60 (100%)	60 (100%)	0	100	100
28	1	46/46 (100%)	45 (98%)	1 (2%)	45	74
29	2	42/46 (91%)	41 (98%)	1 (2%)	43	72
30	3	79/79 (100%)	75 (95%)	4 (5%)	21	48
All	All	3095/3410 (91%)	2951 (95%)	144 (5%)	23	51

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	T	82	THR
30	3	87	ARG
22	U	52	THR
25	X	72	VAL
5	D	52	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 88 such sidechains are listed below:

Mol	Chain	Res	Type
19	R	98	ASN
24	W	27	HIS
19	R	122	GLN
20	S	56	ASN

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Mol	Chain	Res	Type
25	X	22	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	0	2745/2923 (93%)	232 (8%)	30 (1%)
31	9	121/122 (99%)	18 (14%)	1 (0%)
All	All	2866/3045 (94%)	250 (8%)	31 (1%)

5 of 250 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	2718	C
1	0	1685	A
1	0	2791	U
1	0	2541	U

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	PSU	0	2621	1	18,21,22	1.42	2 (11%)	21,30,33	1.27	3 (14%)
1	OMG	0	2588	1	23,26,27	0.30	0	32,38,41	0.37	0
1	UR3	0	2619	1	19,22,23	0.55	0	26,32,35	0.67	1 (3%)
1	1MA	0	628	34,1	21,25,26	0.69	1 (4%)	30,37,40	0.74	1 (3%)
1	OMU	0	2587	34,1	19,22,23	0.32	0	25,31,34	0.43	0

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	PSU	0	2621	1	-	0/7/25/26	0/2/2/2
1	OMG	0	2588	1	-	0/9/27/28	0/3/3/3
1	UR3	0	2619	1	-	0/7/25/26	0/2/2/2
1	1MA	0	628	34,1	-	2/7/25/26	0/3/3/3
1	OMU	0	2587	34,1	-	0/9/27/28	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	0	2621	PSU	C2-N1	4.66	1.42	1.36
1	0	2621	PSU	C6-C5	2.73	1.38	1.35
1	0	628	1MA	C6-N6	2.41	1.33	1.28

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	0	2621	PSU	C6-C5-C4	3.13	120.29	118.17
1	0	2621	PSU	C6-N1-C2	-2.87	120.03	122.69
1	0	628	1MA	N1-C2-N3	2.79	129.31	126.00
1	0	2621	PSU	O2-C2-N1	2.63	125.49	122.79
1	0	2619	UR3	C4-N3-C2	2.61	126.68	124.58

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	0	628	1MA	C2'-C1'-N9-C8
1	0	628	1MA	C2'-C1'-N9-C4

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 oligosaccharides 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	-	41,43,43	0.69	0	43,66,66	2.05	12 (27%)

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	-	-	4/27/74/74	0/5/5/5

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	HMT	O7-C22-C21	4.87	119.71	111.16
37	0	9101	HMT	O4-C19-C20	4.29	119.11	111.24
37	0	9101	HMT	O1-C17-O2	-4.21	101.49	108.09
37	0	9101	HMT	C18-O3-C2	-3.61	110.58	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	0	9101	HMT	O1-C14-C13	3.19	132.10	127.86

There are no chirality outliers.

All (4) torsion outliers are listed below:

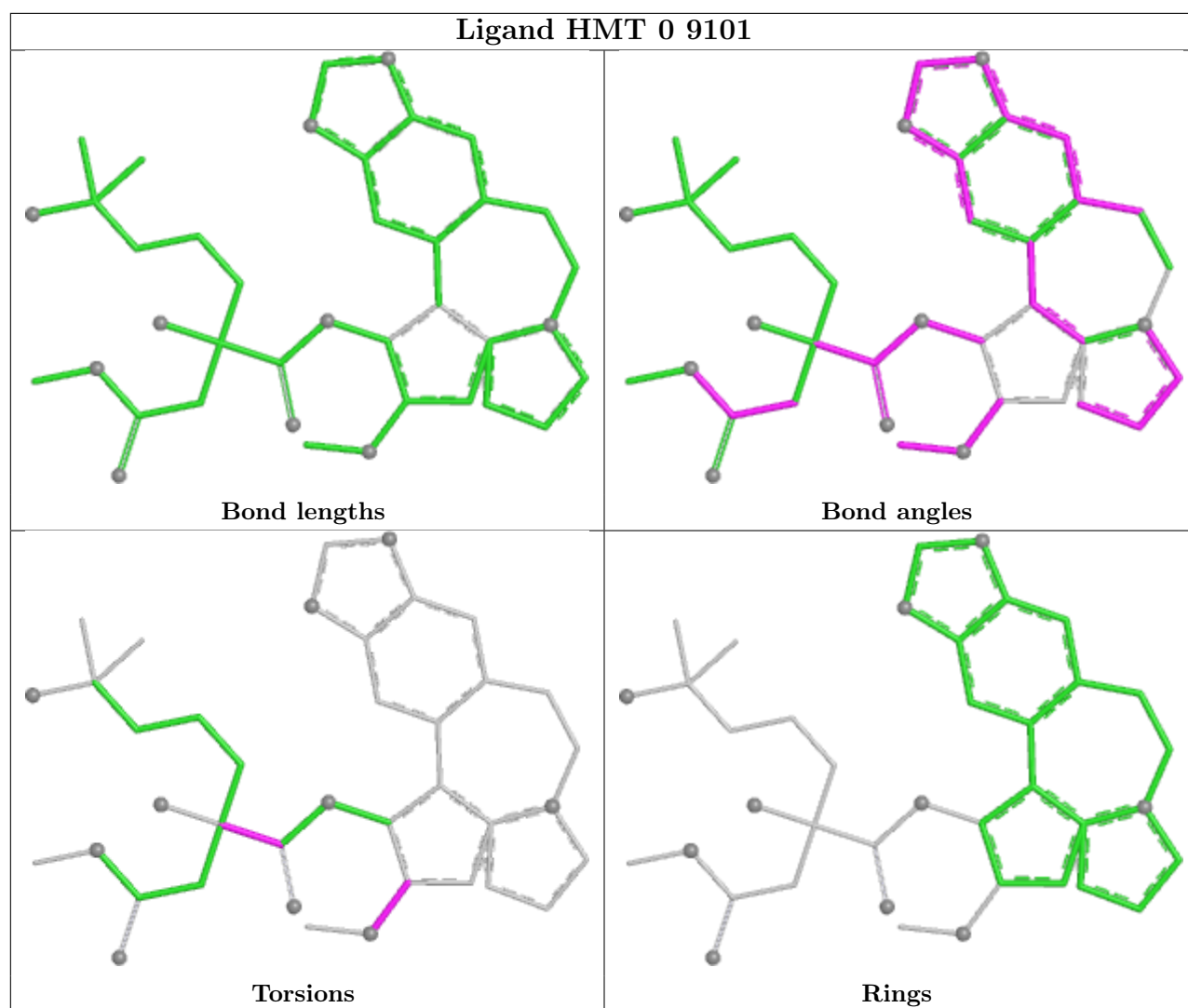
Mol	Chain	Res	Type	Atoms
37	0	9101	HMT	C1-C2-O3-C18
37	0	9101	HMT	C3-C2-O3-C18
37	0	9101	HMT	O5-C19-C20-C24
37	0	9101	HMT	O4-C19-C20-C24

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, 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%)	-0.45	37 (1%) 75 73	22, 50, 99, 170	0
2	A	237/237 (100%)	0.46	13 (5%) 30 27	30, 62, 104, 124	0
3	B	337/337 (100%)	0.39	7 (2%) 63 61	30, 59, 88, 105	0
4	C	246/246 (100%)	0.29	4 (1%) 70 68	25, 51, 78, 88	0
5	D	140/177 (79%)	1.82	49 (35%) 1 1	70, 112, 138, 148	0
6	E	172/172 (100%)	0.80	16 (9%) 14 12	51, 76, 98, 104	0
7	F	119/119 (100%)	1.03	11 (9%) 14 12	58, 83, 116, 132	0
8	G	29/348 (8%)	1.55	10 (34%) 1 1	78, 102, 109, 111	0
9	H	160/177 (90%)	0.61	10 (6%) 26 23	49, 73, 112, 120	0
10	I	70/70 (100%)	2.67	46 (65%) 0 0	140, 157, 176, 177	0
11	J	142/142 (100%)	0.29	4 (2%) 55 51	39, 56, 79, 98	0
12	K	132/132 (100%)	0.27	2 (1%) 72 70	39, 56, 81, 85	0
13	L	145/165 (87%)	0.84	17 (11%) 9 7	30, 76, 128, 140	0
14	M	194/194 (100%)	0.13	1 (0%) 87 86	35, 49, 67, 73	0
15	N	186/186 (100%)	1.00	29 (15%) 5 4	48, 75, 130, 137	0
16	O	115/115 (100%)	0.60	4 (3%) 47 43	42, 61, 79, 88	0
17	P	143/143 (100%)	0.64	8 (5%) 30 26	43, 63, 80, 87	0
18	Q	95/95 (100%)	0.09	0 100 100	40, 53, 67, 79	0
19	R	150/150 (100%)	-0.08	0 100 100	33, 51, 71, 82	0
20	S	81/81 (100%)	0.43	2 (2%) 58 55	49, 68, 90, 99	0
21	T	119/119 (100%)	0.62	6 (5%) 34 30	42, 66, 92, 119	0
22	U	53/53 (100%)	0.51	3 (5%) 29 26	46, 63, 84, 89	0
23	V	65/65 (100%)	1.36	12 (18%) 3 3	62, 87, 128, 136	0
24	W	154/154 (100%)	0.36	0 100 100	38, 56, 73, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	82/82 (100%)	0.64	8 (9%) 13 11	50, 68, 93, 107	0
26	Y	142/142 (100%)	0.15	3 (2%) 63 61	26, 50, 75, 96	0
27	Z	73/73 (100%)	1.58	23 (31%) 1 1	69, 94, 110, 115	0
28	1	56/56 (100%)	-0.36	0 100 100	30, 36, 44, 54	0
29	2	46/50 (92%)	0.78	8 (17%) 4 3	41, 70, 100, 111	0
30	3	92/92 (100%)	0.40	2 (2%) 62 59	42, 70, 83, 95	0
31	9	122/122 (100%)	0.06	4 (3%) 49 45	42, 72, 98, 150	0
All	All	6646/7217 (92%)	0.15	339 (5%) 33 29	22, 58, 112, 177	0

The worst 5 of 339 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
23	V	1	THR	10.8
10	I	128	THR	7.8
5	D	10	PHE	7.1
31	9	1	U	6.1
23	V	39	ALA	6.0

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	UR3	0	2619	21/22	0.97	0.07	40,43,45,50	0
1	OMU	0	2587	21/22	0.98	0.06	35,38,41,42	0
1	OMG	0	2588	24/25	0.98	0.06	35,38,39,41	0
1	1MA	0	628	23/24	0.98	0.06	31,34,35,38	0
1	PSU	0	2621	20/21	0.98	0.06	26,30,42,42	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	0	8573	1/1	0.42	0.54	92,92,92,92	0
36	SR	0	8983	1/1	0.51	0.28	191,191,191,191	0
34	NA	0	8571	1/1	0.52	0.38	96,96,96,96	0
36	SR	9	9003	1/1	0.53	0.23	194,194,194,194	0
36	SR	0	8976	1/1	0.60	0.22	199,199,199,199	0
34	NA	0	8557	1/1	0.63	0.40	77,77,77,77	0
34	NA	0	8561	1/1	0.63	0.95	99,99,99,99	0
36	SR	0	8956	1/1	0.63	0.15	183,183,183,183	0
34	NA	0	8525	1/1	0.64	0.23	70,70,70,70	0
36	SR	0	8959	1/1	0.67	0.17	189,189,189,189	0
32	MG	0	8049	1/1	0.67	0.32	95,95,95,95	0
36	SR	0	9004	1/1	0.69	0.20	200,200,200,200	0
36	SR	0	9001	1/1	0.69	0.18	187,187,187,187	0
36	SR	J	8986	1/1	0.70	0.37	200,200,200,200	0
34	NA	0	8522	1/1	0.71	0.58	96,96,96,96	0
36	SR	0	8923	1/1	0.71	0.25	192,192,192,192	0
36	SR	0	8982	1/1	0.73	0.36	200,200,200,200	0
36	SR	0	8933	1/1	0.73	0.28	159,159,159,159	0
36	SR	0	8944	1/1	0.73	0.18	187,187,187,187	0
36	SR	0	8919	1/1	0.73	0.22	168,168,168,168	0
36	SR	0	8922	1/1	0.73	0.21	158,158,158,158	0
34	NA	0	8570	1/1	0.73	0.28	59,59,59,59	0
36	SR	9	8980	1/1	0.74	0.15	188,188,188,188	0
36	SR	0	8993	1/1	0.74	0.18	186,186,186,186	0
36	SR	0	8947	1/1	0.75	0.23	199,199,199,199	0
36	SR	0	8913	1/1	0.75	0.39	169,169,169,169	0
34	NA	0	8560	1/1	0.75	0.25	73,73,73,73	0
32	MG	0	8063	1/1	0.76	0.30	79,79,79,79	0
36	SR	A	8977	1/1	0.76	0.10	182,182,182,182	0
34	NA	0	8559	1/1	0.76	0.54	98,98,98,98	0
36	SR	9	8978	1/1	0.76	0.21	165,165,165,165	0
36	SR	0	9000	1/1	0.76	0.25	180,180,180,180	0
34	NA	0	8518	1/1	0.76	0.50	96,96,96,96	0
34	NA	0	8546	1/1	0.77	0.47	107,107,107,107	0
36	SR	0	8997	1/1	0.77	0.37	200,200,200,200	0
34	NA	0	8509	1/1	0.77	0.31	71,71,71,71	0
34	NA	0	8574	1/1	0.77	0.51	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	8989	1/1	0.77	0.26	191,191,191,191	0
34	NA	0	8567	1/1	0.78	0.57	81,81,81,81	0
34	NA	0	8511	1/1	0.78	0.35	91,91,91,91	0
32	MG	A	8051	1/1	0.78	0.13	92,92,92,92	0
36	SR	0	8920	1/1	0.78	0.25	200,200,200,200	0
32	MG	0	8083	1/1	0.78	0.16	68,68,68,68	0
36	SR	0	9006	1/1	0.79	0.28	200,200,200,200	0
34	NA	0	8555	1/1	0.79	0.38	59,59,59,59	0
36	SR	0	8996	1/1	0.79	0.27	200,200,200,200	0
36	SR	B	8987	1/1	0.80	0.44	200,200,200,200	0
34	NA	S	8510	1/1	0.80	0.13	51,51,51,51	0
34	NA	0	8548	1/1	0.80	0.33	61,61,61,61	0
36	SR	0	8979	1/1	0.80	0.16	196,196,196,196	0
36	SR	0	8991	1/1	0.80	0.18	199,199,199,199	0
32	MG	0	8092	1/1	0.81	0.31	80,80,80,80	0
36	SR	B	8950	1/1	0.81	0.20	123,123,123,123	0
34	NA	0	8575	1/1	0.81	0.56	100,100,100,100	0
36	SR	0	8924	1/1	0.81	0.22	166,166,166,166	0
33	K	0	8401	1/1	0.81	0.39	130,130,130,130	0
36	SR	0	8975	1/1	0.81	0.19	150,150,150,150	0
36	SR	0	8942	1/1	0.81	0.15	138,138,138,138	0
34	NA	0	8520	1/1	0.82	0.30	60,60,60,60	0
34	NA	0	8501	1/1	0.83	0.16	43,43,43,43	0
36	SR	0	8988	1/1	0.83	0.09	182,182,182,182	0
34	NA	0	8554	1/1	0.83	0.30	72,72,72,72	0
36	SR	0	8927	1/1	0.83	0.18	172,172,172,172	0
36	SR	0	8968	1/1	0.83	0.17	168,168,168,168	0
34	NA	0	8533	1/1	0.83	0.38	73,73,73,73	0
36	SR	0	8938	1/1	0.83	0.17	198,198,198,198	0
34	NA	0	8564	1/1	0.83	0.17	74,74,74,74	0
32	MG	0	8056	1/1	0.83	0.22	67,67,67,67	0
34	NA	0	8523	1/1	0.84	0.15	54,54,54,54	0
36	SR	0	9002	1/1	0.84	0.15	176,176,176,176	0
36	SR	0	8957	1/1	0.84	0.22	200,200,200,200	0
34	NA	0	8541	1/1	0.84	0.19	59,59,59,59	0
36	SR	0	8960	1/1	0.84	0.12	162,162,162,162	0
36	SR	0	8990	1/1	0.84	0.23	161,161,161,161	0
34	NA	9	8572	1/1	0.84	0.12	82,82,82,82	0
36	SR	0	8974	1/1	0.84	0.17	183,183,183,183	0
32	MG	0	8090	1/1	0.84	0.26	96,96,96,96	0
34	NA	0	8531	1/1	0.84	0.25	56,56,56,56	0
36	SR	0	8953	1/1	0.84	0.20	179,179,179,179	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	0	8502	1/1	0.85	0.21	69,69,69,69	0
36	SR	0	8951	1/1	0.85	0.10	144,144,144,144	0
36	SR	0	8916	1/1	0.85	0.19	118,118,118,118	0
36	SR	0	8965	1/1	0.85	0.15	145,145,145,145	0
32	MG	0	8069	1/1	0.85	0.43	82,82,82,82	0
36	SR	0	8971	1/1	0.85	0.21	181,181,181,181	0
36	SR	A	8930	1/1	0.85	0.16	147,147,147,147	0
37	HMT	0	9101	39/39	0.85	0.21	69,75,86,87	0
32	MG	0	8085	1/1	0.86	0.44	89,89,89,89	0
36	SR	0	8995	1/1	0.86	0.17	148,148,148,148	0
36	SR	0	8949	1/1	0.86	0.17	134,134,134,134	0
34	NA	0	8536	1/1	0.86	0.13	56,56,56,56	0
36	SR	F	9005	1/1	0.86	0.11	138,138,138,138	0
36	SR	0	8984	1/1	0.86	0.16	157,157,157,157	0
32	MG	0	8037	1/1	0.86	0.37	83,83,83,83	0
34	NA	Q	8540	1/1	0.86	0.26	67,67,67,67	0
32	MG	9	8040	1/1	0.86	0.35	103,103,103,103	0
34	NA	0	8506	1/1	0.86	0.12	65,65,65,65	0
34	NA	0	8552	1/1	0.87	0.27	73,73,73,73	0
32	MG	9	8074	1/1	0.87	0.20	71,71,71,71	0
36	SR	0	8994	1/1	0.87	0.31	200,200,200,200	0
36	SR	0	8917	1/1	0.88	0.13	117,117,117,117	0
32	MG	0	8053	1/1	0.88	0.25	79,79,79,79	0
34	NA	0	8568	1/1	0.88	0.17	60,60,60,60	0
34	NA	0	8542	1/1	0.88	0.21	52,52,52,52	0
32	MG	0	8031	1/1	0.88	0.17	83,83,83,83	0
34	NA	0	8562	1/1	0.88	0.34	63,63,63,63	0
36	SR	0	8915	1/1	0.88	0.14	128,128,128,128	0
32	MG	0	8080	1/1	0.88	0.11	75,75,75,75	0
36	SR	0	8936	1/1	0.88	0.12	106,106,106,106	0
32	MG	0	8071	1/1	0.89	0.35	72,72,72,72	0
36	SR	0	8967	1/1	0.89	0.15	132,132,132,132	0
32	MG	0	8035	1/1	0.89	0.26	63,63,63,63	0
34	NA	0	8529	1/1	0.89	0.20	46,46,46,46	0
36	SR	0	8928	1/1	0.89	0.18	140,140,140,140	0
34	NA	0	8569	1/1	0.89	0.21	70,70,70,70	0
36	SR	0	8955	1/1	0.89	0.24	200,200,200,200	0
36	SR	0	8934	1/1	0.89	0.23	172,172,172,172	0
34	NA	R	8532	1/1	0.89	0.25	59,59,59,59	0
34	NA	0	8547	1/1	0.89	0.26	49,49,49,49	0
34	NA	0	8556	1/1	0.89	0.24	47,47,47,47	0
36	SR	0	8985	1/1	0.89	0.14	122,122,122,122	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8077	1/1	0.90	0.08	38,38,38,38	0
36	SR	0	8992	1/1	0.90	0.37	132,132,132,132	0
36	SR	0	8931	1/1	0.90	0.11	114,114,114,114	0
36	SR	0	8939	1/1	0.90	0.14	147,147,147,147	0
36	SR	0	8941	1/1	0.90	0.11	113,113,113,113	0
36	SR	0	9007	1/1	0.90	0.37	200,200,200,200	0
36	SR	0	8910	1/1	0.90	0.14	108,108,108,108	0
32	MG	0	8039	1/1	0.90	0.17	56,56,56,56	0
32	MG	0	8030	1/1	0.91	0.29	91,91,91,91	0
36	SR	0	8958	1/1	0.91	0.09	105,105,105,105	0
32	MG	0	8066	1/1	0.91	0.21	62,62,62,62	0
34	NA	0	8519	1/1	0.91	0.11	42,42,42,42	0
36	SR	0	8964	1/1	0.91	0.09	130,130,130,130	0
36	SR	0	8981	1/1	0.91	0.16	159,159,159,159	0
34	NA	0	8507	1/1	0.91	0.15	49,49,49,49	0
34	NA	M	8539	1/1	0.91	0.13	42,42,42,42	0
32	MG	0	8033	1/1	0.91	0.15	54,54,54,54	0
32	MG	T	8057	1/1	0.92	0.18	70,70,70,70	0
36	SR	0	8998	1/1	0.92	0.21	155,155,155,155	0
34	NA	0	8549	1/1	0.92	0.32	64,64,64,64	0
34	NA	0	8551	1/1	0.92	0.16	49,49,49,49	0
32	MG	0	8064	1/1	0.92	0.13	46,46,46,46	0
34	NA	0	8534	1/1	0.92	0.11	44,44,44,44	0
34	NA	9	8543	1/1	0.92	0.26	50,50,50,50	0
36	SR	0	8926	1/1	0.92	0.11	132,132,132,132	0
34	NA	9	8544	1/1	0.92	0.25	68,68,68,68	0
32	MG	0	8078	1/1	0.92	0.13	49,49,49,49	0
35	CL	0	8816	1/1	0.92	0.17	63,63,63,63	0
35	CL	J	8801	1/1	0.92	0.14	70,70,70,70	0
35	CL	J	8802	1/1	0.92	0.12	72,72,72,72	0
36	SR	0	8901	1/1	0.92	0.09	93,93,93,93	0
36	SR	S	8961	1/1	0.92	0.09	141,141,141,141	0
32	MG	0	8020	1/1	0.92	0.30	66,66,66,66	0
32	MG	0	8073	1/1	0.92	0.42	96,96,96,96	0
34	NA	0	8513	1/1	0.92	0.17	53,53,53,53	0
34	NA	0	8514	1/1	0.92	0.10	47,47,47,47	0
32	MG	0	8034	1/1	0.93	0.06	48,48,48,48	0
32	MG	0	8089	1/1	0.93	0.09	45,45,45,45	0
34	NA	0	8537	1/1	0.93	0.06	45,45,45,45	0
34	NA	0	8563	1/1	0.93	0.32	70,70,70,70	0
34	NA	C	8503	1/1	0.93	0.10	40,40,40,40	0
36	SR	0	8962	1/1	0.93	0.21	168,168,168,168	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
36	SR	A	8929	1/1	0.93	0.22	134,134,134,134	0
36	SR	0	8963	1/1	0.93	0.07	132,132,132,132	0
34	NA	J	8538	1/1	0.93	0.14	62,62,62,62	0
36	SR	0	8945	1/1	0.93	0.11	117,117,117,117	0
34	NA	0	8524	1/1	0.93	0.10	57,57,57,57	0
36	SR	0	8948	1/1	0.93	0.10	107,107,107,107	0
36	SR	0	8970	1/1	0.93	0.08	131,131,131,131	0
34	NA	0	8516	1/1	0.93	0.15	39,39,39,39	0
36	SR	1	8952	1/1	0.93	0.09	85,85,85,85	0
36	SR	3	8999	1/1	0.93	0.07	110,110,110,110	0
36	SR	0	8973	1/1	0.93	0.11	139,139,139,139	0
32	MG	0	8024	1/1	0.93	0.10	47,47,47,47	0
32	MG	0	8072	1/1	0.93	0.12	62,62,62,62	0
32	MG	0	8067	1/1	0.93	0.07	35,35,35,35	0
35	CL	A	8809	1/1	0.94	0.21	72,72,72,72	0
36	SR	0	8969	1/1	0.94	0.27	149,149,149,149	0
36	SR	0	8954	1/1	0.94	0.08	109,109,109,109	0
34	NA	0	8508	1/1	0.94	0.10	46,46,46,46	0
34	NA	0	8528	1/1	0.94	0.07	50,50,50,50	0
35	CL	Y	8820	1/1	0.94	0.07	45,45,45,45	0
32	MG	0	8010	1/1	0.94	0.08	52,52,52,52	0
32	MG	0	8059	1/1	0.94	0.13	50,50,50,50	0
36	SR	0	8911	1/1	0.94	0.07	92,92,92,92	0
36	SR	0	8946	1/1	0.94	0.09	117,117,117,117	0
32	MG	0	8075	1/1	0.94	0.13	58,58,58,58	0
34	NA	0	8565	1/1	0.94	0.17	73,73,73,73	0
32	MG	0	8036	1/1	0.94	0.12	50,50,50,50	0
36	SR	0	8966	1/1	0.94	0.10	113,113,113,113	0
32	MG	0	8017	1/1	0.94	0.09	39,39,39,39	0
32	MG	B	8042	1/1	0.95	0.20	60,60,60,60	0
36	SR	0	8914	1/1	0.95	0.10	113,113,113,113	0
32	MG	0	8038	1/1	0.95	0.07	63,63,63,63	0
34	NA	0	8515	1/1	0.95	0.09	43,43,43,43	0
36	SR	0	8972	1/1	0.95	0.22	135,135,135,135	0
32	MG	Y	8086	1/1	0.95	0.06	46,46,46,46	0
36	SR	0	8918	1/1	0.95	0.08	87,87,87,87	0
34	NA	0	8530	1/1	0.95	0.17	56,56,56,56	0
34	NA	0	8550	1/1	0.95	0.19	59,59,59,59	0
36	SR	0	8921	1/1	0.95	0.07	94,94,94,94	0
34	NA	0	8566	1/1	0.95	0.28	47,47,47,47	0
32	MG	2	8060	1/1	0.95	0.12	56,56,56,56	0
35	CL	0	8815	1/1	0.95	0.12	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8082	1/1	0.95	0.12	70,70,70,70	0
34	NA	0	8553	1/1	0.95	0.21	75,75,75,75	0
32	MG	0	8032	1/1	0.95	0.05	41,41,41,41	0
34	NA	0	8535	1/1	0.95	0.15	52,52,52,52	0
35	CL	L	8810	1/1	0.95	0.12	54,54,54,54	0
34	NA	0	8521	1/1	0.95	0.08	67,67,67,67	0
32	MG	0	8044	1/1	0.95	0.06	55,55,55,55	0
36	SR	0	8908	1/1	0.95	0.07	100,100,100,100	0
34	NA	0	8558	1/1	0.95	0.16	50,50,50,50	0
34	NA	0	8512	1/1	0.95	0.23	48,48,48,48	0
34	NA	0	8526	1/1	0.96	0.10	47,47,47,47	0
36	SR	0	8909	1/1	0.96	0.10	100,100,100,100	0
34	NA	0	8545	1/1	0.96	0.09	35,35,35,35	0
34	NA	0	8504	1/1	0.96	0.11	34,34,34,34	0
34	NA	0	8505	1/1	0.96	0.25	42,42,42,42	0
36	SR	0	8935	1/1	0.96	0.07	89,89,89,89	0
36	SR	0	9008	1/1	0.96	0.06	96,96,96,96	0
35	CL	0	8805	1/1	0.96	0.09	70,70,70,70	0
36	SR	0	8937	1/1	0.96	0.07	104,104,104,104	0
32	MG	0	8008	1/1	0.96	0.10	29,29,29,29	0
32	MG	0	8018	1/1	0.96	0.14	39,39,39,39	0
35	CL	0	8817	1/1	0.96	0.06	64,64,64,64	0
35	CL	0	8822	1/1	0.96	0.26	74,74,74,74	0
36	SR	0	8943	1/1	0.96	0.08	97,97,97,97	0
32	MG	0	8055	1/1	0.96	0.10	44,44,44,44	0
32	MG	0	8019	1/1	0.96	0.18	28,28,28,28	0
36	SR	3	8932	1/1	0.96	0.05	84,84,84,84	0
32	MG	0	8070	1/1	0.96	0.12	58,58,58,58	0
33	K	0	8402	1/1	0.96	0.12	65,65,65,65	0
35	CL	O	8808	1/1	0.96	0.12	69,69,69,69	0
32	MG	0	8001	1/1	0.96	0.07	32,32,32,32	0
32	MG	0	8047	1/1	0.96	0.18	61,61,61,61	0
32	MG	0	8079	1/1	0.97	0.16	60,60,60,60	0
32	MG	0	8046	1/1	0.97	0.08	39,39,39,39	0
32	MG	0	8081	1/1	0.97	0.13	63,63,63,63	0
35	CL	B	8819	1/1	0.97	0.09	52,52,52,52	0
32	MG	0	8027	1/1	0.97	0.09	41,41,41,41	0
32	MG	0	8048	1/1	0.97	0.12	28,28,28,28	0
32	MG	0	8062	1/1	0.97	0.18	55,55,55,55	0
36	SR	0	8925	1/1	0.97	0.06	97,97,97,97	0
35	CL	N	8807	1/1	0.97	0.06	68,68,68,68	0
32	MG	0	8087	1/1	0.97	0.06	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8088	1/1	0.97	0.09	42,42,42,42	0
32	MG	0	8016	1/1	0.97	0.15	50,50,50,50	0
36	SR	0	8902	1/1	0.97	0.05	59,59,59,59	0
32	MG	0	8050	1/1	0.97	0.09	48,48,48,48	0
32	MG	0	8091	1/1	0.97	0.15	60,60,60,60	0
32	MG	0	8076	1/1	0.97	0.04	41,41,41,41	0
32	MG	0	8093	1/1	0.97	0.06	42,42,42,42	0
32	MG	0	8052	1/1	0.97	0.08	54,54,54,54	0
34	NA	0	8527	1/1	0.97	0.08	55,55,55,55	0
36	SR	0	8940	1/1	0.97	0.05	84,84,84,84	0
35	CL	0	8813	1/1	0.97	0.06	53,53,53,53	0
32	MG	0	8045	1/1	0.97	0.09	36,36,36,36	0
32	MG	K	8054	1/1	0.97	0.12	44,44,44,44	0
38	CD	Z	8703	1/1	0.97	0.04	98,98,98,98	0
32	MG	0	8012	1/1	0.98	0.09	22,22,22,22	0
32	MG	0	8013	1/1	0.98	0.09	35,35,35,35	0
32	MG	0	8009	1/1	0.98	0.15	31,31,31,31	0
35	CL	J	8821	1/1	0.98	0.04	57,57,57,57	0
32	MG	0	8021	1/1	0.98	0.18	40,40,40,40	0
34	NA	0	8517	1/1	0.98	0.08	38,38,38,38	0
35	CL	0	8803	1/1	0.98	0.10	53,53,53,53	0
32	MG	0	8084	1/1	0.98	0.14	40,40,40,40	0
35	CL	3	8804	1/1	0.98	0.05	65,65,65,65	0
35	CL	0	8811	1/1	0.98	0.06	65,65,65,65	0
36	SR	R	8912	1/1	0.98	0.05	90,90,90,90	0
35	CL	0	8812	1/1	0.98	0.03	46,46,46,46	0
36	SR	0	8904	1/1	0.98	0.06	56,56,56,56	0
32	MG	0	8022	1/1	0.98	0.14	38,38,38,38	0
35	CL	0	8814	1/1	0.98	0.14	49,49,49,49	0
32	MG	0	8041	1/1	0.98	0.13	26,26,26,26	0
32	MG	0	8065	1/1	0.98	0.13	45,45,45,45	0
32	MG	0	8043	1/1	0.98	0.10	45,45,45,45	0
32	MG	0	8011	1/1	0.98	0.12	31,31,31,31	0
38	CD	O	8705	1/1	0.98	0.07	99,99,99,99	0
32	MG	0	8068	1/1	0.98	0.09	57,57,57,57	0
36	SR	0	8907	1/1	0.99	0.04	57,57,57,57	0
32	MG	0	8004	1/1	0.99	0.10	29,29,29,29	0
32	MG	0	8005	1/1	0.99	0.11	34,34,34,34	0
32	MG	0	8006	1/1	0.99	0.11	30,30,30,30	0
32	MG	0	8007	1/1	0.99	0.10	31,31,31,31	0
32	MG	0	8014	1/1	0.99	0.15	30,30,30,30	0
32	MG	0	8023	1/1	0.99	0.10	28,28,28,28	0

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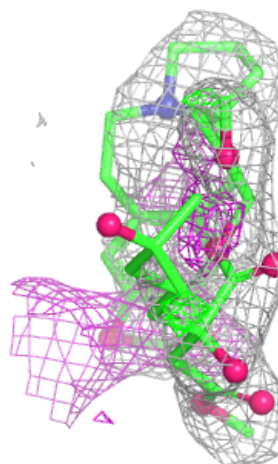
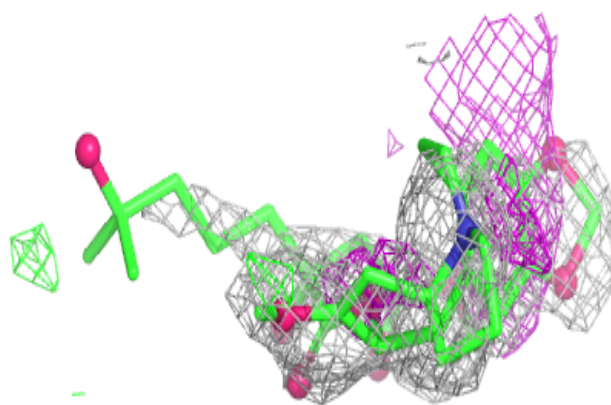
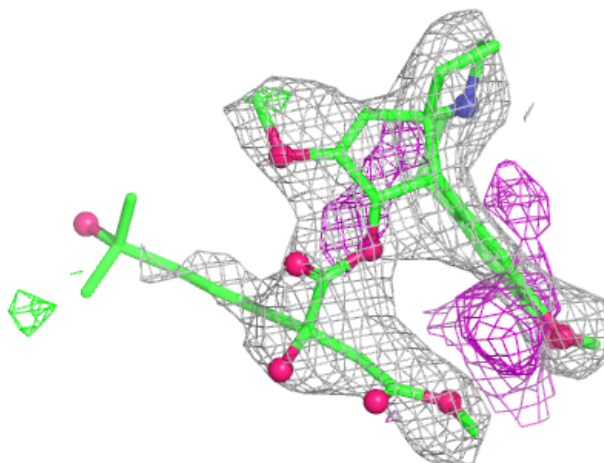
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	0	8015	1/1	0.99	0.11	36,36,36,36	0
32	MG	0	8025	1/1	0.99	0.03	28,28,28,28	0
35	CL	M	8818	1/1	0.99	0.04	46,46,46,46	0
32	MG	0	8026	1/1	0.99	0.07	36,36,36,36	0
32	MG	0	8058	1/1	0.99	0.10	30,30,30,30	0
35	CL	R	8806	1/1	0.99	0.03	47,47,47,47	0
32	MG	0	8002	1/1	0.99	0.05	25,25,25,25	0
32	MG	0	8061	1/1	0.99	0.10	30,30,30,30	0
32	MG	0	8028	1/1	0.99	0.14	33,33,33,33	0
32	MG	0	8029	1/1	0.99	0.18	49,49,49,49	0
36	SR	0	8903	1/1	0.99	0.10	58,58,58,58	0
32	MG	0	8003	1/1	0.99	0.08	34,34,34,34	0
36	SR	0	8905	1/1	0.99	0.14	68,68,68,68	0
36	SR	0	8906	1/1	0.99	0.07	59,59,59,59	0
38	CD	1	8702	1/1	0.99	0.06	57,57,57,57	0
38	CD	3	8704	1/1	0.99	0.02	76,76,76,76	0
38	CD	U	8701	1/1	1.00	0.07	72,72,72,72	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.