



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 11:06 am BST

PDB ID : 1Q81
Title : Crystal Structure of minihelix with 3' puromycin bound to A-site of the 50S ribosomal subunit.
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-20
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

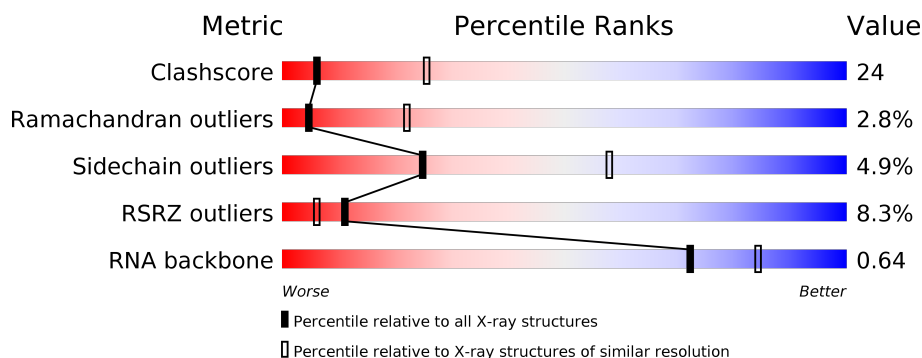
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)
RNA backbone	3102	1065 (3.22-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	2922	<div> <div>2%</div> <div> <div>48%</div> <div>39%</div> <div>7%</div> <div>6%</div> </div> </div>
2	B	122	<div> <div>5%</div> <div> <div>39%</div> <div>48%</div> <div>11%</div> </div> </div>
3	5	2	<div> <div>100%</div> <div>100%</div> </div>
4	C	239	<div> <div>10%</div> <div> <div>52%</div> <div>41%</div> <div>6%</div> </div> </div>
5	D	337	<div> <div>%</div> <div> <div>45%</div> <div>50%</div> <div>6%</div> </div> </div>
6	E	246	<div> <div>%</div> <div> <div>50%</div> <div>46%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	
30	3	48	
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	MG	4	8078	-	-	-	X
32	MG	4	8114	-	-	-	X
32	MG	A	8024	-	-	-	X
32	MG	A	8070	-	-	-	X
32	MG	A	8097	-	-	-	X
34	NA	A	8355	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8384	-	-	-	X
34	NA	B	8351	-	-	-	X
34	NA	S	8386	-	-	-	X
34	NA	T	8312	-	-	-	X
35	CL	4	8504	-	-	-	X
35	CL	A	8515	-	-	-	X
37	CD	4	8404	-	-	-	X
37	CD	P	8405	-	-	-	X

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 98596 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	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

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

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

- Molecule 3 is a RNA chain called minihelix-puromycin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	2	Total	C	N	O	P	0	0	0
			40	18	6	14	2			

- Molecule 4 is a protein called 50S ribosomal protein L2P.

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

- Molecule 5 is a protein called 50S ribosomal protein L3P.

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is a protein called 50S ribosomal protein L4E.

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

- Molecule 7 is a protein called 50S ribosomal protein L5P.

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

- Molecule 8 is a protein called 50S ribosomal protein L6P.

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

- Molecule 9 is a protein called 50S ribosomal protein L7Ae.

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

- Molecule 10 is a protein called Acidic ribosomal protein P0 homolog.

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

- Molecule 12 is a protein called 50S ribosomal protein L13P.

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

- Molecule 13 is a protein called 50S ribosomal protein L14P.

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

- Molecule 14 is a protein called 50S ribosomal protein L15P.

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

- Molecule 16 is a protein called 50S ribosomal protein L18P.

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

- Molecule 17 is a protein called 50S ribosomal protein L18e.

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

- Molecule 18 is a protein called 50S ribosomal protein L19E.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 19 is a protein called 50S ribosomal protein L21e.

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

- Molecule 20 is a protein called 50S ribosomal protein L22P.

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

- Molecule 21 is a protein called 50S ribosomal protein L23P.

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

- Molecule 22 is a protein called 50S ribosomal protein L24P.

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

- Molecule 23 is a protein called 50S ribosomal protein L24E.

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

- Molecule 24 is a protein called 50S ribosomal protein L29P.

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

- Molecule 25 is a protein called 50S ribosomal protein L30P.

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

- Molecule 26 is a protein called 50S ribosomal protein L31e.

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

- Molecule 27 is a protein called 50S ribosomal protein L32E.

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

- Molecule 28 is a protein called L37Ae 50S ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	1	73	Total	C	N	O	S	0	0	0
			563	359	111	86	7			

- Molecule 29 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	2	56	Total	C	N	O	S	0	0	0
			430	258	86	82	4			

- Molecule 30 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	3	46	Total	C	N	O	S	0	0	0
			393	238	86	68	1			

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 31 is a protein called 50S ribosomal protein L44E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	4	92	Total	C	N	O	S	0	0	0
			755	458	153	137	7			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	1	1	Total Mg 1 1	0	0
32	D	1	Total Mg 1 1	0	0
32	B	1	Total Mg 1 1	0	0
32	C	1	Total Mg 1 1	0	0
32	Z	1	Total Mg 1 1	0	0
32	A	108	Total Mg 108 108	0	0
32	4	2	Total Mg 2 2	0	0
32	U	1	Total Mg 1 1	0	0
32	L	1	Total Mg 1 1	0	0

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

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	J	1	Total Na 1 1	0	0
34	K	1	Total Na 1 1	0	0
34	E	1	Total Na 1 1	0	0
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	73	Total Na 73 73	0	0
34	T	1	Total Na 1 1	0	0
34	N	1	Total Na 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Na 1	0	0
34	S	3	Total 3	Na 3	0	0
34	M	1	Total 1	Na 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	P	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	C	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	A	11	Total 11	Cl 11	0	0
35	4	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (three-letter code: PPU) (formula: C₂₂H₃₀N₇O₈P).

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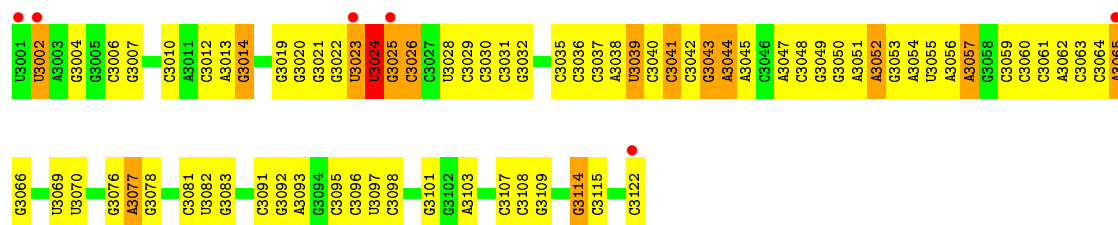
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	D	155	Total 155	O 155	0	0
38	E	171	Total 171	O 171	0	0
38	F	51	Total 51	O 51	0	0
38	G	44	Total 44	O 44	0	0
38	H	26	Total 26	O 26	0	0
38	I	20	Total 20	O 20	0	0
38	J	77	Total 77	O 77	0	0
38	K	55	Total 55	O 55	0	0
38	L	63	Total 63	O 63	0	0
38	M	90	Total 90	O 90	0	0
38	N	125	Total 125	O 125	0	0
38	O	64	Total 64	O 64	0	0
38	P	44	Total 44	O 44	0	0
38	Q	68	Total 68	O 68	0	0
38	R	54	Total 54	O 54	0	0
38	S	83	Total 83	O 83	0	0
38	T	31	Total 31	O 31	0	0
38	U	39	Total 39	O 39	0	0
38	V	26	Total 26	O 26	0	0
38	W	15	Total 15	O 15	0	0
38	X	70	Total 70	O 70	0	0

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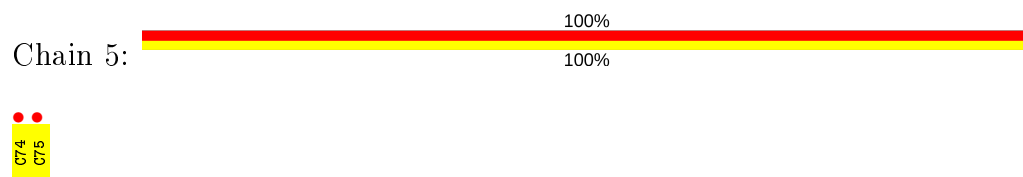
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	Y	30	Total 30	O 30	0	0
38	Z	102	Total 102	O 102	0	0
38	1	38	Total 38	O 38	0	0
38	2	56	Total 56	O 56	0	0
38	3	47	Total 47	O 47	0	0
38	4	72	Total 72	O 72	0	0

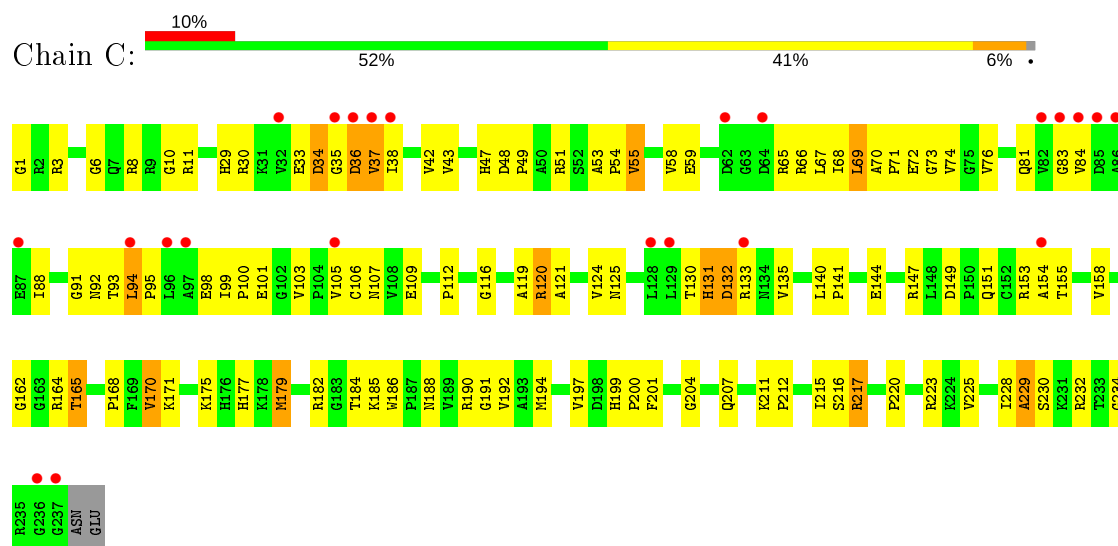
G2025	C1948	C1856	C1772	A1685	U1598	A1515	A1424	G1316	A1215	G1155	U1064	U	U872
C2026	G1949	A1857	G1773	C1695	G1600	C1516	G1425	A1321	G1216	C1156	G1065	G	G873
U2027	G1950	G1687	A1778	G1688	C1602	U1517	C1426			G1157	U1066	U	A874
U2028	G1951		A1779		A1603	A1522	G1430	G1325	G1226	G1158	A1067	C	A875
C2029	U	C1861	A1783	A1691	G1604	G1523	A1434	U1326	G1227	G1159	G1068	C	A876
A2030	A	G1863	C1692	C1692	G1605	U1524	U1435	C1327	C1228	G1160	C1069	C	G877
C2031	C	C1864	U1784	U1784	A1606	U1525	U1435	A1328	C1229	A1161	U1070	C	G878
U2032	U	A1865	A1701	A1701	G1607	A1526	C1436	A1329	U1234	G1162	G1071	C	C884
U2033	U	C1866	U1702	U1702	G1608	A1527	A1436	A1330	G1235	C1163	G1072	C	G885
C2034	U	G1867	G1786	G1786	G1609	A1528	C1439	A1331	A1236	G1164	A1073	C	
U2035	U	G1868	G1787	G1787	G1610	G1529	U1440	A1332	U1237	G1165		G	G892
A2038	A	G1873	G1705	G1705		C1534	G1441	U1333	G1238	G1166	G1080	A	G893
A2039	C	U1874	G1706	G1706		G1535	G1442	C1334	G1239	C1167	A1081	G	A894
C2040	C	U1874	G1707	G1707	A1624	C1536	G1443	G1335		C1168	A1082	A	
G2041	C	G1878	C1708	C1708	U1625	G1540	G1444		A1242	U1170	G1083	G	G902
G2044	U1964	U1879	A1710	A1710	U1626	G1541	G1445	G1340	C1243	U1171	G1084	G	
G2050	G1971	C1882	C1798	A1717	G1629	G1542		A1341	U1244	G1172	G1085	A	G905
G2056	U1972	U1883	C1803	U1722	A1630	G1543		G1342	C1245	A1173	G1086	C	G906
A2054	A1973	G1884	A1804	G1723	A1631	C1545		C1343	A1246	A1174	G1087	U	A907
A2055	G1974	A1885	G1805	U1724	A1632	G1546		G1344		C1175	A1088	C	A908
A2055	A1886	A1886	G1806	G1725	C1633	A1547	C1456	U1345	U1249	C1176	G1094	G	U909
U2064	G1975	U1887	G1807	G1726	G1634	U1548	U1457	U1346	C1250	A1177	U1095	C	C910
C2065	A1978	U1890	C1808	G1727	U1635			G1351	C1253	G1178	U1096	A	C920
C2066	U1980		G1809		G1636	G1552	C1462	A1352		U1180	A1097	C	G921
C2071	C1983	G1901	G1810	G1730	A1637	G1553	A1463	C1353	U1286	A1181	A1098	A	A922
G2072	U1984	G1902	A1811	C1731	G1637	U1554	U1464	C1360	C1267	C1182	A923	C	G924
G2073	U1985	U1903	A1815	A1732	A1641	G1555	A1465	G1363	G1268	C1183	U1109	U1003	
G2074	G1986	G1908	G1816	A1733	A1642	G1556	A1470	G1366	U1270	C1184	G1110	C1004	U932
A2081	C1987	A1909		C1734	C1643	G1557	A1471	C1366	C1271	C1186	U1111	A1005	C933
C2084	U1992	U1910	G1919	G1735	C1644	U1558	U1473	C1377	A1272	U1115	A1114	A1006	C934
A2085	C1993	U1915	A1921	A1736	U1645	U	C1474	A1372	C1273	A1188	U1116	A1007	G935
A2085	A1994	G1916	G1823	A1741	G1652	U1561	G1475	G1376	U1275	A1189	U1117	C1008	C936
A2085	G1995	C1917	C1824	A1742	A1653	C1562	A1476	C1377	C1277	A1191	A1118	A1013	C937
G2084	U1996	G1917	U1825	G1743	G1654	G1563	C1477	G1377	C1278	A1192	A1119	A1014	G941
A2095	G1997	U1918	C1826	G1743	G1655	C1564	U1478	G1378	A1279	A1193	G1120	C1015	U942
A2096	G1998	A1919	G1827	A1747	A1656	C1565	U1479	A1379	U1285	C1194	U1130	U1016	
A2096	C2000	C1920	G1828	A1747	A1657	C1566	C1483	U1380	G1300	G1195	G1131	U1029	G952
A2100	G2001	A1922	A1829	G1751	A1658	A1567	C1484	A1406	C1305	C1196	A1132	G1044	G953
A2101	C2002	G1923		G1752	A1659			A1407	U1306	G1197	A1133	G1044	G956
G2102	U2003	G1925	C1834	C1753	G1660	A1580	A1494	U1408	G1289	U1198	G1134	G1045	
C2105	G2004	G1925	U1835	A1754	G1665	C1574	G1497	G1409	U1298	A1199	U1139	G1052	G960
C2106	C2006		U1838	A1755	C1666	U1577	G1498	U1403	G1299	C1201	C1140	G1055	A961
G2110	U2007	G1929	A1840	G1756	A1667	A1580	U1500	G1409	U1300	A1202	U1149	U1056	C962
G2111	G2008	A1930	C1841	C1762	A1669	G1589	A1501	G1416	G1306	G1203	A1150	A1057	C963
U2115	A2010	C1935	U1845	C1764	A1669	G1589	A1502	G1417	A1307	U1205	G1151	G1059	G968
U2116	U2011	C1936	A1846	G1765	C1675	G1592	U1503	G1417	U1308	U1206	A1150	A1059	U970
U2117	G2013	C1936	A1847	U1766	C1675	C1593	U1504	G1417	U1309	A1207	G1151	G1060	G
G2014	G2014	C1940	A1847	U1767	C1679	C1594	U1506	G1417	U1310	C1208	U1149		
A2015	A1941	A1941	A1852	A1767	C1679	G1595	C1507	C1420	G1312	G1210	A1150	A1057	
C2119	A1942	A1942	C1853	C1768	A1682	G1596	U1507	G1421	A1313	G1211	A1150	A1057	
U2120	C1943	C1943	C1854	U1770	A1684	A1597	G1512	U1422	U1314	C1212	G1151	A1059	
G2121			G1855	U1771	A1684	A1598	C1514	C1423	G1315	G1214	A1154		



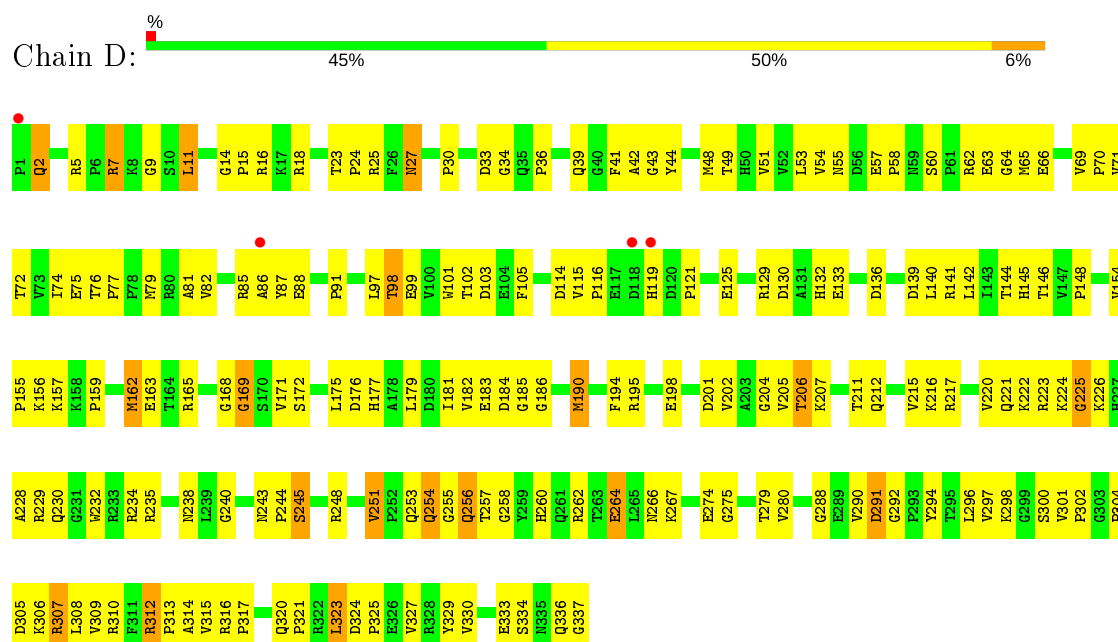
- Molecule 3: minihelix-puromycin



- Molecule 4: 50S ribosomal protein L2P

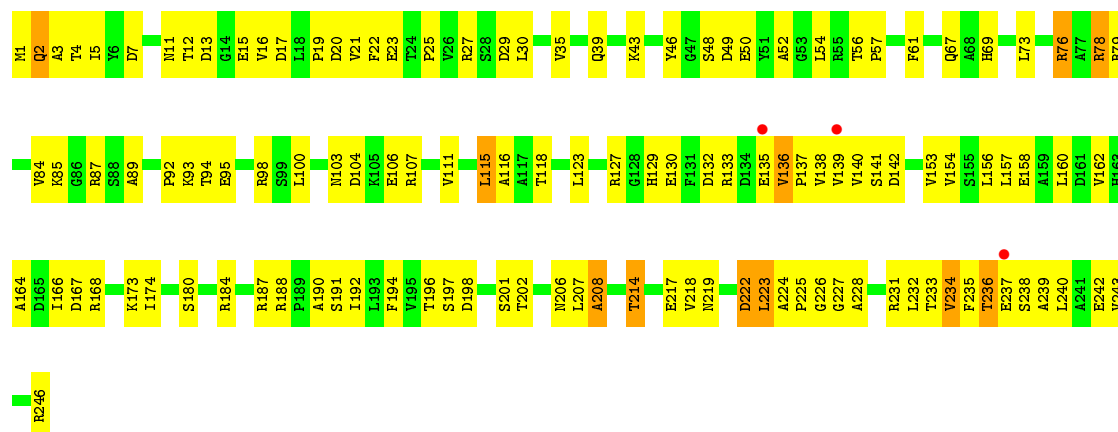


- Molecule 5: 50S ribosomal protein L3P

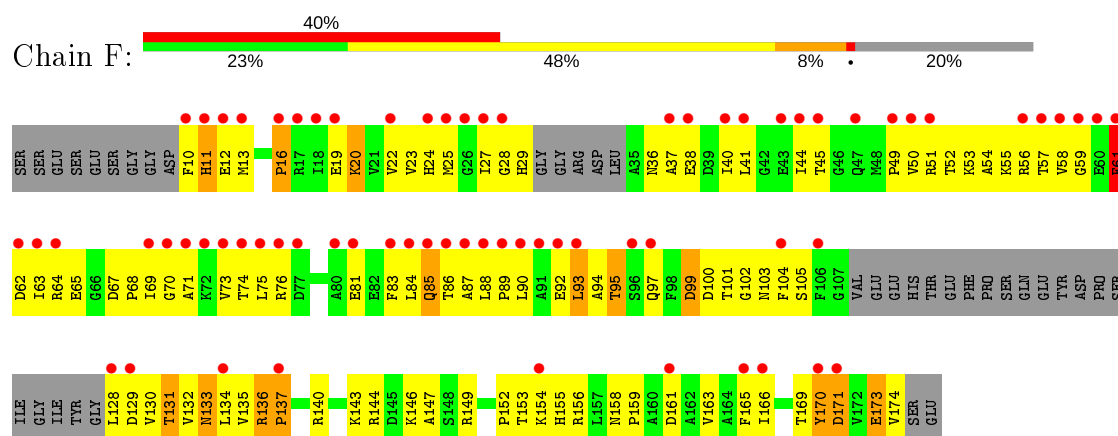


- Molecule 6: 50S ribosomal protein L4E

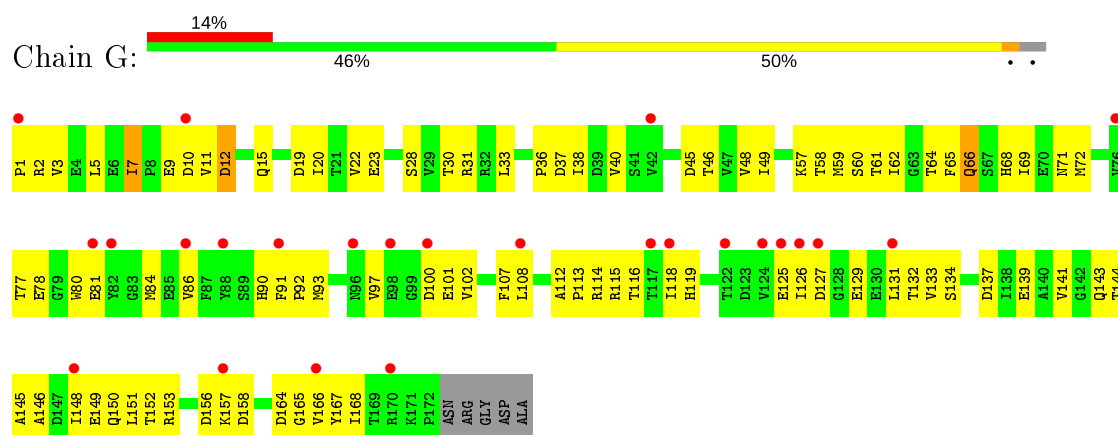




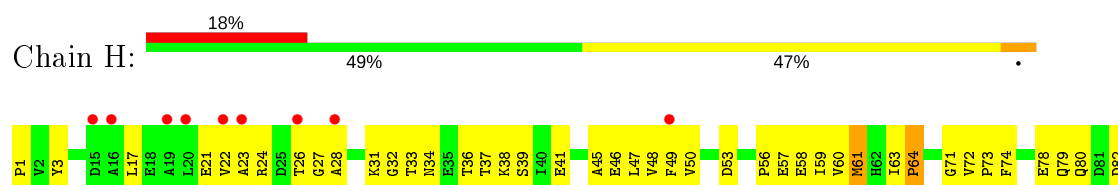
• Molecule 7: 50S ribosomal protein L5P

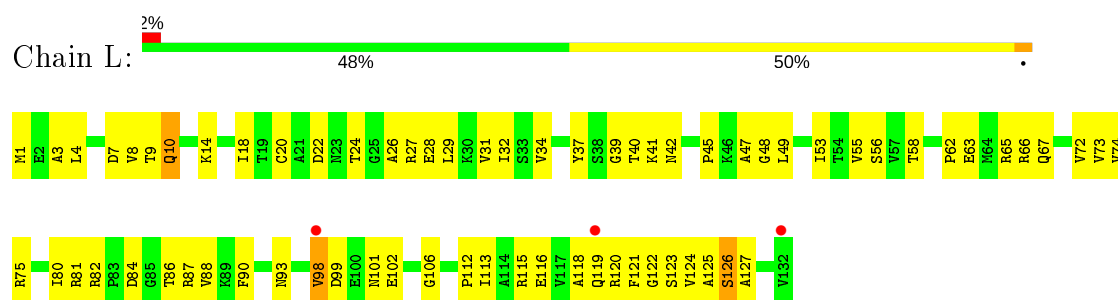


• Molecule 8: 50S ribosomal protein L6P

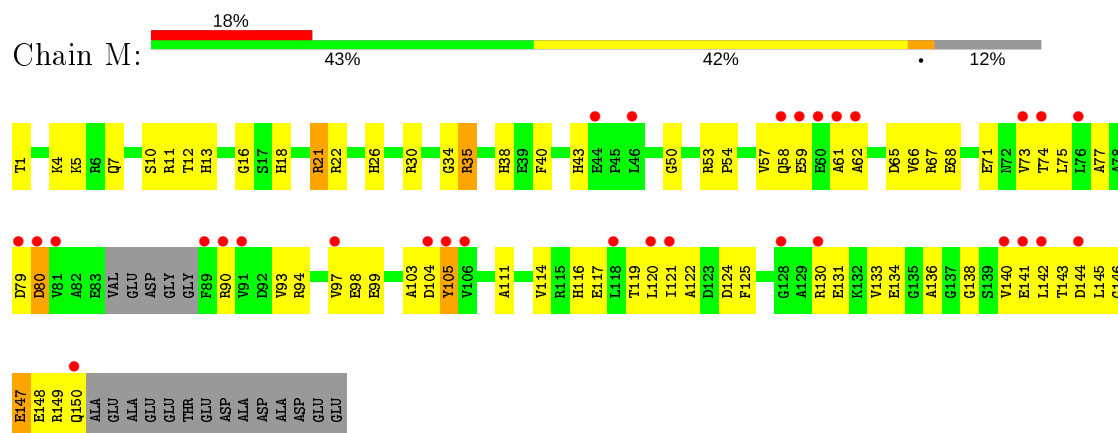


• Molecule 9: 50S ribosomal protein L7Ae

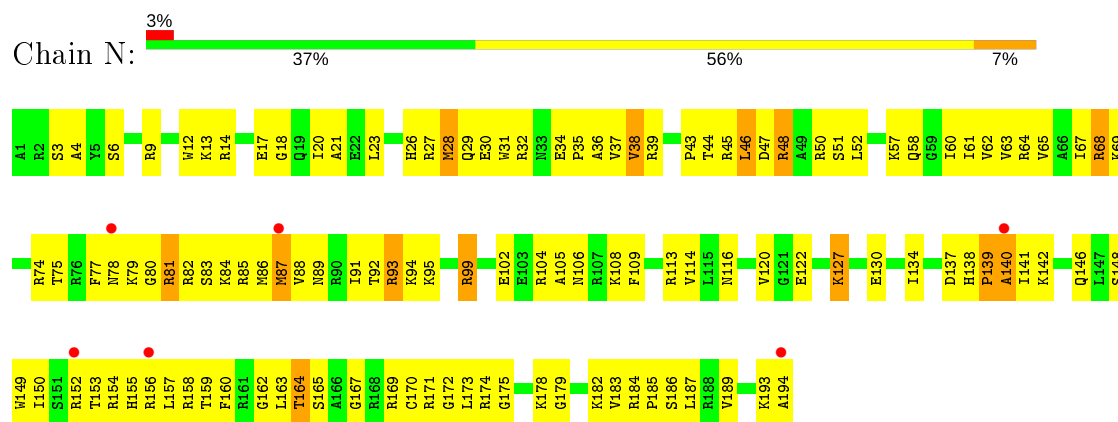




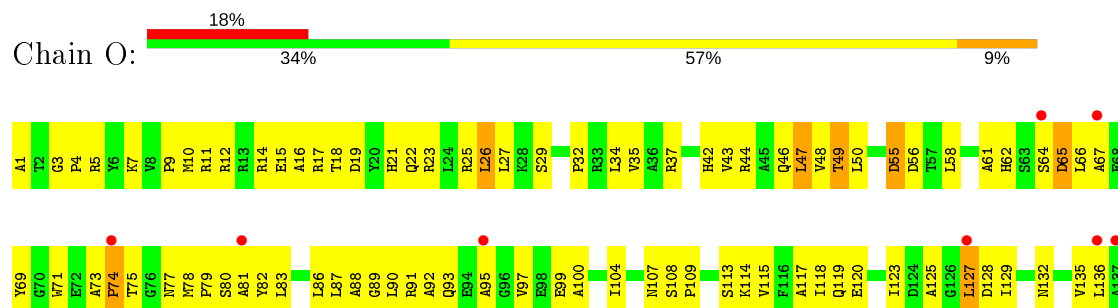
• Molecule 14: 50S ribosomal protein L15P

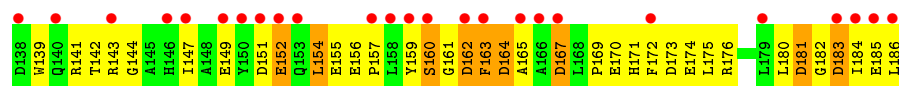


• Molecule 15: L15 Ribosomal Protein

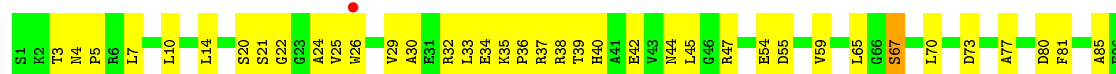


• Molecule 16: 50S ribosomal protein L18P

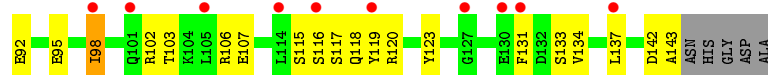




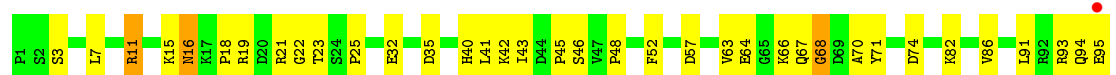
- Molecule 17: 50S ribosomal protein L18e



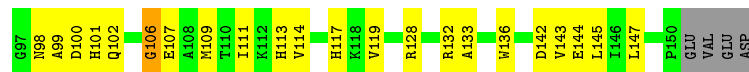
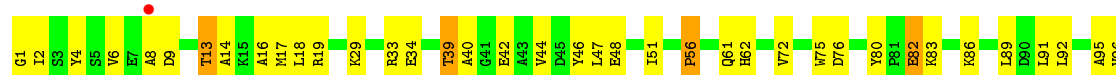
- Molecule 18: 50S ribosomal protein L19E



- Molecule 19: 50S ribosomal protein L21e



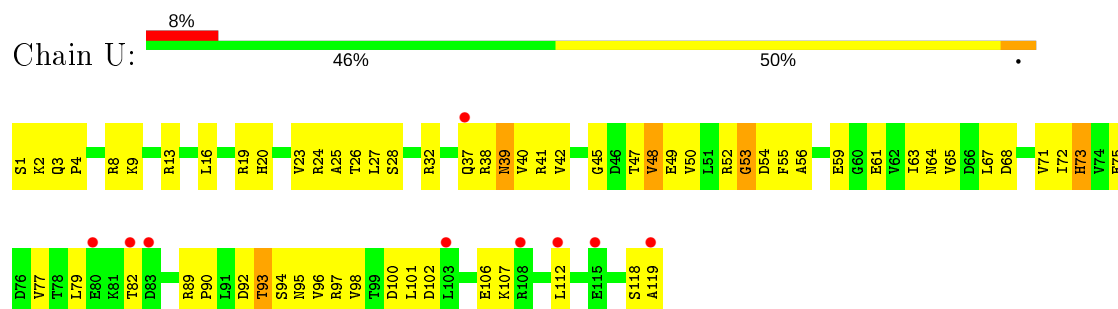
- Molecule 20: 50S ribosomal protein L22P



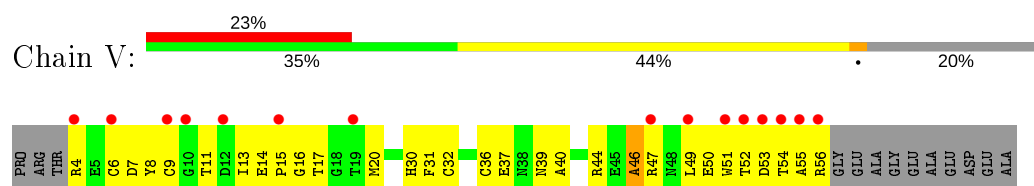
- Molecule 21: 50S ribosomal protein L23P



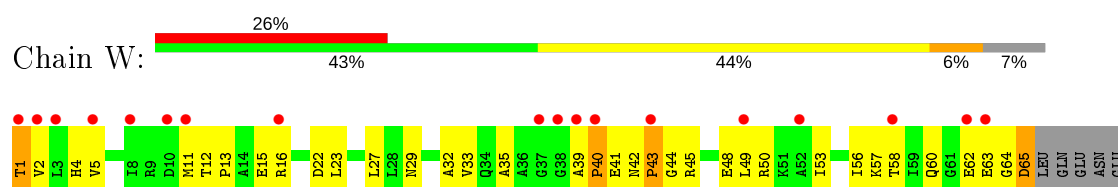
- Molecule 22: 50S ribosomal protein L24P



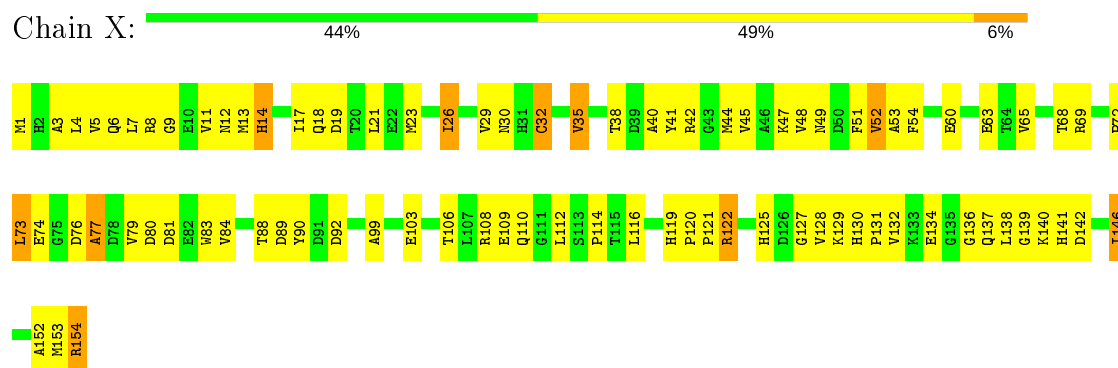
- Molecule 23: 50S ribosomal protein L24E



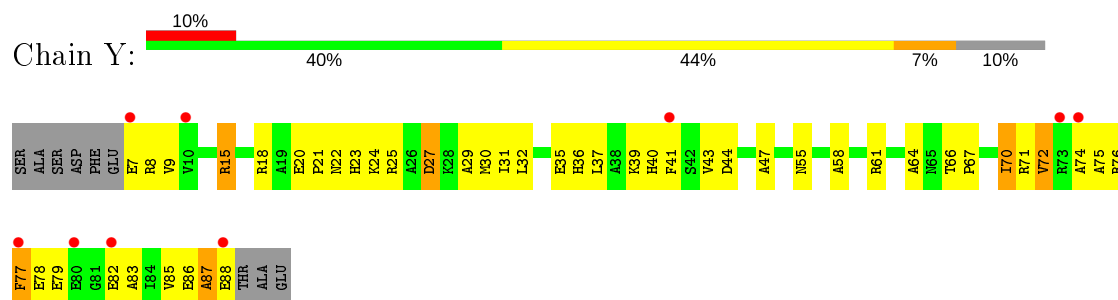
- Molecule 24: 50S ribosomal protein L29P



- Molecule 25: 50S ribosomal protein L30P



- Molecule 26: 50S ribosomal protein L31e



P61	T62	K63	K64	T65	D66	L67	K68	Y69	R70	C71	G72	E73	C74	G75	K76	A77	H78	L79	R80	E81	G82	W83	R84	A85	G86	R87	L88	E89	F90	Q91	E92
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4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.16 Å 301.29 Å 575.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.95 53.80 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.95) 90.6 (53.80-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.80 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.210 , 0.259 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	51.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	98596	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 1.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, K, CD, PPU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.53	6/66076 (0.0%)	0.72	18/103052 (0.0%)
2	B	0.49	0/2905	0.78	3/4528 (0.1%)
3	5	1.19	0/43	0.77	0/64
4	C	0.40	0/1787	0.71	0/2409
5	D	0.39	0/2689	0.69	0/3652
6	E	0.44	0/1883	0.68	0/2551
7	F	0.37	0/1111	0.62	0/1498
8	G	0.38	0/1382	0.62	0/1880
9	H	0.46	1/896 (0.1%)	0.73	3/1219 (0.2%)
10	I	0.42	0/241	0.62	0/324
11	J	0.44	0/1246	0.76	3/1686 (0.2%)
12	K	0.41	0/1135	0.67	0/1530
13	L	0.40	0/1003	0.73	0/1351
14	M	0.41	0/1126	0.72	0/1504
15	N	0.45	0/1633	0.74	2/2180 (0.1%)
16	O	0.36	0/1473	0.69	0/1999
17	P	0.41	0/873	0.71	0/1181
18	Q	0.41	0/1143	0.62	0/1521
19	R	0.42	0/748	0.74	1/1005 (0.1%)
20	S	0.42	0/1172	0.65	0/1578
21	T	0.39	0/648	0.63	0/875
22	U	0.36	0/957	0.66	0/1289
23	V	0.46	0/417	0.65	0/562
24	W	0.33	0/502	0.63	0/675
25	X	0.37	0/1218	0.67	0/1655
26	Y	0.40	0/664	0.66	0/895
27	Z	0.41	0/1146	0.67	0/1536
28	1	0.57	0/575	0.72	0/763
29	2	0.48	0/437	0.69	0/578
30	3	0.35	0/398	0.60	0/527
31	4	0.84	0/771	0.70	0/1024
All	All	0.50	7/98298 (0.0%)	0.71	30/147091 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	58
2	B	1	0
All	All	1	58

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2617	G	C3'-O3'	12.86	1.60	1.42
1	A	2617	G	C4'-O4'	-6.15	1.37	1.45
9	H	3	TYR	CG-CD1	6.05	1.47	1.39
1	A	2618	G	P-OP2	-5.70	1.39	1.49
1	A	2617	G	N9-C8	5.65	1.41	1.37

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1165	G	O5'-P-OP2	10.73	123.58	110.70
1	A	1563	G	C2'-C3'-O3'	9.26	129.87	109.50
2	B	3024	U	C2'-C3'-O3'	9.18	129.70	109.50
9	H	3	TYR	CB-CG-CD2	9.11	126.47	121.00
1	A	1164	U	OP1-P-O3'	-8.57	86.34	105.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	3024	U	C3'

5 of 58 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	A	Sidechain
1	A	176	U	Sidechain
1	A	182	G	Sidechain
1	A	205	U	Sidechain
1	A	214	U	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	59017	0	29805	1413	0
2	B	2600	0	1326	101	0
3	5	40	0	22	7	0
4	C	1754	0	1763	136	0
5	D	2624	0	2533	221	0
6	E	1858	0	1816	138	0
7	F	1094	0	1085	149	0
8	G	1357	0	1266	101	0
9	H	885	0	854	76	0
10	I	240	0	231	24	0
11	J	1215	0	1215	172	0
12	K	1119	0	1098	86	0
13	L	993	0	1027	73	0
14	M	1114	0	1072	76	0
15	N	1605	0	1676	178	0
16	O	1444	0	1401	159	0
17	P	864	0	873	74	0
18	Q	1133	0	1127	64	0
19	R	734	0	728	36	0
20	S	1149	0	1122	76	0
21	T	641	0	605	23	0
22	U	949	0	923	76	0
23	V	410	0	367	46	0
24	W	499	0	511	37	0
25	X	1195	0	1137	111	0
26	Y	654	0	653	53	0
27	Z	1130	0	1133	77	0
28	1	563	0	600	89	0
29	2	430	0	426	24	0
30	3	393	0	406	17	0
31	4	755	0	732	108	0
32	1	1	0	0	0	0
32	4	2	0	0	0	0
32	A	108	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	2	0	0	0	0
34	A	73	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	1	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
35	4	1	0	0	1	0
35	A	11	0	0	3	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	2	0
35	N	1	0	0	1	0
35	O	1	0	0	0	0
35	P	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	1	0	0	0	0
36	5	37	0	28	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	38	0	0	14	0
38	2	56	0	0	9	0
38	3	47	0	0	2	0
38	4	72	0	0	13	0
38	A	5871	0	0	307	0
38	B	147	0	0	14	0
38	C	135	0	0	24	0
38	D	155	0	0	28	0
38	E	171	0	0	31	0
38	F	51	0	0	25	0
38	G	44	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	H	26	0	0	12	0
38	I	20	0	0	6	0
38	J	77	0	0	27	0
38	K	55	0	0	5	0
38	L	63	0	0	14	0
38	M	90	0	0	19	0
38	N	125	0	0	27	0
38	O	64	0	0	26	0
38	P	44	0	0	13	0
38	Q	68	0	0	10	0
38	R	54	0	0	5	0
38	S	83	0	0	9	0
38	T	31	0	0	4	0
38	U	39	0	0	8	0
38	V	26	0	0	7	0
38	W	15	0	0	5	0
38	X	70	0	0	14	0
38	Y	30	0	0	5	0
38	Z	102	0	0	19	0
All	All	98596	0	59561	3672	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 24.

The worst 5 of 3672 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)
2:B:3006:C:H5"	16:O:37:ARG:NH1	1.56	1.19
24:W:12:THR:HG22	24:W:15:GLU:HG3	1.28	1.14
6:E:236:THR:HG22	6:E:239:ALA:H	1.10	1.10
11:J:86:ARG:HH11	11:J:133:ILE:HG13	0.99	1.10
6:E:115:LEU:HD13	6:E:223:LEU:HD21	1.30	1.09

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	235/239 (98%)	199 (85%)	27 (12%)	9 (4%)	3	15
5	D	335/337 (99%)	297 (89%)	28 (8%)	10 (3%)	4	20
6	E	244/246 (99%)	208 (85%)	31 (13%)	5 (2%)	7	30
7	F	134/176 (76%)	98 (73%)	25 (19%)	11 (8%)	1	3
8	G	170/177 (96%)	156 (92%)	13 (8%)	1 (1%)	25	60
9	H	117/119 (98%)	103 (88%)	9 (8%)	5 (4%)	2	12
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	3	14
11	J	152/167 (91%)	128 (84%)	18 (12%)	6 (4%)	3	14
12	K	140/145 (97%)	124 (89%)	11 (8%)	5 (4%)	3	16
13	L	130/132 (98%)	113 (87%)	15 (12%)	2 (2%)	10	38
14	M	141/164 (86%)	114 (81%)	23 (16%)	4 (3%)	5	22
15	N	192/194 (99%)	177 (92%)	10 (5%)	5 (3%)	5	24
16	O	184/186 (99%)	153 (83%)	19 (10%)	12 (6%)	1	5
17	P	113/115 (98%)	105 (93%)	7 (6%)	1 (1%)	17	51
18	Q	141/148 (95%)	129 (92%)	11 (8%)	1 (1%)	22	56
19	R	93/95 (98%)	84 (90%)	9 (10%)	0	100	100
20	S	148/154 (96%)	130 (88%)	14 (10%)	4 (3%)	5	23
21	T	79/84 (94%)	75 (95%)	3 (4%)	1 (1%)	12	41
22	U	117/119 (98%)	106 (91%)	8 (7%)	3 (3%)	5	24
23	V	51/66 (77%)	48 (94%)	1 (2%)	2 (4%)	3	14
24	W	63/70 (90%)	57 (90%)	4 (6%)	2 (3%)	4	19
25	X	152/154 (99%)	142 (93%)	6 (4%)	4 (3%)	5	24
26	Y	80/91 (88%)	69 (86%)	8 (10%)	3 (4%)	3	15
27	Z	140/240 (58%)	134 (96%)	5 (4%)	1 (1%)	22	56
28	1	71/73 (97%)	61 (86%)	9 (13%)	1 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	2	54/56 (96%)	48 (89%)	6 (11%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	82 (91%)	6 (7%)	2 (2%)	6	28
All	All	3633/4235 (86%)	3205 (88%)	327 (9%)	101 (3%)	5	22

5 of 101 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
5	D	206	THR
7	F	93	LEU
7	F	95	THR
7	F	173	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	C	179/181 (99%)	169 (94%)	10 (6%)	21	53
5	D	282/282 (100%)	265 (94%)	17 (6%)	19	50
6	E	193/193 (100%)	178 (92%)	15 (8%)	12	38
7	F	117/147 (80%)	108 (92%)	9 (8%)	13	39
8	G	152/155 (98%)	149 (98%)	3 (2%)	55	80
9	H	92/92 (100%)	90 (98%)	2 (2%)	52	79
10	I	27/283 (10%)	26 (96%)	1 (4%)	34	66
11	J	122/122 (100%)	111 (91%)	11 (9%)	9	32
12	K	118/121 (98%)	110 (93%)	8 (7%)	16	45
13	L	106/106 (100%)	103 (97%)	3 (3%)	43	74
14	M	112/126 (89%)	108 (96%)	4 (4%)	35	67
15	N	166/166 (100%)	156 (94%)	10 (6%)	19	50
16	O	149/149 (100%)	142 (95%)	7 (5%)	26	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	93/93 (100%)	89 (96%)	4 (4%)	29	62
18	Q	113/116 (97%)	110 (97%)	3 (3%)	44	74
19	R	79/79 (100%)	75 (95%)	4 (5%)	24	56
20	S	117/121 (97%)	114 (97%)	3 (3%)	46	75
21	T	71/73 (97%)	71 (100%)	0	100	100
22	U	105/105 (100%)	102 (97%)	3 (3%)	42	73
23	V	44/52 (85%)	44 (100%)	0	100	100
24	W	51/56 (91%)	48 (94%)	3 (6%)	19	50
25	X	130/130 (100%)	122 (94%)	8 (6%)	18	48
26	Y	66/73 (90%)	63 (96%)	3 (4%)	27	61
27	Z	120/195 (62%)	113 (94%)	7 (6%)	20	51
28	1	56/56 (100%)	49 (88%)	7 (12%)	4	17
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	49	77
31	4	79/79 (100%)	76 (96%)	3 (4%)	33	66
All	All	3027/3441 (88%)	2878 (95%)	149 (5%)	25	58

5 of 149 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	150	LYS
15	N	38	VAL
27	Z	235	GLU
12	K	52	GLN
12	K	131	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 90 such sidechains are listed below:

Mol	Chain	Res	Type
12	K	107	ASN
17	P	100	GLN
29	2	28	HIS
13	L	10	GLN
15	N	58	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	246 (8%)	27 (0%)
2	B	121/122 (99%)	17 (14%)	4 (3%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	263 (9%)	31 (1%)

5 of 263 RNA backbone outliers are listed below:

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

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1352	A
1	A	1474	C
2	B	3024	U
1	A	1377	C
1	A	1563	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
36	PPU	5	76	3	32,40,41	2.43	6 (18%)	33,57,60	1.15	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PPU	5	76	3	-	4/21/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	C-N3'	9.69	1.55	1.34
36	5	76	PPU	C10-N6	-4.31	1.35	1.45
36	5	76	PPU	C9-N6	-4.22	1.35	1.45
36	5	76	PPU	CE1-CZ	3.95	1.46	1.38
36	5	76	PPU	CE2-CD2	3.53	1.45	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	76	PPU	C3'-N3'-C	-3.76	117.55	123.21
36	5	76	PPU	CM-OC-CZ	2.11	122.08	117.51
36	5	76	PPU	CA-C-N3'	-2.07	113.28	116.15

There are no chirality outliers.

All (4) torsion outliers are listed below:

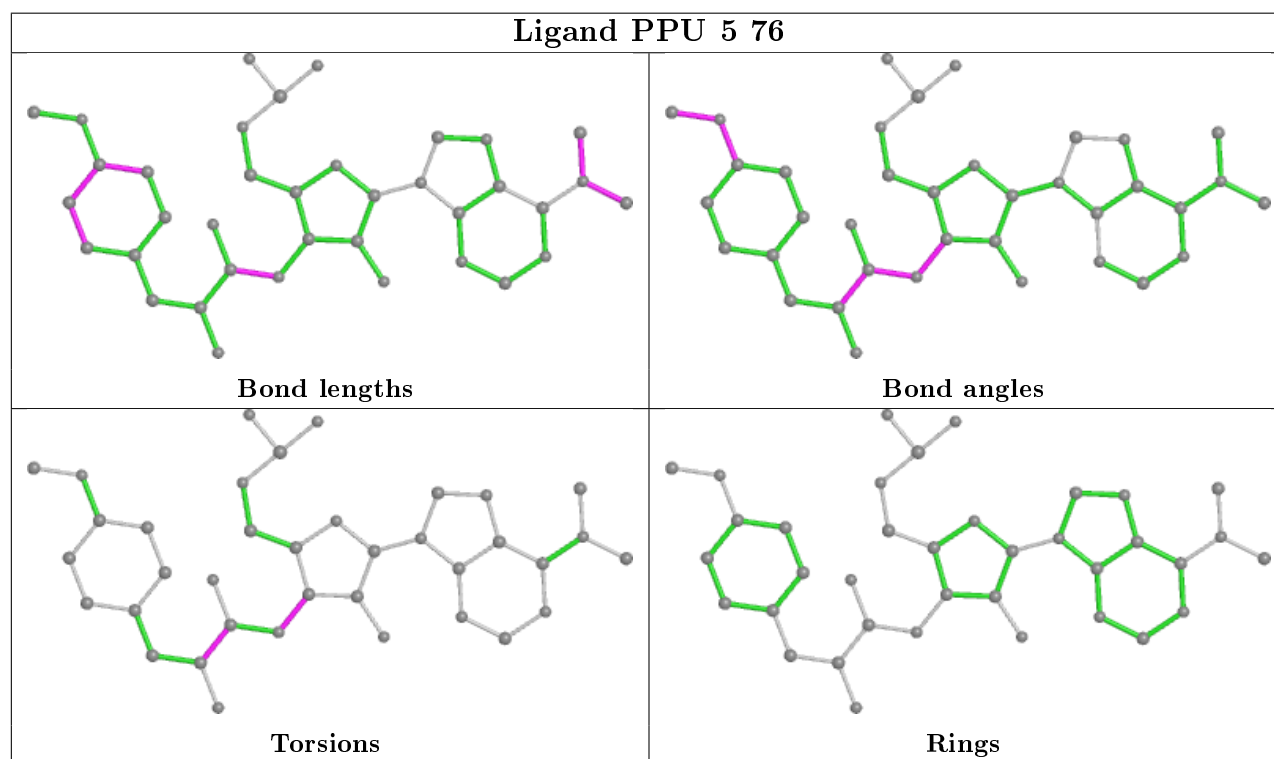
Mol	Chain	Res	Type	Atoms
36	5	76	PPU	O-C-CA-CB
36	5	76	PPU	N3'-C-CA-CB
36	5	76	PPU	C4'-C3'-N3'-C
36	5	76	PPU	C2'-C3'-N3'-C

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	76	PPU	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	2754/2922 (94%)	0.08	70 (2%) 57 40	24, 52, 101, 153	0
2	B	122/122 (100%)	0.27	6 (4%) 29 18	42, 71, 102, 149	0
3	5	2/2 (100%)	2.87	2 (100%) 0 0	96, 96, 96, 111	0
4	C	237/239 (99%)	0.52	23 (9%) 7 4	28, 62, 98, 116	0
5	D	337/337 (100%)	0.26	4 (1%) 79 63	29, 60, 88, 96	0
6	E	246/246 (100%)	0.04	3 (1%) 79 63	27, 53, 76, 87	0
7	F	140/176 (79%)	2.24	70 (50%) 0 0	69, 108, 125, 135	0
8	G	172/177 (97%)	1.03	25 (14%) 2 1	50, 75, 99, 106	0
9	H	119/119 (100%)	0.92	21 (17%) 1 1	59, 82, 106, 110	0
10	I	29/348 (8%)	2.95	19 (65%) 0 0	81, 104, 108, 109	0
11	J	156/167 (93%)	0.50	13 (8%) 11 6	40, 61, 92, 97	0
12	K	142/145 (97%)	0.23	3 (2%) 63 46	40, 55, 75, 83	0
13	L	132/132 (100%)	0.12	3 (2%) 60 43	37, 59, 85, 88	0
14	M	145/164 (88%)	1.10	30 (20%) 1 0	27, 83, 118, 124	0
15	N	194/194 (100%)	0.21	6 (3%) 49 32	34, 54, 73, 81	0
16	O	186/186 (100%)	0.95	33 (17%) 1 1	46, 74, 114, 127	0
17	P	115/115 (100%)	0.34	2 (1%) 70 53	47, 63, 86, 91	0
18	Q	143/148 (96%)	0.59	12 (8%) 11 6	43, 63, 82, 90	0
19	R	95/95 (100%)	0.00	1 (1%) 80 65	40, 52, 61, 75	0
20	S	150/154 (97%)	0.04	1 (0%) 87 76	33, 49, 68, 76	0
21	T	81/84 (96%)	0.36	2 (2%) 57 40	55, 69, 88, 92	0
22	U	119/119 (100%)	0.55	9 (7%) 13 7	45, 61, 82, 91	0
23	V	53/66 (80%)	1.55	15 (28%) 0 0	73, 83, 98, 119	0
24	W	65/70 (92%)	1.52	18 (27%) 0 0	58, 84, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	154/154 (100%)	0.06	0 100 100	43, 55, 73, 83	0
26	Y	82/91 (90%)	0.48	9 (10%) 5 3	43, 64, 88, 102	0
27	Z	142/240 (59%)	0.21	8 (5%) 24 15	33, 51, 74, 92	0
28	1	73/73 (100%)	3.16	40 (54%) 0 0	76, 107, 118, 119	0
29	2	56/56 (100%)	-0.25	0 100 100	29, 37, 45, 48	0
30	3	46/48 (95%)	0.26	3 (6%) 18 11	41, 62, 83, 97	0
31	4	92/92 (100%)	8.53	92 (100%) 0 0	110, 126, 134, 137	0
All	All	6579/7281 (90%)	0.48	543 (8%) 11 6	24, 59, 111, 153	0

The worst 5 of 543 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	4	82	GLY	21.2
31	4	65	THR	20.2
31	4	83	TRP	18.5
31	4	85	ALA	15.1
31	4	62	THR	14.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
34	NA	T	8312	1/1	-0.44	0.49	163,163,163,163	0
35	CL	4	8504	1/1	0.34	0.54	114,114,114,114	0
34	NA	B	8351	1/1	0.46	0.43	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	S	8386	1/1	0.51	0.52	77,77,77,77	0
32	MG	A	8076	1/1	0.53	0.37	123,123,123,123	0
32	MG	A	8070	1/1	0.55	1.20	98,98,98,98	0
32	MG	4	8078	1/1	0.55	0.62	117,117,117,117	0
32	MG	A	8024	1/1	0.59	1.06	84,84,84,84	0
35	CL	A	8510	1/1	0.64	0.30	83,83,83,83	0
32	MG	A	8046	1/1	0.64	0.12	74,74,74,74	0
34	NA	A	8384	1/1	0.65	0.74	105,105,105,105	0
35	CL	A	8515	1/1	0.66	0.51	108,108,108,108	0
32	MG	4	8114	1/1	0.68	0.74	111,111,111,111	0
34	NA	A	8363	1/1	0.69	0.36	56,56,56,56	0
32	MG	A	8097	1/1	0.70	0.45	80,80,80,80	0
34	NA	A	8359	1/1	0.71	0.41	53,53,53,53	0
34	NA	A	8382	1/1	0.72	0.24	44,44,44,44	0
34	NA	A	8355	1/1	0.74	0.41	88,88,88,88	0
32	MG	A	8089	1/1	0.74	0.26	89,89,89,89	0
37	CD	P	8405	1/1	0.77	0.45	202,202,202,202	0
37	CD	4	8404	1/1	0.78	0.46	202,202,202,202	0
34	NA	A	8322	1/1	0.79	0.26	76,76,76,76	0
34	NA	A	8357	1/1	0.79	0.13	43,43,43,43	0
34	NA	A	8377	1/1	0.79	0.55	72,72,72,72	0
34	NA	A	8371	1/1	0.80	0.18	35,35,35,35	0
34	NA	A	8370	1/1	0.80	0.39	82,82,82,82	0
32	MG	A	8106	1/1	0.81	0.09	101,101,101,101	0
32	MG	A	8044	1/1	0.83	0.21	64,64,64,64	0
32	MG	1	8105	1/1	0.83	0.46	80,80,80,80	0
32	MG	A	8068	1/1	0.83	0.08	59,59,59,59	0
34	NA	S	8338	1/1	0.83	0.19	84,84,84,84	0
32	MG	A	8092	1/1	0.84	0.28	105,105,105,105	0
35	CL	O	8507	1/1	0.84	0.18	72,72,72,72	0
37	CD	V	8401	1/1	0.84	0.37	202,202,202,202	0
35	CL	P	8508	1/1	0.84	0.16	99,99,99,99	0
34	NA	A	8350	1/1	0.85	0.23	21,21,21,21	0
36	PPU	5	76	37/38	0.85	0.36	90,95,100,100	0
32	MG	A	8116	1/1	0.85	0.32	117,117,117,117	0
32	MG	A	8099	1/1	0.85	0.19	55,55,55,55	0
34	NA	A	8375	1/1	0.86	0.34	44,44,44,44	0
34	NA	E	8304	1/1	0.86	0.12	23,23,23,23	0
32	MG	A	8051	1/1	0.87	0.16	97,97,97,97	0
32	MG	A	8052	1/1	0.87	0.14	42,42,42,42	0
32	MG	A	8043	1/1	0.87	0.13	67,67,67,67	0
34	NA	A	8344	1/1	0.87	0.09	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8366	1/1	0.88	0.16	38,38,38,38	0
35	CL	C	8509	1/1	0.88	0.26	92,92,92,92	0
32	MG	A	8066	1/1	0.88	0.16	76,76,76,76	0
35	CL	A	8511	1/1	0.88	0.21	73,73,73,73	0
35	CL	A	8514	1/1	0.88	0.19	62,62,62,62	0
34	NA	A	8369	1/1	0.88	0.15	41,41,41,41	0
34	NA	A	8341	1/1	0.88	0.10	28,28,28,28	0
32	MG	A	8111	1/1	0.88	0.25	69,69,69,69	0
32	MG	U	8073	1/1	0.88	0.13	34,34,34,34	0
34	NA	A	8333	1/1	0.88	0.09	25,25,25,25	0
34	NA	A	8319	1/1	0.89	0.11	41,41,41,41	0
34	NA	A	8361	1/1	0.89	0.27	48,48,48,48	0
34	NA	B	8383	1/1	0.89	0.20	52,52,52,52	0
35	CL	A	8505	1/1	0.89	0.14	68,68,68,68	0
34	NA	A	8356	1/1	0.90	0.37	46,46,46,46	0
34	NA	A	8381	1/1	0.90	0.08	35,35,35,35	0
35	CL	S	8506	1/1	0.90	0.16	60,60,60,60	0
34	NA	A	8339	1/1	0.90	0.13	15,15,15,15	0
32	MG	A	8008	1/1	0.90	0.08	50,50,50,50	0
34	NA	A	8306	1/1	0.91	0.40	38,38,38,38	0
35	CL	K	8502	1/1	0.91	0.21	83,83,83,83	0
32	MG	A	8039	1/1	0.91	0.09	66,66,66,66	0
32	MG	A	8040	1/1	0.91	0.17	86,86,86,86	0
32	MG	A	8102	1/1	0.91	0.74	106,106,106,106	0
34	NA	A	8323	1/1	0.91	0.29	55,55,55,55	0
32	MG	A	8071	1/1	0.91	0.07	65,65,65,65	0
32	MG	A	8112	1/1	0.91	0.26	70,70,70,70	0
34	NA	A	8331	1/1	0.91	0.19	37,37,37,37	0
34	NA	A	8314	1/1	0.91	0.26	35,35,35,35	0
37	CD	2	8402	1/1	0.92	0.11	67,67,67,67	0
34	NA	A	8368	1/1	0.92	0.08	22,22,22,22	0
32	MG	A	8047	1/1	0.92	0.21	76,76,76,76	0
35	CL	Z	8520	1/1	0.92	0.15	49,49,49,49	0
34	NA	A	8367	1/1	0.92	0.14	40,40,40,40	0
32	MG	A	8062	1/1	0.92	0.08	32,32,32,32	0
32	MG	A	8085	1/1	0.93	0.18	60,60,60,60	0
32	MG	A	8049	1/1	0.93	0.17	61,61,61,61	0
32	MG	A	8091	1/1	0.93	0.07	53,53,53,53	0
35	CL	A	8512	1/1	0.93	0.11	43,43,43,43	0
32	MG	A	8041	1/1	0.93	0.30	72,72,72,72	0
32	MG	A	8096	1/1	0.93	0.14	55,55,55,55	0
34	NA	A	8342	1/1	0.93	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
35	CL	A	8522	1/1	0.93	0.48	72,72,72,72	0
32	MG	A	8045	1/1	0.93	0.12	69,69,69,69	0
34	NA	A	8340	1/1	0.93	0.38	37,37,37,37	0
32	MG	A	8027	1/1	0.93	0.09	56,56,56,56	0
32	MG	A	8063	1/1	0.93	0.09	82,82,82,82	0
34	NA	A	8317	1/1	0.93	0.12	25,25,25,25	0
34	NA	J	8309	1/1	0.93	0.10	23,23,23,23	0
34	NA	A	8365	1/1	0.93	0.12	21,21,21,21	0
32	MG	A	8082	1/1	0.93	0.10	35,35,35,35	0
34	NA	A	8372	1/1	0.93	0.15	30,30,30,30	0
32	MG	Z	8109	1/1	0.94	0.08	31,31,31,31	0
32	MG	A	8087	1/1	0.94	0.29	42,42,42,42	0
32	MG	A	8101	1/1	0.94	0.09	42,42,42,42	0
32	MG	D	8055	1/1	0.94	0.08	50,50,50,50	0
32	MG	A	8050	1/1	0.94	0.12	62,62,62,62	0
34	NA	A	8325	1/1	0.94	0.17	56,56,56,56	0
34	NA	A	8302	1/1	0.94	0.10	36,36,36,36	0
34	NA	A	8305	1/1	0.94	0.14	22,22,22,22	0
34	NA	A	8364	1/1	0.94	0.16	32,32,32,32	0
32	MG	A	8075	1/1	0.94	0.08	44,44,44,44	0
34	NA	S	8337	1/1	0.94	0.12	57,57,57,57	0
35	CL	K	8521	1/1	0.94	0.15	49,49,49,49	0
32	MG	A	8058	1/1	0.94	0.12	47,47,47,47	0
35	CL	D	8519	1/1	0.94	0.32	68,68,68,68	0
32	MG	A	8098	1/1	0.94	0.26	53,53,53,53	0
32	MG	B	8095	1/1	0.94	0.15	90,90,90,90	0
34	NA	A	8336	1/1	0.94	0.15	72,72,72,72	0
32	MG	A	8001	1/1	0.94	0.12	33,33,33,33	0
34	NA	A	8308	1/1	0.94	0.23	61,61,61,61	0
32	MG	A	8018	1/1	0.94	0.12	26,26,26,26	0
34	NA	A	8379	1/1	0.95	0.13	30,30,30,30	0
32	MG	A	8103	1/1	0.95	0.11	45,45,45,45	0
34	NA	A	8335	1/1	0.95	0.15	50,50,50,50	0
35	CL	A	8517	1/1	0.95	0.29	75,75,75,75	0
32	MG	A	8094	1/1	0.95	0.12	77,77,77,77	0
32	MG	A	8090	1/1	0.95	0.20	81,81,81,81	0
32	MG	A	8032	1/1	0.95	0.11	24,24,24,24	0
34	NA	A	8313	1/1	0.95	0.45	76,76,76,76	0
35	CL	A	8516	1/1	0.95	0.23	57,57,57,57	0
34	NA	A	8374	1/1	0.95	0.12	36,36,36,36	0
32	MG	A	8048	1/1	0.95	0.10	51,51,51,51	0
32	MG	A	8037	1/1	0.95	0.07	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8385	1/1	0.95	0.40	29,29,29,29	0
34	NA	A	8354	1/1	0.95	0.13	20,20,20,20	0
32	MG	A	8020	1/1	0.95	0.09	38,38,38,38	0
32	MG	A	8059	1/1	0.95	0.12	70,70,70,70	0
34	NA	A	8329	1/1	0.95	0.08	47,47,47,47	0
32	MG	A	8100	1/1	0.95	0.11	45,45,45,45	0
32	MG	A	8107	1/1	0.95	0.05	64,64,64,64	0
32	MG	A	8013	1/1	0.95	0.15	27,27,27,27	0
34	NA	A	8349	1/1	0.95	0.18	27,27,27,27	0
34	NA	A	8358	1/1	0.95	0.57	75,75,75,75	0
34	NA	A	8310	1/1	0.95	0.17	35,35,35,35	0
34	NA	A	8320	1/1	0.95	0.10	16,16,16,16	0
32	MG	A	8029	1/1	0.95	0.10	58,58,58,58	0
32	MG	L	8069	1/1	0.96	0.08	65,65,65,65	0
34	NA	A	8373	1/1	0.96	0.07	40,40,40,40	0
34	NA	A	8328	1/1	0.96	0.13	39,39,39,39	0
32	MG	A	8026	1/1	0.96	0.09	19,19,19,19	0
32	MG	A	8056	1/1	0.96	0.12	53,53,53,53	0
34	NA	A	8303	1/1	0.96	0.18	33,33,33,33	0
35	CL	A	8503	1/1	0.96	0.12	65,65,65,65	0
32	MG	C	8065	1/1	0.96	0.13	62,62,62,62	0
34	NA	A	8326	1/1	0.96	0.10	31,31,31,31	0
32	MG	A	8005	1/1	0.96	0.12	39,39,39,39	0
32	MG	A	8006	1/1	0.96	0.09	33,33,33,33	0
33	K	A	8202	1/1	0.96	0.07	43,43,43,43	0
32	MG	A	8036	1/1	0.96	0.06	36,36,36,36	0
32	MG	A	8088	1/1	0.96	0.07	11,11,11,11	0
32	MG	A	8072	1/1	0.96	0.22	64,64,64,64	0
32	MG	A	8028	1/1	0.96	0.06	60,60,60,60	0
34	NA	A	8378	1/1	0.96	0.12	28,28,28,28	0
34	NA	A	8352	1/1	0.96	0.20	36,36,36,36	0
32	MG	A	8077	1/1	0.96	0.16	37,37,37,37	0
33	K	A	8201	1/1	0.96	0.09	53,53,53,53	0
32	MG	A	8108	1/1	0.96	0.10	44,44,44,44	0
32	MG	A	8011	1/1	0.96	0.09	36,36,36,36	0
32	MG	A	8010	1/1	0.96	0.06	37,37,37,37	0
34	NA	A	8332	1/1	0.96	0.17	38,38,38,38	0
34	NA	A	8318	1/1	0.96	0.22	62,62,62,62	0
32	MG	A	8115	1/1	0.96	0.09	41,41,41,41	0
34	NA	A	8360	1/1	0.97	0.15	42,42,42,42	0
32	MG	A	8004	1/1	0.97	0.08	18,18,18,18	0
32	MG	A	8084	1/1	0.97	0.09	65,65,65,65	0

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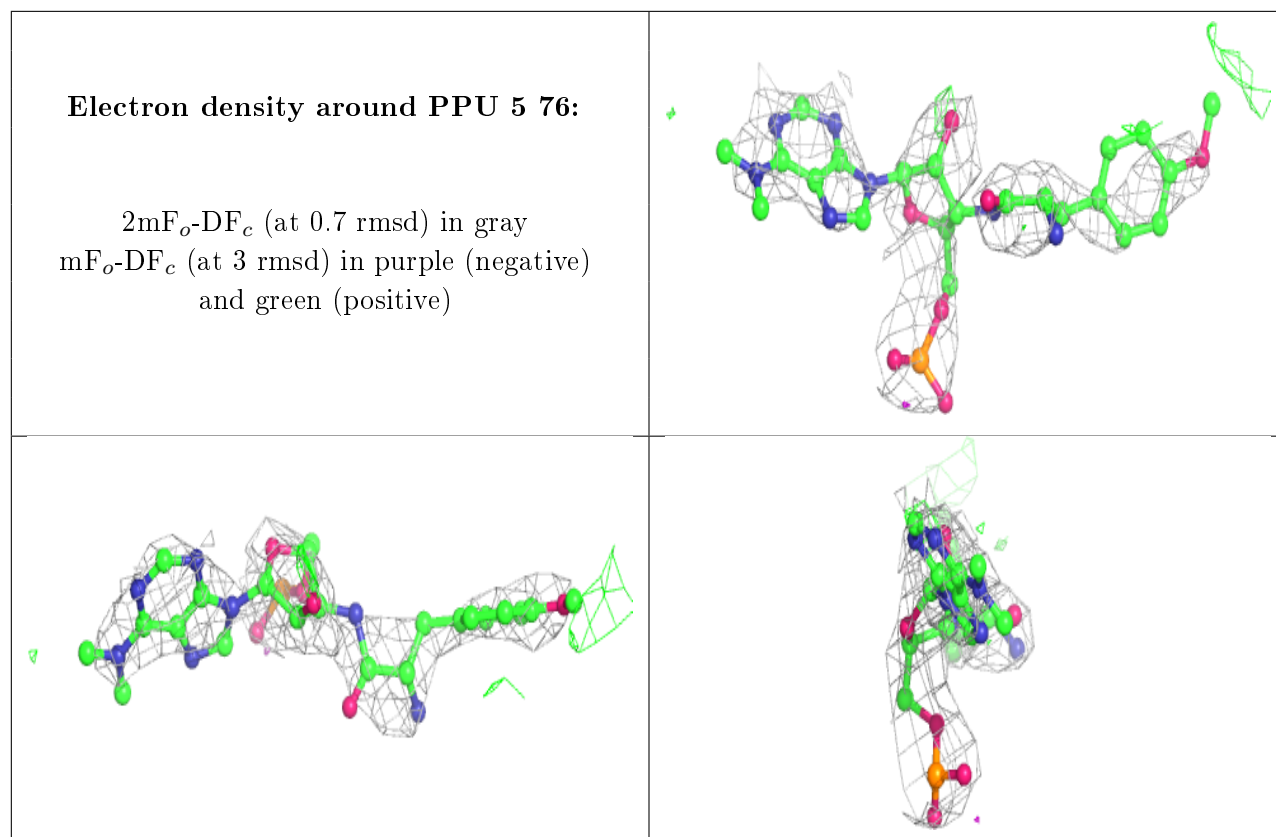
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
34	NA	A	8334	1/1	0.97	0.05	36,36,36,36	0
34	NA	A	8301	1/1	0.97	0.26	27,27,27,27	0
35	CL	A	8513	1/1	0.97	0.13	74,74,74,74	0
32	MG	A	8093	1/1	0.97	0.19	91,91,91,91	0
34	NA	A	8327	1/1	0.97	0.25	18,18,18,18	0
37	CD	1	8403	1/1	0.97	0.14	187,187,187,187	0
32	MG	A	8033	1/1	0.97	0.09	26,26,26,26	0
32	MG	A	8053	1/1	0.97	0.16	86,86,86,86	0
34	NA	A	8324	1/1	0.97	0.06	26,26,26,26	0
34	NA	A	8311	1/1	0.97	0.12	68,68,68,68	0
34	NA	A	8343	1/1	0.97	0.09	17,17,17,17	0
32	MG	A	8023	1/1	0.97	0.07	47,47,47,47	0
34	NA	A	8316	1/1	0.97	0.11	31,31,31,31	0
32	MG	A	8019	1/1	0.97	0.06	27,27,27,27	0
32	MG	A	8061	1/1	0.97	0.07	40,40,40,40	0
34	NA	A	8315	1/1	0.97	0.11	15,15,15,15	0
32	MG	A	8113	1/1	0.97	0.10	40,40,40,40	0
32	MG	A	8009	1/1	0.97	0.08	15,15,15,15	0
34	NA	A	8307	1/1	0.97	0.11	28,28,28,28	0
32	MG	A	8034	1/1	0.97	0.06	32,32,32,32	0
34	NA	R	8348	1/1	0.97	0.11	20,20,20,20	0
32	MG	A	8031	1/1	0.97	0.07	14,14,14,14	0
34	NA	M	8380	1/1	0.98	0.15	43,43,43,43	0
32	MG	A	8060	1/1	0.98	0.12	39,39,39,39	0
32	MG	A	8057	1/1	0.98	0.10	16,16,16,16	0
32	MG	A	8030	1/1	0.98	0.13	31,31,31,31	0
34	NA	A	8321	1/1	0.98	0.23	53,53,53,53	0
32	MG	A	8054	1/1	0.98	0.09	43,43,43,43	0
32	MG	A	8015	1/1	0.98	0.08	35,35,35,35	0
32	MG	A	8086	1/1	0.98	0.14	49,49,49,49	0
32	MG	A	8110	1/1	0.98	0.06	26,26,26,26	0
32	MG	A	8104	1/1	0.98	0.09	40,40,40,40	0
34	NA	C	8345	1/1	0.98	0.15	30,30,30,30	0
34	NA	A	8330	1/1	0.98	0.10	37,37,37,37	0
32	MG	A	8002	1/1	0.98	0.11	26,26,26,26	0
32	MG	A	8067	1/1	0.98	0.15	41,41,41,41	0
32	MG	A	8022	1/1	0.98	0.05	22,22,22,22	0
32	MG	A	8007	1/1	0.98	0.09	22,22,22,22	0
32	MG	A	8012	1/1	0.98	0.14	41,41,41,41	0
32	MG	A	8080	1/1	0.98	0.09	35,35,35,35	0
32	MG	A	8079	1/1	0.98	0.07	19,19,19,19	0
35	CL	N	8518	1/1	0.98	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	MG	A	8083	1/1	0.98	0.07	40,40,40,40	0
32	MG	A	8014	1/1	0.98	0.13	20,20,20,20	0
34	NA	A	8353	1/1	0.98	0.07	15,15,15,15	0
32	MG	A	8003	1/1	0.98	0.19	36,36,36,36	0
32	MG	A	8035	1/1	0.98	0.04	64,64,64,64	0
34	NA	A	8362	1/1	0.98	0.13	45,45,45,45	0
34	NA	A	8376	1/1	0.98	0.12	35,35,35,35	0
32	MG	A	8016	1/1	0.99	0.10	26,26,26,26	0
34	NA	N	8347	1/1	0.99	0.05	21,21,21,21	0
32	MG	A	8117	1/1	0.99	0.06	8,8,8,8	0
32	MG	A	8074	1/1	0.99	0.08	24,24,24,24	0
32	MG	A	8025	1/1	0.99	0.04	57,57,57,57	0
35	CL	K	8501	1/1	0.99	0.10	61,61,61,61	0
32	MG	A	8017	1/1	0.99	0.05	17,17,17,17	0
32	MG	A	8042	1/1	0.99	0.05	17,17,17,17	0
32	MG	A	8064	1/1	0.99	0.11	18,18,18,18	0
32	MG	A	8021	1/1	0.99	0.10	45,45,45,45	0
32	MG	A	8038	1/1	0.99	0.10	30,30,30,30	0
32	MG	A	8081	1/1	0.99	0.13	30,30,30,30	0
34	NA	K	8346	1/1	1.00	0.06	19,19,19,19	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.