



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 11:58 AM UTC

PDB ID : 1Q82 / pdb_00001q82
Title : Crystal Structure of CC-Puromycin bound to the 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 : 2.98 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

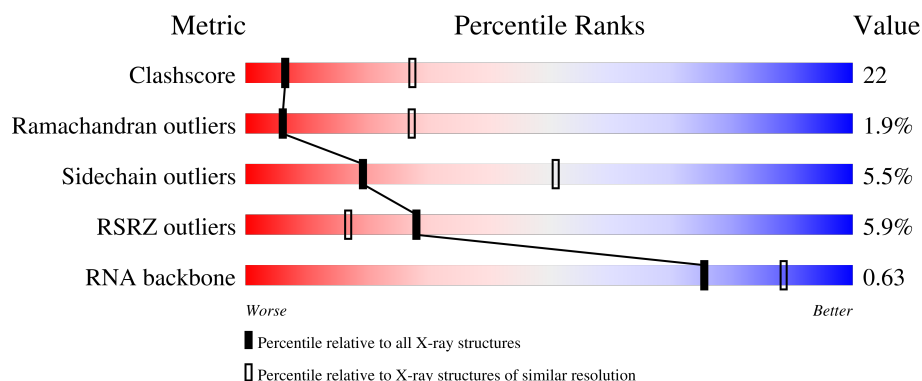
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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.



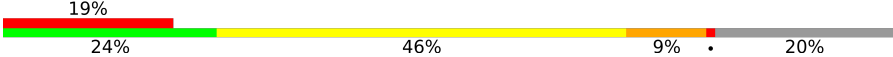
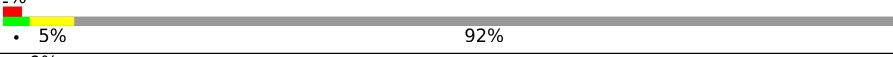
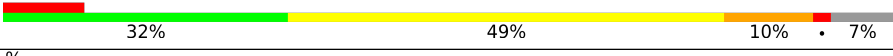
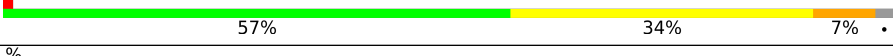
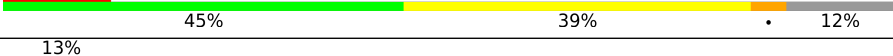
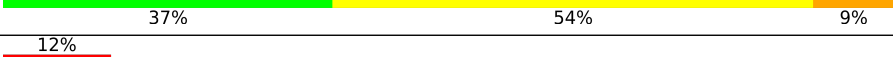
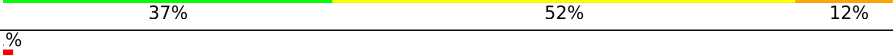
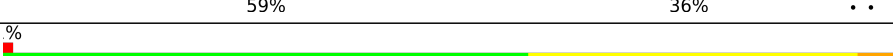
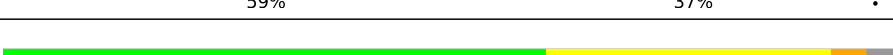
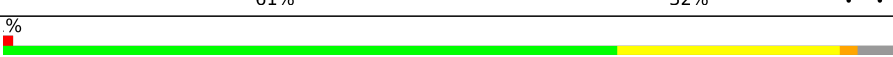
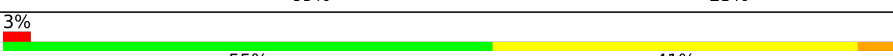
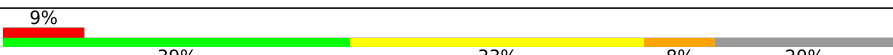
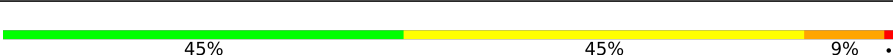
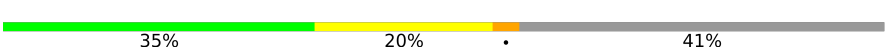
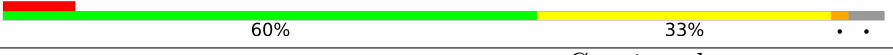
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)
RNA backbone	3983	1013 (3.18-2.78)

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	A	2922	 3% 50% 36% 8% • 6%
2	B	122	 6% 50% 36% 9% 5%
3	5	2	 50% 50%
4	C	239	 6% 51% 43% 6% •
5	D	337	 46% 46% 7%

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Mol	Chain	Length	Quality of chain
6	E	246	
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	

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Mol	Chain	Length	Quality of chain
31	4	92	68% 48% 39% 11%

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	A	8011	-	-	X	-
32	MG	A	8102	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	B	8383	-	-	-	X
35	CL	N	8518	-	-	X	-

2 Entry composition [i](#)

There are 38 unique types of molecules in this entry. The entry contains 98593 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 CC-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		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		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		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	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	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	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	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	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	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 (CCD ID: MG) (formula: Mg).

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

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

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

- Molecule 34 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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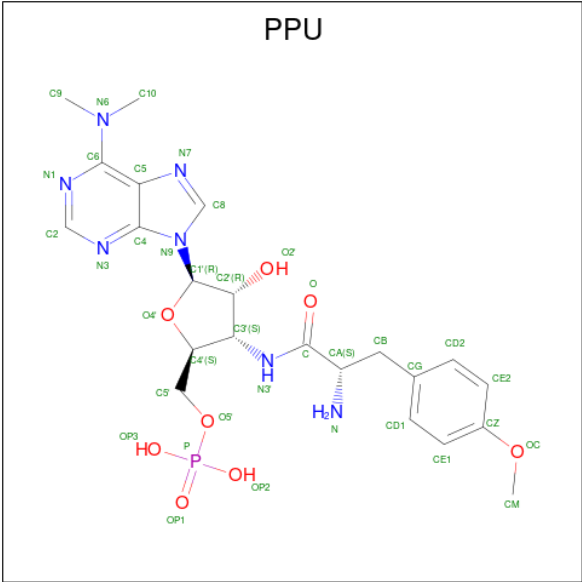
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	R	1	Total 1	Na 1	0	0
34	S	2	Total 2	Na 2	0	0
34	T	1	Total 1	Na 1	0	0
34	U	1	Total 1	Na 1	0	0
34	4	1	Total 1	Na 1	0	0

- Molecule 35 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	7	Total 7	Cl 7	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	4	Total 4	Cl 4	0	0
35	M	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	P	1	Total 1	Cl 1	0	0
35	R	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	2	Total 2	Cl 2	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is PUROMYCIN-5'-MONOPHOSPHATE (CCD ID: PPU) (formula: C₂₂H₃₀N₇O₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	5	1	Total	C	N	O	P	0	0
			37	22	7	7	1		

- Molecule 37 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
37	P	1	Total	Cd	0	0
			1	1		
37	V	1	Total	Cd	0	0
			1	1		
37	1	1	Total	Cd	0	0
			1	1		
37	2	1	Total	Cd	0	0
			1	1		
37	4	1	Total	Cd	0	0
			1	1		

- Molecule 38 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	A	5860	Total	O	0	0
			5860	5860		
38	B	146	Total	O	0	0
			146	146		
38	5	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	C	140	Total 140	O 140	0	0
38	D	146	Total 146	O 146	0	0
38	E	176	Total 176	O 176	0	0
38	F	52	Total 52	O 52	0	0
38	G	45	Total 45	O 45	0	0
38	H	32	Total 32	O 32	0	0
38	I	22	Total 22	O 22	0	0
38	J	78	Total 78	O 78	0	0
38	K	54	Total 54	O 54	0	0
38	L	64	Total 64	O 64	0	0
38	M	86	Total 86	O 86	0	0
38	N	138	Total 138	O 138	0	0
38	O	64	Total 64	O 64	0	0
38	P	44	Total 44	O 44	0	0
38	Q	70	Total 70	O 70	0	0
38	R	57	Total 57	O 57	0	0
38	S	83	Total 83	O 83	0	0
38	T	36	Total 36	O 36	0	0
38	U	38	Total 38	O 38	0	0
38	V	22	Total 22	O 22	0	0
38	W	16	Total 16	O 16	0	0

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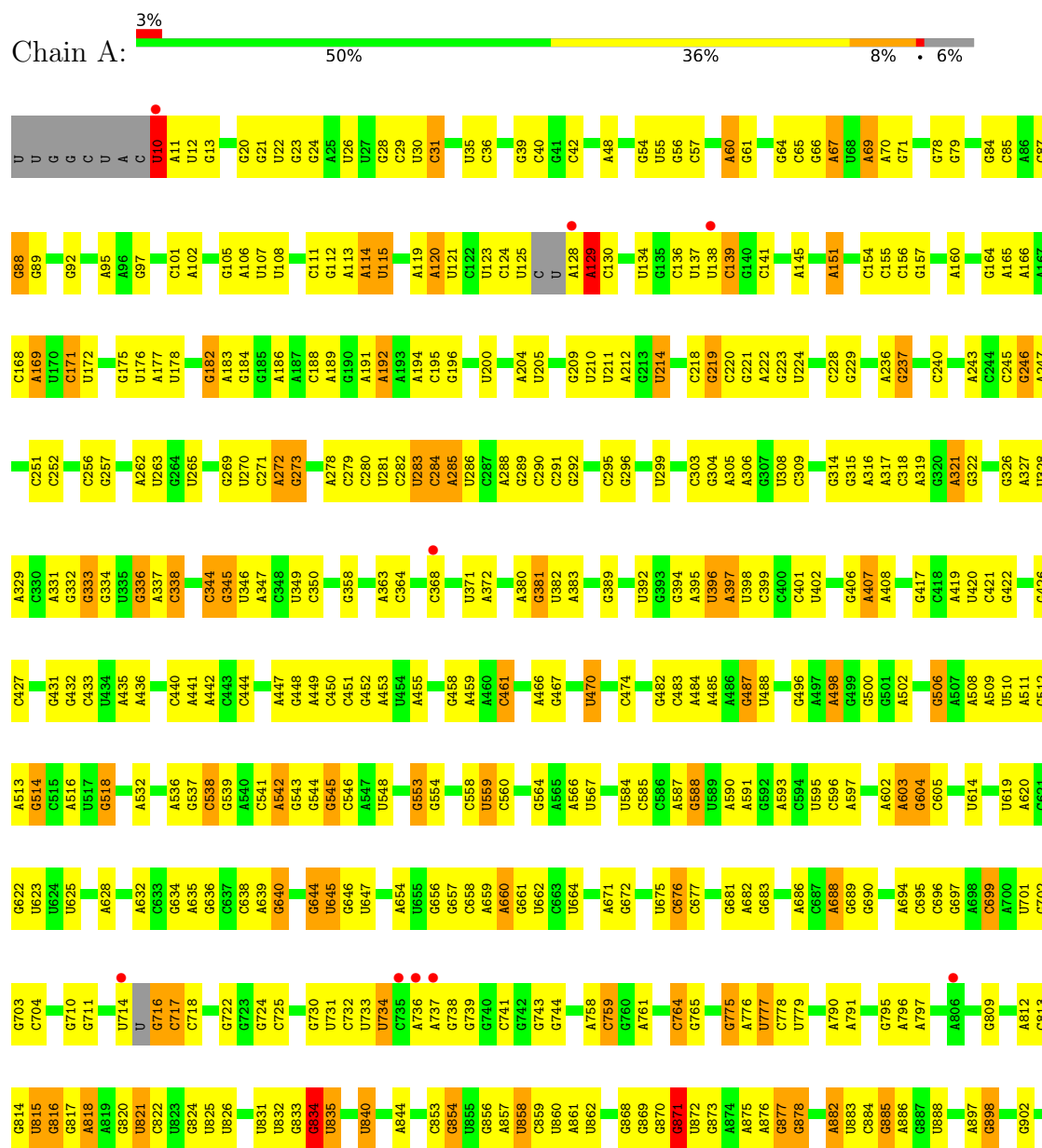
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	X	67	Total 67	O 67	0	0
38	Y	28	Total 28	O 28	0	0
38	Z	100	Total 100	O 100	0	0
38	1	36	Total 36	O 36	0	0
38	2	58	Total 58	O 58	0	0
38	3	37	Total 37	O 37	0	0
38	4	70	Total 70	O 70	0	0

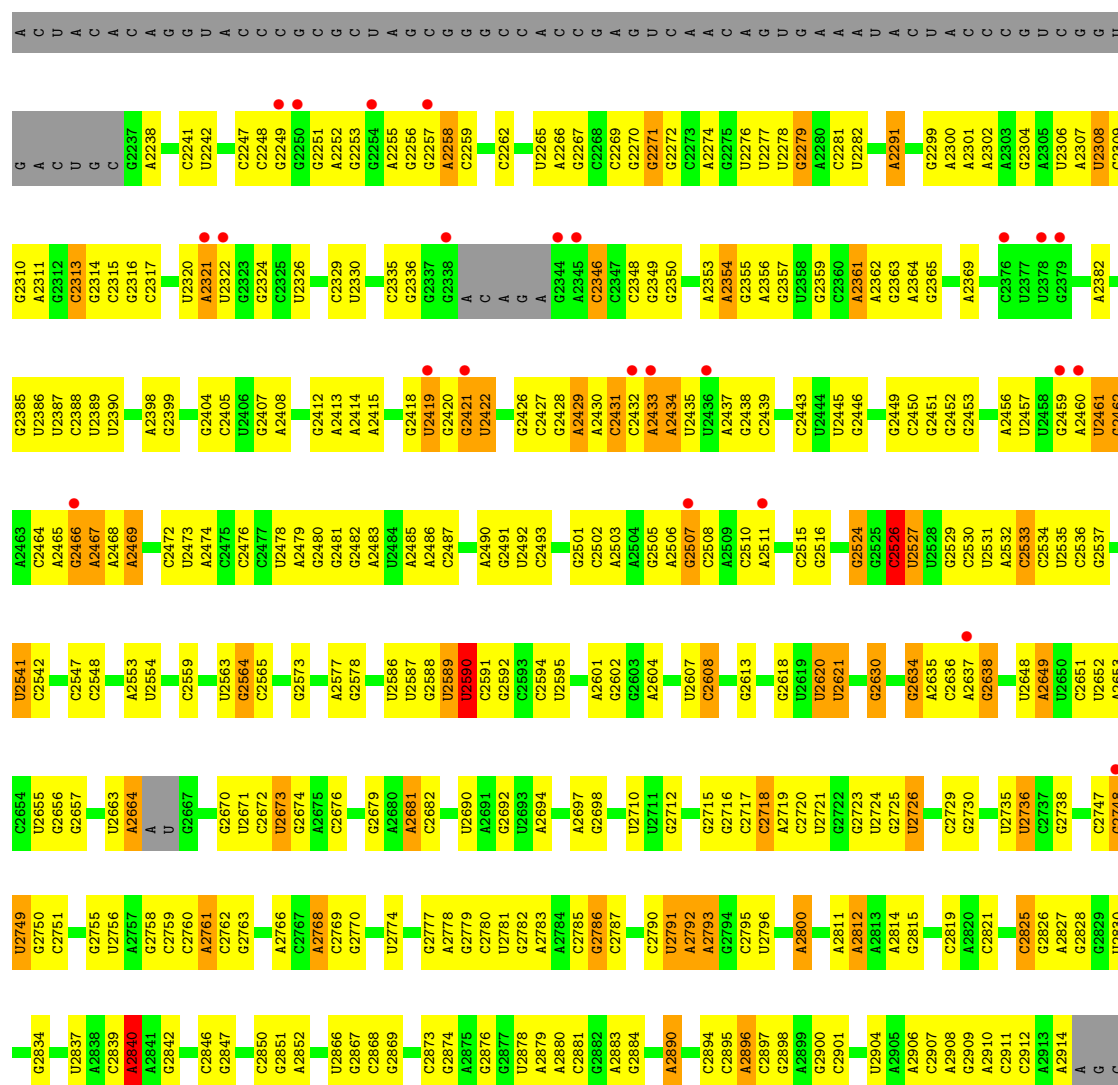
3 Residue-property plots

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

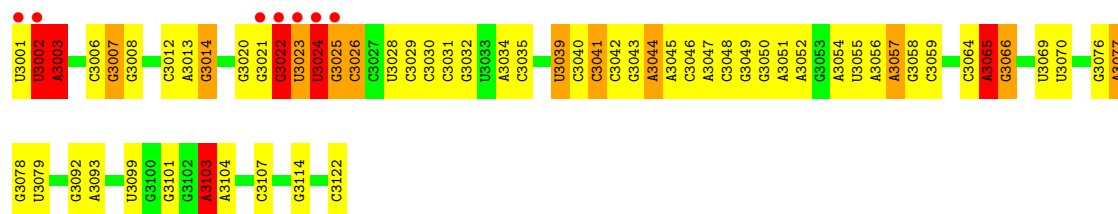
- Molecule 1: 23S ribosomal rna



C2104	A2007	A1909	G1820	G1730	G1643	C1558	A1463	A1358	C1253	U1185	A1086	G	C905
C2105	U2008	A1910	U1825	G1731	C1644	A1559	U1464	A1359	G1260	C1186	G1087	G	C906
C2106	G2009	U1915	U1826	A1732	U1645	U	C1467	C1360	A1261	U1187	A1088	A	G911
U2107	A2010	C1916	G1827	G1733	G1647	U1561	C1467	U1361	G1265	A1188	U	G	A912
A2108	A2011	C1917	G1828	C1734	C1651	G1562	A1471	U1362	U1266	A1189	C	C	A913
U2109	U2012	U1918	A1829	C1735	C1651	G1563	A1472	U1368	U1267	U1190	U	G	U917
G2111	G2013	U1919	A1830	A1736	U1654	C1564	U1473	U1368	C1267	A1191	G	G	G918
A2112	G2014	C1920	C1834	A1737	U1655	C1565	C1474	U1368	U1268	A1192	C	C	U919
G2113	U2016	A1921	U1835	C1738	A1656	C1566	U1475	U1368	U1269	A1193	C	C	C920
C2114	U2016	A1922	U1836	C1738	A1657	G1567	C1477	U1372	U1270	U1194	A	A	G921
U2115	A2019	U1923	A1839	U1741	A1657	U1569	U1478	G1376	U1279	C1196	A	A	G922
U2116	A2022	A1924	A1840	A1742	A1658	U1572	C1483	U1377	U1289	G1197	C999	A	A923
C2119	U2120	G1925	A1845	G1743	A1659	A1573	C1484	U1380	C1289	U1198	U1003	U	G924
U2120	C2026	G1926	U1846	U1749	G1660	C1574	A1485	U1380	U1297	A1200	U	U	G925
G2121	U2027	A1929	A1847	C1750	C1666	C1574	U1488	U1383	U1297	G1121	A1006	A	A926
C2122	U2028	G1930	G1848	G1751	A1667	U1580	U1488	U1384	U1298	A1123	A1007	U	U927
A2123	C2029	A1931	G1849	G1752	U1668	G1589	U1499	G1385	U1299	A1124	C1008	U	A928
G2124	U2033	G1932	U1850	C1753	A1669	U1596	U1500	G1386	U1304	U1125	C1009	U	A929
U2128	U2034	G1933	G1851	A1754	G1670	G1597	A1494	G1387	C1305	C1126	C1010	U	U932
G2134	A2039	C1940	A1852	A1755	U1677	C1593	C1496	U1388	U1306	U1128	A1013	U	G941
A2135	U2047	A1941	G1855	A1759	U1678	C1594	G1497	U1388	A1307	U1129	A1014	U	U942
G2136	G2044	C1943	A1856	C1762	C1680	G1596	U1498	G1389	U1308	U1130	A1015	U	A943
A	C2047	U1951	A1857	U1766	G1681	A1597	U1501	G1391	A1309	G1131	U1016	U	G948
C	U2050	U	U1858	A1767	A1682	A1598	A1502	G1392	U1310	G1132	C1023	U	U949
U	G2050	A	U1859	C1768	G1683	U1599	U1503	A1393	G1311	G1133	G1024	U	G950
G	U2050	C	U1860	C1769	A1684	G1600	A1504	C1394	G1312	U1134	G1025	U	A951
G	G2053	C	C1862	U1770	A1685	G1601	U1505	A1407	G1313	U1135	G1026	U	G952
U	A2054	U	G1868	U1771	C1686	C1602	U1506	U1408	G1314	G1137	U1027	U	G953
C	A2055	U	A1869	G1772	G1687	A1603	C1512	U1412	G1316	G1151	U1028	U	U954
C	U2063	U	C1870	G1773	G1688	G1605	C1513	U1417	G1324	U1217	U1029	U	A955
C	U2064	C	U1871	C1776	C1692	C1609	C1514	G1417	G1325	U1218	G1038	U	G958
G	G2068	A	G1872	A1777	U1696	G1610	A1515	U1422	A1328	G1159	U1041	U	G959
U	C2071	C	G1873	A1778	C1699	G1611	C1516	C1423	A1329	A1161	U1042	U	G960
G	G2072	U	U1874	A1779	C1700	A1612	U1517	A1424	A1330	G1162	C1043	U	A961
U	G2073	U	C1878	C1787	A1701	G1613	G1523	U1427	A1331	U1163	U1044	U	C962
C	A2074	C	A1880	U1788	U1702	G1614	U1524	A1430	G1332	U1164	G1045	U	G968
A	U2081	U	C1881	G1795	G1706	A1615	A1526	G1430	C1333	G1165	C1051	U	G969
G	A2089	U	C1882	A1796	G1707	C1617	A1527	U1434	C1334	U1167	G1052	U	U970
U	U2090	U	A1883	A1797	G1707	A1624	A1528	U1435	U1335	C1168	G1053	U	G
A	G2091	U	A1884	C1798	A1710	U1625	U1530	C1436	A1336	U1169	G1054	U	G
G	G2092	U	A1885	A1804	A1711	A1626	U1531	U1440	U1337	A1171	U1055	C	C
C	U2093	U	U1887	G1805	G1712	G1627	C1534	A1341	G1340	G1173	U1056	C	C
U	G2094	U	G1896	G1806	G1713	C1633	C1535	C1342	C1341	G1174	A1057	U	C
A	A2095	U	U1897	C1715	C1715	U1635	C1536	A1442	U1244	G1175	A1058	U	C
G	A2096	U	G1902	U1813	G1718	G1636	U1543	A1448	G1344	A1177	C1060	U	C
A	U2100	U	G1903	G1814	G1718	G1637	U1544	A1449	A1345	G1178	G1072	U	C
G	A2101	U	A1904	C1816	U1722	U1638	C1545	C1451	U1346	U1180	C	C	C
G	G2102	U	U1907	A1817	G1723	U1641	C1546	U1461	U1347	A1181	A1079	U	G
A	A2103	U	U1908	G1819	C1725	A1642	G1557	C1462	G1351	C1182	C1080	A	G
C		U							A1352	C1251	A1081	A	A



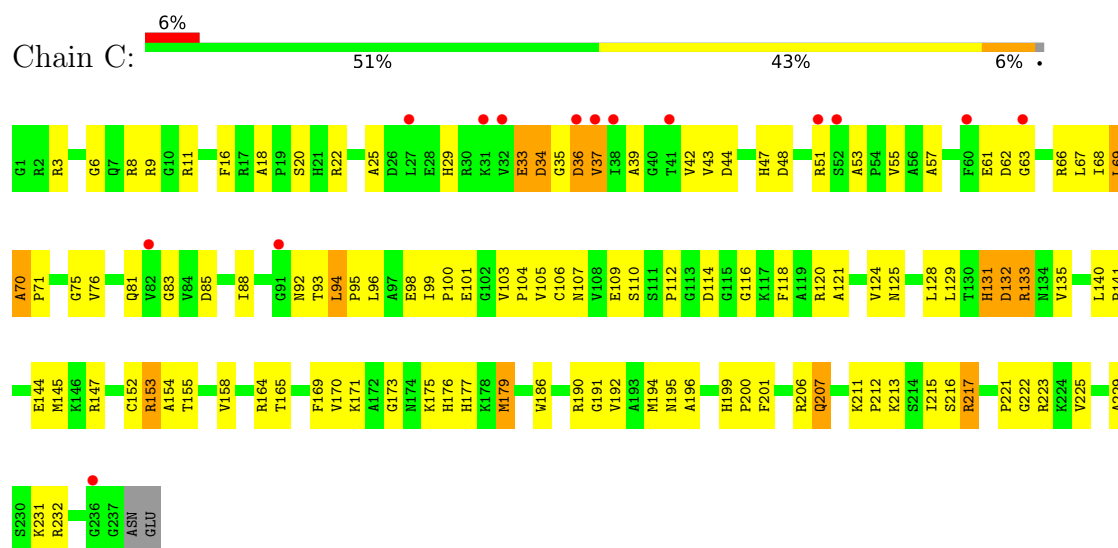
● Molecule 2: 5S ribosomal RNA



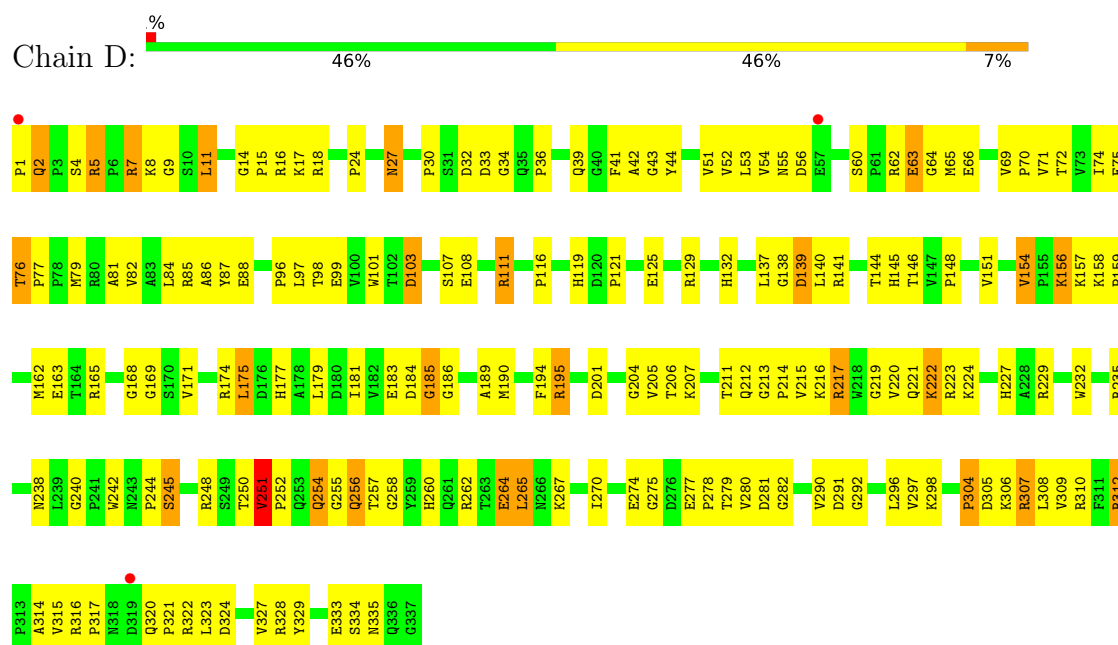
● Molecule 3: CC-puromycin



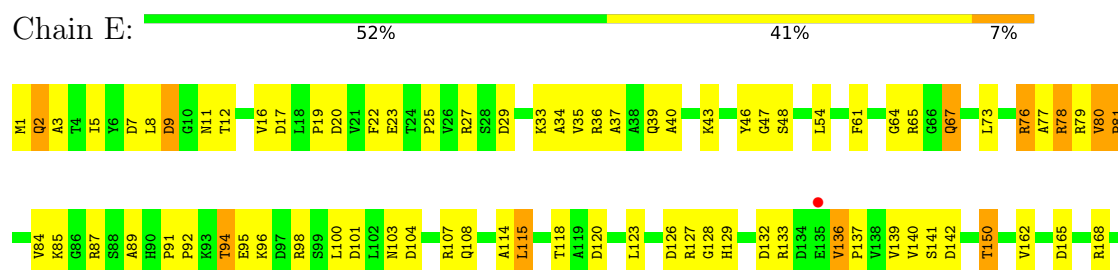
• Molecule 4: 50S ribosomal protein L2P



• Molecule 5: 50S ribosomal protein L3P

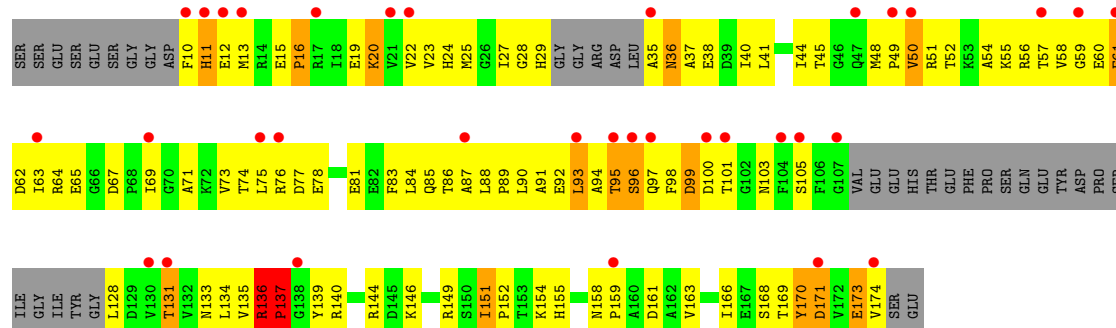


• Molecule 6: 50S ribosomal protein L4E

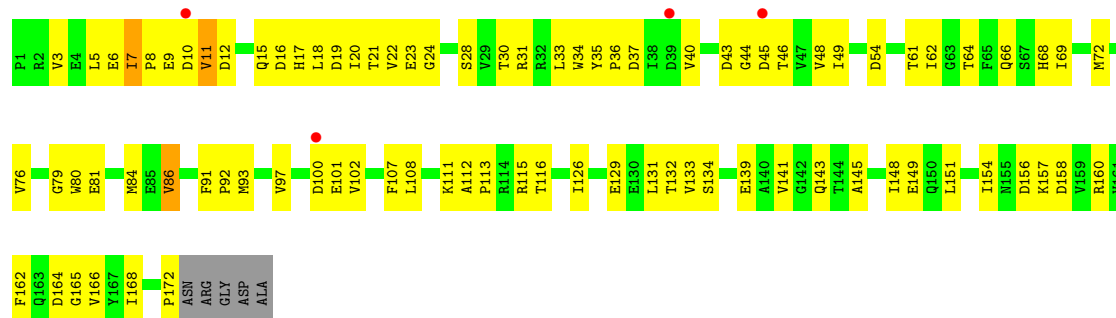




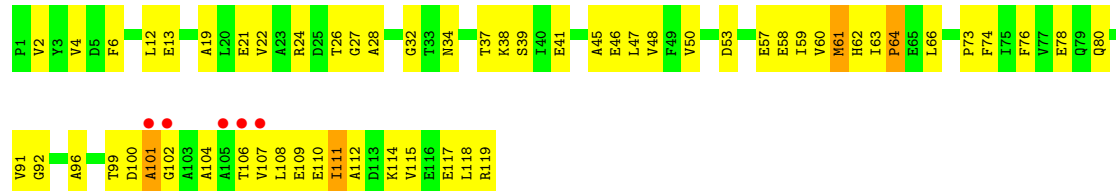
• Molecule 7: 50S ribosomal protein L5P



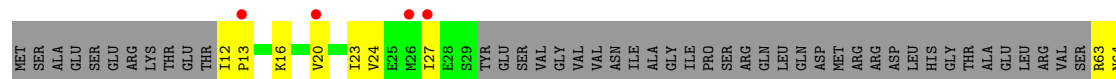
• Molecule 8: 50S ribosomal protein L6P



• Molecule 9: 50S ribosomal protein L7Ae

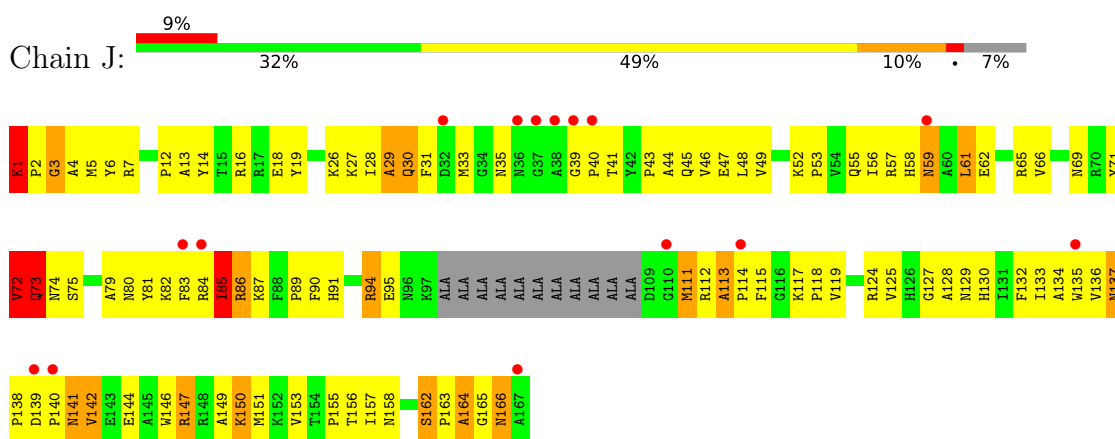


• Molecule 10: Acidic ribosomal protein P0 homolog

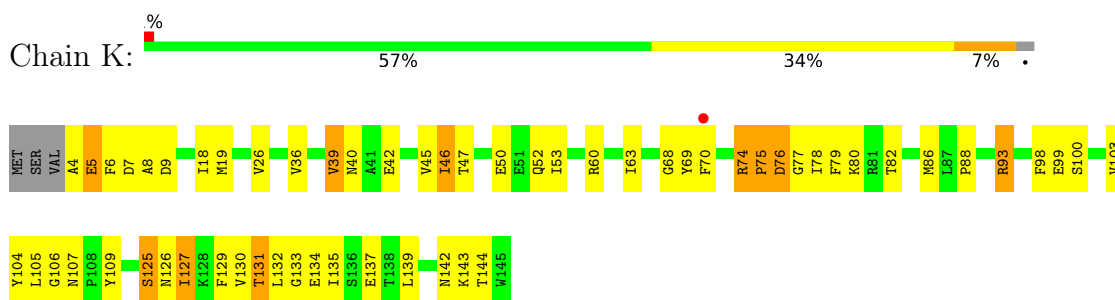




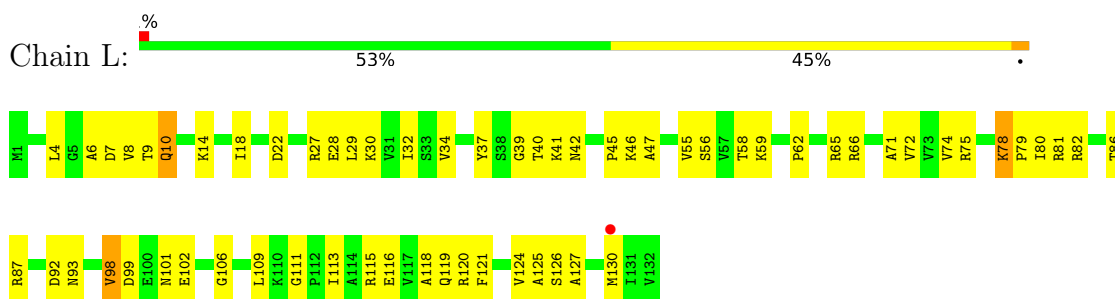
- Molecule 11: L10 Ribosomal Protein



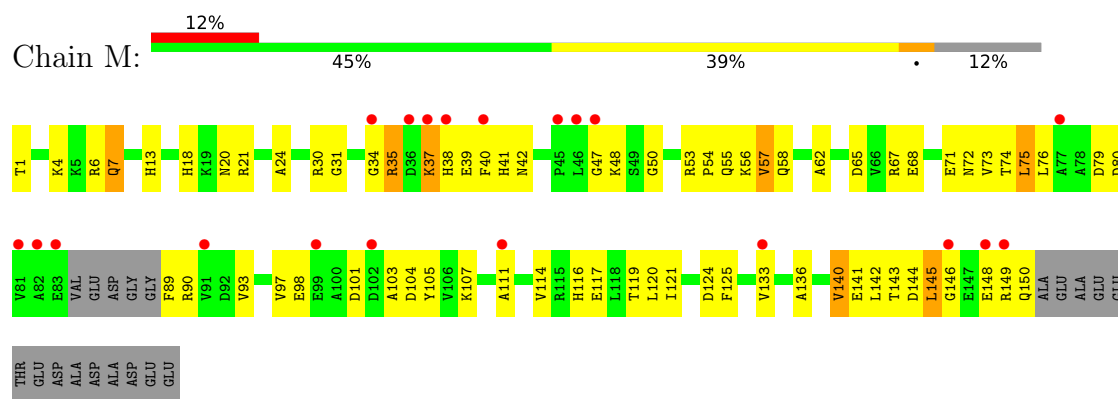
- Molecule 12: 50S ribosomal protein L13P



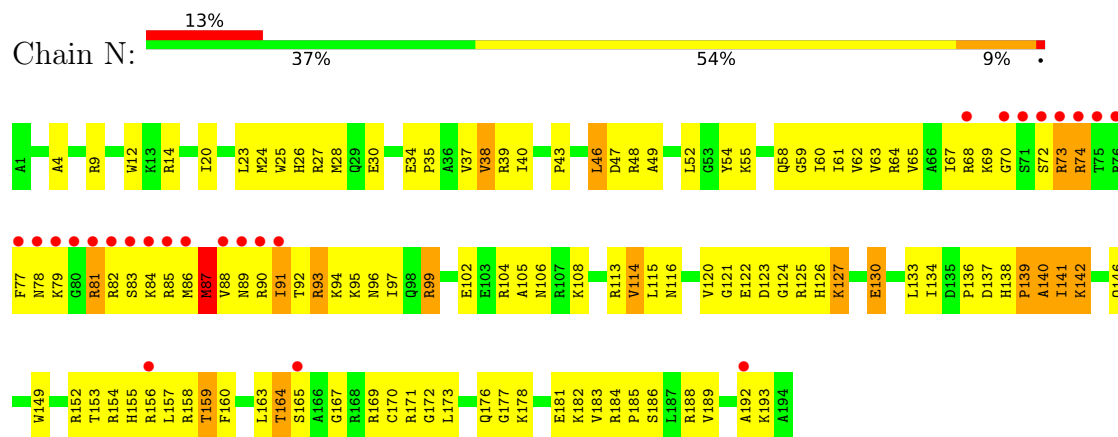
- Molecule 13: 50S ribosomal protein L14P



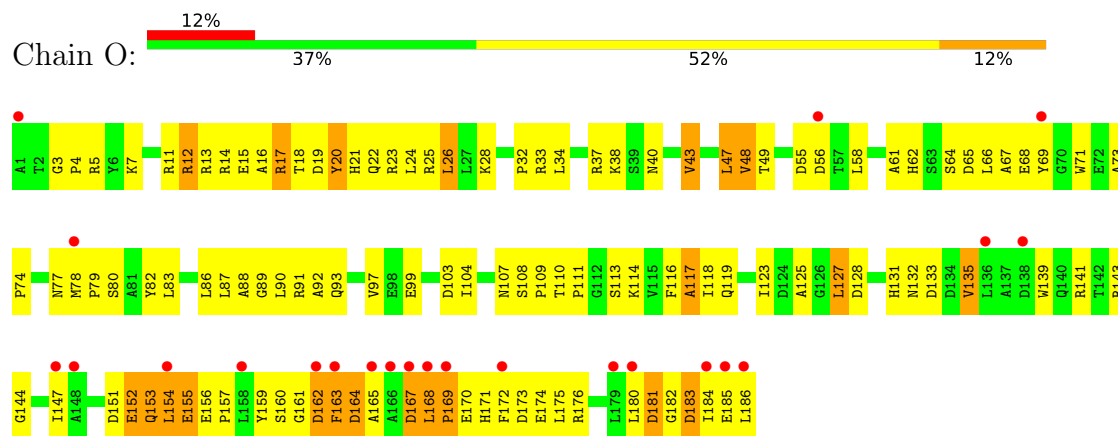
- Molecule 14: 50S ribosomal protein L15P



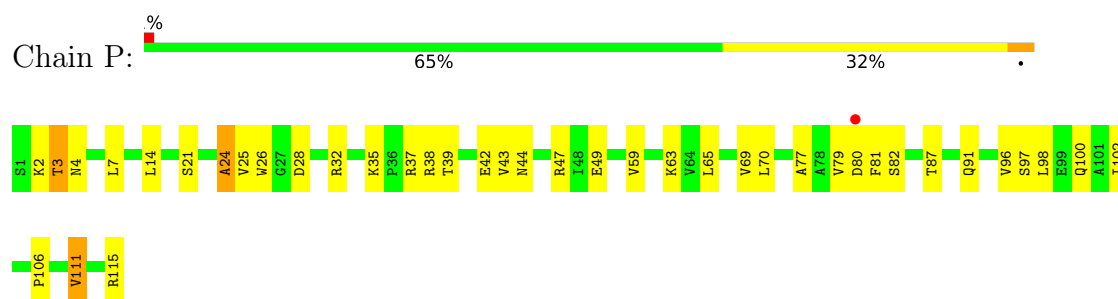
• Molecule 15: L15 Ribosomal Protein



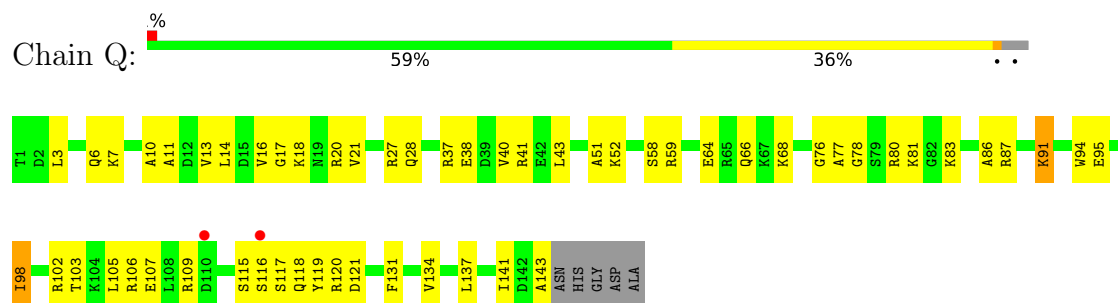
• Molecule 16: 50S ribosomal protein L18P



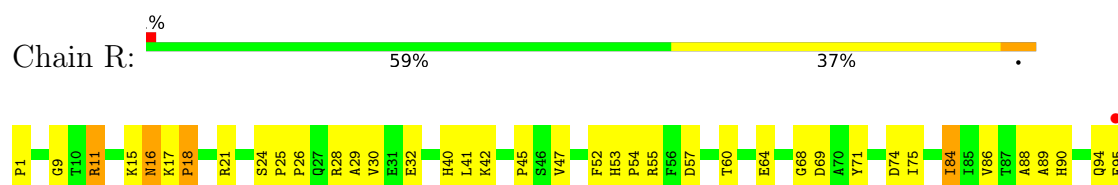
• Molecule 17: 50S ribosomal protein L18e



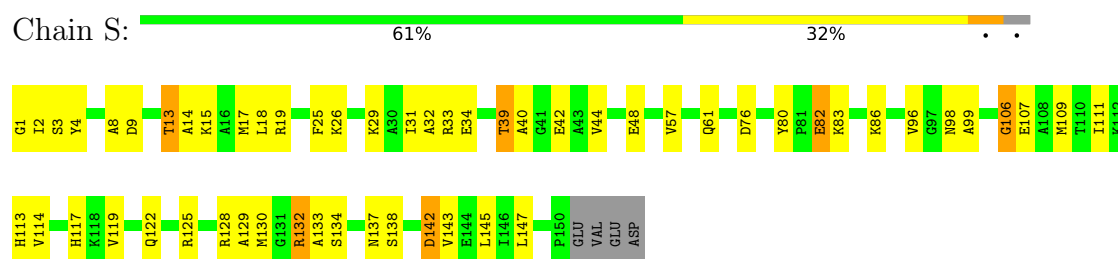
- Molecule 18: 50S ribosomal protein L19E



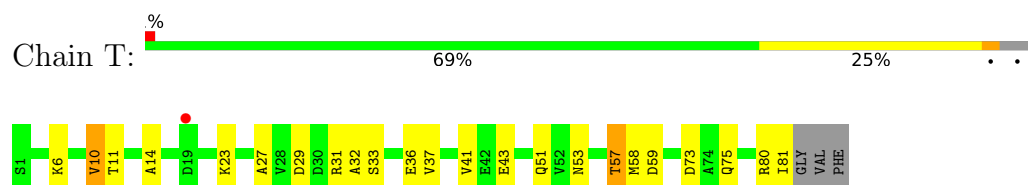
- Molecule 19: 50S ribosomal protein L21e



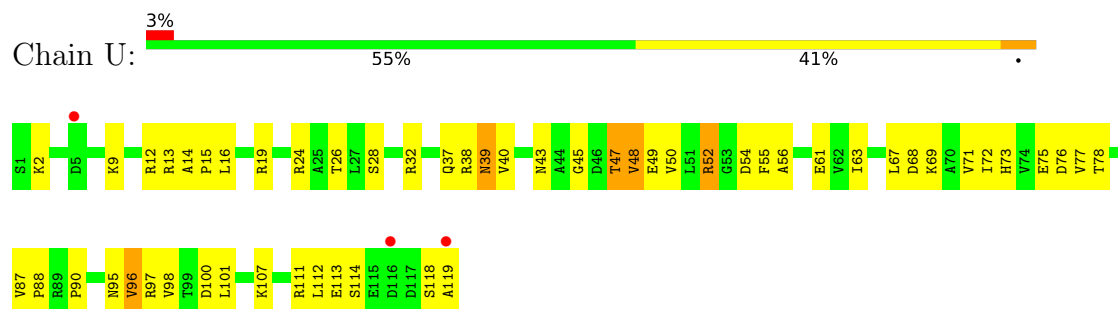
- Molecule 20: 50S ribosomal protein L22P



- Molecule 21: 50S ribosomal protein L23P

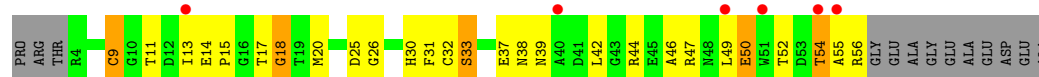


- Molecule 22: 50S ribosomal protein L24P

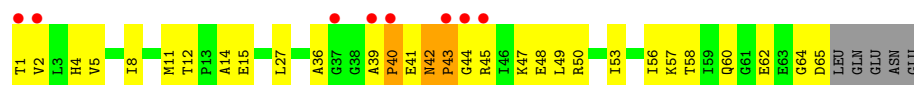


- Molecule 23: 50S ribosomal protein L24E

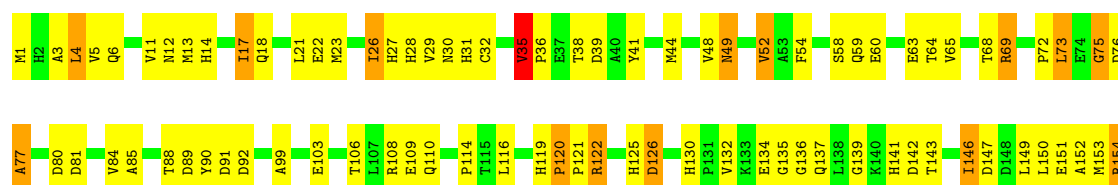




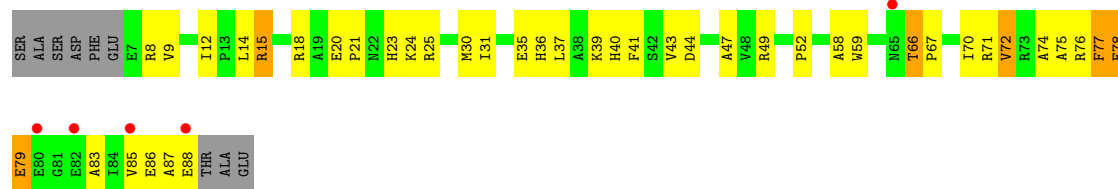
- Molecule 24: 50S ribosomal protein L29P



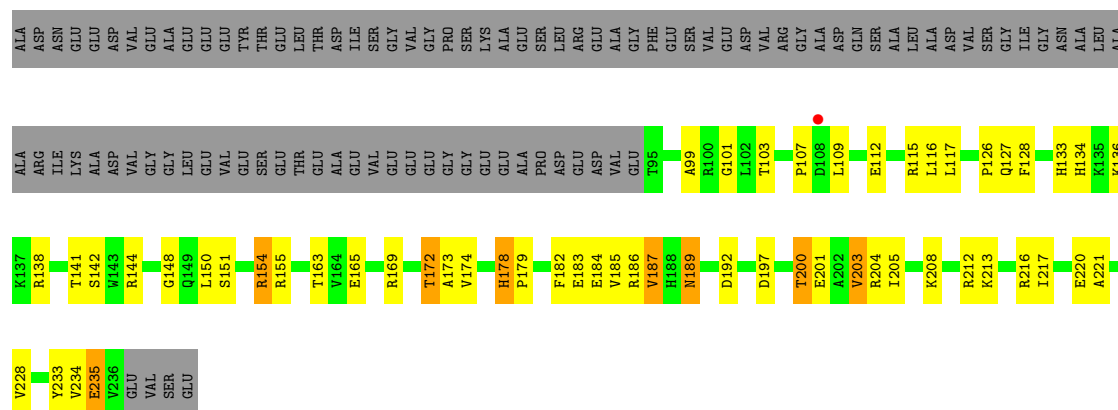
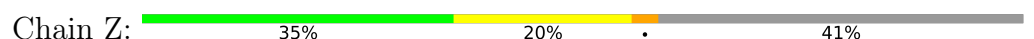
- Molecule 25: 50S ribosomal protein L30P



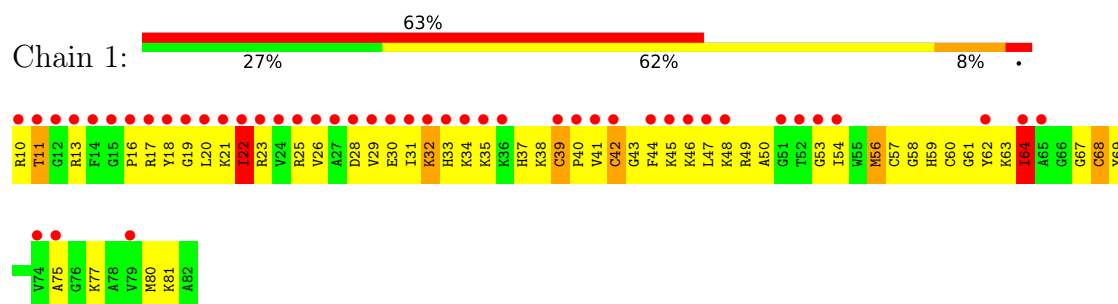
- Molecule 26: 50S ribosomal protein L31e



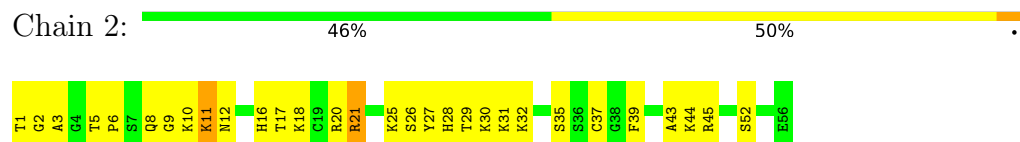
- Molecule 27: 50S ribosomal protein L32E



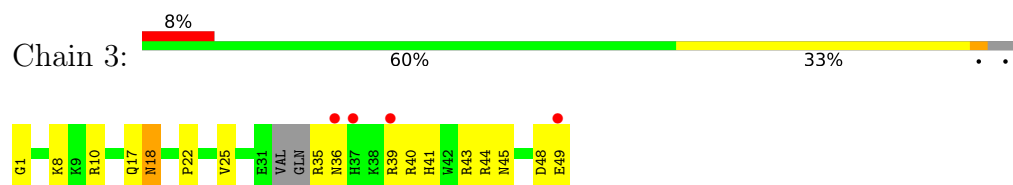
- Molecule 28: L37Ae 50S ribosomal protein



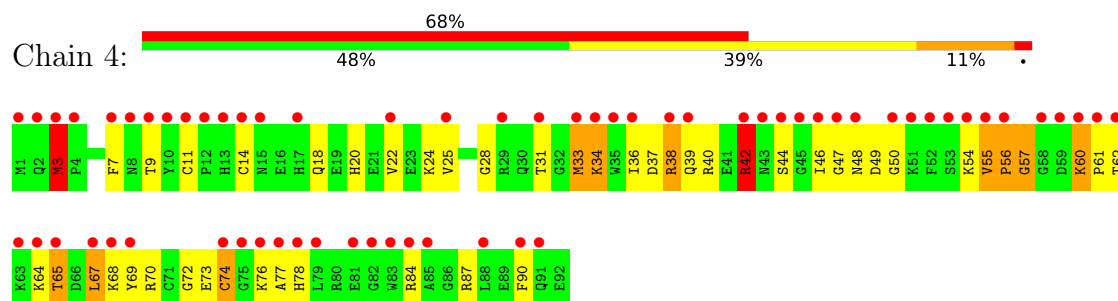
- Molecule 29: 50S ribosomal protein L37e



- Molecule 30: 50S ribosomal protein L39e



- Molecule 31: 50S ribosomal protein L44E



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	213.16Å 301.29Å 575.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.98 20.00 – 2.98	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.98) 91.5 (20.00-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.96Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.251 0.210 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 64.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	98593	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.50	1/66076 (0.0%)	0.72	41/103052 (0.0%)
2	B	0.48	0/2905	0.79	7/4528 (0.2%)
3	5	1.66	0/43	2.37	2/64 (3.1%)
4	C	0.59	0/1787	1.13	8/2409 (0.3%)
5	D	0.58	0/2689	1.11	19/3652 (0.5%)
6	E	0.62	0/1883	1.11	10/2551 (0.4%)
7	F	0.46	0/1111	0.99	6/1498 (0.4%)
8	G	0.57	0/1382	0.96	2/1880 (0.1%)
9	H	0.47	0/896	0.95	2/1219 (0.2%)
10	I	0.49	0/241	0.89	0/324
11	J	0.62	0/1246	1.31	16/1686 (0.9%)
12	K	0.62	0/1135	1.04	6/1530 (0.4%)
13	L	0.60	0/1003	1.16	8/1351 (0.6%)
14	M	0.60	1/1126 (0.1%)	1.13	7/1504 (0.5%)
15	N	0.78	0/1633	1.23	15/2180 (0.7%)
16	O	0.50	0/1473	1.16	12/1999 (0.6%)
17	P	0.61	0/873	1.06	6/1181 (0.5%)
18	Q	0.55	0/1143	0.97	2/1521 (0.1%)
19	R	0.54	0/748	1.16	8/1005 (0.8%)
20	S	0.65	0/1172	1.08	8/1578 (0.5%)
21	T	0.50	0/648	0.99	1/875 (0.1%)
22	U	0.50	0/957	1.09	5/1289 (0.4%)
23	V	0.66	0/417	1.13	4/562 (0.7%)
24	W	0.50	0/502	1.01	2/675 (0.3%)
25	X	0.70	0/1218	1.07	8/1655 (0.5%)
26	Y	0.63	0/664	1.08	1/895 (0.1%)
27	Z	0.59	0/1146	1.05	5/1536 (0.3%)
28	1	0.97	1/575 (0.2%)	1.24	5/763 (0.7%)
29	2	0.65	0/437	1.12	4/578 (0.7%)
30	3	0.58	0/398	0.84	0/527
31	4	1.16	2/771 (0.3%)	1.18	6/1024 (0.6%)
All	All	0.54	5/98298 (0.0%)	0.84	226/147091 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	143
2	B	1	4
All	All	2	147

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	22	ILE	CA-CB	6.87	1.61	1.54
31	4	33	MET	SD-CE	6.71	1.96	1.79
31	4	3	MET	SD-CE	6.48	1.95	1.79
1	A	2487	C	O5'-C5'	6.33	1.51	1.42
14	M	37	LYS	CA-C	5.20	1.55	1.52

The worst 5 of 226 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1164	U	OP1-P-O3'	-14.52	64.43	108.00
1	A	1164	U	OP2-P-O3'	-14.52	64.44	108.00
2	B	3024	U	C2'-C3'-O3'	14.02	130.52	109.50
15	N	141	ILE	N-CA-C	-13.56	100.91	111.90
1	A	1563	G	C2'-C3'-O3'	13.34	129.51	109.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
2	B	3024	U	C3'

5 of 147 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	U	Sidechain
1	A	26	U	Sidechain
1	A	28	G	Sidechain
1	A	48	A	Sidechain
1	A	55	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	29798	1225	0
2	B	2600	0	1326	83	0
3	5	40	0	22	5	0
4	C	1754	0	1763	131	0
5	D	2624	0	2533	194	0
6	E	1858	0	1816	140	0
7	F	1094	0	1085	142	0
8	G	1357	0	1266	91	0
9	H	885	0	854	64	0
10	I	240	0	231	26	0
11	J	1215	0	1215	160	0
12	K	1119	0	1098	74	0
13	L	993	0	1027	71	0
14	M	1114	0	1072	70	0
15	N	1605	0	1676	189	0
16	O	1444	0	1401	143	0
17	P	864	0	873	40	0
18	Q	1133	0	1127	64	0
19	R	734	0	728	29	0
20	S	1149	0	1122	59	0
21	T	641	0	605	28	0
22	U	949	0	923	51	0
23	V	410	0	368	36	0
24	W	499	0	511	27	0
25	X	1195	0	1137	106	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	65	0
28	1	563	0	601	77	0
29	2	430	0	426	40	0
30	3	393	0	406	30	0
31	4	755	0	732	63	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	A	109	0	0	2	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	4	1	0	0	0	0
34	A	71	0	0	0	0
34	B	2	0	0	0	0
34	C	1	0	0	0	0
34	E	1	0	0	0	0
34	J	2	0	0	0	0
34	K	1	0	0	0	0
34	M	1	0	0	0	0
34	N	1	0	0	0	0
34	R	1	0	0	0	0
34	S	2	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	1	0
35	A	7	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	4	0	0	0	0
35	M	1	0	0	0	0
35	N	1	0	0	2	0
35	O	1	0	0	1	0
35	P	1	0	0	0	0
35	R	1	0	0	0	0
35	S	1	0	0	0	0
35	Z	2	0	0	1	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	36	0	0	12	0
38	2	58	0	0	5	0
38	3	37	0	0	4	0
38	4	70	0	0	11	0
38	5	1	0	0	0	0
38	A	5860	0	0	269	0
38	B	146	0	0	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C	140	0	0	15	0
38	D	146	0	0	32	0
38	E	176	0	0	34	0
38	F	52	0	0	21	0
38	G	45	0	0	12	0
38	H	32	0	0	9	0
38	I	22	0	0	8	0
38	J	78	0	0	21	0
38	K	54	0	0	4	0
38	L	64	0	0	15	0
38	M	86	0	0	16	0
38	N	138	0	0	26	0
38	O	64	0	0	19	0
38	P	44	0	0	12	0
38	Q	70	0	0	11	0
38	R	57	0	0	5	0
38	S	83	0	0	11	0
38	T	36	0	0	5	0
38	U	38	0	0	2	0
38	V	22	0	0	5	0
38	W	16	0	0	3	0
38	X	67	0	0	10	0
38	Y	28	0	0	6	0
38	Z	100	0	0	16	0
All	All	98593	0	59556	3265	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 22.

The worst 5 of 3265 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)
11:J:165:GLY:HA3	38:J:8398:HOH:O	1.43	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
15:N:164:THR:HG22	15:N:167:GLY:H	1.10	1.12
1:A:1751:G:H2'	1:A:1752:G:H5''	1.30	1.10
28:1:46:LYS:HD3	28:1:59:HIS:HB2	1.30	1.10

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%)	202 (86%)	29 (12%)	4 (2%)	7	30
5	D	335/337 (99%)	299 (89%)	28 (8%)	8 (2%)	4	22
6	E	244/246 (99%)	222 (91%)	21 (9%)	1 (0%)	30	62
7	F	134/176 (76%)	93 (69%)	29 (22%)	12 (9%)	0	2
8	G	170/177 (96%)	158 (93%)	11 (6%)	1 (1%)	21	53
9	H	117/119 (98%)	100 (86%)	14 (12%)	3 (3%)	4	20
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	2	12
11	J	152/167 (91%)	130 (86%)	17 (11%)	5 (3%)	3	15
12	K	140/145 (97%)	129 (92%)	6 (4%)	5 (4%)	2	14
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	8	33
14	M	141/164 (86%)	122 (86%)	18 (13%)	1 (1%)	18	50
15	N	192/194 (99%)	173 (90%)	18 (9%)	1 (0%)	24	58
16	O	184/186 (99%)	163 (89%)	13 (7%)	8 (4%)	2	11
17	P	113/115 (98%)	107 (95%)	6 (5%)	0	100	100
18	Q	141/148 (95%)	135 (96%)	5 (4%)	1 (1%)	18	50
19	R	93/95 (98%)	85 (91%)	5 (5%)	3 (3%)	3	16
20	S	148/154 (96%)	135 (91%)	12 (8%)	1 (1%)	18	50
21	T	79/84 (94%)	74 (94%)	5 (6%)	0	100	100
22	U	117/119 (98%)	110 (94%)	7 (6%)	0	100	100
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	16
25	X	152/154 (99%)	143 (94%)	7 (5%)	2 (1%)	9	36
26	Y	80/91 (88%)	71 (89%)	6 (8%)	3 (4%)	2	13
27	Z	140/240 (58%)	138 (99%)	2 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	6 (8%)	2 (3%)	4	19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	2	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	84 (93%)	4 (4%)	2 (2%)	5	24
All	All	3633/4235 (86%)	3276 (90%)	289 (8%)	68 (2%)	6	27

5 of 68 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	93	LEU
7	F	95	THR
7	F	137	PRO
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%)	167 (93%)	12 (7%)	15	44
5	D	282/282 (100%)	264 (94%)	18 (6%)	16	45
6	E	193/193 (100%)	176 (91%)	17 (9%)	9	33
7	F	117/147 (80%)	110 (94%)	7 (6%)	17	48
8	G	152/155 (98%)	148 (97%)	4 (3%)	40	70
9	H	92/92 (100%)	91 (99%)	1 (1%)	65	82
10	I	27/283 (10%)	27 (100%)	0	100	100
11	J	122/122 (100%)	108 (88%)	14 (12%)	5	22
12	K	118/121 (98%)	112 (95%)	6 (5%)	21	53
13	L	106/106 (100%)	103 (97%)	3 (3%)	38	69
14	M	112/126 (89%)	108 (96%)	4 (4%)	31	63
15	N	166/166 (100%)	157 (95%)	9 (5%)	20	51
16	O	149/149 (100%)	140 (94%)	9 (6%)	17	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	P	93/93 (100%)	89 (96%)	4 (4%)	26	58
18	Q	113/116 (97%)	110 (97%)	3 (3%)	39	70
19	R	79/79 (100%)	75 (95%)	4 (5%)	21	53
20	S	117/121 (97%)	113 (97%)	4 (3%)	32	64
21	T	71/73 (97%)	70 (99%)	1 (1%)	59	80
22	U	105/105 (100%)	100 (95%)	5 (5%)	23	55
23	V	44/52 (85%)	43 (98%)	1 (2%)	44	72
24	W	51/56 (91%)	50 (98%)	1 (2%)	48	75
25	X	130/130 (100%)	120 (92%)	10 (8%)	12	38
26	Y	66/73 (90%)	62 (94%)	4 (6%)	17	47
27	Z	120/195 (62%)	112 (93%)	8 (7%)	15	44
28	1	56/56 (100%)	49 (88%)	7 (12%)	4	19
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	43	72
31	4	79/79 (100%)	71 (90%)	8 (10%)	7	27
All	All	3027/3441 (88%)	2862 (94%)	165 (6%)	19	51

5 of 165 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	S	13	THR
27	Z	163	THR
21	T	10	VAL
25	X	52	VAL
28	1	22	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 106 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	50	GLN
21	T	53	ASN
30	3	17	GLN
18	Q	73	HIS
20	S	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	255 (9%)	36 (1%)
2	B	121/122 (99%)	20 (16%)	5 (4%)
3	5	1/2 (50%)	0	0
All	All	2869/3046 (94%)	275 (9%)	41 (1%)

5 of 275 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 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2466	G
1	A	2791	U
1	A	2467	A
1	A	2649	A
2	B	3024	U

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 oligosaccharides 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	37,40,41	2.23	13 (35%)	47,57,60	1.52	7 (14%)

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	-	2/25/43/44	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	76	PPU	CB-CG	4.86	1.62	1.51
36	5	76	PPU	C-N3'	4.51	1.43	1.34
36	5	76	PPU	CE2-CD2	-4.26	1.31	1.38
36	5	76	PPU	C10-N6	-4.23	1.36	1.45
36	5	76	PPU	CD1-CG	-3.88	1.31	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	76	PPU	CA-C-N3'	-4.38	110.28	116.21
36	5	76	PPU	C3'-N3'-C	-4.02	117.09	123.20
36	5	76	PPU	CG-CB-CA	-3.98	105.98	114.13
36	5	76	PPU	CM-OC-CZ	3.24	124.45	117.50
36	5	76	PPU	C2-N1-C6	2.71	118.45	111.83

There are no chirality outliers.

All (2) torsion outliers are listed below:

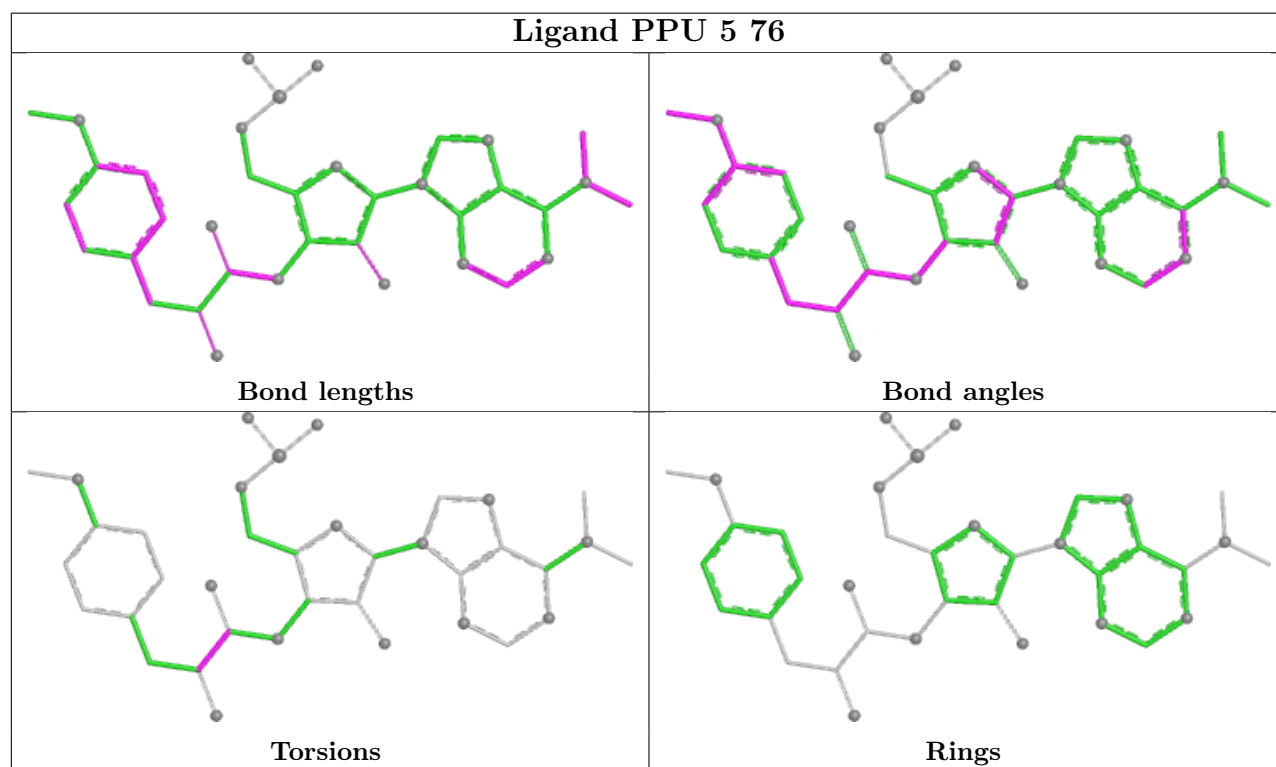
Mol	Chain	Res	Type	Atoms
36	5	76	PPU	O-C-CA-CB
36	5	76	PPU	N3'-C-CA-CB

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%)	-0.12	87 (3%) 50 33	19, 45, 94, 144	0
2	B	122/122 (100%)	0.49	7 (5%) 29 17	33, 67, 97, 147	0
3	5	2/2 (100%)	2.25	1 (50%) 0 0	65, 65, 65, 87	0
4	C	237/239 (99%)	0.41	14 (5%) 28 17	30, 62, 97, 109	0
5	D	337/337 (100%)	0.10	3 (0%) 81 65	22, 50, 77, 89	0
6	E	246/246 (100%)	0.03	1 (0%) 88 79	20, 44, 69, 78	0
7	F	140/176 (79%)	1.52	34 (24%) 2 1	65, 101, 122, 128	0
8	G	172/177 (97%)	0.42	4 (2%) 61 42	38, 62, 84, 89	0
9	H	119/119 (100%)	0.65	5 (4%) 40 25	51, 76, 99, 107	0
10	I	29/348 (8%)	1.52	7 (24%) 2 1	66, 87, 95, 99	0
11	J	156/167 (93%)	0.62	15 (9%) 13 9	35, 59, 82, 89	0
12	K	142/145 (97%)	-0.02	1 (0%) 84 70	32, 44, 67, 78	0
13	L	132/132 (100%)	0.17	1 (0%) 82 67	33, 49, 75, 82	0
14	M	145/164 (88%)	0.89	20 (13%) 6 4	26, 79, 106, 111	0
15	N	194/194 (100%)	0.55	25 (12%) 7 5	28, 47, 106, 118	0
16	O	186/186 (100%)	0.92	23 (12%) 8 6	46, 73, 112, 125	0
17	P	115/115 (100%)	0.27	1 (0%) 81 65	36, 53, 68, 72	0
18	Q	143/148 (96%)	0.26	2 (1%) 73 55	34, 53, 76, 85	0
19	R	95/95 (100%)	0.13	1 (1%) 78 61	36, 47, 63, 82	0
20	S	150/154 (97%)	-0.23	0 100 100	26, 40, 61, 72	0
21	T	81/84 (96%)	0.34	1 (1%) 76 59	44, 62, 82, 88	0
22	U	119/119 (100%)	0.37	3 (2%) 58 39	40, 55, 84, 104	0
23	V	53/66 (80%)	1.27	6 (11%) 10 7	77, 92, 100, 108	0
24	W	65/70 (92%)	0.86	8 (12%) 8 6	46, 76, 111, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	154/154 (100%)	-0.12	0 100 100	28, 42, 59, 70	0
26	Y	82/91 (90%)	0.40	5 (6%) 27 16	37, 53, 77, 91	0
27	Z	142/240 (59%)	-0.15	1 (0%) 84 70	25, 40, 64, 82	0
28	1	73/73 (100%)	2.82	46 (63%) 0 0	93, 115, 125, 127	0
29	2	56/56 (100%)	-0.45	0 100 100	22, 32, 40, 45	0
30	3	46/48 (95%)	0.55	4 (8%) 16 10	34, 63, 96, 105	0
31	4	92/92 (100%)	3.04	63 (68%) 0 0	110, 125, 133, 136	0
All	All	6579/7281 (90%)	0.23	389 (5%) 28 17	19, 52, 105, 147	0

The worst 5 of 389 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	10.2
15	N	80	GLY	8.8
15	N	89	ASN	8.2
31	4	60	LYS	7.2
1	A	1173	A	7.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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
34	NA	B	8351	1/1	0.36	0.16	75,75,75,75	0
34	NA	A	8384	1/1	0.44	0.17	82,82,82,82	0
34	NA	A	8340	1/1	0.45	0.17	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
35	CL	4	8504	1/1	0.46	0.14	101,101,101,101	0
34	NA	T	8312	1/1	0.49	0.16	80,80,80,80	0
34	NA	A	8328	1/1	0.54	0.26	47,47,47,47	0
32	MG	A	8049	1/1	0.63	0.22	95,95,95,95	0
34	NA	A	8302	1/1	0.63	0.16	31,31,31,31	0
34	NA	B	8383	1/1	0.66	0.43	77,77,77,77	0
34	NA	A	8341	1/1	0.66	0.16	55,55,55,55	0
34	NA	A	8381	1/1	0.66	0.10	46,46,46,46	0
34	NA	A	8301	1/1	0.67	0.13	31,31,31,31	0
34	NA	A	8373	1/1	0.68	0.15	54,54,54,54	0
34	NA	A	8382	1/1	0.71	0.47	79,79,79,79	0
34	NA	A	8329	1/1	0.71	0.23	61,61,61,61	0
34	NA	A	8357	1/1	0.71	0.15	49,49,49,49	0
34	NA	A	8365	1/1	0.73	0.28	46,46,46,46	0
34	NA	S	8337	1/1	0.73	0.11	52,52,52,52	0
32	MG	B	8095	1/1	0.74	0.13	72,72,72,72	0
34	NA	A	8352	1/1	0.75	0.15	39,39,39,39	0
34	NA	A	8366	1/1	0.75	0.17	47,47,47,47	0
34	NA	A	8368	1/1	0.75	0.19	56,56,56,56	0
34	NA	A	8332	1/1	0.75	0.22	68,68,68,68	0
32	MG	A	8102	1/1	0.76	0.51	135,135,135,135	0
35	CL	C	8509	1/1	0.76	0.18	86,86,86,86	0
34	NA	A	8363	1/1	0.76	0.22	48,48,48,48	0
34	NA	A	8327	1/1	0.77	0.16	40,40,40,40	0
34	NA	A	8344	1/1	0.77	0.07	27,27,27,27	0
35	CL	M	8510	1/1	0.78	0.22	97,97,97,97	0
37	CD	4	8404	1/1	0.78	0.19	203,203,203,203	0
34	NA	A	8385	1/1	0.79	0.21	46,46,46,46	0
35	CL	A	8522	1/1	0.79	0.38	83,83,83,83	0
32	MG	A	8076	1/1	0.79	0.14	79,79,79,79	0
34	NA	A	8319	1/1	0.79	0.11	44,44,44,44	0
34	NA	A	8374	1/1	0.79	0.35	60,60,60,60	0
34	NA	S	8386	1/1	0.79	0.23	70,70,70,70	0
34	NA	A	8356	1/1	0.80	0.29	57,57,57,57	0
34	NA	A	8377	1/1	0.81	0.40	86,86,86,86	0
32	MG	A	8045	1/1	0.81	0.09	50,50,50,50	0
37	CD	1	8403	1/1	0.81	0.16	203,203,203,203	0
34	NA	A	8371	1/1	0.81	0.27	54,54,54,54	0
34	NA	A	8354	1/1	0.82	0.14	51,51,51,51	0
32	MG	1	8105	1/1	0.83	0.14	58,58,58,58	0
32	MG	A	8067	1/1	0.83	0.14	41,41,41,41	0
32	MG	A	8114	1/1	0.83	0.31	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8355	1/1	0.83	0.30	64,64,64,64	0
35	CL	D	8519	1/1	0.83	0.17	70,70,70,70	0
34	NA	A	8303	1/1	0.83	0.18	51,51,51,51	0
32	MG	A	8089	1/1	0.83	0.10	82,82,82,82	0
34	NA	R	8348	1/1	0.83	0.10	57,57,57,57	0
34	NA	A	8326	1/1	0.83	0.20	60,60,60,60	0
32	MG	A	8046	1/1	0.84	0.07	53,53,53,53	0
34	NA	A	8362	1/1	0.84	0.36	74,74,74,74	0
35	CL	N	8518	1/1	0.84	0.11	46,46,46,46	0
35	CL	K	8502	1/1	0.85	0.11	71,71,71,71	0
32	MG	A	8101	1/1	0.85	0.10	50,50,50,50	0
32	MG	A	8050	1/1	0.85	0.07	52,52,52,52	0
34	NA	A	8379	1/1	0.86	0.13	48,48,48,48	0
34	NA	A	8307	1/1	0.86	0.15	58,58,58,58	0
32	MG	A	8092	1/1	0.86	0.20	91,91,91,91	0
32	MG	A	8047	1/1	0.86	0.08	31,31,31,31	0
32	MG	A	8024	1/1	0.86	0.37	110,110,110,110	0
34	NA	A	8378	1/1	0.87	0.24	52,52,52,52	0
34	NA	A	8316	1/1	0.87	0.13	45,45,45,45	0
34	NA	J	8309	1/1	0.87	0.13	42,42,42,42	0
32	MG	A	8116	1/1	0.87	0.10	55,55,55,55	0
35	CL	A	8505	1/1	0.88	0.18	74,74,74,74	0
34	NA	A	8318	1/1	0.88	0.15	43,43,43,43	0
35	CL	R	8511	1/1	0.88	0.13	67,67,67,67	0
32	MG	A	8066	1/1	0.88	0.11	65,65,65,65	0
34	NA	A	8331	1/1	0.88	0.34	76,76,76,76	0
34	NA	A	8372	1/1	0.88	0.24	80,80,80,80	0
34	NA	A	8308	1/1	0.89	0.16	63,63,63,63	0
32	MG	A	8057	1/1	0.89	0.10	46,46,46,46	0
32	MG	U	8073	1/1	0.90	0.06	48,48,48,48	0
32	MG	A	8093	1/1	0.90	0.13	44,44,44,44	0
36	PPU	5	76	37/38	0.90	0.14	60,64,69,71	0
32	MG	A	8075	1/1	0.90	0.08	45,45,45,45	0
35	CL	O	8507	1/1	0.90	0.09	65,65,65,65	0
32	MG	4	8078	1/1	0.91	0.08	74,74,74,74	0
32	MG	A	8111	1/1	0.91	0.07	61,61,61,61	0
34	NA	A	8310	1/1	0.91	0.17	40,40,40,40	0
35	CL	K	8516	1/1	0.91	0.15	61,61,61,61	0
32	MG	A	8070	1/1	0.91	0.23	69,69,69,69	0
32	MG	A	8053	1/1	0.91	0.10	41,41,41,41	0
32	MG	A	8090	1/1	0.92	0.18	70,70,70,70	0
34	NA	A	8306	1/1	0.92	0.18	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8370	1/1	0.92	0.22	52,52,52,52	0
34	NA	A	8321	1/1	0.92	0.15	48,48,48,48	0
34	NA	A	8358	1/1	0.92	0.25	105,105,105,105	0
35	CL	A	8503	1/1	0.92	0.12	57,57,57,57	0
34	NA	A	8349	1/1	0.92	0.16	67,67,67,67	0
34	NA	A	8334	1/1	0.92	0.10	46,46,46,46	0
34	NA	A	8335	1/1	0.92	0.16	57,57,57,57	0
34	NA	C	8345	1/1	0.92	0.08	35,35,35,35	0
32	MG	A	8042	1/1	0.93	0.07	34,34,34,34	0
32	MG	A	8117	1/1	0.93	0.05	33,33,33,33	0
32	MG	A	8088	1/1	0.93	0.09	65,65,65,65	0
34	NA	A	8375	1/1	0.93	0.17	55,55,55,55	0
32	MG	D	8055	1/1	0.93	0.09	81,81,81,81	0
32	MG	A	8051	1/1	0.93	0.09	86,86,86,86	0
32	MG	A	8062	1/1	0.93	0.07	49,49,49,49	0
34	NA	A	8330	1/1	0.93	0.08	35,35,35,35	0
35	CL	S	8506	1/1	0.93	0.10	60,60,60,60	0
34	NA	4	8369	1/1	0.93	0.28	66,66,66,66	0
34	NA	A	8353	1/1	0.93	0.15	53,53,53,53	0
32	MG	A	8113	1/1	0.93	0.07	54,54,54,54	0
32	MG	A	8064	1/1	0.93	0.16	24,24,24,24	0
35	CL	K	8501	1/1	0.94	0.08	58,58,58,58	0
34	NA	A	8339	1/1	0.94	0.06	30,30,30,30	0
32	MG	A	8041	1/1	0.94	0.06	55,55,55,55	0
35	CL	K	8521	1/1	0.94	0.10	60,60,60,60	0
32	MG	A	8103	1/1	0.94	0.07	45,45,45,45	0
34	NA	A	8342	1/1	0.94	0.06	28,28,28,28	0
34	NA	A	8325	1/1	0.94	0.16	40,40,40,40	0
34	NA	A	8313	1/1	0.94	0.09	74,74,74,74	0
34	NA	A	8350	1/1	0.94	0.11	37,37,37,37	0
35	CL	Z	8517	1/1	0.94	0.07	61,61,61,61	0
35	CL	Z	8520	1/1	0.94	0.10	35,35,35,35	0
35	CL	A	8515	1/1	0.94	0.16	68,68,68,68	0
33	K	A	8202	1/1	0.94	0.12	89,89,89,89	0
37	CD	V	8401	1/1	0.94	0.12	129,129,129,129	0
32	MG	Z	8109	1/1	0.94	0.07	38,38,38,38	0
34	NA	J	8322	1/1	0.94	0.24	72,72,72,72	0
32	MG	A	8082	1/1	0.95	0.07	56,56,56,56	0
33	K	A	8201	1/1	0.95	0.22	71,71,71,71	0
32	MG	A	8096	1/1	0.95	0.09	51,51,51,51	0
34	NA	A	8333	1/1	0.95	0.13	33,33,33,33	0
32	MG	A	8100	1/1	0.95	0.13	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	K	8346	1/1	0.95	0.08	37,37,37,37	0
34	NA	N	8347	1/1	0.95	0.05	24,24,24,24	0
32	MG	A	8023	1/1	0.95	0.07	45,45,45,45	0
34	NA	A	8323	1/1	0.95	0.13	45,45,45,45	0
32	MG	A	8071	1/1	0.95	0.04	93,93,93,93	0
34	NA	A	8360	1/1	0.95	0.16	61,61,61,61	0
34	NA	U	8343	1/1	0.95	0.04	27,27,27,27	0
34	NA	A	8361	1/1	0.95	0.13	62,62,62,62	0
32	MG	A	8043	1/1	0.95	0.06	32,32,32,32	0
32	MG	A	8104	1/1	0.95	0.06	52,52,52,52	0
35	CL	A	8513	1/1	0.95	0.09	56,56,56,56	0
32	MG	A	8052	1/1	0.95	0.06	51,51,51,51	0
32	MG	A	8112	1/1	0.95	0.12	57,57,57,57	0
32	MG	A	8040	1/1	0.96	0.17	100,100,100,100	0
34	NA	A	8338	1/1	0.96	0.05	44,44,44,44	0
32	MG	A	8094	1/1	0.96	0.11	65,65,65,65	0
34	NA	A	8314	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8008	1/1	0.96	0.09	42,42,42,42	0
35	CL	P	8508	1/1	0.96	0.07	82,82,82,82	0
35	CL	A	8512	1/1	0.96	0.07	31,31,31,31	0
34	NA	A	8305	1/1	0.96	0.06	27,27,27,27	0
35	CL	A	8514	1/1	0.96	0.08	50,50,50,50	0
32	MG	A	8106	1/1	0.96	0.07	76,76,76,76	0
34	NA	A	8320	1/1	0.96	0.08	42,42,42,42	0
32	MG	A	8044	1/1	0.96	0.09	54,54,54,54	0
32	MG	A	8087	1/1	0.96	0.05	49,49,49,49	0
34	NA	A	8324	1/1	0.96	0.17	51,51,51,51	0
34	NA	A	8367	1/1	0.96	0.08	43,43,43,43	0
32	MG	A	8039	1/1	0.97	0.06	51,51,51,51	0
32	MG	A	8014	1/1	0.97	0.06	20,20,20,20	0
32	MG	A	8115	1/1	0.97	0.07	59,59,59,59	0
32	MG	A	8108	1/1	0.97	0.06	53,53,53,53	0
32	MG	A	8056	1/1	0.97	0.04	56,56,56,56	0
34	NA	A	8336	1/1	0.97	0.03	49,49,49,49	0
37	CD	P	8405	1/1	0.97	0.04	89,89,89,89	0
32	MG	A	8099	1/1	0.97	0.09	68,68,68,68	0
34	NA	A	8359	1/1	0.97	0.15	60,60,60,60	0
34	NA	E	8304	1/1	0.97	0.05	25,25,25,25	0
32	MG	A	8059	1/1	0.98	0.04	47,47,47,47	0
34	NA	A	8315	1/1	0.98	0.08	43,43,43,43	0
32	MG	A	8060	1/1	0.98	0.09	44,44,44,44	0
34	NA	A	8317	1/1	0.98	0.03	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8376	1/1	0.98	0.09	79,79,79,79	0
32	MG	A	8034	1/1	0.98	0.04	36,36,36,36	0
32	MG	A	8063	1/1	0.98	0.05	85,85,85,85	0
32	MG	A	8035	1/1	0.98	0.04	48,48,48,48	0
32	MG	A	8005	1/1	0.98	0.04	38,38,38,38	0
32	MG	L	8069	1/1	0.98	0.03	81,81,81,81	0
32	MG	A	8019	1/1	0.98	0.07	30,30,30,30	0
32	MG	A	8097	1/1	0.98	0.09	32,32,32,32	0
32	MG	A	8098	1/1	0.98	0.12	33,33,33,33	0
32	MG	A	8068	1/1	0.98	0.04	46,46,46,46	0
32	MG	A	8022	1/1	0.98	0.05	32,32,32,32	0
32	MG	A	8002	1/1	0.98	0.05	36,36,36,36	0
32	MG	A	8072	1/1	0.98	0.04	53,53,53,53	0
32	MG	A	8012	1/1	0.98	0.05	44,44,44,44	0
32	MG	A	8054	1/1	0.98	0.05	33,33,33,33	0
34	NA	M	8380	1/1	0.98	0.06	65,65,65,65	0
34	NA	A	8364	1/1	0.98	0.12	54,54,54,54	0
32	MG	A	8079	1/1	0.98	0.05	48,48,48,48	0
32	MG	A	8027	1/1	0.98	0.04	54,54,54,54	0
32	MG	A	8110	1/1	0.98	0.09	30,30,30,30	0
32	MG	A	8083	1/1	0.98	0.07	37,37,37,37	0
32	MG	A	8085	1/1	0.98	0.06	95,95,95,95	0
32	MG	A	8029	1/1	0.98	0.03	38,38,38,38	0
32	MG	A	8017	1/1	0.99	0.08	35,35,35,35	0
32	MG	A	8018	1/1	0.99	0.03	42,42,42,42	0
32	MG	A	8091	1/1	0.99	0.06	67,67,67,67	0
32	MG	A	8061	1/1	0.99	0.04	45,45,45,45	0
32	MG	A	8006	1/1	0.99	0.04	57,57,57,57	0
32	MG	A	8021	1/1	0.99	0.03	32,32,32,32	0
32	MG	A	8003	1/1	0.99	0.03	23,23,23,23	0
32	MG	A	8010	1/1	0.99	0.03	30,30,30,30	0
32	MG	A	8004	1/1	0.99	0.05	53,53,53,53	0
32	MG	A	8026	1/1	0.99	0.02	33,33,33,33	0
32	MG	A	8013	1/1	0.99	0.04	42,42,42,42	0
32	MG	A	8048	1/1	0.99	0.03	33,33,33,33	0
32	MG	A	8028	1/1	0.99	0.04	37,37,37,37	0
32	MG	A	8074	1/1	0.99	0.05	42,42,42,42	0
32	MG	A	8001	1/1	0.99	0.03	33,33,33,33	0
34	NA	A	8311	1/1	0.99	0.04	31,31,31,31	0
32	MG	A	8030	1/1	0.99	0.04	34,34,34,34	0
32	MG	A	8107	1/1	0.99	0.03	36,36,36,36	0
32	MG	A	8077	1/1	0.99	0.04	32,32,32,32	0

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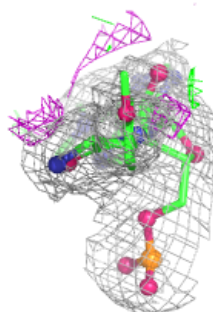
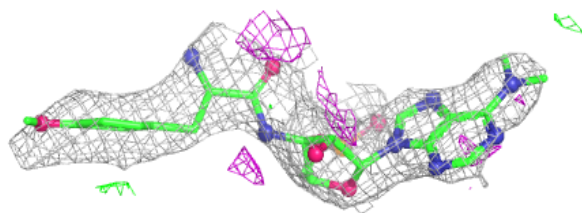
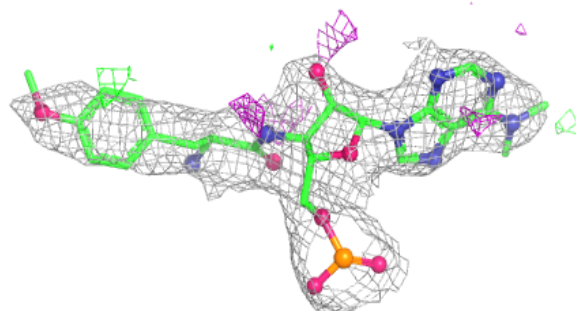
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8032	1/1	0.99	0.07	34,34,34,34	0
32	MG	A	8080	1/1	0.99	0.04	35,35,35,35	0
32	MG	A	8081	1/1	0.99	0.03	39,39,39,39	0
32	MG	A	8015	1/1	0.99	0.03	50,50,50,50	0
32	MG	A	8016	1/1	0.99	0.03	36,36,36,36	0
32	MG	A	8084	1/1	0.99	0.07	50,50,50,50	0
32	MG	A	8036	1/1	0.99	0.04	38,38,38,38	0
32	MG	A	8086	1/1	0.99	0.04	49,49,49,49	0
32	MG	A	8037	1/1	0.99	0.05	43,43,43,43	0
32	MG	C	8065	1/1	0.99	0.03	68,68,68,68	0
32	MG	A	8058	1/1	0.99	0.07	39,39,39,39	0
32	MG	A	8033	1/1	1.00	0.03	25,25,25,25	0
32	MG	A	8009	1/1	1.00	0.02	32,32,32,32	0
32	MG	A	8007	1/1	1.00	0.06	28,28,28,28	0
32	MG	A	8020	1/1	1.00	0.04	46,46,46,46	0
32	MG	A	8025	1/1	1.00	0.02	40,40,40,40	0
32	MG	A	8038	1/1	1.00	0.04	33,33,33,33	0
32	MG	A	8031	1/1	1.00	0.02	32,32,32,32	0
37	CD	2	8402	1/1	1.00	0.03	57,57,57,57	0
32	MG	A	8011	1/1	1.00	0.04	24,24,24,24	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 PPU 5 76:

$2mF_o-DF_c$ (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.