



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:00 AM UTC

PDB ID : 1M90 / pdb_00001m90
Title : Co-crystal structure of CCA-Phe-caproic acid-biotin and sparsomycin bound to the 50S ribosomal subunit
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2002-07-26
Resolution : 2.80 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

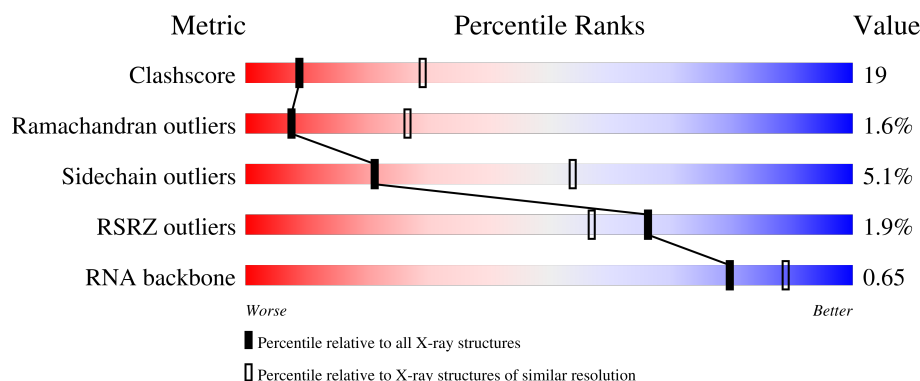
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)
RNA backbone	3983	1114 (3.00-2.60)

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	% 59% 30% 6% 6%
2	B	122	4% 49% 39% 10%
3	5	3	67% 33%
4	C	239	% 58% 33% 8%
5	D	337	% 47% 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	58% 35% 7% •

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98611 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 RRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2754	Total	C	N	O	P	0	0	0
			59017	26346	10878	19048	2745			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	C	U	conflict	GB 3377779

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

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 CCA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

- Molecule 4 is a protein called RIBOSOMAL PROTEIN L2.

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 RIBOSOMAL PROTEIN L3.

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 RIBOSOMAL PROTEIN L4.

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 RIBOSOMAL PROTEIN L5.

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 RIBOSOMAL PROTEIN L6.

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 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 RIBOSOMAL PROTEIN L10.

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 RIBOSOMAL PROTEIN L10E.

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 RIBOSOMAL PROTEIN L13.

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 RIBOSOMAL PROTEIN L14.

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 RIBOSOMAL PROTEIN L15.

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 RIBOSOMAL PROTEIN L15E.

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 RIBOSOMAL PROTEIN L18.

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 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 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 RIBOSOMAL PROTEIN L21E.

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

- Molecule 20 is a protein called RIBOSOMAL PROTEIN L22.

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

- Molecule 21 is a protein called RIBOSOMAL PROTEIN L23.

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

- Molecule 22 is a protein called RIBOSOMAL PROTEIN L24.

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

- Molecule 23 is a protein called RIBOSOMAL PROTEIN L24E.

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

- Molecule 24 is a protein called RIBOSOMAL PROTEIN L29.

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

- Molecule 25 is a protein called RIBOSOMAL PROTEIN L30.

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

- Molecule 26 is a protein called 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 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 RIBOSOMAL PROTEIN L37Ae.

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 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 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 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	111	Total	Mg	0	0
			111	111		
32	B	1	Total	Mg	0	0
			1	1		
32	5	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	1	1	Total	Mg	0	0
			1	1		
32	4	1	Total	Mg	0	0
			1	1		

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

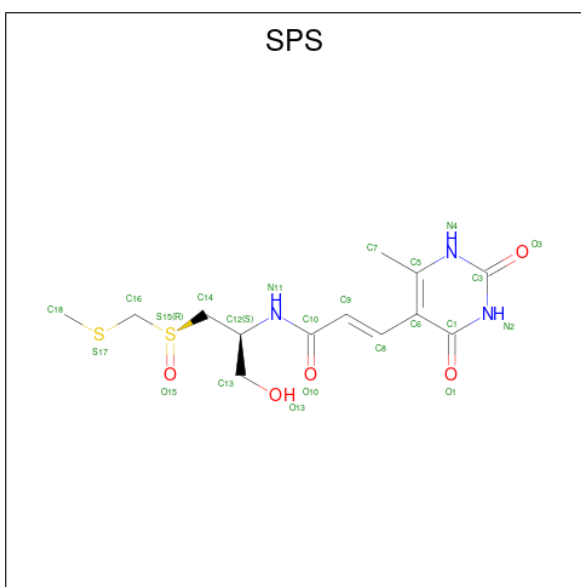
- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

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

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

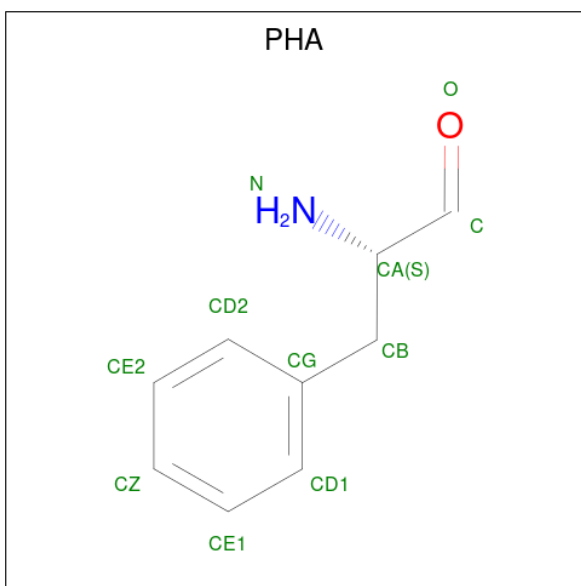
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	10	Total 10	Cl 10	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0
35	Z	1	Total 1	Cl 1	0	0
35	4	1	Total 1	Cl 1	0	0

- Molecule 36 is SPARSOMYCIN (CCD ID: SPS) (formula: C₁₃H₁₉N₃O₅S₂).



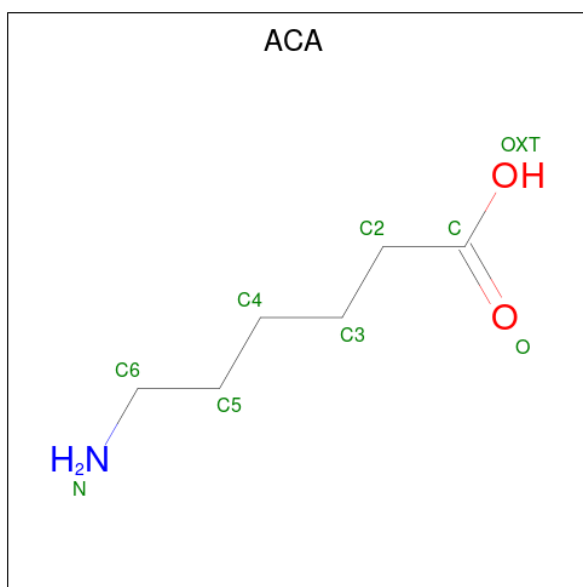
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
36	5	1	Total	C	N	O	S	0	0
			23	13	3	5	2		

- Molecule 37 is PHENYLALANINAL (CCD ID: PHA) (formula: $C_9H_{11}NO$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
37	5	1	Total	C	N	O	0	0
			11	9	1	1		

- Molecule 38 is 6-AMINOHEXANOIC ACID (CCD ID: ACA) (formula: $C_6H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
38	5	1	Total	C	N	O	0	0
			8	6	1	1		

- Molecule 39 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
39	P	1	Total	Cd	0	0
			1	1		
39	V	1	Total	Cd	0	0
			1	1		
39	1	1	Total	Cd	0	0
			1	1		
39	2	1	Total	Cd	0	0
			1	1		
39	4	1	Total	Cd	0	0
			1	1		

- Molecule 40 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	A	5920	Total	O	0	0
			5920	5920		
40	B	136	Total	O	0	0
			136	136		
40	5	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	C	119	Total 119	O 119	0	0
40	D	142	Total 142	O 142	0	0
40	E	172	Total 172	O 172	0	0
40	F	51	Total 51	O 51	0	0
40	G	44	Total 44	O 44	0	0
40	H	28	Total 28	O 28	0	0
40	I	21	Total 21	O 21	0	0
40	J	75	Total 75	O 75	0	0
40	K	56	Total 56	O 56	0	0
40	L	61	Total 61	O 61	0	0
40	M	86	Total 86	O 86	0	0
40	N	125	Total 125	O 125	0	0
40	O	69	Total 69	O 69	0	0
40	P	43	Total 43	O 43	0	0
40	Q	67	Total 67	O 67	0	0
40	R	49	Total 49	O 49	0	0
40	S	83	Total 83	O 83	0	0
40	T	35	Total 35	O 35	0	0
40	U	37	Total 37	O 37	0	0
40	V	24	Total 24	O 24	0	0
40	W	16	Total 16	O 16	0	0

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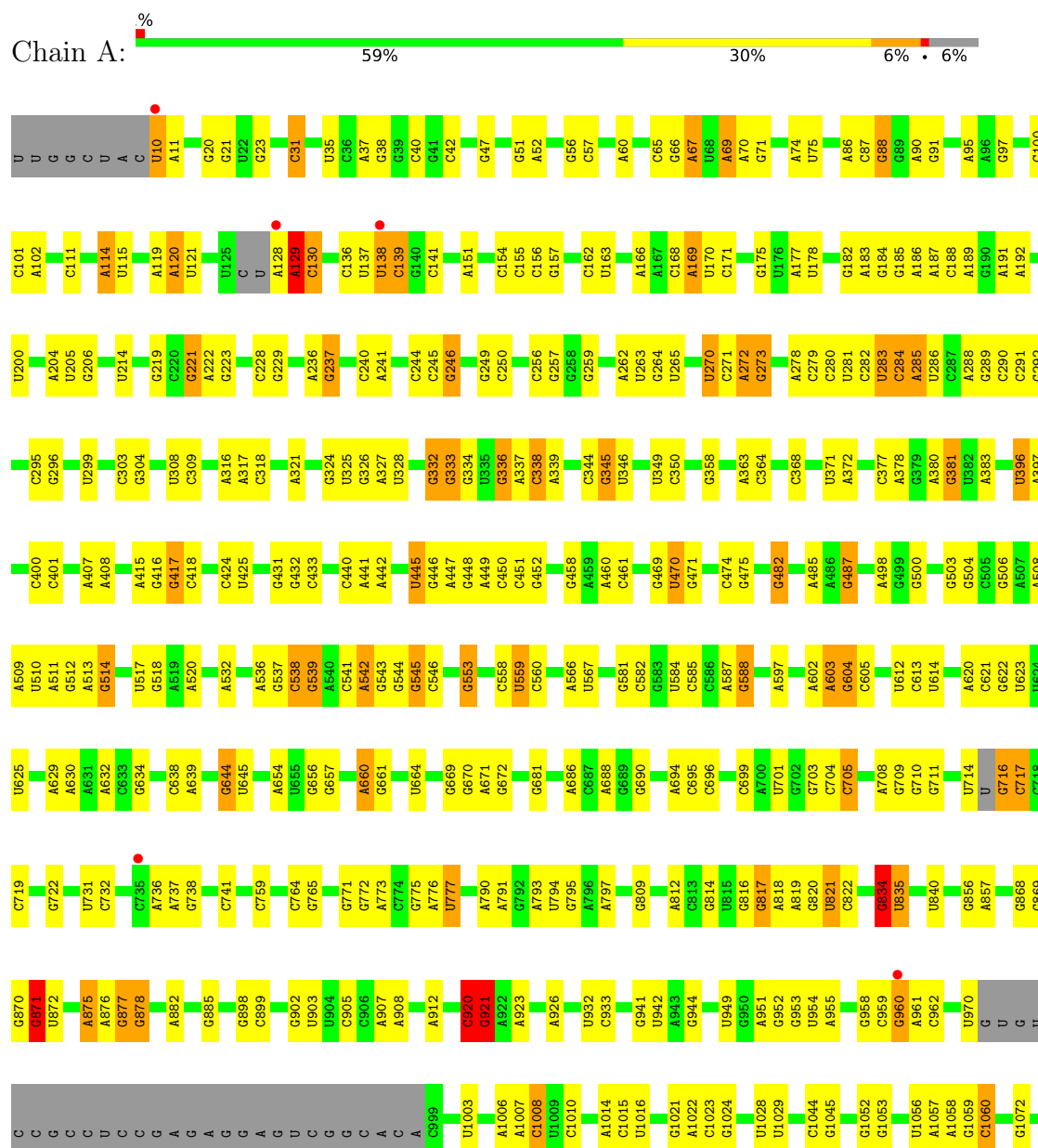
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
40	X	71	Total 71	O 71	0	0
40	Y	31	Total 31	O 31	0	0
40	Z	92	Total 92	O 92	0	0
40	1	36	Total 36	O 36	0	0
40	2	55	Total 55	O 55	0	0
40	3	40	Total 40	O 40	0	0
40	4	73	Total 73	O 73	0	0

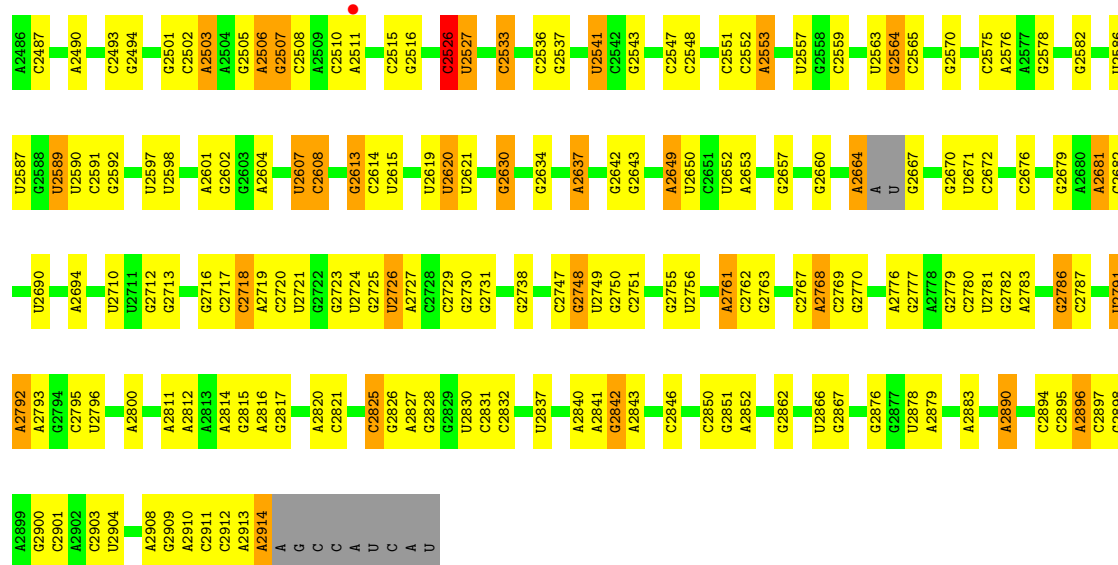
3 Residue-property plots

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.

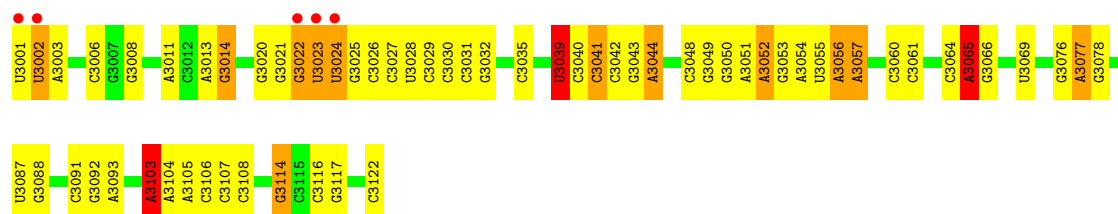
• Molecule 1: 23S rRNA



U2387	A2300	G	C2061	G1828	U1722	A1603	C1477	A1246	G1175	A1078
C2388	A2301	U	A2062	G1829	G1723	G1604	U1478	A1368	C1176	A1079
A2401	A2302	G	U2063	A1830	U1724	G1605	C1482	C1360	A1177	C1080
A2402	A2303	A	U2064	U1835	C1725	G1609	A1483	C1372	U1180	A1081
C2403	C2310	A	G2068	U1836	G1730	G1610	C1484	A1375	C1181	A1086
A2408	C2309	C	U2069	A1840	C1731	C1613	A1485	C1376	C1182	G1087
G2412	C2313	A	G2070	U1845	A1732	G1614	U1488	C1377	C1184	A1088
A2413	G2314	A	C2071	A1846	A1733	A1615	C1489	C1384	U1185	U1095
A2414	C2315	A	U2072	U1847	C1734	U1626	A1494	C1384	C1186	A1098
A2415	G2316	G	G2073	A1848	C1735	U1627	G1497	A1393	U1187	G1099
G2416	C2317	C	A2074	U1849	A1736	A1628	U1497	C1394	A1188	A1099
U2419	U2320	G	U2078	C1856	U1741	G1627	U1500	A1398	A1189	U1109
G2420	A2321	G	G2079	A1857	A1742	A1630	U1503	C1398	G1190	G1110
G2421	G2324	G	G2080	U1858	G1743	U1633	U1506	A1406	A1191	A1114
U2422	C2325	A	A2081	C1862	G1744	C1634	U1515	A1407	A1192	U1115
C2423	U2326	C	C2088	C1863	G1745	U1635	C1516	A1413	A1193	U1116
U2424	G2327	U	A2089	C1864	U1751	G1636	U1529	A1414	A1194	U1117
A2425	C2329	A	G2090	G1867	C1752	A1637	U1529	G1417	G1195	G1118
G2426	U2330	C	G2091	G1868	G1753	U1637	U1529	U1418	C1196	U1119
C2427	U2330	U	G2092	U1874	A1754	A1641	U1529	U1418	G1197	U1120
G2428	G2338	C	G2093	U1875	G1755	A1642	U1529	U1418	C1201	G1121
A2434	A	G	G2094	U1876	G1756	U1642	U1529	U1418	U1205	U1122
U2435	C	C	A2095	G1877	U1761	U1654	U1529	U1418	U1206	A1123
U2436	G	A	G2096	G1878	U1762	U1655	U1529	U1418	A1207	C1129
G2438	G	G	A2101	U1879	C1763	G1656	U1529	U1418	C1208	U1130
C2443	A	U	G2102	C1880	U1766	A1657	U1529	U1418	C1209	G1131
G2453	G2344	C	A2103	U1881	U1766	C1666	U1529	U1418	G1210	A1132
U2456	A2345	C	C2104	C1882	U1766	C1667	U1529	U1418	C1211	U1133
U2457	C2346	C	U2107	U1883	U1771	U1667	U1529	U1418	C1212	G1134
U2457	G	G	G2108	G1884	C1772	A1669	U1529	U1418	G1213	G1135
G2462	G2251	C	G2110	U1887	G1773	U1670	U1529	U1418	G1214	U1136
A2463	A2252	C	G2111	U1891	A1778	C1675	U1529	U1418	G1215	U1137
A2464	G2253	U	G2112	G1891	A1779	U1676	U1529	U1418	G1216	G1138
A2465	G2254	A	U2115	U1902	A1783	A1677	U1529	U1418	G1217	U1139
A2466	G2255	G	U2116	U1903	U1784	U1678	U1529	U1418	G1218	U1140
A2467	G2256	C	G2117	A1904	U1785	C1679	U1529	U1418	G1219	G1151
A2468	G2257	C	G2118	A1909	U1786	U1680	U1529	U1418	G1220	G1158
A2469	A2258	G	G2119	U1910	G1787	C1681	U1529	U1418	C1221	G1159
U2472	U2265	G	G2120	A1919	U1788	G1682	U1529	U1418	C1222	A1161
U2473	A2266	C	A2010	U1920	G1789	U1683	U1529	U1418	C1223	G1162
A2474	G2267	C	U2011	A1921	G1798	A1684	U1529	U1418	C1224	U1163
C2475	C2268	A	G2012	U1922	C1798	U1685	U1529	U1418	C1225	G1164
A2476	G2269	C	G2013	A1923	U1804	C1686	U1529	U1418	G1226	G1165
C2477	G2270	C	U2014	U1924	G1805	C1687	U1529	U1418	C1227	U1166
U2478	G2271	G	A2015	G1926	G1806	C1688	U1529	U1418	C1228	G1167
A2479	G2272	A	U2016	U1927	U1807	C1689	U1529	U1418	C1229	C1168
G2480	C2273	C	G2033	C1928	G1809	U1692	U1529	U1418	C1230	U1169
U2483	U2281	A	U2034	G1929	A1815	C1699	U1529	U1418	C1231	U1170
U2484	U2282	C	G2044	C1930	G1820	U1700	U1529	U1418	C1232	A1171
A2485	A2291	A	A2054	A1941	G1820	A1701	U1529	U1418	C1233	G1172
		U	A2055	A1942	G1820	U1702	U1529	U1418	C1234	G1173
		A		C1943	G1820	U1702	U1529	U1418	C1235	A1174



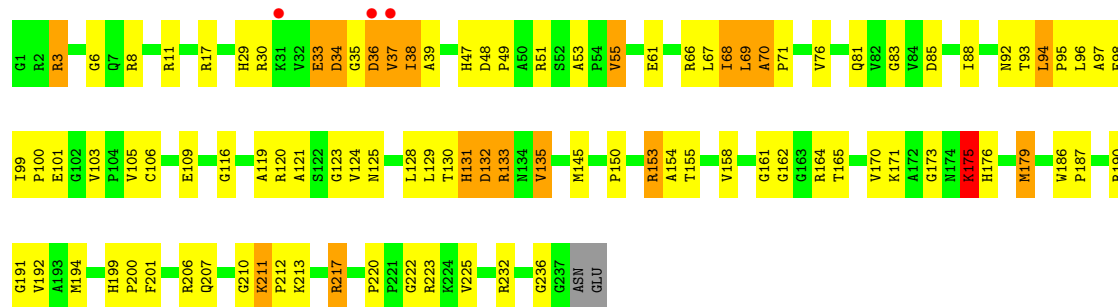
• Molecule 2: 5S RRNA



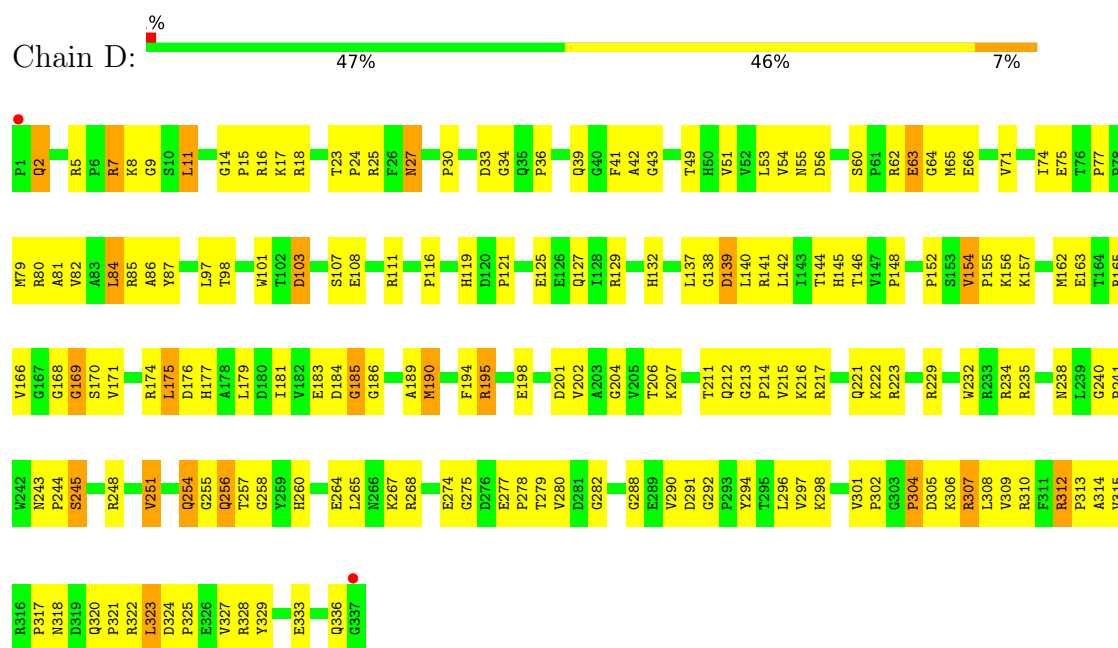
• Molecule 3: CCA



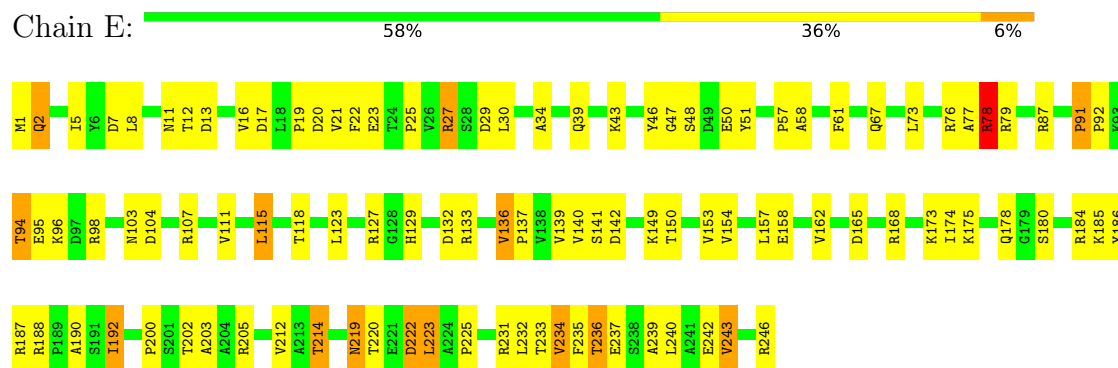
• Molecule 4: RIBOSOMAL PROTEIN L2



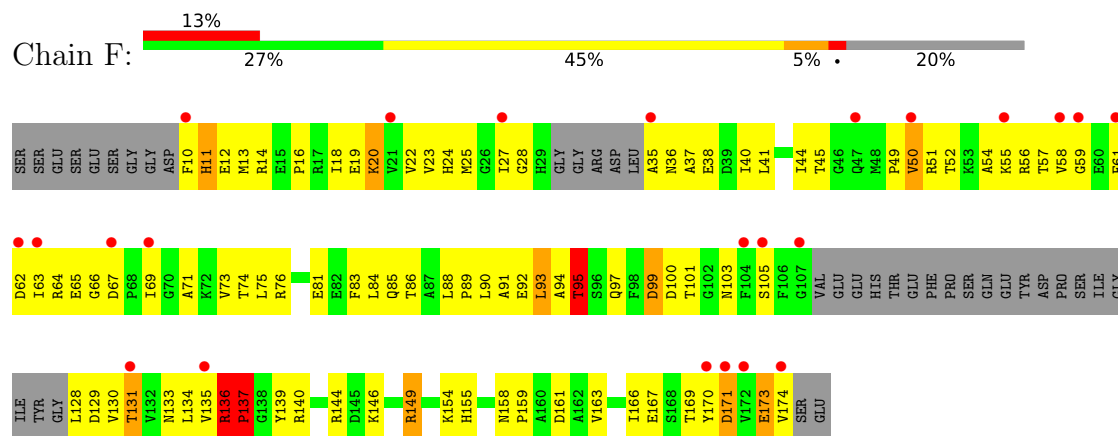
• Molecule 5: RIBOSOMAL PROTEIN L3



• Molecule 6: RIBOSOMAL PROTEIN L4



• Molecule 7: RIBOSOMAL PROTEIN L5

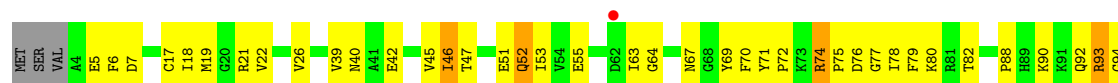


• Molecule 8: RIBOSOMAL PROTEIN L6

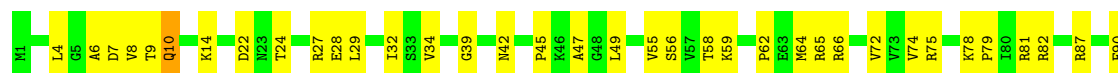




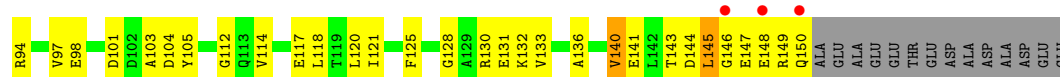
• Molecule 12: RIBOSOMAL PROTEIN L13



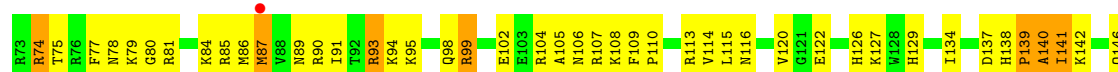
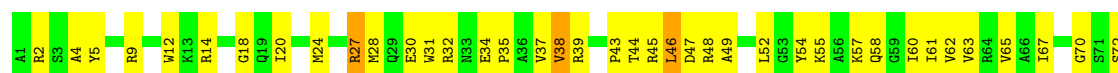
• Molecule 13: RIBOSOMAL PROTEIN L14



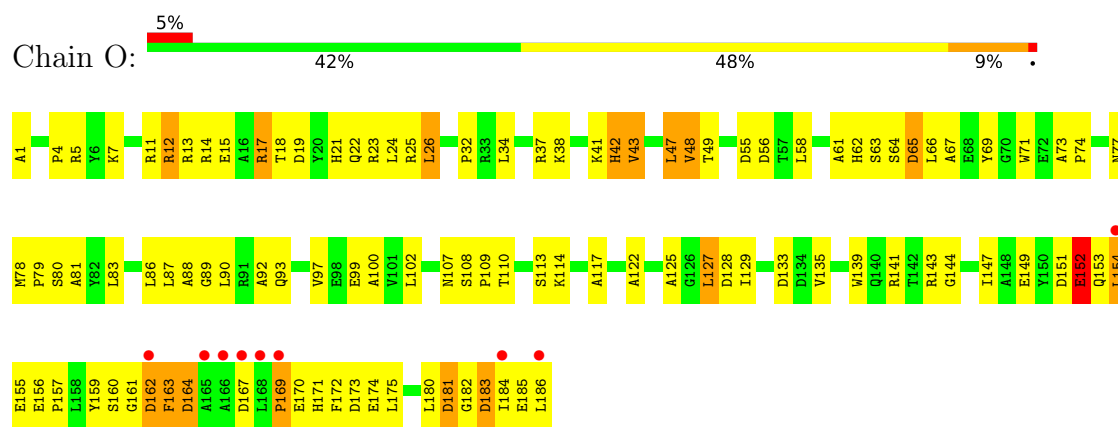
• Molecule 14: RIBOSOMAL PROTEIN L15



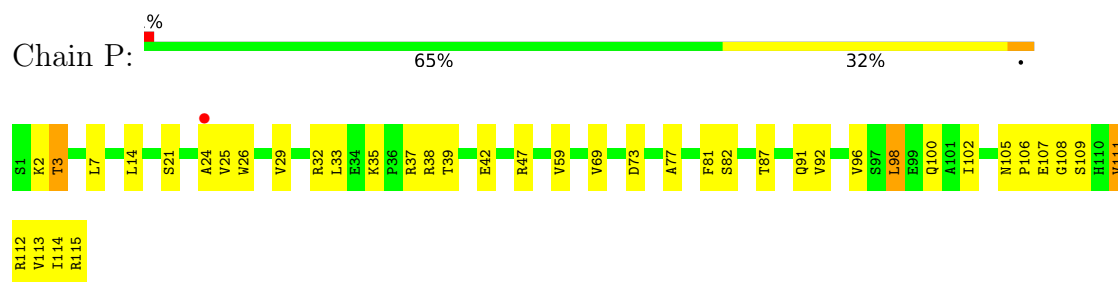
• Molecule 15: RIBOSOMAL PROTEIN L15E



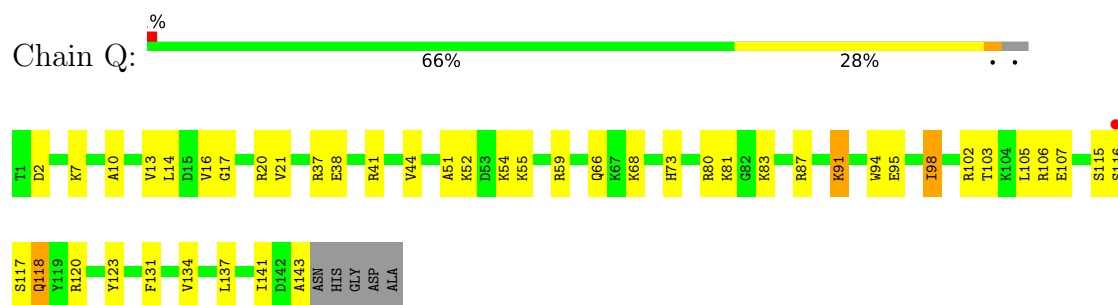
• Molecule 16: RIBOSOMAL PROTEIN L18



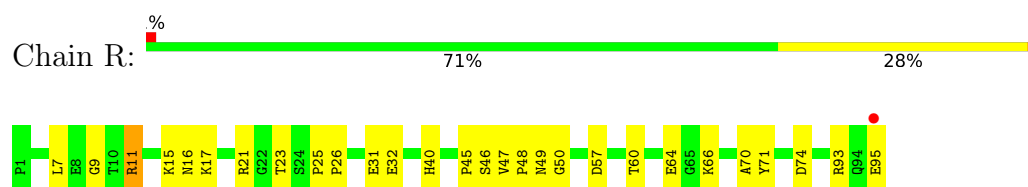
• Molecule 17: RIBOSOMAL PROTEIN L18E



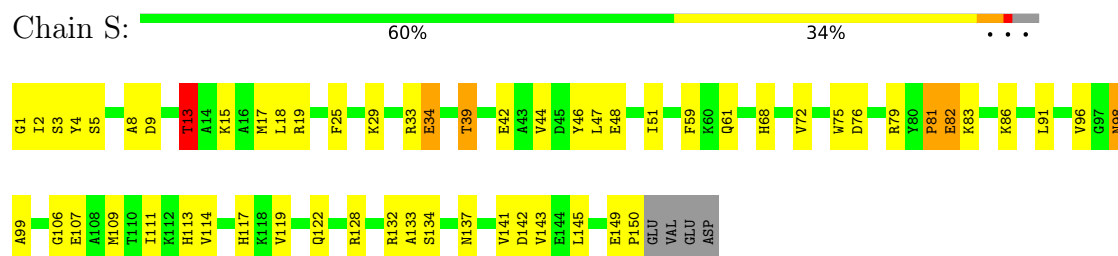
• Molecule 18: RIBOSOMAL PROTEIN L19E



• Molecule 19: RIBOSOMAL PROTEIN L21E



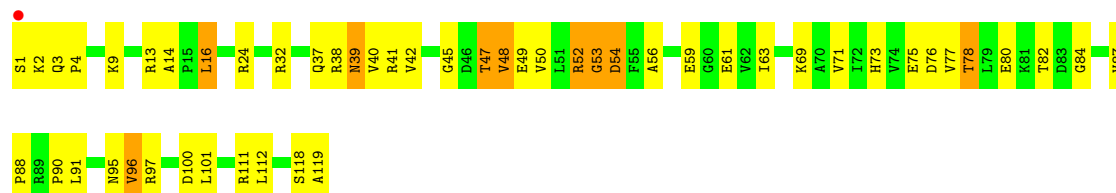
• Molecule 20: RIBOSOMAL PROTEIN L22



- Molecule 21: RIBOSOMAL PROTEIN L23



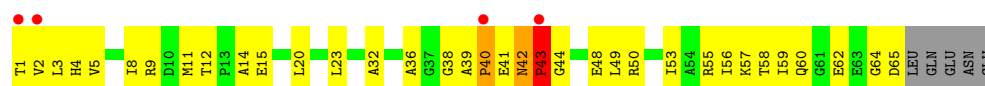
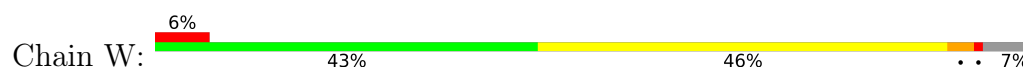
- Molecule 22: RIBOSOMAL PROTEIN L24



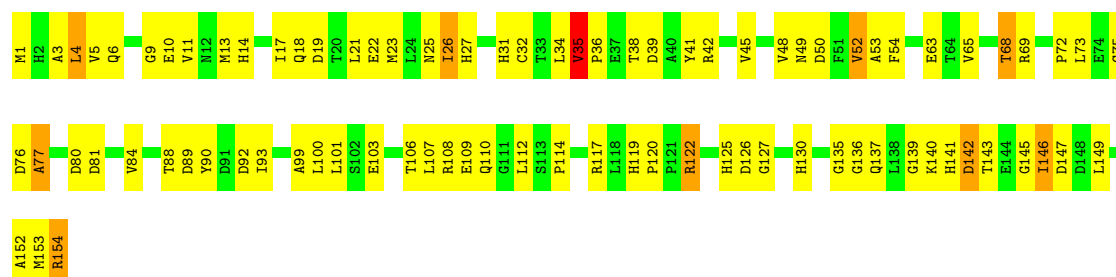
- Molecule 23: RIBOSOMAL PROTEIN L24E



- Molecule 24: RIBOSOMAL PROTEIN L29

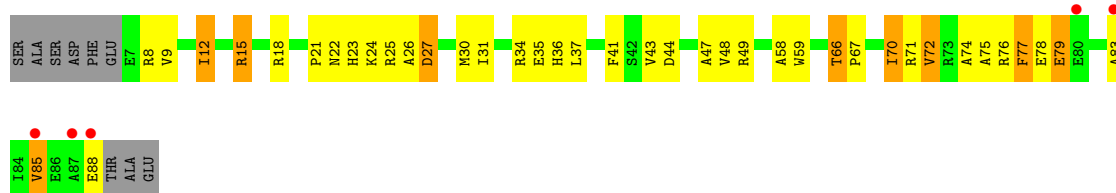


- Molecule 25: RIBOSOMAL PROTEIN L30

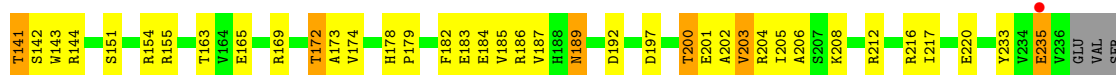
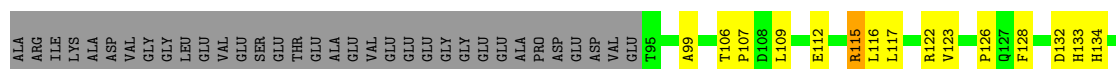


- Molecule 26: RIBOSOMAL PROTEIN L31E

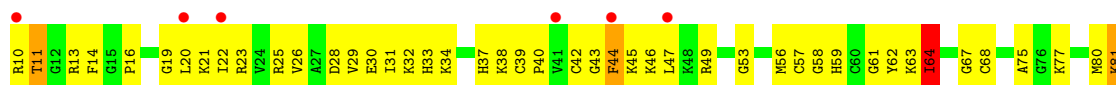




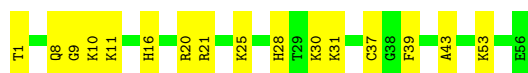
- Molecule 27: RIBOSOMAL PROTEIN L32E



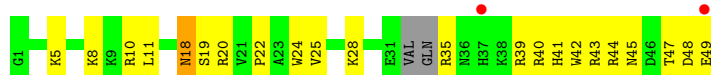
- Molecule 28: RIBOSOMAL PROTEIN L37Ae



- Molecule 29: RIBOSOMAL PROTEIN L37E

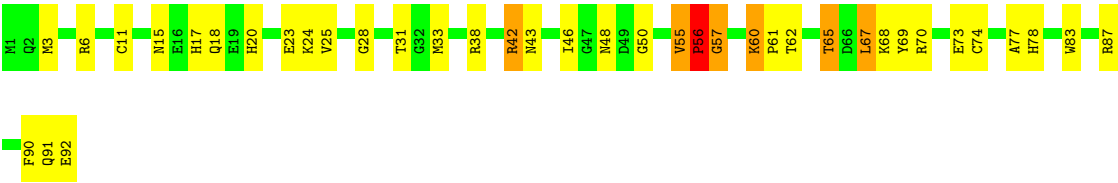


- Molecule 30: RIBOSOMAL PROTEIN L39E



- Molecule 31: 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	211.66Å 299.77Å 573.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (20.00-2.80) 94.1 (20.00-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.181 , 0.222 0.179 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	44.1	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	98611	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% 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, K, CL, SPS, ACA, NA, CD, PHA

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	0.39	0/66076	0.63	31/103052 (0.0%)
2	B	0.46	0/2905	0.71	4/4528 (0.1%)
3	5	0.61	0/65	1.47	1/99 (1.0%)
4	C	0.44	0/1787	1.02	6/2409 (0.2%)
5	D	0.44	0/2689	1.02	12/3652 (0.3%)
6	E	0.51	0/1883	1.01	7/2551 (0.3%)
7	F	0.40	0/1111	0.95	4/1498 (0.3%)
8	G	0.40	0/1382	0.90	3/1880 (0.2%)
9	H	0.41	0/896	0.90	1/1219 (0.1%)
10	I	0.37	0/241	0.78	0/324
11	J	0.49	0/1246	1.19	9/1686 (0.5%)
12	K	0.45	0/1135	0.92	1/1530 (0.1%)
13	L	0.43	0/1003	1.01	3/1351 (0.2%)
14	M	0.41	0/1126	1.00	4/1504 (0.3%)
15	N	0.51	0/1633	1.05	7/2180 (0.3%)
16	O	0.40	0/1473	1.06	10/1999 (0.5%)
17	P	0.47	0/873	0.94	3/1181 (0.3%)
18	Q	0.43	0/1143	0.89	1/1521 (0.1%)
19	R	0.48	0/748	1.07	5/1005 (0.5%)
20	S	0.47	0/1172	1.00	7/1578 (0.4%)
21	T	0.40	0/648	0.89	4/875 (0.5%)
22	U	0.41	0/957	1.01	6/1289 (0.5%)
23	V	0.38	0/417	0.87	0/562
24	W	0.39	0/502	0.98	2/675 (0.3%)
25	X	0.49	0/1218	1.04	9/1655 (0.5%)
26	Y	0.47	0/664	0.98	3/895 (0.3%)
27	Z	0.48	0/1146	0.99	5/1536 (0.3%)
28	1	0.48	0/575	1.02	1/763 (0.1%)
29	2	0.51	0/437	0.93	1/578 (0.2%)
30	3	0.43	0/398	0.80	0/527
31	4	0.45	0/771	0.99	6/1024 (0.6%)
All	All	0.41	0/98320	0.75	156/147126 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	58
2	B	0	3
All	All	1	61

There are no bond length outliers.

The worst 5 of 156 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1563	G	C2'-C3'-O3'	14.11	130.67	109.50
1	A	1164	U	OP1-P-O3'	-13.73	66.80	108.00
1	A	1164	U	OP2-P-O3'	-13.06	68.82	108.00
11	J	74	ASN	N-CA-C	-13.02	94.08	113.61
1	A	1979	G	C2'-C3'-O3'	11.35	126.52	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'

5 of 61 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	221	G	Sidechain
1	A	246	G	Sidechain
1	A	270	U	Sidechain
1	A	332	G	Sidechain
1	A	333	G	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	901	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2600	0	1326	74	0
3	5	59	0	34	2	0
4	C	1754	0	1763	137	0
5	D	2624	0	2533	187	0
6	E	1858	0	1816	119	0
7	F	1094	0	1085	134	0
8	G	1357	0	1266	82	0
9	H	885	0	854	64	0
10	I	240	0	231	23	0
11	J	1215	0	1215	157	0
12	K	1119	0	1098	70	0
13	L	993	0	1027	62	0
14	M	1114	0	1072	63	0
15	N	1605	0	1676	165	0
16	O	1444	0	1401	132	0
17	P	864	0	873	42	0
18	Q	1133	0	1127	51	0
19	R	734	0	728	22	0
20	S	1149	0	1122	66	0
21	T	641	0	605	20	0
22	U	949	0	923	49	0
23	V	410	0	364	32	0
24	W	499	0	511	36	0
25	X	1195	0	1137	108	0
26	Y	654	0	653	46	0
27	Z	1130	0	1133	62	0
28	1	563	0	597	60	0
29	2	430	0	426	24	0
30	3	393	0	406	30	0
31	4	755	0	728	37	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	5	1	0	0	0	0
32	A	111	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	L	1	0	0	0	0
32	U	1	0	0	0	0
32	Z	1	0	0	0	0
33	A	73	0	0	0	0
33	B	2	0	0	0	0
33	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	E	1	0	0	0	0
33	J	1	0	0	0	0
33	K	1	0	0	0	0
33	M	1	0	0	0	0
33	N	1	0	0	0	0
33	R	1	0	0	0	0
33	S	2	0	0	0	0
33	T	1	0	0	0	0
33	U	1	0	0	0	0
34	A	2	0	0	0	0
35	4	1	0	0	0	0
35	A	10	0	0	0	0
35	C	1	0	0	0	0
35	D	1	0	0	0	0
35	K	3	0	0	1	0
35	M	1	0	0	0	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	23	0	19	5	0
37	5	11	0	8	0	0
38	5	8	0	6	0	0
39	1	1	0	0	0	0
39	2	1	0	0	0	0
39	4	1	0	0	0	0
39	P	1	0	0	0	0
39	V	1	0	0	0	0
40	1	36	0	0	8	0
40	2	55	0	0	3	0
40	3	40	0	0	6	0
40	4	73	0	0	10	0
40	5	1	0	0	0	0
40	A	5920	0	0	192	0
40	B	136	0	0	11	0
40	C	119	0	0	26	0
40	D	142	0	0	31	0
40	E	172	0	0	28	0
40	F	51	0	0	24	0
40	G	44	0	0	8	0
40	H	28	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	I	21	0	0	6	0
40	J	75	0	0	23	0
40	K	56	0	0	5	0
40	L	61	0	0	14	0
40	M	86	0	0	19	0
40	N	125	0	0	21	0
40	O	69	0	0	17	0
40	P	43	0	0	7	0
40	Q	67	0	0	1	0
40	R	49	0	0	3	0
40	S	83	0	0	11	0
40	T	35	0	0	5	0
40	U	37	0	0	4	0
40	V	24	0	0	5	0
40	W	16	0	0	2	0
40	X	71	0	0	12	0
40	Y	31	0	0	5	0
40	Z	92	0	0	14	0
All	All	98611	0	59568	2788	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 19.

The worst 5 of 2788 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)
6:E:236:THR:HG22	6:E:239:ALA:H	1.04	1.16
1:A:1160:G:H5'	1:A:1161:A:H5'	1.22	1.15
1:A:1134:G:H4'	11:J:151:MET:HE1	1.27	1.15
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.63	1.13
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.30	1.12

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%)	209 (89%)	21 (9%)	5 (2%)	5	20
5	D	335/337 (99%)	303 (90%)	25 (8%)	7 (2%)	5	20
6	E	244/246 (99%)	218 (89%)	25 (10%)	1 (0%)	30	60
7	F	134/176 (76%)	98 (73%)	28 (21%)	8 (6%)	1	3
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	21	51
9	H	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	4	15
10	I	25/348 (7%)	24 (96%)	1 (4%)	0	100	100
11	J	152/167 (91%)	133 (88%)	13 (9%)	6 (4%)	2	8
12	K	140/145 (97%)	126 (90%)	11 (8%)	3 (2%)	5	20
13	L	130/132 (98%)	118 (91%)	10 (8%)	2 (2%)	8	28
14	M	141/164 (86%)	120 (85%)	19 (14%)	2 (1%)	9	30
15	N	192/194 (99%)	174 (91%)	16 (8%)	2 (1%)	12	38
16	O	184/186 (99%)	167 (91%)	11 (6%)	6 (3%)	3	11
17	P	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	Q	141/148 (95%)	137 (97%)	3 (2%)	1 (1%)	18	47
19	R	93/95 (98%)	85 (91%)	8 (9%)	0	100	100
20	S	148/154 (96%)	140 (95%)	7 (5%)	1 (1%)	18	47
21	T	79/84 (94%)	75 (95%)	4 (5%)	0	100	100
22	U	117/119 (98%)	111 (95%)	5 (4%)	1 (1%)	14	41
23	V	51/66 (77%)	47 (92%)	4 (8%)	0	100	100
24	W	63/70 (90%)	58 (92%)	3 (5%)	2 (3%)	3	11
25	X	152/154 (99%)	147 (97%)	3 (2%)	2 (1%)	9	31
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	4	16
27	Z	140/240 (58%)	139 (99%)	1 (1%)	0	100	100
28	1	71/73 (97%)	63 (89%)	7 (10%)	1 (1%)	9	30
29	2	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
30	3	42/48 (88%)	42 (100%)	0	0	100	100
31	4	90/92 (98%)	85 (94%)	3 (3%)	2 (2%)	5	19
All	All	3633/4235 (86%)	3313 (91%)	262 (7%)	58 (2%)	7	27

5 of 58 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
7	F	20	LYS
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%)	167 (93%)	12 (7%)	15	42
5	D	282/282 (100%)	263 (93%)	19 (7%)	15	42
6	E	193/193 (100%)	177 (92%)	16 (8%)	10	32
7	F	117/147 (80%)	109 (93%)	8 (7%)	14	42
8	G	152/155 (98%)	148 (97%)	4 (3%)	40	75
9	H	92/92 (100%)	90 (98%)	2 (2%)	45	78
10	I	27/283 (10%)	26 (96%)	1 (4%)	30	65
11	J	122/122 (100%)	107 (88%)	15 (12%)	4	16
12	K	118/121 (98%)	110 (93%)	8 (7%)	14	42
13	L	106/106 (100%)	103 (97%)	3 (3%)	38	73
14	M	112/126 (89%)	109 (97%)	3 (3%)	39	74
15	N	166/166 (100%)	160 (96%)	6 (4%)	31	66
16	O	149/149 (100%)	140 (94%)	9 (6%)	17	47
17	P	93/93 (100%)	90 (97%)	3 (3%)	34	70
18	Q	113/116 (97%)	110 (97%)	3 (3%)	39	74
19	R	79/79 (100%)	75 (95%)	4 (5%)	21	54
20	S	117/121 (97%)	114 (97%)	3 (3%)	40	75
21	T	71/73 (97%)	70 (99%)	1 (1%)	59	85
22	U	105/105 (100%)	101 (96%)	4 (4%)	29	64
23	V	44/52 (85%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
24	W	51/56 (91%)	50 (98%)	1 (2%)	48 80
25	X	130/130 (100%)	121 (93%)	9 (7%)	14 41
26	Y	66/73 (90%)	60 (91%)	6 (9%)	9 28
27	Z	120/195 (62%)	113 (94%)	7 (6%)	18 49
28	1	56/56 (100%)	53 (95%)	3 (5%)	20 51
29	2	46/46 (100%)	46 (100%)	0	100 100
30	3	42/44 (96%)	41 (98%)	1 (2%)	43 77
31	4	79/79 (100%)	76 (96%)	3 (4%)	29 64
All	All	3027/3441 (88%)	2873 (95%)	154 (5%)	21 54

5 of 154 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	R	95	GLU
27	Z	189	ASN
21	T	10	VAL
25	X	122	ARG
30	3	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 103 such sidechains are listed below:

Mol	Chain	Res	Type
18	Q	50	GLN
21	T	53	ASN
30	3	45	ASN
18	Q	73	HIS
20	S	94	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	250 (9%)	38 (1%)
2	B	121/122 (99%)	15 (12%)	3 (2%)
3	5	2/3 (66%)	1 (50%)	0
All	All	2870/3047 (94%)	266 (9%)	41 (1%)

5 of 266 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	2011	A
1	A	2726	U
1	A	2313	C
1	A	2536	C
1	A	2791	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 237 ligands modelled in this entry, 234 are monoatomic - leaving 3 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	$\# Z > 2$
38	ACA	5	9078	37	6,7,8	1.24	1 (16%)	5,6,8	0.86	0
37	PHA	5	9077	38,3	10,11,11	0.82	0	8,13,13	0.45	0
36	SPS	5	9080	32	20,23,23	1.86	4 (20%)	23,30,30	2.33	10 (43%)

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
38	ACA	5	9078	37	-	1/5/5/6	-
37	PHA	5	9077	38,3	-	2/5/6/6	0/1/1/1
36	SPS	5	9080	32	-	5/15/18/18	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	5	9080	SPS	C6-C1	5.31	1.54	1.45
36	5	9080	SPS	C16-S17	-3.47	1.76	1.79
36	5	9080	SPS	C9-C10	-3.17	1.41	1.48
36	5	9080	SPS	O15-S15	-2.43	1.41	1.50
38	5	9078	ACA	C3-C2	-2.23	1.42	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	5	9080	SPS	C7-C5-N4	5.18	119.44	113.42
36	5	9080	SPS	N4-C3-N2	4.55	122.89	115.74
36	5	9080	SPS	C7-C5-C6	-4.42	120.75	126.47
36	5	9080	SPS	C1-N2-C3	-3.95	120.94	126.37
36	5	9080	SPS	O15-S15-C16	2.55	109.50	106.47

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

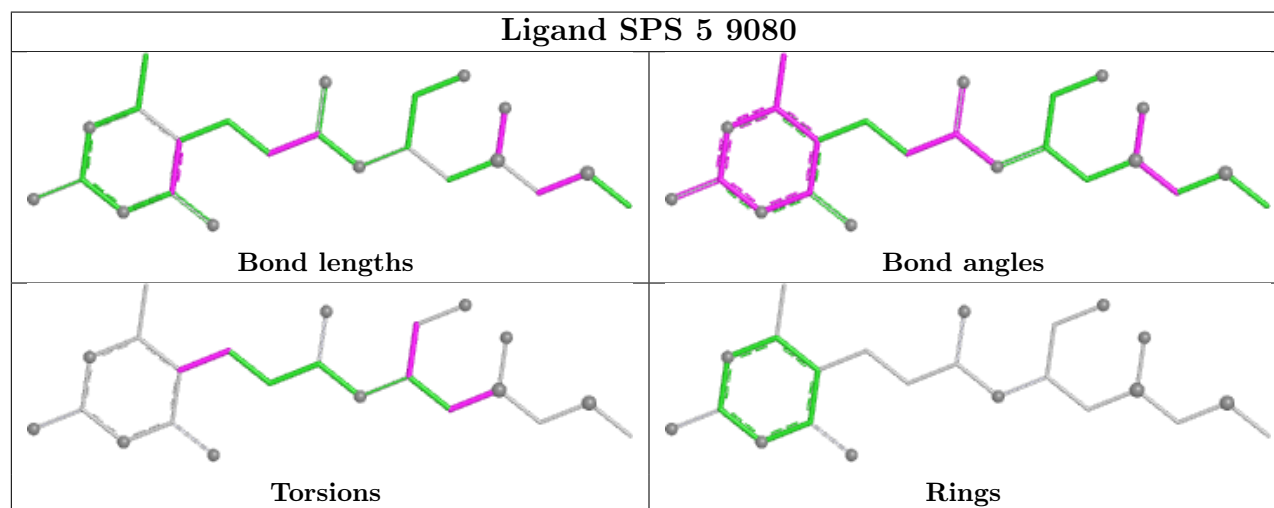
Mol	Chain	Res	Type	Atoms
36	5	9080	SPS	N11-C12-C13-O13
36	5	9080	SPS	C14-C12-C13-O13
36	5	9080	SPS	C12-C14-S15-O15
36	5	9080	SPS	C12-C14-S15-C16
37	5	9077	PHA	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	9080	SPS	5	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%)	-0.50	36 (1%) 75 66	18, 43, 87, 135	0
2	B	122/122 (100%)	0.04	5 (4%) 41 33	35, 60, 87, 145	0
3	5	3/3 (100%)	-0.65	0 100 100	33, 33, 35, 36	0
4	C	237/239 (99%)	-0.21	3 (1%) 75 66	24, 47, 79, 101	0
5	D	337/337 (100%)	-0.07	2 (0%) 85 80	25, 53, 79, 88	0
6	E	246/246 (100%)	-0.25	0 100 100	21, 42, 64, 75	0
7	F	140/176 (79%)	1.12	23 (16%) 4 3	51, 94, 112, 118	0
8	G	172/177 (97%)	0.31	4 (2%) 61 51	44, 67, 85, 92	0
9	H	119/119 (100%)	0.33	2 (1%) 69 60	45, 66, 91, 97	0
10	I	29/348 (8%)	0.98	2 (6%) 23 16	66, 85, 93, 96	0
11	J	156/167 (93%)	0.16	6 (3%) 44 35	34, 52, 77, 80	0
12	K	142/145 (97%)	-0.15	1 (0%) 84 77	33, 49, 68, 86	0
13	L	132/132 (100%)	-0.09	1 (0%) 82 75	31, 50, 70, 80	0
14	M	145/164 (88%)	0.09	6 (4%) 41 33	20, 60, 98, 111	0
15	N	194/194 (100%)	-0.25	3 (1%) 72 63	28, 39, 58, 68	0
16	O	186/186 (100%)	0.34	9 (4%) 35 28	36, 59, 99, 111	0
17	P	115/115 (100%)	0.04	1 (0%) 81 74	35, 49, 67, 77	0
18	Q	143/148 (96%)	-0.05	1 (0%) 84 77	36, 52, 64, 74	0
19	R	95/95 (100%)	-0.27	1 (1%) 78 70	29, 40, 54, 70	0
20	S	150/154 (97%)	-0.50	0 100 100	29, 41, 61, 70	0
21	T	81/84 (96%)	-0.16	1 (1%) 76 68	40, 54, 73, 80	0
22	U	119/119 (100%)	-0.03	1 (0%) 82 75	36, 52, 76, 90	0
23	V	53/66 (80%)	0.06	0 100 100	39, 53, 69, 77	0
24	W	65/70 (92%)	0.41	4 (6%) 26 20	49, 68, 105, 110	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	X	154/154 (100%)	-0.23	0 100 100	32, 45, 63, 72	0
26	Y	82/91 (90%)	0.16	5 (6%) 27 20	40, 57, 79, 99	0
27	Z	142/240 (59%)	-0.33	1 (0%) 84 77	24, 41, 65, 82	0
28	1	73/73 (100%)	0.56	6 (8%) 17 13	46, 60, 71, 79	0
29	2	56/56 (100%)	-0.78	0 100 100	24, 29, 35, 43	0
30	3	46/48 (95%)	0.16	2 (4%) 40 31	31, 57, 84, 98	0
31	4	92/92 (100%)	-0.16	0 100 100	31, 51, 64, 78	0
All	All	6580/7282 (90%)	-0.21	126 (1%) 66 57	18, 48, 88, 145	0

The worst 5 of 126 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	7.0
16	O	162	ASP	5.0
7	F	10	PHE	4.6
5	D	1	PRO	4.5
8	G	10	ASP	4.4

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
38	ACA	5	9078	8/9	0.63	0.28	45,53,55,55	0
33	NA	A	8329	1/1	0.66	0.14	54,54,54,54	0
33	NA	S	8386	1/1	0.68	0.37	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	T	8312	1/1	0.75	0.16	79,79,79,79	0
33	NA	B	8351	1/1	0.75	0.11	78,78,78,78	0
33	NA	A	8324	1/1	0.77	0.23	55,55,55,55	0
32	MG	A	8050	1/1	0.77	0.09	64,64,64,64	0
33	NA	A	8307	1/1	0.78	0.11	46,46,46,46	0
32	MG	A	8024	1/1	0.80	0.36	89,89,89,89	0
32	MG	A	8087	1/1	0.82	0.15	63,63,63,63	0
33	NA	A	8371	1/1	0.82	0.38	61,61,61,61	0
33	NA	A	8357	1/1	0.83	0.14	53,53,53,53	0
33	NA	A	8385	1/1	0.84	0.23	50,50,50,50	0
33	NA	A	8384	1/1	0.84	0.12	75,75,75,75	0
33	NA	J	8322	1/1	0.84	0.21	61,61,61,61	0
33	NA	A	8310	1/1	0.85	0.12	39,39,39,39	0
32	MG	B	8095	1/1	0.85	0.17	70,70,70,70	0
32	MG	A	8113	1/1	0.85	0.11	43,43,43,43	0
39	CD	P	8405	1/1	0.85	0.14	174,174,174,174	0
33	NA	A	8364	1/1	0.86	0.14	39,39,39,39	0
32	MG	A	8049	1/1	0.86	0.13	77,77,77,77	0
33	NA	A	8333	1/1	0.86	0.15	33,33,33,33	0
33	NA	A	8352	1/1	0.86	0.25	71,71,71,71	0
32	MG	A	8066	1/1	0.86	0.13	84,84,84,84	0
33	NA	C	8345	1/1	0.87	0.09	44,44,44,44	0
33	NA	A	8341	1/1	0.87	0.08	41,41,41,41	0
33	NA	A	8373	1/1	0.87	0.14	50,50,50,50	0
32	MG	A	8092	1/1	0.87	0.14	79,79,79,79	0
32	MG	A	8106	1/1	0.87	0.06	52,52,52,52	0
33	NA	A	8311	1/1	0.87	0.13	55,55,55,55	0
33	NA	A	8366	1/1	0.88	0.16	68,68,68,68	0
33	NA	A	8362	1/1	0.88	0.20	64,64,64,64	0
32	MG	A	8099	1/1	0.89	0.10	48,48,48,48	0
33	NA	A	8363	1/1	0.89	0.13	49,49,49,49	0
32	MG	A	8076	1/1	0.89	0.07	50,50,50,50	0
32	MG	1	8105	1/1	0.89	0.08	32,32,32,32	0
33	NA	A	8368	1/1	0.89	0.14	56,56,56,56	0
33	NA	B	8383	1/1	0.89	0.19	69,69,69,69	0
33	NA	A	8313	1/1	0.90	0.07	62,62,62,62	0
33	NA	A	8355	1/1	0.90	0.14	56,56,56,56	0
32	MG	A	8053	1/1	0.91	0.06	50,50,50,50	0
32	MG	A	8047	1/1	0.91	0.09	66,66,66,66	0
32	MG	A	8116	1/1	0.91	0.05	51,51,51,51	0
33	NA	M	8380	1/1	0.91	0.16	64,64,64,64	0
33	NA	A	8382	1/1	0.91	0.24	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
33	NA	A	8365	1/1	0.91	0.20	43,43,43,43	0
33	NA	A	8340	1/1	0.91	0.11	44,44,44,44	0
33	NA	A	8367	1/1	0.91	0.11	44,44,44,44	0
32	MG	A	8114	1/1	0.92	0.11	54,54,54,54	0
33	NA	E	8304	1/1	0.92	0.09	33,33,33,33	0
33	NA	U	8343	1/1	0.92	0.07	33,33,33,33	0
32	MG	A	8041	1/1	0.92	0.06	53,53,53,53	0
32	MG	A	8070	1/1	0.92	0.07	47,47,47,47	0
33	NA	A	8317	1/1	0.93	0.04	45,45,45,45	0
32	MG	A	8082	1/1	0.93	0.12	53,53,53,53	0
33	NA	A	8314	1/1	0.93	0.07	38,38,38,38	0
35	CL	A	8511	1/1	0.93	0.06	48,48,48,48	0
35	CL	K	8502	1/1	0.93	0.06	66,66,66,66	0
35	CL	4	8504	1/1	0.93	0.09	67,67,67,67	0
36	SPS	5	9080	23/23	0.93	0.10	30,33,47,49	0
37	PHA	5	9077	11/11	0.93	0.13	41,45,52,53	0
33	NA	A	8370	1/1	0.93	0.28	57,57,57,57	0
33	NA	A	8359	1/1	0.93	0.14	40,40,40,40	0
32	MG	A	8064	1/1	0.94	0.09	31,31,31,31	0
33	NA	A	8326	1/1	0.94	0.13	37,37,37,37	0
33	NA	A	8328	1/1	0.94	0.17	34,34,34,34	0
33	NA	A	8374	1/1	0.94	0.21	53,53,53,53	0
33	NA	A	8377	1/1	0.94	0.24	66,66,66,66	0
32	MG	A	8044	1/1	0.94	0.08	36,36,36,36	0
35	CL	A	8513	1/1	0.94	0.08	50,50,50,50	0
35	CL	A	8517	1/1	0.94	0.08	59,59,59,59	0
33	NA	A	8332	1/1	0.94	0.10	29,29,29,29	0
32	MG	A	8117	1/1	0.94	0.06	25,25,25,25	0
33	NA	A	8335	1/1	0.94	0.09	43,43,43,43	0
32	MG	A	8046	1/1	0.94	0.07	47,47,47,47	0
32	MG	A	8090	1/1	0.94	0.13	70,70,70,70	0
33	NA	A	8301	1/1	0.94	0.09	46,46,46,46	0
32	MG	A	8119	1/1	0.95	0.07	41,41,41,41	0
32	MG	A	8042	1/1	0.95	0.05	31,31,31,31	0
32	MG	A	8100	1/1	0.95	0.10	65,65,65,65	0
32	MG	A	8103	1/1	0.95	0.11	61,61,61,61	0
33	NA	A	8334	1/1	0.95	0.10	32,32,32,32	0
33	NA	A	8316	1/1	0.95	0.06	40,40,40,40	0
33	NA	S	8337	1/1	0.95	0.05	28,28,28,28	0
33	NA	A	8339	1/1	0.95	0.05	22,22,22,22	0
33	NA	A	8306	1/1	0.95	0.20	32,32,32,32	0
33	NA	A	8318	1/1	0.95	0.19	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	K	A	8391	1/1	0.95	0.18	48,48,48,48	0
33	NA	A	8349	1/1	0.95	0.06	41,41,41,41	0
33	NA	A	8350	1/1	0.95	0.08	32,32,32,32	0
35	CL	A	8515	1/1	0.95	0.18	65,65,65,65	0
35	CL	A	8516	1/1	0.95	0.10	56,56,56,56	0
33	NA	A	8375	1/1	0.95	0.27	47,47,47,47	0
35	CL	C	8509	1/1	0.95	0.08	56,56,56,56	0
33	NA	A	8319	1/1	0.95	0.06	36,36,36,36	0
35	CL	O	8507	1/1	0.95	0.08	59,59,59,59	0
33	NA	A	8378	1/1	0.95	0.16	47,47,47,47	0
33	NA	A	8379	1/1	0.95	0.11	45,45,45,45	0
33	NA	A	8321	1/1	0.95	0.14	54,54,54,54	0
32	MG	A	8067	1/1	0.95	0.08	43,43,43,43	0
33	NA	A	8308	1/1	0.95	0.06	43,43,43,43	0
33	NA	A	8302	1/1	0.96	0.06	46,46,46,46	0
32	MG	A	8062	1/1	0.96	0.05	48,48,48,48	0
32	MG	A	8101	1/1	0.96	0.07	52,52,52,52	0
33	NA	N	8347	1/1	0.96	0.04	23,23,23,23	0
32	MG	A	8045	1/1	0.96	0.11	56,56,56,56	0
33	NA	A	8323	1/1	0.96	0.13	42,42,42,42	0
33	NA	A	8369	1/1	0.96	0.09	49,49,49,49	0
33	NA	A	8342	1/1	0.96	0.08	40,40,40,40	0
33	NA	A	8309	1/1	0.96	0.06	32,32,32,32	0
35	CL	A	8505	1/1	0.96	0.06	49,49,49,49	0
33	NA	A	8372	1/1	0.96	0.12	58,58,58,58	0
32	MG	A	8094	1/1	0.96	0.10	63,63,63,63	0
32	MG	L	8069	1/1	0.96	0.06	50,50,50,50	0
33	NA	A	8354	1/1	0.96	0.05	34,34,34,34	0
32	MG	U	8073	1/1	0.96	0.04	46,46,46,46	0
35	CL	A	8522	1/1	0.96	0.22	55,55,55,55	0
33	NA	A	8356	1/1	0.96	0.12	47,47,47,47	0
35	CL	K	8501	1/1	0.96	0.08	55,55,55,55	0
33	NA	A	8330	1/1	0.96	0.05	34,34,34,34	0
33	NA	A	8358	1/1	0.96	0.26	82,82,82,82	0
35	CL	P	8508	1/1	0.96	0.07	62,62,62,62	0
35	CL	Z	8520	1/1	0.96	0.05	42,42,42,42	0
33	NA	A	8331	1/1	0.96	0.12	31,31,31,31	0
33	NA	A	8360	1/1	0.96	0.13	39,39,39,39	0
33	NA	A	8361	1/1	0.96	0.06	47,47,47,47	0
32	MG	A	8096	1/1	0.96	0.04	46,46,46,46	0
32	MG	A	8089	1/1	0.96	0.05	58,58,58,58	0
35	CL	A	8503	1/1	0.97	0.04	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8093	1/1	0.97	0.06	49,49,49,49	0
32	MG	A	8088	1/1	0.97	0.07	30,30,30,30	0
35	CL	A	8512	1/1	0.97	0.06	47,47,47,47	0
32	MG	A	8108	1/1	0.97	0.08	60,60,60,60	0
32	MG	A	8057	1/1	0.97	0.06	40,40,40,40	0
33	NA	A	8336	1/1	0.97	0.05	53,53,53,53	0
33	NA	A	8338	1/1	0.97	0.03	41,41,41,41	0
32	MG	A	8098	1/1	0.97	0.06	36,36,36,36	0
33	NA	A	8327	1/1	0.97	0.04	41,41,41,41	0
33	NA	K	8346	1/1	0.97	0.05	40,40,40,40	0
32	MG	A	8068	1/1	0.97	0.05	50,50,50,50	0
35	CL	K	8521	1/1	0.97	0.08	50,50,50,50	0
33	NA	A	8305	1/1	0.97	0.05	35,35,35,35	0
33	NA	R	8348	1/1	0.97	0.04	42,42,42,42	0
33	NA	A	8376	1/1	0.97	0.11	47,47,47,47	0
33	NA	A	8344	1/1	0.97	0.04	25,25,25,25	0
32	MG	A	8091	1/1	0.97	0.05	69,69,69,69	0
32	MG	A	8052	1/1	0.97	0.05	40,40,40,40	0
34	K	A	8390	1/1	0.97	0.19	70,70,70,70	0
33	NA	A	8381	1/1	0.97	0.06	44,44,44,44	0
32	MG	A	8097	1/1	0.98	0.09	28,28,28,28	0
32	MG	A	8022	1/1	0.98	0.09	40,40,40,40	0
32	MG	A	8012	1/1	0.98	0.04	28,28,28,28	0
33	NA	A	8315	1/1	0.98	0.07	32,32,32,32	0
35	CL	A	8514	1/1	0.98	0.04	46,46,46,46	0
32	MG	A	8043	1/1	0.98	0.05	39,39,39,39	0
32	MG	A	8059	1/1	0.98	0.08	35,35,35,35	0
32	MG	A	8102	1/1	0.98	0.07	45,45,45,45	0
32	MG	Z	8109	1/1	0.98	0.05	33,33,33,33	0
33	NA	A	8320	1/1	0.98	0.09	38,38,38,38	0
32	MG	A	8061	1/1	0.98	0.04	34,34,34,34	0
32	MG	A	8104	1/1	0.98	0.16	52,52,52,52	0
32	MG	A	8051	1/1	0.98	0.06	57,57,57,57	0
35	CL	M	8510	1/1	0.98	0.08	47,47,47,47	0
33	NA	A	8303	1/1	0.98	0.07	43,43,43,43	0
33	NA	A	8353	1/1	0.98	0.04	23,23,23,23	0
35	CL	S	8506	1/1	0.98	0.03	46,46,46,46	0
32	MG	A	8107	1/1	0.98	0.03	43,43,43,43	0
32	MG	A	8081	1/1	0.98	0.03	43,43,43,43	0
32	MG	A	8111	1/1	0.98	0.04	51,51,51,51	0
32	MG	A	8112	1/1	0.98	0.15	28,28,28,28	0
32	MG	A	8063	1/1	0.98	0.05	73,73,73,73	0

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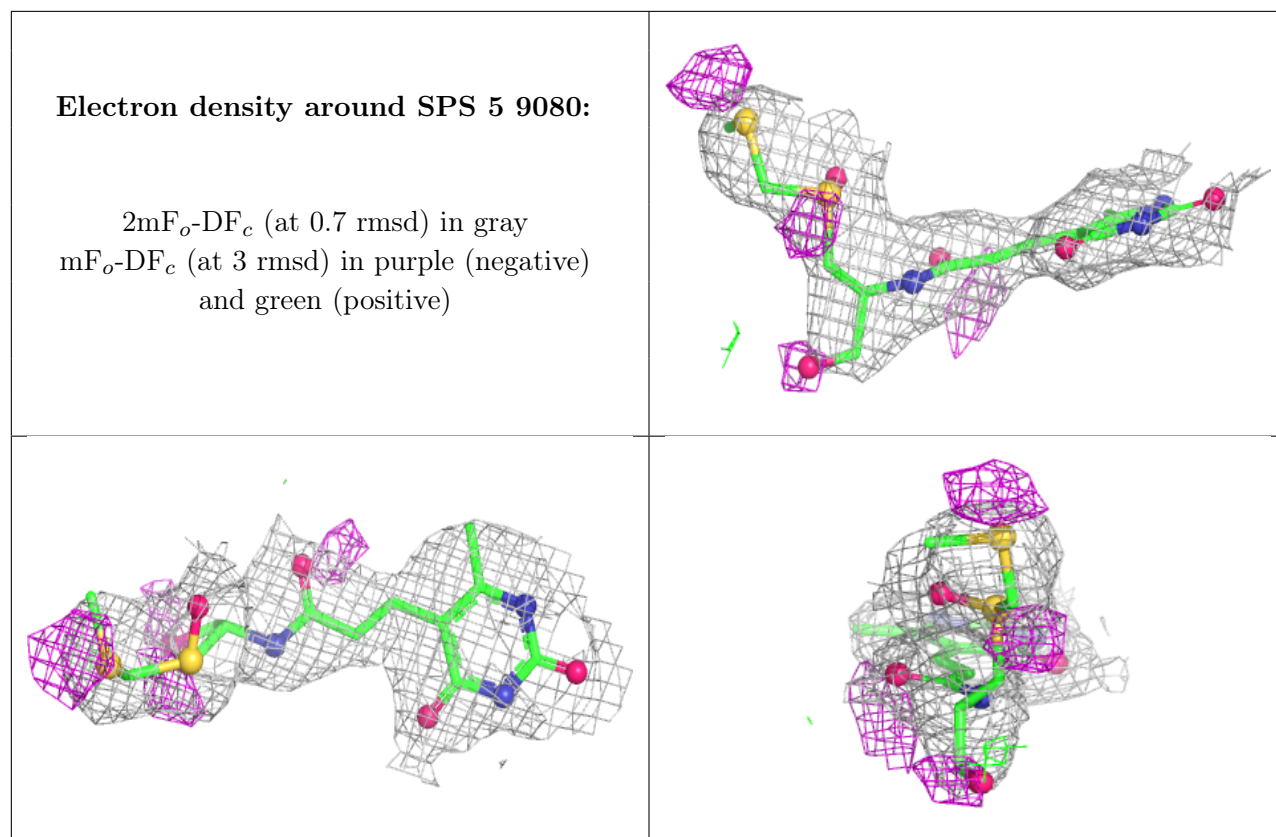
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8083	1/1	0.98	0.04	41,41,41,41	0
32	MG	A	8075	1/1	0.99	0.04	37,37,37,37	0
32	MG	A	8008	1/1	0.99	0.03	35,35,35,35	0
32	MG	5	8118	1/1	0.99	0.03	29,29,29,29	0
32	MG	A	8079	1/1	0.99	0.03	27,27,27,27	0
32	MG	A	8080	1/1	0.99	0.04	36,36,36,36	0
32	MG	A	8010	1/1	0.99	0.04	35,35,35,35	0
32	MG	A	8011	1/1	0.99	0.03	26,26,26,26	0
32	MG	4	8078	1/1	0.99	0.05	41,41,41,41	0
32	MG	A	8003	1/1	0.99	0.03	26,26,26,26	0
32	MG	A	8085	1/1	0.99	0.03	45,45,45,45	0
32	MG	A	8086	1/1	0.99	0.06	45,45,45,45	0
32	MG	A	8013	1/1	0.99	0.03	32,32,32,32	0
32	MG	A	8014	1/1	0.99	0.07	25,25,25,25	0
32	MG	A	8016	1/1	0.99	0.03	39,39,39,39	0
32	MG	A	8048	1/1	0.99	0.07	58,58,58,58	0
32	MG	A	8019	1/1	0.99	0.04	29,29,29,29	0
32	MG	A	8021	1/1	0.99	0.03	33,33,33,33	0
32	MG	A	8005	1/1	0.99	0.02	33,33,33,33	0
32	MG	A	8023	1/1	0.99	0.02	39,39,39,39	0
32	MG	A	8007	1/1	0.99	0.04	16,16,16,16	0
32	MG	A	8054	1/1	0.99	0.03	24,24,24,24	0
32	MG	A	8055	1/1	0.99	0.03	43,43,43,43	0
32	MG	A	8025	1/1	0.99	0.03	40,40,40,40	0
32	MG	A	8058	1/1	0.99	0.04	37,37,37,37	0
32	MG	A	8027	1/1	0.99	0.03	49,49,49,49	0
32	MG	A	8060	1/1	0.99	0.03	42,42,42,42	0
32	MG	A	8028	1/1	0.99	0.02	34,34,34,34	0
35	CL	D	8519	1/1	0.99	0.10	40,40,40,40	0
32	MG	A	8031	1/1	0.99	0.02	27,27,27,27	0
32	MG	A	8032	1/1	0.99	0.06	28,28,28,28	0
33	NA	A	8325	1/1	0.99	0.07	50,50,50,50	0
32	MG	A	8033	1/1	0.99	0.02	28,28,28,28	0
35	CL	N	8518	1/1	0.99	0.07	39,39,39,39	0
32	MG	A	8035	1/1	0.99	0.03	52,52,52,52	0
32	MG	A	8110	1/1	0.99	0.10	35,35,35,35	0
32	MG	A	8037	1/1	0.99	0.04	34,34,34,34	0
32	MG	A	8039	1/1	0.99	0.04	42,42,42,42	0
32	MG	A	8040	1/1	0.99	0.03	53,53,53,53	0
32	MG	A	8071	1/1	0.99	0.04	63,63,63,63	0
32	MG	A	8115	1/1	0.99	0.04	42,42,42,42	0
32	MG	A	8072	1/1	0.99	0.03	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8074	1/1	0.99	0.03	29,29,29,29	0
39	CD	1	8403	1/1	0.99	0.02	62,62,62,62	0
39	CD	2	8402	1/1	0.99	0.04	56,56,56,56	0
39	CD	4	8404	1/1	0.99	0.03	57,57,57,57	0
32	MG	A	8009	1/1	1.00	0.04	26,26,26,26	0
32	MG	A	8038	1/1	1.00	0.03	27,27,27,27	0
32	MG	A	8015	1/1	1.00	0.01	29,29,29,29	0
32	MG	A	8002	1/1	1.00	0.05	28,28,28,28	0
32	MG	A	8056	1/1	1.00	0.03	39,39,39,39	0
32	MG	A	8026	1/1	1.00	0.02	26,26,26,26	0
32	MG	A	8077	1/1	1.00	0.03	27,27,27,27	0
32	MG	A	8017	1/1	1.00	0.05	19,19,19,19	0
32	MG	A	8018	1/1	1.00	0.04	31,31,31,31	0
32	MG	A	8029	1/1	1.00	0.02	41,41,41,41	0
32	MG	C	8065	1/1	1.00	0.03	31,31,31,31	0
32	MG	A	8030	1/1	1.00	0.02	32,32,32,32	0
32	MG	A	8006	1/1	1.00	0.04	30,30,30,30	0
32	MG	A	8084	1/1	1.00	0.09	40,40,40,40	0
32	MG	A	8020	1/1	1.00	0.05	28,28,28,28	0
32	MG	A	8001	1/1	1.00	0.02	27,27,27,27	0
39	CD	V	8401	1/1	1.00	0.02	62,62,62,62	0
32	MG	A	8034	1/1	1.00	0.02	33,33,33,33	0
32	MG	A	8004	1/1	1.00	0.02	26,26,26,26	0
32	MG	A	8036	1/1	1.00	0.04	32,32,32,32	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.