



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 12:18 AM UTC

PDB ID : 1Q86 / pdb_00001q86
Title : Crystal structure of CCA-Phe-cap-biotin bound simultaneously at half occupancy to both the A-site and P-site of the the 50S ribosomal Subunit.
Authors : Hansen, J.L.; Schmeing, T.M.; Moore, P.B.; Steitz, T.A.
Deposited on : 2003-08-20
Resolution : 3.00 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
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

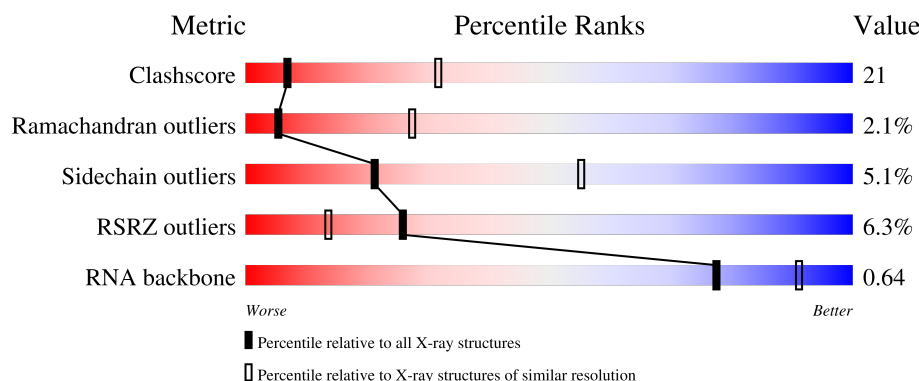
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	7% 53% 35% 6% 6%
2	B	122	5% 48% 39% 11% .
3	5	3	100% 33% 67%
3	6	3	100% 33% 67%
4	C	239	% 55% 35% 9% .

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Mol	Chain	Length	Quality of chain
5	D	337	
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	

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Mol	Chain	Length	Quality of chain
30	3	48	
31	4	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
34	NA	A	8324	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8375	-	-	-	X
36	PHA	6	77	-	-	-	X

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 98659 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 CCA-phenylalanine-carboxylic-acid-biotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	5	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			
3	6	3	Total	C	N	O	P	0	0	0
			59	28	11	18	2			

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP P20279
D	310	ARG	PHE	conflict	UNP P20279

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- 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	0	0	0
			1149	713	209	223	4			

- 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	0	0	0
			641	389	111	138	3			

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

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 50S 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 50S ribosomal protein L29P.

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 50S ribosomal protein L30P.

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 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	108	Total	Mg	0	0
			108	108		
32	B	1	Total	Mg	0	0
			1	1		
32	6	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	D	2	Total	Mg	0	0
			2	2		
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 POTASSIUM ION (CCD ID: K) (formula: K).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	A	70	Total	Na	0	0
			70	70		
34	B	2	Total	Na	0	0
			2	2		
34	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	E	1	Total 1	Na 1	0	0
34	J	2	Total 2	Na 2	0	0
34	K	1	Total 1	Na 1	0	0
34	M	1	Total 1	Na 1	0	0
34	N	2	Total 2	Na 2	0	0
34	R	1	Total 1	Na 1	0	0
34	S	3	Total 3	Na 3	0	0
34	T	1	Total 1	Na 1	0	0
34	U	1	Total 1	Na 1	0	0

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

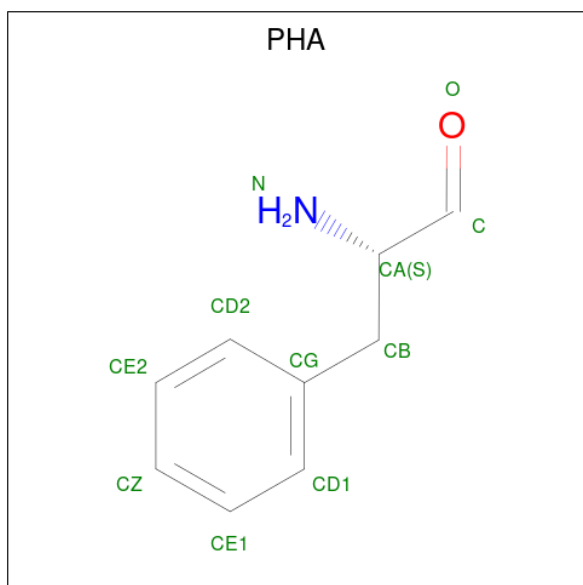
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	A	9	Total 9	Cl 9	0	0
35	C	1	Total 1	Cl 1	0	0
35	D	1	Total 1	Cl 1	0	0
35	K	3	Total 3	Cl 3	0	0
35	L	1	Total 1	Cl 1	0	0
35	M	1	Total 1	Cl 1	0	0
35	N	1	Total 1	Cl 1	0	0
35	O	1	Total 1	Cl 1	0	0
35	P	1	Total 1	Cl 1	0	0
35	S	1	Total 1	Cl 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
35	Z	1	Total	Cl	0	0
			1	1		
35	4	1	Total	Cl	0	0
			1	1		

- Molecule 36 is PHENYLALANINAL (CCD ID: PHA) (formula: C₉H₁₁NO).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
36	5	1	Total	C	N	O	0	0
			11	9	1	1		
36	6	1	Total	C	O		0	0
			10	9	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	5892	Total 5892	O 5892	0	0
38	B	139	Total 139	O 139	0	0
38	C	116	Total 116	O 116	0	0
38	D	149	Total 149	O 149	0	0
38	E	173	Total 173	O 173	0	0
38	F	52	Total 52	O 52	0	0
38	G	43	Total 43	O 43	0	0
38	H	27	Total 27	O 27	0	0
38	I	21	Total 21	O 21	0	0
38	J	77	Total 77	O 77	0	0
38	K	54	Total 54	O 54	0	0
38	L	62	Total 62	O 62	0	0
38	M	82	Total 82	O 82	0	0
38	N	139	Total 139	O 139	0	0
38	O	70	Total 70	O 70	0	0
38	P	43	Total 43	O 43	0	0
38	Q	67	Total 67	O 67	0	0
38	R	54	Total 54	O 54	0	0
38	S	84	Total 84	O 84	0	0
38	T	37	Total 37	O 37	0	0
38	U	44	Total 44	O 44	0	0

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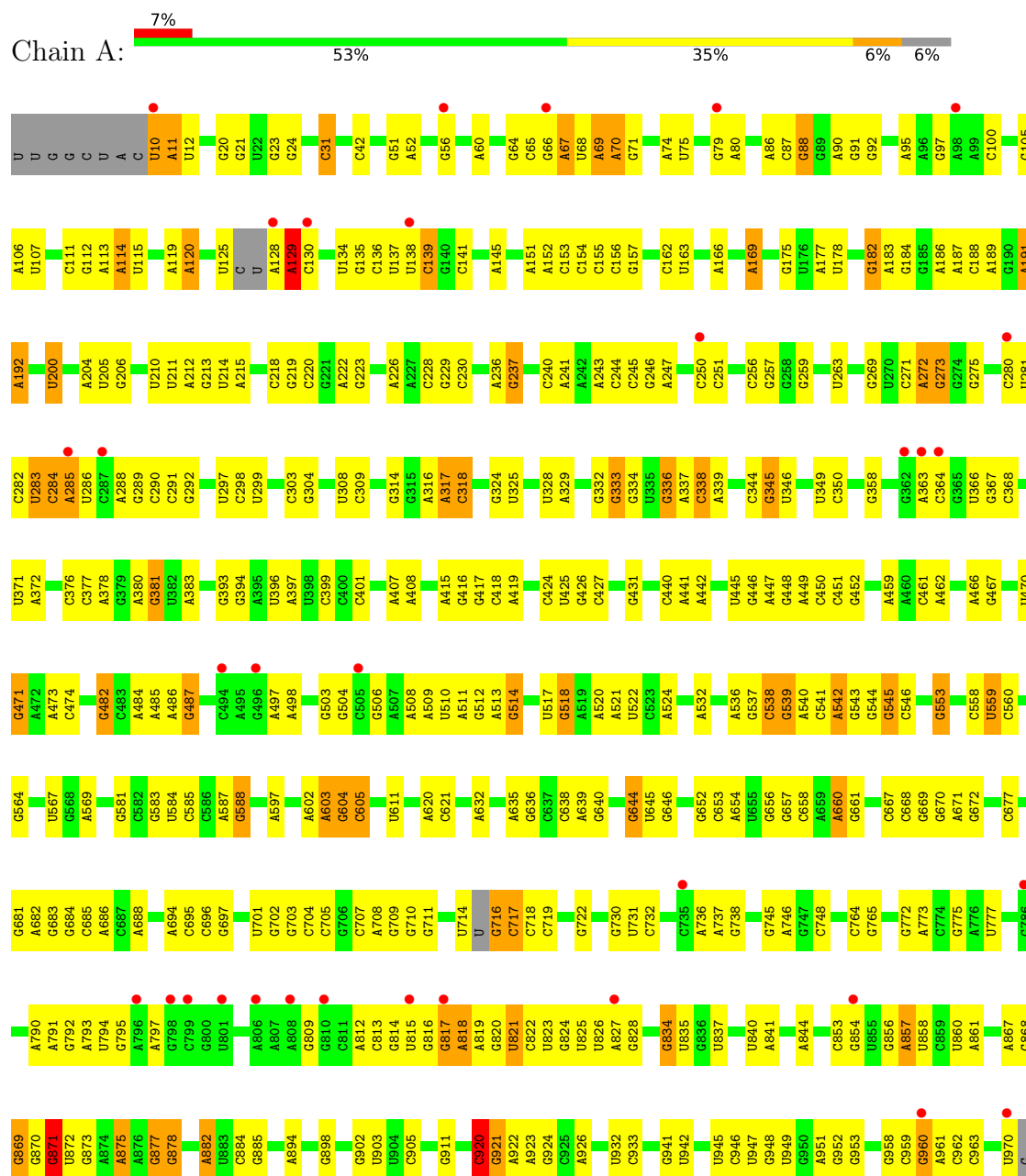
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
38	V	24	Total 24	O 24	0	0
38	W	14	Total 14	O 14	0	0
38	X	71	Total 71	O 71	0	0
38	Y	31	Total 31	O 31	0	0
38	Z	93	Total 93	O 93	0	0
38	1	37	Total 37	O 37	0	0
38	2	63	Total 63	O 63	0	0
38	3	41	Total 41	O 41	0	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.

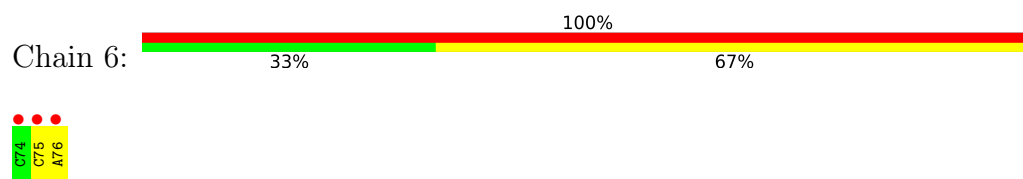
- Molecule 1: 23S ribosomal rna



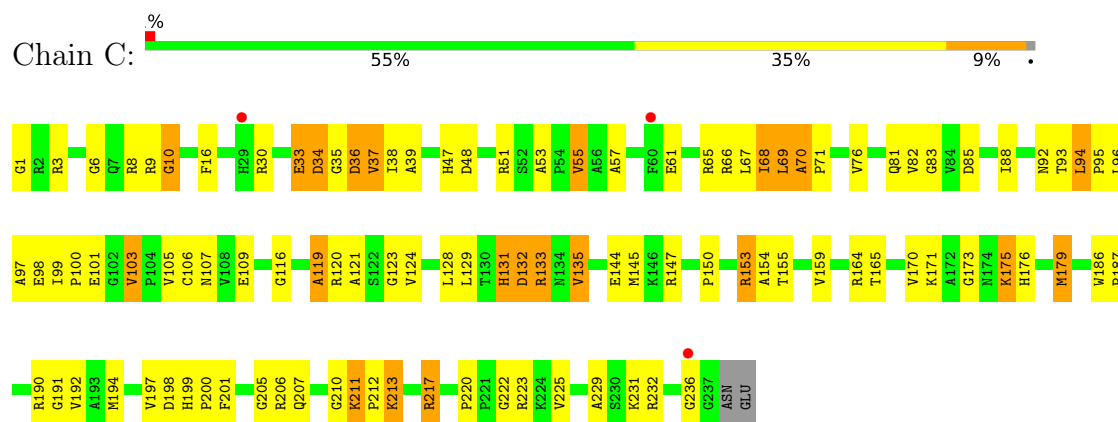
G	U2032	C1940	U1835	U1761	C1675	U1596	G1510	U1435	G1325	G1226	G1160	A1058	U
G	G2033	C1941	A1840	C1762	C1679	A1598	C1513	C1436	A1328	C1229	A1161	G1059	G
U	C2034	A1942	C1841	C1763	C1680	A1599	C1514	G1438	A1329	G1437	G1162	C1060	U
C	C2035	C1943	C1842	C1764	C1681	A1603	U1517	U1439	C1332	A1231	G1163	U1064	C
C	G2044	G1947	A1845	U1766	G1682	G1604	U1518	U1440	U1333	A1232	G1165	G1065	C
C	G2045	C1948	A1846	C1767	G1683	G1605	U1519	G1441	U1334	A1233	G1166	U1066	C
C	G2046	A1949	A1847	C1768	G1684	A1606	U1520	G1442	C1335	U1234	G1167	A1067	C
A	G2050	U1850	A1848	C1769	A1685	A1607	U1521	G1443	C1336	U1235	G1168	G1068	U
U	U2060	U1851	C1856	U1770	A1686	G1610	U1522	G1444	C1337	U1236	U1169	C1069	C
U	U2061	C1857	C1857	C1772	C1687	G1611	A1527	G1445	C1338	U1237	U1170	G1072	C
U	A2054	A1852	A1852	C1773	C1688	G1612	A1528	U1446	C1339	G1238	A1171	G	G
C	U2064	C1853	C1853	U1774	C1689	G1613	A1529	U1447	G1340	G1239	A1172	A	C
C	A2067	G1854	C1854	A1778	C1690	G1614	A1530	G1448	G1341	A1240	A1173	A1078	G
G	G2068	A1855	C1855	A1779	C1691	G1615	U1531	G1449	A1342	C1241	A1174	A1079	A
C	U2069	A1856	C1856	C1780	C1692	A1616	G1532	C1450	A1343	U1242	A1175	C1080	G
C	G2070	A1857	C1857	A1701	C1693	A1617	G1533	C1451	A1344	U1243	A1176	A1081	A
U	U2071	C1858	C1858	U1702	C1694	G1618	G1534	G1452	C1360	U1244	A1177	G	C
U	C2072	C1859	C1859	U1703	C1695	G1619	U1535	G1453	C1361	C1245	A1178	A1086	G
U	C2073	C1860	C1860	U1704	C1696	G1620	U1536	G1454	C1362	A1246	G1179	A1087	U
A	U2078	G1861	C1861	G1785	G1707	G1621	G1537	G1455	C1363	U1249	C1180	A1088	C
G	G2079	C1862	C1862	G1786	C1708	G1622	U1538	G1456	C1364	C1250	A1181	G	G
G	A2081	G1863	C1863	C1787	C1709	G1623	U1539	U1457	A1372	C1251	A1182	A1097	C
U	U2074	C1864	C1864	U1788	C1710	A1624	U1540	A1458	A1373	A1252	G1183	A1098	C
A	U2075	G1865	C1865	G1789	A1711	U1625	G1541	C1462	C1374	C1253	C1184	A1099	A
G	U2076	G1866	C1866	C1790	A1712	A1626	U1542	C1463	C1375	U1254	U1185	G	C
G	G2090	G1867	C1867	C1791	C1713	G1627	U1543	G1464	C1376	C1262	U1186	U1109	A
G	A2082	G1868	C1868	U1792	C1714	G1628	U1544	G1465	C1377	U1263	U1187	G1110	C
C	U2091	G1869	C1869	G1793	C1715	G1629	U1545	C1466	C1378	U1264	A1188	U1003	U
A	G2092	G1870	C1870	G1794	C1716	A1631	U1546	A1470	C1379	U1265	A1189	A1006	A
A	U2093	G1871	C1871	G1795	C1717	A1632	U1547	A1471	C1380	C1266	A1190	A1007	C
C	U2094	G1872	C1872	G1796	C1718	A1633	U1548	A1472	C1381	C1267	A1191	C1008	C
C	A2095	G1873	C1873	G1797	C1719	A1634	U1549	C1473	C1382	U1268	A1192	U1009	C
C	G2096	G1874	C1874	G1798	C1720	A1635	U1550	C1474	C1383	C1269	A1193	G1119	C
A	U2097	G1875	C1875	G1799	C1721	A1636	U1551	C1475	C1384	U1270	A1194	U1120	C
A	G2098	G1876	C1876	G1800	C1722	A1637	U1552	C1476	C1385	A1271	G1195	U1010	C
C	U2099	G1877	C1877	G1801	C1723	A1638	U1553	C1477	C1386	C1272	C1196	A1014	C
C	A2101	G1878	C1878	G1802	C1724	A1639	U1554	C1478	C1387	C1273	G1197	C1015	C
C	G2102	G1879	C1879	G1803	C1725	A1640	U1555	C1479	C1388	A1278	U1198	U1016	C
A	A2103	G1880	C1880	G1804	C1726	A1641	U1556	C1480	C1389	U1279	A1199	A1020	C
G	C2104	G1881	C1881	G1805	C1727	A1642	U1557	C1481	C1390	C1285	C1201	G1127	C
G	U2107	G1882	C1882	G1806	C1728	A1643	U1558	C1482	C1391	U1286	A1202	C1128	C
U	A2108	G1883	C1883	G1807	C1729	A1644	U1559	C1483	C1392	A1287	G1203	U1130	C
C	U2109	G1884	C1884	G1808	C1730	A1645	U1560	C1484	C1393	C1288	A1204	A1132	C
C	G2110	G1885	C1885	G1809	C1731	A1646	U1561	C1485	C1394	U1290	G1205	G1133	C
C	C2111	G1886	C1886	G1810	C1732	A1647	U1562	C1486	C1395	G1293	A1206	U1028	C
G	U2115	G1887	C1887	G1811	C1733	A1648	U1563	C1487	C1396	U1294	C1207	U1029	C
C	U2116	G1888	C1888	G1812	C1734	A1649	U1564	C1488	C1397	U1295	A1208	G1039	C
U	U2117	G1889	C1889	G1813	C1735	A1650	U1565	C1489	C1398	U1296	C1209	G1136	C
U	G2128	G1890	C1890	G1814	C1736	A1651	U1566	C1490	C1399	U1297	G1210	G1137	C
G	U2129	G1891	C1891	G1815	C1737	A1652	U1567	C1491	C1400	U1298	C1211	G1138	C
G	C2130	G1892	C1892	G1816	C1738	A1653	U1568	C1492	C1401	G1299	C1212	C1140	C
C	U2131	G1893	C1893	G1817	C1739	A1654	U1569	C1493	C1402	U1304	C1213	G1151	C
C	G2132	G1894	C1894	G1818	C1740	A1655	U1570	C1494	C1403	C1305	G1214	C1052	C
C	A2133	G1895	C1895	G1819	C1741	A1656	U1571	C1495	C1404	U1306	G1215	G1053	C
C	U2134	G1896	C1896	G1820	C1742	A1657	U1572	C1496	C1405	G1311	G1216	G1054	C
C	G2135	G1897	C1897	G1821	C1743	A1658	U1573	C1497	C1406	G1312	G1217	U1056	C
C	U2136	G1898	C1898	G1822	C1744	A1659	U1574	C1498	C1407	G1313	G1218	U1057	C
C	A2137	G1899	C1899	G1823	C1745	A1660	U1575	C1499	C1408	U1307	C1219	G1152	C
C	U2138	G1900	C1900	G1824	C1746	A1661	U1576	C1500	C1409	U1308	C1220	G1153	C
C	G2139	G1901	C1901	G1825	C1747	A1662	U1577	C1501	C1410	U1309	C1221	G1154	C
C	U2140	G1902	C1902	G1826	C1748	A1663	U1578	C1502	C1411	U1310	C1222	G1155	C
C	A2141	G1903	C1903	G1827	C1749	A1664	U1579	C1503	C1412	G1315	G1223	U1058	C
C	U2142	G1904	C1904	G1828	C1750	A1665	U1580	C1504	C1413	U1316	G1224	U1059	C
C	U2143	G1905	C1905	G1829	C1751	A1666	U1581	C1505	C1414	U1317	G1225	U1060	C
C	U2144	G1906	C1906	G1830	C1752	A1667	U1582	C1506	C1415	U1318	G1226	U1061	C
C	A2145	G1907	C1907	G1831	C1753	A1668	U1583	C1507	C1416	U1319	G1227	U1062	C
C	U2146	G1908	C1908	G1832	C1754	A1669	U1584	C1508	C1417	U1320	G1228	U1063	C
C	U2147	G1909	C1909	G1833	C1755	A1670	U1585	C1509	C1418	U1321	G1229	U1064	C
C	U2148	G1910	C1910	G1834	C1756	A1671	U1586	C1510	C1419	U1322	G1230	U1065	C
C	U2149	G1911	C1911	G1835	C1757	A1672	U1587	C1511	C1420	U1323	G1231	U1066	C
C	U2150	G1912	C1912	G1836	C1758	A1673	U1588	C1512	C1421	U1324	G1232	U1067	C
C	U2151	G1913	C1913	G1837	C1759	A1674	U1589	C1513	C1422	U1325	G1233	U1068	C
C	U2152	G1914	C1914	G1838	C1760	A1675	U1590	C1514	C1423	U1326	G1234	U1069	C
C	U2153	G1915	C1915	G1839	C1761	A1676	U1591	C1515	C1424	U1327	G1235	U1070	C
C	U2154	G1916	C1916	G1840	C1762	A1677	U1592	C1516	C1425	U1328	G1236	U1071	C
C	U2155	G1917	C1917	G1841	C1763	A1678	U1593	C1517	C1426	U1329	G1237	U1072	C
C	U2156	G1918	C1918	G1842	C1764	A1679	U1594	C1518	C1427	U1330	G1238	U1073	C
C	U2157	G1919	C1919	G1843	C1765	A1680	U1595	C1519	C1428	U1331	G1239	U1074	C
C	U2158	G1920	C1920	G1844	C1766	A1681	U1596	C1520	C1429	U1332	G1240	U1075	C
C	U2159	G1921	C1921	G1845	C1767	A1682	U1597	C1521	C1430	U1333	G1241	U1076	C
C	U2160	G1922	C1922	G1846	C1768	A1683	U1598	C1522	C1431	U1334	G1242	U1077	C
C	U2161	G1923	C1923	G1847	C1769	A1684	U1599	C1523	C1432	U1335	G1243	U1078	C
C	U2162	G1924	C1924	G1848	C1770	A1685	U1600	C1524	C1433	U1336	G1244	U1079	C
C	U2163	G1925	C1925	G1849	C1771	A1686	U1601	C1525	C1434	U1337	G1245	U1080	C
C	U2164	G1926	C1926	G1850	C1772	A1687	U1602	C1526	C1435	U1338	G1246	U1081	C
C	U2165	G1927	C1927	G1851	C1773	A1688	U1603	C1527	C1436	U1339	G1247	U1082	C
C	U2166	G1928	C1928	G1852	C1774	A1689	U1604	C1528	C1437	U1340	G1248	U1083	C
C	U2167	G1929	C1929	G1853	C1775	A1690	U1605	C1529	C1438	U1341	G1249	U1084	C
C	U2168	G1930	C1930	G1854	C1776	A1691	U1606	C1530	C1439	U1342	G1250	U1085	C
C	U2169	G1931	C1931	G1855	C1777	A1692	U1607	C1531	C1440	U1343	G1251	U1086	C
C	U2170	G1932	C1932	G1856	C1778	A1693	U1608	C1532	C1441	U1344	G1252	U1087	C
C	U2171	G1933	C1933	G1857	C1779	A1694	U1609	C1533	C1442	U1345	G1253	U1088	C
C	U2172	G1934	C1934	G1858	C1780	A1695	U1610	C1534	C1443	U1346	G1254	U1089	C
C	U2173	G1935	C1935	G1859	C1781	A1696	U1611	C1535	C1444	U1347	G1255	U1090	C
C	U2174	G1936	C1936	G1860	C1782	A1697	U1612	C1536	C1445	U1348	G1256	U1091	C
C	U2175	G1937	C1937	G1861	C1783	A1698	U1613	C1537	C1446	U1349	G1257	U1092	C
C	U2176	G1938	C1938	G1862	C1784	A1699	U161						



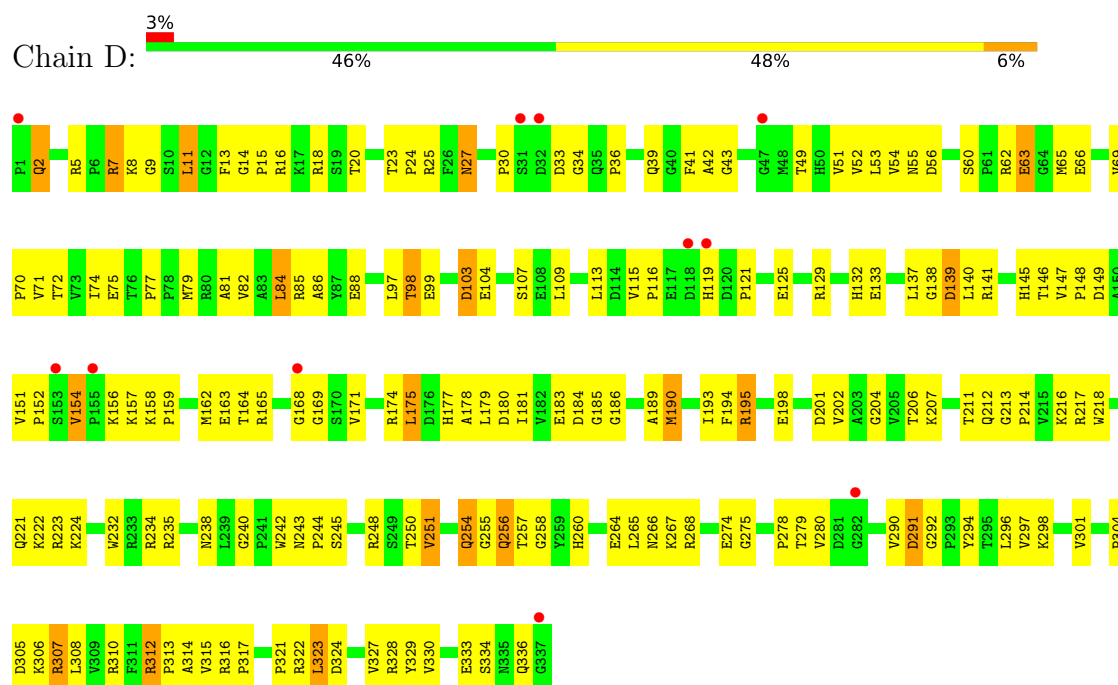
- Molecule 3: CCA-phenylalanine-cariotic-acid-biotin



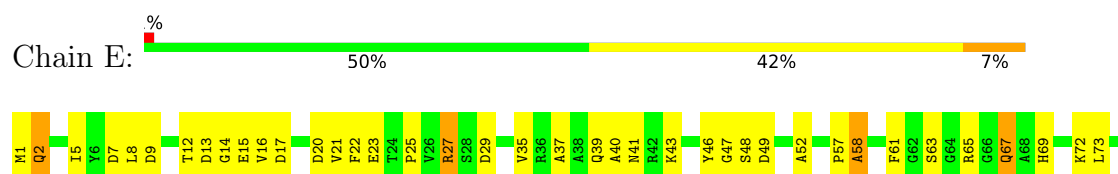
- Molecule 4: 50S ribosomal protein L2P

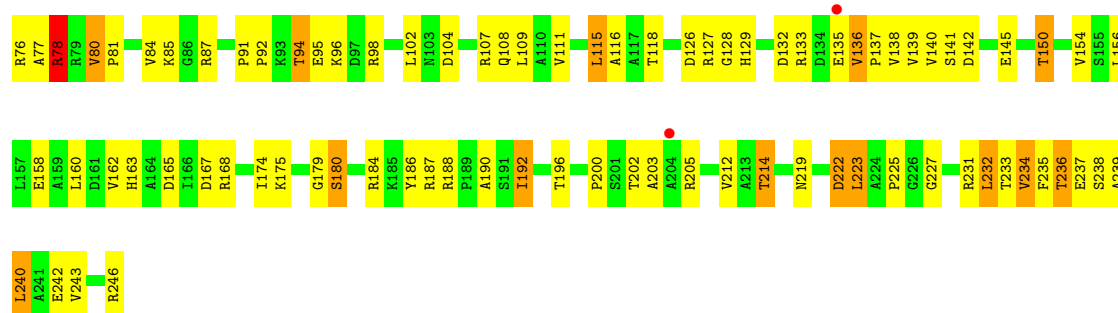


- Molecule 5: 50S ribosomal protein L3P

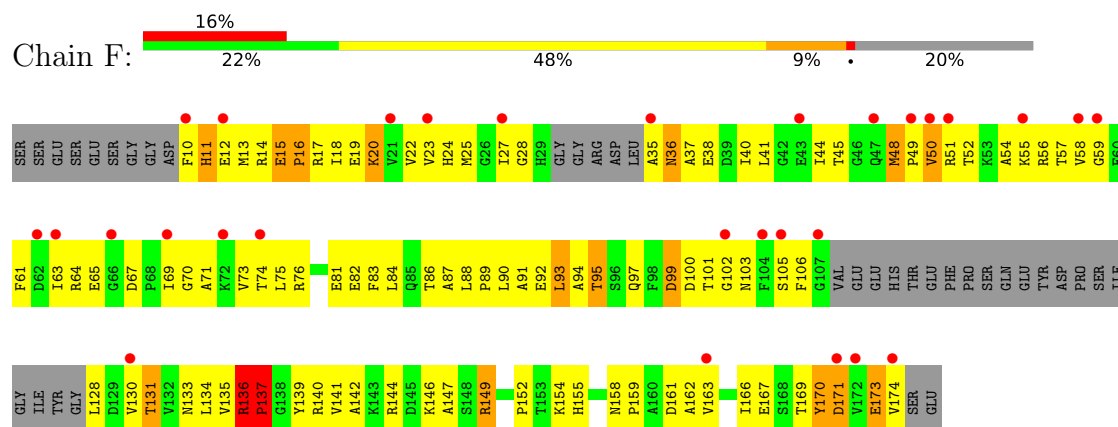


- Molecule 6: 50S ribosomal protein L4E

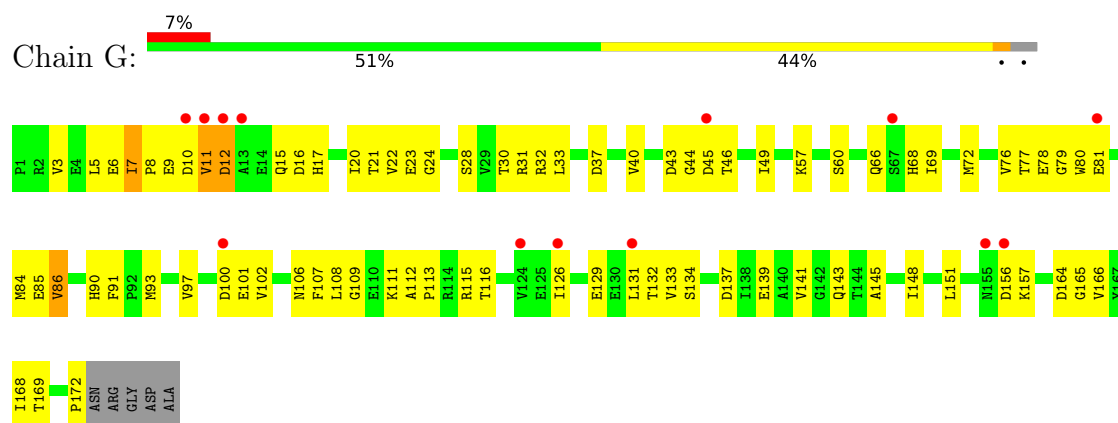




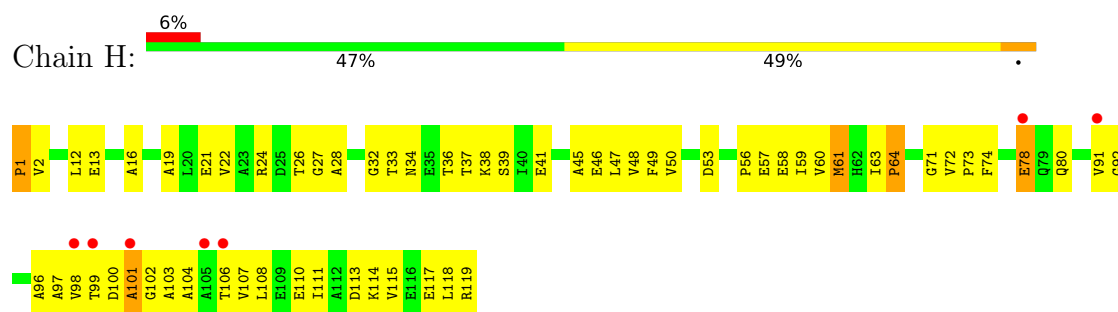
• Molecule 7: 50S ribosomal protein L5P



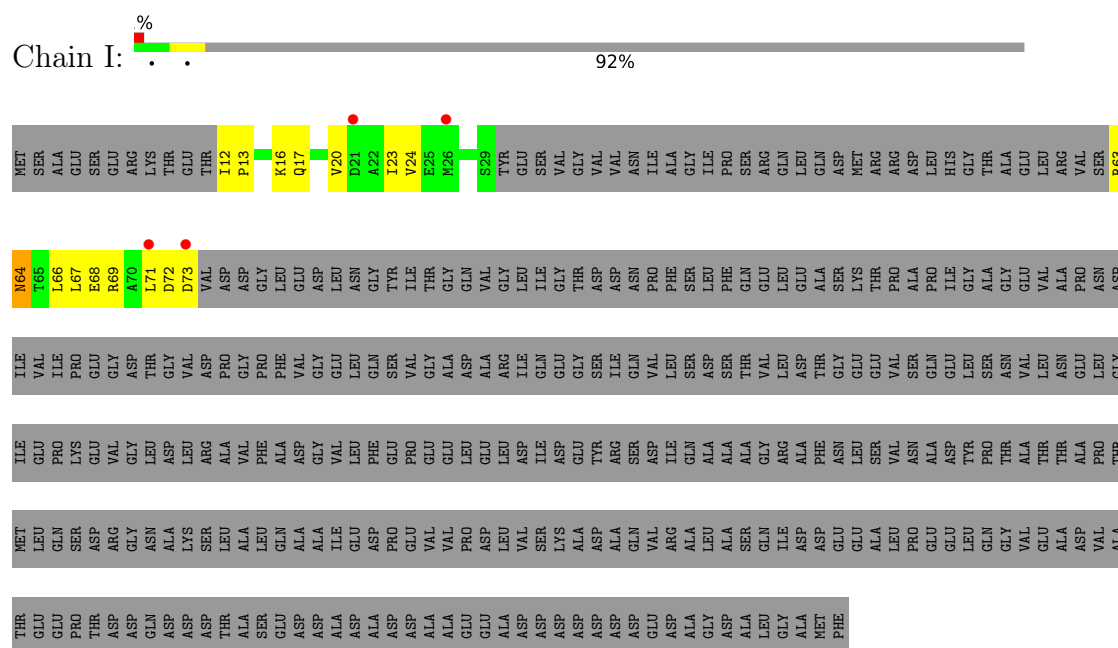
• Molecule 8: 50S ribosomal protein L6P



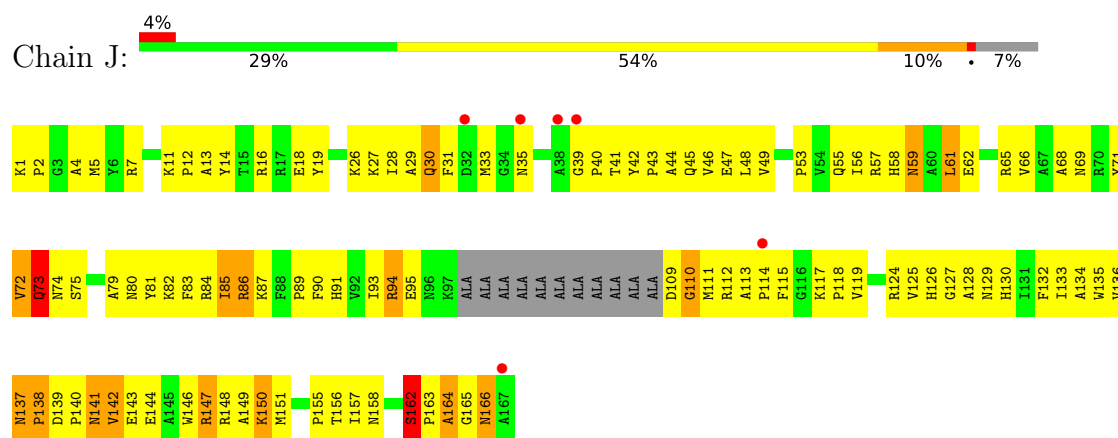
• Molecule 9: 50S ribosomal protein L7Ae



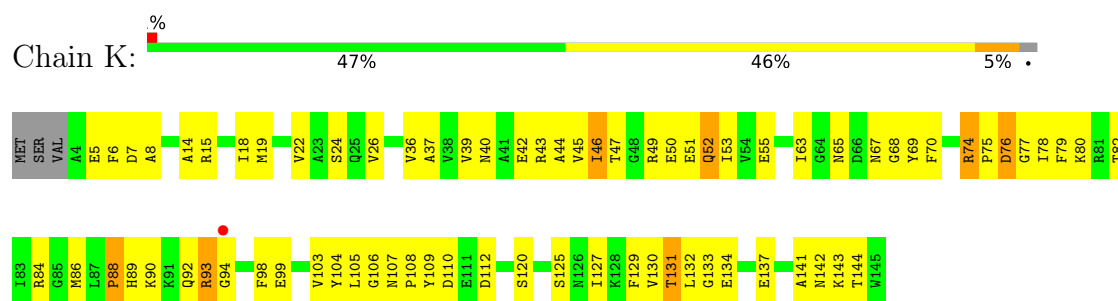
• Molecule 10: Acidic ribosomal protein P0 homolog



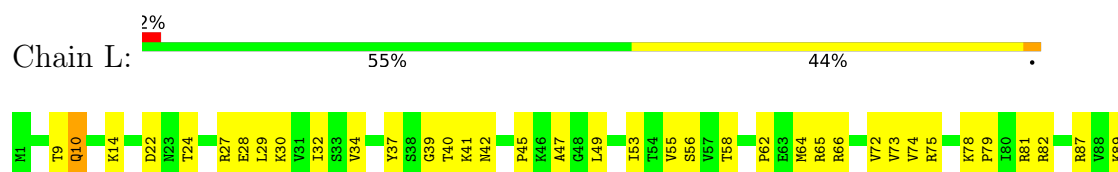
- Molecule 11: L10 Ribosomal Protein



- Molecule 12: 50S ribosomal protein L13P

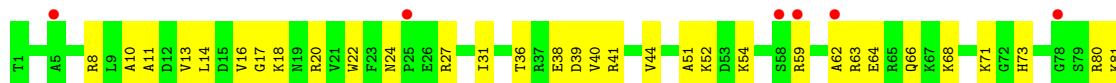


- Molecule 13: 50S ribosomal protein L14P





• Molecule 18: 50S ribosomal protein L19E



• Molecule 19: 50S ribosomal protein L21e



• Molecule 20: 50S ribosomal protein L22P

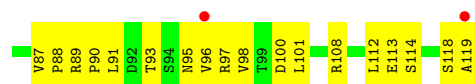


• Molecule 21: 50S ribosomal protein L23P



• Molecule 22: 50S ribosomal protein L24P

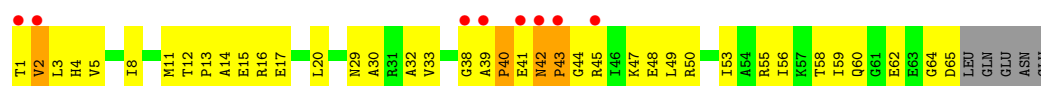




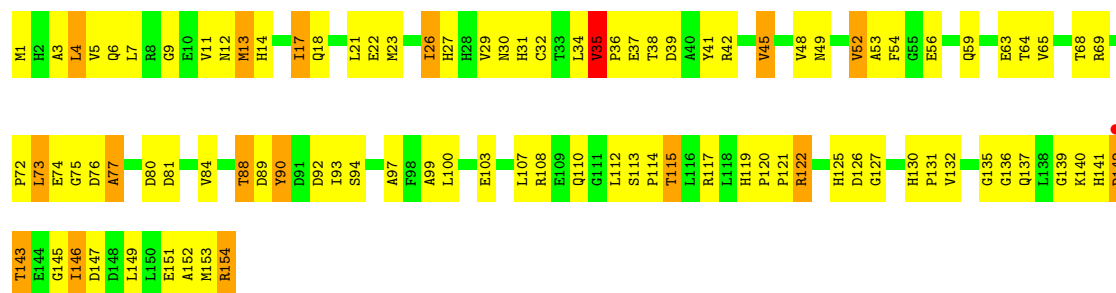
- Molecule 23: 50S ribosomal protein L24E



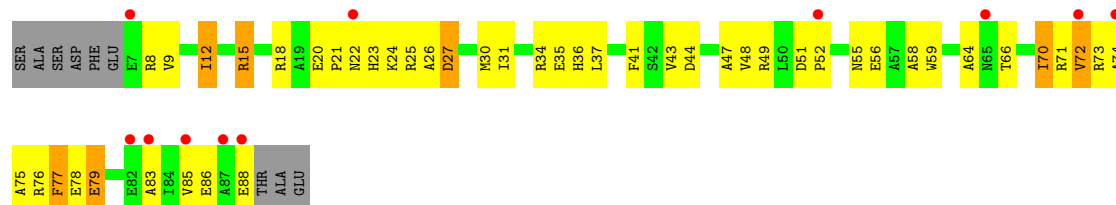
- Molecule 24: 50S ribosomal protein L29P



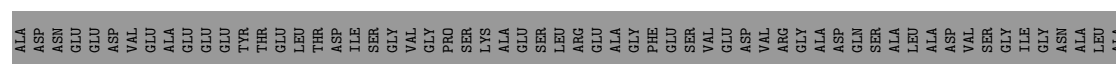
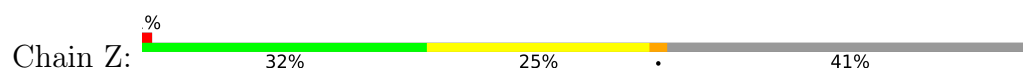
- Molecule 25: 50S ribosomal protein L30P

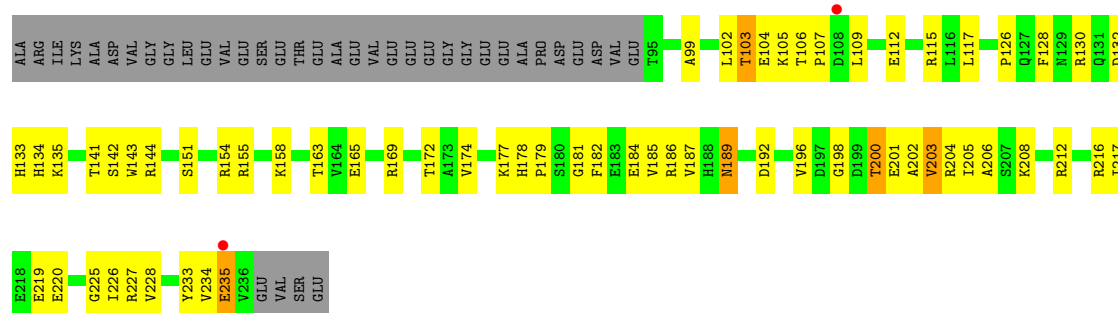


- Molecule 26: 50S ribosomal protein L31e

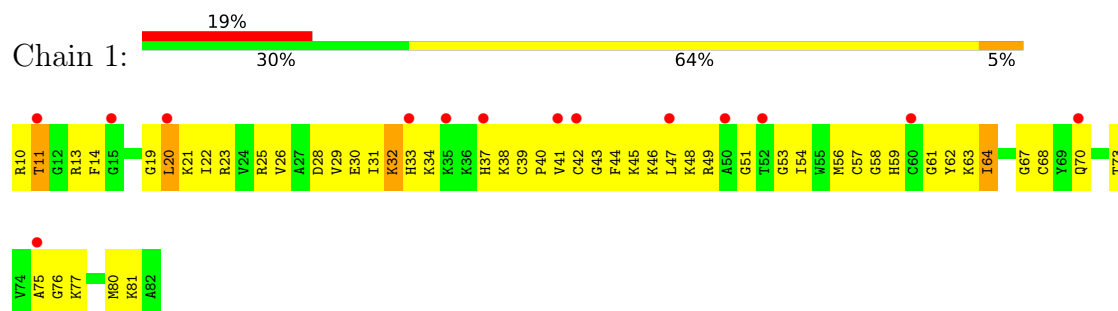


- Molecule 27: 50S ribosomal protein L32E

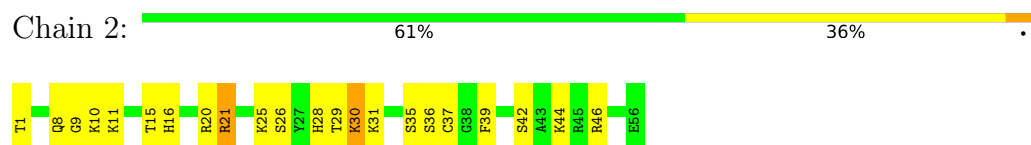




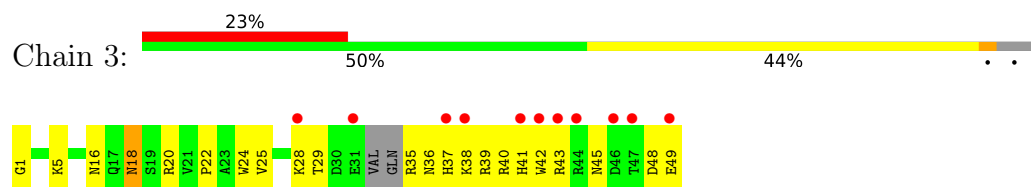
• Molecule 28: L37Ae 50S ribosomal protein



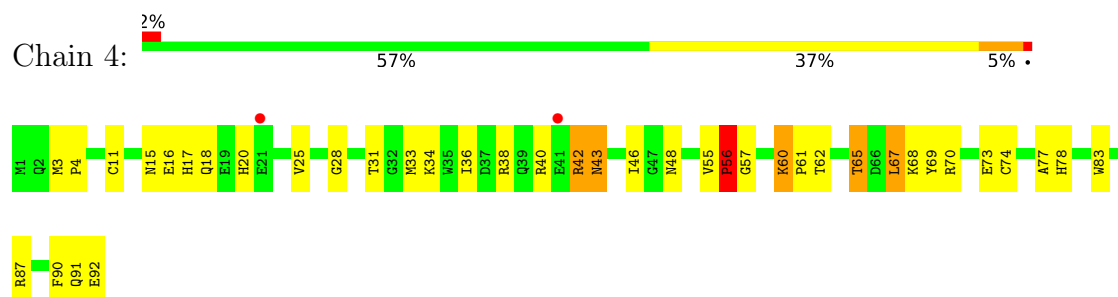
• Molecule 29: 50S ribosomal protein L37e



• 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 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-3.00) 95.3 (20.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.264 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 71.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	98659	wwPDB-VP
Average B, all atoms (Å ²)	53.0	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: CL, NA, CD, PHA, 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	0.40	0/66076	0.63	32/103052 (0.0%)
2	B	0.38	0/2905	0.70	6/4528 (0.1%)
3	5	0.65	0/65	1.05	0/99
3	6	1.57	1/65 (1.5%)	1.36	1/99 (1.0%)
4	C	0.43	0/1787	1.02	7/2409 (0.3%)
5	D	0.43	0/2689	1.00	16/3652 (0.4%)
6	E	0.48	0/1883	1.01	9/2551 (0.4%)
7	F	0.38	0/1111	0.96	7/1498 (0.5%)
8	G	0.40	0/1382	0.91	1/1880 (0.1%)
9	H	0.38	0/896	0.91	2/1219 (0.2%)
10	I	0.42	0/241	0.82	0/324
11	J	0.50	0/1246	1.27	13/1686 (0.8%)
12	K	0.46	0/1135	0.94	5/1530 (0.3%)
13	L	0.43	0/1003	1.02	0/1351
14	M	0.38	0/1126	1.00	5/1504 (0.3%)
15	N	0.48	0/1633	1.04	9/2180 (0.4%)
16	O	0.38	0/1473	1.06	12/1999 (0.6%)
17	P	0.45	0/873	0.94	3/1181 (0.3%)
18	Q	0.43	0/1143	0.87	2/1521 (0.1%)
19	R	0.46	0/748	1.06	6/1005 (0.6%)
20	S	0.47	0/1172	0.98	4/1578 (0.3%)
21	T	0.39	0/648	0.92	2/875 (0.2%)
22	U	0.40	0/957	0.98	5/1289 (0.4%)
23	V	0.41	0/417	0.92	1/562 (0.2%)
24	W	0.36	0/502	1.01	3/675 (0.4%)
25	X	0.49	0/1218	1.04	7/1655 (0.4%)
26	Y	0.46	0/664	0.97	2/895 (0.2%)
27	Z	0.45	0/1146	0.97	2/1536 (0.1%)
28	1	0.46	0/575	0.97	1/763 (0.1%)
29	2	0.44	0/437	0.93	2/578 (0.3%)
30	3	0.36	0/398	0.77	0/527
31	4	0.45	0/771	0.95	5/1024 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	1/98385 (0.0%)	0.75	170/147225 (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	2	50
2	B	1	3
3	6	0	1
25	X	0	1
All	All	3	55

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	75	C	O5'-C5'	7.55	1.53	1.42

The worst 5 of 170 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	J	74	ASN	N-CA-C	-15.05	92.57	114.39
1	A	1563	G	C2'-C3'-O3'	13.82	130.23	109.50
2	B	3024	U	C2'-C3'-O3'	13.45	129.68	109.50
11	J	141	ASN	N-CA-C	-12.69	97.49	113.23
15	N	141	ILE	N-CA-C	-12.19	101.88	112.12

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1563	G	C3'
1	A	2616	G	C3'
2	B	3024	U	C3'

5 of 55 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	182	G	Sidechain
1	A	333	G	Sidechain
1	A	471	G	Sidechain

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Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	482	G	Sidechain
1	A	518	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	1079	0
2	B	2600	0	1326	85	0
3	5	59	0	34	1	0
3	6	59	0	34	0	0
4	C	1754	0	1763	119	0
5	D	2624	0	2533	191	0
6	E	1858	0	1816	137	0
7	F	1094	0	1085	149	0
8	G	1357	0	1266	81	0
9	H	885	0	854	75	0
10	I	240	0	231	24	0
11	J	1215	0	1215	179	0
12	K	1119	0	1098	77	0
13	L	993	0	1027	77	0
14	M	1114	0	1072	73	0
15	N	1605	0	1676	193	0
16	O	1444	0	1401	133	0
17	P	864	0	873	57	0
18	Q	1133	0	1127	64	0
19	R	734	0	729	27	0
20	S	1149	0	1122	66	0
21	T	641	0	605	32	0
22	U	949	0	923	64	0
23	V	410	0	364	37	0
24	W	499	0	511	37	0
25	X	1195	0	1137	122	0
26	Y	654	0	653	52	0
27	Z	1130	0	1133	70	0
28	1	563	0	597	66	0
29	2	430	0	426	29	0
30	3	393	0	406	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	4	755	0	728	39	0
32	1	1	0	0	0	0
32	4	1	0	0	0	0
32	6	1	0	0	0	0
32	A	108	0	0	0	0
32	B	1	0	0	0	0
32	C	1	0	0	0	0
32	D	2	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	2	0	0	0	0
34	A	70	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	2	0	0	0	0
34	R	1	0	0	0	0
34	S	3	0	0	0	0
34	T	1	0	0	0	0
34	U	1	0	0	0	0
35	4	1	0	0	0	0
35	A	9	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	L	1	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	11	0	10	0	0
36	6	10	0	7	0	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	V	1	0	0	0	0
38	1	37	0	0	13	0
38	2	63	0	0	5	0
38	3	41	0	0	5	0
38	4	70	0	0	10	0
38	A	5892	0	0	227	0
38	B	139	0	0	14	0
38	C	116	0	0	13	0
38	D	149	0	0	30	0
38	E	173	0	0	37	0
38	F	52	0	0	23	0
38	G	43	0	0	12	0
38	H	27	0	0	11	0
38	I	21	0	0	6	0
38	J	77	0	0	23	0
38	K	54	0	0	5	0
38	L	62	0	0	12	0
38	M	82	0	0	18	0
38	N	139	0	0	24	0
38	O	70	0	0	17	0
38	P	43	0	0	14	0
38	Q	67	0	0	5	0
38	R	54	0	0	5	0
38	S	84	0	0	6	0
38	T	37	0	0	6	0
38	U	44	0	0	8	0
38	V	24	0	0	5	0
38	W	14	0	0	3	0
38	X	71	0	0	15	0
38	Y	31	0	0	5	0
38	Z	93	0	0	13	0
All	All	98659	0	59587	3187	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 21.

The worst 5 of 3187 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	1.05	1.18
11:J:45:GLN:HB3	11:J:163:PRO:HD2	1.31	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:86:ARG:NH1	11:J:133:ILE:HG13	1.64	1.11
1:A:1119:G:H2'	12:K:52:GLN:HE22	1.10	1.10
20:S:99:ALA:HB1	20:S:109:MET:HE1	1.27	1.10

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	27 (12%)	6 (3%)	4	23
5	D	335/337 (99%)	291 (87%)	36 (11%)	8 (2%)	4	24
6	E	244/246 (99%)	210 (86%)	31 (13%)	3 (1%)	10	40
7	F	134/176 (76%)	95 (71%)	28 (21%)	11 (8%)	0	3
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	21	56
9	H	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	3	17
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	2	14
11	J	152/167 (91%)	129 (85%)	18 (12%)	5 (3%)	3	17
12	K	140/145 (97%)	126 (90%)	8 (6%)	6 (4%)	2	12
13	L	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	8	35
14	M	141/164 (86%)	117 (83%)	22 (16%)	2 (1%)	9	36
15	N	192/194 (99%)	164 (85%)	25 (13%)	3 (2%)	7	34
16	O	184/186 (99%)	160 (87%)	17 (9%)	7 (4%)	2	15
17	P	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
18	Q	141/148 (95%)	132 (94%)	8 (6%)	1 (1%)	18	53
19	R	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	11	43
20	S	148/154 (96%)	134 (90%)	14 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	T	79/84 (94%)	71 (90%)	8 (10%)	0	100	100
22	U	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	7	32
23	V	51/66 (77%)	44 (86%)	6 (12%)	1 (2%)	6	28
24	W	63/70 (90%)	55 (87%)	5 (8%)	3 (5%)	2	11
25	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	9	38
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	4	23
27	Z	140/240 (58%)	135 (96%)	5 (4%)	0	100	100
28	1	71/73 (97%)	59 (83%)	10 (14%)	2 (3%)	4	21
29	2	54/56 (96%)	51 (94%)	3 (6%)	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	26
All	All	3633/4235 (86%)	3206 (88%)	352 (10%)	75 (2%)	5	27

5 of 75 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	D	139	ASP
5	D	184	ASP
6	E	8	LEU
7	F	93	LEU
7	F	95	THR

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	46
5	D	282/282 (100%)	264 (94%)	18 (6%)	16	48
6	E	193/193 (100%)	177 (92%)	16 (8%)	10	37
7	F	117/147 (80%)	109 (93%)	8 (7%)	14	45
8	G	152/155 (98%)	148 (97%)	4 (3%)	40	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	H	92/92 (100%)	89 (97%)	3 (3%)	33	67
10	I	27/283 (10%)	26 (96%)	1 (4%)	30	64
11	J	122/122 (100%)	109 (89%)	13 (11%)	6	26
12	K	118/121 (98%)	109 (92%)	9 (8%)	12	41
13	L	106/106 (100%)	104 (98%)	2 (2%)	50	76
14	M	112/126 (89%)	110 (98%)	2 (2%)	51	77
15	N	166/166 (100%)	159 (96%)	7 (4%)	26	61
16	O	149/149 (100%)	142 (95%)	7 (5%)	23	58
17	P	93/93 (100%)	91 (98%)	2 (2%)	45	74
18	Q	113/116 (97%)	109 (96%)	4 (4%)	32	65
19	R	79/79 (100%)	75 (95%)	4 (5%)	21	55
20	S	117/121 (97%)	113 (97%)	4 (3%)	32	66
21	T	71/73 (97%)	70 (99%)	1 (1%)	59	80
22	U	105/105 (100%)	100 (95%)	5 (5%)	23	57
23	V	44/52 (85%)	43 (98%)	1 (2%)	44	74
24	W	51/56 (91%)	50 (98%)	1 (2%)	48	76
25	X	130/130 (100%)	118 (91%)	12 (9%)	8	33
26	Y	66/73 (90%)	61 (92%)	5 (8%)	12	41
27	Z	120/195 (62%)	113 (94%)	7 (6%)	18	51
28	1	56/56 (100%)	54 (96%)	2 (4%)	31	65
29	2	46/46 (100%)	46 (100%)	0	100	100
30	3	42/44 (96%)	41 (98%)	1 (2%)	43	73
31	4	79/79 (100%)	76 (96%)	3 (4%)	29	63
All	All	3027/3441 (88%)	2873 (95%)	154 (5%)	21	55

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

Mol	Chain	Res	Type
20	S	143	VAL
27	Z	172	THR
22	U	39	ASN
25	X	73	LEU
30	3	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 113 such sidechains are listed below:

Mol	Chain	Res	Type
16	O	93	GLN
31	4	30	GLN
20	S	98	ASN
31	4	18	GLN
28	1	37	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	248 (9%)	32 (1%)
2	B	121/122 (99%)	16 (13%)	3 (2%)
3	5	2/3 (66%)	1 (50%)	0
3	6	2/3 (66%)	0	0
All	All	2872/3050 (94%)	265 (9%)	35 (1%)

5 of 265 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 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2616	G
1	A	2649	A
2	B	3024	U
1	A	1080	C
1	A	898	G

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 235 ligands modelled in this entry, 233 are monoatomic - leaving 2 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	PHA	6	77	3	9,10,11	0.69	0	11,11,13	0.46	0
36	PHA	5	77	3	10,11,11	0.90	0	8,13,13	1.00	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	PHA	6	77	3	-	2/4/4/6	0/1/1/1
36	PHA	5	77	3	-	3/5/6/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	6	77	PHA	O-C-CA-CB
36	5	77	PHA	CA-CB-CG-CD2
36	5	77	PHA	CA-CB-CG-CD1
36	6	77	PHA	C-CA-CB-CG
36	5	77	PHA	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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%)	0.81	218 (7%) 18 10	19, 47, 95, 154	0
2	B	122/122 (100%)	0.51	6 (4%) 35 18	30, 62, 92, 154	0
3	5	3/3 (100%)	4.72	3 (100%) 0 0	14, 14, 16, 17	3 (100%)
3	6	3/3 (100%)	3.65	3 (100%) 0 0	8, 8, 9, 15	3 (100%)
4	C	237/239 (99%)	0.76	3 (1%) 75 53	27, 52, 91, 115	0
5	D	337/337 (100%)	0.80	11 (3%) 49 28	26, 55, 84, 96	0
6	E	246/246 (100%)	0.33	2 (0%) 82 64	19, 47, 71, 80	0
7	F	140/176 (79%)	1.27	29 (20%) 2 2	53, 101, 124, 131	0
8	G	172/177 (97%)	0.73	13 (7%) 20 10	41, 68, 91, 99	0
9	H	119/119 (100%)	0.96	7 (5%) 28 14	53, 77, 104, 111	0
10	I	29/348 (8%)	1.04	4 (13%) 6 4	66, 86, 97, 103	0
11	J	156/167 (93%)	0.41	6 (3%) 44 24	30, 52, 77, 81	0
12	K	142/145 (97%)	0.37	1 (0%) 84 66	34, 47, 71, 90	0
13	L	132/132 (100%)	0.78	2 (1%) 72 49	31, 53, 78, 86	0
14	M	145/164 (88%)	0.55	5 (3%) 48 27	21, 67, 108, 116	0
15	N	194/194 (100%)	0.53	8 (4%) 41 23	30, 47, 68, 80	0
16	O	186/186 (100%)	0.64	14 (7%) 20 10	35, 65, 112, 125	0
17	P	115/115 (100%)	0.42	1 (0%) 81 61	36, 54, 74, 83	0
18	Q	143/148 (96%)	1.14	16 (11%) 10 6	36, 57, 71, 80	0
19	R	95/95 (100%)	0.10	0 100 100	32, 42, 57, 73	0
20	S	150/154 (97%)	0.55	2 (1%) 75 53	29, 43, 64, 75	0
21	T	81/84 (96%)	0.98	5 (6%) 26 14	41, 62, 81, 85	0
22	U	119/119 (100%)	0.73	5 (4%) 40 22	38, 60, 86, 105	0
23	V	53/66 (80%)	1.12	5 (9%) 14 7	42, 53, 71, 80	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
24	W	65/70 (92%)	1.25	8 (12%) 8 5	56, 79, 120, 125	0
25	X	154/154 (100%)	0.04	1 (0%) 85 69	29, 45, 62, 74	0
26	Y	82/91 (90%)	1.12	11 (13%) 7 4	42, 56, 79, 100	0
27	Z	142/240 (59%)	0.28	2 (1%) 73 51	25, 45, 67, 86	0
28	1	73/73 (100%)	1.32	14 (19%) 3 2	43, 61, 76, 81	0
29	2	56/56 (100%)	0.40	0 100 100	24, 33, 39, 41	0
30	3	46/48 (95%)	1.26	11 (23%) 2 1	34, 65, 118, 126	0
31	4	92/92 (100%)	0.48	2 (2%) 62 39	39, 55, 69, 78	0
All	All	6583/7285 (90%)	0.73	418 (6%) 26 13	8, 52, 97, 154	6 (0%)

The worst 5 of 418 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	11.1
5	D	1	PRO	6.4
3	5	74	C	5.6
2	B	3025	G	5.2
1	A	1173	A	5.2

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	A	8329	1/1	0.34	0.17	65,65,65,65	0
34	NA	B	8351	1/1	0.47	0.24	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8315	1/1	0.49	0.21	29,29,29,29	0
32	MG	A	8041	1/1	0.51	0.17	79,79,79,79	0
34	NA	A	8384	1/1	0.52	0.32	101,101,101,101	0
34	NA	A	8366	1/1	0.52	0.24	51,51,51,51	0
32	MG	6	8118	1/1	0.53	0.29	61,61,61,61	0
34	NA	T	8312	1/1	0.56	0.20	108,108,108,108	0
34	NA	A	8344	1/1	0.59	0.04	17,17,17,17	0
34	NA	S	8386	1/1	0.60	0.22	63,63,63,63	0
36	PHA	5	77	11/11	0.61	0.38	24,25,29,29	11
34	NA	A	8354	1/1	0.63	0.20	31,31,31,31	0
34	NA	A	8340	1/1	0.64	0.18	38,38,38,38	0
34	NA	A	8328	1/1	0.67	0.27	54,54,54,54	0
36	PHA	6	77	10/11	0.67	0.40	35,38,41,41	10
32	MG	A	8044	1/1	0.70	0.13	50,50,50,50	0
34	NA	A	8385	1/1	0.71	0.14	43,43,43,43	0
32	MG	A	8046	1/1	0.71	0.15	45,45,45,45	0
34	NA	A	8359	1/1	0.71	0.43	48,48,48,48	0
32	MG	A	8116	1/1	0.72	0.13	67,67,67,67	0
34	NA	A	8350	1/1	0.72	0.22	36,36,36,36	0
34	NA	A	8310	1/1	0.72	0.14	33,33,33,33	0
34	NA	A	8367	1/1	0.76	0.16	48,48,48,48	0
34	NA	A	8377	1/1	0.76	0.30	76,76,76,76	0
34	NA	A	8361	1/1	0.76	0.18	48,48,48,48	0
34	NA	A	8330	1/1	0.77	0.11	42,42,42,42	0
34	NA	A	8336	1/1	0.77	0.10	41,41,41,41	0
34	NA	A	8324	1/1	0.77	0.46	58,58,58,58	0
32	MG	A	8092	1/1	0.78	0.20	92,92,92,92	0
34	NA	A	8356	1/1	0.78	0.34	44,44,44,44	0
34	NA	A	8307	1/1	0.78	0.17	53,53,53,53	0
34	NA	A	8375	1/1	0.78	0.50	63,63,63,63	0
34	NA	A	8302	1/1	0.79	0.16	39,39,39,39	0
32	MG	A	8111	1/1	0.79	0.14	67,67,67,67	0
34	NA	A	8373	1/1	0.79	0.19	45,45,45,45	0
34	NA	A	8363	1/1	0.79	0.17	46,46,46,46	0
35	CL	A	8514	1/1	0.80	0.17	55,55,55,55	0
32	MG	A	8024	1/1	0.80	0.37	95,95,95,95	0
34	NA	K	8346	1/1	0.80	0.10	33,33,33,33	0
32	MG	A	8089	1/1	0.81	0.15	60,60,60,60	0
32	MG	A	8067	1/1	0.81	0.18	55,55,55,55	0
32	MG	A	8117	1/1	0.82	0.11	26,26,26,26	0
32	MG	A	8049	1/1	0.82	0.10	67,67,67,67	0
34	NA	S	8337	1/1	0.82	0.10	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8357	1/1	0.82	0.16	53,53,53,53	0
34	NA	A	8316	1/1	0.82	0.18	30,30,30,30	0
34	NA	A	8360	1/1	0.82	0.26	45,45,45,45	0
34	NA	A	8320	1/1	0.82	0.16	24,24,24,24	0
34	NA	A	8353	1/1	0.82	0.07	26,26,26,26	0
35	CL	K	8502	1/1	0.83	0.08	62,62,62,62	0
32	MG	A	8082	1/1	0.83	0.16	51,51,51,51	0
34	NA	A	8327	1/1	0.83	0.13	34,34,34,34	0
34	NA	A	8370	1/1	0.84	0.20	50,50,50,50	0
34	NA	A	8382	1/1	0.84	0.21	54,54,54,54	0
34	NA	N	8365	1/1	0.84	0.27	46,46,46,46	0
32	MG	Z	8109	1/1	0.84	0.06	28,28,28,28	0
34	NA	A	8368	1/1	0.84	0.30	69,69,69,69	0
34	NA	S	8338	1/1	0.85	0.11	48,48,48,48	0
34	NA	A	8313	1/1	0.85	0.09	44,44,44,44	0
34	NA	A	8371	1/1	0.85	0.51	62,62,62,62	0
35	CL	A	8511	1/1	0.85	0.14	65,65,65,65	0
32	MG	A	8070	1/1	0.85	0.19	36,36,36,36	0
32	MG	A	8045	1/1	0.85	0.12	52,52,52,52	0
35	CL	L	8512	1/1	0.85	0.15	47,47,47,47	0
34	NA	A	8311	1/1	0.85	0.15	52,52,52,52	0
34	NA	A	8369	1/1	0.85	0.28	59,59,59,59	0
34	NA	A	8372	1/1	0.86	0.19	55,55,55,55	0
34	NA	A	8308	1/1	0.86	0.23	49,49,49,49	0
32	MG	A	8050	1/1	0.86	0.11	65,65,65,65	0
32	MG	A	8075	1/1	0.86	0.14	64,64,64,64	0
34	NA	A	8317	1/1	0.86	0.10	63,63,63,63	0
35	CL	A	8513	1/1	0.87	0.12	50,50,50,50	0
32	MG	A	8101	1/1	0.87	0.17	54,54,54,54	0
34	NA	A	8374	1/1	0.87	0.21	60,60,60,60	0
32	MG	A	8076	1/1	0.87	0.12	37,37,37,37	0
35	CL	M	8510	1/1	0.87	0.16	57,57,57,57	0
32	MG	A	8094	1/1	0.87	0.11	67,67,67,67	0
32	MG	A	8100	1/1	0.87	0.16	53,53,53,53	0
34	NA	N	8347	1/1	0.88	0.07	36,36,36,36	0
34	NA	A	8362	1/1	0.88	0.20	70,70,70,70	0
35	CL	A	8522	1/1	0.88	0.28	78,78,78,78	0
32	MG	A	8080	1/1	0.88	0.09	33,33,33,33	0
32	MG	A	8097	1/1	0.88	0.08	27,27,27,27	0
34	NA	A	8301	1/1	0.88	0.05	26,26,26,26	0
35	CL	P	8508	1/1	0.88	0.13	72,72,72,72	0
32	MG	A	8106	1/1	0.88	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	NA	A	8303	1/1	0.88	0.18	55,55,55,55	0
37	CD	P	8405	1/1	0.88	0.12	184,184,184,184	0
32	MG	A	8098	1/1	0.89	0.14	28,28,28,28	0
32	MG	A	8035	1/1	0.89	0.10	54,54,54,54	0
32	MG	A	8087	1/1	0.89	0.08	56,56,56,56	0
32	MG	A	8051	1/1	0.89	0.10	87,87,87,87	0
35	CL	C	8509	1/1	0.89	0.11	55,55,55,55	0
35	CL	K	8501	1/1	0.89	0.10	69,69,69,69	0
34	NA	A	8325	1/1	0.89	0.14	49,49,49,49	0
32	MG	A	8053	1/1	0.89	0.07	39,39,39,39	0
32	MG	A	8112	1/1	0.89	0.17	43,43,43,43	0
35	CL	O	8507	1/1	0.89	0.09	63,63,63,63	0
32	MG	A	8115	1/1	0.89	0.07	36,36,36,36	0
32	MG	A	8058	1/1	0.89	0.09	33,33,33,33	0
32	MG	A	8096	1/1	0.89	0.12	46,46,46,46	0
32	MG	A	8064	1/1	0.89	0.09	29,29,29,29	0
37	CD	V	8401	1/1	0.89	0.06	69,69,69,69	0
32	MG	A	8043	1/1	0.90	0.11	38,38,38,38	0
32	MG	A	8016	1/1	0.90	0.08	38,38,38,38	0
32	MG	A	8042	1/1	0.90	0.07	35,35,35,35	0
32	MG	A	8081	1/1	0.90	0.08	51,51,51,51	0
35	CL	N	8518	1/1	0.90	0.12	41,41,41,41	0
34	NA	A	8333	1/1	0.90	0.09	24,24,24,24	0
32	MG	A	8099	1/1	0.90	0.09	32,32,32,32	0
34	NA	A	8321	1/1	0.90	0.18	49,49,49,49	0
35	CL	A	8516	1/1	0.90	0.11	51,51,51,51	0
32	MG	1	8105	1/1	0.90	0.17	30,30,30,30	0
33	K	A	8201	1/1	0.90	0.19	76,76,76,76	0
37	CD	1	8403	1/1	0.90	0.06	60,60,60,60	0
34	NA	A	8323	1/1	0.91	0.11	34,34,34,34	0
34	NA	A	8342	1/1	0.91	0.14	34,34,34,34	0
32	MG	A	8059	1/1	0.91	0.09	65,65,65,65	0
34	NA	A	8364	1/1	0.91	0.20	39,39,39,39	0
32	MG	A	8071	1/1	0.91	0.09	80,80,80,80	0
32	MG	A	8061	1/1	0.91	0.07	25,25,25,25	0
35	CL	S	8506	1/1	0.91	0.15	41,41,41,41	0
35	CL	4	8504	1/1	0.91	0.08	56,56,56,56	0
32	MG	C	8065	1/1	0.91	0.10	40,40,40,40	0
32	MG	U	8073	1/1	0.91	0.07	52,52,52,52	0
34	NA	A	8318	1/1	0.91	0.27	37,37,37,37	0
32	MG	A	8114	1/1	0.91	0.07	51,51,51,51	0
32	MG	A	8090	1/1	0.91	0.23	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8037	1/1	0.92	0.09	46,46,46,46	0
32	MG	A	8039	1/1	0.92	0.08	52,52,52,52	0
34	NA	A	8379	1/1	0.92	0.12	34,34,34,34	0
32	MG	A	8088	1/1	0.92	0.19	23,23,23,23	0
34	NA	U	8343	1/1	0.92	0.12	23,23,23,23	0
32	MG	A	8040	1/1	0.92	0.08	71,71,71,71	0
32	MG	A	8029	1/1	0.92	0.08	53,53,53,53	0
35	CL	Z	8520	1/1	0.92	0.07	39,39,39,39	0
32	MG	A	8091	1/1	0.92	0.07	53,53,53,53	0
35	CL	A	8515	1/1	0.92	0.26	85,85,85,85	0
34	NA	J	8309	1/1	0.92	0.07	31,31,31,31	0
34	NA	A	8326	1/1	0.92	0.21	54,54,54,54	0
34	NA	A	8305	1/1	0.92	0.11	27,27,27,27	0
34	NA	A	8306	1/1	0.92	0.29	42,42,42,42	0
34	NA	A	8319	1/1	0.93	0.10	33,33,33,33	0
32	MG	A	8054	1/1	0.93	0.08	37,37,37,37	0
34	NA	A	8341	1/1	0.93	0.06	28,28,28,28	0
32	MG	A	8102	1/1	0.93	0.07	53,53,53,53	0
34	NA	B	8383	1/1	0.93	0.21	72,72,72,72	0
34	NA	C	8345	1/1	0.93	0.08	48,48,48,48	0
35	CL	K	8521	1/1	0.93	0.07	51,51,51,51	0
32	MG	A	8103	1/1	0.93	0.13	73,73,73,73	0
32	MG	A	8011	1/1	0.93	0.07	37,37,37,37	0
32	MG	A	8062	1/1	0.93	0.05	61,61,61,61	0
34	NA	A	8376	1/1	0.94	0.11	42,42,42,42	0
32	MG	D	8055	1/1	0.94	0.11	34,34,34,34	0
32	MG	D	8056	1/1	0.94	0.07	44,44,44,44	0
34	NA	A	8381	1/1	0.94	0.11	54,54,54,54	0
32	MG	A	8104	1/1	0.94	0.10	51,51,51,51	0
34	NA	A	8314	1/1	0.94	0.09	21,21,21,21	0
32	MG	A	8068	1/1	0.94	0.07	58,58,58,58	0
34	NA	A	8331	1/1	0.94	0.12	34,34,34,34	0
34	NA	A	8332	1/1	0.94	0.21	35,35,35,35	0
32	MG	A	8084	1/1	0.94	0.09	56,56,56,56	0
34	NA	A	8334	1/1	0.94	0.11	46,46,46,46	0
32	MG	A	8006	1/1	0.94	0.07	34,34,34,34	0
32	MG	A	8052	1/1	0.94	0.07	39,39,39,39	0
32	MG	A	8022	1/1	0.94	0.08	17,17,17,17	0
32	MG	A	8063	1/1	0.94	0.07	54,54,54,54	0
32	MG	A	8013	1/1	0.94	0.08	45,45,45,45	0
32	MG	B	8095	1/1	0.94	0.09	69,69,69,69	0
32	MG	A	8015	1/1	0.94	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
32	MG	A	8093	1/1	0.94	0.07	48,48,48,48	0
35	CL	A	8503	1/1	0.94	0.10	47,47,47,47	0
35	CL	A	8505	1/1	0.94	0.08	60,60,60,60	0
34	NA	A	8355	1/1	0.94	0.17	72,72,72,72	0
34	NA	A	8349	1/1	0.95	0.06	40,40,40,40	0
32	MG	A	8014	1/1	0.95	0.06	21,21,21,21	0
34	NA	A	8352	1/1	0.95	0.20	51,51,51,51	0
32	MG	A	8113	1/1	0.95	0.06	43,43,43,43	0
35	CL	A	8517	1/1	0.95	0.11	61,61,61,61	0
32	MG	A	8085	1/1	0.95	0.07	61,61,61,61	0
34	NA	A	8378	1/1	0.95	0.16	46,46,46,46	0
35	CL	D	8519	1/1	0.95	0.12	47,47,47,47	0
34	NA	E	8304	1/1	0.95	0.06	39,39,39,39	0
32	MG	A	8110	1/1	0.95	0.08	29,29,29,29	0
32	MG	A	8021	1/1	0.95	0.07	22,22,22,22	0
34	NA	M	8380	1/1	0.95	0.18	61,61,61,61	0
37	CD	2	8402	1/1	0.95	0.05	64,64,64,64	0
32	MG	A	8048	1/1	0.96	0.08	57,57,57,57	0
32	MG	A	8010	1/1	0.96	0.07	26,26,26,26	0
34	NA	R	8348	1/1	0.96	0.04	29,29,29,29	0
34	NA	A	8335	1/1	0.96	0.11	58,58,58,58	0
32	MG	A	8108	1/1	0.96	0.14	72,72,72,72	0
34	NA	A	8339	1/1	0.96	0.08	14,14,14,14	0
32	MG	A	8019	1/1	0.96	0.11	15,15,15,15	0
32	MG	4	8078	1/1	0.96	0.08	63,63,63,63	0
32	MG	A	8023	1/1	0.96	0.06	34,34,34,34	0
34	NA	J	8322	1/1	0.96	0.39	68,68,68,68	0
34	NA	A	8358	1/1	0.96	0.22	113,113,113,113	0
33	K	A	8202	1/1	0.96	0.06	53,53,53,53	0
32	MG	A	8020	1/1	0.97	0.06	27,27,27,27	0
32	MG	A	8032	1/1	0.97	0.05	24,24,24,24	0
32	MG	A	8003	1/1	0.97	0.06	29,29,29,29	0
32	MG	A	8066	1/1	0.97	0.07	72,72,72,72	0
32	MG	A	8001	1/1	0.97	0.05	23,23,23,23	0
32	MG	A	8012	1/1	0.97	0.05	33,33,33,33	0
32	MG	A	8057	1/1	0.97	0.04	34,34,34,34	0
32	MG	A	8047	1/1	0.97	0.10	58,58,58,58	0
32	MG	A	8007	1/1	0.97	0.04	19,19,19,19	0
32	MG	A	8060	1/1	0.97	0.07	49,49,49,49	0
32	MG	A	8077	1/1	0.97	0.04	33,33,33,33	0
32	MG	A	8028	1/1	0.97	0.08	30,30,30,30	0
32	MG	L	8069	1/1	0.98	0.04	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	8038	1/1	0.98	0.04	29,29,29,29	0
32	MG	A	8009	1/1	0.98	0.06	15,15,15,15	0
32	MG	A	8030	1/1	0.98	0.05	23,23,23,23	0
32	MG	A	8031	1/1	0.98	0.06	19,19,19,19	0
32	MG	A	8083	1/1	0.98	0.04	43,43,43,43	0
32	MG	A	8004	1/1	0.98	0.05	28,28,28,28	0
32	MG	A	8033	1/1	0.98	0.06	22,22,22,22	0
32	MG	A	8086	1/1	0.98	0.09	49,49,49,49	0
32	MG	A	8027	1/1	0.98	0.09	35,35,35,35	0
32	MG	A	8008	1/1	0.98	0.05	20,20,20,20	0
37	CD	4	8404	1/1	0.98	0.03	63,63,63,63	0
32	MG	A	8036	1/1	0.99	0.04	27,27,27,27	0
32	MG	A	8005	1/1	0.99	0.02	32,32,32,32	0
32	MG	A	8002	1/1	0.99	0.03	33,33,33,33	0
32	MG	A	8079	1/1	0.99	0.03	27,27,27,27	0
32	MG	A	8025	1/1	0.99	0.03	63,63,63,63	0
32	MG	A	8026	1/1	0.99	0.03	20,20,20,20	0
32	MG	A	8017	1/1	0.99	0.05	24,24,24,24	0
32	MG	A	8107	1/1	0.99	0.04	39,39,39,39	0
32	MG	A	8034	1/1	0.99	0.05	24,24,24,24	0
32	MG	A	8018	1/1	0.99	0.03	44,44,44,44	0
32	MG	A	8072	1/1	0.99	0.07	44,44,44,44	0
32	MG	A	8074	1/1	0.99	0.04	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.