wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 01:28 pm GMT

PDB ID	:	4WCE
Title	:	The crystal structure of the large ribosomal subunit of Staphylococcus aureus
Authors	:	Eyal, Z.; Matzov, D.; Krupkin, M.; Wekselman, I.; Zimmerman, E.; Rozenberg, H.; Bashan, A.; Yonath, A.
Deposited on	:	2014-09-04
Resolution	:	3.53 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 (i) 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 (1)) were used in the production of this report:

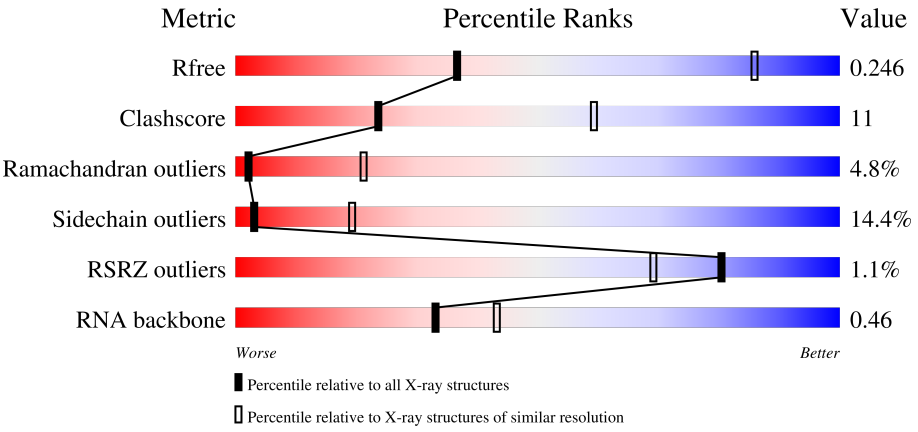
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)
RNA backbone	3102	1003 (4.02-3.00)

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 <=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	X	2923	44% 37% 11% • 7%
2	Y	114	48% 43% 6% •
3	A	277	% 66% 24% 6% •
4	B	220	57% 35% 6% •

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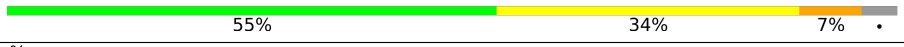
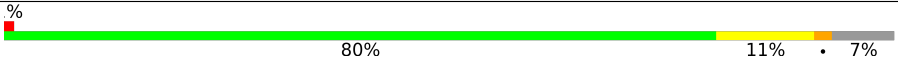
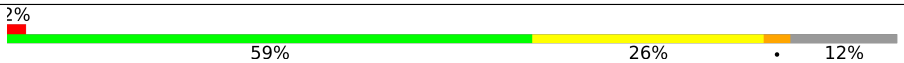
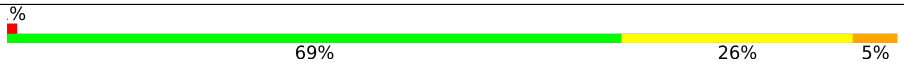
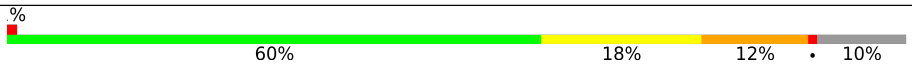
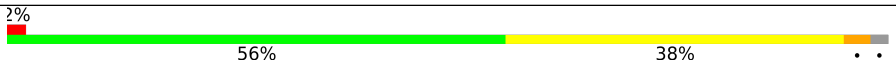
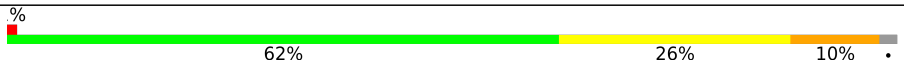
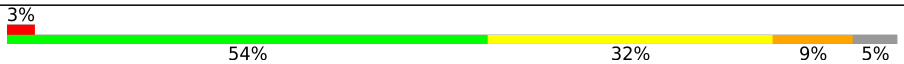
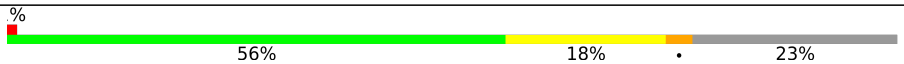
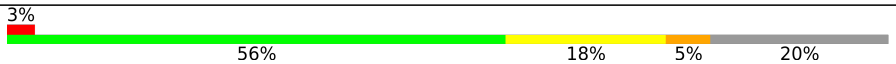
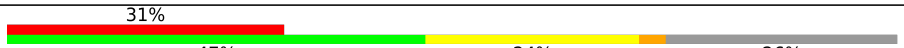
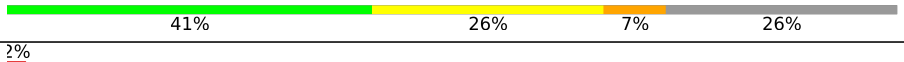
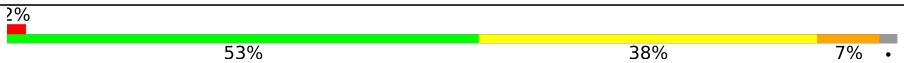
Mol	Chain	Length	Quality of chain
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	146	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	MN	B	303	-	-	-	X
30	MN	X	3050	-	-	-	X
30	MN	X	3053	-	-	-	X
30	MN	X	3308	-	-	-	X
31	MG	X	3013	-	-	-	X
31	MG	X	3113	-	-	-	X
31	MG	X	3173	-	-	-	X
34	EOH	X	3317	-	-	-	X

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 81909 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
			Total	C	N	O	P			
1	X	2708	58077	25928	10647	18794	2708	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	Y	114	2430	1086	436	794	114	0	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	269	1686	1024	333	324	5	0	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	B	215	1558	976	291	286	5	0	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	C	199	1320	818	249	251	2	0	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	D	166	866	523	166	175	2	0	0	0

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	156	Total	C	N	O	S	0	0	0
			970	596	177	195	2			

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1106	693	204	206	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			859	527	170	161	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	141	Total	C	N	O	S	0	0	0
			1068	684	198	183	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			908	557	177	173	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	110	Total	C	N	O	0	0	0
			705	433	137	135			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total 826	C 521	N 164	O 141	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total 932	C 587	N 187	O 154	S 4	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total 751	C 477	N 138	O 135	S 1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total 862	C 537	N 164	O 158	S 3	0	0	0

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	89	Total 626	C 394	N 113	O 116	S 3	0	0	0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	100	Total 683	C 424	N 127	O 131	S 1	0	0	0

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total 1097	C 690	N 191	O 214	S 2	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O	0	0	0
			568	352	110	106			

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	U	46	Total	C	N	O	0	0	0
			300	182	65	53			

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O	0	0	0
			486	299	89	98			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	58	Total	C	N	O	S	0	0	0
			449	279	84	85	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	44	Total	C	N	O	S	0	0	0
			362	222	86	53	1			

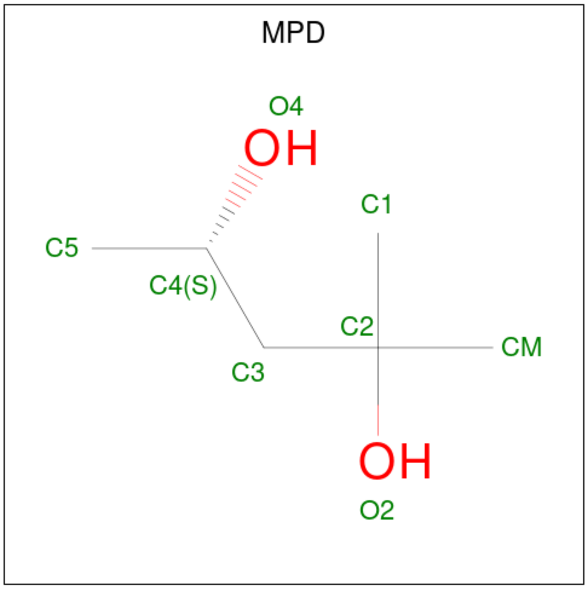
- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			420	260	84	74	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	4	37	277	173	58	41	5	0	0	0

- Molecule 29 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0
29	X	1	8	6	2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	X	1	Total C O 8 6 2	0	0
29	Z	1	Total C O 8 6 2	0	0

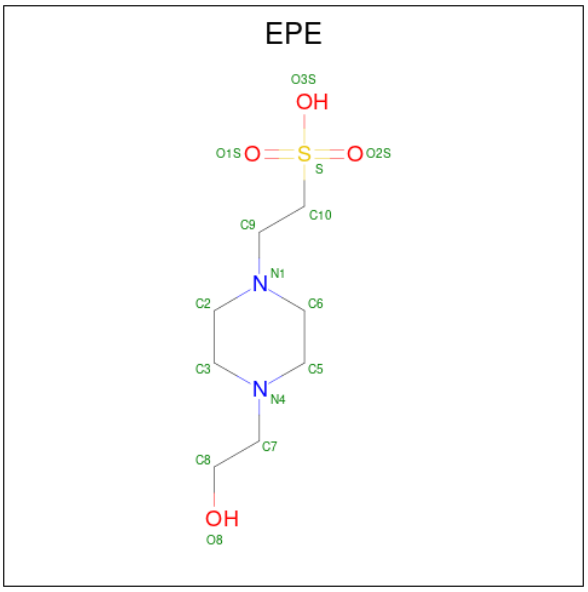
- Molecule 30 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	X	223	Total Mn 223 223	0	0
30	Y	2	Total Mn 2 2	0	0
30	B	1	Total Mn 1 1	0	0
30	I	2	Total Mn 2 2	0	0
30	J	1	Total Mn 1 1	0	0
30	R	2	Total Mn 2 2	0	0

- Molecule 31 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

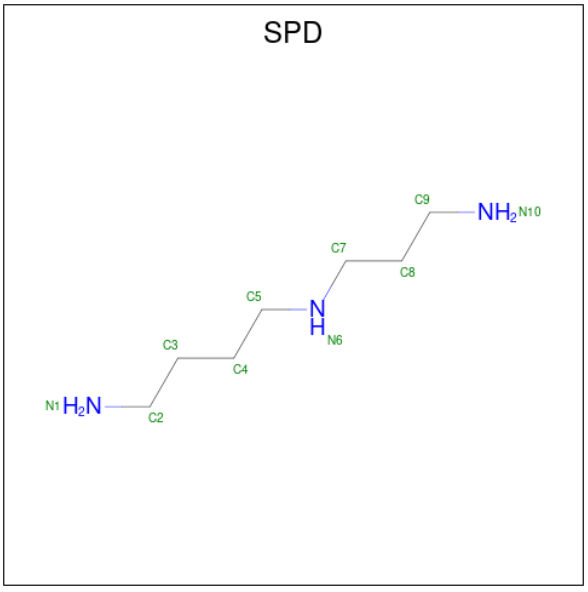
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
31	X	80	Total Mg 80 80	0	0
31	Y	3	Total Mg 3 3	0	0
31	B	2	Total Mg 2 2	0	0
31	C	1	Total Mg 1 1	0	0
31	G	3	Total Mg 3 3	0	0
31	I	1	Total Mg 1 1	0	0
31	O	1	Total Mg 1 1	0	0

- Molecule 32 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	X	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 33 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			
33	X	1	Total	C	N		0	0
			10	7	3			

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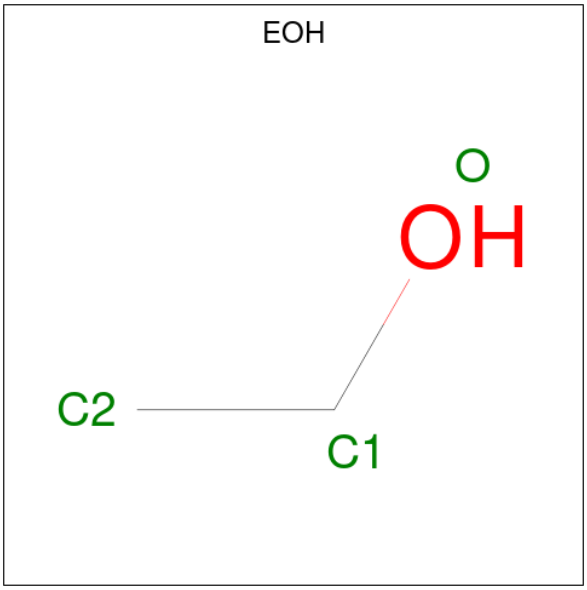
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
33	X	1	Total C N 10 7 3	0	0

- Molecule 34 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



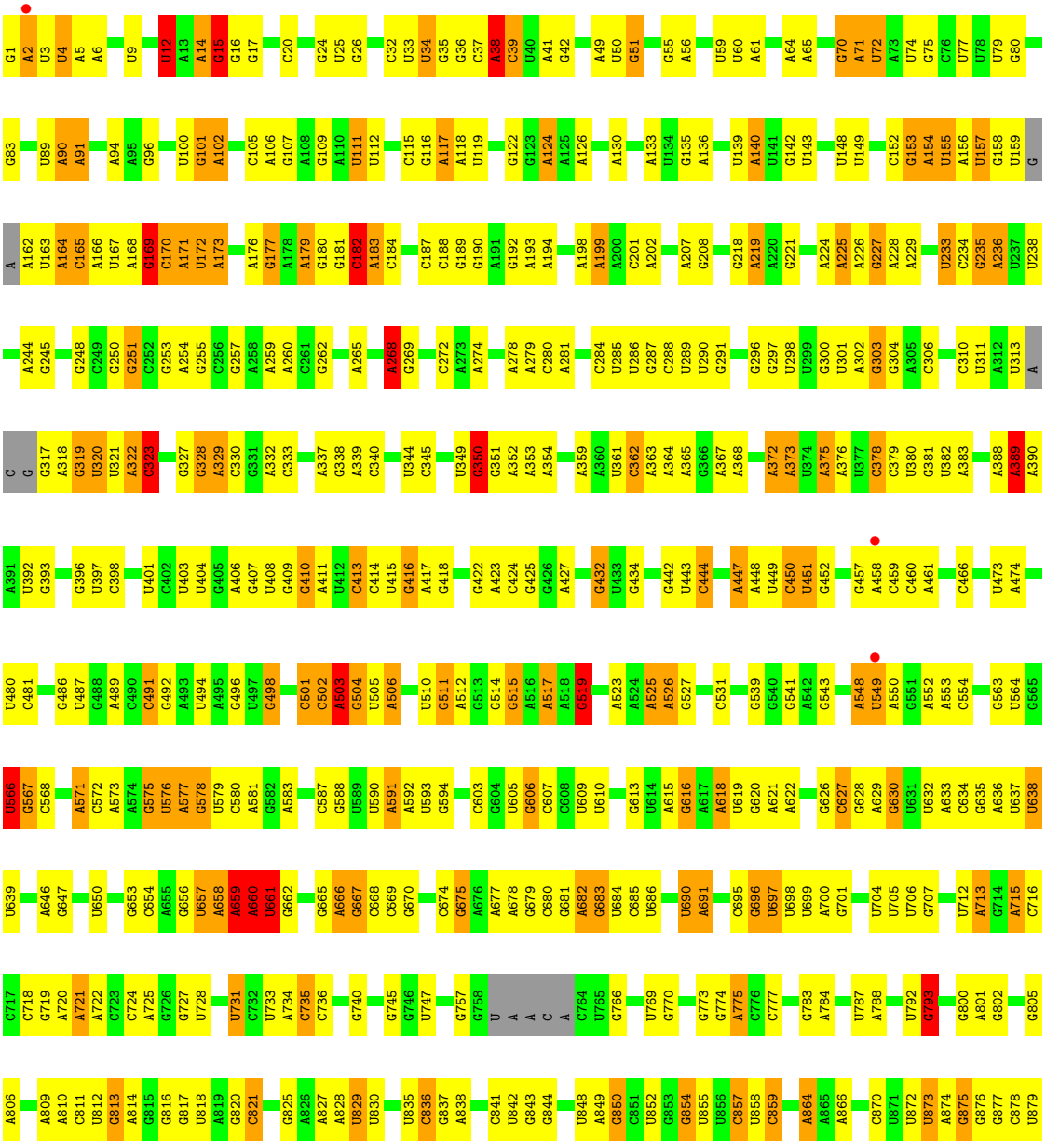
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	X	1	Total C O 3 2 1	0	0
34	X	1	Total C O 3 2 1	0	0
34	X	1	Total C O 3 2 1	0	0
34	X	1	Total C O 3 2 1	0	0
34	X	1	Total C O 3 2 1	0	0
34	X	1	Total C O 3 2 1	0	0
34	X	1	Total C O 3 2 1	0	0

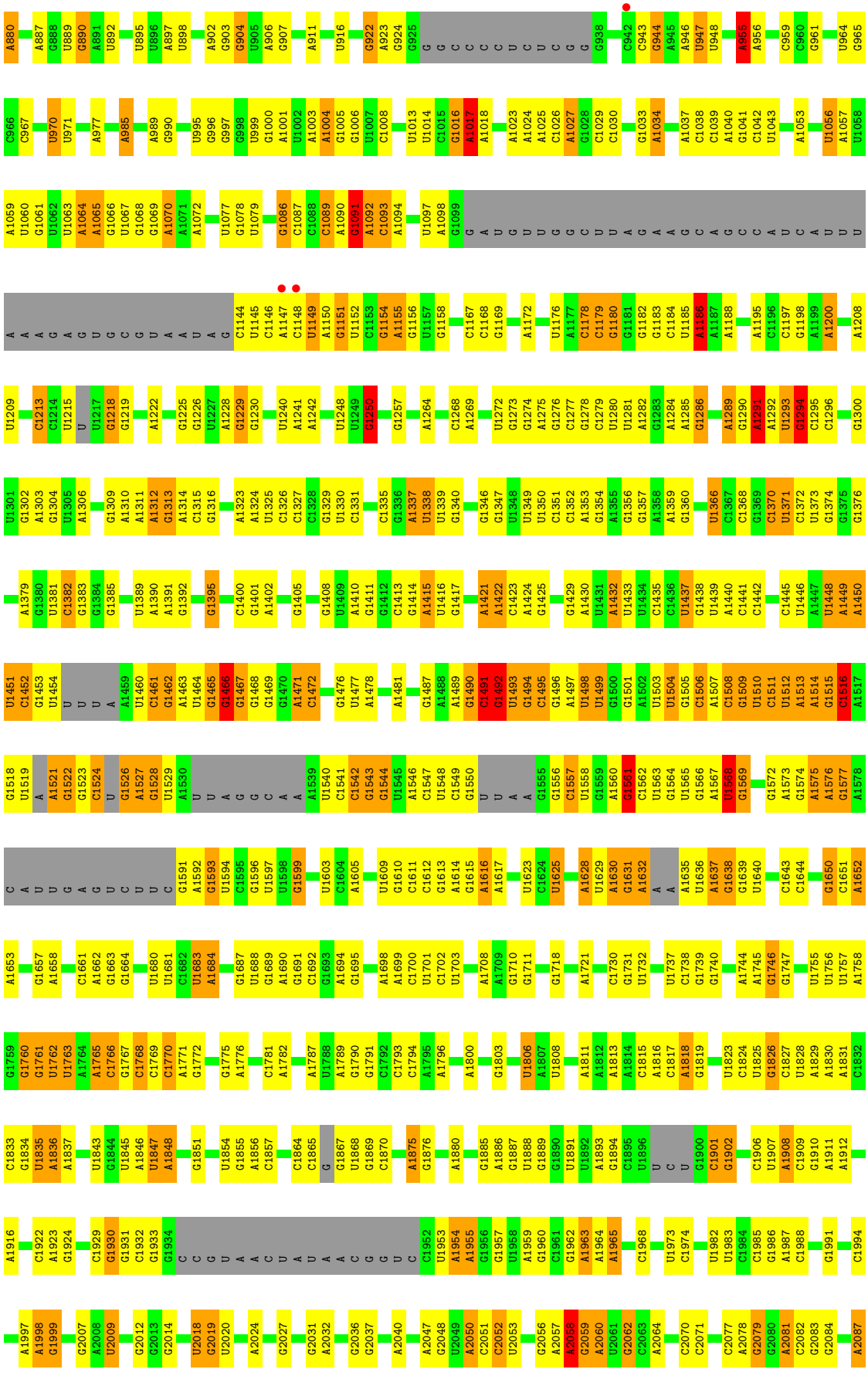
3 Residue-property plots (i)

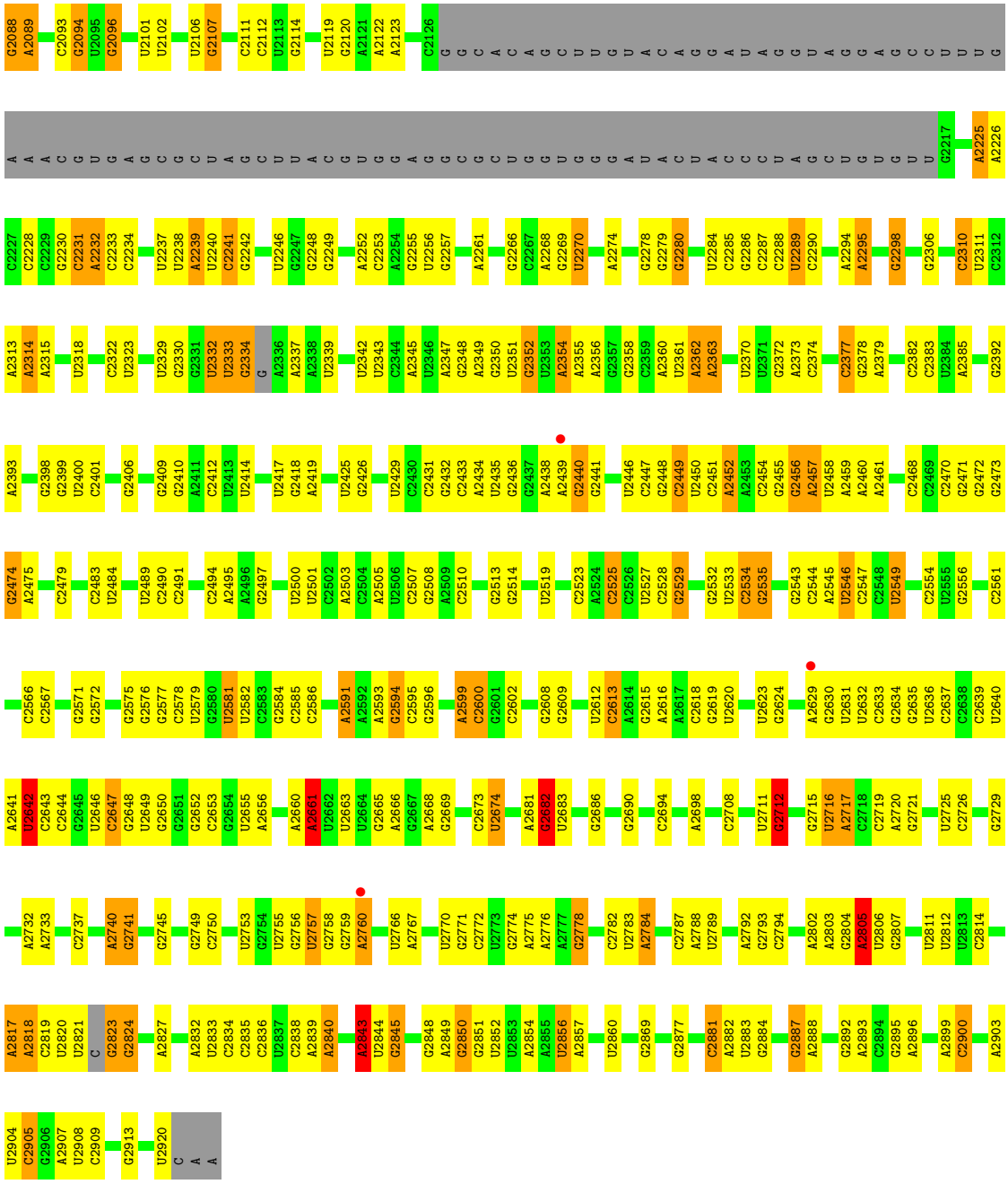
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: 23S rRNA

Chain X:




A880 A887 G888 U889 G890 A891 U892 U895 U896 A897 U898 A902 G903 G904 U905 A906 G907 A911 U916 G922 A923 G924 G925 G938 C942 C943 G944 A945 A946 U947 U948 A955 A956 C959 C960 G961 U964 G965
C966 C967 U970 U971 A977 A985 A989 G990 U995 G996 G997 G998 U999 G1000 A1001 U1002 A1003 A1004 G1005 G1006 U1007 C1008 U1013 U1014 C1015 G1016 A1017 A1018 A1023 A1024 A1025 C1026 A1027 G1028 C1029 C1030 G1033 A1034 A1037 C1038 C1039 A1040 G1041 C1042 U1043 A1053 U1056 A1057 U1058
A1059 U1060 G1061 U1062 U1063 A1064 A1065 G1066 U1067 G1068 G1069 A1070 A1071 A1072 U1077 G1078 U1079 G1086 C1087 C1088 C1089 A1090 G1091 A1092 C1093 A1094 U1097 A1098 G1099 G
A C1144 A U1145 A C1146 G A1147 A C1148 A U1149 G A1150 U G1151 C U1152 G C1153 G C1154 U A1155 G A1156 U A1157 A G1158 A C1167 A C1168 A G1169 A1172 A1176 A1177 C1178 C1179 G1180 U1181 G1182 G1183 A1184 G1185 C A1186 A A1187 G A1188 C A1195 A C1196 A C1197 U G1198 C A1199 U A1200 U A1208
U1209 C1213 C1214 U1215 U A1217 G1218 G1219 A1222 G1225 G1226 U1227 A1228 G1229 G1230 U1240 A1241 A1242 U1248 U1249 G1250 G1257 A1264 C1268 A1269 U1272 G1273 G1274 A1275 G1276 C1277 G1278 C1279 U1280 U1281 A1282 G1283 A1284 A1285 G1286 A1289 G1290 A1291 A1292 U1293 G1294 C1295 C1296 G1300
U1301 G1302 A1303 G1304 U1305 A1306 G1309 A1310 A1311 A1312 G1313 A1314 C1315 G1316 A1323 A1324 U1325 C1326 C1327 C1328 G1329 U1330 C1331 C1335 G1336 A1337 U1338 U1339 G1340 G1346 G1347 U1348 U1349 U1350 C1351 C1352 A1353 G1354 A1355 G1356 G1357 A1358 A1359 G1360 U1366 C1367 C1368 G1369 C1370 U1371 C1372 U1373 G1374 G1375 G1376
A1379 G1380 U1381 C1382 G1383 G1384 G1385 U1389 A1390 A1391 G1392 G1395 C1400 G1401 A1402 G1405 G1408 U1409 A1410 G1411 G1412 C1413 G1414 A1415 U1416 G1417 A1421 A1422 C1423 A1424 G1425 G1429 A1430 U1431 A1432 U1433 U1434 C1435 C1436 U1437 G1438 U1439 A1440 C1441 C1442 C1445 U1446 A1447 U1448 A1449 A1450
U1451 C1452 G1453 U1454 U U U A1459 U1460 C1461 G1462 A1463 U1464 G1465 G1466 G1467 G1468 G1469 G1470 A1471 C1472 G1476 U1477 A1478 A1481 G1487 A1488 A1489 G1490 C1491 G1492 U1493 G1494 C1495 G1496 A1497 U1498 U1499 G1500 G1501 A1502 U1503 U1504 U1505 C1506 A1507 C1508 G1509 U1510 C1511 U1512 A1513 A1514 G1515 C1516 A1517
G1518 U1519 A A1521 G1522 G1523 C1524 U G1526 A1527 G1528 U1529 A1530 U U U A G C A A1539 U1540 C1541 C1542 G1543 G1544 U1545 A1546 C1547 U1548 C1549 G1550 U U A A G1555 C1556 C1557 U1558 G1559 A1560 G1561 C1562 U1563 G1564 U1565 G1566 A1567 U1568 G1569 G1572 A1573 G1574 A1575 A1576 G1577 A1578
C A U U G A G U C U U C G1591 A1592 G1593 U1594 C1595 G1596 U1597 U1598 G1599 U1603 C1604 A1605 U1609 G1610 C1611 C1612 G1613 A1614 G1615 A1616 A1617 U1623 C1624 U1625 A1628 U1629 A1630 G1631 A1632 A A A1635 U1636 A1637 G1638 G1639 U1640 C1643 C1644 G1650 C1651 A1652
A1653 G1657 A1658 C1661 A1662 G1663 G1664 U1680 U1681 C1682 U1683 A1684 G1687 U1688 G1689 A1690 G1691 C1692 G1693 A1694 G1695 A1698 A1699 C1700 U1701 C1702 U1703 A1708 A1709 G1710 G1711 G1718 A1721 C1730 G1731 U1732 U1737 C1738 G1739 G1740 A1744 A1745 G1746 G1747 U1755 U1756 U1757 A1758
G1759 G1760 G1761 U1762 U1763 A1764 A1765 C1766 G1767 C1768 C1769 C1770 A1771 G1772 G1775 A1776 C1781 A1782 A1787 U1788 A1789 G1790 G1791 C1792 C1793 C1794 A1795 A1796 A1800 G1803 U1806 A1807 U1808 A1811 A1812 A1813 A1814 C1815 A1816 C1817 A1818 G1819 U1823 C1824 U1825 G1826 C1827 U1828 A1829 A1830 A1831 C1832
C1833 G1834 U1835 A1836 A1837 U1843 G1844 U1845 A1846 U1847 A1848 G1851 U1854 G1855 A1856 C1857 C1864 C1865 G A1867 U1868 G1869 C1870 A1875 G1876 A1880 G1885 A1886 G1887 U1888 G1889 C1890 U1891 U1892 A1893 G1894 C1895 U1896 U C U G1900 C1901 G1902 C1906 U1907 A1908 C1909 G1910 A1911 A1912
A1916 C1922 A1923 G1924 C1929 G1930 G1931 C1932 G1933 G1934 C C G U A A C U A U A A C G G U C C1952 U1953 A1954 A1955 G1956 G1957 U1958 A1959 G1960 C1961 G1962 A1963 A1964 A1965 C1968 U1973 C1974 U1982 U1983 C1984 C1985 G1986 A1987 C1988 G1991 C1994
A1997 A1998 G1999 G2007 A2008 U2009 G2012 G2013 G2014 U2018 G2019 U2020 A2024 G2027 G2031 A2032 G2036 G2037 A2040 A2047 G2048 U2049 A2050 C2051 C2052 U2053 G2056 A2057 A2058 G2059 A2060 U2061 G2062 C2063 A2064 C2070 C2071 C2077 A2078 G2079 G2080 A2081 C2082 G2083 G2084 A2087

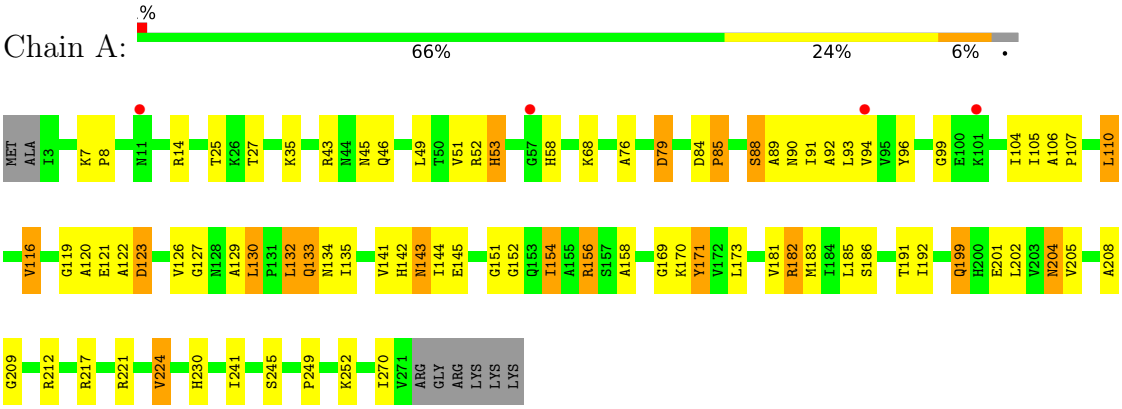


• Molecule 2: 5S rRNA

Chain Y:

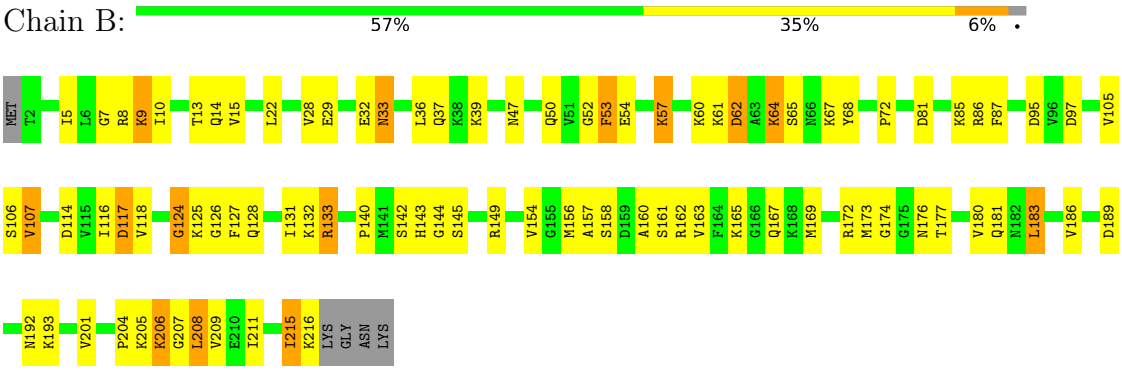
• Molecule 3: 50S ribosomal protein L2

Chain A:



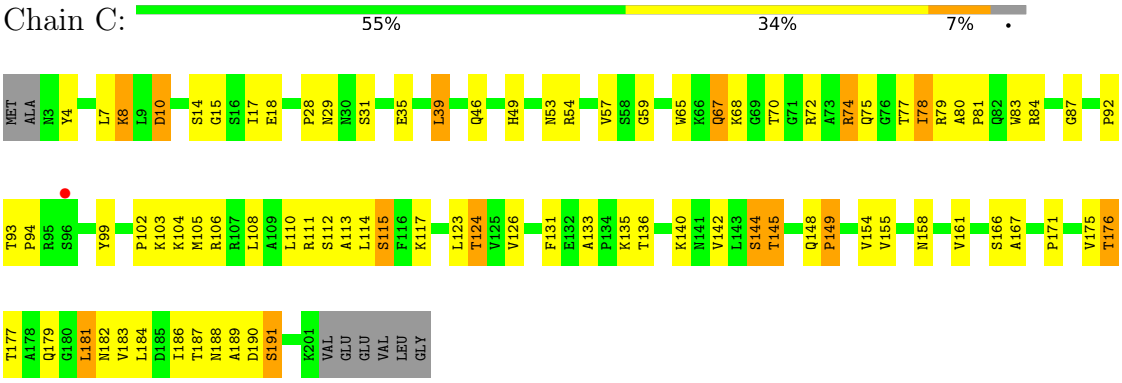
• Molecule 4: 50S ribosomal protein L3

Chain B:



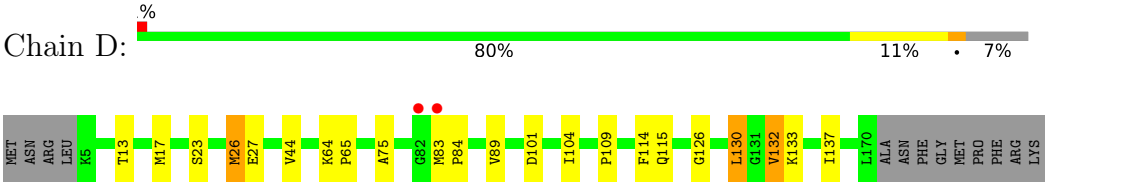
• Molecule 5: 50S ribosomal protein L4

Chain C:



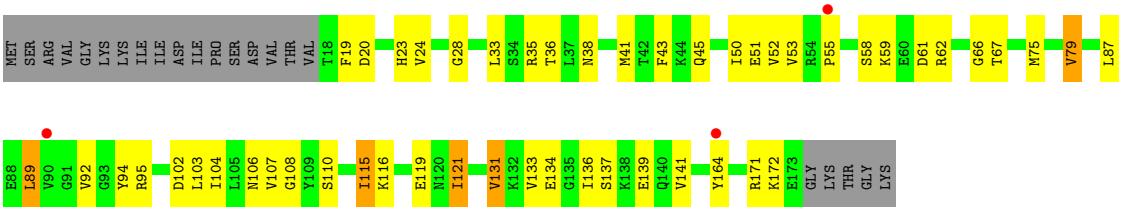
• Molecule 6: 50S ribosomal protein L5

Chain D:



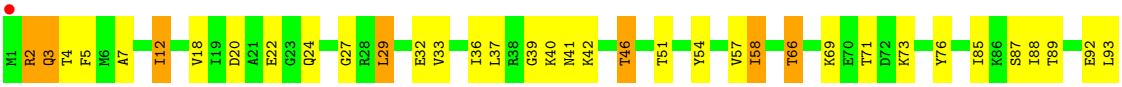
• Molecule 7: 50S ribosomal protein L6

Chain E:



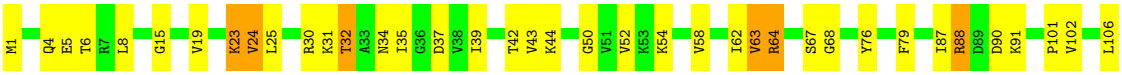
• Molecule 8: 50S ribosomal protein L13

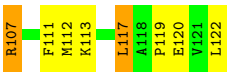
Chain G:



• Molecule 9: 50S ribosomal protein L14

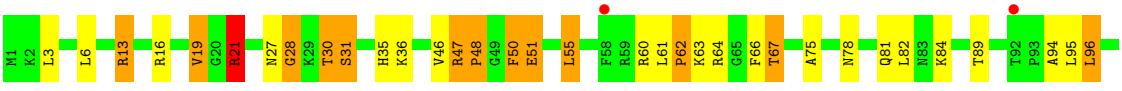
Chain H:

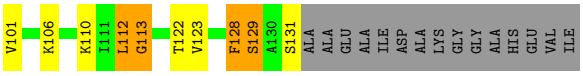




• Molecule 10: 50S ribosomal protein L15

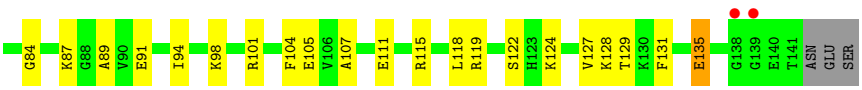
Chain I:





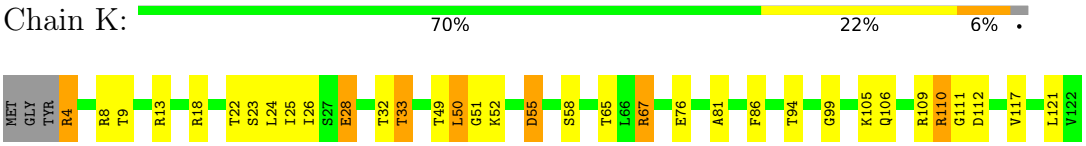
• Molecule 11: 50S ribosomal protein L16

Chain J:



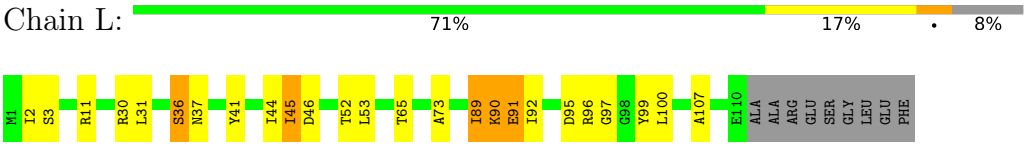
• Molecule 12: 50S ribosomal protein L17

Chain K:



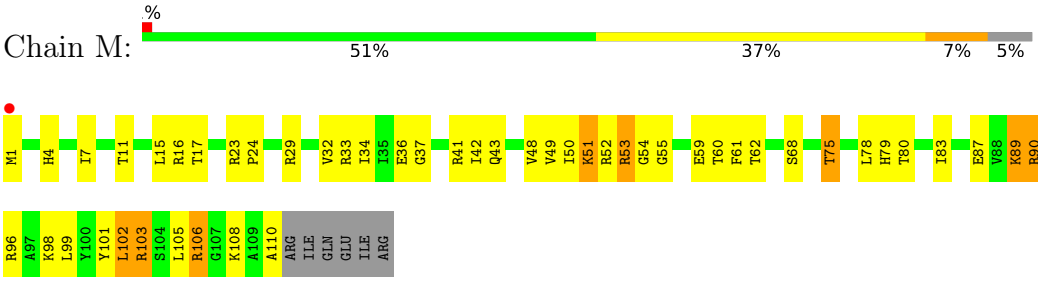
• Molecule 13: 50S ribosomal protein L18

Chain L:



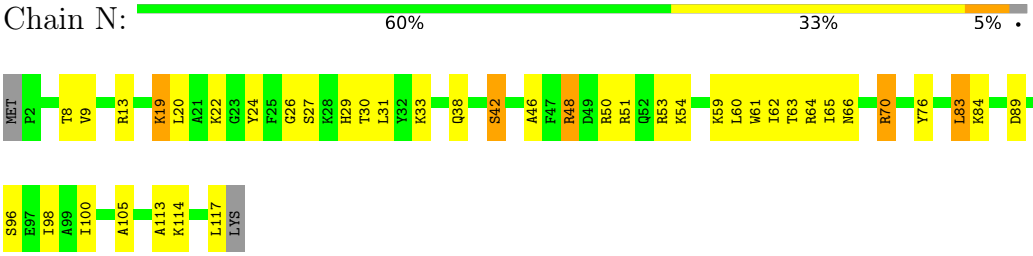
• Molecule 14: 50S ribosomal protein L19

Chain M:



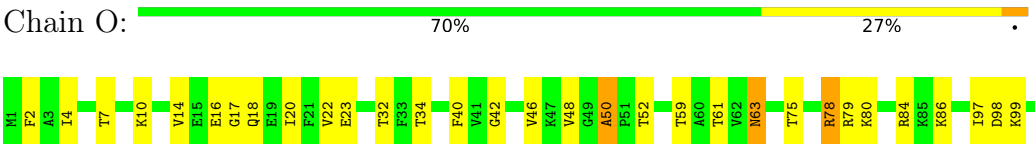
• Molecule 15: 50S ribosomal protein L20

Chain N:



• Molecule 16: 50S ribosomal protein L21

Chain O:

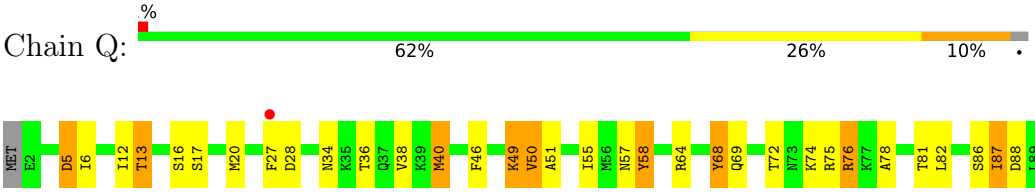


• Molecule 17: 50S ribosomal protein L22

Chain P:

• Molecule 18: 50S ribosomal protein L23

Chain Q:

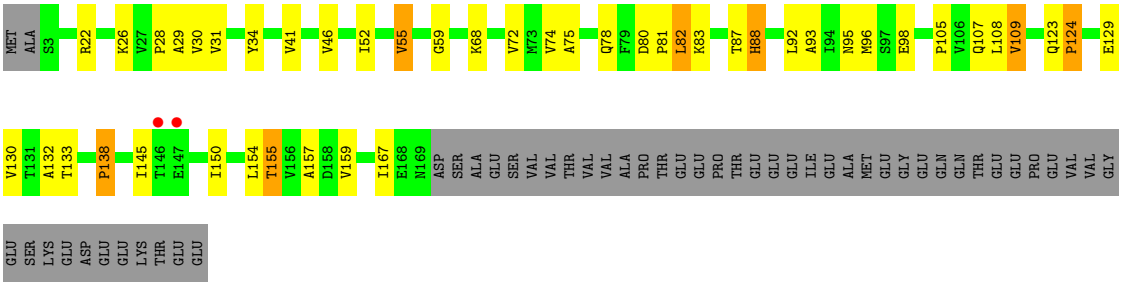


• Molecule 19: 50S ribosomal protein L24

Chain R:

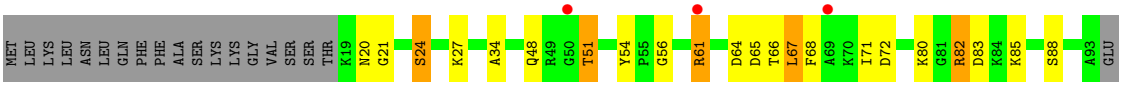
• Molecule 20: 50S ribosomal protein L25

Chain S:



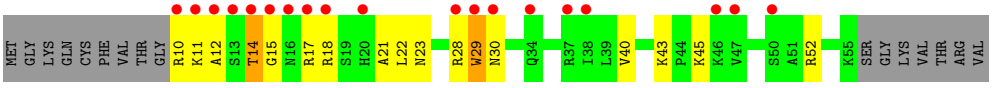
• Molecule 21: 50S ribosomal protein L27

Chain T:



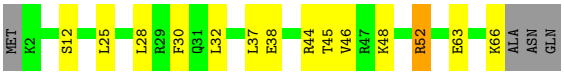
• Molecule 22: 50S ribosomal protein L28

Chain U:



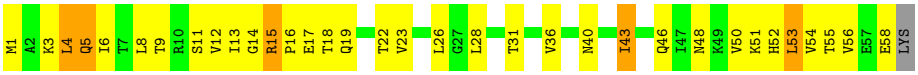
• Molecule 23: 50S ribosomal protein L29

Chain V:



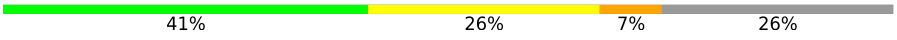
• Molecule 24: 50S ribosomal protein L30

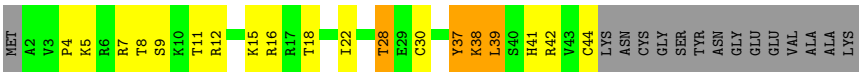
Chain W:



• Molecule 25: 50S ribosomal protein L32

Chain Z:



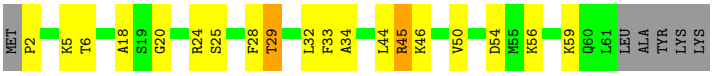


• Molecule 26: 50S ribosomal protein L34

Chain 2:

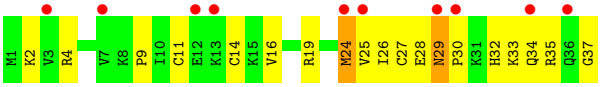
• Molecule 27: 50S ribosomal protein L35

Chain 3:



• Molecule 28: 50S ribosomal protein L36

Chain 4:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α, β, γ	279.76Å 279.76Å 872.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.74 – 3.53 49.74 – 3.53	Depositor EDS
% Data completeness (in resolution range)	96.0 (49.74-3.53) 96.0 (49.74-3.53)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.202 , 0.246 0.202 , 0.246	Depositor DCC
R_{free} test set	11858 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	108.0	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.21 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	81909	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.29% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MPD, EOH, EPE, MG, SPD, MN

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	X	0.64	12/65032 (0.0%)	1.16	279/101388 (0.3%)
2	Y	0.56	0/2717	1.14	17/4232 (0.4%)
3	A	0.25	0/1717	0.55	0/2361
4	B	0.32	0/1581	0.62	0/2129
5	C	0.48	0/1338	0.72	0/1831
6	D	0.23	0/869	0.48	0/1205
7	E	0.27	0/982	0.51	0/1354
8	G	0.37	0/1128	0.58	0/1525
9	H	0.28	0/891	0.53	0/1203
10	I	0.58	0/868	0.91	1/1172 (0.1%)
11	J	0.30	0/1092	0.54	0/1473
12	K	0.31	0/911	0.59	0/1219
13	L	0.25	0/711	0.54	0/970
14	M	0.51	0/838	0.76	0/1132
15	N	0.38	0/944	0.59	0/1252
16	O	0.30	0/761	0.58	1/1022 (0.1%)
17	P	0.55	0/870	0.78	0/1171
18	Q	0.40	0/633	0.66	0/859
19	R	0.27	0/688	0.59	0/930
20	S	0.28	0/1109	0.58	0/1522
21	T	0.26	0/574	0.48	0/763
22	U	0.28	0/305	0.55	0/419
23	V	0.29	0/487	0.53	0/654
24	W	0.54	0/451	0.69	0/607
25	Z	0.48	0/345	0.67	0/460
26	2	0.47	0/366	0.65	0/480
27	3	0.32	0/424	0.66	0/566
28	4	0.39	0/280	0.63	0/371
All	All	0.59	12/88912 (0.0%)	1.07	298/134270 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
7	E	0	1
27	3	0	1
All	All	0	3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1289	A	N9-C4	-8.14	1.32	1.37
1	X	1065	A	N9-C4	-6.85	1.33	1.37
1	X	350	G	N9-C4	6.79	1.43	1.38
1	X	2845	G	N9-C4	-6.28	1.32	1.38
1	X	1186	A	N9-C4	-6.07	1.34	1.37

The worst 5 of 298 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	2845	G	N3-C4-C5	11.31	134.26	128.60
1	X	955	A	N1-C6-N6	11.28	125.37	118.60
1	X	350	G	N3-C4-C5	-10.89	123.15	128.60
2	Y	86	C	N3-C2-O2	-10.49	114.56	121.90
1	X	1065	A	C2-N3-C4	-9.90	105.65	110.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	3	24	ARG	Peptide
3	A	52	ARG	Peptide
7	E	119	GLU	Peptide

5.2 Too-close contacts (i)

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	X	58077	0	29209	849	0
2	Y	2430	0	1229	48	0
3	A	1686	0	1350	48	0
4	B	1558	0	1545	60	0
5	C	1320	0	1171	54	0
6	D	866	0	470	8	0
7	E	970	0	741	23	0
8	G	1106	0	1072	31	0
9	H	884	0	902	26	0
10	I	859	0	772	37	0
11	J	1068	0	1078	42	0
12	K	908	0	935	28	0
13	L	705	0	589	10	0
14	M	826	0	831	41	0
15	N	932	0	995	37	0
16	O	751	0	743	14	0
17	P	862	0	920	37	0
18	Q	626	0	567	21	0
19	R	683	0	661	21	0
20	S	1097	0	956	18	0
21	T	568	0	575	11	0
22	U	300	0	231	9	0
23	V	486	0	469	6	0
24	W	449	0	490	25	0
25	Z	339	0	350	19	0
26	2	362	0	398	14	0
27	3	420	0	405	7	0
28	4	277	0	301	17	0
29	X	88	0	154	14	0
29	Z	8	0	14	0	0
30	B	1	0	0	0	0
30	I	2	0	0	0	0
30	J	1	0	0	0	0
30	R	2	0	0	0	0
30	X	223	0	0	0	0
30	Y	2	0	0	0	0
31	B	2	0	0	0	0
31	C	1	0	0	0	0
31	G	3	0	0	0	0
31	I	1	0	0	0	0
31	O	1	0	0	0	0
31	X	80	0	0	0	0
31	Y	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	X	15	0	17	0	0
33	X	40	0	76	0	0
34	X	21	0	42	0	0
All	All	81909	0	50258	1401	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 11.

The worst 5 of 1401 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:2231:C:HO2'	1:X:2232:A:H8	1.06	0.97
2:Y:80:A:H61	2:Y:91:C:H42	1.05	0.94
2:Y:79:C:H42	2:Y:92:G:H1	1.06	0.94
1:X:1487:G:H1	1:X:1597:U:H3	1.17	0.93
26:2:36:ARG:HG3	26:2:43:LEU:HD21	1.52	0.90

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
3	A	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1 15
4	B	213/220 (97%)	182 (85%)	18 (8%)	13 (6%)	1 16
5	C	197/207 (95%)	169 (86%)	20 (10%)	8 (4%)	3 25
6	D	164/179 (92%)	134 (82%)	19 (12%)	11 (7%)	1 15
7	E	154/178 (86%)	112 (73%)	27 (18%)	15 (10%)	0 8
8	G	143/145 (99%)	129 (90%)	12 (8%)	2 (1%)	11 47
9	H	120/122 (98%)	109 (91%)	8 (7%)	3 (2%)	5 35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
10	I	129/146 (88%)	91 (70%)	25 (19%)	13 (10%)	0 7
11	J	139/144 (96%)	124 (89%)	9 (6%)	6 (4%)	2 23
12	K	117/122 (96%)	101 (86%)	15 (13%)	1 (1%)	17 57
13	L	108/119 (91%)	88 (82%)	15 (14%)	5 (5%)	2 22
14	M	108/116 (93%)	93 (86%)	11 (10%)	4 (4%)	3 28
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100 100
16	O	100/102 (98%)	85 (85%)	11 (11%)	4 (4%)	3 25
17	P	110/117 (94%)	107 (97%)	3 (3%)	0	100 100
18	Q	87/91 (96%)	78 (90%)	7 (8%)	2 (2%)	6 37
19	R	98/105 (93%)	76 (78%)	18 (18%)	4 (4%)	3 25
20	S	165/217 (76%)	130 (79%)	19 (12%)	16 (10%)	0 8
21	T	73/94 (78%)	65 (89%)	7 (10%)	1 (1%)	11 47
22	U	44/62 (71%)	31 (70%)	9 (20%)	4 (9%)	1 9
23	V	63/69 (91%)	58 (92%)	4 (6%)	1 (2%)	9 45
24	W	56/59 (95%)	53 (95%)	3 (5%)	0	100 100
25	Z	41/58 (71%)	38 (93%)	3 (7%)	0	100 100
26	2	42/45 (93%)	38 (90%)	2 (5%)	2 (5%)	2 21
27	3	58/66 (88%)	46 (79%)	4 (7%)	8 (14%)	0 4
28	4	35/37 (95%)	32 (91%)	2 (6%)	1 (3%)	4 33
All	All	2945/3215 (92%)	2499 (85%)	304 (10%)	142 (5%)	2 21

5 of 142 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	27	THR
3	A	51	VAL
3	A	120	ALA
3	A	126	VAL
3	A	141	VAL

5.3.2 Protein sidechains (i)

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
3	A	120/224 (54%)	101 (84%)	19 (16%)	2 16
4	B	153/177 (86%)	136 (89%)	17 (11%)	6 29
5	C	106/169 (63%)	88 (83%)	18 (17%)	2 12
6	D	18/158 (11%)	17 (94%)	1 (6%)	21 55
7	E	67/155 (43%)	58 (87%)	9 (13%)	4 22
8	G	111/123 (90%)	101 (91%)	10 (9%)	9 38
9	H	91/100 (91%)	78 (86%)	13 (14%)	3 20
10	I	67/112 (60%)	52 (78%)	15 (22%)	1 5
11	J	103/119 (87%)	91 (88%)	12 (12%)	5 27
12	K	91/102 (89%)	81 (89%)	10 (11%)	6 30
13	L	47/95 (50%)	39 (83%)	8 (17%)	2 12
14	M	80/102 (78%)	66 (82%)	14 (18%)	2 11
15	N	93/98 (95%)	79 (85%)	14 (15%)	3 18
16	O	71/86 (83%)	60 (84%)	11 (16%)	2 17
17	P	91/94 (97%)	84 (92%)	7 (8%)	13 43
18	Q	53/82 (65%)	39 (74%)	14 (26%)	0 3
19	R	63/90 (70%)	46 (73%)	17 (27%)	0 3
20	S	91/190 (48%)	83 (91%)	8 (9%)	10 39
21	T	56/75 (75%)	48 (86%)	8 (14%)	3 20
22	U	18/52 (35%)	17 (94%)	1 (6%)	21 55
23	V	47/62 (76%)	42 (89%)	5 (11%)	6 31
24	W	52/53 (98%)	40 (77%)	12 (23%)	1 5
25	Z	38/51 (74%)	30 (79%)	8 (21%)	1 6
26	2	37/40 (92%)	32 (86%)	5 (14%)	4 21
27	3	37/57 (65%)	33 (89%)	4 (11%)	6 30
28	4	30/35 (86%)	27 (90%)	3 (10%)	7 33
All	All	1831/2701 (68%)	1568 (86%)	263 (14%)	3 19

5 of 263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	W	1	MET
24	W	18	THR
28	4	24	MET
10	I	89	THR
10	I	67	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	X	2691/2923 (92%)	627 (23%)	18 (0%)
2	Y	113/114 (99%)	13 (11%)	0
All	All	2804/3037 (92%)	640 (22%)	18 (0%)

5 of 640 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	X	2	A
1	X	4	U
1	X	9	U
1	X	12	U
1	X	14	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	X	1576	A
1	X	2823	G
1	X	2457	A
1	X	1503	U
1	X	1575	A

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 346 ligands modelled in this entry, 322 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
34	EOH	X	3319	-	2,2,2	0.50	0	1,1,1	0.76	0
29	MPD	X	3001	-	7,7,7	0.33	0	9,10,10	0.45	0
29	MPD	X	3004	-	7,7,7	0.58	0	9,10,10	0.19	0
29	MPD	X	3010	-	7,7,7	0.63	0	9,10,10	0.35	0
33	SPD	X	3315	-	9,9,9	0.23	0	8,8,8	0.23	0
29	MPD	X	3009	-	7,7,7	0.66	0	9,10,10	0.25	0
29	MPD	X	3006	-	7,7,7	0.46	0	9,10,10	0.10	0
34	EOH	X	3320	-	2,2,2	0.58	0	1,1,1	0.63	0
29	MPD	Z	101	-	7,7,7	0.30	0	9,10,10	0.36	0
29	MPD	X	3011	-	7,7,7	0.88	0	9,10,10	0.45	0
34	EOH	X	3317	-	2,2,2	0.53	0	1,1,1	0.66	0
29	MPD	X	3008	-	7,7,7	0.69	0	9,10,10	0.32	0
33	SPD	X	3312	-	9,9,9	0.28	0	8,8,8	0.34	0
34	EOH	X	3322	-	2,2,2	0.54	0	1,1,1	0.66	0
34	EOH	X	3318	-	2,2,2	0.56	0	1,1,1	0.64	0
34	EOH	X	3321	-	2,2,2	0.58	0	1,1,1	0.62	0
32	EPE	X	3311	-	15,15,15	1.27	1 (6%)	18,20,20	0.45	0
29	MPD	X	3002	-	7,7,7	0.96	1 (14%)	9,10,10	0.53	0
33	SPD	X	3313	-	9,9,9	0.19	0	8,8,8	0.27	0
34	EOH	X	3316	-	2,2,2	0.67	0	1,1,1	0.41	0
33	SPD	X	3314	-	9,9,9	0.14	0	8,8,8	0.22	0
29	MPD	X	3003	-	7,7,7	0.30	0	9,10,10	0.37	0
29	MPD	X	3005	-	7,7,7	0.67	0	9,10,10	0.23	0
29	MPD	X	3007	-	7,7,7	0.79	0	9,10,10	0.41	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
33	SPD	X	3313	-	-	2/7/7/7	-
29	MPD	X	3001	-	-	0/5/5/5	-
29	MPD	X	3004	-	-	0/5/5/5	-
29	MPD	X	3010	-	-	3/5/5/5	-
33	SPD	X	3315	-	-	2/7/7/7	-
29	MPD	X	3008	-	-	1/5/5/5	-
29	MPD	X	3009	-	-	1/5/5/5	-
29	MPD	X	3006	-	-	1/5/5/5	-
33	SPD	X	3312	-	-	1/7/7/7	-
29	MPD	Z	101	-	-	3/5/5/5	-
29	MPD	X	3011	-	-	2/5/5/5	-
32	EPE	X	3311	-	-	6/9/19/19	0/1/1/1
33	SPD	X	3314	-	-	2/7/7/7	-
29	MPD	X	3003	-	-	3/5/5/5	-
29	MPD	X	3005	-	-	3/5/5/5	-
29	MPD	X	3007	-	-	5/5/5/5	-
29	MPD	X	3002	-	-	2/5/5/5	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	X	3311	EPE	C10-S	-4.67	1.70	1.77
29	X	3002	MPD	C3-C2	2.32	1.60	1.53

There are no bond angle outliers.

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	X	3002	MPD	C2-C3-C4-O4
29	X	3003	MPD	C2-C3-C4-C5
29	X	3006	MPD	C2-C3-C4-C5
29	X	3007	MPD	C2-C3-C4-O4
29	X	3009	MPD	C2-C3-C4-C5

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	X	3011	MPD	1	0
29	X	3008	MPD	1	0
29	X	3003	MPD	4	0
29	X	3005	MPD	4	0
29	X	3007	MPD	4	0

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, 95^{th} 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	X	2708/2923 (92%)	-0.47	9 (0%) 94 89	11, 51, 139, 230	0
2	Y	114/114 (100%)	-0.66	0 100 100	22, 67, 115, 151	0
3	A	269/277 (97%)	-0.24	4 (1%) 73 61	43, 74, 106, 136	0
4	B	215/220 (97%)	-0.32	0 100 100	12, 28, 66, 97	0
5	C	199/207 (96%)	-0.53	1 (0%) 91 84	12, 35, 71, 107	0
6	D	166/179 (92%)	-0.41	2 (1%) 79 67	80, 102, 132, 150	0
7	E	156/178 (87%)	-0.26	3 (1%) 66 53	61, 86, 120, 131	0
8	G	145/145 (100%)	-0.28	1 (0%) 87 79	9, 26, 58, 114	0
9	H	122/122 (100%)	-0.39	0 100 100	17, 41, 74, 102	0
10	I	131/146 (89%)	-0.11	2 (1%) 73 61	14, 47, 91, 108	0
11	J	141/144 (97%)	-0.04	3 (2%) 63 50	25, 43, 97, 121	0
12	K	119/122 (97%)	-0.44	0 100 100	14, 37, 86, 97	0
13	L	110/119 (92%)	-0.50	0 100 100	39, 62, 92, 111	0
14	M	110/116 (94%)	-0.48	1 (0%) 84 73	23, 43, 89, 115	0
15	N	116/118 (98%)	-0.54	0 100 100	6, 21, 59, 69	0
16	O	102/102 (100%)	-0.57	0 100 100	7, 35, 75, 92	0
17	P	112/117 (95%)	-0.35	0 100 100	7, 21, 86, 125	0
18	Q	89/91 (97%)	-0.22	1 (1%) 80 69	39, 60, 93, 108	0
19	R	100/105 (95%)	0.18	3 (3%) 50 37	43, 66, 122, 142	0
20	S	167/217 (76%)	-0.19	2 (1%) 79 67	42, 61, 120, 130	0
21	T	75/94 (79%)	0.20	3 (4%) 38 28	21, 39, 81, 102	0
22	U	46/62 (74%)	1.90	19 (41%) 0 0	60, 91, 122, 130	0
23	V	65/69 (94%)	-0.29	0 100 100	48, 71, 105, 119	0
24	W	58/59 (98%)	-0.11	0 100 100	12, 24, 72, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
25	Z	43/58 (74%)	-0.39	0 100 100	11, 20, 99, 127	0
26	2	44/45 (97%)	0.01	1 (2%) 60 46	19, 41, 73, 93	0
27	3	60/66 (90%)	-0.43	0 100 100	10, 32, 69, 83	0
28	4	37/37 (100%)	1.54	10 (27%) 0 0	39, 60, 89, 103	0
All	All	5819/6252 (93%)	-0.35	65 (1%) 80 69	6, 51, 123, 230	0

The worst 5 of 65 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	U	13	SER	6.3
22	U	12	ALA	6.1
22	U	14	THR	5.3
22	U	11	LYS	5.1
20	S	146	THR	4.1

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 monosaccharides 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
30	MN	X	3308	1/1	0.39	0.74	92,92,92,92	0
31	MG	G	203	1/1	0.47	0.33	17,17,17,17	0
30	MN	X	3055	1/1	0.62	0.21	94,94,94,94	0
30	MN	X	3053	1/1	0.63	0.54	89,89,89,89	0
31	MG	X	3113	1/1	0.66	1.07	45,45,45,45	0
30	MN	X	3132	1/1	0.67	0.16	97,97,97,97	0
31	MG	X	3083	1/1	0.70	0.34	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3044	1/1	0.70	0.24	94,94,94,94	0
30	MN	B	303	1/1	0.70	0.74	102,102,102,102	0
30	MN	X	3213	1/1	0.71	0.23	95,95,95,95	0
31	MG	X	3173	1/1	0.71	1.13	26,26,26,26	0
30	MN	X	3057	1/1	0.71	0.20	71,71,71,71	0
34	EOH	X	3317	3/3	0.71	0.51	46,46,46,46	0
30	MN	X	3133	1/1	0.72	0.31	98,98,98,98	0
31	MG	X	3034	1/1	0.73	0.39	18,18,18,18	0
30	MN	X	3168	1/1	0.73	0.21	74,74,74,74	0
30	MN	X	3222	1/1	0.73	0.35	71,71,71,71	0
30	MN	X	3015	1/1	0.74	0.38	75,75,75,75	0
30	MN	X	3050	1/1	0.74	0.47	99,99,99,99	0
31	MG	X	3016	1/1	0.74	0.39	23,23,23,23	0
30	MN	X	3148	1/1	0.75	0.25	79,79,79,79	0
31	MG	X	3013	1/1	0.76	0.83	30,30,30,30	0
31	MG	X	3084	1/1	0.76	0.14	14,14,14,14	0
33	SPD	X	3312	10/10	0.77	0.29	47,47,47,47	0
30	MN	X	3182	1/1	0.77	0.38	107,107,107,107	0
30	MN	X	3121	1/1	0.78	0.31	88,88,88,88	0
31	MG	X	3023	1/1	0.78	0.29	37,37,37,37	0
29	MPD	X	3008	8/8	0.79	0.35	70,70,70,70	0
30	MN	X	3143	1/1	0.79	0.18	94,94,94,94	0
30	MN	X	3128	1/1	0.79	0.16	84,84,84,84	0
30	MN	X	3066	1/1	0.79	0.12	56,56,56,56	0
31	MG	X	3175	1/1	0.80	0.30	0,0,0,0	0
30	MN	X	3111	1/1	0.80	0.13	99,99,99,99	0
31	MG	X	3137	1/1	0.80	0.92	17,17,17,17	0
30	MN	J	201	1/1	0.80	0.20	78,78,78,78	0
30	MN	X	3124	1/1	0.81	0.11	77,77,77,77	0
30	MN	X	3220	1/1	0.81	0.43	68,68,68,68	0
30	MN	X	3126	1/1	0.81	0.24	77,77,77,77	0
30	MN	X	3293	1/1	0.81	0.19	70,70,70,70	0
29	MPD	X	3010	8/8	0.81	0.33	87,87,87,87	0
31	MG	X	3298	1/1	0.82	1.02	23,23,23,23	0
30	MN	X	3130	1/1	0.82	0.13	102,102,102,102	0
30	MN	X	3140	1/1	0.82	0.17	71,71,71,71	0
31	MG	X	3114	1/1	0.82	0.57	36,36,36,36	0
30	MN	X	3052	1/1	0.83	0.21	71,71,71,71	0
30	MN	X	3123	1/1	0.83	0.42	97,97,97,97	0
30	MN	X	3254	1/1	0.83	0.23	48,48,48,48	0
30	MN	X	3076	1/1	0.83	0.09	74,74,74,74	0
29	MPD	X	3002	8/8	0.83	0.32	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3135	1/1	0.83	0.14	94,94,94,94	0
31	MG	X	3109	1/1	0.83	0.70	24,24,24,24	0
30	MN	X	3138	1/1	0.83	0.10	112,112,112,112	0
34	EOH	X	3318	3/3	0.83	0.27	47,47,47,47	0
30	MN	X	3122	1/1	0.84	0.50	89,89,89,89	0
31	MG	X	3093	1/1	0.84	0.27	21,21,21,21	0
31	MG	X	3095	1/1	0.84	0.34	26,26,26,26	0
30	MN	X	3090	1/1	0.84	0.35	96,96,96,96	0
30	MN	X	3042	1/1	0.84	0.11	104,104,104,104	0
33	SPD	X	3315	10/10	0.84	0.31	46,46,46,46	0
31	MG	X	3079	1/1	0.84	0.74	27,27,27,27	0
30	MN	X	3059	1/1	0.84	0.10	61,61,61,61	0
29	MPD	X	3006	8/8	0.85	0.18	88,88,88,88	0
31	MG	X	3106	1/1	0.85	0.22	37,37,37,37	0
30	MN	X	3125	1/1	0.85	0.32	79,79,79,79	0
30	MN	I	202	1/1	0.85	0.25	64,64,64,64	0
30	MN	X	3158	1/1	0.85	0.22	62,62,62,62	0
34	EOH	X	3316	3/3	0.85	0.40	10,10,10,10	0
30	MN	X	3131	1/1	0.85	0.48	89,89,89,89	0
29	MPD	X	3011	8/8	0.85	0.24	39,39,39,39	0
31	MG	G	201	1/1	0.86	0.20	19,19,19,19	0
31	MG	X	3294	1/1	0.86	0.34	37,37,37,37	0
30	MN	X	3268	1/1	0.86	0.29	27,27,27,27	0
33	SPD	X	3313	10/10	0.86	0.29	30,30,30,30	0
31	MG	X	3302	1/1	0.87	0.30	20,20,20,20	0
33	SPD	X	3314	10/10	0.87	0.48	26,26,26,26	0
31	MG	Y	203	1/1	0.87	0.76	21,21,21,21	0
30	MN	X	3068	1/1	0.87	0.21	70,70,70,70	0
31	MG	X	3172	1/1	0.87	0.79	27,27,27,27	0
30	MN	X	3118	1/1	0.87	0.31	101,101,101,101	0
30	MN	Y	202	1/1	0.88	0.14	57,57,57,57	0
31	MG	X	3174	1/1	0.88	0.31	5,5,5,5	0
31	MG	X	3082	1/1	0.88	0.17	31,31,31,31	0
30	MN	X	3276	1/1	0.88	0.17	42,42,42,42	0
30	MN	X	3183	1/1	0.88	0.15	41,41,41,41	0
30	MN	X	3073	1/1	0.88	0.14	86,86,86,86	0
31	MG	Y	201	1/1	0.88	0.11	34,34,34,34	0
31	MG	X	3039	1/1	0.88	0.30	7,7,7,7	0
31	MG	Y	205	1/1	0.88	0.14	12,12,12,12	0
34	EOH	X	3320	3/3	0.88	0.28	28,28,28,28	0
34	EOH	X	3321	3/3	0.88	0.30	18,18,18,18	0
31	MG	X	3031	1/1	0.89	0.33	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3074	1/1	0.89	0.06	78,78,78,78	0
31	MG	X	3035	1/1	0.89	0.34	23,23,23,23	0
30	MN	X	3223	1/1	0.89	0.24	60,60,60,60	0
31	MG	B	301	1/1	0.89	0.14	0,0,0,0	0
30	MN	X	3216	1/1	0.89	0.19	54,54,54,54	0
30	MN	X	3169	1/1	0.89	0.67	78,78,78,78	0
30	MN	X	3273	1/1	0.89	0.27	41,41,41,41	0
30	MN	X	3127	1/1	0.90	0.13	44,44,44,44	0
31	MG	X	3097	1/1	0.90	0.23	14,14,14,14	0
30	MN	X	3155	1/1	0.90	0.38	87,87,87,87	0
29	MPD	Z	101	8/8	0.90	0.35	48,48,48,48	0
30	MN	X	3290	1/1	0.90	0.18	89,89,89,89	0
31	MG	X	3305	1/1	0.90	0.91	15,15,15,15	0
30	MN	X	3192	1/1	0.90	0.32	84,84,84,84	0
30	MN	X	3244	1/1	0.90	0.18	57,57,57,57	0
31	MG	X	3028	1/1	0.90	0.30	34,34,34,34	0
34	EOH	X	3319	3/3	0.90	0.19	47,47,47,47	0
30	MN	X	3146	1/1	0.90	0.23	101,101,101,101	0
31	MG	C	301	1/1	0.90	0.25	2,2,2,2	0
31	MG	X	3115	1/1	0.91	0.72	1,1,1,1	1
31	MG	X	3022	1/1	0.91	0.60	25,25,25,25	0
30	MN	X	3178	1/1	0.91	0.46	78,78,78,78	0
31	MG	X	3026	1/1	0.91	0.61	18,18,18,18	0
31	MG	X	3085	1/1	0.91	0.21	9,9,9,9	0
30	MN	X	3041	1/1	0.91	0.22	84,84,84,84	0
30	MN	X	3134	1/1	0.91	0.18	58,58,58,58	0
30	MN	X	3058	1/1	0.91	0.14	64,64,64,64	0
31	MG	X	3300	1/1	0.91	0.16	11,11,11,11	0
31	MG	X	3098	1/1	0.91	0.33	14,14,14,14	0
30	MN	X	3288	1/1	0.91	0.11	55,55,55,55	0
31	MG	X	3038	1/1	0.91	0.29	23,23,23,23	0
30	MN	X	3067	1/1	0.91	0.19	51,51,51,51	0
30	MN	X	3250	1/1	0.91	0.27	80,80,80,80	0
34	EOH	X	3322	3/3	0.91	0.47	34,34,34,34	0
30	MN	X	3230	1/1	0.92	0.28	65,65,65,65	0
30	MN	X	3233	1/1	0.92	0.26	63,63,63,63	0
30	MN	X	3063	1/1	0.92	0.13	60,60,60,60	0
30	MN	X	3199	1/1	0.92	0.36	51,51,51,51	0
30	MN	X	3207	1/1	0.92	0.44	62,62,62,62	0
31	MG	I	201	1/1	0.92	0.26	0,0,0,0	0
31	MG	O	201	1/1	0.92	0.28	7,7,7,7	0
30	MN	X	3255	1/1	0.92	0.56	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3065	1/1	0.92	0.10	60,60,60,60	0
30	MN	X	3117	1/1	0.92	0.25	80,80,80,80	0
29	MPD	X	3004	8/8	0.92	0.34	73,73,73,73	0
31	MG	X	3297	1/1	0.92	0.31	5,5,5,5	0
29	MPD	X	3009	8/8	0.92	0.15	76,76,76,76	0
30	MN	X	3186	1/1	0.92	0.29	51,51,51,51	0
31	MG	X	3103	1/1	0.92	0.45	3,3,3,3	0
30	MN	X	3226	1/1	0.92	0.33	89,89,89,89	0
31	MG	X	3107	1/1	0.92	0.59	18,18,18,18	0
30	MN	X	3227	1/1	0.92	0.17	57,57,57,57	0
31	MG	X	3018	1/1	0.93	0.47	15,15,15,15	0
31	MG	X	3136	1/1	0.93	0.34	27,27,27,27	0
31	MG	X	3019	1/1	0.93	0.25	15,15,15,15	0
30	MN	X	3231	1/1	0.93	0.24	74,74,74,74	0
30	MN	X	3072	1/1	0.93	0.17	80,80,80,80	0
30	MN	X	3291	1/1	0.93	0.52	94,94,94,94	0
30	MN	X	3061	1/1	0.93	0.12	63,63,63,63	0
30	MN	X	3149	1/1	0.93	0.27	94,94,94,94	0
31	MG	X	3100	1/1	0.93	0.21	17,17,17,17	0
30	MN	X	3202	1/1	0.93	0.23	54,54,54,54	0
31	MG	X	3299	1/1	0.93	0.26	5,5,5,5	0
30	MN	X	3119	1/1	0.93	0.15	63,63,63,63	0
30	MN	X	3211	1/1	0.93	0.20	60,60,60,60	0
31	MG	X	3304	1/1	0.93	0.78	15,15,15,15	0
30	MN	X	3269	1/1	0.93	0.24	36,36,36,36	0
31	MG	X	3309	1/1	0.93	0.24	20,20,20,20	0
30	MN	X	3229	1/1	0.93	0.13	79,79,79,79	0
30	MN	X	3046	1/1	0.93	0.30	94,94,94,94	0
30	MN	X	3162	1/1	0.94	0.31	43,43,43,43	0
30	MN	X	3218	1/1	0.94	0.31	65,65,65,65	0
31	MG	X	3303	1/1	0.94	0.25	4,4,4,4	0
30	MN	X	3261	1/1	0.94	0.16	30,30,30,30	0
30	MN	X	3263	1/1	0.94	0.33	52,52,52,52	0
31	MG	X	3099	1/1	0.94	0.14	26,26,26,26	0
31	MG	X	3310	1/1	0.94	0.13	15,15,15,15	0
31	MG	X	3021	1/1	0.94	0.18	21,21,21,21	0
30	MN	X	3267	1/1	0.94	0.31	48,48,48,48	0
30	MN	X	3187	1/1	0.94	0.28	74,74,74,74	0
30	MN	X	3221	1/1	0.94	0.12	46,46,46,46	0
31	MG	X	3108	1/1	0.94	0.10	12,12,12,12	0
31	MG	X	3027	1/1	0.94	0.19	29,29,29,29	0
31	MG	G	202	1/1	0.94	0.37	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3188	1/1	0.94	0.45	87,87,87,87	0
30	MN	X	3191	1/1	0.94	0.15	51,51,51,51	0
31	MG	X	3032	1/1	0.94	0.25	21,21,21,21	0
30	MN	X	3224	1/1	0.94	0.25	53,53,53,53	0
30	MN	X	3054	1/1	0.94	0.28	86,86,86,86	0
30	MN	X	3069	1/1	0.94	0.14	68,68,68,68	0
30	MN	X	3157	1/1	0.94	0.22	68,68,68,68	0
29	MPD	X	3001	8/8	0.94	0.14	33,33,33,33	0
30	MN	X	3208	1/1	0.94	0.25	37,37,37,37	0
30	MN	X	3209	1/1	0.94	0.20	24,24,24,24	0
31	MG	X	3295	1/1	0.94	0.68	18,18,18,18	0
30	MN	X	3160	1/1	0.94	0.18	45,45,45,45	0
30	MN	X	3184	1/1	0.94	0.36	88,88,88,88	0
31	MG	X	3089	1/1	0.94	0.15	13,13,13,13	0
30	MN	X	3142	1/1	0.95	0.39	72,72,72,72	0
29	MPD	X	3005	8/8	0.95	0.17	65,65,65,65	0
31	MG	X	3176	1/1	0.95	0.16	14,14,14,14	0
30	MN	X	3040	1/1	0.95	0.19	74,74,74,74	0
30	MN	X	3265	1/1	0.95	0.24	43,43,43,43	0
31	MG	X	3036	1/1	0.95	0.14	8,8,8,8	0
31	MG	X	3105	1/1	0.95	0.24	35,35,35,35	0
32	EPE	X	3311	15/15	0.95	0.18	57,57,57,57	0
30	MN	X	3048	1/1	0.95	0.10	59,59,59,59	0
30	MN	X	3171	1/1	0.95	0.15	86,86,86,86	0
30	MN	X	3177	1/1	0.95	0.21	82,82,82,82	0
30	MN	X	3070	1/1	0.95	0.10	78,78,78,78	0
30	MN	X	3179	1/1	0.95	0.21	83,83,83,83	0
30	MN	X	3153	1/1	0.95	0.29	95,95,95,95	0
30	MN	X	3110	1/1	0.95	0.13	96,96,96,96	0
31	MG	X	3087	1/1	0.95	0.32	51,51,51,51	0
30	MN	X	3156	1/1	0.95	0.22	53,53,53,53	0
30	MN	X	3129	1/1	0.95	0.07	73,73,73,73	0
30	MN	X	3049	1/1	0.95	0.39	82,82,82,82	0
30	MN	X	3196	1/1	0.96	0.33	51,51,51,51	0
30	MN	X	3071	1/1	0.96	0.08	69,69,69,69	0
30	MN	X	3025	1/1	0.96	0.21	52,52,52,52	0
30	MN	X	3206	1/1	0.96	0.45	57,57,57,57	0
30	MN	X	3240	1/1	0.96	0.19	28,28,28,28	0
31	MG	X	3307	1/1	0.96	0.04	21,21,21,21	0
31	MG	X	3102	1/1	0.96	0.34	6,6,6,6	0
30	MN	X	3281	1/1	0.96	0.17	40,40,40,40	0
31	MG	X	3104	1/1	0.96	0.32	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3120	1/1	0.96	0.17	55,55,55,55	0
30	MN	X	3180	1/1	0.96	0.54	76,76,76,76	0
30	MN	X	3252	1/1	0.96	0.30	17,17,17,17	0
30	MN	X	3112	1/1	0.96	0.06	54,54,54,54	0
30	MN	X	3225	1/1	0.96	0.41	41,41,41,41	0
30	MN	X	3324	1/1	0.96	0.18	12,12,12,12	0
31	MG	X	3037	1/1	0.96	0.12	11,11,11,11	0
30	MN	X	3325	1/1	0.96	0.22	59,59,59,59	0
30	MN	X	3258	1/1	0.96	0.22	35,35,35,35	0
30	MN	X	3259	1/1	0.96	0.15	13,13,13,13	0
30	MN	X	3260	1/1	0.96	0.30	40,40,40,40	0
29	MPD	X	3007	8/8	0.96	0.28	9,9,9,9	0
30	MN	R	201	1/1	0.96	0.10	63,63,63,63	0
30	MN	R	202	1/1	0.96	0.23	58,58,58,58	0
31	MG	X	3086	1/1	0.96	0.10	26,26,26,26	0
30	MN	X	3262	1/1	0.96	0.22	50,50,50,50	0
30	MN	X	3194	1/1	0.96	0.17	31,31,31,31	0
31	MG	X	3296	1/1	0.96	0.47	9,9,9,9	0
31	MG	X	3091	1/1	0.96	0.43	30,30,30,30	0
31	MG	X	3092	1/1	0.96	0.15	20,20,20,20	0
30	MN	X	3228	1/1	0.96	0.34	85,85,85,85	0
29	MPD	X	3003	8/8	0.97	0.19	21,21,21,21	0
30	MN	X	3278	1/1	0.97	0.30	35,35,35,35	0
30	MN	X	3024	1/1	0.97	0.43	107,107,107,107	0
30	MN	X	3282	1/1	0.97	0.21	49,49,49,49	0
30	MN	X	3287	1/1	0.97	0.31	78,78,78,78	0
30	MN	X	3141	1/1	0.97	0.35	69,69,69,69	0
30	MN	X	3289	1/1	0.97	0.28	57,57,57,57	0
30	MN	X	3236	1/1	0.97	0.15	36,36,36,36	0
31	MG	X	3080	1/1	0.97	0.19	33,33,33,33	0
30	MN	X	3239	1/1	0.97	0.36	15,15,15,15	0
30	MN	X	3292	1/1	0.97	0.28	99,99,99,99	0
30	MN	X	3181	1/1	0.97	0.19	39,39,39,39	0
30	MN	X	3241	1/1	0.97	0.28	20,20,20,20	0
30	MN	X	3323	1/1	0.97	0.15	42,42,42,42	0
30	MN	X	3242	1/1	0.97	0.30	22,22,22,22	0
31	MG	X	3306	1/1	0.97	0.06	29,29,29,29	0
31	MG	X	3088	1/1	0.97	0.13	36,36,36,36	0
30	MN	X	3075	1/1	0.97	0.11	76,76,76,76	0
30	MN	X	3212	1/1	0.97	0.27	56,56,56,56	0
30	MN	Y	204	1/1	0.97	0.11	63,63,63,63	0
30	MN	X	3012	1/1	0.97	0.31	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3253	1/1	0.97	0.34	26,26,26,26	0
30	MN	I	203	1/1	0.97	0.22	33,33,33,33	0
30	MN	X	3159	1/1	0.97	0.15	42,42,42,42	0
30	MN	X	3078	1/1	0.97	0.19	78,78,78,78	0
30	MN	X	3219	1/1	0.97	0.31	53,53,53,53	0
30	MN	X	3147	1/1	0.97	0.12	82,82,82,82	0
30	MN	X	3165	1/1	0.97	0.16	63,63,63,63	0
30	MN	X	3166	1/1	0.97	0.23	62,62,62,62	0
30	MN	X	3014	1/1	0.97	0.20	12,12,12,12	0
31	MG	X	3020	1/1	0.97	0.25	20,20,20,20	0
30	MN	X	3193	1/1	0.97	0.18	33,33,33,33	0
30	MN	X	3047	1/1	0.97	0.20	69,69,69,69	0
30	MN	X	3266	1/1	0.97	0.18	22,22,22,22	0
30	MN	X	3170	1/1	0.97	0.10	54,54,54,54	0
30	MN	X	3151	1/1	0.97	0.17	44,44,44,44	0
30	MN	X	3152	1/1	0.97	0.29	68,68,68,68	0
31	MG	X	3029	1/1	0.97	0.39	19,19,19,19	0
31	MG	X	3030	1/1	0.97	0.21	15,15,15,15	0
31	MG	X	3144	1/1	0.97	0.18	8,8,8,8	0
30	MN	X	3204	1/1	0.97	0.16	21,21,21,21	0
30	MN	X	3256	1/1	0.98	0.22	13,13,13,13	0
30	MN	X	3197	1/1	0.98	0.24	34,34,34,34	0
30	MN	X	3214	1/1	0.98	0.11	81,81,81,81	0
31	MG	X	3101	1/1	0.98	0.35	9,9,9,9	0
30	MN	X	3163	1/1	0.98	0.16	61,61,61,61	0
30	MN	X	3232	1/1	0.98	0.30	55,55,55,55	0
31	MG	X	3033	1/1	0.98	0.19	19,19,19,19	0
30	MN	X	3217	1/1	0.98	0.27	38,38,38,38	0
30	MN	X	3235	1/1	0.98	0.39	40,40,40,40	0
30	MN	X	3164	1/1	0.98	0.23	48,48,48,48	0
30	MN	X	3238	1/1	0.98	0.22	34,34,34,34	0
30	MN	X	3203	1/1	0.98	0.37	27,27,27,27	0
31	MG	B	302	1/1	0.98	0.11	4,4,4,4	0
30	MN	X	3051	1/1	0.98	0.18	67,67,67,67	0
30	MN	X	3205	1/1	0.98	0.27	61,61,61,61	0
30	MN	X	3272	1/1	0.98	0.36	44,44,44,44	0
31	MG	X	3081	1/1	0.98	0.07	36,36,36,36	0
30	MN	X	3077	1/1	0.98	0.20	78,78,78,78	0
30	MN	X	3274	1/1	0.98	0.10	36,36,36,36	0
30	MN	X	3017	1/1	0.98	0.36	103,103,103,103	0
30	MN	X	3277	1/1	0.98	0.17	35,35,35,35	0
30	MN	X	3060	1/1	0.98	0.15	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3280	1/1	0.98	0.27	39,39,39,39	0
30	MN	X	3251	1/1	0.98	0.19	8,8,8,8	0
30	MN	X	3161	1/1	0.98	0.23	46,46,46,46	0
30	MN	X	3283	1/1	0.98	0.34	14,14,14,14	0
30	MN	X	3285	1/1	0.98	0.21	85,85,85,85	0
30	MN	X	3210	1/1	0.98	0.20	57,57,57,57	0
30	MN	X	3195	1/1	0.98	0.21	30,30,30,30	0
31	MG	X	3096	1/1	0.98	0.24	9,9,9,9	0
30	MN	X	3043	1/1	0.98	0.11	61,61,61,61	0
30	MN	X	3245	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3246	1/1	0.99	0.19	13,13,13,13	0
30	MN	X	3275	1/1	0.99	0.18	30,30,30,30	0
30	MN	X	3247	1/1	0.99	0.25	25,25,25,25	0
31	MG	X	3301	1/1	0.99	0.13	8,8,8,8	0
31	MG	X	3094	1/1	0.99	0.16	5,5,5,5	0
30	MN	X	3248	1/1	0.99	0.28	37,37,37,37	0
30	MN	X	3249	1/1	0.99	0.21	51,51,51,51	0
30	MN	X	3279	1/1	0.99	0.25	25,25,25,25	0
30	MN	X	3145	1/1	0.99	0.16	51,51,51,51	0
30	MN	X	3139	1/1	0.99	0.29	97,97,97,97	0
30	MN	X	3185	1/1	0.99	0.21	28,28,28,28	0
30	MN	X	3198	1/1	0.99	0.20	64,64,64,64	0
30	MN	X	3284	1/1	0.99	0.15	21,21,21,21	0
30	MN	X	3154	1/1	0.99	0.22	40,40,40,40	0
30	MN	X	3286	1/1	0.99	0.31	57,57,57,57	0
30	MN	X	3215	1/1	0.99	0.28	26,26,26,26	0
30	MN	X	3200	1/1	0.99	0.26	37,37,37,37	0
30	MN	X	3257	1/1	0.99	0.23	25,25,25,25	0
30	MN	X	3201	1/1	0.99	0.20	40,40,40,40	0
30	MN	X	3234	1/1	0.99	0.18	17,17,17,17	0
30	MN	X	3056	1/1	0.99	0.19	61,61,61,61	0
30	MN	X	3064	1/1	0.99	0.14	68,68,68,68	0
30	MN	X	3237	1/1	0.99	0.23	47,47,47,47	0
31	MG	X	3116	1/1	0.99	0.13	20,20,20,20	0
30	MN	X	3189	1/1	0.99	0.30	64,64,64,64	0
30	MN	X	3264	1/1	0.99	0.33	52,52,52,52	0
30	MN	X	3190	1/1	0.99	0.41	59,59,59,59	0
30	MN	X	3326	1/1	0.99	0.17	57,57,57,57	0
30	MN	X	3045	1/1	0.99	0.28	3,3,3,3	0
30	MN	X	3150	1/1	0.99	0.13	50,50,50,50	0
30	MN	X	3167	1/1	0.99	0.20	57,57,57,57	0
30	MN	X	3243	1/1	0.99	0.42	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
30	MN	X	3270	1/1	0.99	0.16	30,30,30,30	0
30	MN	X	3271	1/1	0.99	0.25	17,17,17,17	0
30	MN	X	3062	1/1	0.99	0.16	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.