wwPDB X-ray Structure Validation Summary Report (i)

Jan 31, 2016 – 09:51 PM GMT

PDB ID	:	1Q86
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

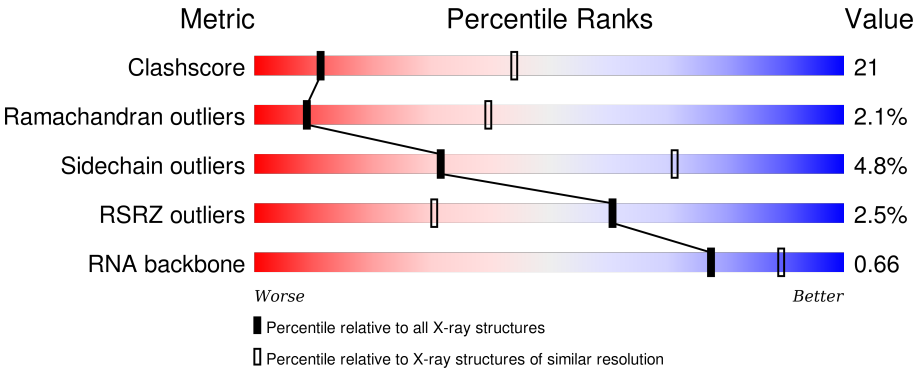
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	A	2922	2% 53% 35% 5% 6%
2	B	122	5% 48% 39% 11% •
3	5	3	33% 33% 33% 33%
3	6	3	100% 100%
4	C	239	3% 57% 36% 6% •

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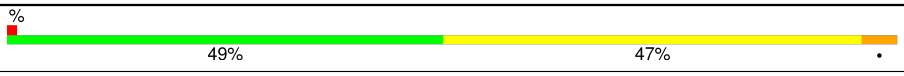
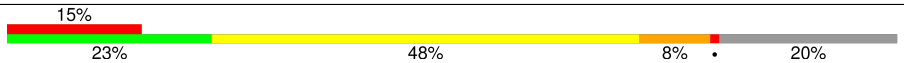
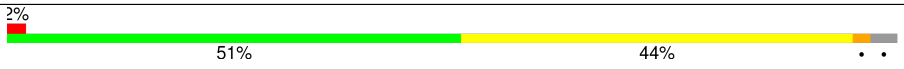
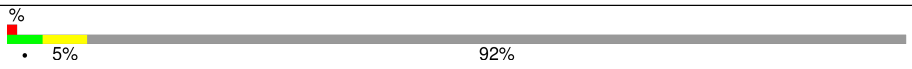
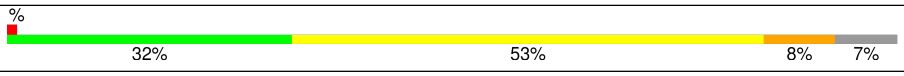
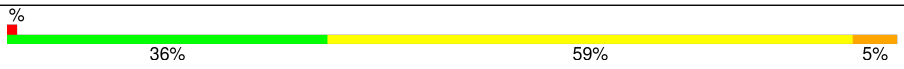
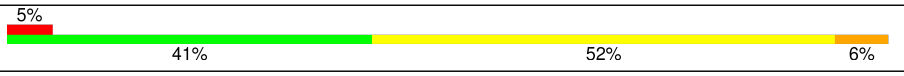
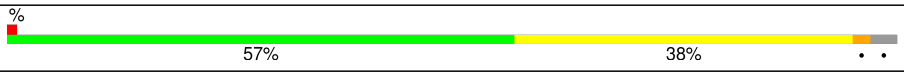
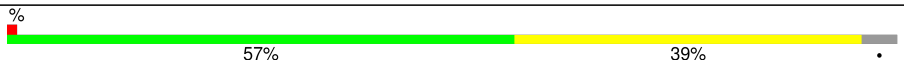
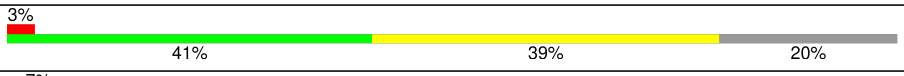
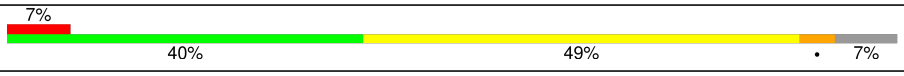
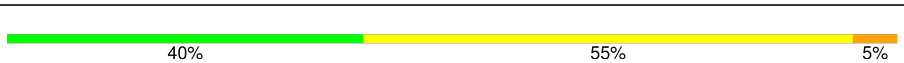
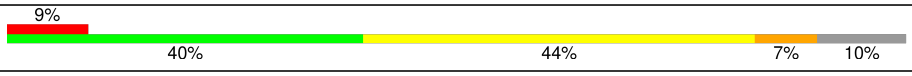
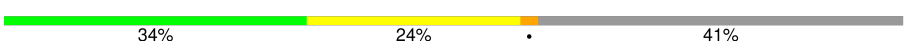
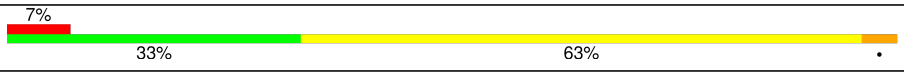
Mol	Chain	Length	Quality of chain
5	D	337	
6	E	246	
7	F	176	
8	G	177	
9	H	119	
10	I	348	
11	J	167	
12	K	145	
13	L	132	
14	M	164	
15	N	194	
16	O	186	
17	P	115	
18	Q	148	
19	R	95	
20	S	154	
21	T	84	
22	U	119	
23	V	66	
24	W	70	
25	X	154	
26	Y	91	
27	Z	240	
28	1	73	
29	2	56	

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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
32	MG	6	8118	-	-	-	X
32	MG	A	8049	-	-	-	X
32	MG	A	8112	-	-	-	X
33	K	A	8201	-	-	-	X
34	NA	A	8305	-	-	-	X
34	NA	A	8320	-	-	-	X
34	NA	A	8321	-	-	-	X
34	NA	A	8323	-	-	-	X
34	NA	A	8325	-	-	-	X
34	NA	A	8326	-	-	-	X
34	NA	A	8332	-	-	-	X
34	NA	A	8339	-	-	-	X
34	NA	A	8340	-	-	-	X
34	NA	A	8350	-	-	-	X
34	NA	A	8356	-	-	-	X
34	NA	A	8359	-	-	-	X
34	NA	A	8361	-	-	-	X
34	NA	A	8362	-	-	-	X
34	NA	A	8366	-	-	-	X
34	NA	A	8367	-	-	-	X
34	NA	A	8371	-	-	-	X
34	NA	A	8372	-	-	-	X
34	NA	A	8373	-	-	-	X
34	NA	A	8374	-	-	-	X
34	NA	A	8376	-	-	-	X
34	NA	A	8377	-	-	-	X
34	NA	A	8378	-	-	-	X
34	NA	A	8382	-	-	-	X
34	NA	B	8383	-	-	-	X
34	NA	K	8346	-	-	-	X
34	NA	M	8380	-	-	-	X
34	NA	N	8365	-	-	-	X
34	NA	S	8386	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
35	CL	A	8515	-	-	-	X
35	CL	D	8519	-	-	-	X
36	PHA	5	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
			Total	C	N	O	P			
1	A	2754	59017	26346	10878	19048	2745	0	0	0

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

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

- Molecule 3 is a RNA chain called CCA-phenylalanine-cariotic-acid-biotin.

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

- Molecule 11 is a protein called L10 Ribosomal Protein.

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

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

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

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

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

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

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

- Molecule 15 is a protein called L15 Ribosomal Protein.

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	R	95	Total	C	N	O	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	0	0	0
			1130	686	228	216			

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	1	1	Total	Mg	0	0
			1	1		
32	D	2	Total	Mg	0	0
			2	2		
32	B	1	Total	Mg	0	0
			1	1		
32	C	1	Total	Mg	0	0
			1	1		
32	6	1	Total	Mg	0	0
			1	1		
32	Z	1	Total	Mg	0	0
			1	1		
32	A	108	Total	Mg	0	0
			108	108		
32	4	1	Total	Mg	0	0
			1	1		
32	U	1	Total	Mg	0	0
			1	1		
32	L	1	Total	Mg	0	0
			1	1		

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
34	J	2	Total	Na	0	0
			2	2		
34	K	1	Total	Na	0	0
			1	1		
34	E	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
34	B	2	Total Na 2 2	0	0
34	C	1	Total Na 1 1	0	0
34	A	70	Total Na 70 70	0	0
34	T	1	Total Na 1 1	0	0
34	N	2	Total Na 2 2	0	0
34	U	1	Total Na 1 1	0	0
34	R	1	Total Na 1 1	0	0
34	S	3	Total Na 3 3	0	0
34	M	1	Total Na 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	P	1	Total Cl 1 1	0	0
35	D	1	Total Cl 1 1	0	0
35	K	3	Total Cl 3 3	0	0
35	C	1	Total Cl 1 1	0	0
35	Z	1	Total Cl 1 1	0	0
35	A	9	Total Cl 9 9	0	0
35	4	1	Total Cl 1 1	0	0
35	N	1	Total Cl 1 1	0	0
35	O	1	Total Cl 1 1	0	0
35	L	1	Total Cl 1 1	0	0

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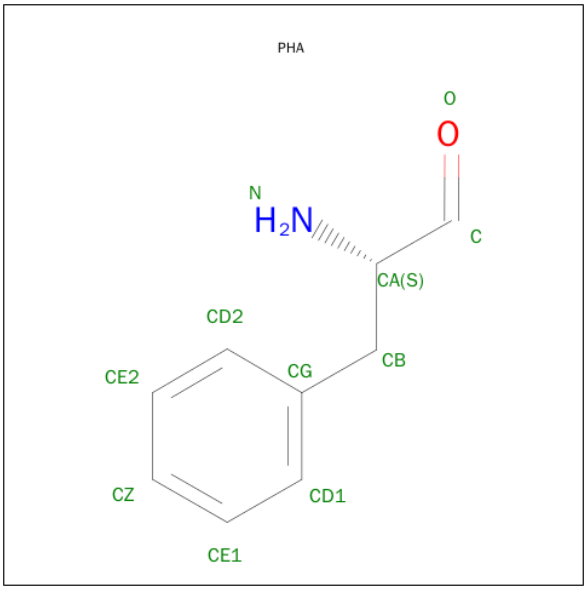
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
35	S	1	Total Cl 1 1	0	0
35	M	1	Total Cl 1 1	0	0

- Molecule 36 is PHENYLALANINAL (three-letter code: PHA) (formula: $C_9H_{11}NO$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
36	5	1	Total C N O 11 9 1 1	0	0
36	6	1	Total C O 10 9 1	0	0

- Molecule 37 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 38 is water.

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

Continued on next page...

Continued from previous page...

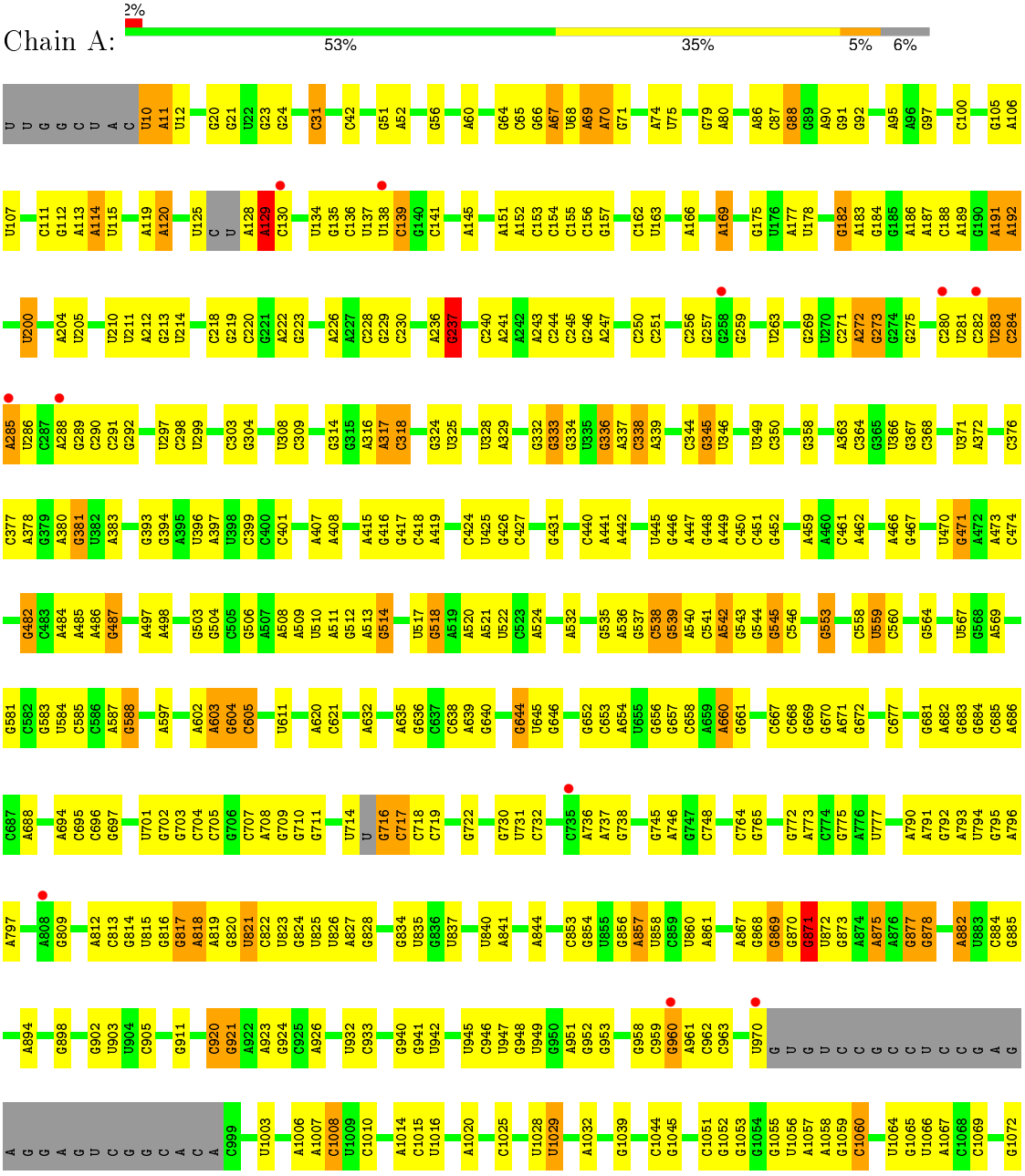
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
38	V	24	Total O 24 24	0	0
38	W	14	Total O 14 14	0	0
38	X	71	Total O 71 71	0	0
38	Y	31	Total O 31 31	0	0
38	Z	93	Total O 93 93	0	0
38	1	37	Total O 37 37	0	0
38	2	63	Total O 63 63	0	0
38	3	41	Total O 41 41	0	0
38	4	70	Total O 70 70	0	0

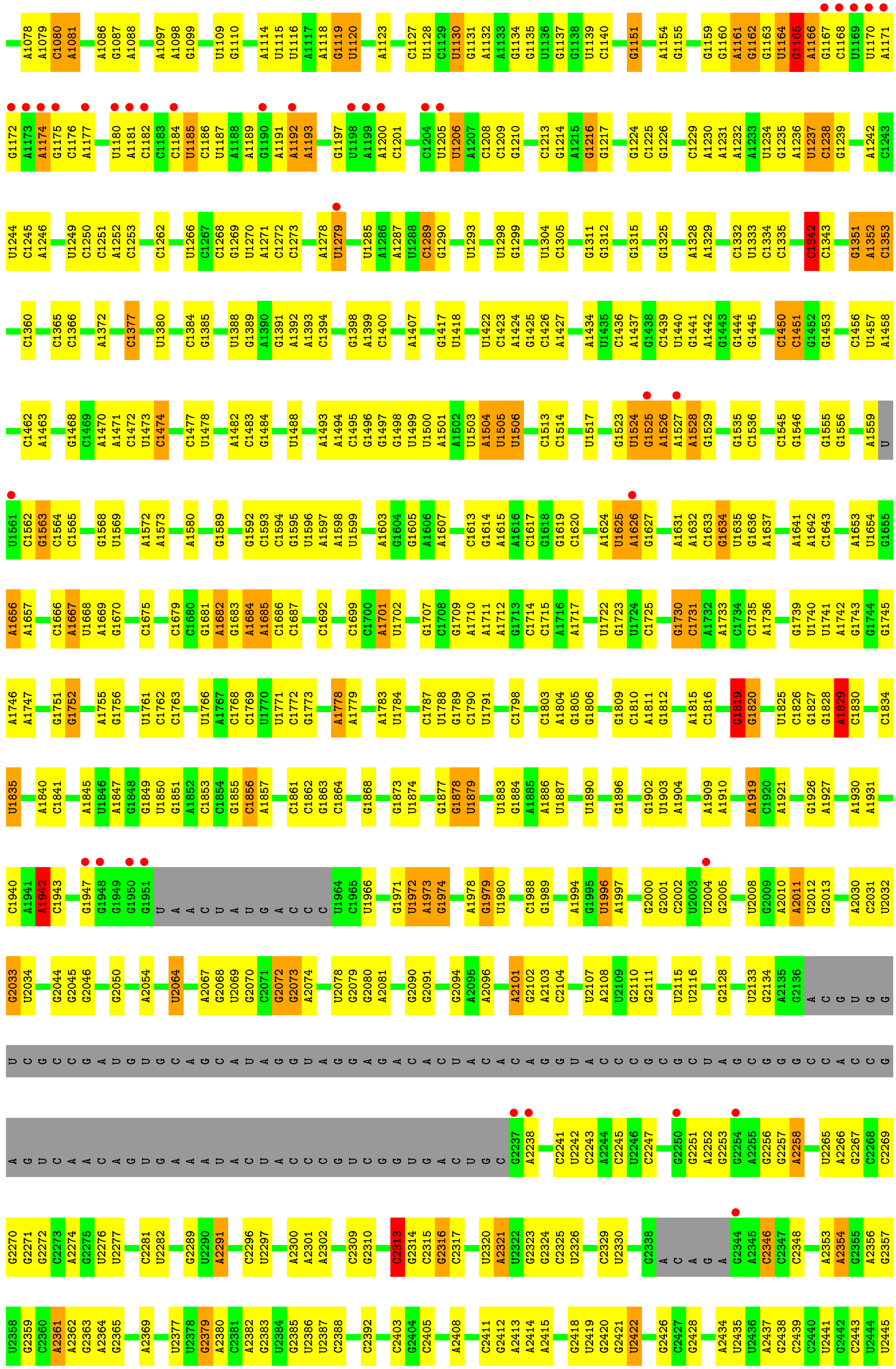
3 Residue-property plots (i)

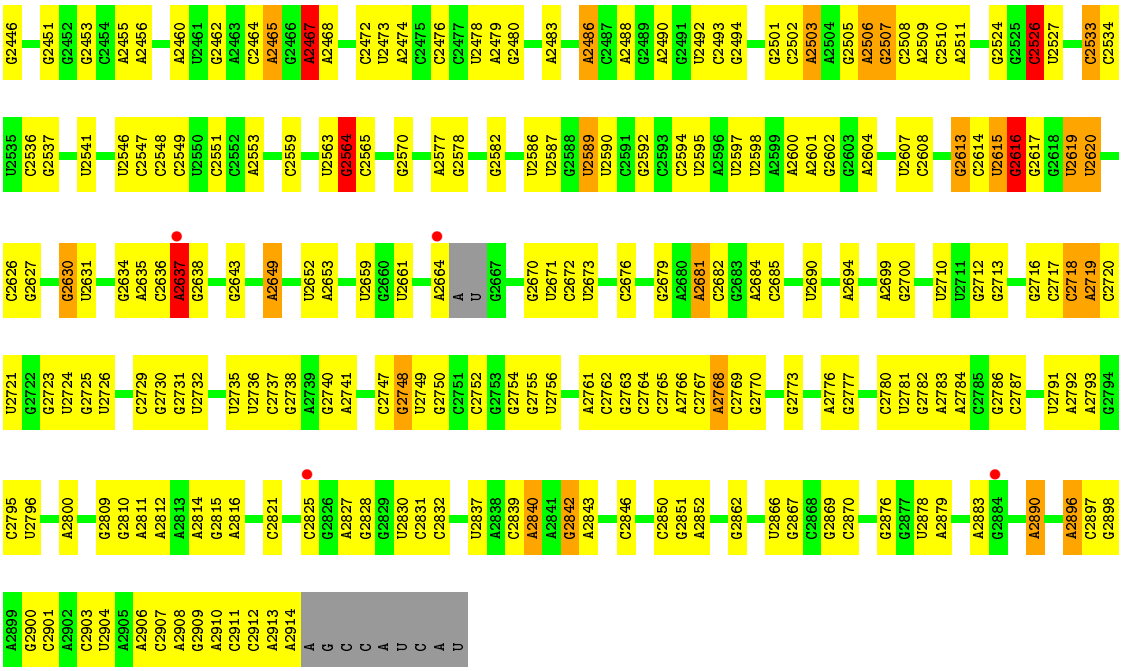
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

Chain A:

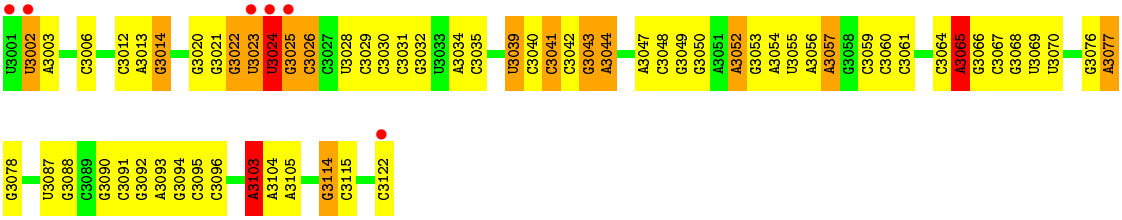



A1078 A1079 C1080 A1081 A1086 G1087 A1088 A1097 A1098 G1099 U1109 G1110 A1114 U1115 U1116 A1117 A1118 G1119 U1120 A1123 C1127 U1128 C1129 U1130 G1131 A1132 A1133 G1134 G1135 U1136 G1137 G1138 U1139 C1140 G1151 A1154 G1155 G1159 G1160 A1161 G1162 G1163 U1164 G1165 A1166 G1167 C1168 U1169 U1170 A1171
G1172 A1173 A1174 G1175 C1176 A1177 U1180 A1181 C1182 C1183 C1184 U1185 C1186 U1187 A1188 A1189 G1190 A1191 A1192 A1193 G1197 U1198 A1199 A1200 C1201 C1204 U1205 U1206 A1207 C1208 C1209 G1210 C1213 G1214 A1215 G1216 G1217 G1224 C1225 G1226 C1229 A1230 A1231 A1232 A1233 U1234 G1235 A1236 U1237 C1238 G1239 A1242 C1243
U1244 C1245 A1246 U1249 C1250 C1251 A1252 C1253 C1262 U1266 C1267 C1268 G1269 U1270 A1271 C1272 C1273 A1278 U1279 U1285 A1286 A1287 U1288 C1289 G1290 U1293 U1298 G1299 U1304 C1305 G1311 G1312 G1315 G1325 A1328 A1329 C1332 U1333 C1334 C1335 C1342 C1343 G1351 A1352 C1353
C1360 C1365 C1366 A1372 C1377 U1380 C1384 G1385 U1388 G1389 A1390 G1391 A1392 A1393 C1394 G1398 A1399 C1400 A1407 G1417 U1418 U1422 C1423 A1424 G1425 C1426 A1427 A1434 U1435 C1436 A1437 G1438 C1439 U1440 G1441 A1442 G1443 G1444 G1445 C1450 C1451 G1452 G1453 C1456 U1457 A1458
C1462 A1463 G1468 G1469 A1470 A1471 C1472 U1473 C1474 C1477 U1478 A1482 C1483 G1484 U1488 A1493 A1494 C1495 G1496 G1497 G1498 U1499 U1500 A1501 A1502 U1503 A1504 U1505 U1506 C1513 C1514 U1517 G1523 U1524 G1525 A1526 A1527 A1528 G1529 G1535 C1536 C1545 G1546 G1555 G1556 A1559 U
U1561 C1562 G1563 C1564 C1565 G1568 U1569 A1572 A1573 A1580 G1589 G1592 C1593 C1594 G1595 U1596 A1597 A1598 U1599 A1603 G1604 G1605 A1606 A1607 C1613 G1614 A1615 A1616 C1617 G1618 G1619 C1620 A1624 C1625 A1626 G1627 A1631 A1632 C1633 G1634 U1635 G1636 A1637 A1641 A1642 C1643 A1653 U1654 G1655
A1656 A1657 C1666 A1667 U1668 A1669 G1670 C1675 C1679 C1680 G1681 A1682 G1683 A1684 A1685 C1686 C1687 C1692 C1699 C1700 A1701 U1702 G1707 C1708 G1709 A1710 A1711 A1712 G1713 C1714 C1715 A1716 A1717 U1722 G1723 U1724 C1725 G1730 C1731 A1732 A1733 C1734 C1735 A1736 G1739 U1740 U1741 A1742 G1743 G1744 G1745
A1746 A1747 G1751 G1752 A1755 G1756 U1761 C1762 C1763 U1766 A1767 C1768 C1769 U1770 U1771 C1772 G1773 A1778 A1779 A1783 U1784 C1787 U1788 G1789 C1790 U1791 C1798 C1803 A1804 G1805 G1806 G1809 C1810 A1811 G1812 A1815 C1816 G1819 G1820 U1825 C1826 G1827 G1828 A1829 C1830 C1834
U1835 A1840 C1841 A1845 U1846 A1847 G1848 G1849 U1850 G1851 A1852 C1853 C1854 G1855 C1856 A1857 C1861 C1862 G1863 C1864 G1868 G1873 U1874 G1877 G1878 U1879 U1883 G1884 A1885 C1886 U1887 U1890 G1896 G1902 U1903 A1904 A1909 A1910 A1919 C1920 A1921 G1926 A1927 A1930 A1931
C1940 A1941 A1942 C1943 G1947 G1948 G1949 G1950 G1951 U A A C U A U G A C C C U1964 C1965 U1966 G1971 U1972 A1973 G1974 A1978 G1979 U1980 C1988 G1989 A1994 G1995 U1996 A1997 G2000 G2001 C2002 U2003 U2004 G2005 U2008 G2009 A2010 A2011 U2012 G2013 A2030 C2031 U2032
G2033 U2034 G2044 G2045 G2046 G2050 A2054 U2064 A2067 G2068 U2069 G2070 C2071 G2072 G2073 A2074 U2078 G2079 G2080 A2081 G2090 G2091 G2094 A2095 A2096 A2101 G2102 A2103 C2104 U2107 A2108 U2109 G2110 G2111 U2115 U2116 G2128 U2133 G2134 A2135 G2136 A C G U G G
U C G C C G A U G U G C A G C A U A G G U A G G A G A C A C U A C A C A G G U A C C C G C G C U A G C G G G C C A C C G
A G U C A A C A G U G A A A U A C U A C C C G U C G G U G A C U G C G2237 A2238 C2241 U2242 C2243 A2244 C2245 U2246 C2247 G2250 G2251 A2252 G2253 G2254 A2255 G2256 G2257 A2258 U2265 A2266 G2267 C2268 C2269
G2270 G2271 G2272 C2273 A2274 G2275 U2276 U2277 C2281 U2282 G2289 U2290 A2291 C2296 U2297 A2300 A2301 A2302 C2309 G2310 C2313 G2314 C2315 G2316 C2317 U2320 A2321 U2322 G2323 G2324 C2325 U2326 C2329 U2330 G2338 A C A G A G2344 A2345 C2346 C2347 C2348 A2353 A2354 G2355 A2356 G2357
U2358 G2359 C2360 A2361 A2362 G2363 A2364 G2365 A2369 U2377 U2378 G2379 A2380 C2381 A2382 G2383 U2384 G2385 U2386 U2387 C2388 C2392 C2403 G2404 C2405 A2408 C2411 G2412 A2413 A2414 A2415 G2418 U2419 G2420 G2421 U2422 G2426 C2427 G2428 A2434 U2435 U2436 A2437 G2438 C2439 C2440 U2441 G2442 C2443 U2444 U2445



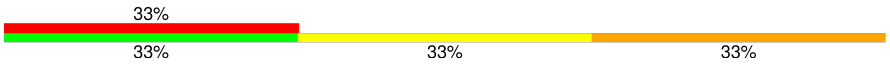
• Molecule 2: 5S ribosomal RNA

Chain B:



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

Chain 5:

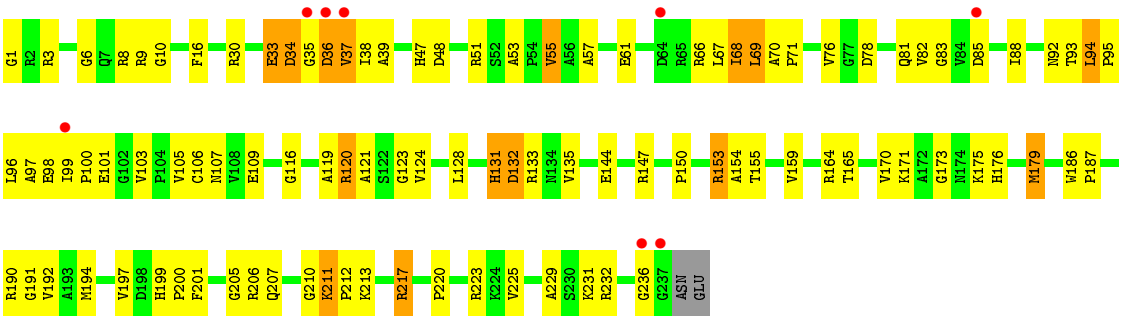


• Molecule 3: CCA-phenylalanine-cariotic-acid-biotin

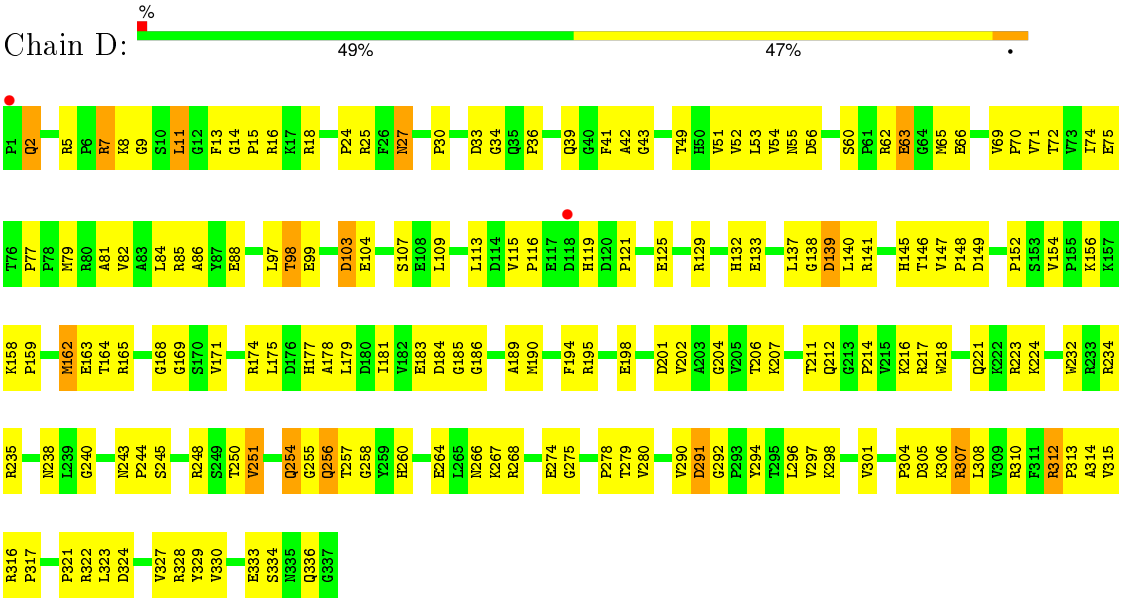
Chain 6:

• Molecule 4: 50S ribosomal protein L2P

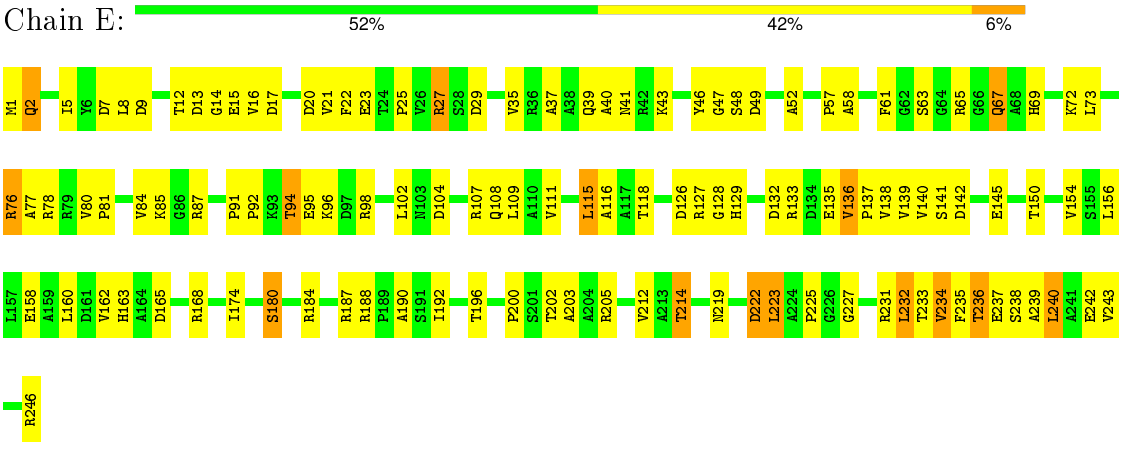
Chain C:



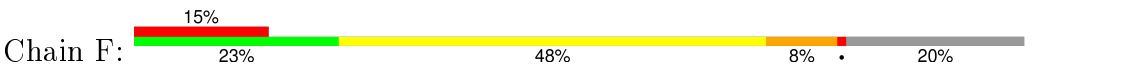
- Molecule 5: 50S ribosomal protein L3P

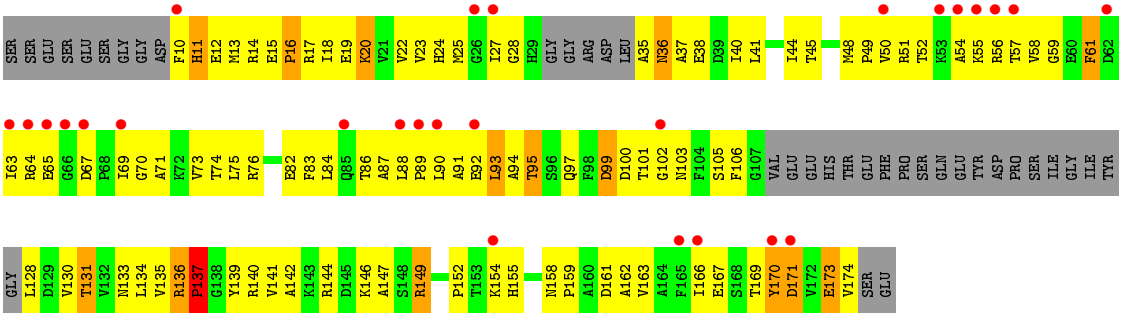


- Molecule 6: 50S ribosomal protein L4E



- Molecule 7: 50S ribosomal protein L5P





- Molecule 8: 50S ribosomal protein L6P

Chain G:

- Molecule 9: 50S ribosomal protein L7Ae

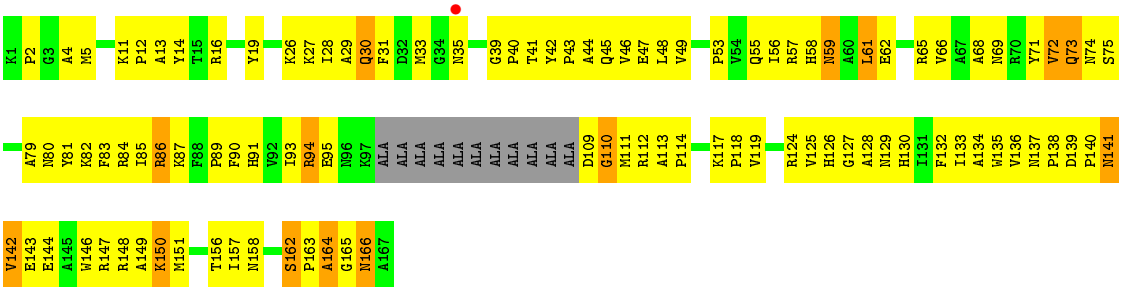
Chain H:

- Molecule 10: Acidic ribosomal protein P0 homolog

Chain I:

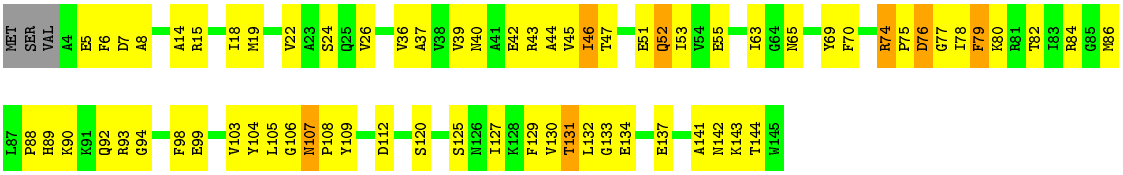
- Molecule 11: L10 Ribosomal Protein

Chain J:



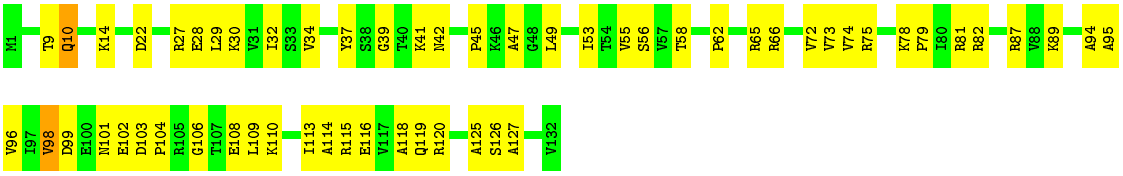
- Molecule 12: 50S ribosomal protein L13P

Chain K:



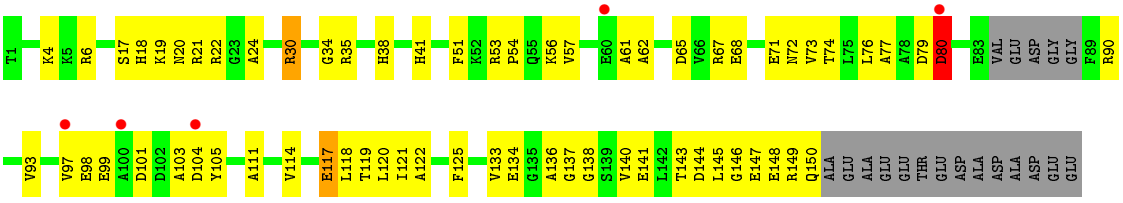
- Molecule 13: 50S ribosomal protein L14P

Chain L:



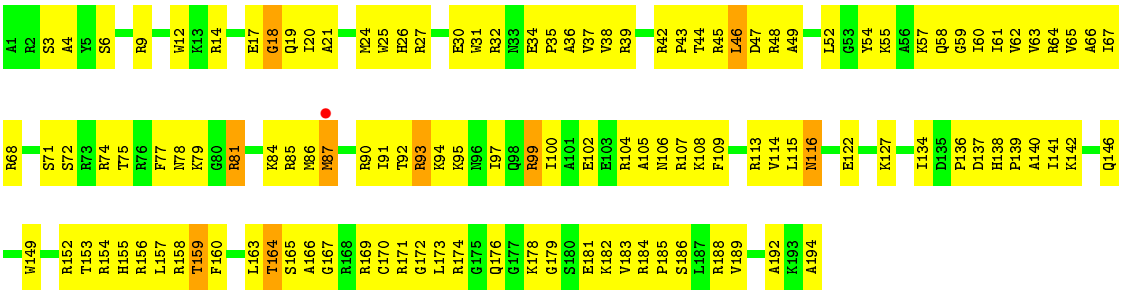
- Molecule 14: 50S ribosomal protein L15P

Chain M:



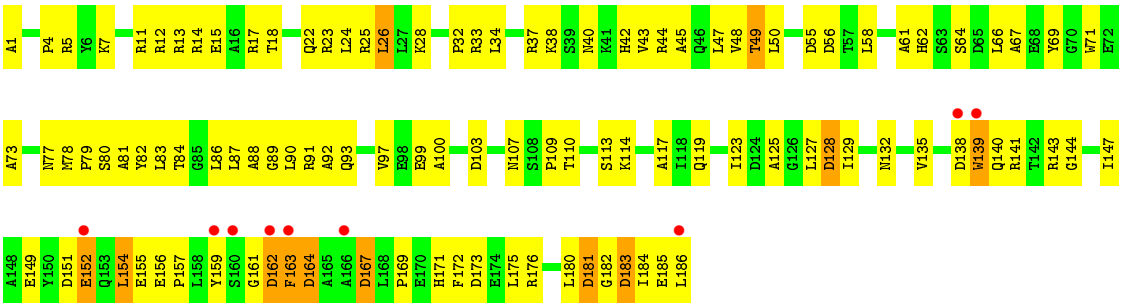
- Molecule 15: L15 Ribosomal Protein

Chain N:



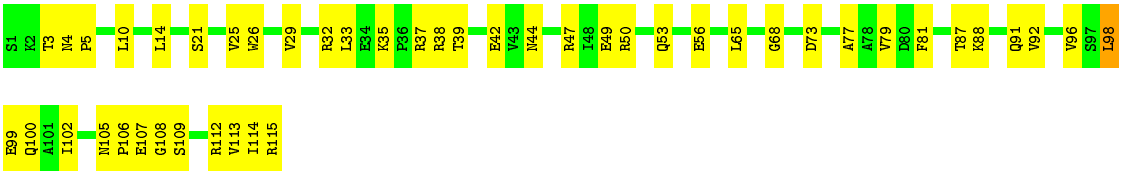
• Molecule 16: 50S ribosomal protein L18P

Chain O:



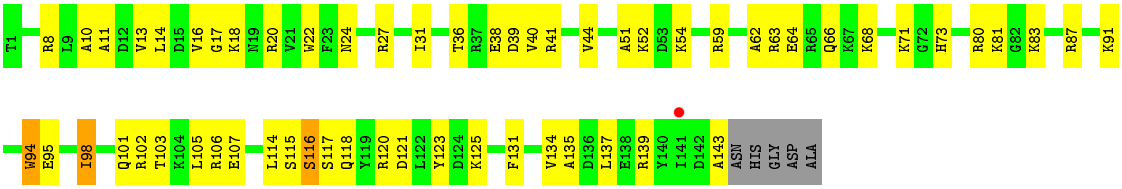
• Molecule 17: 50S ribosomal protein L18e

Chain P:



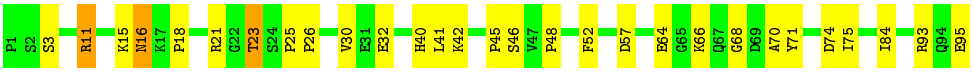
• Molecule 18: 50S ribosomal protein L19E

Chain Q:



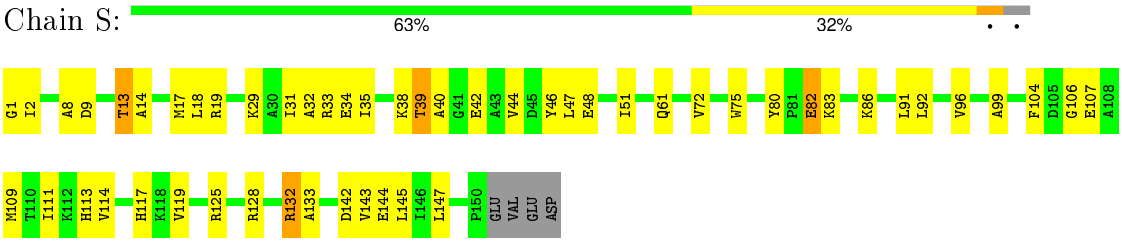
• Molecule 19: 50S ribosomal protein L21e

Chain R:



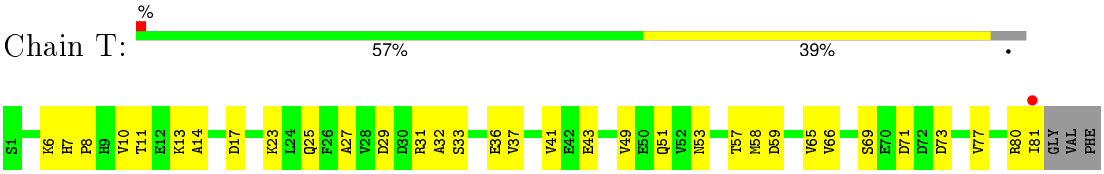
• Molecule 20: 50S ribosomal protein L22P

Chain S:



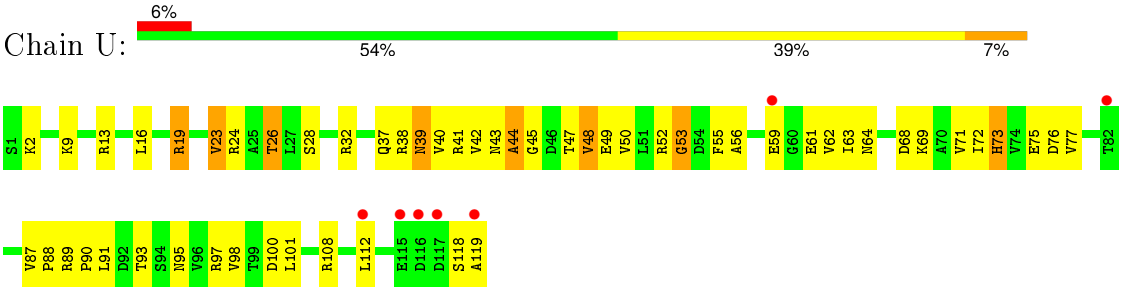
• Molecule 21: 50S ribosomal protein L23P

Chain T:



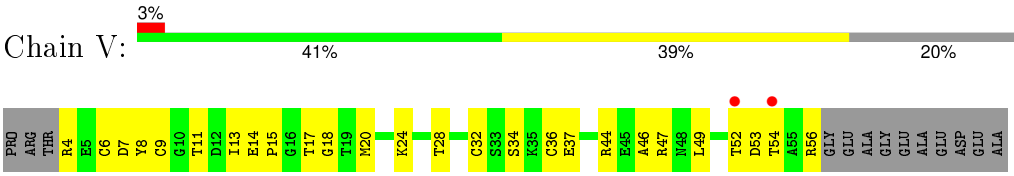
• Molecule 22: 50S ribosomal protein L24P

Chain U:



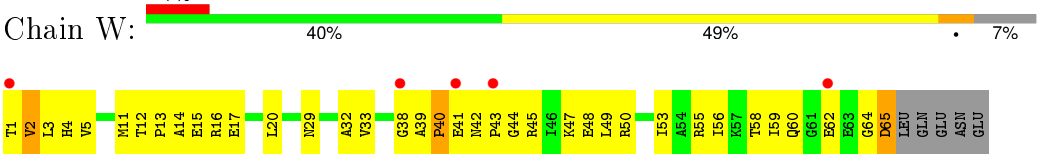
• Molecule 23: 50S ribosomal protein L24E

Chain V:



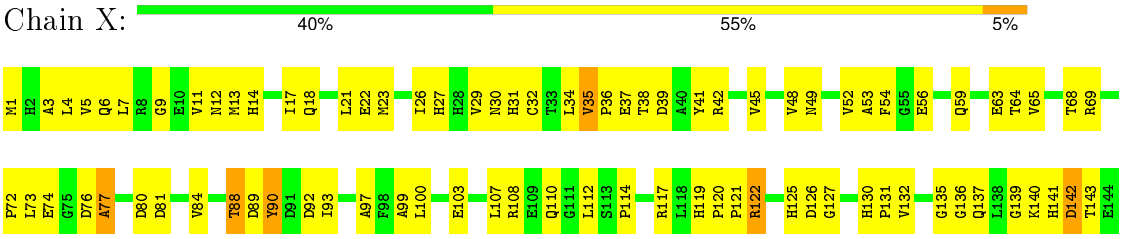
• Molecule 24: 50S ribosomal protein L29P

Chain W:



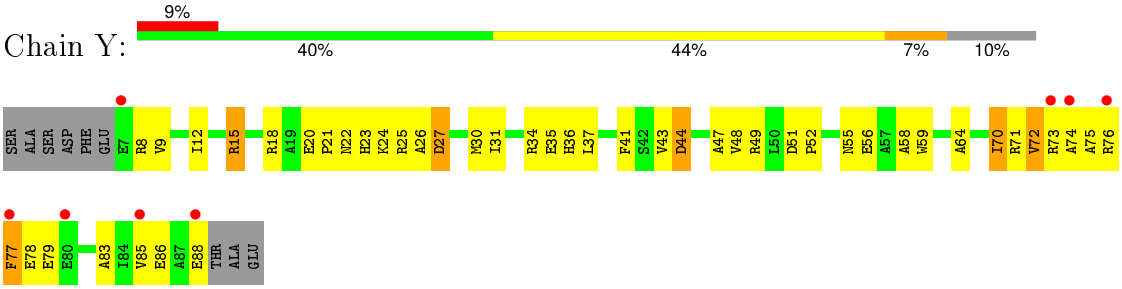
• Molecule 25: 50S ribosomal protein L30P

Chain X:



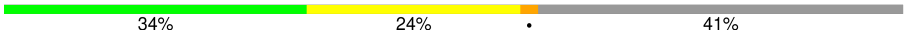
• Molecule 26: 50S ribosomal protein L31e

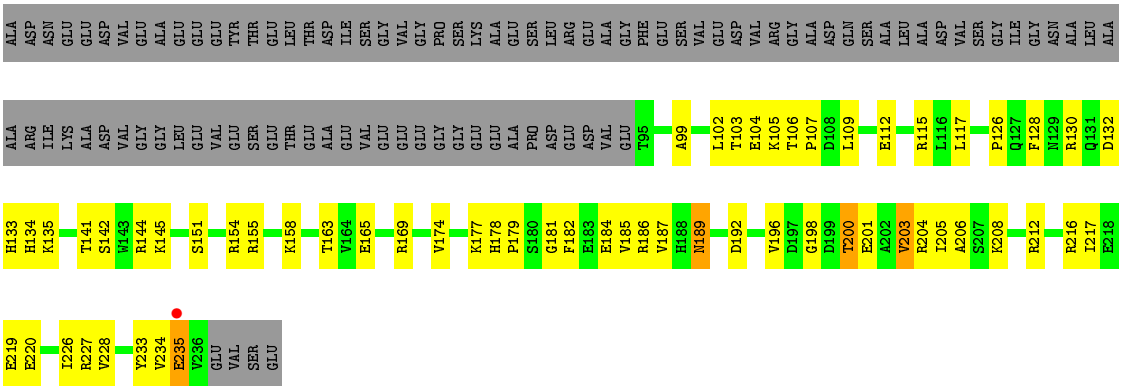
Chain Y:



• Molecule 27: 50S ribosomal protein L32E

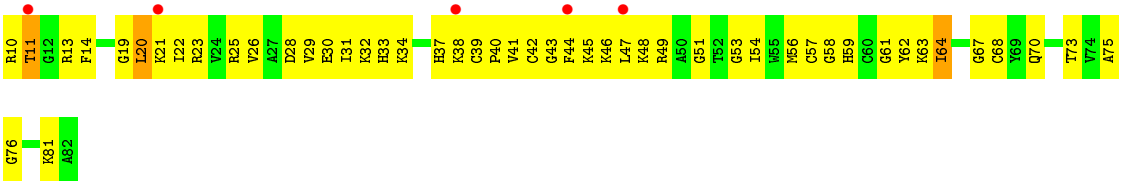
Chain Z:





• Molecule 28: L37Ae 50S ribosomal protein

Chain 1:

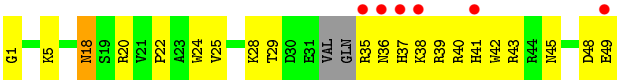


• Molecule 29: 50S ribosomal protein L37e

Chain 2:

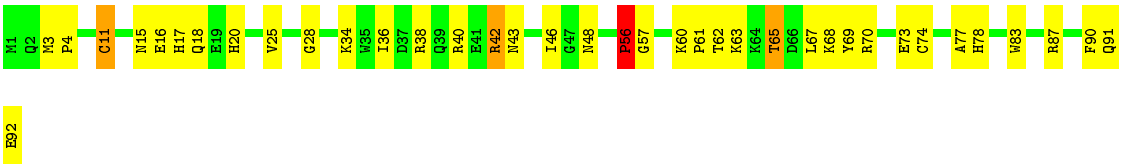
• Molecule 30: 50S ribosomal protein L39e

Chain 3:



- Molecule 31: 50S ribosomal protein L44E

Chain 4:



4 Data and refinement statistics (i)

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 49.62 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.6 (20.00-3.00) 92.8 (49.62-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.264 0.235 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	47.1	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 70.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 447539 reflections	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, NA, PHA, CD, 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	0.41	1/66076 (0.0%)	0.70	24/103052 (0.0%)
2	B	0.37	0/2905	0.75	4/4528 (0.1%)
3	5	0.67	0/65	0.86	0/99
3	6	1.66	2/65 (3.1%)	1.27	0/99
4	C	0.32	0/1787	0.65	0/2409
5	D	0.34	0/2689	0.64	0/3652
6	E	0.38	0/1883	0.65	0/2551
7	F	0.32	0/1111	0.59	0/1498
8	G	0.33	0/1382	0.59	0/1880
9	H	0.31	0/896	0.58	0/1219
10	I	0.29	0/241	0.50	0/324
11	J	0.40	0/1246	0.77	4/1686 (0.2%)
12	K	0.38	0/1135	0.63	0/1530
13	L	0.35	0/1003	0.68	0/1351
14	M	0.32	0/1126	0.65	0/1504
15	N	0.38	0/1633	0.68	0/2180
16	O	0.29	0/1473	0.64	0/1999
17	P	0.34	0/873	0.61	0/1181
18	Q	0.34	0/1143	0.54	0/1521
19	R	0.37	0/748	0.69	1/1005 (0.1%)
20	S	0.36	0/1172	0.67	0/1578
21	T	0.33	0/648	0.58	0/875
22	U	0.31	0/957	0.62	0/1289
23	V	0.33	0/417	0.59	0/562
24	W	0.29	0/502	0.56	0/675
25	X	0.35	0/1218	0.64	0/1655
26	Y	0.35	0/664	0.60	0/895
27	Z	0.36	0/1146	0.65	0/1536
28	1	0.37	0/575	0.69	0/763
29	2	0.37	0/437	0.63	0/578
30	3	0.30	0/398	0.52	0/527
31	4	0.41	0/771	0.62	0/1024

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.39	3/98385 (0.0%)	0.68	33/147225 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	50
2	B	1	3
3	6	0	1
25	X	0	1
All	All	3	55

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	6	75	C	O5'-C5'	5.83	1.53	1.44
1	A	2620	U	N1-C6	5.47	1.42	1.38
3	6	74	C	C2'-O2'	5.05	1.48	1.41

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1563	G	C2'-C3'-O3'	9.42	130.23	109.50
2	B	3024	U	C2'-C3'-O3'	9.17	129.68	109.50
1	A	2637	A	C4'-C3'-O3'	-7.22	94.24	109.40
2	B	3103	A	C5'-C4'-O4'	7.11	117.63	109.10
11	J	74	ASN	N-CA-C	-6.83	92.57	111.00

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

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Mol	Chain	Res	Type	Group
1	A	333	G	Sidechain
1	A	471	G	Sidechain
1	A	482	G	Sidechain
1	A	518	G	Sidechain

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	A	59017	0	29805	1077	0
2	B	2600	0	1326	84	0
3	5	59	0	34	4	0
3	6	59	0	34	0	0
4	C	1754	0	1763	112	0
5	D	2624	0	2533	183	0
6	E	1858	0	1816	135	0
7	F	1094	0	1085	146	0
8	G	1357	0	1266	77	0
9	H	885	0	854	71	0
10	I	240	0	231	23	0
11	J	1215	0	1215	170	0
12	K	1119	0	1098	77	0
13	L	993	0	1027	72	0
14	M	1114	0	1072	66	0
15	N	1605	0	1676	182	0
16	O	1444	0	1401	129	0
17	P	864	0	873	53	0
18	Q	1133	0	1127	62	0
19	R	734	0	729	26	0
20	S	1149	0	1122	67	0
21	T	641	0	605	31	0
22	U	949	0	923	62	0
23	V	410	0	364	35	0
24	W	499	0	511	33	0
25	X	1195	0	1137	118	0
26	Y	654	0	653	51	0
27	Z	1130	0	1133	71	0
28	1	563	0	597	66	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	2	430	0	426	28	0
30	3	393	0	406	32	0
31	4	755	0	728	40	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	5	0
36	6	10	0	7	4	0
37	1	1	0	0	0	0
37	2	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	4	1	0	0	0	0
37	P	1	0	0	0	0
37	V	1	0	0	0	0
38	1	37	0	0	14	0
38	2	63	0	0	4	0
38	3	41	0	0	3	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	12	0
38	D	149	0	0	30	0
38	E	173	0	0	37	0
38	F	52	0	0	22	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	11	0
38	M	82	0	0	18	0
38	N	139	0	0	23	0
38	O	70	0	0	17	0
38	P	43	0	0	13	0
38	Q	67	0	0	5	0
38	R	54	0	0	5	0
38	S	84	0	0	7	0
38	T	37	0	0	6	0
38	U	44	0	0	7	0
38	V	24	0	0	5	0
38	W	14	0	0	3	0
38	X	71	0	0	14	0
38	Y	31	0	0	5	0
38	Z	93	0	0	14	0
All	All	98659	0	59587	3106	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 3106 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
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
1:A:156:C:H5"	15:N:171:ARG:HD3	1.29	1.09

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%)	7 33
5	D	335/337 (99%)	291 (87%)	36 (11%)	8 (2%)	7 35
6	E	244/246 (99%)	210 (86%)	31 (13%)	3 (1%)	16 56
7	F	134/176 (76%)	95 (71%)	28 (21%)	11 (8%)	1 5
8	G	170/177 (96%)	159 (94%)	10 (6%)	1 (1%)	30 72
9	H	117/119 (98%)	100 (86%)	13 (11%)	4 (3%)	5 25
10	I	25/348 (7%)	23 (92%)	1 (4%)	1 (4%)	4 21
11	J	152/167 (91%)	129 (85%)	18 (12%)	5 (3%)	5 26
12	K	140/145 (97%)	126 (90%)	8 (6%)	6 (4%)	3 19
13	L	130/132 (98%)	115 (88%)	13 (10%)	2 (2%)	13 50
14	M	141/164 (86%)	117 (83%)	22 (16%)	2 (1%)	14 51
15	N	192/194 (99%)	164 (85%)	25 (13%)	3 (2%)	12 48
16	O	184/186 (99%)	160 (87%)	17 (9%)	7 (4%)	4 22
17	P	113/115 (98%)	105 (93%)	8 (7%)	0	100 100
18	Q	141/148 (95%)	132 (94%)	8 (6%)	1 (1%)	26 70
19	R	93/95 (98%)	88 (95%)	4 (4%)	1 (1%)	17 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
20	S	148/154 (96%)	134 (90%)	14 (10%)	0	100 100
21	T	79/84 (94%)	71 (90%)	8 (10%)	0	100 100
22	U	117/119 (98%)	103 (88%)	12 (10%)	2 (2%)	11 46
23	V	51/66 (77%)	44 (86%)	6 (12%)	1 (2%)	9 41
24	W	63/70 (90%)	55 (87%)	5 (8%)	3 (5%)	3 17
25	X	152/154 (99%)	142 (93%)	8 (5%)	2 (1%)	15 53
26	Y	80/91 (88%)	70 (88%)	8 (10%)	2 (2%)	7 34
27	Z	140/240 (58%)	135 (96%)	5 (4%)	0	100 100
28	1	71/73 (97%)	59 (83%)	10 (14%)	2 (3%)	6 30
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%)	8 38
All	All	3633/4235 (86%)	3206 (88%)	352 (10%)	75 (2%)	9 40

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 (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
4	C	179/181 (99%)	166 (93%)	13 (7%)	17 52
5	D	282/282 (100%)	267 (95%)	15 (5%)	28 67
6	E	193/193 (100%)	177 (92%)	16 (8%)	14 46
7	F	117/147 (80%)	108 (92%)	9 (8%)	16 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	G	152/155 (98%)	147 (97%)	5 (3%)	45 82
9	H	92/92 (100%)	91 (99%)	1 (1%)	80 94
10	I	27/283 (10%)	27 (100%)	0	100 100
11	J	122/122 (100%)	111 (91%)	11 (9%)	12 41
12	K	118/121 (98%)	107 (91%)	11 (9%)	11 39
13	L	106/106 (100%)	104 (98%)	2 (2%)	65 90
14	M	112/126 (89%)	107 (96%)	5 (4%)	34 74
15	N	166/166 (100%)	157 (95%)	9 (5%)	27 66
16	O	149/149 (100%)	144 (97%)	5 (3%)	44 81
17	P	93/93 (100%)	92 (99%)	1 (1%)	80 94
18	Q	113/116 (97%)	109 (96%)	4 (4%)	43 80
19	R	79/79 (100%)	75 (95%)	4 (5%)	29 69
20	S	117/121 (97%)	113 (97%)	4 (3%)	44 81
21	T	71/73 (97%)	70 (99%)	1 (1%)	74 93
22	U	105/105 (100%)	99 (94%)	6 (6%)	25 64
23	V	44/52 (85%)	44 (100%)	0	100 100
24	W	51/56 (91%)	50 (98%)	1 (2%)	63 89
25	X	130/130 (100%)	124 (95%)	6 (5%)	33 73
26	Y	66/73 (90%)	61 (92%)	5 (8%)	16 51
27	Z	120/195 (62%)	115 (96%)	5 (4%)	36 76
28	1	56/56 (100%)	54 (96%)	2 (4%)	42 79
29	2	46/46 (100%)	46 (100%)	0	100 100
30	3	42/44 (96%)	41 (98%)	1 (2%)	57 87
31	4	79/79 (100%)	75 (95%)	4 (5%)	29 69
All	All	3027/3441 (88%)	2881 (95%)	146 (5%)	31 71

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	J	94	ARG
13	L	10	GLN
27	Z	163	THR
11	J	142	VAL
12	K	76	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 97 such sidechains are listed below:

Mol	Chain	Res	Type
13	L	10	GLN
18	Q	66	GLN
29	2	28	HIS
14	M	41	HIS
15	N	176	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2747/2922 (94%)	244 (8%)	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%)	261 (9%)	35 (1%)

5 of 261 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	1352	A
1	A	1667	A
2	B	3024	U
1	A	1377	C
1	A	1450	C

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

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	5	77	3	10,11,11	0.85	0	10,13,13	1.01	0
36	PHA	6	77	3	10,10,11	0.71	0	10,11,13	0.38	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	5	77	3	-	0/4/6/6	0/1/1/1
36	PHA	6	77	3	-	0/3/4/6	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
36	5	77	PHA	5	0
36	6	77	PHA	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	A	2754/2922 (94%)	0.18	51 (1%) 70 41	19, 47, 95, 154	0
2	B	122/122 (100%)	0.16	6 (4%) 33 13	30, 62, 92, 154	0
3	5	3/3 (100%)	1.71	1 (33%) 0 0	29, 29, 31, 35	3 (100%)
3	6	3/3 (100%)	2.49	3 (100%) 0 0	15, 15, 17, 31	3 (100%)
4	C	237/239 (99%)	0.24	8 (3%) 49 21	27, 52, 91, 115	0
5	D	337/337 (100%)	0.06	2 (0%) 90 73	26, 55, 84, 96	0
6	E	246/246 (100%)	-0.20	0 100 100	19, 47, 71, 80	0
7	F	140/176 (79%)	1.00	27 (19%) 2 1	53, 101, 124, 131	0
8	G	172/177 (97%)	0.32	4 (2%) 64 33	41, 68, 91, 99	0
9	H	119/119 (100%)	0.50	5 (4%) 40 16	53, 77, 104, 111	0
10	I	29/348 (8%)	1.28	4 (13%) 4 1	66, 86, 97, 103	0
11	J	156/167 (93%)	-0.07	1 (0%) 90 73	30, 52, 77, 81	0
12	K	142/145 (97%)	-0.17	0 100 100	34, 47, 71, 90	0
13	L	132/132 (100%)	0.01	0 100 100	31, 53, 78, 86	0
14	M	145/164 (88%)	0.10	5 (3%) 49 21	21, 67, 108, 117	0
15	N	194/194 (100%)	-0.02	1 (0%) 91 76	30, 47, 68, 80	0
16	O	186/186 (100%)	0.19	9 (4%) 34 14	35, 65, 112, 125	0
17	P	115/115 (100%)	-0.09	0 100 100	36, 54, 74, 83	0
18	Q	143/148 (96%)	0.42	1 (0%) 89 70	36, 57, 71, 80	0
19	R	95/95 (100%)	-0.25	0 100 100	32, 42, 57, 73	0
20	S	150/154 (97%)	-0.01	0 100 100	29, 43, 64, 75	0
21	T	81/84 (96%)	0.26	1 (1%) 81 55	41, 62, 81, 85	0
22	U	119/119 (100%)	0.39	7 (5%) 26 10	38, 60, 86, 105	0
23	V	53/66 (80%)	0.41	2 (3%) 44 18	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%)	0.88	5 (7%) 16 6	56, 79, 120, 125	0
25	X	154/154 (100%)	-0.38	0 100 100	29, 45, 62, 74	0
26	Y	82/91 (90%)	0.55	8 (9%) 10 4	42, 56, 79, 100	0
27	Z	142/240 (59%)	-0.10	1 (0%) 89 70	25, 45, 67, 86	0
28	1	73/73 (100%)	0.34	5 (6%) 20 7	43, 61, 76, 81	0
29	2	56/56 (100%)	-0.26	0 100 100	24, 33, 39, 41	0
30	3	46/48 (95%)	0.89	6 (13%) 5 2	35, 65, 118, 126	0
31	4	92/92 (100%)	0.06	0 100 100	39, 55, 69, 78	0
All	All	6583/7285 (90%)	0.16	163 (2%) 61 30	15, 52, 97, 154	6 (0%)

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
24	W	1	THR	12.4
2	B	3001	U	7.8
1	A	2237	G	5.4
1	A	1172	G	5.3
7	F	66	GLY	5.3

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
34	NA	A	8356	1/1	0.90	0.70	32.93	44,44,44,44	0
34	NA	A	8326	1/1	0.86	1.04	30.44	54,54,54,54	0
34	NA	A	8371	1/1	0.90	0.53	28.08	62,62,62,62	0
34	NA	A	8359	1/1	0.62	0.74	26.75	48,48,48,48	0
35	CL	A	8515	1/1	0.82	0.57	23.73	85,85,85,85	0
34	NA	A	8372	1/1	0.64	0.56	19.68	55,55,55,55	0
34	NA	A	8350	1/1	0.77	0.44	18.00	36,36,36,36	0
34	NA	A	8378	1/1	0.93	0.59	14.70	46,46,46,46	0
34	NA	A	8377	1/1	0.74	0.41	14.05	76,76,76,76	0
34	NA	A	8367	1/1	0.97	0.36	13.83	48,48,48,48	0
34	NA	S	8386	1/1	0.35	0.80	13.43	63,63,63,63	0
34	NA	A	8320	1/1	0.80	0.25	13.11	24,24,24,24	0
34	NA	A	8340	1/1	0.77	0.31	11.38	38,38,38,38	0
34	NA	A	8362	1/1	0.95	0.30	11.14	70,70,70,70	0
34	NA	A	8321	1/1	0.91	0.40	10.74	49,49,49,49	0
34	NA	A	8374	1/1	0.79	0.28	9.52	60,60,60,60	0
34	NA	B	8383	1/1	0.88	0.28	6.70	72,72,72,72	0
33	K	A	8201	1/1	0.89	0.32	6.18	76,76,76,76	0
34	NA	A	8332	1/1	0.93	0.28	6.04	35,35,35,35	0
34	NA	A	8325	1/1	0.92	0.25	5.25	49,49,49,49	0
34	NA	N	8365	1/1	0.87	0.49	4.90	46,46,46,46	0
34	NA	A	8361	1/1	0.92	0.27	4.86	48,48,48,48	0
34	NA	A	8323	1/1	0.91	0.30	4.71	34,34,34,34	0
34	NA	A	8373	1/1	0.85	0.40	4.70	45,45,45,45	0
32	MG	A	8112	1/1	0.87	0.27	4.21	43,43,43,43	0
34	NA	A	8339	1/1	0.97	0.22	4.10	14,14,14,14	0
32	MG	6	8118	1/1	0.65	0.68	3.58	61,61,61,61	0
36	PHA	5	77	11/11	0.70	0.51	3.44	24,25,29,29	11
34	NA	M	8380	1/1	0.94	0.27	3.36	61,61,61,61	0
35	CL	D	8519	1/1	0.93	0.27	2.78	47,47,47,47	0
34	NA	A	8305	1/1	0.86	0.21	2.78	27,27,27,27	0
34	NA	A	8376	1/1	0.92	0.21	2.42	42,42,42,42	0
34	NA	A	8366	1/1	0.45	0.24	2.41	51,51,51,51	0
32	MG	A	8049	1/1	0.91	0.24	2.37	67,67,67,67	0
34	NA	K	8346	1/1	0.85	0.30	2.24	33,33,33,33	0
34	NA	A	8382	1/1	0.71	0.25	2.15	54,54,54,54	0
32	MG	A	8067	1/1	0.91	0.28	1.79	55,55,55,55	0
34	NA	A	8303	1/1	0.92	0.22	1.76	55,55,55,55	0
34	NA	A	8327	1/1	0.74	0.21	1.59	34,34,34,34	0
32	MG	A	8044	1/1	0.75	0.20	1.57	50,50,50,50	0
32	MG	A	8064	1/1	0.92	0.20	1.52	29,29,29,29	0
34	NA	A	8335	1/1	0.92	0.21	1.41	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
34	NA	A	8368	1/1	0.80	0.22	1.10	69,69,69,69	0
34	NA	A	8324	1/1	0.59	0.31	1.09	58,58,58,58	0
35	CL	P	8508	1/1	0.72	0.22	0.86	72,72,72,72	0
32	MG	A	8059	1/1	0.73	0.20	0.60	65,65,65,65	0
34	NA	S	8338	1/1	0.85	0.23	0.38	48,48,48,48	0
35	CL	4	8504	1/1	0.90	0.27	0.26	56,56,56,56	0
34	NA	A	8364	1/1	0.94	0.19	0.12	39,39,39,39	0
34	NA	A	8314	1/1	0.91	0.17	-0.26	21,21,21,21	0
35	CL	M	8510	1/1	0.90	0.19	-0.64	57,57,57,57	0
32	MG	A	8071	1/1	0.76	0.19	-0.71	80,80,80,80	0
35	CL	K	8521	1/1	0.90	0.19	-0.80	51,51,51,51	0
34	NA	A	8317	1/1	0.66	0.19	-0.84	63,63,63,63	0
34	NA	A	8381	1/1	0.83	0.16	-1.07	54,54,54,54	0
34	NA	N	8347	1/1	0.89	0.16	-1.07	36,36,36,36	0
35	CL	A	8505	1/1	0.87	0.16	-1.20	60,60,60,60	0
34	NA	S	8337	1/1	0.89	0.18	-1.21	45,45,45,45	0
32	MG	A	8096	1/1	0.75	0.18	-1.27	46,46,46,46	0
34	NA	U	8343	1/1	0.93	0.18	-1.41	23,23,23,23	0
32	MG	U	8073	1/1	0.68	0.27	-1.50	52,52,52,52	0
34	NA	C	8345	1/1	0.84	0.18	-1.51	48,48,48,48	0
32	MG	4	8078	1/1	0.73	0.12	-1.61	63,63,63,63	0
34	NA	E	8304	1/1	0.92	0.18	-1.84	39,39,39,39	0
34	NA	A	8353	1/1	0.89	0.13	-1.92	26,26,26,26	0
37	CD	4	8404	1/1	0.97	0.08	-2.00	63,63,63,63	0
37	CD	1	8403	1/1	0.86	0.09	-2.16	60,60,60,60	0
35	CL	L	8512	1/1	0.82	0.15	-2.26	47,47,47,47	0
32	MG	C	8065	1/1	0.58	0.16	-2.35	40,40,40,40	0
32	MG	A	8107	1/1	0.96	0.06	-2.41	39,39,39,39	0
34	NA	A	8333	1/1	0.87	0.11	-2.52	24,24,24,24	0
34	NA	J	8309	1/1	0.96	0.12	-2.55	31,31,31,31	0
37	CD	V	8401	1/1	0.89	0.07	-2.60	69,69,69,69	0
32	MG	A	8058	1/1	0.84	0.15	-2.67	33,33,33,33	0
35	CL	N	8518	1/1	0.96	0.12	-2.70	41,41,41,41	0
32	MG	D	8056	1/1	0.92	0.14	-2.87	44,44,44,44	0
32	MG	Z	8109	1/1	0.83	0.11	-2.90	28,28,28,28	0
32	MG	A	8052	1/1	0.96	0.12	-2.92	39,39,39,39	0
32	MG	A	8014	1/1	0.93	0.12	-2.95	21,21,21,21	0
32	MG	A	8108	1/1	0.94	0.12	-2.95	72,72,72,72	0
32	MG	D	8055	1/1	0.89	0.09	-3.19	34,34,34,34	0
34	NA	A	8331	1/1	0.94	0.12	-3.19	34,34,34,34	0
32	MG	A	8013	1/1	0.89	0.15	-3.22	45,45,45,45	0
32	MG	A	8012	1/1	0.98	0.10	-3.30	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8027	1/1	0.98	0.07	-3.37	35,35,35,35	0
32	MG	A	8015	1/1	0.84	0.09	-3.55	38,38,38,38	0
32	MG	A	8080	1/1	0.72	0.14	-3.90	33,33,33,33	0
37	CD	2	8402	1/1	0.94	0.07	-3.98	64,64,64,64	0
34	NA	R	8348	1/1	0.99	0.10	-4.03	29,29,29,29	0
32	MG	A	8074	1/1	0.96	0.05	-4.15	15,15,15,15	0
32	MG	A	8003	1/1	0.96	0.10	-4.27	29,29,29,29	0
32	MG	A	8054	1/1	0.82	0.12	-4.45	37,37,37,37	0
32	MG	A	8077	1/1	0.93	0.11	-4.48	33,33,33,33	0
32	MG	A	8039	1/1	0.87	0.10	-4.52	52,52,52,52	0
32	MG	A	8091	1/1	0.79	0.09	-4.56	53,53,53,53	0
34	NA	A	8379	1/1	0.90	0.12	-5.22	34,34,34,34	0
32	MG	A	8057	1/1	0.94	0.10	-5.31	34,34,34,34	0
34	NA	A	8308	1/1	0.93	0.12	-5.85	49,49,49,49	0
32	MG	A	8020	1/1	0.89	0.14	-5.92	27,27,27,27	0
32	MG	A	8032	1/1	0.87	0.09	-5.97	24,24,24,24	0
32	MG	A	8004	1/1	0.91	0.09	-6.10	28,28,28,28	0
32	MG	A	8001	1/1	0.91	0.09	-6.28	23,23,23,23	0
32	MG	A	8017	1/1	0.97	0.04	-6.58	24,24,24,24	0
32	MG	A	8053	1/1	0.93	0.12	-6.72	39,39,39,39	0
32	MG	A	8002	1/1	0.95	0.07	-6.84	33,33,33,33	0
32	MG	A	8038	1/1	0.97	0.09	-6.89	29,29,29,29	0
32	MG	A	8060	1/1	0.94	0.10	-7.07	49,49,49,49	0
32	MG	A	8018	1/1	0.93	0.09	-7.24	44,44,44,44	0
32	MG	A	8007	1/1	0.91	0.09	-7.61	19,19,19,19	0
32	MG	A	8035	1/1	0.77	0.11	-7.83	54,54,54,54	0
34	NA	A	8344	1/1	0.94	0.09	-8.42	17,17,17,17	0
32	MG	A	8062	1/1	0.87	0.09	-9.12	61,61,61,61	0
33	K	A	8202	1/1	0.98	0.08	-9.85	53,53,53,53	0
32	MG	A	8006	1/1	0.86	0.09	-10.67	34,34,34,34	0
32	MG	A	8033	1/1	0.91	0.06	-12.13	22,22,22,22	0
32	MG	A	8019	1/1	0.82	0.09	-13.03	15,15,15,15	0
32	MG	A	8084	1/1	0.82	0.14	-13.42	56,56,56,56	0
32	MG	A	8010	1/1	0.89	0.09	-16.64	26,26,26,26	0
32	MG	A	8008	1/1	0.91	0.07	-17.80	20,20,20,20	0
36	PHA	6	77	10/11	0.69	0.42	-	35,38,41,41	10
32	MG	A	8037	1/1	0.87	0.12	-	46,46,46,46	0
34	NA	A	8334	1/1	0.91	0.11	-	46,46,46,46	0
32	MG	A	8100	1/1	0.92	0.25	-	53,53,53,53	0
32	MG	A	8031	1/1	0.96	0.11	-	19,19,19,19	0
32	MG	A	8115	1/1	0.74	0.20	-	36,36,36,36	0
32	MG	A	8079	1/1	0.96	0.07	-	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8113	1/1	0.70	0.18	-	43,43,43,43	0
34	NA	A	8349	1/1	0.95	0.20	-	40,40,40,40	0
32	MG	A	8117	1/1	0.81	0.13	-	26,26,26,26	0
34	NA	A	8355	1/1	0.90	0.65	-	72,72,72,72	0
34	NA	A	8369	1/1	0.60	0.38	-	59,59,59,59	0
35	CL	O	8507	1/1	0.90	0.34	-	63,63,63,63	0
32	MG	A	8021	1/1	0.85	0.11	-	22,22,22,22	0
34	NA	A	8370	1/1	0.79	0.30	-	50,50,50,50	0
32	MG	A	8034	1/1	0.97	0.05	-	24,24,24,24	0
35	CL	A	8516	1/1	0.87	0.19	-	51,51,51,51	0
34	NA	A	8301	1/1	0.91	0.14	-	26,26,26,26	0
32	MG	A	8081	1/1	0.76	0.09	-	51,51,51,51	0
32	MG	A	8045	1/1	0.86	0.19	-	52,52,52,52	0
32	MG	A	8005	1/1	0.95	0.10	-	32,32,32,32	0
32	MG	A	8051	1/1	0.96	0.22	-	87,87,87,87	0
32	MG	A	8063	1/1	0.85	0.10	-	54,54,54,54	0
32	MG	A	8106	1/1	0.59	0.17	-	45,45,45,45	0
34	NA	A	8329	1/1	0.74	0.38	-	65,65,65,65	0
34	NA	A	8342	1/1	0.86	0.21	-	34,34,34,34	0
32	MG	A	8082	1/1	0.90	0.27	-	51,51,51,51	0
32	MG	A	8097	1/1	0.92	0.12	-	27,27,27,27	0
35	CL	S	8506	1/1	0.92	0.22	-	41,41,41,41	0
32	MG	A	8104	1/1	0.76	0.29	-	51,51,51,51	0
32	MG	B	8095	1/1	0.91	0.10	-	69,69,69,69	0
34	NA	A	8316	1/1	0.85	0.23	-	30,30,30,30	0
32	MG	A	8028	1/1	0.89	0.06	-	30,30,30,30	0
32	MG	A	8025	1/1	0.95	0.09	-	63,63,63,63	0
32	MG	A	8042	1/1	0.93	0.10	-	35,35,35,35	0
32	MG	A	8094	1/1	0.86	0.15	-	67,67,67,67	0
35	CL	A	8503	1/1	0.90	0.24	-	47,47,47,47	0
32	MG	A	8026	1/1	0.96	0.10	-	20,20,20,20	0
32	MG	A	8102	1/1	0.90	0.09	-	53,53,53,53	0
35	CL	K	8502	1/1	0.89	0.14	-	62,62,62,62	0
32	MG	A	8030	1/1	0.88	0.10	-	23,23,23,23	0
32	MG	A	8070	1/1	0.91	0.28	-	36,36,36,36	0
32	MG	L	8069	1/1	0.91	0.09	-	56,56,56,56	0
34	NA	A	8302	1/1	0.91	0.34	-	39,39,39,39	0
34	NA	A	8306	1/1	0.88	0.84	-	42,42,42,42	0
34	NA	A	8318	1/1	0.87	0.61	-	37,37,37,37	0
32	MG	A	8092	1/1	0.78	0.33	-	92,92,92,92	0
35	CL	A	8511	1/1	0.84	0.19	-	65,65,65,65	0
34	NA	B	8351	1/1	0.69	0.30	-	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8110	1/1	0.75	0.14	-	29,29,29,29	0
32	MG	A	8036	1/1	0.94	0.10	-	27,27,27,27	0
34	NA	A	8310	1/1	0.80	0.38	-	33,33,33,33	0
32	MG	A	8083	1/1	0.95	0.05	-	43,43,43,43	0
32	MG	A	8022	1/1	0.90	0.06	-	17,17,17,17	0
32	MG	A	8043	1/1	0.91	0.16	-	38,38,38,38	0
35	CL	A	8522	1/1	0.92	0.31	-	78,78,78,78	0
32	MG	A	8016	1/1	0.75	0.22	-	38,38,38,38	0
32	MG	A	8090	1/1	0.78	0.35	-	62,62,62,62	0
35	CL	A	8517	1/1	0.96	0.10	-	61,61,61,61	0
32	MG	A	8024	1/1	0.65	0.81	-	95,95,95,95	0
32	MG	A	8023	1/1	0.94	0.08	-	34,34,34,34	0
32	MG	A	8093	1/1	0.96	0.12	-	48,48,48,48	0
34	NA	A	8341	1/1	0.96	0.11	-	28,28,28,28	0
34	NA	A	8385	1/1	0.62	0.28	-	43,43,43,43	0
34	NA	A	8375	1/1	0.78	0.73	-	63,63,63,63	0
34	NA	J	8322	1/1	0.77	0.31	-	68,68,68,68	0
32	MG	A	8041	1/1	0.56	0.21	-	79,79,79,79	0
32	MG	A	8088	1/1	0.86	0.21	-	23,23,23,23	0
32	MG	A	8066	1/1	0.88	0.11	-	72,72,72,72	0
34	NA	A	8357	1/1	0.81	0.09	-	53,53,53,53	0
32	MG	A	8029	1/1	0.64	0.15	-	53,53,53,53	0
34	NA	A	8384	1/1	0.23	0.69	-	101,101,101,101	0
32	MG	A	8061	1/1	0.87	0.11	-	25,25,25,25	0
34	NA	A	8319	1/1	0.77	0.15	-	33,33,33,33	0
32	MG	1	8105	1/1	0.67	0.46	-	30,30,30,30	0
32	MG	A	8111	1/1	0.79	0.15	-	67,67,67,67	0
34	NA	A	8328	1/1	0.76	0.55	-	54,54,54,54	0
34	NA	A	8354	1/1	0.79	0.54	-	31,31,31,31	0
34	NA	A	8311	1/1	0.92	0.17	-	52,52,52,52	0
34	NA	A	8358	1/1	0.83	0.45	-	113,113,113,113	0
32	MG	A	8103	1/1	0.94	0.13	-	73,73,73,73	0
35	CL	A	8514	1/1	0.76	0.29	-	55,55,55,55	0
32	MG	A	8116	1/1	0.79	0.12	-	67,67,67,67	0
32	MG	A	8040	1/1	0.65	0.17	-	71,71,71,71	0
35	CL	A	8513	1/1	0.94	0.13	-	50,50,50,50	0
34	NA	A	8307	1/1	0.79	0.24	-	53,53,53,53	0
34	NA	A	8330	1/1	0.81	0.40	-	42,42,42,42	0
32	MG	A	8047	1/1	0.95	0.17	-	58,58,58,58	0
35	CL	Z	8520	1/1	0.89	0.12	-	39,39,39,39	0
32	MG	A	8076	1/1	0.54	0.16	-	37,37,37,37	0
35	CL	K	8501	1/1	0.79	0.13	-	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
32	MG	A	8086	1/1	0.86	0.16	-	49,49,49,49	0
32	MG	A	8089	1/1	0.91	0.21	-	60,60,60,60	0
35	CL	C	8509	1/1	0.96	0.17	-	55,55,55,55	0
32	MG	A	8087	1/1	0.88	0.10	-	56,56,56,56	0
32	MG	A	8085	1/1	0.91	0.17	-	61,61,61,61	0
32	MG	A	8075	1/1	0.84	0.15	-	64,64,64,64	0
32	MG	A	8072	1/1	0.95	0.14	-	44,44,44,44	0
32	MG	A	8099	1/1	0.89	0.15	-	32,32,32,32	0
32	MG	A	8011	1/1	0.73	0.10	-	37,37,37,37	0
32	MG	A	8101	1/1	0.94	0.22	-	54,54,54,54	0
34	NA	A	8315	1/1	0.92	0.30	-	29,29,29,29	0
32	MG	A	8048	1/1	0.91	0.09	-	57,57,57,57	0
34	NA	A	8313	1/1	0.82	0.23	-	44,44,44,44	0
34	NA	A	8360	1/1	0.90	0.46	-	45,45,45,45	0
34	NA	T	8312	1/1	0.71	0.47	-	108,108,108,108	0
34	NA	A	8352	1/1	0.74	0.44	-	51,51,51,51	0
37	CD	P	8405	1/1	0.72	0.12	-	184,184,184,184	0
32	MG	A	8114	1/1	0.46	0.29	-	51,51,51,51	0
34	NA	A	8363	1/1	0.94	0.20	-	46,46,46,46	0
32	MG	A	8050	1/1	0.94	0.09	-	65,65,65,65	0
32	MG	A	8046	1/1	0.39	0.18	-	45,45,45,45	0
32	MG	A	8009	1/1	0.84	0.08	-	15,15,15,15	0
34	NA	A	8336	1/1	0.79	0.18	-	41,41,41,41	0
32	MG	A	8068	1/1	0.84	0.16	-	58,58,58,58	0
32	MG	A	8098	1/1	0.94	0.20	-	28,28,28,28	0

6.5 Other polymers (i)

There are no such residues in this entry.