wwPDB EM Validation Summary Report ⓘ

Apr 16, 2024 – 02:51 am BST

PDB ID	:	7Q4K
EMDB ID	:	EMD-13805
Title	:	Erythromycin-stalled Escherichia coli 70S ribosome with streptococcal MsrDL nascent chain
Authors	:	Fostier, C.R.; Ousalem, F.; Soufari, H.; Leroy, E.C.; Ngo, S.; Innis, A.; Hashem, Y.; Boel, G.
Deposited on	:	2021-10-31
Resolution	:	3.00 Å(reported)

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

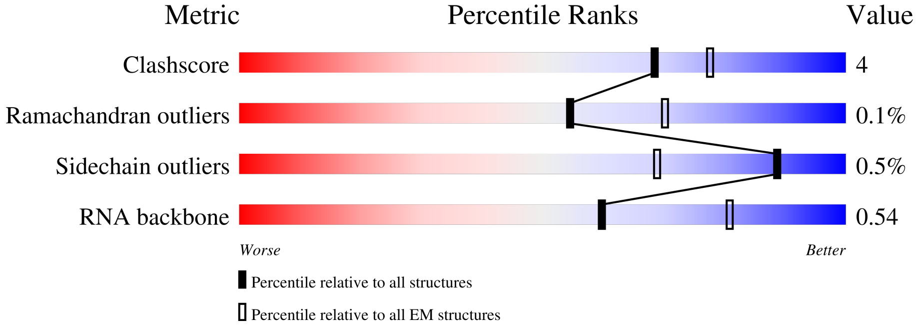
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

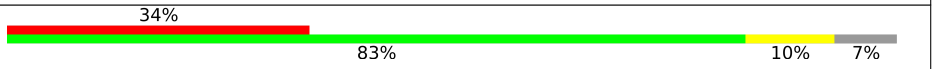
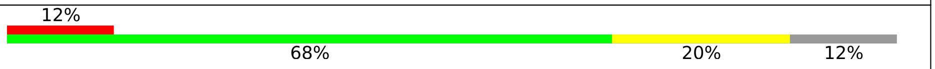
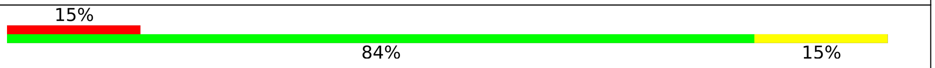
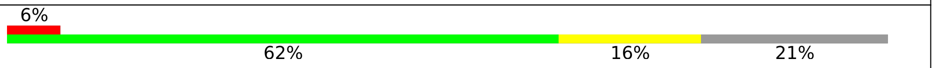
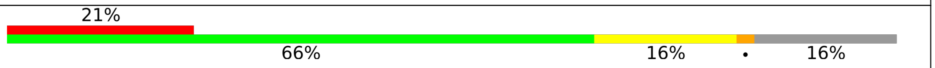
The reported resolution of this entry is 3.00 Å.

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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1534	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	135	
7	AG	179	

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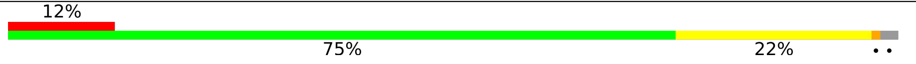
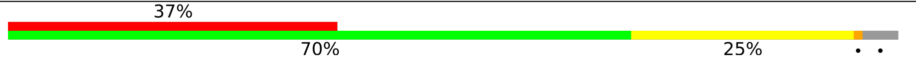
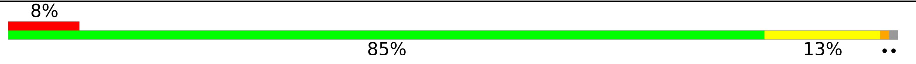
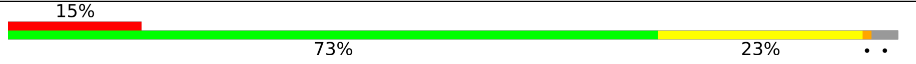
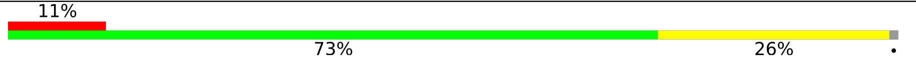
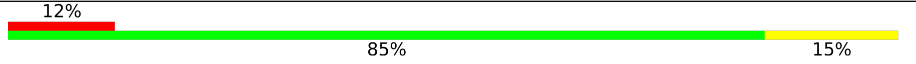
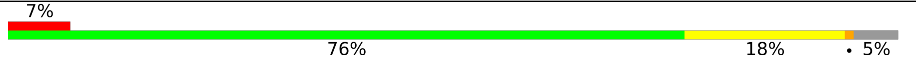
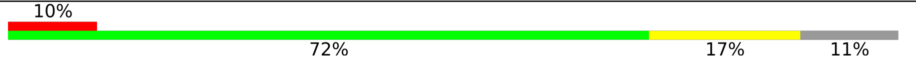
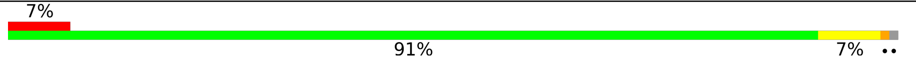
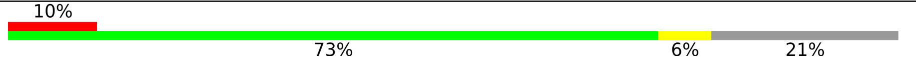
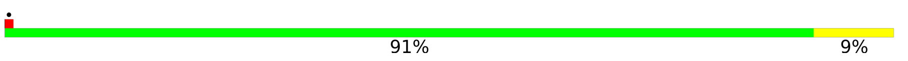
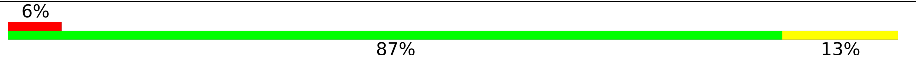
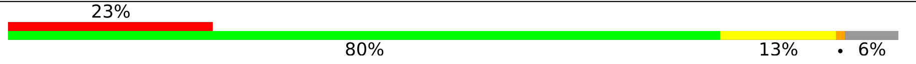
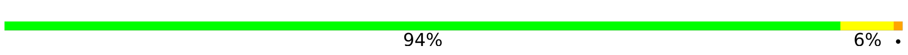
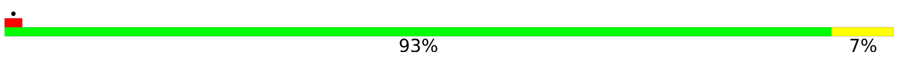
Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2903	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	

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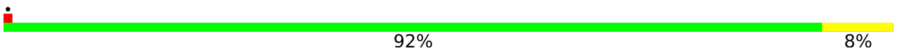
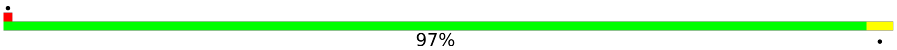
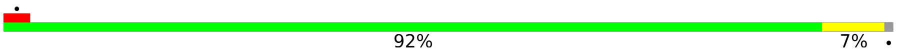
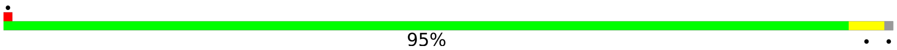
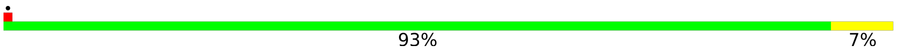
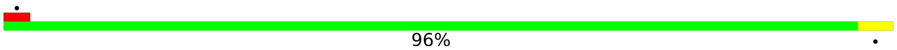
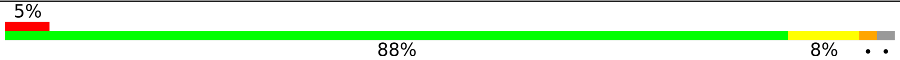
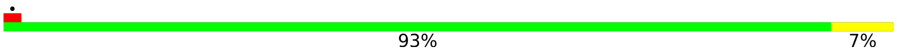
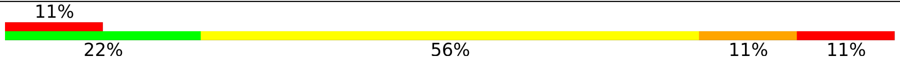
Mol	Chain	Length	Quality of chain
33	BL	144	
34	BM	136	
35	BN	127	
36	BO	117	
37	BP	115	
38	BQ	118	
39	BR	103	
40	BS	110	
41	BT	100	
42	BU	104	
43	BV	94	
44	BW	85	
45	BX	78	
46	BY	63	
47	BZ	59	
48	B0	57	
49	B1	55	
50	B2	46	
51	B3	65	
52	B4	38	
53	D1	6	
54	D2	77	
55	D3	76	
56	D4	9	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 146607 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AN	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AN	35	ALA	-	insertion	UNP C3SR07

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AO	88	714	439	144	130	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AP	82	649	406	128	114	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AQ	80	648	411	121	113	3	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	AR	55	455	288	86	81	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	AS	82	656	419	125	110	2	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BE	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	BF	177	1410	899	249	256	6	0	0

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	BG	176	1323	832	243	246	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	BH	149	1110	699	197	213	1	0	0

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	BI	66	522	323	99	94	6	0	0

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	BJ	142	1129	714	212	199	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	BK	123	946	593	181	166	6	0	0

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	BL	144	1053	654	207	190	2	0	0

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	BM	136	1075	686	205	178	6	0	0

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	BN	118	945	585	194	161	5	0	0

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	BO	117	900	557	179	163	1	0	0

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	BP	114	917	574	179	163	1	0	0

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
38	BQ	117	947	604	192	151	0	0

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	BR	103	816	516	153	145	2	0	0

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	BS	110	857	532	166	156	3	0	0

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	BT	93	738	466	139	131	2	0	0

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	BU	102	779	492	146	141	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	BV	94	753	479	137	134	3	0	0

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BW	76	580	359	117	103	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	BX	77	625	388	129	106	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BY	62	501	308	98	94	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	BZ	58	449	281	87	79	2	0	0

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B0	56	Total 444	C 269	N 94	O 80	S 1	0	0

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	B1	51	Total 414	C 266	N 76	O 72	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	46	Total 377	C 228	N 90	O 57	S 2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B3	64	Total 504	C 323	N 105	O 74	S 2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	38	Total 302	C 185	N 65	O 48	S 4	0	0

- Molecule 53 is a protein called MsrDL: FME-TYR-LEU-ILE-PHE-MET.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	D1	6	Total 57	C 41	N 6	O 8	S 2	0	0

- Molecule 54 is a RNA chain called Met-tRNA (P site).

Mol	Chain	Residues	Atoms						AltConf	Trace
54	D2	76	Total 1634	C 733	N 290	O 534	P 76	S 1	0	0

- Molecule 55 is a RNA chain called Phe-tRNA (E site).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	D3	75	Total 1604	C 715	N 288	O 525	P 75	S 1	0	0

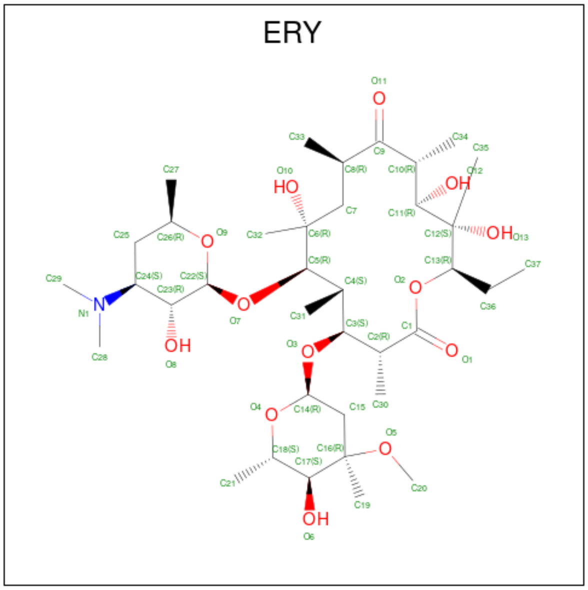
- Molecule 56 is a RNA chain called MsrDL mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	D4	9	Total 189	C 85	N 31	O 64	P 9	0	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	AA	35	Total 35	Mg 35	0
57	BA	134	Total 134	Mg 134	0
57	BC	1	Total 1	Mg 1	0
57	BD	1	Total 1	Mg 1	0
57	D2	1	Total 1	Mg 1	0

- Molecule 58 is ERYTHROMYCIN A (three-letter code: ERY) (formula: $C_{37}H_{67}NO_{13}$).



Mol	Chain	Residues	Atoms	AltConf
58	BA	1	Total C N O 51 37 1 13	0

- Molecule 59 is water.

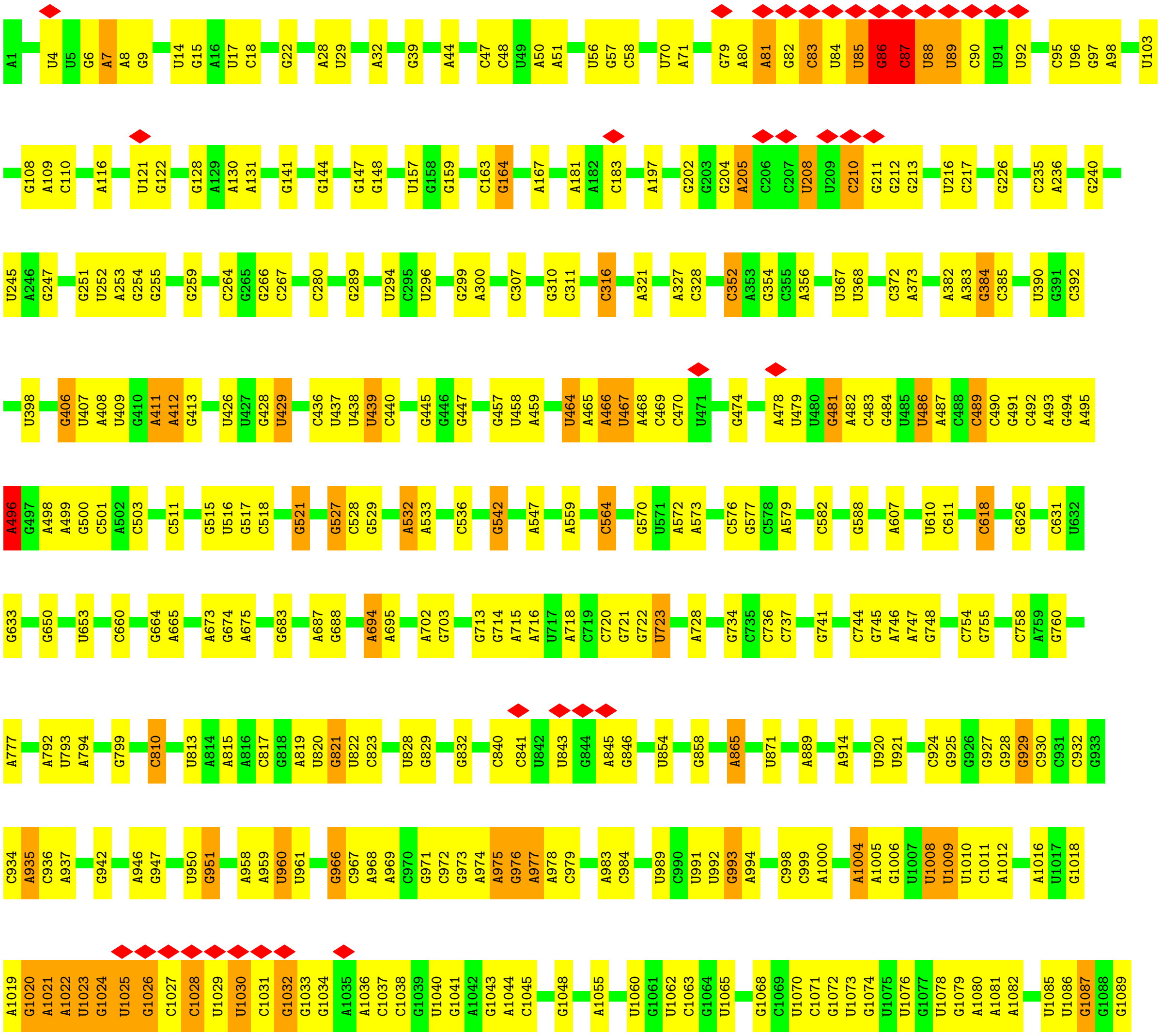
Mol	Chain	Residues	Atoms	AltConf
59	AA	166	Total O 166 166	0
59	AK	2	Total O 2 2	0
59	AM	1	Total O 1 1	0
59	AN	2	Total O 2 2	0
59	AQ	1	Total O 1 1	0
59	BA	614	Total O 614 614	0
59	BC	6	Total O 6 6	0
59	BD	3	Total O 3 3	0
59	BE	1	Total O 1 1	0
59	BJ	1	Total O 1 1	0
59	BL	1	Total O 1 1	0
59	BN	2	Total O 2 2	0

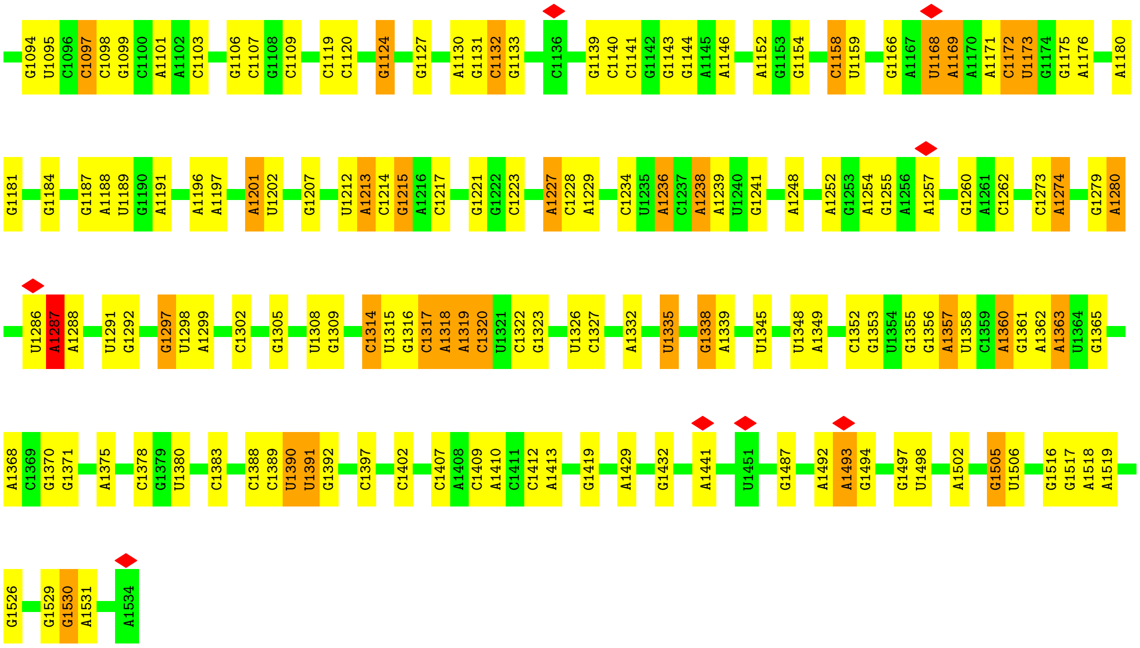
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: 16S rRNA

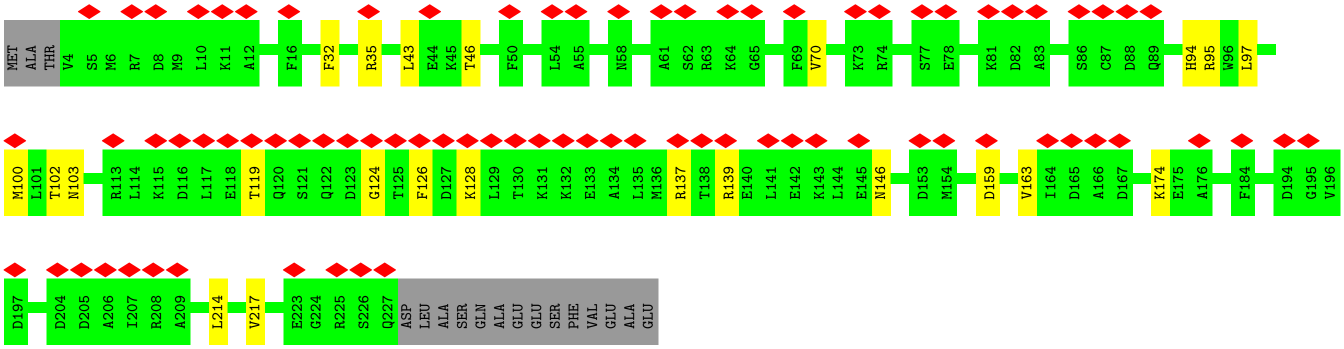
Chain AA:





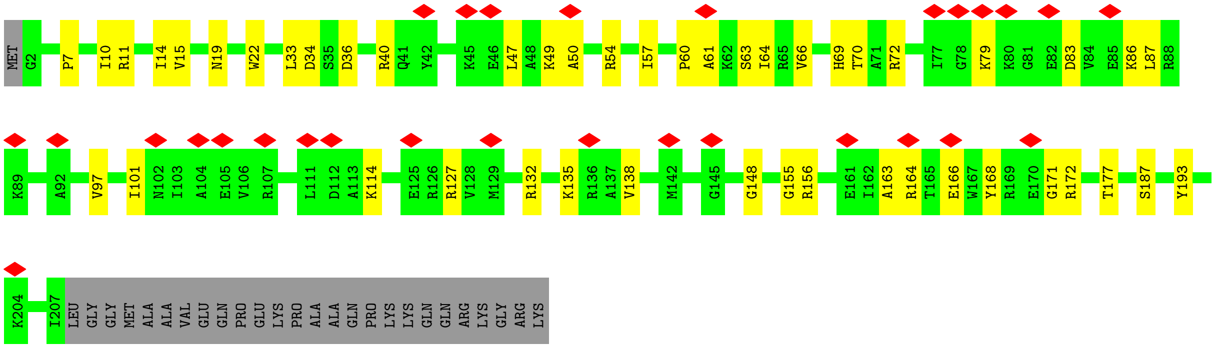
- Molecule 2: 30S ribosomal protein S2

Chain AB:



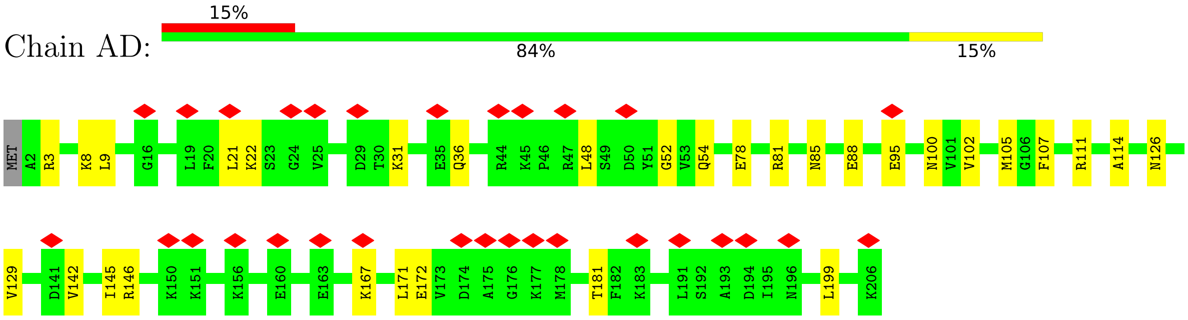
- Molecule 3: 30S ribosomal protein S3

Chain AC:



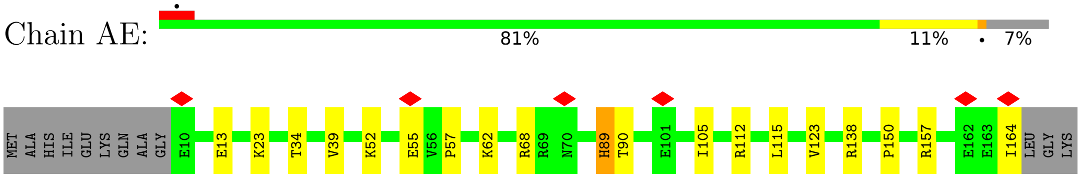
- Molecule 4: 30S ribosomal protein S4

Chain AD:



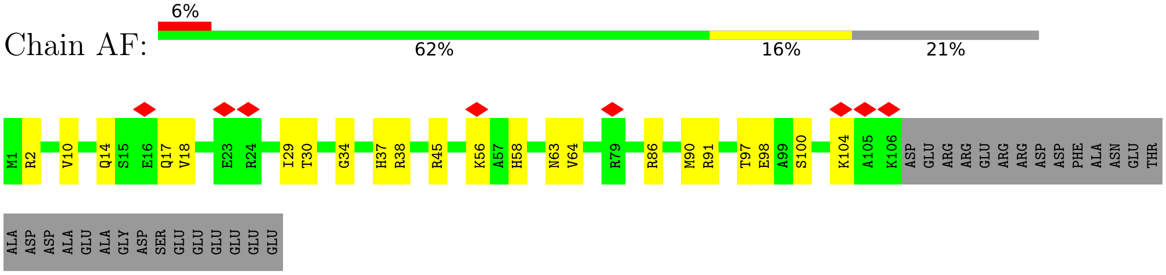
- Molecule 5: 30S ribosomal protein S5

Chain AE:



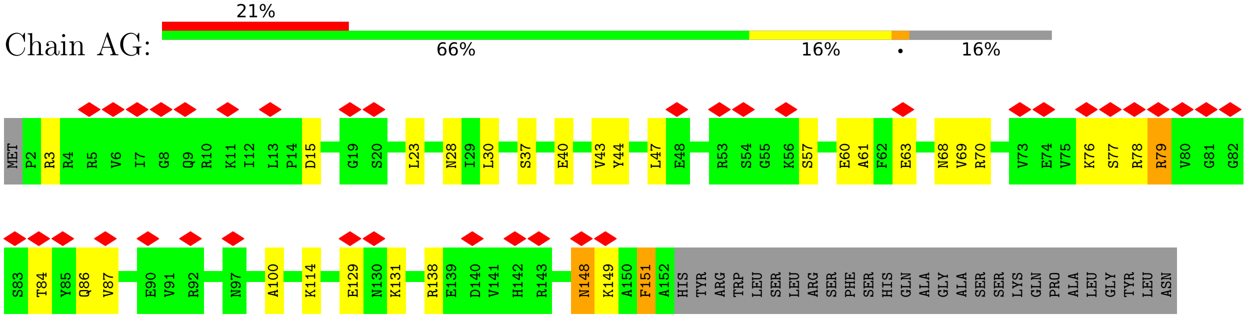
- Molecule 6: 30S ribosomal protein S6

Chain AF:



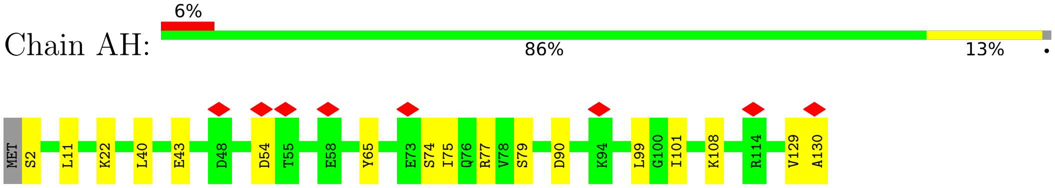
- Molecule 7: 30S ribosomal protein S7

Chain AG:



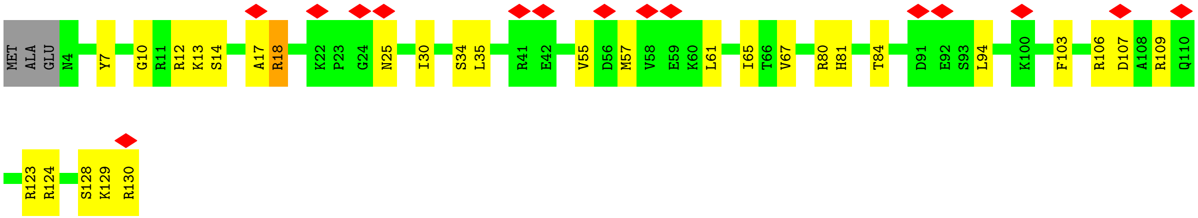
- Molecule 8: 30S ribosomal protein S8

Chain AH:



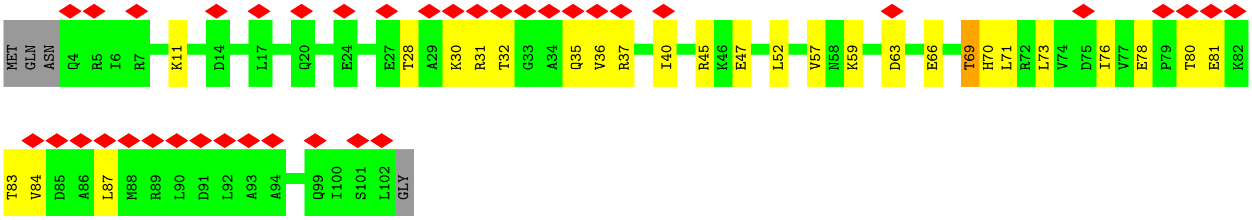
- Molecule 9: 30S ribosomal protein S9

Chain AI:



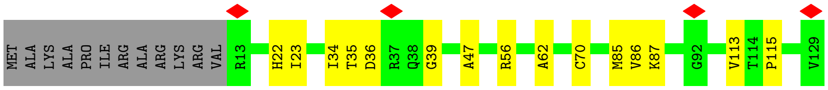
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



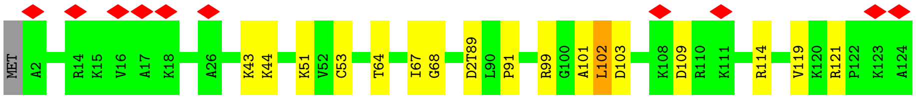
- Molecule 11: 30S ribosomal protein S11

Chain AK:



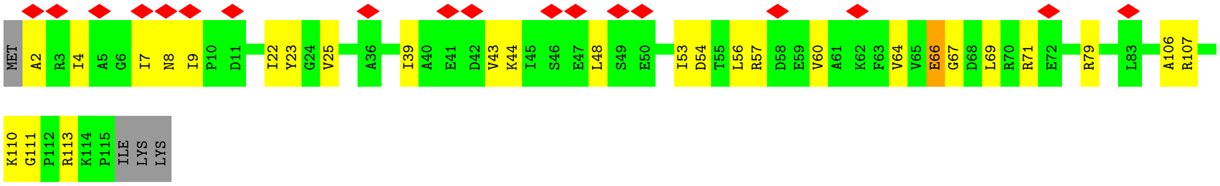
- Molecule 12: 30S ribosomal protein S12

Chain AL:



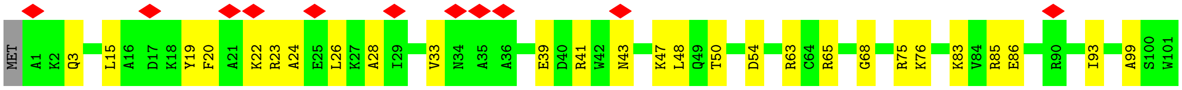
- Molecule 13: 30S ribosomal protein S13

Chain AM:



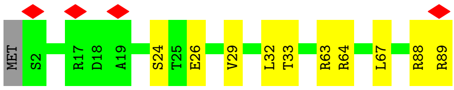
- Molecule 14: 30S ribosomal protein S14

Chain AN:



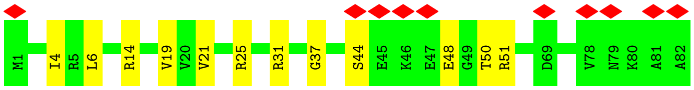
- Molecule 15: 30S ribosomal protein S15

Chain AO:



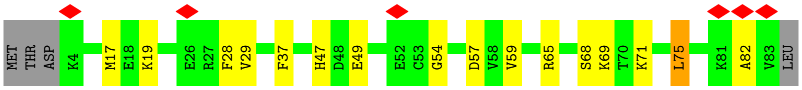
- Molecule 16: 30S ribosomal protein S16

Chain AP:



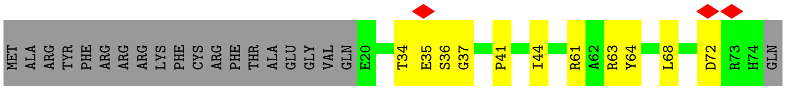
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



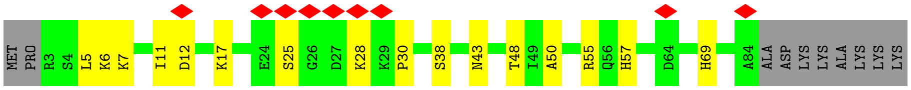
- Molecule 18: 30S ribosomal protein S18

Chain AR:



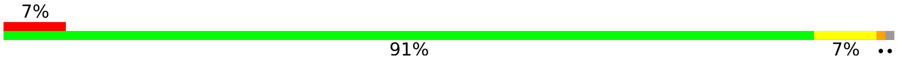
- Molecule 19: 30S ribosomal protein S19

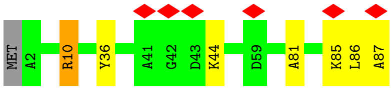
Chain AS:



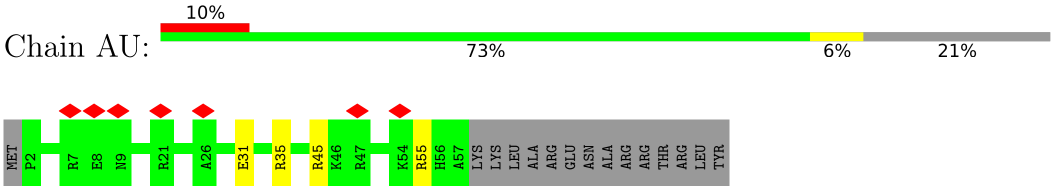
- Molecule 20: 30S ribosomal protein S20

Chain AT:

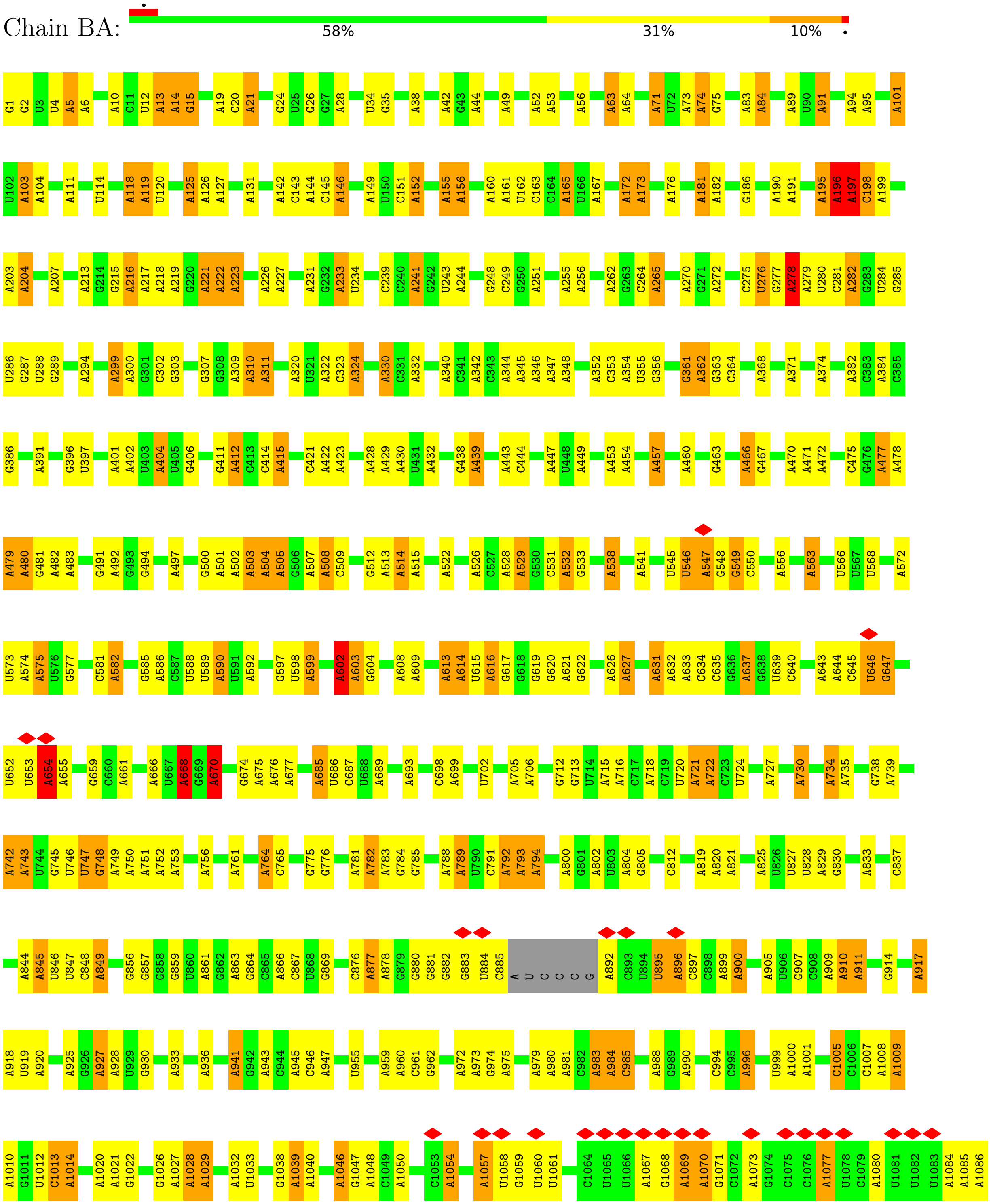


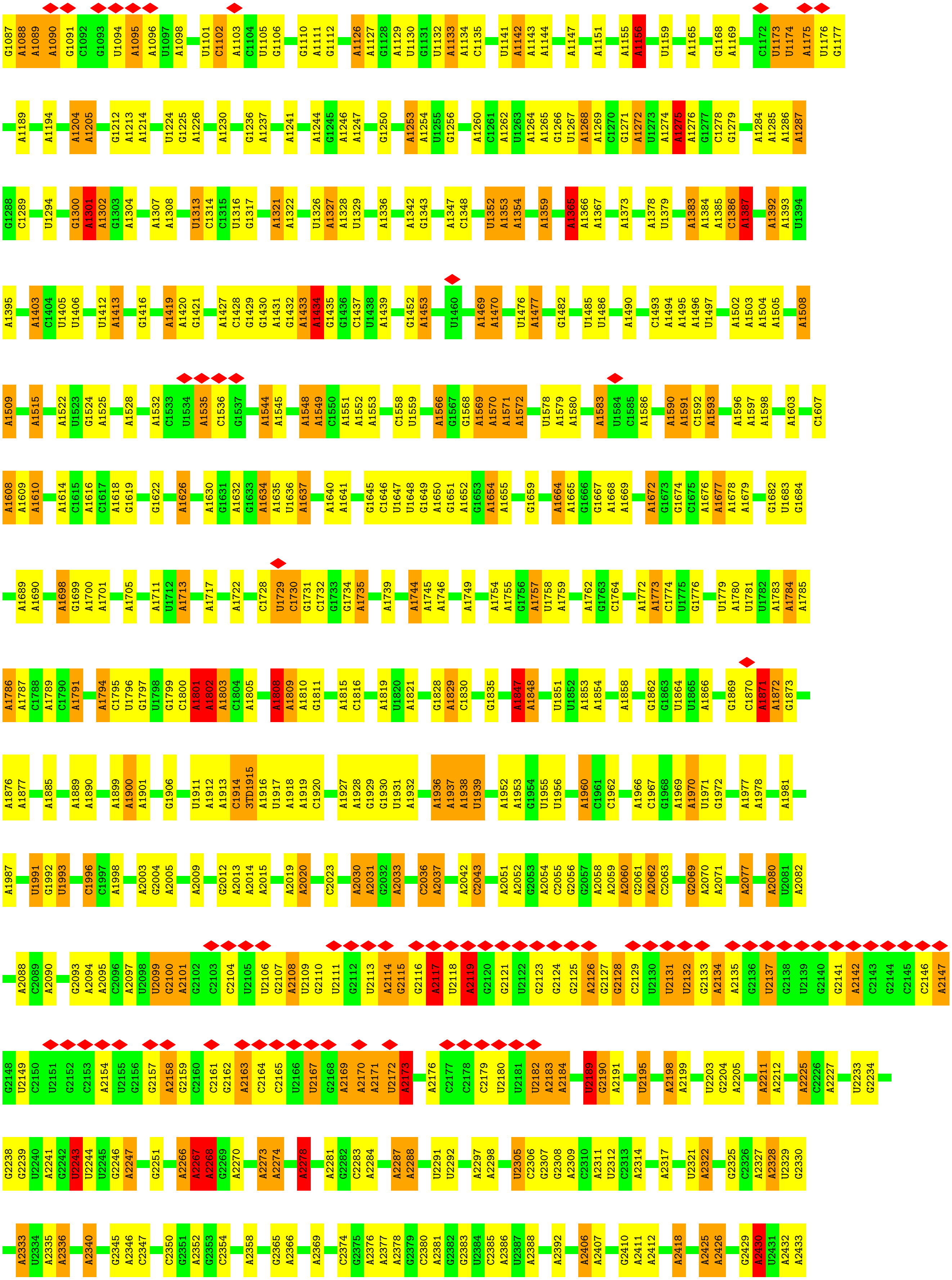


- Molecule 21: 30S ribosomal protein S21



- Molecule 22: 23S rRNA

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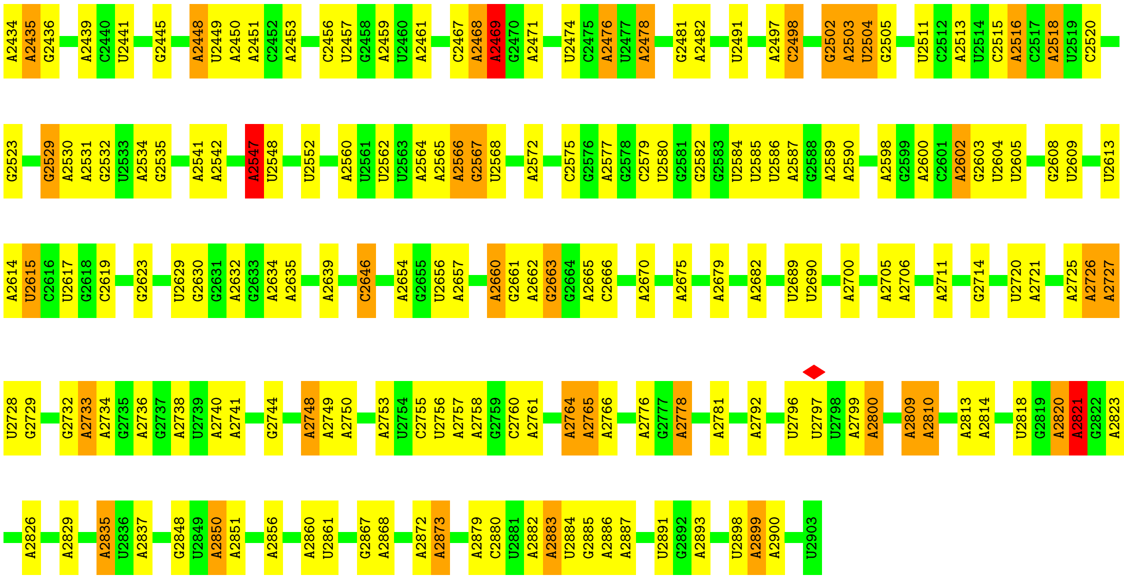
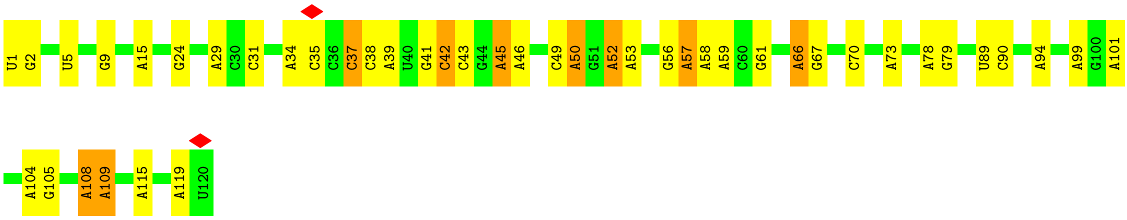
A1189 A1194 A1204 A1205 G1212 A1213 A1214 U1224 G1225 A1226 A1230 G1236 A1237 A1241 A1244 G1245 A1246 A1247 G1250 A1253 A1254 U1255 G1256 A1260 C1261 A1262 U1263 A1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 C1278 G1279 A1284 A1285 A1286 A1287
G1288 C1289 U1294 G1300 A1301 A1302 G1303 A1304 A1307 A1308 U1313 C1314 C1315 U1316 G1317 A1321 A1322 U1326 A1327 A1328 U1329 A1336 A1342 G1343 A1347 C1348 U1352 A1353 A1354 A1359 A1365 A1366 A1367 A1373 A1378 U1379 A1383 A1384 A1385 C1386 A1387 A1392 A1393 U1394
A1395 A1403 C1404 U1405 U1406 U1412 A1413 G1416 A1419 A1420 G1421 A1427 C1428 G1429 G1430 A1431 G1432 A1433 A1434 G1435 G1436 C1437 U1438 A1439 G1452 A1453 U1460 A1469 A1470 U1476 A1477 G1482 U1485 U1486 A1490 C1493 A1494 A1495 A1496 U1497 A1502 A1503 A1504 A1505 A1508
A1509 A1515 A1522 U1523 G1524 A1525 A1528 A1532 C1533 U1534 A1535 C1536 G1537 A1544 A1545 A1548 A1549 C1550 A1551 A1552 A1553 C1558 U1559 A1566 G1567 G1568 A1569 A1570 A1571 A1572 U1578 A1579 A1580 A1583 U1584 C1585 A1586 A1590 A1591 C1592 A1593 A1596 A1597 A1598 A1603 C1607
A1608 A1609 A1610 A1614 C1615 A1616 C1617 A1618 G1619 G1622 A1626 A1630 G1631 A1632 G1633 A1634 A1635 U1636 A1637 A1640 A1641 G1645 C1646 U1647 U1648 G1649 A1650 G1651 A1652 G1653 A1654 A1655 G1659 A1664 A1665 G1666 G1667 A1668 A1669 A1672 G1673 G1674 C1675 A1676 A1677 A1678 A1679 G1682 U1683 G1684
A1689 A1690 A1698 G1699 A1700 A1701 A1705 A1711 U1712 A1713 A1717 A1722 C1728 U1729 C1730 G1731 C1732 G1733 G1734 A1735 A1739 A1744 A1745 A1746 A1749 A1754 A1755 G1756 A1757 U1758 A1759 A1762 G1763 C1764 A1772 A1773 C1774 U1775 G1776 U1779 A1780 U1781 U1782 A1783 A1784 A1785
A1786 A1787 C1788 A1789 C1790 A1791 A1794 C1795 U1796 G1797 U1798 G1799 C1800 A1801 A1802 A1803 C1804 A1805 A1808 A1809 A1810 G1811 A1815 C1816 A1819 U1820 A1821 G1828 A1829 C1830 G1835 A1847 A1848 U1851 U1852 A1853 A1854 A1858 G1862 G1863 U1864 U1865 A1866 G1869 C1870 A1871 A1872 G1873
A1876 A1877 A1885 A1889 A1890 A1899 A1900 A1901 G1906 U1911 A1912 A1913 C1914 3TD1915 A1916 U1917 A1918 A1919 C1920 A1927 A1928 G1929 G1930 U1931 A1932 A1936 A1937 A1938 U1939 A1952 A1953 G1954 U1955 U1956 A1960 C1961 C1962 A1966 C1967 G1968 A1969 A1970 U1971 G1972 A1977 A1978 A1981
A1987 U1991 G1992 U1993 C1996 C1997 A1998 A2003 G2004 A2005 A2009 G2012 A2013 A2014 A2015 A2019 A2020 C2023 A2030 A2031 G2032 A2033 C2036 A2037 A2042 C2043 A2051 A2052 G2053 A2054 C2055 G2056 G2057 A2058 A2059 A2060 G2061 A2062 C2063 G2069 A2070 A2071 A2077 A2080 U2081 A2082
A2088 C2089 A2090 G2093 A2094 A2095 C2096 A2097 U2098 U2099 G2100 A2101 G2102 C2103 C2104 U2105 U2106 G2107 A2108 U2109 G2110 U2111 G2112 U2113 A2114 G2115 G2116 A2117 U2118 A2119 G2120 G2121 U2122 G2123 G2124 G2125 A2126 G2127 G2128 C2129 U2130 U2131 U2132 G2133 A2134 A2135 G2136 U2137 G2138 U2139 G2140 G2141 A2142 C2143 G2144 C2145 C2146 A2147
G2148 U2149 C2150 U2151 G2152 C2153 A2154 U2155 G2156 G2157 A2158 G2159 C2160 C2161 G2162 A2163 C2164 C2165 U2166 U2167 G2168 A2169 A2170 A2171 U2172 A2173 A2176 C2177 C2178 C2179 U2180 U2181 U2182 A2183 A2184 U2189 G2190 A2191 U2195 A2198 A2199 U2203 G2204 A2205 A2211 A2212 A2225 C2226 A2227 U2233 G2234
G2238 G2239 U2240 A2241 G2242 U2243 U2244 U2245 G2246 A2247 G2251 A2266 A2267 A2268 G2269 A2270 A2273 A2274 A2278 A2281 G2282 C2283 A2284 A2287 A2288 U2291 U2292 A2297 A2298 U2305 C2306 G2307 G2308 A2309 C2310 A2311 U2312 C2313 A2314 A2317 U2321 A2322 G2325 C2326 A2327 A2328 U2329 G2330
A2333 U2334 A2335 A2336 A2340 G2345 A2346 C2347 C2350 G2351 A2352 G2353 C2354 A2358 G2365 A2366 A2369 C2374 G2375 A2376 A2377 A2378 G2379 C2380 A2381 G2382 U2383 U2384 C2385 A2386 U2387 A2388 A2392 A2406 A2407 G2410 A2411 A2412 A2418 A2425 A2426 G2429 A2430 U2431 A2432 A2433



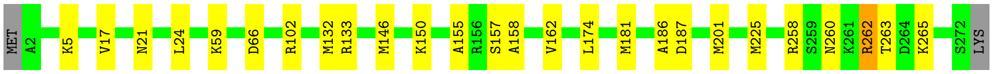
- Molecule 23: 5S rRNA

Chain BB:



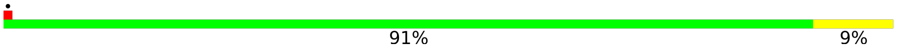
- Molecule 24: 50S ribosomal protein L2

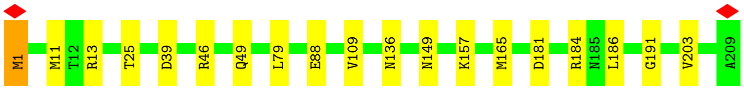
Chain BC:



- Molecule 25: 50S ribosomal protein L3

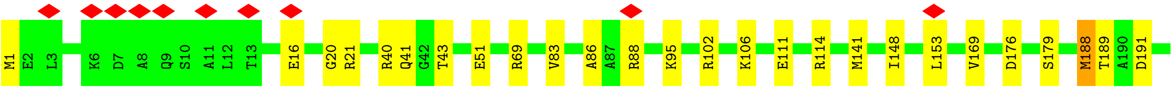
Chain BD:

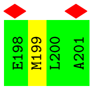




- Molecule 26: 50S ribosomal protein L4

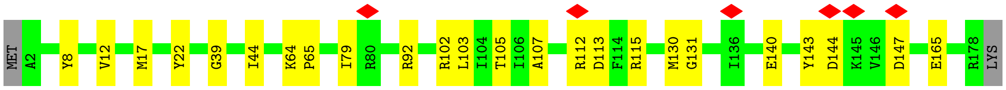
Chain BE:





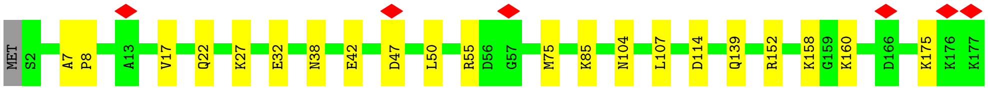
- Molecule 27: 50S ribosomal protein L5

Chain BF:



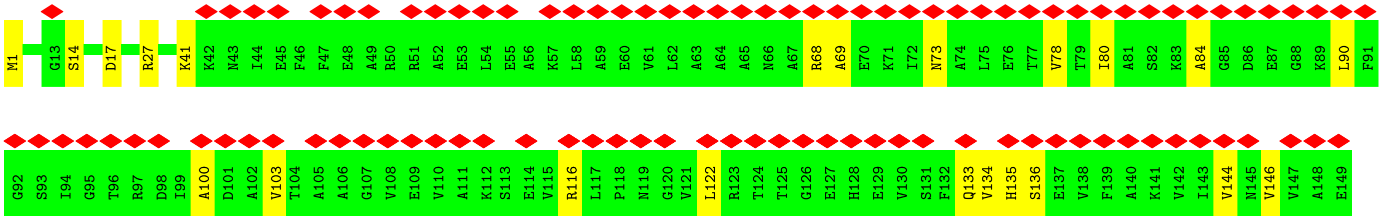
- Molecule 28: 50S ribosomal protein L6

Chain BG:



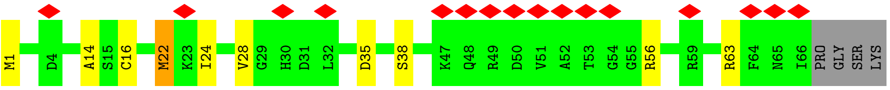
- Molecule 29: 50S ribosomal protein L9

Chain BH:



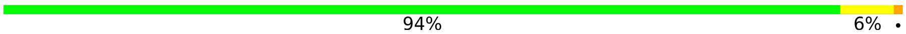
- Molecule 30: 50S ribosomal protein L31

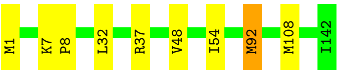
Chain BI:



- Molecule 31: 50S ribosomal protein L13

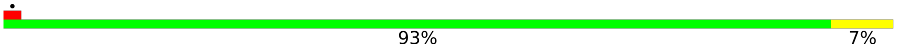
Chain BJ:

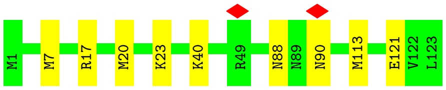




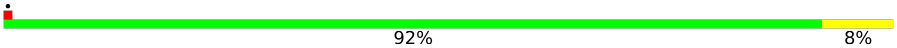
- Molecule 32: 50S ribosomal protein L14

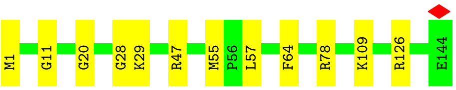
Chain BK:





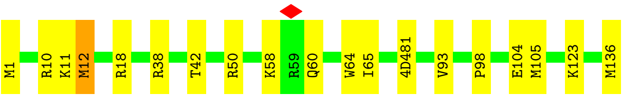
- Molecule 33: 50S ribosomal protein L15

Chain BL:




- Molecule 34: 50S ribosomal protein L16

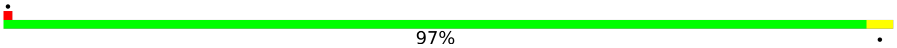
Chain BM:

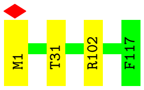



- Molecule 35: 50S ribosomal protein L17

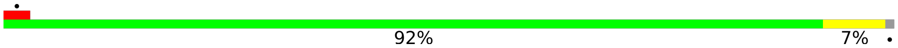
Chain BN:

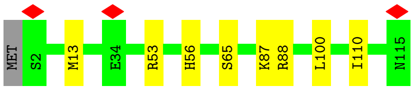

- Molecule 36: 50S ribosomal protein L18

Chain BO:


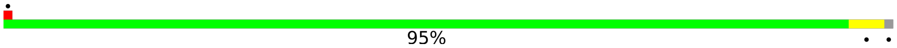


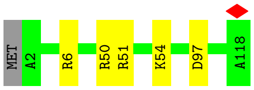
- Molecule 37: 50S ribosomal protein L19

Chain BP:




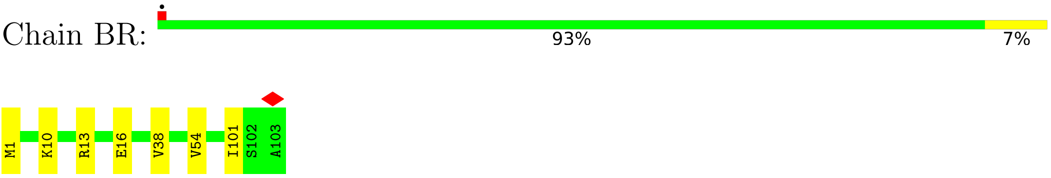
- Molecule 38: 50S ribosomal protein L20

Chain BQ:




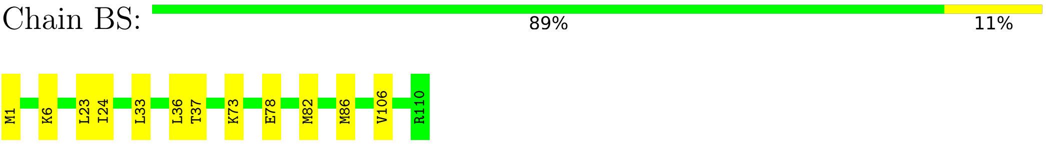
- Molecule 39: 50S ribosomal protein L21

Chain BR:



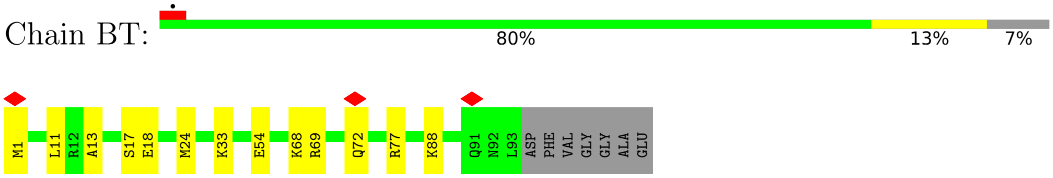
- Molecule 40: 50S ribosomal protein L22

Chain BS:



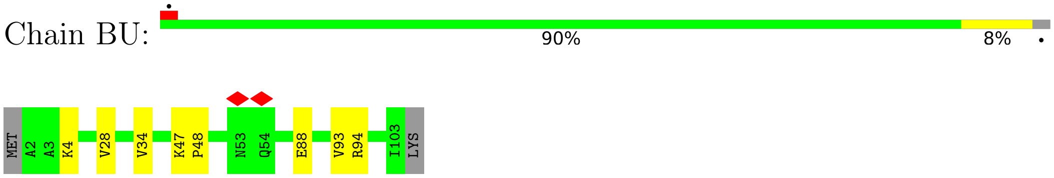
- Molecule 41: 50S ribosomal protein L23

Chain BT:



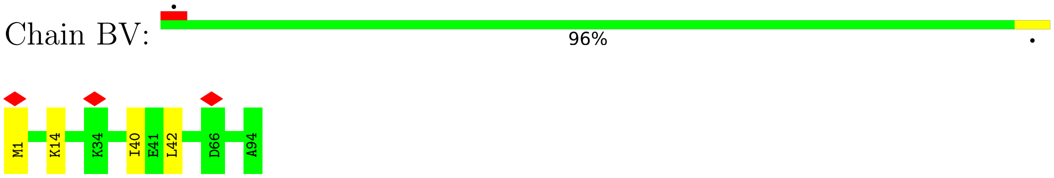
- Molecule 42: 50S ribosomal protein L24

Chain BU:



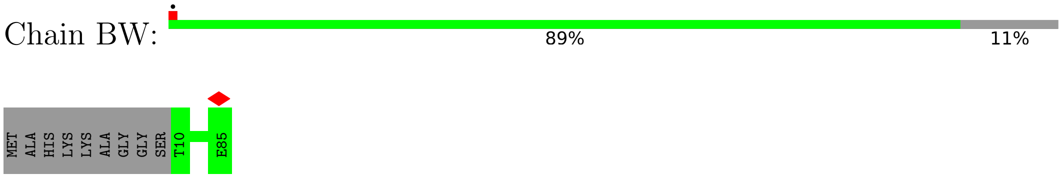
- Molecule 43: 50S ribosomal protein L25

Chain BV:



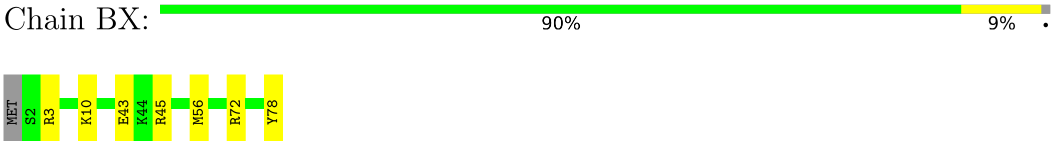
- Molecule 44: 50S ribosomal protein L27

Chain BW:

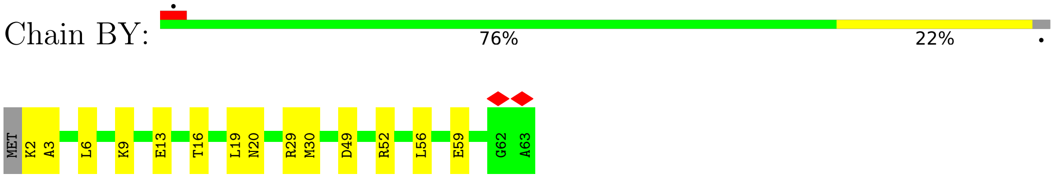


- Molecule 45: 50S ribosomal protein L28

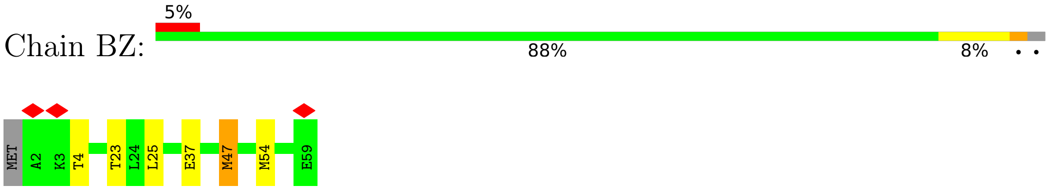
Chain BX:



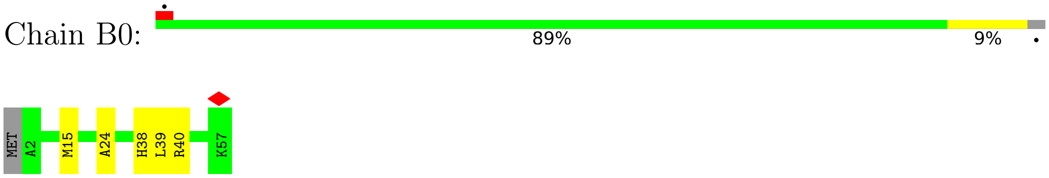
- Molecule 46: 50S ribosomal protein L29



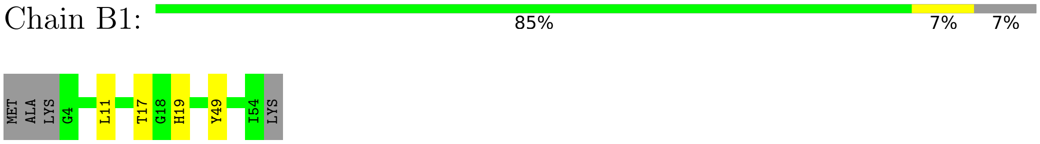
- Molecule 47: 50S ribosomal protein L30



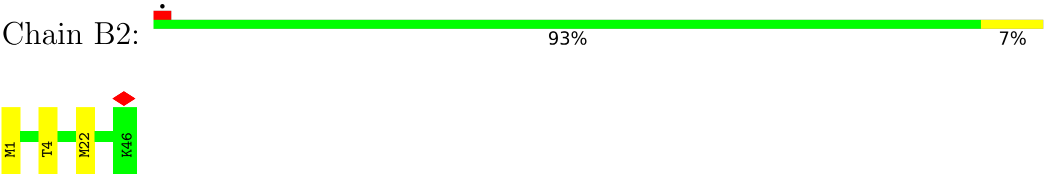
- Molecule 48: 50S ribosomal protein L32



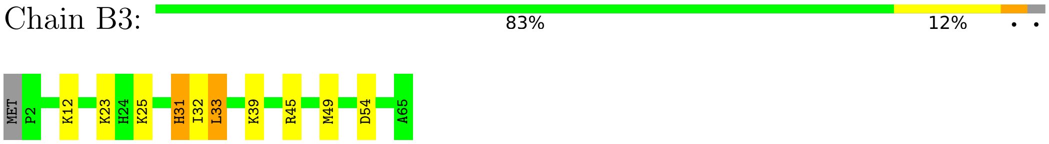
- Molecule 49: 50S ribosomal protein L33



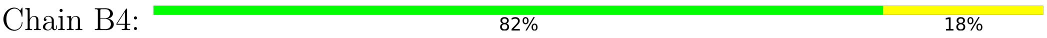
- Molecule 50: 50S ribosomal protein L34

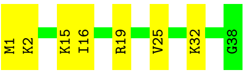


- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



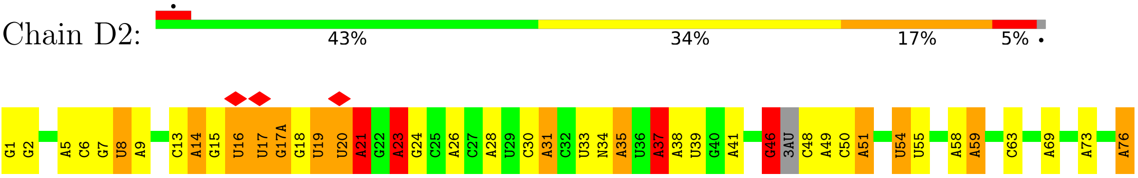


- Molecule 53: MsrDL: FME-TYR-LEU-ILE-PHE-MET

Chain D1:

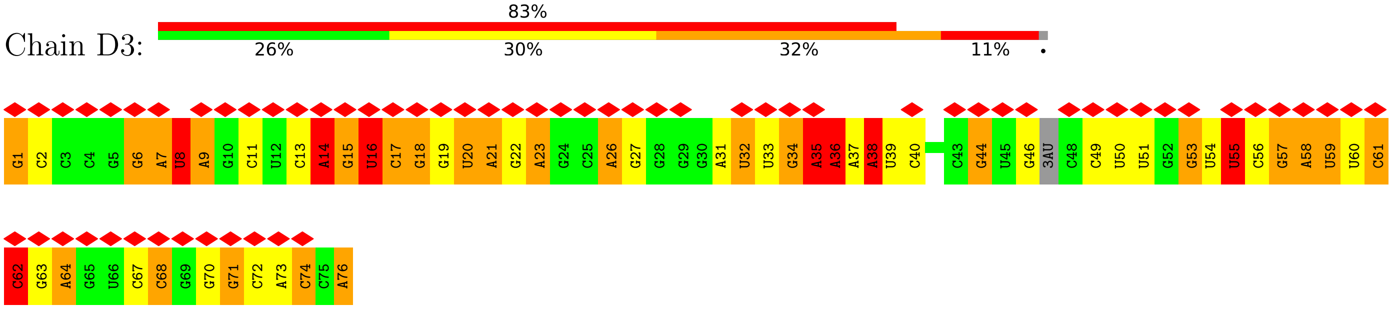
- Molecule 54: Met-tRNA (P site)

Chain D2:



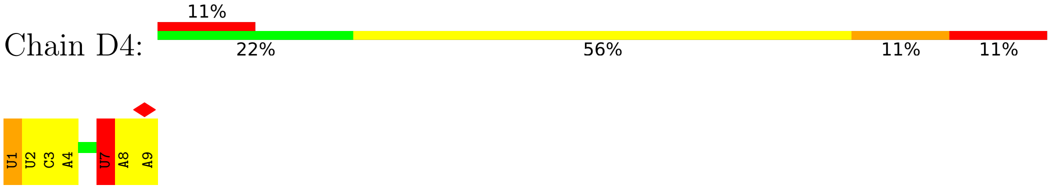
- Molecule 55: Phe-tRNA (E site)

Chain D3:



- Molecule 56: MsrDL mRNA

Chain D4:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose $(e^-/\text{Å}^2)$	64	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	23.089	Depositor
Minimum map value	-11.414	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.85	Depositor
Map size (Å)	414.0, 414.0, 414.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 2MG, PSU, 3TD, D2T, MA6, 1MG, OMG, G7M, MEQ, T6A, 2MA, FME, 4AC, 4D4, 4OC, 6MZ, H2U, 5MU, 5MC, UR3, ERY, OMC, MG, 4SU

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	AA	1.42	48/36593 (0.1%)	1.10	110/57081 (0.2%)
2	AB	0.41	0/1784	0.57	0/2403
3	AC	0.70	0/1651	0.64	0/2225
4	AD	0.59	0/1665	0.59	0/2227
5	AE	0.58	0/1157	0.59	0/1557
6	AF	0.50	0/881	0.60	0/1189
7	AG	0.55	0/1195	0.62	0/1602
8	AH	0.57	0/989	0.57	0/1326
9	AI	0.77	0/1034	0.70	0/1375
10	AJ	0.68	0/805	0.68	0/1089
11	AK	0.51	0/893	0.58	0/1205
12	AL	0.62	0/960	0.78	5/1286 (0.4%)
13	AM	0.62	0/892	0.70	0/1193
14	AN	0.74	0/811	0.67	0/1081
15	AO	0.49	0/722	0.53	0/964
16	AP	0.60	0/659	0.72	1/884 (0.1%)
17	AQ	0.57	0/657	0.61	1/881 (0.1%)
18	AR	0.60	0/462	0.60	0/621
19	AS	0.75	0/672	0.67	0/904
20	AT	0.44	0/676	0.54	1/895 (0.1%)
21	AU	0.50	0/472	0.52	0/627
22	BA	2.27	2742/69099 (4.0%)	3.49	8699/107794 (8.1%)
23	BB	1.94	90/2872 (3.1%)	3.02	275/4478 (6.1%)
24	BC	0.41	0/2121	0.59	5/2852 (0.2%)
25	BD	0.41	0/1576	0.57	3/2119 (0.1%)
26	BE	0.35	0/1571	0.58	5/2113 (0.2%)
27	BF	0.31	0/1434	0.57	2/1926 (0.1%)
28	BG	0.32	0/1343	0.49	1/1816 (0.1%)
29	BH	0.30	0/1121	0.63	2/1515 (0.1%)
30	BI	0.31	0/531	0.61	2/709 (0.3%)
31	BJ	0.38	0/1152	0.55	3/1551 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	BK	0.38	0/955	0.61	3/1279 (0.2%)
33	BL	0.36	0/1062	0.57	2/1413 (0.1%)
34	BM	0.39	0/1081	0.60	4/1443 (0.3%)
35	BN	0.36	0/958	0.60	3/1281 (0.2%)
36	BO	0.33	0/910	0.49	1/1219 (0.1%)
37	BP	0.39	0/929	0.52	1/1242 (0.1%)
38	BQ	0.42	0/960	0.46	0/1278
39	BR	0.39	0/829	0.57	1/1107 (0.1%)
40	BS	0.35	0/864	0.58	3/1156 (0.3%)
41	BT	0.36	0/744	0.57	2/994 (0.2%)
42	BU	0.34	0/787	0.50	0/1051
43	BV	0.34	0/766	0.56	1/1025 (0.1%)
44	BW	0.39	0/587	0.46	0/776
45	BX	0.39	0/635	0.57	1/848 (0.1%)
46	BY	0.28	0/502	0.48	1/667 (0.1%)
47	BZ	0.35	0/453	0.61	2/605 (0.3%)
48	B0	0.40	0/450	0.55	1/599 (0.2%)
49	B1	0.34	0/421	0.51	0/561
50	B2	0.37	0/380	0.64	2/498 (0.4%)
51	B3	0.36	0/513	0.67	1/676 (0.1%)
52	B4	0.39	0/303	0.57	1/397 (0.3%)
53	D1	0.62	0/48	0.74	0/63
54	D2	2.31	72/1531 (4.7%)	3.60	211/2380 (8.9%)
55	D3	2.07	54/1636 (3.3%)	3.39	194/2547 (7.6%)
56	D4	0.89	0/210	1.35	7/324 (2.2%)
All	All	1.72	3006/156964 (1.9%)	2.53	9557/234917 (4.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AC	0	1
5	AE	0	1
29	BH	0	1
51	B3	0	1
All	All	0	4

The worst 5 of 3006 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1872	A	C6-N6	17.23	1.47	1.33
55	D3	23	A	C6-N6	17.03	1.47	1.33
22	BA	1086	A	C6-N6	17.01	1.47	1.33
22	BA	2101	A	C6-N6	16.98	1.47	1.33
22	BA	1420	A	C6-N6	16.97	1.47	1.33

The worst 5 of 9557 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	BA	1021	A	C2-N3-C4	22.58	121.89	110.60
22	BA	783	A	C2-N3-C4	22.43	121.82	110.60
22	BA	1515	A	N1-C6-N6	-22.17	105.30	118.60
22	BA	2765	A	C2-N3-C4	21.64	121.42	110.60
22	BA	1392	A	C2-N3-C4	21.64	121.42	110.60

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AC	60	PRO	Peptide
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide
29	BH	41	LYS	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16591	184	0
2	AB	1753	0	1780	19	0
3	AC	1624	0	1696	37	0
4	AD	1643	0	1707	19	0
5	AE	1144	0	1184	13	0
6	AF	862	0	864	13	0
7	AG	1181	0	1238	25	0
8	AH	979	0	1031	11	0
9	AI	1022	0	1070	24	0
10	AJ	795	0	836	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	AK	877	0	887	12	0
12	AL	957	0	1017	8	0
13	AM	883	0	941	66	0
14	AN	799	0	841	18	0
15	AO	714	0	734	10	0
16	AP	649	0	666	11	0
17	AQ	648	0	691	11	0
18	AR	455	0	478	11	0
19	AS	656	0	679	21	0
20	AT	670	0	719	4	0
21	AU	465	0	491	4	0
22	BA	62209	0	31307	228	0
23	BB	2569	0	1301	7	0
24	BC	2082	0	2154	13	0
25	BD	1566	0	1618	10	0
26	BE	1552	0	1619	13	0
27	BF	1410	0	1444	37	0
28	BG	1323	0	1371	12	0
29	BH	1110	0	1148	9	0
30	BI	522	0	522	15	0
31	BJ	1129	0	1162	4	0
32	BK	946	0	1023	4	0
33	BL	1053	0	1129	8	0
34	BM	1075	0	1155	9	0
35	BN	945	0	989	5	0
36	BO	900	0	935	1	0
37	BP	917	0	962	6	0
38	BQ	947	0	1019	4	0
39	BR	816	0	839	4	0
40	BS	857	0	922	6	0
41	BT	738	0	807	7	0
42	BU	779	0	831	4	0
43	BV	753	0	780	2	0
44	BW	580	0	594	0	0
45	BX	625	0	652	4	0
46	BY	501	0	531	8	0
47	BZ	449	0	488	3	0
48	B0	444	0	458	3	0
49	B1	414	0	442	2	0
50	B2	377	0	418	1	0
51	B3	504	0	572	8	0
52	B4	302	0	343	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	D1	57	0	59	7	0
54	D2	1634	0	842	18	0
55	D3	1604	0	817	29	0
56	D4	189	0	96	13	0
57	AA	35	0	0	1	0
57	BA	134	0	0	1	0
57	BC	1	0	0	0	0
57	BD	1	0	0	0	0
57	D2	1	0	0	0	0
58	BA	51	0	67	4	0
59	AA	166	0	0	4	0
59	AK	2	0	0	0	0
59	AM	1	0	0	0	0
59	AN	2	0	0	0	0
59	AQ	1	0	0	0	0
59	BA	614	0	0	4	0
59	BC	6	0	0	0	0
59	BD	3	0	0	0	0
59	BE	1	0	0	0	0
59	BJ	1	0	0	0	0
59	BL	1	0	0	0	0
59	BN	2	0	0	0	0
All	All	146607	0	97557	882	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 4.

The worst 5 of 882 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)
13:AM:7:ILE:HD12	27:BF:112:ARG:CD	1.04	1.50
13:AM:7:ILE:CD1	27:BF:112:ARG:HD2	1.36	1.48
13:AM:7:ILE:CD1	27:BF:112:ARG:CD	1.89	1.44
13:AM:7:ILE:HD12	27:BF:112:ARG:CG	1.51	1.40
13:AM:43:VAL:CG1	13:AM:48:LEU:HD11	1.54	1.37

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
2	AB	222/241 (92%)	207 (93%)	15 (7%)	0	100	100
3	AC	204/233 (88%)	192 (94%)	11 (5%)	1 (0%)	29	68
4	AD	203/206 (98%)	192 (95%)	11 (5%)	0	100	100
5	AE	153/167 (92%)	143 (94%)	10 (6%)	0	100	100
6	AF	104/135 (77%)	100 (96%)	4 (4%)	0	100	100
7	AG	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
8	AH	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
9	AI	125/130 (96%)	110 (88%)	14 (11%)	1 (1%)	19	57
10	AJ	97/103 (94%)	92 (95%)	4 (4%)	1 (1%)	15	53
11	AK	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
12	AL	120/124 (97%)	111 (92%)	8 (7%)	1 (1%)	19	57
13	AM	112/118 (95%)	102 (91%)	9 (8%)	1 (1%)	17	55
14	AN	99/102 (97%)	83 (84%)	16 (16%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	AP	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	AR	53/75 (71%)	50 (94%)	3 (6%)	0	100	100
19	AS	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
24	BC	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
25	BD	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	29	68
26	BE	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
27	BF	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
28	BG	174/177 (98%)	168 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
32	BK	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	BL	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
34	BM	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	BN	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
36	BO	115/117 (98%)	114 (99%)	1 (1%)	0	100	100
37	BP	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
40	BS	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
41	BT	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
42	BU	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
43	BV	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
44	BW	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	BX	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	BY	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
47	BZ	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
48	B0	54/57 (95%)	54 (100%)	0	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	44 (100%)	0	0	100	100
51	B3	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	4	22
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	D1	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	5579/5920 (94%)	5322 (95%)	249 (4%)	8 (0%)	54	85

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	AL	102	LEU
25	BD	149	ASN
51	B3	32	ILE

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Mol	Chain	Res	Type
10	AJ	57	VAL
51	B3	33	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	
2	AB	186/199 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	169 (99%)	1 (1%)	86	95
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	119 (96%)	5 (4%)	31	68
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	103 (98%)	2 (2%)	57	84
10	AJ	87/90 (97%)	86 (99%)	1 (1%)	73	90
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	102/103 (99%)	101 (99%)	1 (1%)	76	91
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	76/77 (99%)	76 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	73 (99%)	1 (1%)	67	88
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67	88
20	AT	65/66 (98%)	64 (98%)	1 (2%)	65	87
21	AU	48/61 (79%)	48 (100%)	0	100	100
24	BC	216/218 (99%)	215 (100%)	1 (0%)	88	96
25	BD	163/163 (100%)	162 (99%)	1 (1%)	86	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BE	165/165 (100%)	164 (99%)	1 (1%)	86	95
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	113 (99%)	1 (1%)	78	92
30	BI	59/62 (95%)	58 (98%)	1 (2%)	60	85
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	78	92
32	BK	104/104 (100%)	104 (100%)	0	100	100
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	107 (99%)	1 (1%)	78	92
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	87 (100%)	0	100	100
37	BP	99/100 (99%)	99 (100%)	0	100	100
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	46 (98%)	1 (2%)	53	82
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	D1	5/5 (100%)	5 (100%)	0	100	100
All	All	4638/4832 (96%)	4617 (100%)	21 (0%)	89	96

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	BD	1	MET
30	BI	16	CYS
48	B0	40	ARG
31	BJ	92	MET
29	BH	27	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
24	BC	260	ASN
28	BG	104	ASN
49	B1	45	GLN
28	BG	22	GLN
28	BG	139	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	267 (17%)	4 (0%)
22	BA	2891/2903 (99%)	413 (14%)	16 (0%)
23	BB	119/120 (99%)	15 (12%)	0
54	D2	73/77 (94%)	17 (23%)	3 (4%)
55	D3	74/76 (97%)	43 (58%)	3 (4%)
56	D4	8/9 (88%)	4 (50%)	0
All	All	4695/4719 (99%)	759 (16%)	26 (0%)

5 of 759 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	14	U

5 of 26 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	1900	A
22	BA	2468	A
55	D3	8	4SU

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Mol	Chain	Res	Type
22	BA	2189	U
22	BA	2602	A

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

58 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
54	H2U	D2	20	54	18,21,22	3.02	5 (27%)	21,30,33	2.12	5 (23%)
22	PSU	BA	2504	22	18,21,22	1.06	1 (5%)	22,30,33	1.74	4 (18%)
1	MA6	AA	1519	1	18,26,27	1.25	1 (5%)	19,38,41	4.21	3 (15%)
1	G7M	AA	527	1	20,26,27	2.10	6 (30%)	17,39,42	1.22	1 (5%)
22	2MG	BA	2445	22	18,26,27	2.56	6 (33%)	16,38,41	1.53	4 (25%)
22	6MZ	BA	1618	22	18,25,26	2.00	3 (16%)	16,36,39	2.15	3 (18%)
55	4SU	D3	8	55	18,21,22	3.69	8 (44%)	26,30,33	2.24	5 (19%)
54	H2U	D2	19	54	18,21,22	3.27	4 (22%)	21,30,33	1.77	5 (23%)
22	PSU	BA	1911	22	18,21,22	1.02	1 (5%)	22,30,33	1.85	4 (18%)
22	OMC	BA	2498	57,22	19,22,23	2.73	7 (36%)	26,31,34	0.98	1 (3%)
22	PSU	BA	955	22	18,21,22	1.09	1 (5%)	22,30,33	1.78	4 (18%)
54	PSU	D2	39	54	18,21,22	0.93	1 (5%)	22,30,33	1.66	4 (18%)
55	H2U	D3	16	55	18,21,22	3.19	5 (27%)	21,30,33	1.65	4 (19%)
22	3TD	BA	1915	22	18,22,23	4.18	6 (33%)	22,32,35	1.69	3 (13%)
54	PSU	D2	55	54	18,21,22	1.06	1 (5%)	22,30,33	1.79	4 (18%)
1	2MG	AA	1516	1	18,26,27	2.40	6 (33%)	16,38,41	1.63	4 (25%)
22	5MU	BA	747	22	19,22,23	4.72	7 (36%)	28,32,35	3.70	9 (32%)
1	PSU	AA	516	57,1	18,21,22	1.03	3 (16%)	22,30,33	1.92	4 (18%)
54	5MU	D2	54	54	19,22,23	4.83	7 (36%)	28,32,35	3.68	9 (32%)
55	PSU	D3	55	55	18,21,22	1.15	1 (5%)	22,30,33	1.63	4 (18%)
22	6MZ	BA	2030	22	18,25,26	1.92	2 (11%)	16,36,39	2.91	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
53	FME	D1	1	53	8,9,10	0.59	0	7,9,11	1.10	1 (14%)
34	4D4	BM	81	34	9,11,12	2.03	2 (22%)	8,13,15	1.97	3 (37%)
22	1MG	BA	745	22	18,26,27	2.54	5 (27%)	19,39,42	1.52	3 (15%)
1	2MG	AA	1207	1	18,26,27	2.45	6 (33%)	16,38,41	1.50	2 (12%)
22	PSU	BA	2580	22	18,21,22	1.10	3 (16%)	22,30,33	1.90	5 (22%)
22	PSU	BA	2604	22	18,21,22	1.02	1 (5%)	22,30,33	1.72	4 (18%)
54	OMG	D2	17(A)	54	18,26,27	2.65	8 (44%)	19,38,41	1.55	4 (21%)
54	G7M	D2	46	54	20,26,27	2.23	7 (35%)	17,39,42	1.15	1 (5%)
54	H2U	D2	17	54	18,21,22	3.06	5 (27%)	21,30,33	2.03	5 (23%)
54	4AC	D2	34	54	21,24,25	3.25	9 (42%)	29,34,37	2.03	9 (31%)
1	2MG	AA	966	1	18,26,27	2.36	5 (27%)	16,38,41	1.61	4 (25%)
12	D2T	AL	89	12	7,9,10	1.37	1 (14%)	6,11,13	1.45	0
22	5MU	BA	1939	22	19,22,23	4.66	7 (36%)	28,32,35	3.72	9 (32%)
22	OMU	BA	2552	22	19,22,23	2.99	8 (42%)	26,31,34	1.78	5 (19%)
1	5MC	AA	1407	1	18,22,23	3.18	7 (38%)	26,32,35	1.05	1 (3%)
55	H2U	D3	20	55	18,21,22	3.15	5 (27%)	21,30,33	1.90	4 (19%)
55	PSU	D3	32	55	18,21,22	1.11	1 (5%)	22,30,33	1.72	5 (22%)
1	UR3	AA	1498	1	19,22,23	2.60	6 (31%)	26,32,35	1.28	2 (7%)
22	2MG	BA	1835	22	18,26,27	2.56	6 (33%)	16,38,41	1.51	4 (25%)
1	4OC	AA	1402	1	20,23,24	2.89	8 (40%)	26,32,35	0.97	1 (3%)
22	PSU	BA	1917	22	18,21,22	1.00	1 (5%)	22,30,33	1.65	4 (18%)
54	H2U	D2	16	54	18,21,22	3.21	5 (27%)	21,30,33	1.77	5 (23%)
22	2MA	BA	2503	57,22	17,25,26	2.31	5 (29%)	17,37,40	1.40	3 (17%)
1	MA6	AA	1518	1	18,26,27	1.18	1 (5%)	19,38,41	4.21	3 (15%)
22	PSU	BA	2457	22	18,21,22	1.00	1 (5%)	22,30,33	1.91	4 (18%)
22	PSU	BA	2605	22	18,21,22	0.99	1 (5%)	22,30,33	1.77	3 (13%)
1	5MC	AA	967	1	18,22,23	3.25	7 (38%)	26,32,35	1.15	1 (3%)
25	MEQ	BD	150	25	8,9,10	0.93	0	5,10,12	0.75	0
55	PSU	D3	39	55	18,21,22	1.06	1 (5%)	22,30,33	1.74	5 (22%)
22	OMG	BA	2251	54,22	18,26,27	2.44	8 (44%)	19,38,41	1.48	4 (21%)
22	H2U	BA	2449	22	18,21,22	2.86	5 (27%)	21,30,33	2.01	5 (23%)
54	4SU	D2	8	54	18,21,22	3.61	8 (44%)	26,30,33	2.14	5 (19%)
22	5MC	BA	1962	22	18,22,23	3.31	7 (38%)	26,32,35	1.02	2 (7%)
22	G7M	BA	2069	22	20,26,27	2.16	7 (35%)	17,39,42	1.20	3 (17%)
54	T6A	D2	37	54	27,34,35	1.10	3 (11%)	29,49,52	2.17	8 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert > 2$	Counts	RMSZ	$\#\lvert Z\rvert > 2$
22	PSU	BA	746	57,22	18,21,22	1.08	1 (5%)	22,30,33	1.69	4 (18%)
55	5MU	D3	54	55	19,22,23	4.88	7 (36%)	28,32,35	3.58	9 (32%)

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
54	H2U	D2	20	54	-	3/7/38/39	0/2/2/2
22	PSU	BA	2504	22	-	2/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3
22	6MZ	BA	1618	22	-	2/5/27/28	0/3/3/3
55	4SU	D3	8	55	-	7/7/25/26	0/2/2/2
54	H2U	D2	19	54	-	6/7/38/39	0/2/2/2
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	OMC	BA	2498	57,22	-	1/9/27/28	0/2/2/2
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
54	PSU	D2	39	54	-	3/7/25/26	0/2/2/2
55	H2U	D3	16	55	-	2/7/38/39	0/2/2/2
22	3TD	BA	1915	22	-	0/7/25/26	0/2/2/2
54	PSU	D2	55	54	-	0/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
22	5MU	BA	747	22	-	0/7/25/26	0/2/2/2
1	PSU	AA	516	57,1	-	0/7/25/26	0/2/2/2
54	5MU	D2	54	54	-	2/7/25/26	0/2/2/2
55	PSU	D3	55	55	-	4/7/25/26	0/2/2/2
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
53	FME	D1	1	53	-	3/7/9/11	-
34	4D4	BM	81	34	-	3/11/12/14	-
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
54	OMG	D2	17(A)	54	-	0/5/27/28	0/3/3/3
54	G7M	D2	46	54	-	2/3/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	H2U	D2	17	54	-	1/7/38/39	0/2/2/2
54	4AC	D2	34	54	-	5/11/29/30	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
12	D2T	AL	89	12	-	1/7/12/14	-
22	5MU	BA	1939	22	-	2/7/25/26	0/2/2/2
22	OMU	BA	2552	22	-	0/9/27/28	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
55	H2U	D3	20	55	-	4/7/38/39	0/2/2/2
55	PSU	D3	32	55	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	1	-	2/9/29/30	0/2/2/2
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
54	H2U	D2	16	54	-	5/7/38/39	0/2/2/2
22	2MA	BA	2503	57,22	-	2/3/25/26	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
25	MEQ	BD	150	25	-	3/8/9/11	-
55	PSU	D3	39	55	-	0/7/25/26	0/2/2/2
22	OMG	BA	2251	54,22	-	0/5/27/28	0/3/3/3
22	H2U	BA	2449	22	-	0/7/38/39	0/2/2/2
54	4SU	D2	8	54	-	2/7/25/26	0/2/2/2
22	5MC	BA	1962	22	-	0/7/25/26	0/2/2/2
22	G7M	BA	2069	22	-	3/3/25/26	0/3/3/3
54	T6A	D2	37	54	-	7/19/41/42	0/3/3/3
22	PSU	BA	746	57,22	-	1/7/25/26	0/2/2/2
55	5MU	D3	54	55	-	2/7/25/26	0/2/2/2

The worst 5 of 250 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	12.07	1.49	1.35
54	D2	54	5MU	C2-N1	11.23	1.56	1.38
55	D3	54	5MU	C2-N1	11.22	1.56	1.38
55	D3	54	5MU	C6-N1	10.79	1.56	1.38
55	D3	16	H2U	C2-N1	10.54	1.50	1.35

The worst 5 of 227 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	C1'-N9-C4	12.74	149.02	126.64
54	D2	54	5MU	C5-C4-N3	12.41	125.90	115.31
22	BA	1939	5MU	C5-C4-N3	12.30	125.81	115.31
22	BA	747	5MU	C5-C4-N3	12.19	125.72	115.31
55	D3	54	5MU	C5-C4-N3	12.13	125.66	115.31

There are no chirality outliers.

5 of 94 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
1	AA	1519	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	D3	8	4SU	1	0
55	D3	16	H2U	6	0
22	BA	1915	3TD	1	0
55	D3	55	PSU	1	0
22	BA	2030	6MZ	1	0
53	D1	1	FME	5	0
54	D2	46	G7M	1	0
55	D3	32	PSU	1	0
22	BA	2503	2MA	1	0
54	D2	37	T6A	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 173 ligands modelled in this entry, 172 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	ERY	BA	3001	-	53,53,53	0.43	0	82,82,82	0.95	5 (6%)

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
58	ERY	BA	3001	-	-	7/72/107/107	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	BA	3001	ERY	C12-C11-C10	-4.27	111.08	116.43
58	BA	3001	ERY	O5-C16-C15	-2.64	108.73	112.96
58	BA	3001	ERY	O7-C5-C6	2.33	109.26	106.39
58	BA	3001	ERY	C16-C15-C14	-2.30	111.08	115.07
58	BA	3001	ERY	C6-C5-C4	-2.12	111.04	114.05

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	BA	3001	ERY	C23-C24-N1-C29
58	BA	3001	ERY	C25-C24-N1-C28
58	BA	3001	ERY	C23-C24-N1-C28
58	BA	3001	ERY	C25-C24-N1-C29
58	BA	3001	ERY	O2-C13-C36-C37

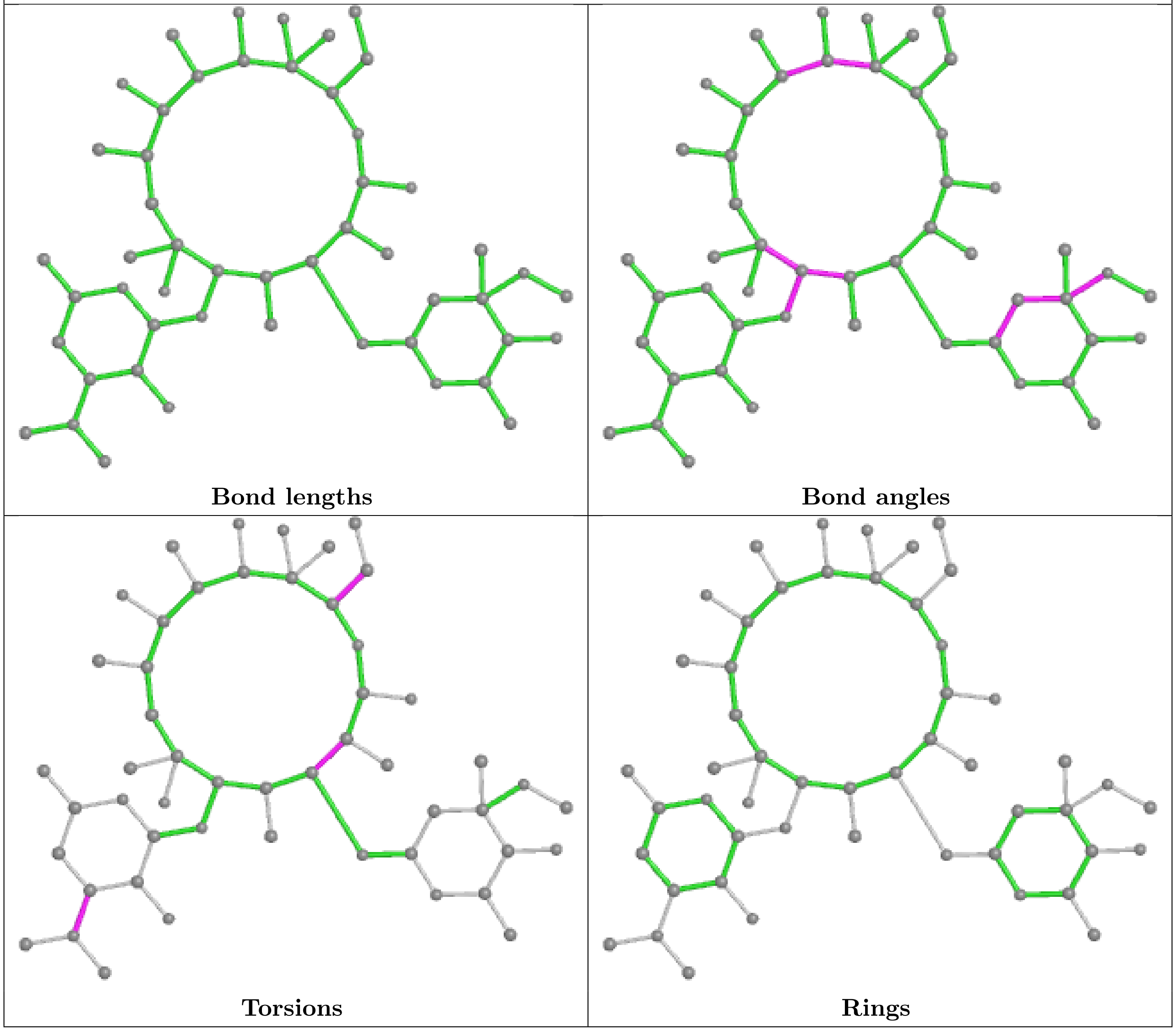
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	BA	3001	ERY	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ERY BA 3001



Bond lengths

Bond angles

Torsions

Rings

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.

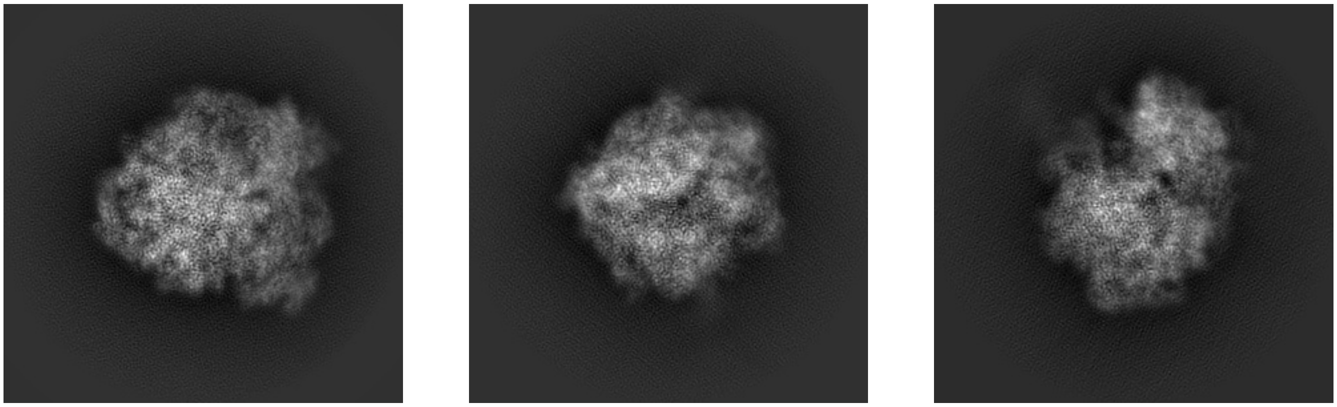
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-13805. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

6.1.1 Primary map

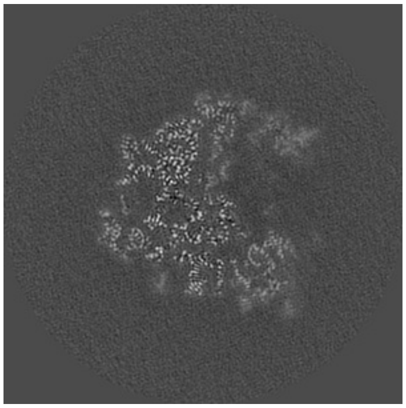


X Y Z

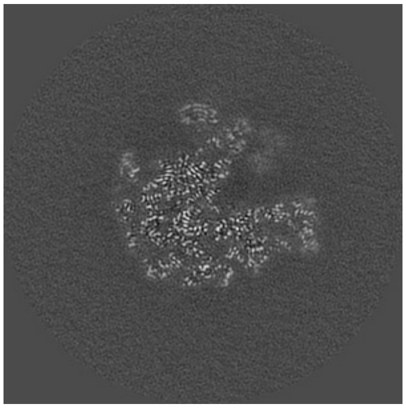
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

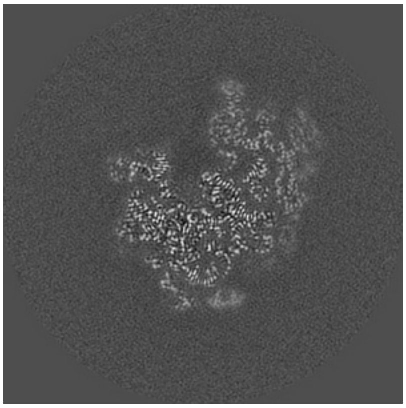
6.2.1 Primary map



X Index: 180



Y Index: 180

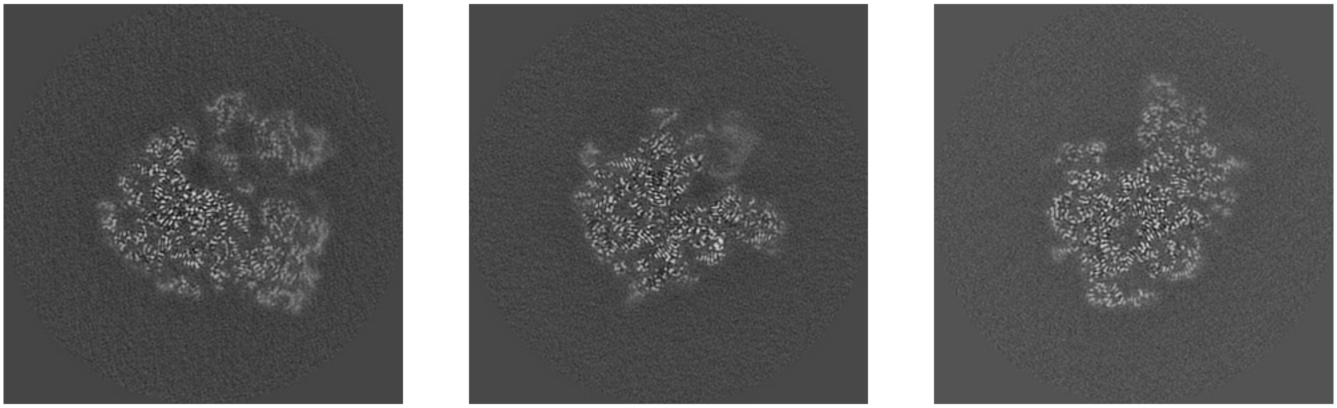


Z Index: 180

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

6.3.1 Primary map

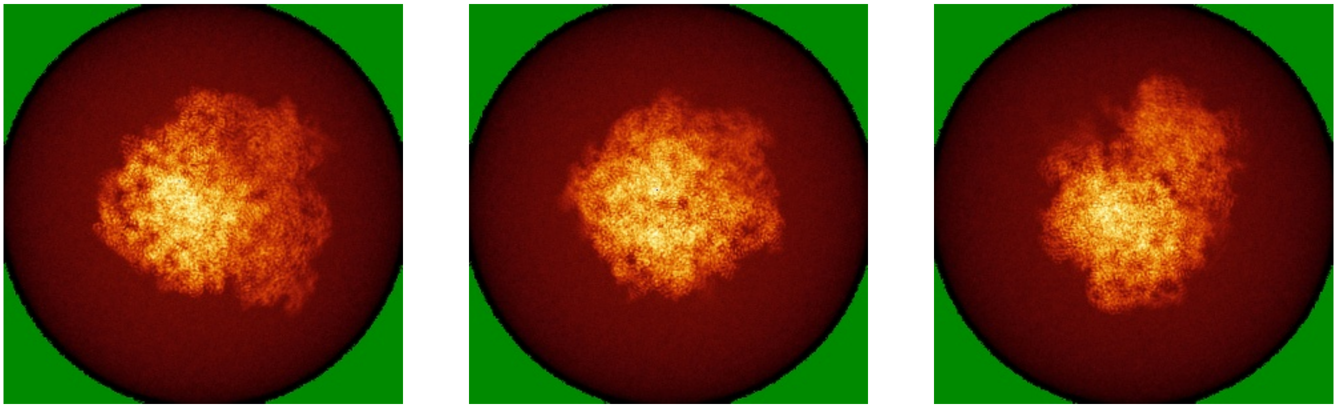


X Index: 190 Y Index: 172 Z Index: 169

The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map

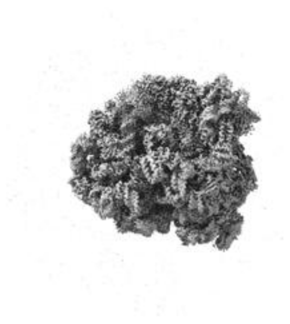


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

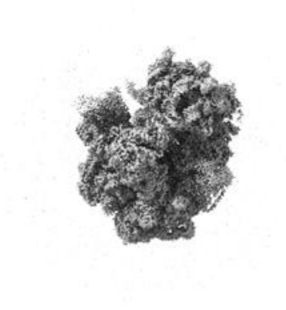
6.5 Orthogonal surface views

6.5.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.85. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

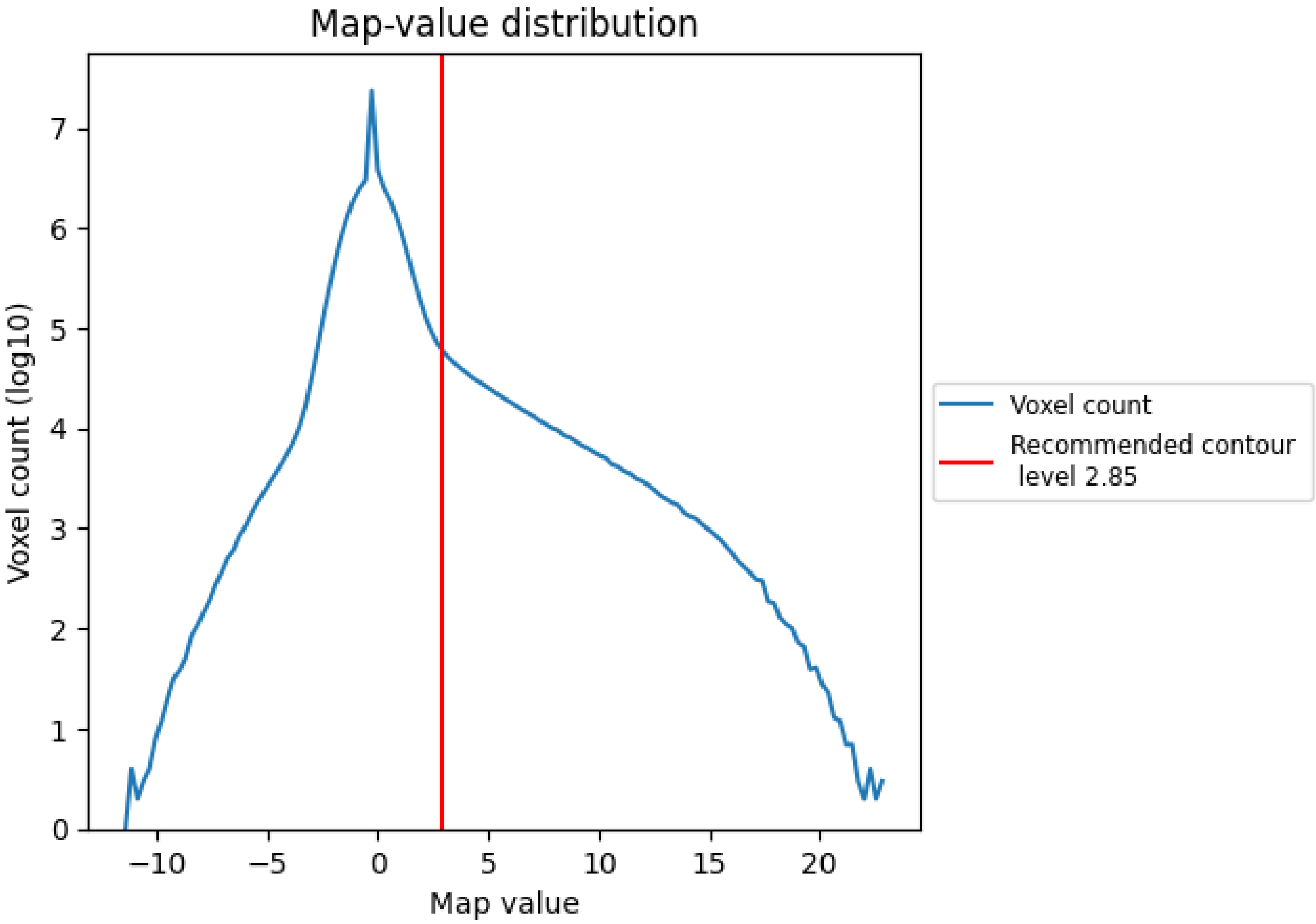
6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

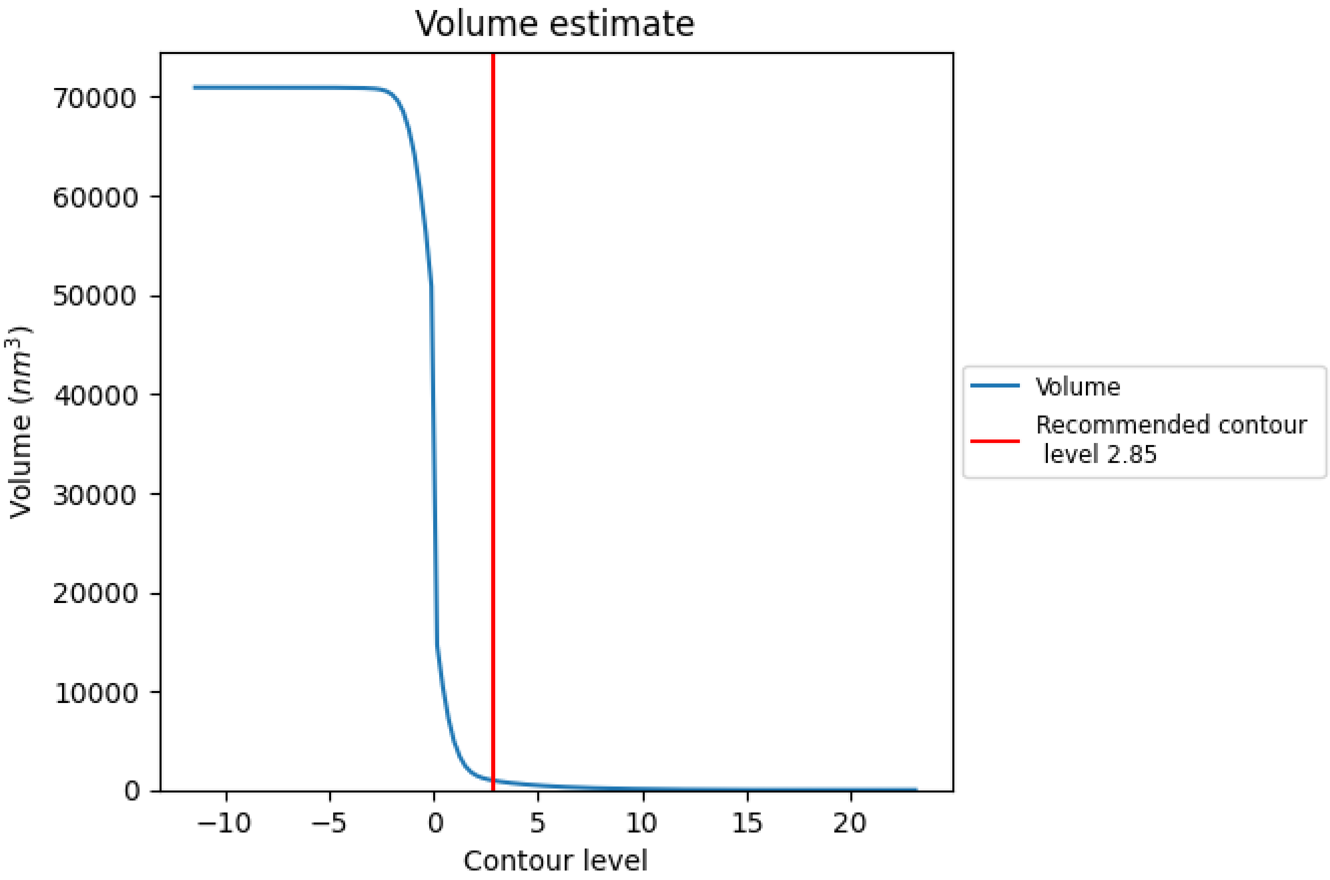
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

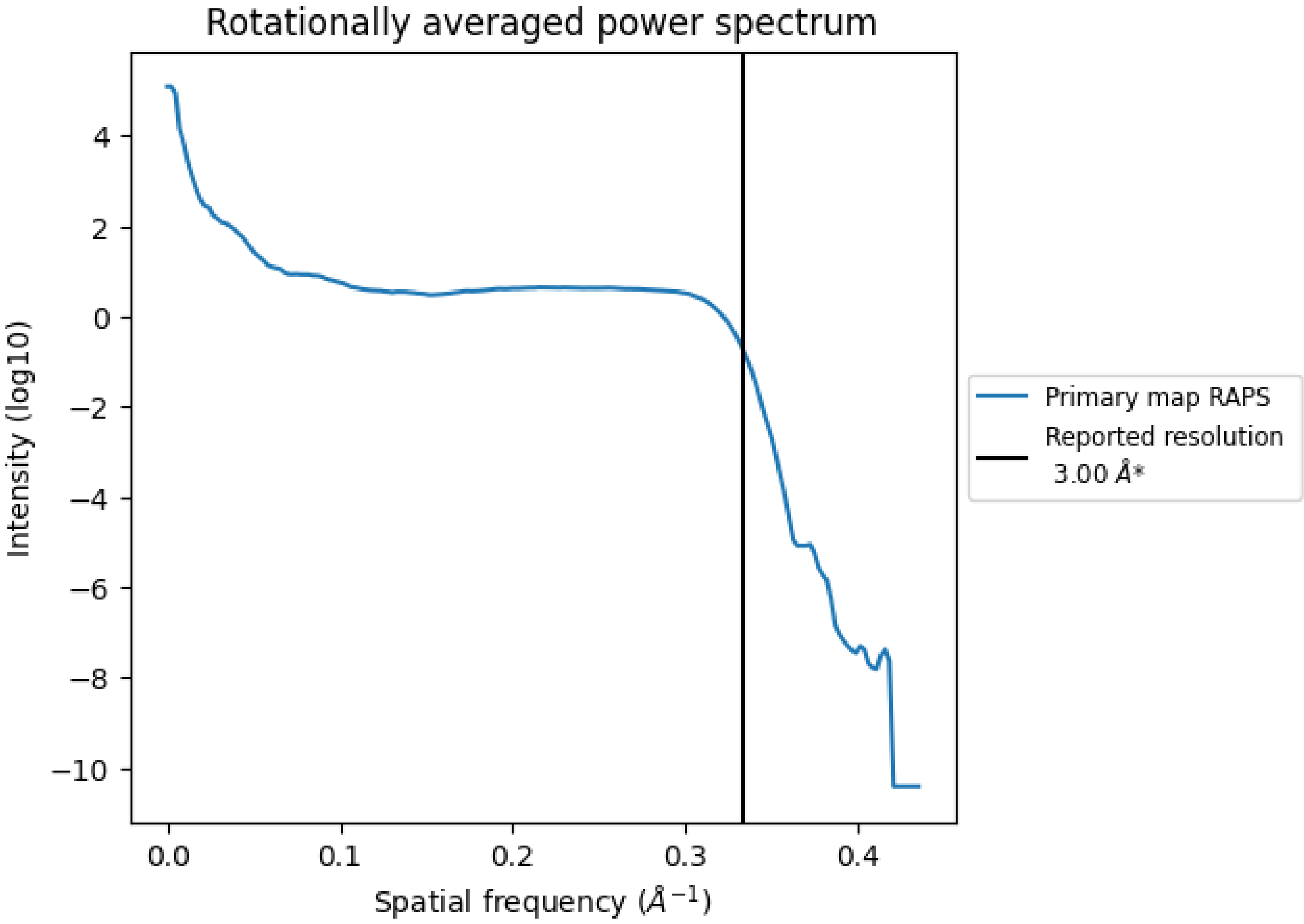
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 959 nm^3; this corresponds to an approximate mass of 866 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

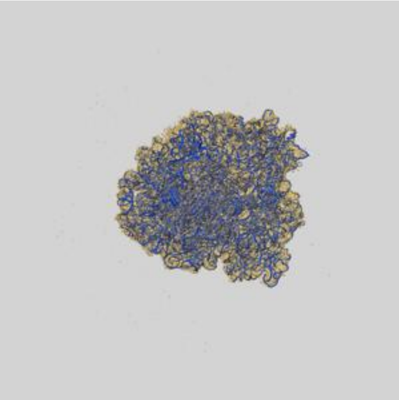
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

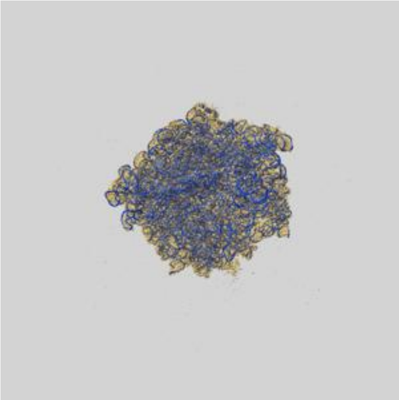
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-13805 and PDB model 7Q4K. Per-residue inclusion information can be found in section 3 on page 15.

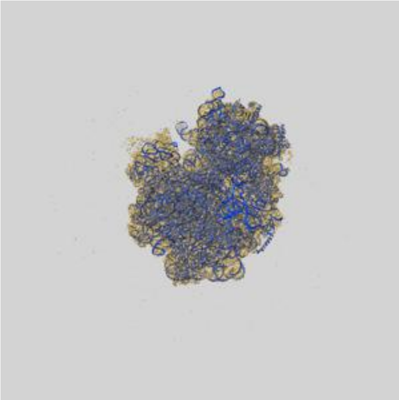
9.1 Map-model overlay (i)



X



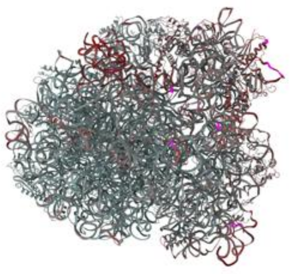
Y



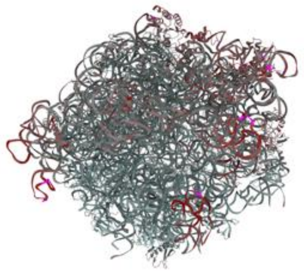
Z

The images above show the 3D surface view of the map at the recommended contour level 2.85 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

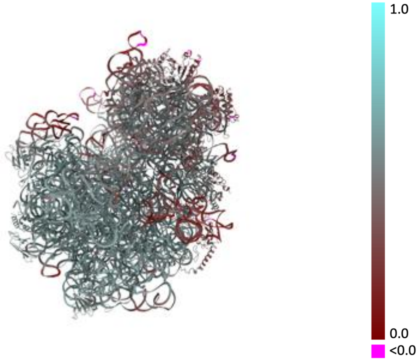
9.2 Q-score mapped to coordinate model ⓘ



X



Y



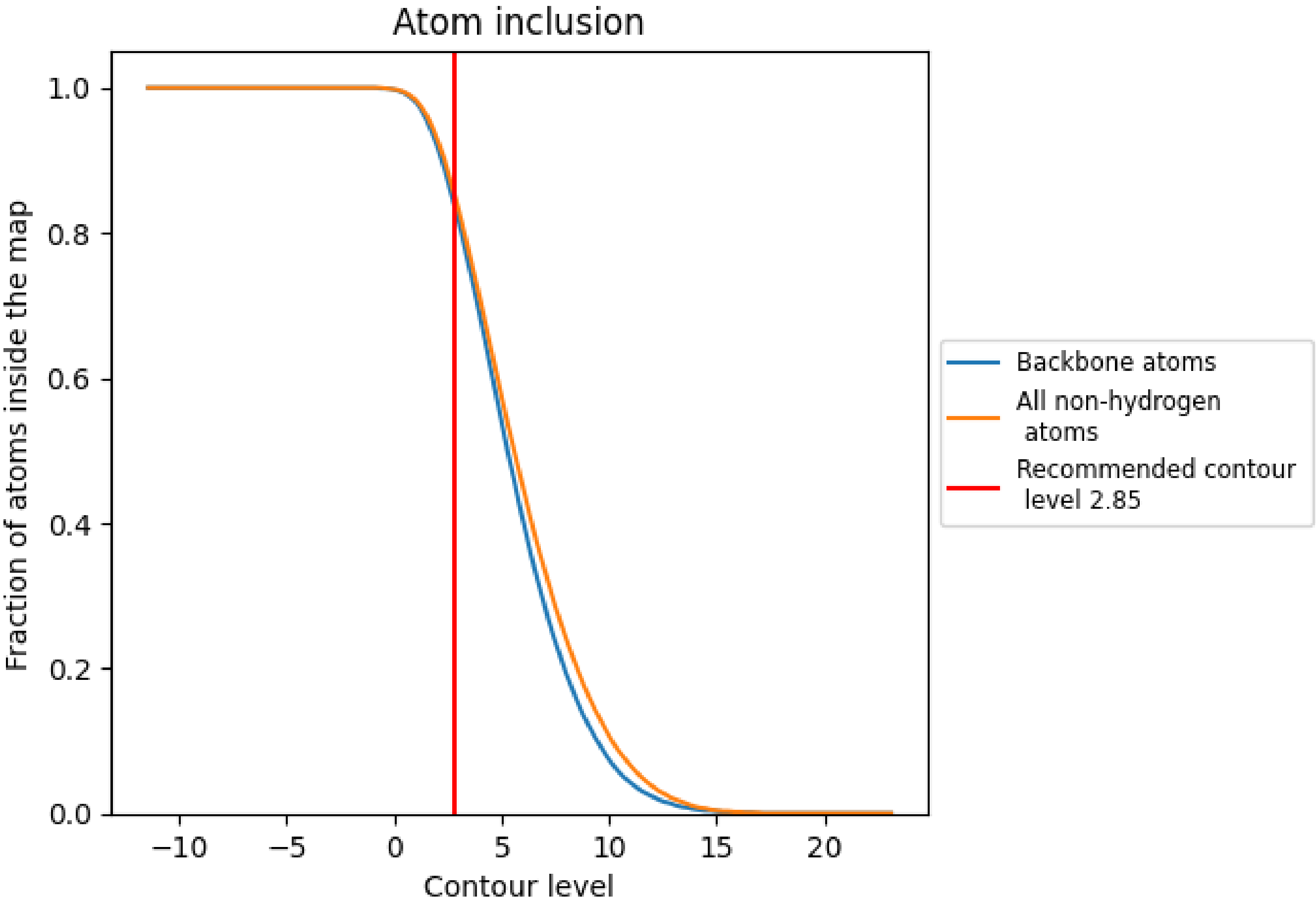
Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model ⓘ

This section was not generated.

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (2.85) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8490	0.5140
AA	0.8790	0.4770
AB	0.4950	0.3570
AC	0.6150	0.4030
AD	0.6160	0.4130
AE	0.7280	0.4880
AF	0.6710	0.4290
AG	0.5470	0.3450
AH	0.7160	0.4960
AI	0.6330	0.3880
AJ	0.5050	0.3260
AK	0.7350	0.4870
AL	0.7280	0.5090
AM	0.6490	0.3910
AN	0.6760	0.4110
AO	0.7590	0.4920
AP	0.7030	0.4730
AQ	0.6710	0.4810
AR	0.7390	0.4760
AS	0.6550	0.4090
AT	0.7360	0.4740
AU	0.6080	0.4160
B0	0.8600	0.5770
B1	0.8080	0.5600
B2	0.8840	0.5990
B3	0.9180	0.5890
B4	0.8870	0.5830
BA	0.9240	0.5500
BB	0.9420	0.5430
BC	0.8800	0.5770
BD	0.8780	0.5810
BE	0.8180	0.5560
BF	0.7400	0.4930
BG	0.7810	0.5250
BH	0.3300	0.4060

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Chain	Atom inclusion	Q-score
BI	0.5700	0.3970
BJ	0.8900	0.5850
BK	0.8360	0.5700
BL	0.8560	0.5630
BM	0.8630	0.5740
BN	0.9320	0.5940
BO	0.8520	0.5480
BP	0.8420	0.5740
BQ	0.9000	0.5860
BR	0.8630	0.5730
BS	0.8730	0.5780
BT	0.8120	0.5570
BU	0.8270	0.5500
BV	0.8360	0.5560
BW	0.8920	0.5760
BX	0.8650	0.5680
BY	0.8240	0.5540
BZ	0.8440	0.5680
D1	0.7680	0.5620
D2	0.7750	0.4750
D3	0.1840	0.3060
D4	0.7090	0.4500