



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:00 PM BST

PDB ID : 4V6V  
EMDB ID: : EMD-5562  
Title : Tetracycline resistance protein Tet(O) bound to the ribosome  
Authors : Li, W.; Atkinson, G.C.; Thakor, N.S.; Allas, U.; Lu, C.; Chan, K.Y.; Tenson, T.; Schulten, K.; Wilson, K.S.; Hauryliuk, V.; Frank, J.  
Deposited on : 2013-02-25  
Resolution : 9.80 Å(reported)  
Based on PDB ID : 2I2U, 2I2V

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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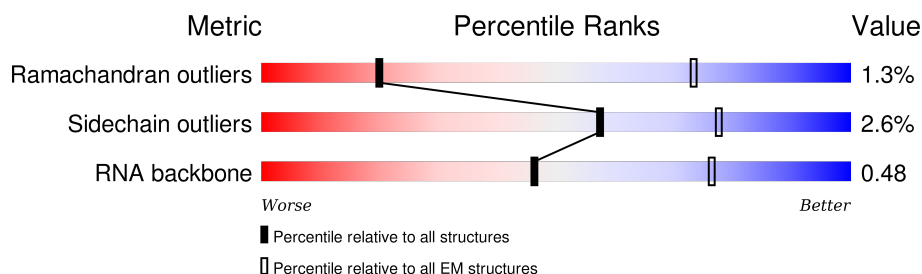
MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

# 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 9.80 Å.

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




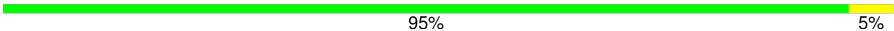







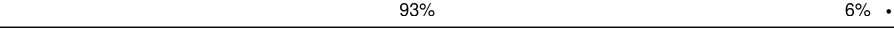

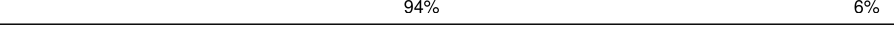

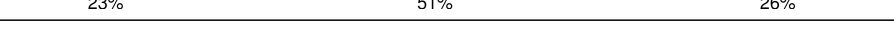

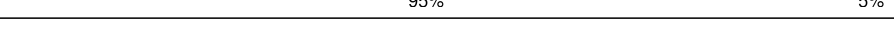
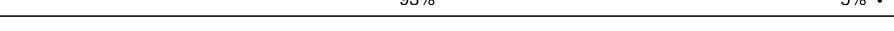
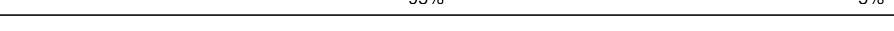

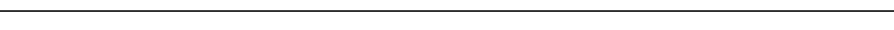

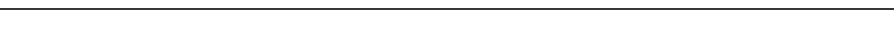
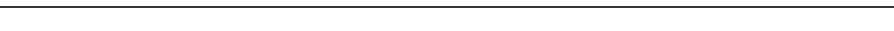


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AJ	103	89% 10% .
2	AK	128	91% 8% .
3	AL	123	89% 9% .
4	AM	117	87% 13%
5	AN	100	89% 11%
6	AO	88	91% 7% ..
7	AP	82	88% 11% .
8	AQ	83	93% 6% .
9	AR	74	82% 16% .





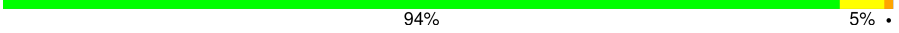
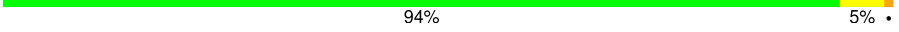
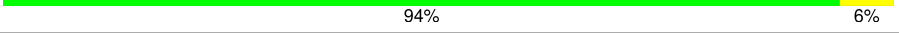





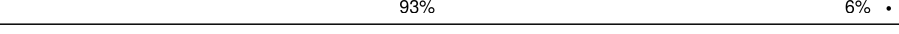
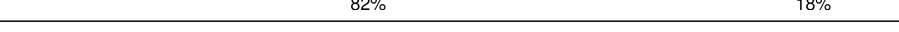
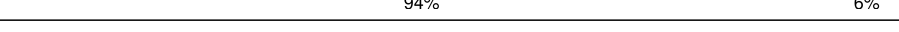
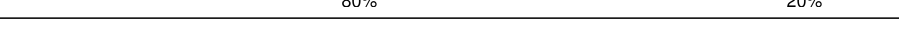



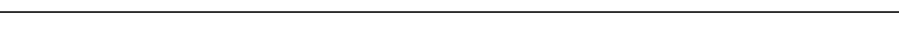




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Mol	Chain	Length	Quality of chain
10	AS	91	 87% 13%
11	AB	240	 95% 5%
12	AT	86	 93% 7%
13	AU	70	 77% 20% .
14	AC	232	 91% 9%
15	AD	205	 90% 9% .
16	AE	166	 92% 8% .
17	AF	135	 90% 9% .
18	AG	178	 90% 9% .
19	AH	129	 93% 6% .
20	AI	129	 87% 12% .
21	A1	639	 94% 6%
22	AA	1542	 16% 57% 24% .
23	A2	47	 23% 51% 26%
24	A3	77	 17% 57% 26%
25	BC	234	 95% 5%
26	BJ	164	 93% 5% .
27	BK	141	 95% 5%
28	BN	142	 87% 12% .
29	BO	123	 84% 13% ..
30	BP	144	 88% 10% .
31	BQ	136	 87% 13%
32	BR	127	 84% 15% .
33	BS	117	 91% 9%
34	BT	114	 89% 11% .

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Mol	Chain	Length	Quality of chain
35	BD	272	 88% 11% .
36	BU	117	 85% 13% .
37	BV	103	 88% 12%
38	BW	110	 90% 8% .
39	BX	100	 94% 5% .
40	BY	103	 94% 5% .
41	BZ	94	 94% 6%
42	B0	84	 85% 12% .
43	B1	77	 87% 10% .
44	B2	63	 92% 6% .
45	BE	209	 92% 7%
46	B3	58	 90% 10%
47	B4	70	 93% 6% .
48	B5	56	 82% 18%
49	B6	54	 94% 6%
50	B7	46	 80% 20%
51	B8	64	 89% 9% .
52	B9	38	 87% 13%
53	BF	201	 92% 7% .
54	BG	178	 88% 11% .
55	BH	176	 92% 6% .
56	BL	149	 95% 5%
57	BA	2904	 15% 57% 24% .
58	Ba	120	 18% 64% 17% .

## 2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 154956 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 protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AJ	103	Total	C	N	O	S	0	0
			794	483	158	151	2		

- Molecule 2 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AK	128	Total	C	N	O	S	0	0
			923	553	196	171	3		

- Molecule 3 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AL	123	Total	C	N	O	S	0	0
			923	558	196	165	4		

- Molecule 4 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AM	117	Total	C	N	O	S	0	0
			876	530	183	160	3		

- Molecule 5 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AN	100	Total	C	N	O	S	0	0
			771	465	164	139	3		

- Molecule 6 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AO	88	Total	C	N	O	S	0	0
			690	414	146	129	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AO	79	ARG	GLN	CONFLICT	UNP P0ADZ4

- Molecule 7 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AP	82	Total	C	N	O	S	0	0
			620	377	128	114	1		

- Molecule 8 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AQ	83	Total	C	N	O	S	0	0
			657	410	124	120	3		

- Molecule 9 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AR	74	Total	C	N	O	S	0	0
			603	372	123	107	1		

- Molecule 10 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AS	91	Total	C	N	O	S	0	0
			708	445	139	122	2		

- Molecule 11 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AB	240	Total	C	N	O	S	0	0
			1805	1113	332	352	8		

- Molecule 12 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AT	86	Total	C	N	O	S	0	0
			636	380	138	115	3		

- Molecule 13 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AU	70	Total	C	N	O	S	0	0
			564	340	125	98	1		

- Molecule 14 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AC	232	Total	C	N	O	S	0	0
			1761	1088	346	323	4		

- Molecule 15 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AD	205	Total	C	N	O	S	0	0
			1587	970	315	298	4		

- Molecule 16 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AE	166	Total	C	N	O	S	0	0
			1182	718	232	226	6		

- Molecule 17 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AF	135	Total	C	N	O	S	0	0
			1061	637	198	219	7		

- Molecule 18 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AG	178	Total	C	N	O	S	0	0
			1347	821	269	253	4		

- Molecule 19 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AH	129	Total	C	N	O	S	0	0
			948	585	173	184	6		

- Molecule 20 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AI	129	Total	C	N	O	S	0	0
			1000	606	208	183	3		

- Molecule 21 is a protein called Tetracycline resistance protein TetO.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	A1	639	Total	C	N	O	S	0	0
			4989	3146	850	966	27		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A1	227	ILE	THR	CONFLICT	UNP P10952

- Molecule 22 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	A2	47	Total	C	N	O	P	0	0
			993	445	167	335	46		

- Molecule 24 is a RNA chain called P-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	A3	77	Total	C	N	O	P	S	0	0
			1640	734	297	533	75	1		

- Molecule 25 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BC	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

- Molecule 26 is a protein called 50S ribosomal protein L10.



Mol	Chain	Residues	Atoms					AltConf	Trace
26	BJ	164	Total	C	N	O	S	0	0
			1233	776	220	231	6		

- Molecule 27 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BK	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 28 is a protein called 50S ribosomal protein L13.

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

- Molecule 29 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BO	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 30 is a protein called 50S ribosomal protein L15.

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

- Molecule 31 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BQ	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 32 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BR	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

- Molecule 33 is a protein called 50S ribosomal protein L18.

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

- Molecule 34 is a protein called 50S ribosomal protein L19.

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

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

- Molecule 36 is a protein called 50S ribosomal protein L20.

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

- Molecule 37 is a protein called 50S ribosomal protein L21.

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

- Molecule 38 is a protein called 50S ribosomal protein L22.

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

- Molecule 39 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BX	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 40 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BY	103	Total	C	N	O		
			789	498	148	143	0	0

- Molecule 41 is a protein called 50S ribosomal protein L25.

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

- Molecule 42 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	B0	84	Total	C	N	O	S	
			634	391	129	113	1	0

- Molecule 43 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	B1	77	Total	C	N	O	S	
			625	388	129	106	2	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	B2	63	Total	C	N	O	S	
			509	313	99	95	2	0

- Molecule 45 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	BE	209	Total	C	N	O	S	
			1565	979	288	294	4	0

- Molecule 46 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	B3	58	Total	C	N	O	S	
			449	281	87	79	2	0

- Molecule 47 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B4	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B5	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B6	54	Total	C	N	O	S	0	0
			441	284	81	76			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B7	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B8	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B9	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called 50S ribosomal protein L4.

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

- Molecule 54 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BG	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 55 is a protein called 50S ribosomal protein L6.

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

- Molecule 56 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BL	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 57 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BA	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

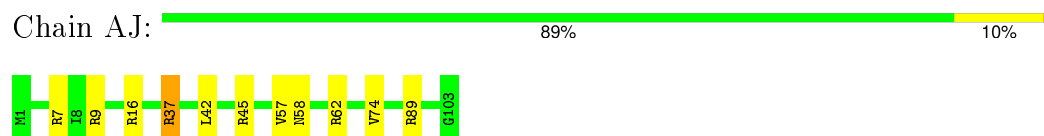
- Molecule 58 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Ba	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

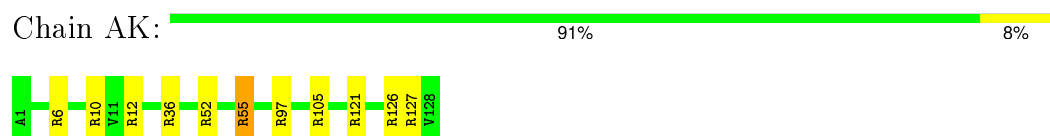
### 3 Residue-property plots [i](#)

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. 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. 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.

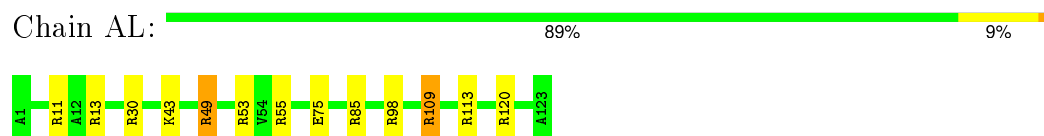
- Molecule 1: 30S ribosomal protein S10



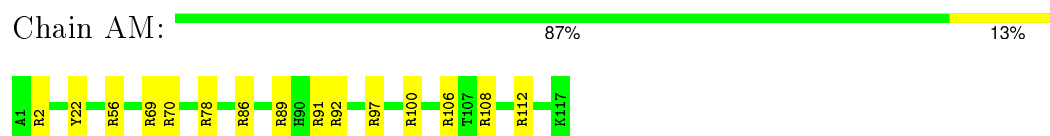
- Molecule 2: 30S ribosomal protein S11



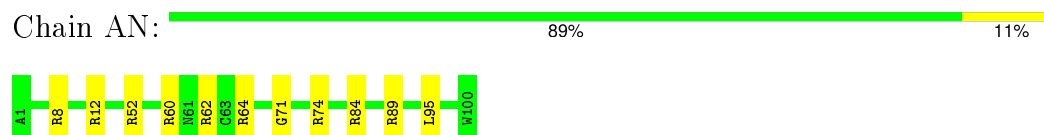
- Molecule 3: 30S ribosomal protein S12



- Molecule 4: 30S ribosomal protein S13



- Molecule 5: 30S ribosomal protein S14



- Molecule 6: 30S ribosomal protein S15





- Molecule 7: 30S ribosomal protein S16

Chain AP: 88% 11%



- Molecule 8: 30S ribosomal protein S17

Chain AQ: 93% 6%



- Molecule 9: 30S ribosomal protein S18

Chain AR: 82% 16%



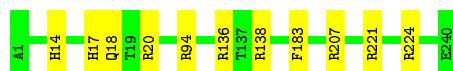
- Molecule 10: 30S ribosomal protein S19

Chain AS: 87% 13%



- Molecule 11: 30S ribosomal protein S2

Chain AB: 95% 5%



- Molecule 12: 30S ribosomal protein S20

Chain AT: 93% 7%

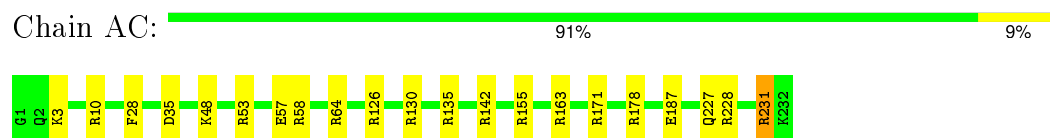


- Molecule 13: 30S ribosomal protein S21

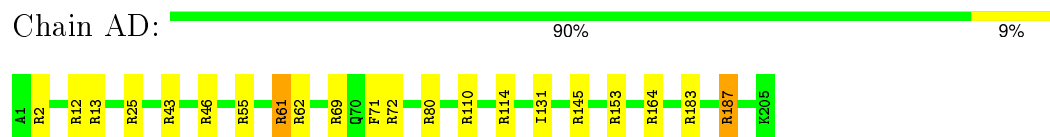
Chain AU: 77% 20%



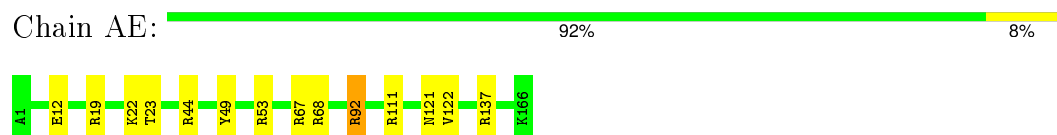
- Molecule 14: 30S ribosomal protein S3



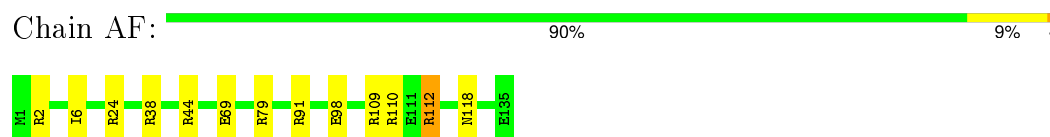
- Molecule 15: 30S ribosomal protein S4



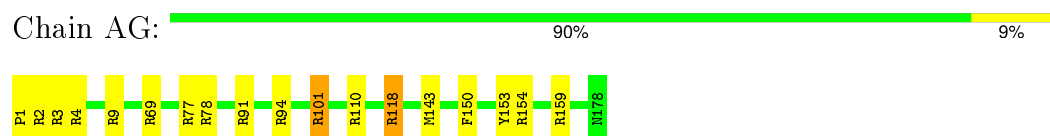
- Molecule 16: 30S ribosomal protein S5



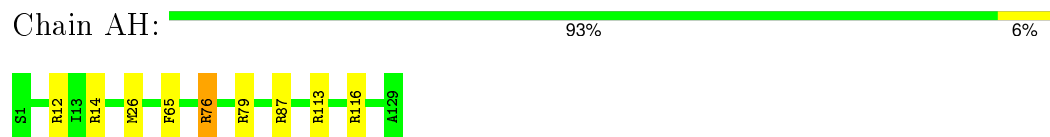
- Molecule 17: 30S ribosomal protein S6



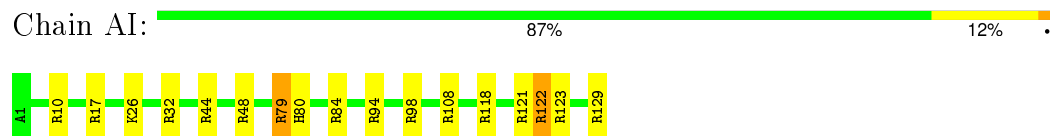
- Molecule 18: 30S ribosomal protein S7



- Molecule 19: 30S ribosomal protein S8



- Molecule 20: 30S ribosomal protein S9



- Molecule 21: Tetracycline resistance protein TetO



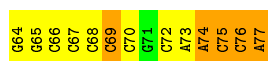


C1482	C1483	C1484	C1485	C1486	C1487	C1488	C1489	C1490	C1491	C1492	C1493	C1494	C1495	C1496	C1497	C1498	C1499	C1500	C1501	C1502	C1503	C1504	C1505	C1506	C1507	C1508	C1509	C1510	C1511	C1512	C1513	C1514	C1515	C1516	C1517	C1518	C1519	C1520	C1521	C1522	C1523	C1524	C1525	C1526	C1527	C1528	C1529	C1530	C1531	C1532	C1533	C1534	C1535	C1536	C1537	C1538	C1539	C1540	C1541	C1542	C1543	C1544	C1545	C1546	C1547	C1548	C1549	C1550	C1551	C1552	C1553	C1554	C1555	C1556	C1557	C1558	C1559	C1560	C1561	C1562	C1563	C1564	C1565	C1566	C1567	C1568	C1569	C1570	C1571	C1572	C1573	C1574	C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640	C1641	C1642	C1643	C1644	C1645	C1646	C1647	C1648	C1649	C1650	C1651	C1652	C1653	C1654	C1655	C1656	C1657	C1658	C1659	C1660	C1661	C1662	C1663	C1664	C1665	C1666	C1667	C1668	C1669	C1670	C1671	C1672	C1673	C1674	C1675	C1676	C1677	C1678	C1679	C1680	C1681	C1682	C1683	C1684	C1685	C1686	C1687	C1688	C1689	C1690	C1691	C1692	C1693	C1694	C1695	C1696	C1697	C1698	C1699	C1700	C1701	C1702	C1703	C1704	C1705	C1706	C1707	C1708	C1709	C1710	C1711	C1712	C1713	C1714	C1715	C1716	C1717	C1718	C1719	C1720	C1721	C1722	C1723	C1724	C1725	C1726	C1727	C1728	C1729	C1730	C1731	C1732	C1733	C1734	C1735	C1736	C1737	C1738	C1739	C1740	C1741	C1742	C1743	C1744	C1745	C1746	C1747	C1748	C1749	C1750	C1751	C1752	C1753	C1754	C1755	C1756	C1757	C1758	C1759	C1760	C1761	C1762	C1763	C1764	C1765	C1766	C1767	C1768	C1769	C1770	C1771	C1772	C1773	C1774	C1775	C1776	C1777	C1778	C1779	C1780	C1781	C1782	C1783	C1784	C1785	C1786	C1787	C1788	C1789	C1790	C1791	C1792	C1793	C1794	C1795	C1796	C1797	C1798	C1799	C1800	C1801	C1802	C1803	C1804	C1805	C1806	C1807	C1808	C1809	C1810	C1811	C1812	C1813	C1814	C1815	C1816	C1817	C1818	C1819	C1820	C1821	C1822	C1823	C1824	C1825	C1826	C1827	C1828	C1829	C1830	C1831	C1832	C1833	C1834	C1835	C1836	C1837	C1838	C1839	C1840	C1841	C1842	C1843	C1844	C1845	C1846	C1847	C1848	C1849	C1850	C1851	C1852	C1853	C1854	C1855	C1856	C1857	C1858	C1859	C1860	C1861	C1862	C1863	C1864	C1865	C1866	C1867	C1868	C1869	C1870	C1871	C1872	C1873	C1874	C1875	C1876	C1877	C1878	C1879	C1880	C1881	C1882	C1883	C1884	C1885	C1886	C1887	C1888	C1889	C1890	C1891	C1892	C1893	C1894	C1895	C1896	C1897	C1898	C1899	C1900	C1901	C1902	C1903	C1904	C1905	C1906	C1907	C1908	C1909	C1910	C1911	C1912	C1913	C1914	C1915	C1916	C1917	C1918	C1919	C1920	C1921	C1922	C1923	C1924	C1925	C1926	C1927	C1928	C1929	C1930	C1931	C1932	C1933	C1934	C1935	C1936	C1937	C1938	C1939	C1940	C1941	C1942	C1943	C1944	C1945	C1946	C1947	C1948	C1949	C1950	C1951	C1952	C1953	C1954	C1955	C1956	C1957	C1958	C1959	C1960	C1961	C1962	C1963	C1964	C1965	C1966	C1967	C1968	C1969	C1970	C1971	C1972	C1973	C1974	C1975	C1976	C1977	C1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	C2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	C2130	C2131	C2132	C2133	C2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2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- Molecule 23: mRNA

Chain A2: 23% 51% 26%

A13	G14	G15	A16	U17	A18	A19	G20	U21	G22	G23	A24	U25	U26	A27	U28	G29	U30		A33	U34	G35	U36		U39	G40	A41		U44	G45	C46	C47	C48	U49	U50	C51	U52		A55	G56	C57	C58	A59
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- Molecule 25: 50S ribosomal protein L1

Chain BC: 95% 5%



- Molecule 26: 50S ribosomal protein L10

Chain BJ: 93% 5%



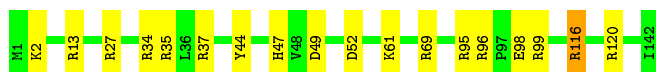
- Molecule 27: 50S ribosomal protein L11

Chain BK: 95% 5%



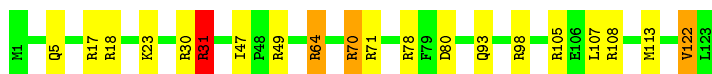
- Molecule 28: 50S ribosomal protein L13

Chain BN: 87% 12%



- Molecule 29: 50S ribosomal protein L14

Chain BO: 84% 13%



- Molecule 30: 50S ribosomal protein L15

Chain BP: 88% 10%




- Molecule 31: 50S ribosomal protein L16

Chain BQ: 87% 13%



- Molecule 32: 50S ribosomal protein L17

Chain BR:  84% 15%



- Molecule 33: 50S ribosomal protein L18

Chain BS:  91% 9%




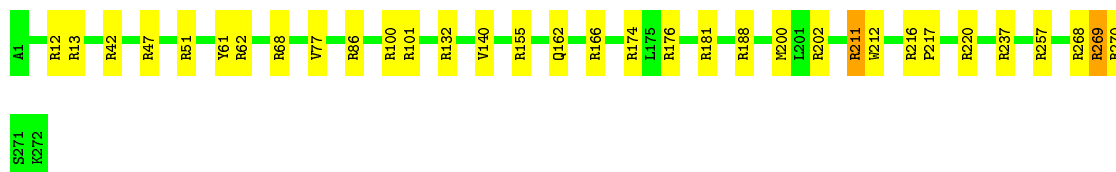
- Molecule 34: 50S ribosomal protein L19

Chain BT:  89% 11%




- Molecule 35: 50S ribosomal protein L2

Chain BD:  88% 11%




- Molecule 36: 50S ribosomal protein L20

Chain BU:  85% 13%



- Molecule 37: 50S ribosomal protein L21

Chain BV:  88% 12%



- Molecule 38: 50S ribosomal protein L22

Chain BW:  90% 8%



- Molecule 39: 50S ribosomal protein L23

Chain BX:  94% 5% •



- Molecule 40: 50S ribosomal protein L24

Chain BY:  94% 5% •




- Molecule 41: 50S ribosomal protein L25

Chain BZ:  94% 6% •




- Molecule 42: 50S ribosomal protein L27

Chain B0:  85% 12% •



- Molecule 43: 50S ribosomal protein L28

Chain B1:  87% 10% •



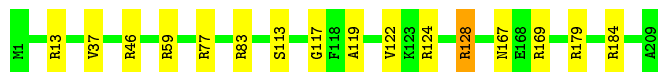
- Molecule 44: 50S ribosomal protein L29

Chain B2:  92% 6% •



- Molecule 45: 50S ribosomal protein L3

Chain BE:  92% 7% •



- Molecule 46: 50S ribosomal protein L30

Chain B3:  90% 10%




- Molecule 47: 50S ribosomal protein L31

Chain B4:  93% 6%



- Molecule 48: 50S ribosomal protein L32

Chain B5:  82% 18%




- Molecule 49: 50S ribosomal protein L33

Chain B6:  94% 6%



- Molecule 50: 50S ribosomal protein L34

Chain B7:  80% 20%



- Molecule 51: 50S ribosomal protein L35

Chain B8:  89% 9%



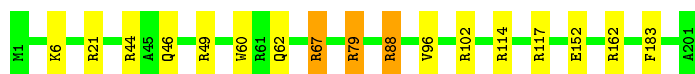
- Molecule 52: 50S ribosomal protein L36

Chain B9:  87% 13%



- Molecule 53: 50S ribosomal protein L4

Chain BF:  92% 7%



- Molecule 54: 50S ribosomal protein L5

Chain BG: 88% 11%



- Molecule 55: 50S ribosomal protein L6

Chain BH: 92% 6%



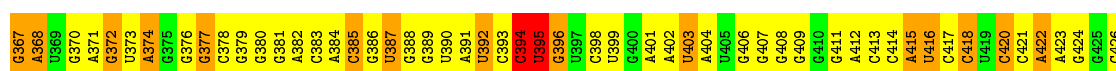
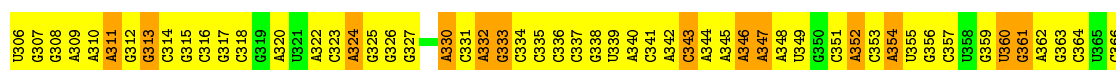
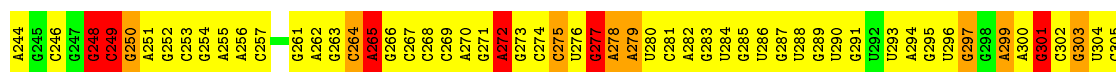
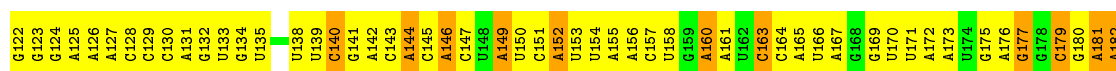
- Molecule 56: 50S ribosomal protein L9

Chain BL: 95% 5%



- Molecule 57: 23S ribosomal RNA

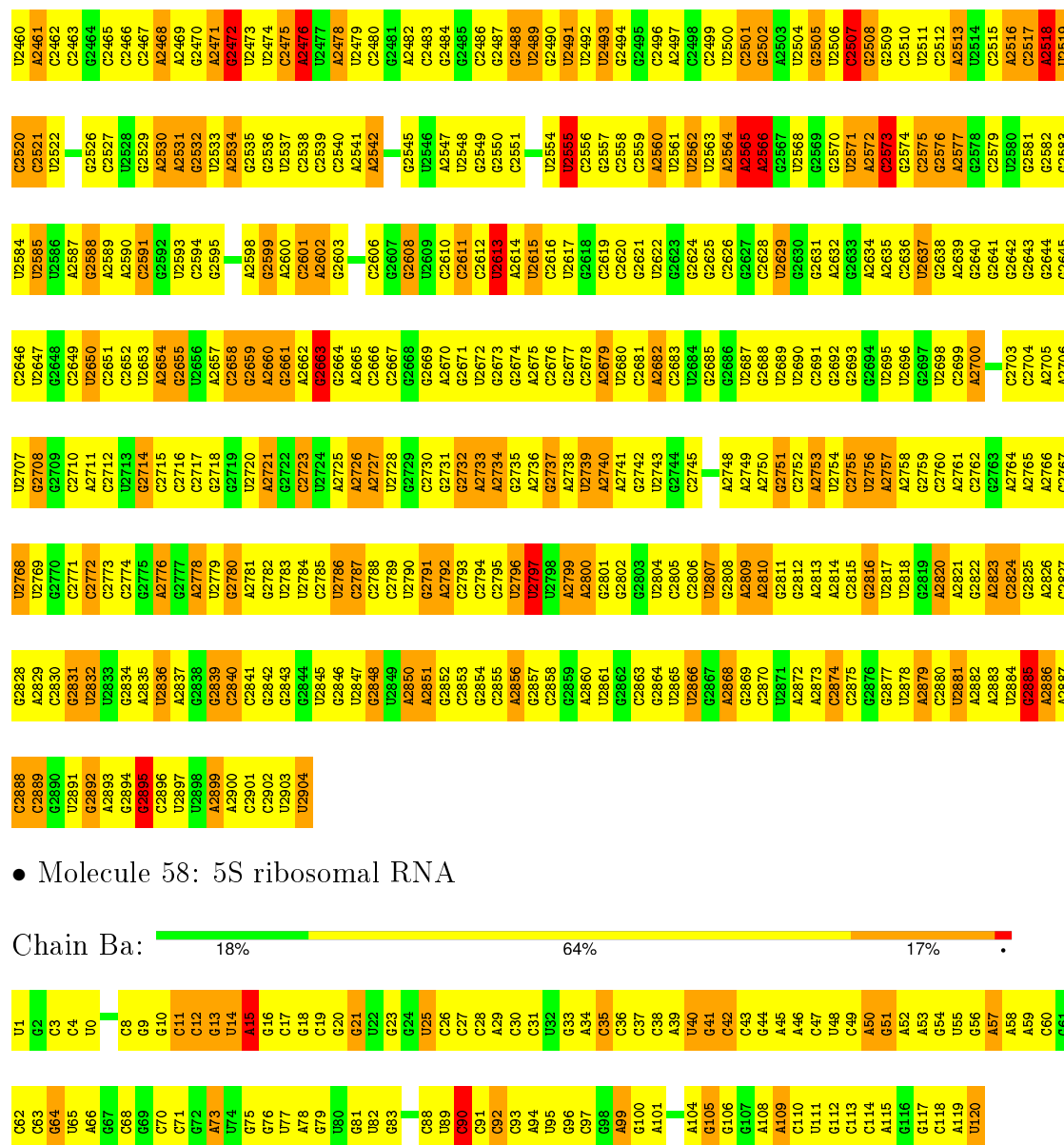
Chain BA: 15% 57% 24%



U1412	C1348	A1287	U1224	C1164	C1104	C1044	A983	A920	U860	A800	C732	A670	A608	G548	C487
A1413	C1349	G1288	G1225	A1165	U1105	C1045	A984	C921	A861	G801	G733	C671	A609	G549	G488
C1414	C1350	C1289	A1226	G1166	G1106	A1046	C985	C922	G862	A802	A734	C672	A610	C550	G489
U1415	C1351	G1227	G1227	C1167	G1107	G1047	C986	G923	A863	U803	A735	C673	C611	G551	C490
G1416	U1352	G1291	G1228	G1168	U1108	A1048	C987	G924	G864	A804	C736	G674	G612	U552	G491
C1417	A1353	G1292	G1229	A1169	C1109	C1049	C988	A925	C565	G805	C737	A675	G613	G553	A492
G1418	A1354	C1293	A1230	C1170	G1110	A1050	C989	G926	A866	C806	G738	A676	A614	U554	A493
A1419	G1355	U1294	U1231	C1171	A1111	G1051	A990	A927	C867	U807	A739	A677	U615	G555	
A1420	G1356	C1295	G1232	C1172	G1112	C1052	C991	A928	U868	G808	C740	C678	A616	G496	
G1421	C1357	G1296	C1233	U1173	U1113	A1053	C992	U929	G869	G809	U741	C679	G617	A556	A497
G1422	G1358	A1297	U1174	U1174	C1114	A1054	C993	G930	U870	U810	U742	C680	G618	U557	G498
G1423	A1359	C1298	G1235	A1175	G1115	G1055	C994	U931	U871	U811	U743		G619	U499	
G1424	G1360	G1299	U1236	U1176	G1116	G1056	C995	U932	U872	C812	U744		G620	C560	G500
G1425	G1361	G1300	A1237	G1177	C1117	A1057	A996	A933	C873	U813		U683	A621	C561	A501
G1426	C1362	A1301	G1238	C1178	C1118	U1058	C997	U934	G874	C814	U747	A685	A622	U562	A502
A1427	C1363	G1302		G1179	U1119	U1059	C998	C935	G875	C815	G748	U686	C623	A563	A503
C1428	G1364	A1303	A1241	U1180	G1120	U1060	U999	A936	C876	C816	A749	U687	C624	C564	A504
	A1365	G1304	U1242	U1181	C1121	G1062	A1001	C937	A877	C817	A750	U688	G625	C565	A505
A1431	A1366	C1305	C1243	G1182	G1122	G1063	G1002		A878	G818	A751	G689	A626	U566	G506
G1432	A1367	C1306	A1244	U1183	C1123	C1064	G1003	G940	G879	A819	A752	G690	A627	U567	A507
A1433	G1368	A1307	G1245	U1184	G1124	U1065	G1004	A941	G880	A821	A753	C691	G628	U568	A508
A1434	G1369	A1308	A1246	G1185	G1125	U1066	U1005	G942	G881	A822	U754	C692	G629	U569	C509
G1435	C1370	G1309	G1186	G1187	A1126	U1067	C1006	A943	G882	G822	U755	A693	G630	G570	C510
		G1310	G1248	G1187	A1127	A1067	C1007	C944	G883	C823	A756	U694	A631	U571	U511
C1437	A1373	G1311		U1188	G1128	G1068	C1007	A945	U884	U824	G757		A632	A572	G512
U1438	G1374	U1312	C1251	A1189	A1129	A1069	A1008	C946	C885	A825	C758		A633	U573	A513
A1439	U1375	U1313	G1252	G1190	U1130	A1070	A1009	A947	A886	U826		C698	C634	A574	A514
U1440	C1376	C1314	A1253	G1191	G1131	G1071	A1010	C948	U887	G827	A761	A699	C635	A575	A515
G1441	G1377	C1315	A1254	G1192	U1132	C1072	G1012	G949	C888	U828		G700	C636	U576	C516
U1442	A1378	G1316	U1255	G1193	A1133	A1073	U1013	G950	C889	A829	A764	G701	A637	G577	C517
U1443	U1379	G1317	G1256	A1194	A1134	G1074	C1013	C951	C890	G830	C765	U702	G638	G578	G518
		U1318	C1257	G1195	C1135	C1075	A1014	G952	G891	C831	U766	U703	U639	G579	U519
	G1382	C1319	U1258	G1196	G1136	C1076	U1015	G953	A892	U832	U767	G704	C640	U580	G520
G1447	A1383	G1320	G1197	G1197	G1137	A1077	G1016	G954	C933	A833	G768	A705	U641	C581	U521
G1448	A1384	A1321	A1260	U1198	G1138	U1078	G1017	U955	U894	G834	U769	A706	U642	A522	A522
G1449	A1385	A1322	C1261	U1199	G1139	C1079	U1018	G956	U895	C835	G770	G707	A643	G583	C523
G1450	G1386	C1323	A1262	G1200	C1140	A1080	U1019	C957	A896	G836	G771	G708	A644	G584	G524
C1451	A1387	G1324	U1263	U1201	U1141	U1081	A1020	U958	C937	C837	C772	U709	C645	G585	U525
G1452	G1388	U1325	A1264	G1202	A1142	U1082	A1021	A959	C938	C838		U710	U646	A586	A526
A1453		U1326	A1265	G1203	A1143	U1083	G1022	A960	C939	U839	G776	G711	G647	C587	C527
C1454	A1392	A1327	G1266	A1204	A1144	A1084	U1023	C961	A900	C840	U779	G713	C650	U588	A528
G1455	A1393	A1328	U1267	A1205	C1145	A1085	G1024	G962	C901	G841	U780	U714	G651	A590	A529
U1456	U1394	U1329	A1268	G1206	C1146	A1086	G1025	U963	C902	U842	G780	A715	U652	A591	G530
U1457	A1395	C1330	A1269	C1207	A1147	G1087	G1026	C964	C903	G843	A781	A716	U653	A592	G531
U1458	U1396	C1331	C1270	C1208	U1148	A1088	A1027	C965	G904	A844	A782	A717	U654	U593	A532
G1459	C1397	G1332	G1271	U1209	G1149	A1089	A1028	G966	A905	A845	A783	C717	A655	U594	G533
U1460	G1398	G1333	A1272	G1210	C1150	A1090	A1029	U967	U906	U846	G784	A718	A656	U594	U534
C1461	C1399	G1334	U1273	A1211	A1151	G1091	C1030	C968	G907	U847	G785	C719	G656	C595	G535
C1462	U1400	C1335	A1274	G1212	C1152	C1092	G1031	G969	C908	C848	G786	U720	U657	U596	G536
C1463	G1401	A1336	A1275	A1213	C1153	G1093	A1032	U970	A909	A849	C787	A721	U658	G597	G537
G1464	U1402	G1337	A1276	A1214	G1154	U1094	U1033	G971	A910	U850	A788	A722	G659	U598	A538
G1465	A1403		G1277	G1215	A1155	A1095	G1034	A972	A911	C851	A789	C723	C660	A599	G539
U1466	C1404	G1340	C1278	G1216	A1156	A1096	U1035	A973	C912	U852	U790	U724	A661	G600	C540
U1467	U1405	G1341	U1217	U1217	G1157	U1097	G1036	G974	U913	C853	G791	G725		C601	A541
U1468	U1406	A1342	G1218	U1158	A1158	A1098	G1037	A975	G914	C854	A792	G726	G664	A602	C542
A1469	G1407	G1343	U1219	U1159	C1159	G1099	G1038		C915	G855	A793	A727	U665	A603	G543
A1470	G1408	U1344	G1283	G1220	G1160	C1100	A1039	A979	G916	G856	A794	G728	A866	G604	G544
G1471	U1409	C1345	A1284	C1221	C1161	U1101	A1040	A980	A917	G857	A795	G729	U667	G605	U545
C1472	G1410	G1346	U1222	C1102	G1162	U1102	A981	A981	A918	G858	C796	A730	A668	U606	U546
G1473		A1347	G1223		G1163	A1103	C1043	C982	U919	G859		C731	G669	U607	A547



U2398	A2385	G2148	U2086	C2025	U1963	A1900	G1840	U1779	G1718	U1657	A1597	C1536	U1474
G2399	A2386	U2149	G2087	U2026	G1964	A1901	U1841	A1780	G1719	C1658	A1598	G1537	G1475
G2400	G2337	C2150	A2088	G2027	G1965	C1902	G1842	U1781	G1720	G1659	U1599	G1538	U1476
U2401	C2338	U2151	C2089	U2028	A1966	G1903	G1843	U1782	G1721	G1660	C1600	U1539	A1477
U2402	C2339	G2152	C2090	A2031	G1967	G1904	G1844	A1784	G1722	G1661	U1602	G1540	G1478
C2403	C2340	C2153	C2091	G2032	G1968	G1905	G1845	U1785	G1723	U1662	A1603	C1541	G1479
U2404	G2341	A2154	U2092	G2033	A1969	G1906	G1846	A1786	G1724	G1663	A1604	U1542	C1480
G2405	G2342	U2155	G2093	U2034	A1970	G1907	A1847	U1787	U1725	A1664	G1543	U1481	
A2406			A2094	U2034	U1971	C1908	A1848	A1788	G1726	A1665	A1544	G1482	
A2407	A2158	U2219	A2095	G2035	G1972	C1909	G1850	C1788	C1727	G1666	C1606	A1545	U1483
U2408	G2159	U2220	C2096	G2036	G1973		G1851	U1789	G1728	G1667	C1607	G1546	U1484
G2409	C2160	G2221	A2097	A2037	C1974		U1851	C1790	U1729	A1668	A1608	U1547	U1485
U2410	C2161	C2222	U2098	G2038	G1975	A1912	U1852	A1791	C1730	A1669	A1609	U1548	U1486
A2411	G2162	G2223	U2099	U2039	U1976	C1914	A1853	G1792	G1731	C1670	A1610	A1549	U1487
A2412	A2163	G2224	G2100	G2040	A1977	G1915	A1854	C1793	G1732	A1671	C1611	C1550	
G2413	C2164	U2221	A2101	U2041	A1978	A1916	U1855	A1794	G1733	A1672	A1551	C1488	
G2414	C2165	G2226	C2103	A2042	U1917	U1918	U1856	C1795	G1734	G1673	A1614	A1552	G1491
A2415	A2227	U2227	C2108	C2043	A1981	A1918	G1857	U1796	A1735	G1674	A1615	U1553	
G2416	U2167	C2228	C2104	C2045	U1982	A1919	A1858	G1797	U1736	C1675	U1554	G1492	
C2417	G2168	U2229	U2105	C2046	C1985	C1920	U1859	U1798	G1737	A1676	A1616	G1555	C1493
U2418	A2169	G2230	U2106	G2046	C1986	G1921	G1860	G1799	G1738	A1677	C1556	C1557	A1494
G2419	C2170	U2231	G2107	C2047	A1987	U1922	G1861	A1800	A1739	A1678	G1618	C1557	A1495
C2420	A2171	C2232	A2108	G2048	G1988	U1923	G1862	A1801	G1740	A1679	G1619	C1558	A1496
G2421	U2172	U2233	U2109	G2049	G1989	C1924	G1863	A1802	C1741	U1680	G1620	U1559	U1497
A2422	C2173	G2234	G2110	C2050	G1990	C1925	U1864	A1803	U1742	G1681	U1621	G1560	C1498
U2423	C2174	G2235	U2111	A2051	C1990	U1926	U1865	C1804	G1743	G1682	G1622	C1561	
C2424	C2175	U2236	G2112	A2052	U1991	A1927	A1866	A1805	A1744	U1683	G1623		A1502
G2425	G2237	G2237	U2113	G2053	G1992	A1928	G1867	A1745	U1624	U1684	U1624	C1564	A1503
A2426	C2177	C2177	A2114	A2054	U1993	G1929	C1868	G1807	A1746	C1685	C1625	C1565	A1504
G2427	G2238	C2178	G2115	C2055	C1994	G1930	G1869	A1808	U1747	C1686	A1626	A1566	
G2428	A2366	C2179	G2116	G2056	U1995	U1931	C1870	A1809	C1748	G1687	G1627	G1567	A1505
G2429	G2367	U2180	A2117	G2057	C1996	A1932	A1871	A1810	A1749	U1688	G1628	U1568	U1506
C2430	C2368	U2181	U2118	A2058	C1997	G1933	A1872	G1811	G1750	A1689	U1629	A1569	C1507
U2431	A2369	A2182	A2119	A2059	A1998	U1934	C1873	A1812	U1751	A1690	A1630	A1570	A1508
A2432	G2367	C2183	G2120	A2060	G1999	G1935	C1874	G1813	G1752	C1691	A1631	A1571	
A2433	U2185	U2185	G2121	G2061	C2000	A1936	G1875	G1814	G1753	U1693	A1632	A1572	
A2434	G2186	G2186	U2122	C2063	C2001	A1937	A1876	A1754	A1755	U1694	G1633	C1574	G1512
A2435			A2126	C2064	G2002	A1938	A1877	G1756	G1756	G1695	A1634		U1513
G2436	U2187	C2245	G2127	C2065	A2003	U1939	G1878	G1817	A1757	G1696	A1635	C1575	G1514
G2437	U2188	C2246	G2128	G2066	G2004	U1940	C1879	U1818	U1758	G1697	U1636	U1576	A1515
A2438	G2190	G2250	C2129	A2067	A2005	C1941	U1880	A1819	A1759	C1637	A1637	C1577	G1516
G2439	A2191	G2251	U2130	U2068	C2006	G1942	C1881	U1820	A1758	C1638	A1578	U1578	G1517
C2440	U2192	G2252	U2131	G2069	U2007	U1943	U1882	A1821	G1760	G1698	C1639	A1579	G1518
U2441	G2193	G2253	U2132	A2070	C2008	U1944	U1883	C1822	G1761	A1700	A1640	A1580	G1519
C2442	C2194	G2254	G2133	G2071	A2009	G1945	G1884	G1823	A1763	A1701	A1641	G1581	U1520
C2443	U2195	C2258	A2134	A2072	G2010	U1946	U1885	G1824	G1763	G1702	G1642	C1582	G1521
G2444	C2196	U2259	G2135	C2073	U2011	C1947	U1886	U1825	C1764	G1703	G1643	U1583	U1522
G2445	G2197	C2260	G2136	U2074	G2012	G1948	C1887	G1826	U1765	A1705	G1644	U1584	U1523
A2446	A2198	C2261	U2137	U2075	A2013		G1888	U1827		G1706	G1645	A1585	G1524
U2449	C2199	U2262	G2138	U2076	A2014	A1952	A1889	G1828	G1768	C1706	C1646	A1586	A1525
A2450	C2200	C2263	U2139	A2077	A2015	A1953	A1890	A1829	U1769	G1707	U1647	G1587	C1526
U2451	G2201	C2264	G2140	C2078	U2016	G1954	G1891	U1770	G1770	U1648	U1648	G1588	G1527
C2452	U2202	G2265	C2141	U2079	U2017	U1955	C1892	G1831	C1771	U1709	G1649	U1589	A1528
A2453	A2266	U2203	A2142	A2080	G2018	U1956	C1893	A1832	A1772	G1710	A1650	A1590	G1529
	G2267	G2204	C2143	U2081	A2019	C1957	C1894	C1833	A1773	A1711	G1651	A1591	G1530
	A2267	G2205	C2144	A2082	A2020	C1958	C1895		C1774	U1712	A1652	C1592	G1531
C2456	A2205	G2144	G2144	A2082	C2021	G1959	G1896	C1836	U1775	A1713	G1653	A1593	A1532
U2457	C2206	C2145	C2146	G2083	U2022	U1960	G1897	C1837	G1776		A1654	U1594	U1533
G2458	C2207	C2146	G2084	C2083	C2023	A1961	U1898	C1838	U1777	U1716	A1655	C1595	U1534
A2459	C2208	A2147	U2085	G2085	C2024	C1962	A1899	G1839	U1778		C1656	A1596	



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	98000	Depositor
Resolution determination method	FSC	Depositor
CTF correction method	group defocus	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	10	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 3TD, OMG, 5MC, MA6, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, 4SU, 7MG, 5MU, 1MG, PSU

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  >2	RMSZ	# Z  >2
1	AJ	0.75	0/742	1.26	7/941 (0.7%)
10	AS	0.77	0/687	1.27	10/880 (1.1%)
11	AB	0.74	0/1703	1.07	9/2161 (0.4%)
12	AT	0.75	0/574	1.25	12/694 (1.7%)
13	AU	0.94	0/520	1.61	15/636 (2.4%)
14	AC	0.75	0/1669	1.15	16/2122 (0.8%)
15	AD	0.80	0/1497	1.29	19/1890 (1.0%)
16	AE	0.73	0/1110	1.14	9/1405 (0.6%)
17	AF	0.79	0/1001	1.23	11/1268 (0.9%)
18	AG	0.79	0/1263	1.33	16/1590 (1.0%)
19	AH	0.72	0/896	1.11	7/1141 (0.6%)
2	AK	0.79	0/856	1.39	14/1069 (1.3%)
20	AI	0.85	0/940	1.37	19/1180 (1.6%)
21	A1	0.76	0/4864	1.12	24/6363 (0.4%)
22	AA	1.47	6/36769 (0.0%)	2.38	2673/57354 (4.7%)
23	A2	1.48	0/1108	2.31	71/1724 (4.1%)
24	A3	1.49	0/1717	2.41	129/2675 (4.8%)
25	BC	0.68	0/1748	0.98	4/2355 (0.2%)
26	BJ	0.73	0/1247	1.15	10/1679 (0.6%)
27	BK	0.67	0/1046	1.00	4/1410 (0.3%)
28	BN	0.75	0/1152	1.11	11/1551 (0.7%)
29	BO	0.74	0/956	1.20	13/1279 (1.0%)
3	AL	0.79	0/873	1.30	12/1110 (1.1%)
30	BP	0.79	0/1062	1.36	15/1413 (1.1%)
31	BQ	0.78	0/1093	1.24	13/1460 (0.9%)
32	BR	0.79	0/1021	1.35	17/1364 (1.2%)
33	BS	0.76	0/910	1.23	14/1219 (1.1%)
34	BT	0.77	0/929	1.25	10/1242 (0.8%)
35	BD	0.75	0/2131	1.25	32/2863 (1.1%)
36	BU	0.80	0/960	1.29	15/1278 (1.2%)
37	BV	0.76	0/829	1.18	9/1107 (0.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	BW	0.67	0/864	1.10	12/1156 (1.0%)
39	BX	0.69	0/794	1.10	3/1060 (0.3%)
4	AM	0.79	0/817	1.45	20/1022 (2.0%)
40	BY	0.69	0/797	1.04	4/1062 (0.4%)
41	BZ	0.73	0/766	1.11	6/1025 (0.6%)
42	B0	0.79	0/642	1.25	8/848 (0.9%)
43	B1	0.79	0/635	1.37	13/848 (1.5%)
44	B2	0.71	0/510	1.17	6/677 (0.9%)
45	BE	0.72	0/1586	1.14	15/2134 (0.7%)
46	B3	0.72	0/453	1.29	9/605 (1.5%)
47	B4	0.75	0/559	1.06	5/745 (0.7%)
48	B5	0.79	0/450	1.38	9/599 (1.5%)
49	B6	0.73	0/448	1.02	3/594 (0.5%)
5	AN	0.82	0/715	1.37	10/883 (1.1%)
50	B7	0.84	0/380	1.47	10/498 (2.0%)
51	B8	0.76	0/513	1.28	9/676 (1.3%)
52	B9	0.71	0/303	1.16	3/397 (0.8%)
53	BF	0.71	0/1571	1.09	13/2113 (0.6%)
54	BG	0.77	0/1444	1.18	10/1937 (0.5%)
55	BH	0.72	0/1343	1.08	7/1816 (0.4%)
56	BL	0.70	0/1122	1.05	8/1515 (0.5%)
57	BA	1.47	5/69280 (0.0%)	2.39	5083/108078 (4.7%)
58	Ba	1.46	0/2869	2.35	208/4474 (4.6%)
6	AO	0.76	0/646	1.22	8/813 (1.0%)
7	AP	0.83	0/572	1.39	11/711 (1.5%)
8	AQ	0.72	0/636	1.16	6/822 (0.7%)
9	AR	0.92	0/568	1.46	12/713 (1.7%)
All	All	1.28	11/165156 (0.0%)	2.11	8751/244244 (3.6%)

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
10	AS	0	1
15	AD	0	1
18	AG	0	2
21	A1	0	2
22	AA	0	350
23	A2	0	5
24	A3	0	15

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	BJ	0	1
28	BN	0	2
29	BO	0	1
3	AL	0	1
32	BR	0	1
34	BT	0	1
35	BD	0	1
36	BU	0	2
38	BW	0	1
40	BY	0	1
42	B0	0	1
51	B8	0	1
55	BH	0	2
57	BA	0	660
58	Ba	0	15
6	AO	0	1
7	AP	0	1
9	AR	0	1
All	All	0	1070

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AA	1223	C	C4-N4	-5.72	1.28	1.33
22	AA	1226	C	O3'-P	-5.66	1.54	1.61
22	AA	1432	G	C2-N2	-5.45	1.29	1.34
57	BA	823	C	C4-N4	-5.35	1.29	1.33
22	AA	1497	G	C2-N2	-5.32	1.29	1.34

The worst 5 of 8751 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	AE	111	ARG	NE-CZ-NH1	15.27	127.93	120.30
57	BA	1073	A	N1-C6-N6	-14.45	109.93	118.60
26	BJ	55	ARG	NE-CZ-NH1	14.31	127.46	120.30
57	BA	423	A	N1-C6-N6	-14.03	110.18	118.60
7	AP	70	ARG	NE-CZ-NH1	13.34	126.97	120.30

There are no chirality outliers.

5 of 1070 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AL	109	ARG	Sidechain
6	AO	88	ARG	Sidechain
7	AP	25	ARG	Sidechain
9	AR	2	ARG	Sidechain
10	AS	79	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AJ	794	0	803	0	0
2	AK	923	0	912	0	0
3	AL	923	0	954	0	0
4	AM	876	0	910	0	0
5	AN	771	0	777	0	0
6	AO	690	0	691	0	0
7	AP	620	0	611	0	0
8	AQ	657	0	687	0	0
9	AR	603	0	602	0	0
10	AS	708	0	732	0	0
11	AB	1805	0	1750	0	0
12	AT	636	0	652	0	0
13	AU	564	0	579	0	0
14	AC	1761	0	1793	0	0
15	AD	1587	0	1596	0	0
16	AE	1182	0	1185	0	0
17	AF	1061	0	971	0	0
18	AG	1347	0	1347	0	0
19	AH	948	0	975	0	0
20	AI	1000	0	1011	0	0
21	A1	4989	0	4915	0	0
22	AA	33089	0	16668	0	0
23	A2	993	0	501	0	0
24	A3	1640	0	845	0	0
25	BC	1733	0	1824	0	0
26	BJ	1233	0	1283	0	0
27	BK	1032	0	1088	0	0
28	BN	1129	0	1162	0	0
29	BO	947	0	1023	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	BP	1053	0	1129	0	0
31	BQ	1074	0	1157	0	0
32	BR	1008	0	1045	0	0
33	BS	900	0	935	0	0
34	BT	917	0	965	0	0
35	BD	2092	0	2170	0	0
36	BU	947	0	1022	0	0
37	BV	816	0	839	0	0
38	BW	857	0	922	0	0
39	BX	787	0	846	0	0
40	BY	789	0	847	0	0
41	BZ	753	0	780	0	0
42	B0	634	0	656	0	0
43	B1	625	0	655	0	0
44	B2	509	0	543	0	0
45	BE	1565	0	1616	0	0
46	B3	449	0	491	0	0
47	B4	549	0	552	0	0
48	B5	444	0	461	0	0
49	B6	441	0	485	0	0
50	B7	377	0	418	0	0
51	B8	504	0	574	0	0
52	B9	302	0	343	0	0
53	BF	1552	0	1619	0	0
54	BG	1420	0	1460	0	0
55	BH	1323	0	1374	0	0
56	BL	1111	0	1148	0	0
57	BA	62351	0	31378	0	0
58	Ba	2566	0	1302	0	0
All	All	154956	0	106579	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	
1	AJ	44/103 (43%)	40 (91%)	1 (2%)	3 (7%)	1	23
2	AK	57/128 (44%)	52 (91%)	5 (9%)	0	100	100
3	AL	64/123 (52%)	54 (84%)	8 (12%)	2 (3%)	5	42
4	AM	56/117 (48%)	51 (91%)	4 (7%)	1 (2%)	11	53
5	AN	41/100 (41%)	37 (90%)	3 (7%)	1 (2%)	7	47
6	AO	44/88 (50%)	43 (98%)	1 (2%)	0	100	100
7	AP	34/82 (42%)	31 (91%)	3 (9%)	0	100	100
8	AQ	52/83 (63%)	48 (92%)	4 (8%)	0	100	100
9	AR	36/74 (49%)	34 (94%)	2 (6%)	0	100	100
10	AS	54/91 (59%)	53 (98%)	1 (2%)	0	100	100
11	AB	123/240 (51%)	114 (93%)	7 (6%)	2 (2%)	12	56
12	AT	32/86 (37%)	30 (94%)	2 (6%)	0	100	100
13	AU	24/70 (34%)	18 (75%)	3 (12%)	3 (12%)	0	8
14	AC	126/232 (54%)	122 (97%)	4 (3%)	0	100	100
15	AD	107/205 (52%)	102 (95%)	5 (5%)	0	100	100
16	AE	89/166 (54%)	84 (94%)	4 (4%)	1 (1%)	17	63
17	AF	65/135 (48%)	61 (94%)	4 (6%)	0	100	100
18	AG	84/178 (47%)	79 (94%)	5 (6%)	0	100	100
19	AH	77/129 (60%)	70 (91%)	7 (9%)	0	100	100
20	AI	69/129 (54%)	63 (91%)	6 (9%)	0	100	100
21	A1	434/639 (68%)	390 (90%)	38 (9%)	6 (1%)	14	58
25	BC	232/234 (99%)	213 (92%)	18 (8%)	1 (0%)	39	80
26	BJ	162/164 (99%)	158 (98%)	3 (2%)	1 (1%)	30	74
27	BK	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
28	BN	140/142 (99%)	131 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BO	121/123 (98%)	107 (88%)	11 (9%)	3 (2%)	7	46
30	BP	142/144 (99%)	127 (89%)	13 (9%)	2 (1%)	14	58
31	BQ	134/136 (98%)	126 (94%)	6 (4%)	2 (2%)	13	57
32	BR	125/127 (98%)	112 (90%)	11 (9%)	2 (2%)	12	56
33	BS	115/117 (98%)	115 (100%)	0	0	100	100
34	BT	112/114 (98%)	107 (96%)	3 (3%)	2 (2%)	11	53
35	BD	270/272 (99%)	252 (93%)	15 (6%)	3 (1%)	17	63
36	BU	115/117 (98%)	108 (94%)	5 (4%)	2 (2%)	11	55
37	BV	101/103 (98%)	94 (93%)	4 (4%)	3 (3%)	5	42
38	BW	108/110 (98%)	103 (95%)	4 (4%)	1 (1%)	21	67
39	BX	98/100 (98%)	83 (85%)	12 (12%)	3 (3%)	5	42
40	BY	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
41	BZ	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
42	B0	82/84 (98%)	72 (88%)	6 (7%)	4 (5%)	3	31
43	B1	75/77 (97%)	69 (92%)	5 (7%)	1 (1%)	15	60
44	B2	61/63 (97%)	54 (88%)	7 (12%)	0	100	100
45	BE	207/209 (99%)	181 (87%)	20 (10%)	6 (3%)	6	43
46	B3	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
47	B4	68/70 (97%)	62 (91%)	6 (9%)	0	100	100
48	B5	54/56 (96%)	50 (93%)	3 (6%)	1 (2%)	10	52
49	B6	52/54 (96%)	51 (98%)	1 (2%)	0	100	100
50	B7	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B8	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
52	B9	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	2	28
53	BF	199/201 (99%)	186 (94%)	7 (4%)	6 (3%)	5	42
54	BG	176/178 (99%)	155 (88%)	15 (8%)	6 (3%)	5	40
55	BH	174/176 (99%)	157 (90%)	14 (8%)	3 (2%)	11	55
56	BL	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	26	71
All	All	5512/7062 (78%)	5089 (92%)	349 (6%)	74 (1%)	20	60

5 of 74 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
21	A1	242	THR
21	A1	493	LYS
32	BR	13	ASN
35	BD	140	VAL
42	B0	40	ARG

### 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	
1	AJ	90/90 (100%)	88 (98%)	2 (2%)	60	83
2	AK	98/98 (100%)	97 (99%)	1 (1%)	82	92
3	AL	103/103 (100%)	102 (99%)	1 (1%)	82	92
4	AM	95/95 (100%)	95 (100%)	0	100	100
5	AN	83/83 (100%)	82 (99%)	1 (1%)	78	90
6	AO	76/76 (100%)	74 (97%)	2 (3%)	54	80
7	AP	65/65 (100%)	64 (98%)	1 (2%)	72	88
8	AQ	77/77 (100%)	75 (97%)	2 (3%)	54	80
9	AR	64/64 (100%)	62 (97%)	2 (3%)	47	77
10	AS	78/78 (100%)	74 (95%)	4 (5%)	29	66
11	AB	198/198 (100%)	196 (99%)	2 (1%)	82	92
12	AT	65/65 (100%)	65 (100%)	0	100	100
13	AU	60/60 (100%)	58 (97%)	2 (3%)	45	76
14	AC	189/189 (100%)	181 (96%)	8 (4%)	36	70
15	AD	172/172 (100%)	168 (98%)	4 (2%)	58	83
16	AE	125/125 (100%)	119 (95%)	6 (5%)	31	67
17	AF	116/116 (100%)	111 (96%)	5 (4%)	35	70
18	AG	146/146 (100%)	143 (98%)	3 (2%)	61	84
19	AH	104/104 (100%)	101 (97%)	3 (3%)	50	78
20	AI	106/106 (100%)	102 (96%)	4 (4%)	40	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	A1	568/568 (100%)	559 (98%)	9 (2%)	70	88
25	BC	181/181 (100%)	174 (96%)	7 (4%)	39	72
26	BJ	122/122 (100%)	120 (98%)	2 (2%)	70	88
27	BK	109/109 (100%)	106 (97%)	3 (3%)	51	78
28	BN	116/116 (100%)	110 (95%)	6 (5%)	29	65
29	BO	104/104 (100%)	95 (91%)	9 (9%)	13	45
30	BP	103/103 (100%)	96 (93%)	7 (7%)	20	57
31	BQ	109/109 (100%)	105 (96%)	4 (4%)	41	73
32	BR	103/103 (100%)	100 (97%)	3 (3%)	50	78
33	BS	87/87 (100%)	86 (99%)	1 (1%)	80	91
34	BT	99/99 (100%)	97 (98%)	2 (2%)	63	85
35	BD	217/217 (100%)	212 (98%)	5 (2%)	58	83
36	BU	89/89 (100%)	86 (97%)	3 (3%)	44	75
37	BV	84/84 (100%)	83 (99%)	1 (1%)	78	90
38	BW	93/93 (100%)	90 (97%)	3 (3%)	46	76
39	BX	84/84 (100%)	83 (99%)	1 (1%)	78	90
40	BY	84/84 (100%)	82 (98%)	2 (2%)	57	82
41	BZ	78/78 (100%)	77 (99%)	1 (1%)	76	89
42	B0	62/62 (100%)	56 (90%)	6 (10%)	10	40
43	B1	67/67 (100%)	66 (98%)	1 (2%)	72	88
44	B2	55/55 (100%)	54 (98%)	1 (2%)	66	87
45	BE	164/164 (100%)	163 (99%)	1 (1%)	90	95
46	B3	48/48 (100%)	48 (100%)	0	100	100
47	B4	62/62 (100%)	61 (98%)	1 (2%)	70	88
48	B5	47/47 (100%)	45 (96%)	2 (4%)	35	70
49	B6	48/48 (100%)	48 (100%)	0	100	100
50	B7	38/38 (100%)	37 (97%)	1 (3%)	54	80
51	B8	51/51 (100%)	51 (100%)	0	100	100
52	B9	34/34 (100%)	34 (100%)	0	100	100
53	BF	165/165 (100%)	161 (98%)	4 (2%)	57	82
54	BG	149/149 (100%)	141 (95%)	8 (5%)	27	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	BH	137/137 (100%)	132 (96%)	5 (4%)	42	74
56	BL	114/114 (100%)	114 (100%)	0	100	100
All	All	5781/5781 (100%)	5629 (97%)	152 (3%)	57	80

5 of 152 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	BC	234	ASN
29	BO	80	ASP
54	BG	65	LEU
26	BJ	94	LEU
28	BN	49	ASP

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AA	1538/1542 (99%)	194 (12%)	57 (3%)
23	A2	46/47 (97%)	13 (28%)	1 (2%)
24	A3	75/77 (97%)	12 (16%)	2 (2%)
57	BA	2899/2904 (99%)	404 (13%)	115 (3%)
58	Ba	119/120 (99%)	11 (9%)	0
All	All	4677/4690 (99%)	634 (13%)	175 (3%)

5 of 634 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
22	AA	2	A
22	AA	3	A
22	AA	5	U
22	AA	6	G
22	AA	7	A

5 of 175 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
57	BA	544	C
57	BA	958	U

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Mol	Chain	Res	Type
57	BA	2447	G
57	BA	561	G
57	BA	718	A

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

39 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	$\# Z  > 2$
24	H2U	A3	21	24	17,21,22	1.08	2 (11%)	23,30,33	1.09	2 (8%)
24	OMC	A3	33	24	15,22,23	1.04	1 (6%)	20,31,34	0.79	0
24	5MU	A3	55	24	13,22,23	0.99	1 (7%)	16,32,35	4.63	2 (12%)
24	PSU	A3	56	24	15,21,22	1.10	2 (13%)	16,30,33	3.45	4 (25%)
24	4SU	A3	8	24	12,21,22	1.04	1 (8%)	15,30,33	1.64	1 (6%)
22	2MG	AA	1207	22	18,26,27	1.07	1 (5%)	21,38,41	2.60	5 (23%)
22	4OC	AA	1402	22	15,23,24	0.94	1 (6%)	21,32,35	1.56	4 (19%)
22	5MC	AA	1407	22	14,22,23	1.11	1 (7%)	17,32,35	1.17	1 (5%)
22	UR3	AA	1498	22	13,22,23	0.82	0	18,32,35	1.12	1 (5%)
22	2MG	AA	1516	22	18,26,27	1.05	1 (5%)	21,38,41	2.75	7 (33%)
22	MA6	AA	1518	22	18,26,27	0.82	1 (5%)	15,38,41	1.36	1 (6%)
22	MA6	AA	1519	22	18,26,27	0.83	1 (5%)	15,38,41	1.35	1 (6%)
22	PSU	AA	516	22	15,21,22	1.08	2 (13%)	16,30,33	3.48	4 (25%)
22	7MG	AA	527	22	20,26,27	2.14	4 (20%)	23,39,42	2.11	2 (8%)
22	2MG	AA	966	22	18,26,27	1.11	1 (5%)	21,38,41	2.53	4 (19%)
22	5MC	AA	967	22	14,22,23	1.04	1 (7%)	17,32,35	1.25	2 (11%)
57	6MZ	BA	1618	57	17,25,26	0.86	0	15,36,39	1.46	2 (13%)
57	2MG	BA	1835	57	18,26,27	1.08	1 (5%)	21,38,41	2.48	5 (23%)
57	PSU	BA	1911	57	15,21,22	1.09	2 (13%)	16,30,33	3.65	3 (18%)
57	3TD	BA	1915	57	15,22,23	0.99	0	17,32,35	1.70	3 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
57	PSU	BA	1917	57	15,21,22	1.07	2 (13%)	16,30,33	3.53	3 (18%)
57	5MU	BA	1939	57	13,22,23	1.01	1 (7%)	16,32,35	4.36	3 (18%)
57	5MC	BA	1962	57	14,22,23	1.11	1 (7%)	17,32,35	1.46	3 (17%)
57	6MZ	BA	2030	57	17,25,26	0.85	0	15,36,39	1.35	2 (13%)
57	7MG	BA	2069	57	20,26,27	2.14	3 (15%)	23,39,42	2.20	2 (8%)
57	OMG	BA	2251	57	18,26,27	1.11	1 (5%)	21,38,41	2.54	5 (23%)
57	2MG	BA	2445	57	18,26,27	1.02	1 (5%)	21,38,41	2.59	6 (28%)
57	H2U	BA	2449	57	17,21,22	1.20	2 (11%)	23,30,33	1.02	0
57	PSU	BA	2457	57	15,21,22	1.10	2 (13%)	16,30,33	3.49	3 (18%)
57	OMC	BA	2498	57	15,22,23	1.11	1 (6%)	20,31,34	0.90	0
57	2MA	BA	2503	57	17,25,26	0.95	0	18,37,40	2.28	4 (22%)
57	PSU	BA	2504	57	15,21,22	1.06	2 (13%)	16,30,33	3.44	2 (12%)
57	OMU	BA	2552	57	14,22,23	1.09	2 (14%)	19,31,34	2.70	3 (15%)
57	PSU	BA	2580	57	15,21,22	1.09	2 (13%)	16,30,33	3.83	4 (25%)
57	PSU	BA	2605	57	15,21,22	1.03	2 (13%)	16,30,33	3.90	5 (31%)
57	1MG	BA	745	57	17,26,27	1.00	0	19,39,42	1.54	2 (10%)
57	PSU	BA	746	57	15,21,22	1.08	2 (13%)	16,30,33	3.57	4 (25%)
57	5MU	BA	747	57	13,22,23	1.05	1 (7%)	16,32,35	4.34	3 (18%)
57	PSU	BA	955	57	15,21,22	1.08	2 (13%)	16,30,33	3.34	4 (25%)

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
24	H2U	A3	21	24	-	0/7/38/39	0/2/2/2
24	OMC	A3	33	24	-	0/5/27/28	0/2/2/2
24	5MU	A3	55	24	-	0/3/25/26	0/2/2/2
24	PSU	A3	56	24	-	0/7/25/26	0/2/2/2
24	4SU	A3	8	24	-	0/3/25/26	0/2/2/2
22	2MG	AA	1207	22	-	0/5/27/28	0/3/3/3
22	4OC	AA	1402	22	-	0/7/29/30	0/2/2/2
22	5MC	AA	1407	22	-	0/3/25/26	0/2/2/2
22	UR3	AA	1498	22	-	0/3/25/26	0/2/2/2
22	2MG	AA	1516	22	-	0/5/27/28	0/3/3/3
22	MA6	AA	1518	22	-	0/7/29/30	0/3/3/3
22	MA6	AA	1519	22	-	0/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	AA	516	22	-	0/7/25/26	0/2/2/2
22	7MG	AA	527	22	-	0/7/37/38	0/3/3/3
22	2MG	AA	966	22	-	0/5/27/28	0/3/3/3
22	5MC	AA	967	22	-	0/3/25/26	0/2/2/2
57	6MZ	BA	1618	57	-	0/5/27/28	0/3/3/3
57	2MG	BA	1835	57	-	0/5/27/28	0/3/3/3
57	PSU	BA	1911	57	-	0/7/25/26	0/2/2/2
57	3TD	BA	1915	57	-	0/7/25/26	0/2/2/2
57	PSU	BA	1917	57	-	0/7/25/26	0/2/2/2
57	5MU	BA	1939	57	-	0/3/25/26	0/2/2/2
57	5MC	BA	1962	57	-	0/3/25/26	0/2/2/2
57	6MZ	BA	2030	57	-	0/5/27/28	0/3/3/3
57	7MG	BA	2069	57	-	0/7/37/38	0/3/3/3
57	OMG	BA	2251	57	-	0/5/27/28	0/3/3/3
57	2MG	BA	2445	57	-	0/5/27/28	0/3/3/3
57	H2U	BA	2449	57	-	0/7/38/39	0/2/2/2
57	PSU	BA	2457	57	-	0/7/25/26	0/2/2/2
57	OMC	BA	2498	57	-	0/5/27/28	0/2/2/2
57	2MA	BA	2503	57	-	0/3/25/26	0/3/3/3
57	PSU	BA	2504	57	-	0/7/25/26	0/2/2/2
57	OMU	BA	2552	57	-	0/5/27/28	0/2/2/2
57	PSU	BA	2580	57	-	0/7/25/26	0/2/2/2
57	PSU	BA	2605	57	-	0/7/25/26	0/2/2/2
57	1MG	BA	745	57	-	0/3/25/26	0/3/3/3
57	PSU	BA	746	57	-	0/7/25/26	0/2/2/2
57	5MU	BA	747	57	-	0/3/25/26	0/2/2/2
57	PSU	BA	955	57	-	0/7/25/26	0/2/2/2

The worst 5 of 51 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	BA	2069	7MG	C8-N9	-7.87	1.34	1.45
22	AA	527	7MG	C8-N9	-7.74	1.34	1.45
57	BA	2449	H2U	C4-N3	-3.25	1.32	1.37
24	A3	21	H2U	C4-N3	-2.88	1.33	1.37
57	BA	2449	H2U	C2-N3	-2.82	1.32	1.38

The worst 5 of 112 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A3	55	5MU	C5-C4-N3	-12.66	114.73	125.35
57	BA	1939	5MU	C5-C4-N3	-12.14	115.16	125.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	BA	747	5MU	C5-C4-N3	-12.11	115.18	125.35
57	BA	2251	OMG	C5-C6-N1	-7.74	113.40	123.52
22	AA	1516	2MG	C5-C6-N1	-7.54	113.67	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.