



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 26, 2020 – 01:09 AM BST

PDB ID : 4V4J  
Title : Interactions and Dynamics of the Shine-Dalgarno Helix in the 70S Ribosome.  
Authors : Korostelev, A.; Trakhanov, S.; Asahara, H.; Laurberg, M.; Noller, H.F.  
Deposited on : 2007-07-18  
Resolution : 3.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

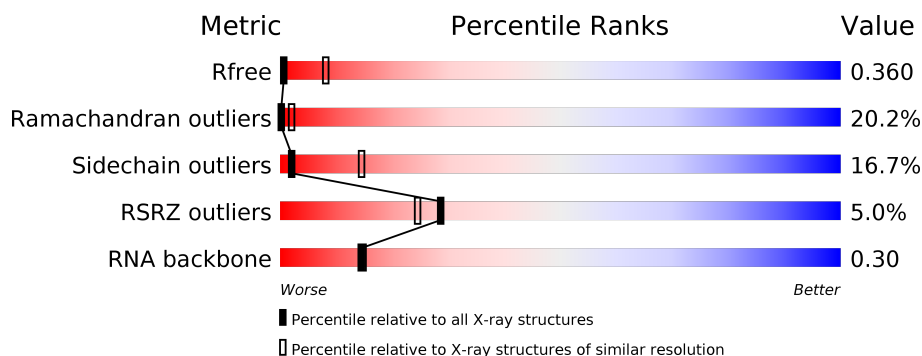
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.83 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1242 (4.08-3.60)
Ramachandran outliers	138981	1003 (4.06-3.62)
Sidechain outliers	138945	1266 (4.08-3.60)
RSRZ outliers	127900	1149 (4.08-3.60)
RNA backbone	3102	1038 (4.68-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	w	2889	<div> <div>4%</div> <div>65%</div> <div>33%</div> <div>.</div> </div>
2	x	120	<div> <div>61%</div> <div>38%</div> <div>.</div> </div>
3	A	229	<div> <div>3%</div> <div>40%</div> <div>13%</div> <div>45%</div> <div>.</div> </div>
4	B	276	<div> <div>7%</div> <div>62%</div> <div>34%</div> <div>..</div> </div>
5	C	206	<div> <div>6%</div> <div>60%</div> <div>33%</div> <div>..</div> </div>
6	D	205	<div> <div>60%</div> <div>32%</div> <div>5%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
7	E	182	
8	F	180	
9	G	148	
10	H	140	
11	I	122	
12	J	150	
13	K	141	
14	L	118	
15	M	112	
16	N	146	
17	O	118	
18	P	101	
19	Q	113	
20	R	96	
21	S	110	
22	T	206	
23	U	85	
24	V	98	
25	W	72	
26	X	60	
27	Y	60	
28	Z	49	
29	a	65	
30	b	37	
31	y	1522	

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Mol	Chain	Length	Quality of chain
32	z	77	
33	2	76	
34	3	18	
35	c	256	
36	d	239	
37	e	209	
38	f	162	
39	g	101	
40	h	156	
41	i	138	
42	j	128	
43	k	105	
44	l	129	
45	m	132	
46	n	126	
47	o	61	
48	p	89	
49	q	88	
50	r	105	
51	s	88	
52	t	93	
53	u	106	
54	v	27	

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 147125 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	w	2889	Total	C	N	O	P	0	0	0
			62213	27690	11624	20011	2888			

- Molecule 2 is a RNA chain called 5S LARGE SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	x	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	127	Total	C	N	O	S	0	0	0
			996	627	184	184	1			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	201	Total	C	N	O	S	0	0	0
			1541	974	295	267	5			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	194	Total	C	N	O	S	0	0	0
			1517	969	283	263	2			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	180	Total	C	N	O	S	0	0	0
			1468	938	267	259	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	173	Total	C	N	O	S	0	0	0
			1319	839	245	234	1			

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	148	Total	C	N	O	S	0	0	0
			1156	737	204	214	1			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	138	Total	C	N	O	S	0	0	0
			1103	712	206	182	3			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	24	VAL	MET	CONFLICT	UNP Q72IN1

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	I	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	137	Total	C	N	O	S	0	0	0
			1089	698	207	177	7			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	106	Total	C	N	O	S	0	0	0
			846	534	168	144				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	137	Total	C	N	O	S	0	0	0
			1143	713	234	195	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	109	Total	C	N	O	S	0	0	0
			868	547	170	150	1			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	R	92	Total	C	N	O			
			725	471	131	123	0	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	S	103	Total	C	N	O	S		
			793	510	151	126	6	0	0

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
22	T	185	Total	C	N	O	S		
			1475	941	262	269	3	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	U	76	Total	C	N	O	S		
			605	376	126	102	1	0	0

- Molecule 24 is a protein called LSU ribosomal protein L28P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
24	V	88	Total	C	N	O			
			694	435	141	118		0	0

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	W	62	Total	C	N	O	S		
			520	325	102	91	2	0	0

- Molecule 26 is a protein called LSU ribosomal protein L30P.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	X	60	Total	C	N	O	S		
			477	303	91	82	1	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	Y	56	Total	C	N	O	S	0	0	0
			436	275	84	72	5			

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	Z	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	a	63	Total	C	N	O	S	0	0	0
			507	326	101	78	2			

- Molecule 30 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	b	35	Total	C	N	O	S	0	0	0
			294	181	66	44	3			

- Molecule 31 is a RNA chain called 16S RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	y	1514	Total	C	N	O	P	0	0	0
			32546	14494	6022	10517	1513			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	466	G	C	CONFLICT	GB 155076

- Molecule 32 is a RNA chain called P-site tRNA<sup>f</sup>MET.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	z	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 33 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	2	76	Total	C	N	O	P	0	0	0
			1621	725	293	528	75			

- Molecule 34 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	3	18	Total	C	N	O	P	0	0	0
			390	176	80	117	17			

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	c	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	d	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	e	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	f	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	g	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	h	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	i	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	j	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	k	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	l	116	Total	C	N	O	S	0	0	0
			864	537	164	160	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	m	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	n	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	o	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	p	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	q	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	r	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	s	81	Total	C	N	O	0	0	0
			668	423	135	110			

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	t	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	u	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

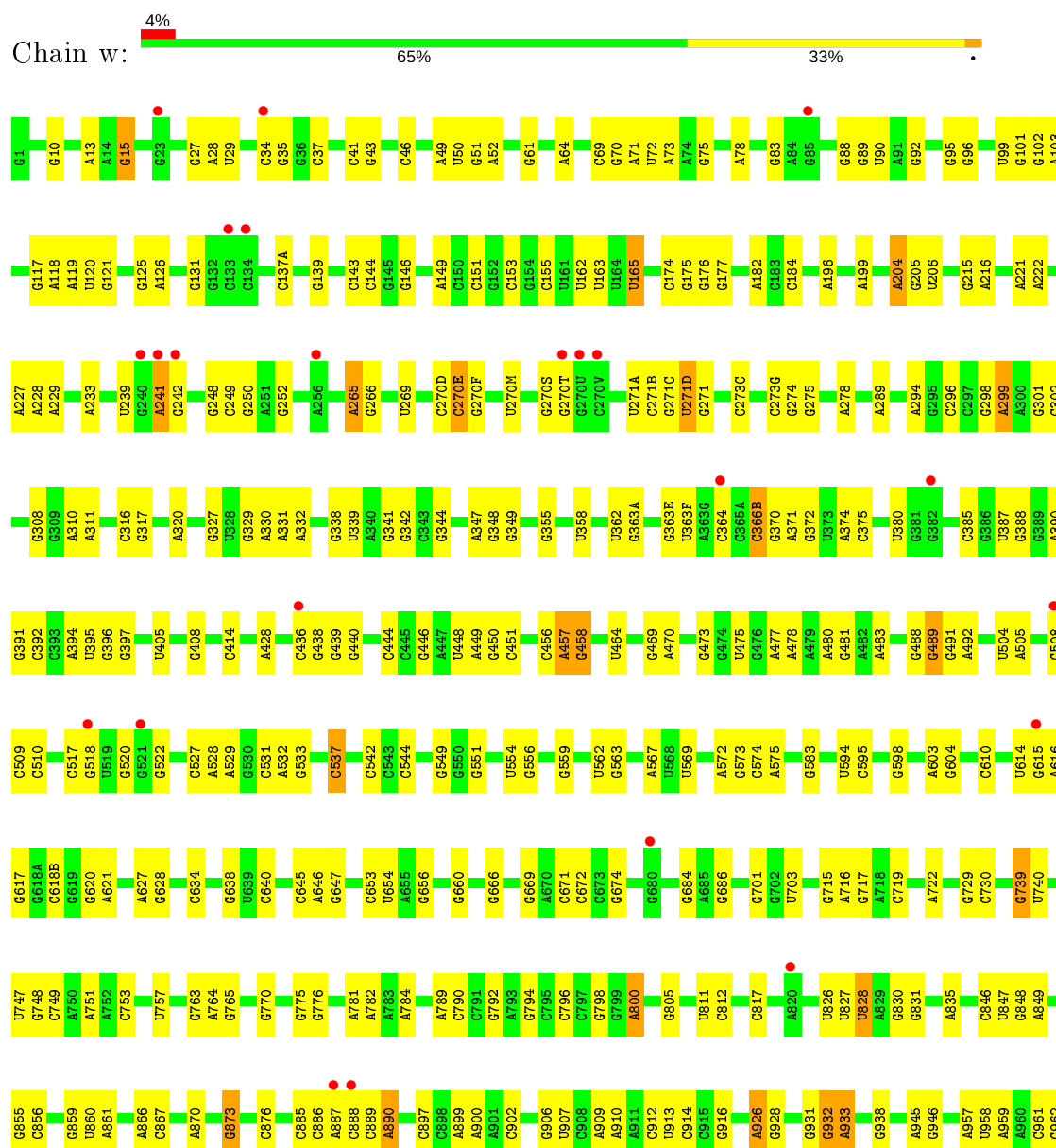
- Molecule 54 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	v	24	Total	C	N	O	0	0	0
			208	128	50	30			

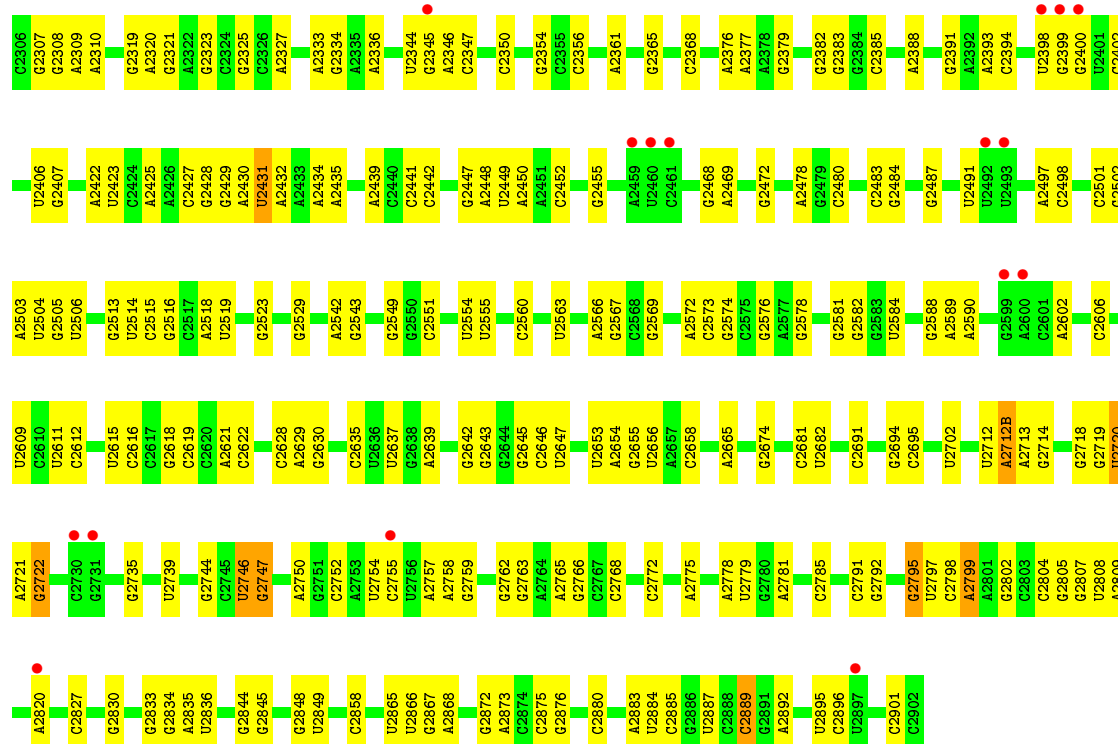
### 3 Residue-property plots [i](#)

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

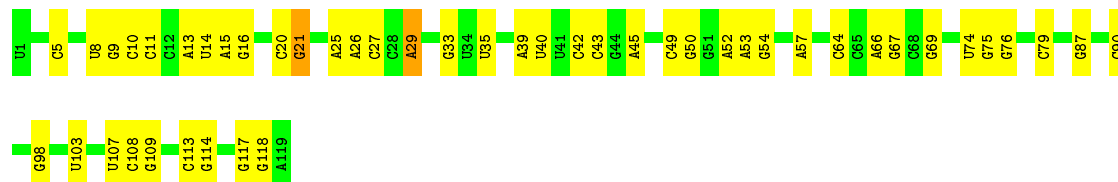
#### • Molecule 1: 23S LARGE SUBUNIT RIBOSOMAL RNA



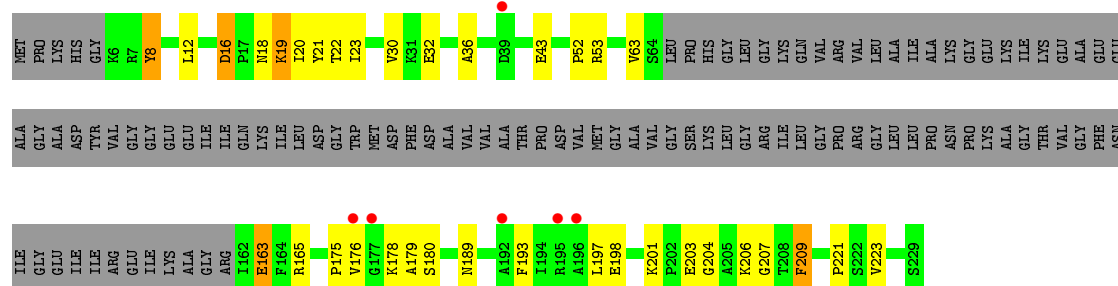
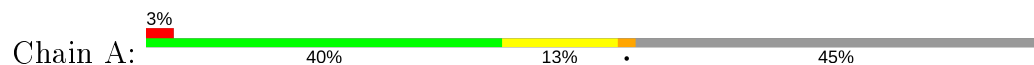
C2188	G1987	G1863	G1760	G1560	G1471	G1356	G1248	C1161	G1059	U963
C2189	C1988	U1864	C1761	A1567	G1472	A1359	U1249	C1166	U1060	C964
C2190	C1989	G1869	A1762	G1568	G1473	A1360	C1251	G1170	U1061	C965
C2191	U1991	A1372	G1764	A1569	C1474	G1361	G1252	G1171	G1062	G966
C2192	G1992	G1878	A1773	A1570	G1478	C1362	A1253	G1176	A1067	G972
C2193	U1993	C1879	C1774	U1576	G1479	A1365	G1256	U1175	G1068	A973
C2194	G1997	A1885	G1775	C1577	G1480	A1366	G1257	G1176	A1069	G974A
C2195	G1998	C1886	G1776	U1578	U1481	A1367	A1265	A1177	A1070	C974B
A2199	A2001	C1887	U1777	A1579	G1483	G1368	G1266	C1178	G1071	G975
C2205	G2002	G1888	A1780	A1580	G1484	G1369	U1267	C1179	C1072	G976
G2211	G2010	A1889	C1781	C1582	G1485	A1378	G1271	C1180	C1079	G977
A2212	U2011	G1782	G1785	A1585	A1486	A1379	A1272	C1181	C1080	A980
G2215	G2012	C1786	A1786	A1586	G1487	A1384	U1273	G1182	U1083	A981
C2216	A2013	U1787	G1788	U1590	U1488	A1385	A1274	G1186	G1087	A983
G2217	A2014	A1801	A1789	G1591	U1489	A1386	A1275	G1187	A1088	G989
G2218	G2120	A1802	U1792	G1592	G1491	A1387	G1277	U1188	G1089	A990
G2219	A2020	C1800	G1793	G1593	A1496	A1388	A1276	G1189	A1095	C991
G2224	G2023	G1801	U1699	G1594	U1497	C1398	G1278	A1194	U1096	C992
A2225	G2024	G1802	A1700	G1595	U1498	A1395	G1279	G1195	U1097	G993
C2226	C2026	A1802	U1698	A1596	C1501	A1404	U1288	C1196	A1098	A996
G2228	A2031	C1806	U1692	C1599	C1502	G1416	U1289	G1197	G1099	G997
G2239	G2032	G1807	C1694	C1600	C1506	C1417	C1295	U1198	A1111	C1006
U2243	G2033	U1808	C1694	A1603	A1508	G1418	G1296	U1199	G1112	C1007
C2248	U2034	A1810	G1699	A1603	A1509	A1419	G1297	C1200	G1008	A1009
G2251	G2035	G1811	A1700	C1607	A1510	U1420	G1298	C1201	G1115	A1010
G2257	C2040	A1812	G1707	A1608	U1516	G1426	G1299	G1202	G1116	A1010
C2258	U2041	G1816	C1712	A1610	U1517	G1427	U1300	G1203	G1117	G1011
G2259	C2042	G1817	U1716	A1613	G1518	C1428	A1301	A1204	A1126	U1012
C2260	C2043	U1818	U1717	A1614	U1520	A1434	A1302	U1205	G1014	C1013
C2264	C2050	A1821	G1718	C1615	G1522	G1435	G1305	G1208	G1015	G1016
A2269	A2051	A1822	U1719	C1616	U1521	C1436	G1310	G1209	G1016	G1017
G2274	G2052	G1823	G1720	C1617	G1522	U1437	U1313	U1211	A1129	A1020
C2275	C2055	G1824	G1721	A1618	G1534	U1438	A1320	G1212	U1130	A1021
G2276	G2056	A1825	U1722	C1625	U1535	A1444B	A1321	C1221	G1135	A1022
C2283	A2057	G1826	C1733	G1626	A1536	C1445	A1326	C1221A	G1024	G1023
A2287	C2063	A1829	U1734	G1627	C1537	G1448	G1325	C1224	G1139	U1025
A2288	G2066	G1836	G1742	G1628	G1538	A1449	U1329	G1227	C1140	G1026
G2289	U2067	C1837	G1743	C1630B	U1543	G1450	U1329	G1228	A1142B	U1033
C2290	G2068	G1838	G1746	G1633	C1544	C1451	G1339	G1229	A1143	G1034
C2294	U2069	G1839	G1747	A1634	U1545	A1453	U1340	A1237	A1148	G1042
C2297	C2076	C1843	G1748	G1635	A1546	G1454	G1341	G1238	G1043	C1043
G2304	G2076	C1847	C1754	C1636	C1547	G1458	G1343	G1239	C1152	A1045
A2305	U2076	A1847	A1755	U1639	G1555	G1459	G1347	U1240	A1155	A1046
G2305	A2077	G1858	G1756	C1640	A1558	A1460	G1348	G1244	A1156	G1047
G2306	C1983	A1859	U1757	A1641	G1559	G1461	A1349	A1247	G1157	A1054
G2307	G2080	G1759	A1759	G1642		C1467				



- Molecule 2: 5S LARGE SUBUNIT RIBOSOMAL RNA



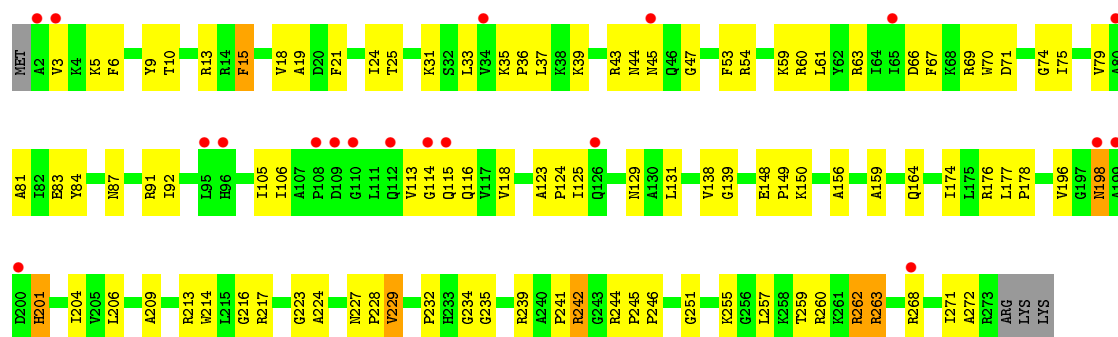
- Molecule 3: 50S ribosomal protein L1



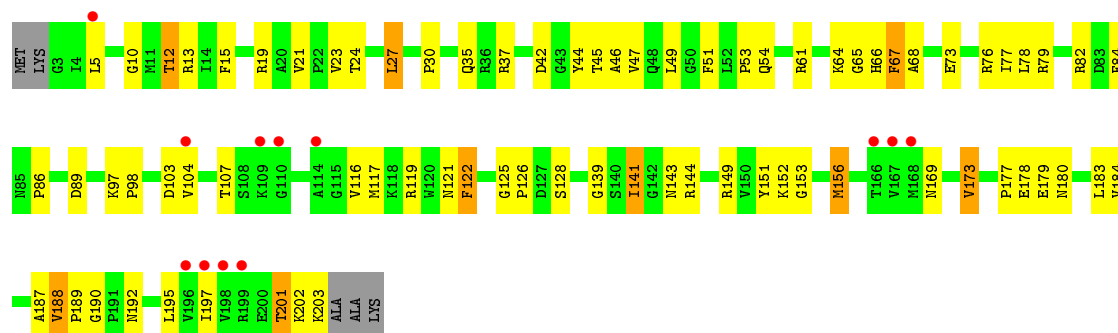
- Molecule 4: 50S ribosomal protein L2



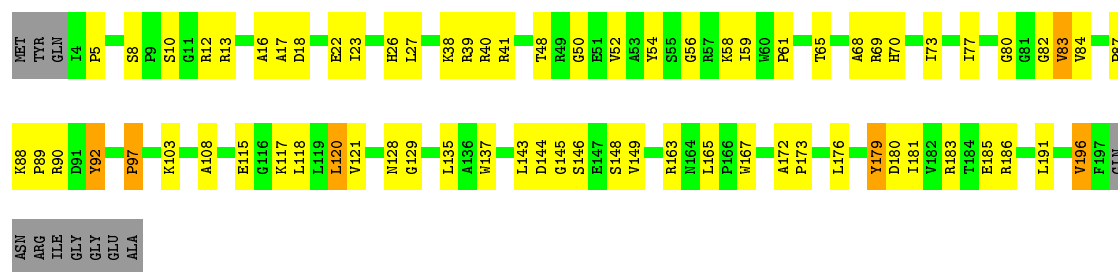




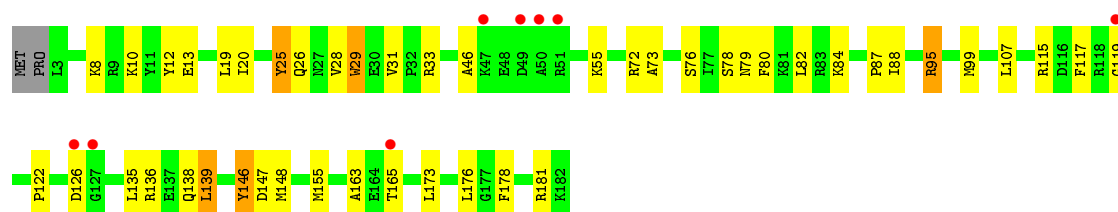
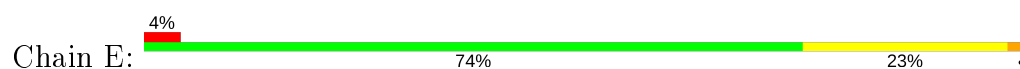
• Molecule 5: 50S ribosomal protein L3



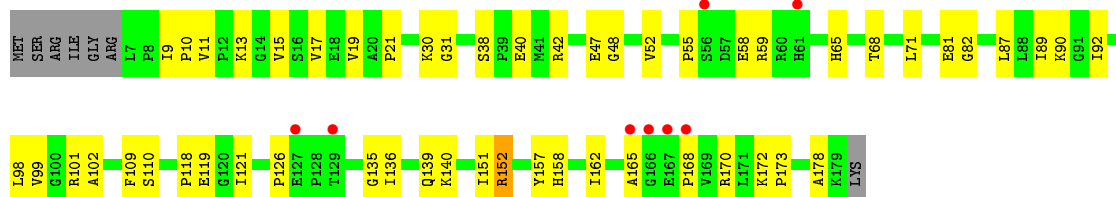
• Molecule 6: 50S ribosomal protein L4



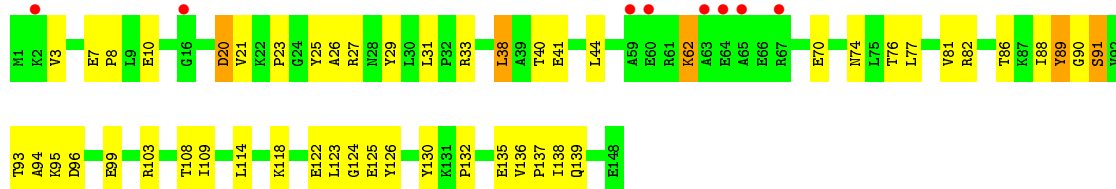
• Molecule 7: 50S ribosomal protein L5



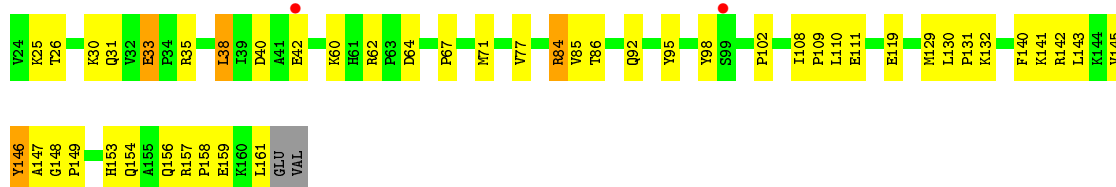
• Molecule 8: 50S ribosomal protein L6



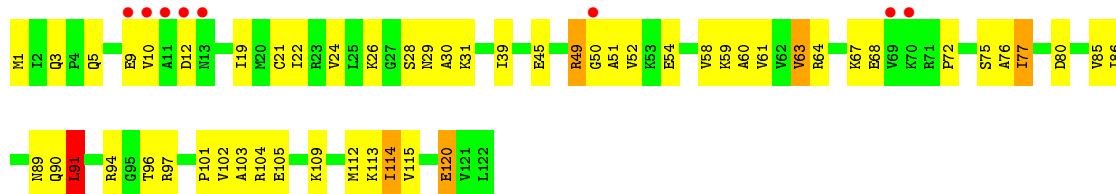
- Molecule 9: 50S ribosomal protein L9



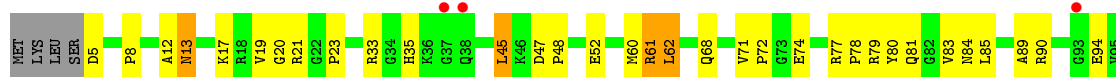
- Molecule 10: 50S ribosomal protein L13

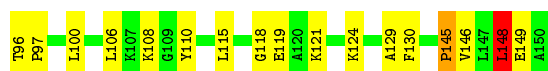


- Molecule 11: 50S ribosomal protein L14

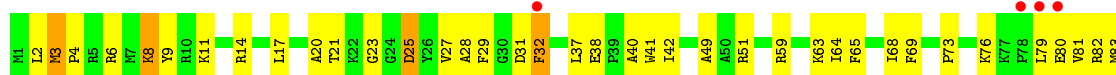


- Molecule 12: 50S ribosomal protein L15

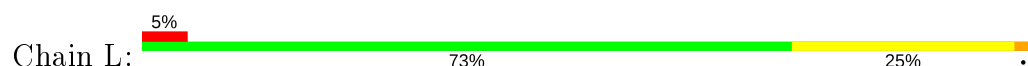




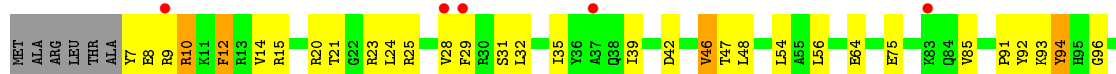
- Molecule 13: 50S ribosomal protein L16



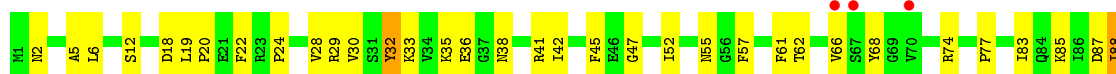
- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19

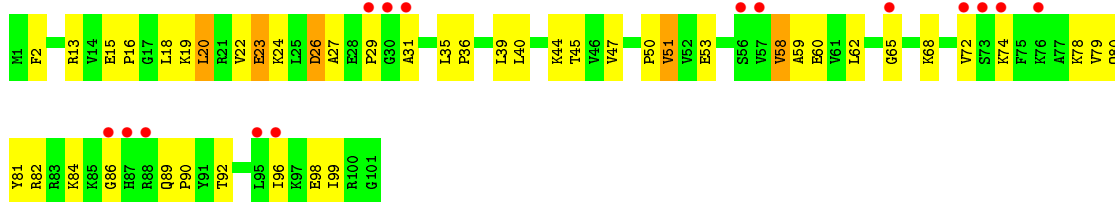


- Molecule 17: 50S ribosomal protein L20

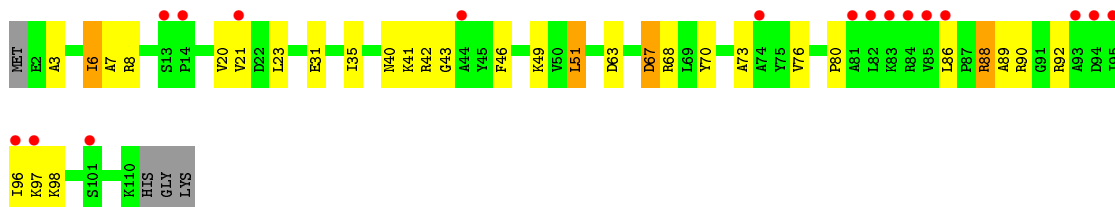




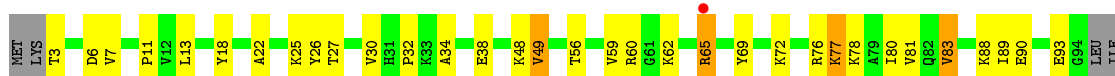
- Molecule 18: 50S ribosomal protein L21



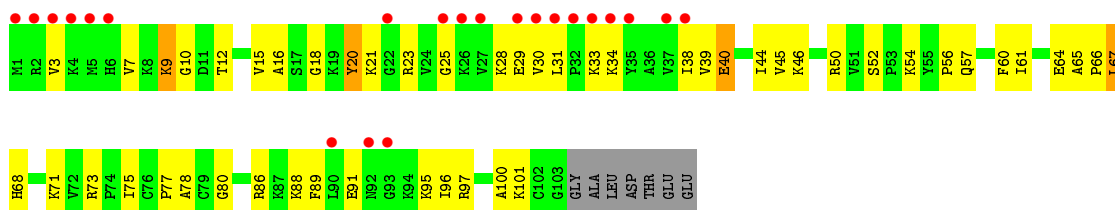
- Molecule 19: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L23

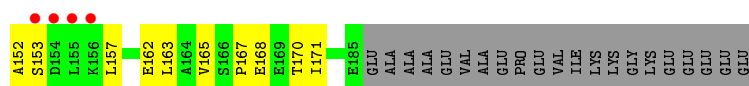


- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25





- Molecule 23: 50S ribosomal protein L27



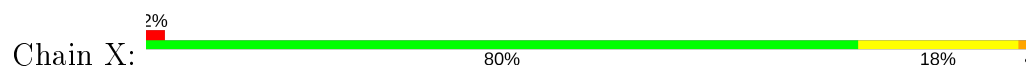
- Molecule 24: LSU ribosomal protein L28P



- Molecule 25: 50S ribosomal protein L29



- Molecule 26: LSU ribosomal protein L30P



- Molecule 27: 50S ribosomal protein L32



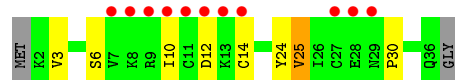
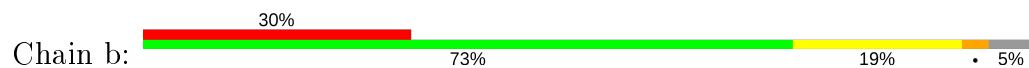
- Molecule 28: 50S ribosomal protein L34



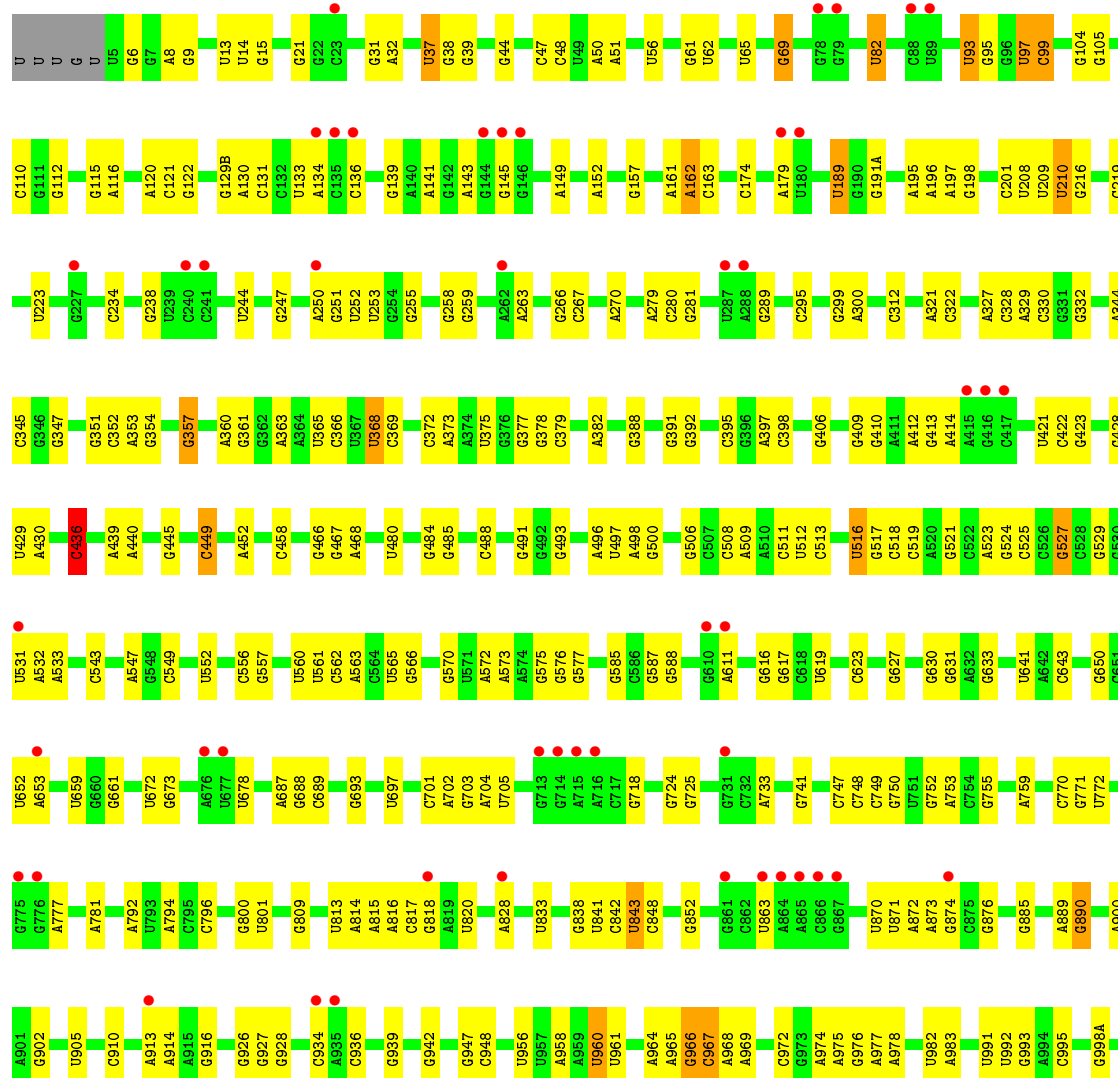
- Molecule 29: 50S ribosomal protein L35

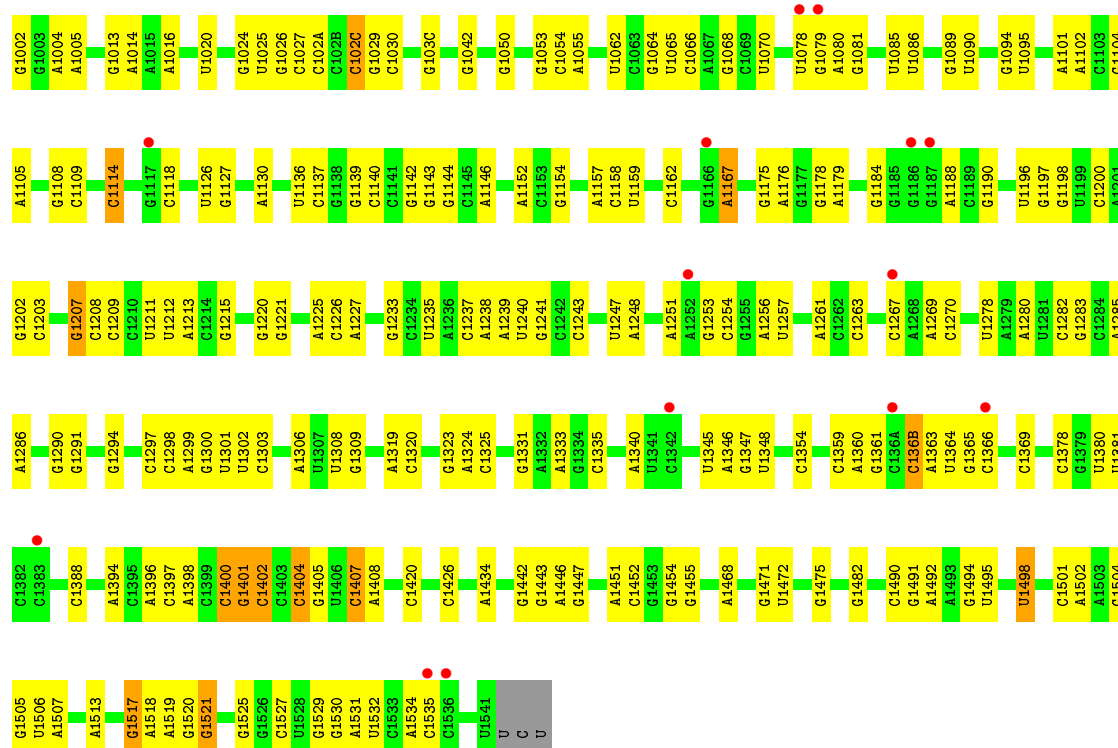


• Molecule 30: 50S ribosomal protein L36

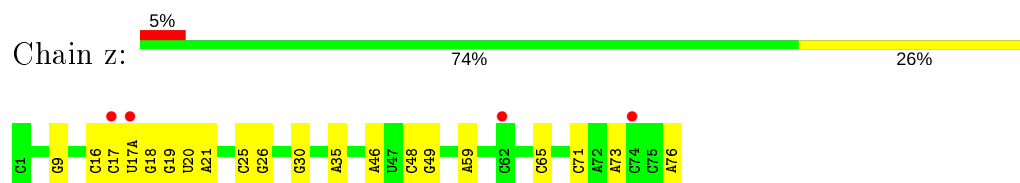


• Molecule 31: 16S RNA

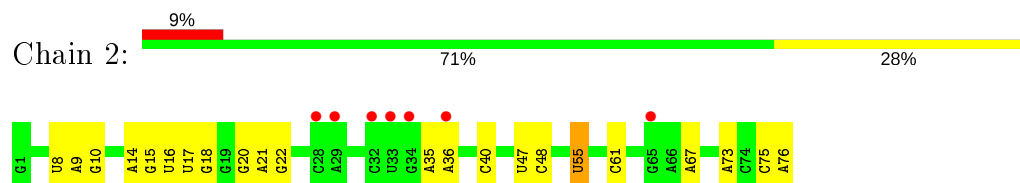




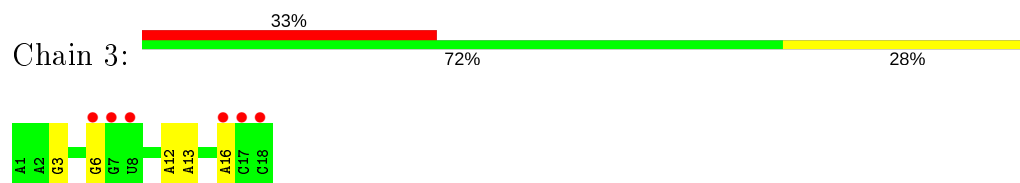
• Molecule 32: P-site tRNA<sup>f</sup>MET



• Molecule 33: E-site tRNA

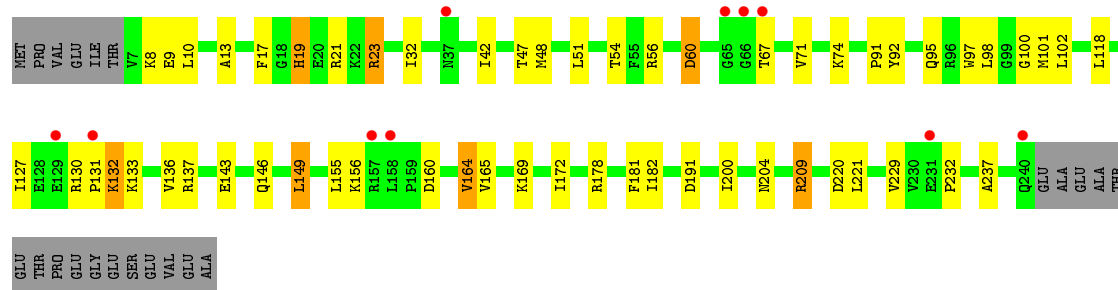


• Molecule 34: MRNA

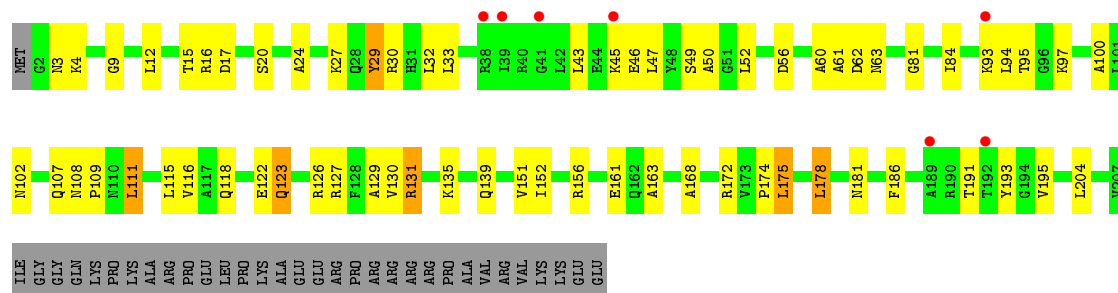


• Molecule 35: 30S ribosomal protein S2

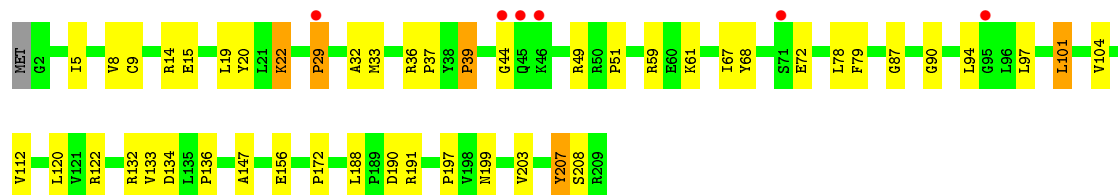
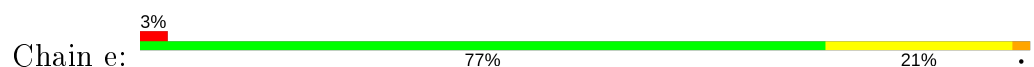




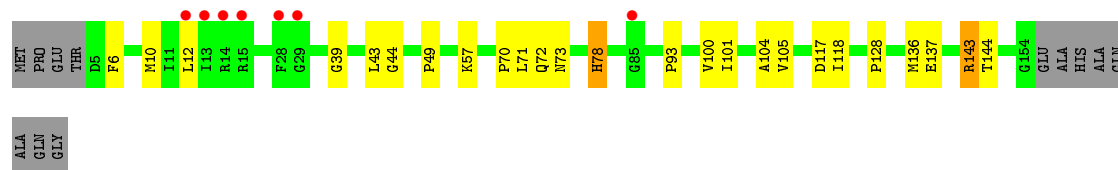
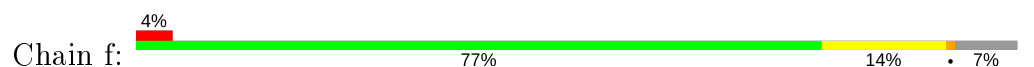
- Molecule 36: 30S ribosomal protein S3



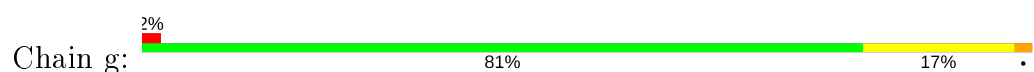
- Molecule 37: 30S ribosomal protein S4



- Molecule 38: 30S ribosomal protein S5

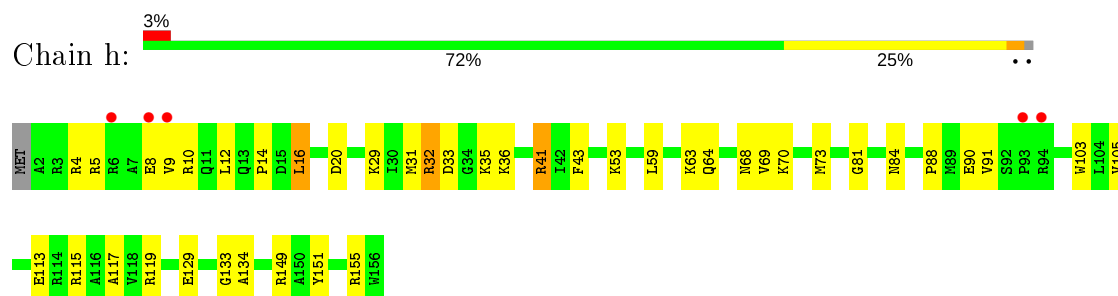


- Molecule 39: 30S ribosomal protein S6

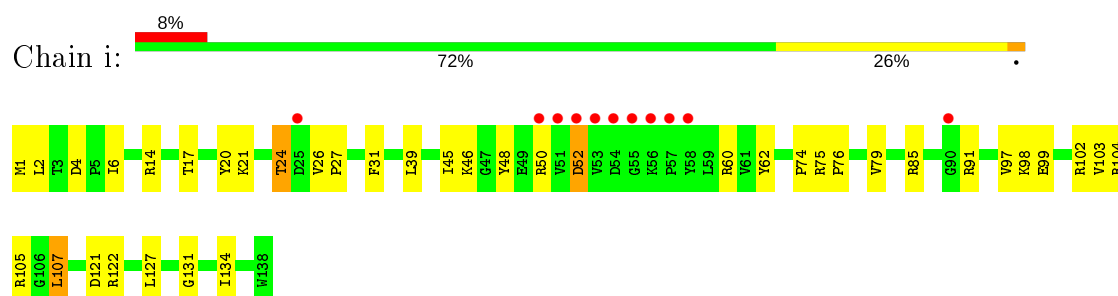




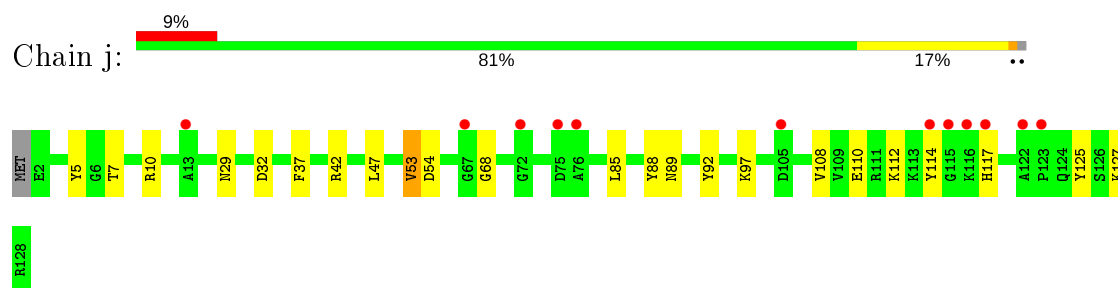
- Molecule 40: 30S ribosomal protein S7



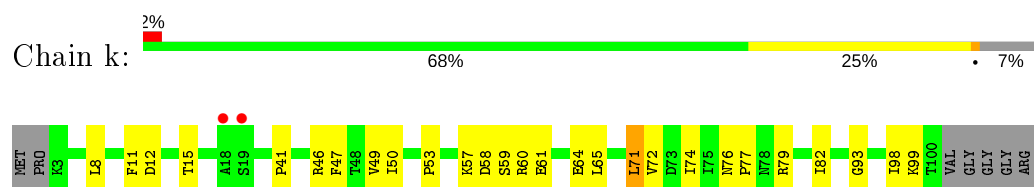
- Molecule 41: 30S ribosomal protein S8



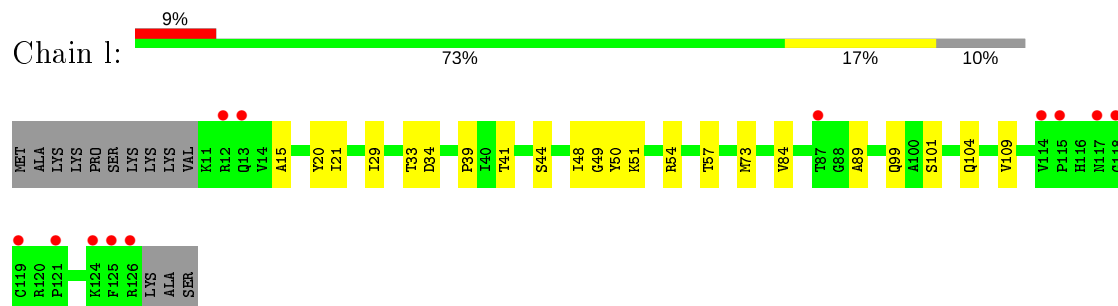
- Molecule 42: 30S ribosomal protein S9



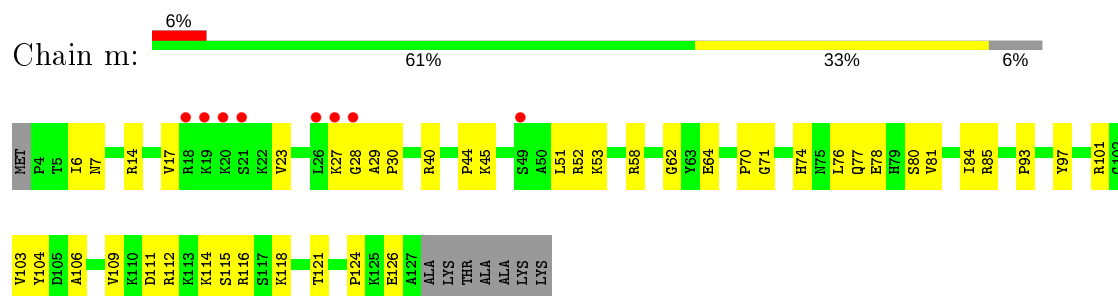
- Molecule 43: 30S ribosomal protein S10



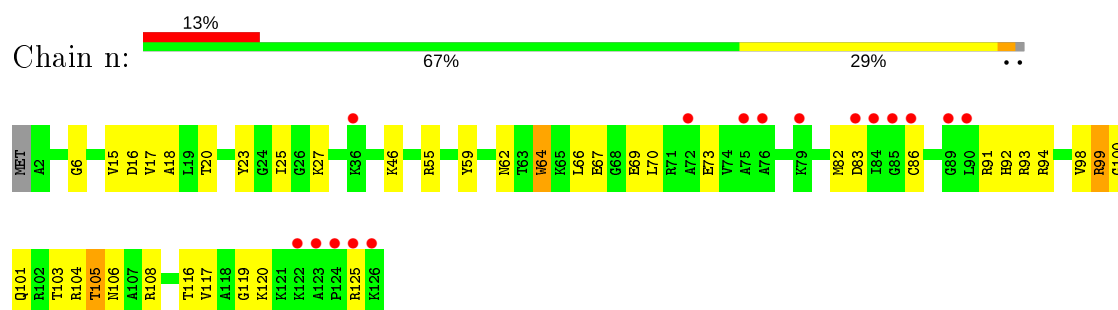
- Molecule 44: 30S ribosomal protein S11



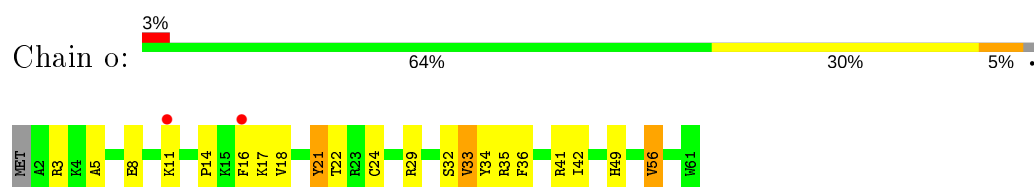
- Molecule 45: 30S ribosomal protein S12



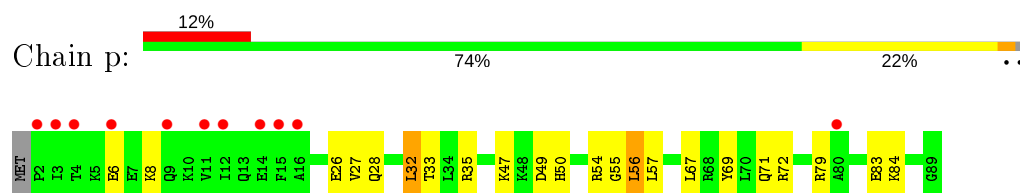
- Molecule 46: 30S ribosomal protein S13



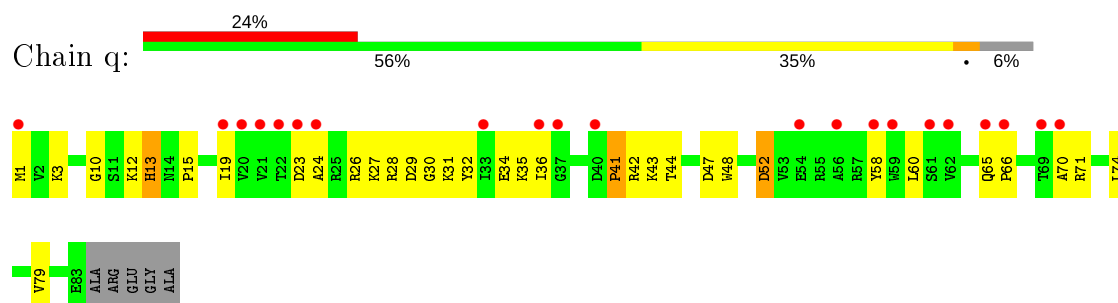
- Molecule 47: 30S ribosomal protein S14 type Z



- Molecule 48: 30S ribosomal protein S15

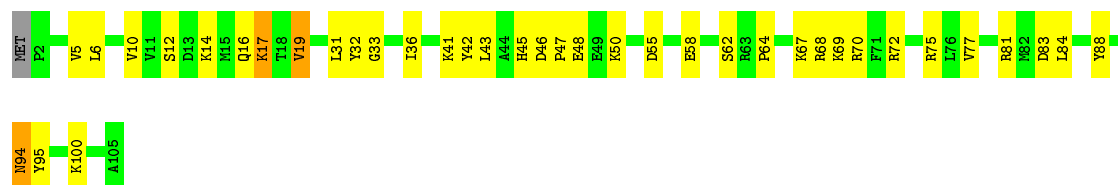


- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17

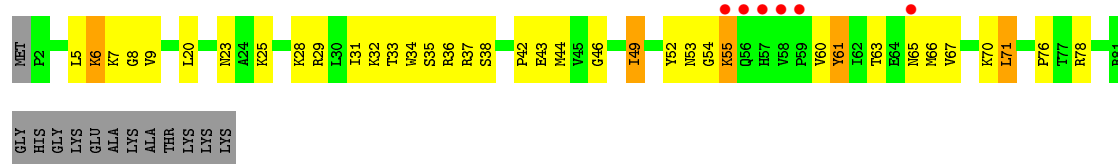




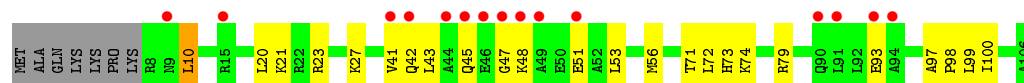
- Molecule 51: 30S ribosomal protein S18



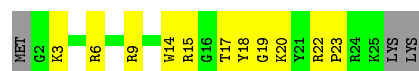
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein Thx



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	507.21Å 507.21Å 692.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.83 78.70 – 3.70	Depositor EDS
% Data completeness (in resolution range)	81.7 (30.00-3.83) 68.4 (78.70-3.70)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.43 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, $R_{free}$	0.327 , 0.351 0.340 , 0.360	Depositor DCC
$R_{free}$ test set	10300 reflections (2.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.5	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.07 , -110.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.22$ , $\langle L^2 \rangle = 0.07$	Xtriage
Estimated twinning fraction	0.267 for -1/2*h+1/2*k-1/2*l, 1/2*h-1/2*k-1/2*l, -h-k 0.260 for -1/2*h-1/2*k+1/2*l, -1/2*h-1/2*k-1/2*l, h-k	Xtriage
$F_o, F_c$ correlation	0.69	EDS
Total number of atoms	147125	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	1.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 2MG, 5MC, M2G, 7MG, 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  > 5$	RMSZ	# $ Z  > 5$
1	w	1.00	42/69679 (0.1%)	1.03	92/108779 (0.1%)
2	x	0.65	1/2878 (0.0%)	0.90	1/4490 (0.0%)
3	A	0.53	0/1015	0.63	0/1369
4	B	0.53	0/2165	0.70	0/2919
5	C	0.56	0/1574	0.69	0/2125
6	D	0.58	0/1551	0.69	0/2101
7	E	0.58	0/1492	0.72	1/2006 (0.0%)
8	F	0.56	0/1345	0.70	0/1819
9	G	0.51	0/1171	0.70	0/1583
10	H	0.54	0/1130	0.71	1/1525 (0.1%)
11	I	0.57	0/942	0.74	1/1268 (0.1%)
12	J	0.57	0/1131	0.76	1/1504 (0.1%)
13	K	0.58	0/1110	0.74	1/1483 (0.1%)
14	L	0.49	0/982	0.69	0/1312
15	M	0.51	0/856	0.63	0/1138
16	N	0.56	0/1157	0.72	0/1544
17	O	0.53	0/982	0.64	0/1306
18	P	0.58	0/790	0.69	0/1057
19	Q	0.51	0/878	0.74	1/1179 (0.1%)
20	R	0.60	0/739	0.75	0/993
21	S	0.61	0/806	0.70	0/1074
22	T	0.54	0/1507	0.66	0/2045
23	U	0.56	0/613	0.75	0/816
24	V	0.64	0/701	0.71	0/932
25	W	0.53	0/522	0.75	0/690
26	X	0.51	0/482	0.66	0/646
27	Y	0.53	0/449	0.69	0/606
28	Z	0.52	0/426	0.65	0/561
29	a	0.56	0/515	0.70	0/679
30	b	0.60	0/297	0.63	0/392
31	y	0.72	23/36178 (0.1%)	0.93	44/56463 (0.1%)
32	z	0.62	0/1831	0.88	0/2853

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	2	0.65	0/1791	0.85	0/2791
34	3	0.63	0/439	0.90	0/684
35	c	0.56	0/1935	0.67	0/2609
36	d	0.51	0/1636	0.68	0/2205
37	e	0.55	0/1733	0.68	1/2318 (0.0%)
38	f	0.60	0/1162	0.68	0/1564
39	g	0.55	0/856	0.70	0/1154
40	h	0.54	0/1276	0.63	0/1709
41	i	0.51	0/1136	0.68	0/1527
42	j	0.58	0/1029	0.66	0/1378
43	k	0.59	0/807	0.66	0/1085
44	l	0.58	0/879	0.64	0/1187
45	m	0.55	0/986	0.75	0/1320
46	n	0.54	0/1008	0.68	0/1347
47	o	0.52	0/501	0.67	0/664
48	p	0.50	0/745	0.64	0/992
49	q	0.57	0/716	0.70	0/963
50	r	0.55	0/870	0.71	0/1159
51	s	0.60	0/675	0.67	0/894
52	t	0.59	0/661	0.68	1/890 (0.1%)
53	u	0.46	0/764	0.65	0/1006
54	v	0.58	0/212	0.60	0/277
All	All	0.81	66/159711 (0.0%)	0.92	145/238980 (0.1%)

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	41	C	O3'-P	43.37	2.13	1.61
1	w	1506	C	O3'-P	40.09	2.09	1.61
1	w	489	G	O3'-P	39.72	2.08	1.61
1	w	1448(B)	A	O3'-P	38.61	2.07	1.61
1	w	436	C	O3'-P	36.62	2.05	1.61
1	w	554	U	O3'-P	36.54	2.04	1.61
1	w	1743	G	O3'-P	36.44	2.04	1.61
1	w	1712	C	O3'-P	36.33	2.04	1.61
1	w	2213	U	O3'-P	35.61	2.03	1.61
1	w	366(B)	C	O3'-P	35.53	2.03	1.61
1	w	2712(B)	A	O3'-P	35.29	2.03	1.61
1	w	890	A	O3'-P	34.85	2.02	1.61
1	w	926	A	O3'-P	34.47	2.02	1.61
1	w	155	C	O3'-P	34.19	2.02	1.61
1	w	1583	A	O3'-P	33.94	2.01	1.61

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	99	U	O3'-P	33.39	2.01	1.61
1	w	1718	G	O3'-P	33.29	2.01	1.61
1	w	1481	U	O3'-P	31.86	1.99	1.61
1	w	1451	C	O3'-P	31.83	1.99	1.61
1	w	1735	U	O3'-P	31.62	1.99	1.61
1	w	537	C	O3'-P	31.45	1.98	1.61
1	w	1864	U	O3'-P	30.27	1.97	1.61
1	w	1171	G	O3'-P	30.16	1.97	1.61
1	w	1546(B)	C	O3'-P	29.62	1.96	1.61
1	w	1630(B)	C	O3'-P	29.10	1.96	1.61
1	w	1872	A	O3'-P	28.59	1.95	1.61
1	w	1142(B)	A	O3'-P	28.49	1.95	1.61
1	w	2219	G	O3'-P	28.38	1.95	1.61
1	w	1221(A)	C	O3'-P	27.85	1.94	1.61
1	w	165	U	O3'-P	27.37	1.94	1.61
1	w	1444(B)	A	O3'-P	26.83	1.93	1.61
1	w	1133	U	O3'-P	25.03	1.91	1.61
31	y	201	C	O3'-P	23.92	1.89	1.61
1	w	2199	A	O3'-P	21.55	1.87	1.61
31	y	97	U	O3'-P	18.57	1.83	1.61
1	w	2799	A	O3'-P	17.20	1.81	1.61
1	w	2746	U	O5'-C5'	16.23	1.70	1.44
1	w	2795	G	O3'-P	15.55	1.79	1.61
31	y	99	C	O3'-P	15.40	1.79	1.61
31	y	103(C)	G	O3'-P	15.38	1.79	1.61
31	y	1455	G	O3'-P	14.53	1.78	1.61
31	y	843	U	O3'-P	13.63	1.77	1.61
31	y	136(B)	C	O3'-P	13.10	1.76	1.61
31	y	458	C	O3'-P	13.00	1.76	1.61
31	y	1498	U	C4-O4	12.92	1.33	1.23
31	y	102(C)	C	O3'-P	12.51	1.76	1.61
1	w	2746	U	O3'-P	11.80	1.75	1.61
31	y	838	G	O3'-P	11.41	1.74	1.61
1	w	2889	C	O3'-P	11.28	1.74	1.61
31	y	93	U	O3'-P	9.74	1.72	1.61
31	y	1167	A	O3'-P	8.96	1.72	1.61
1	w	2747	G	P-O5'	8.92	1.68	1.59
31	y	1402	C	P-O5'	8.88	1.68	1.59
1	w	2746	U	P-O5'	8.37	1.68	1.59
1	w	2722	G	O5'-C5'	7.90	1.57	1.44
31	y	1402	C	O5'-C5'	7.66	1.56	1.44
31	y	99	C	P-O5'	7.37	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	1402	C	C4-N4	7.28	1.40	1.33
31	y	69	G	O3'-P	7.14	1.69	1.61
1	w	2720	U	O5'-C5'	6.96	1.55	1.44
2	x	29	A	P-O5'	5.49	1.65	1.59
31	y	97	U	O5'-C5'	5.49	1.53	1.44
31	y	449	C	O5'-C5'	5.45	1.53	1.44
31	y	162	A	O5'-C5'	5.27	1.52	1.44
31	y	1114	C	O5'-C5'	5.08	1.52	1.44
31	y	37	U	O5'-C5'	5.02	1.52	1.44

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	2712(B)	A	P-O3'-C3'	-23.05	92.04	119.70
1	w	489	G	P-O3'-C3'	-18.72	97.23	119.70
31	y	97	U	P-O3'-C3'	-16.92	99.40	119.70
1	w	41	C	P-O3'-C3'	-15.29	101.35	119.70
1	w	1712	C	P-O3'-C3'	-15.07	101.61	119.70
31	y	99	C	P-O3'-C3'	-15.02	101.68	119.70
1	w	155	C	P-O3'-C3'	-13.31	103.73	119.70
1	w	537	C	P-O3'-C3'	-12.70	104.46	119.70
1	w	1718	G	P-O3'-C3'	-12.30	104.94	119.70
1	w	2746	U	P-O5'-C5'	-11.99	101.71	120.90
31	y	136(B)	C	P-O3'-C3'	-11.73	105.63	119.70
1	w	436	C	P-O3'-C3'	-11.65	105.72	119.70
1	w	99	U	P-O3'-C3'	-11.53	105.86	119.70
1	w	2393	A	N9-C1'-C2'	-11.49	99.07	114.00
31	y	201	C	P-O3'-C3'	-10.95	106.56	119.70
31	y	93	U	P-O3'-C3'	-10.73	106.83	119.70
1	w	1735	U	P-O3'-C3'	-10.67	106.90	119.70
1	w	1506	C	P-O3'-C3'	-10.31	107.32	119.70
1	w	1133	U	P-O3'-C3'	-10.18	107.49	119.70
31	y	838	G	P-O3'-C3'	-10.06	107.63	119.70
1	w	890	A	P-O3'-C3'	-9.59	108.19	119.70
1	w	1221(A)	C	P-O3'-C3'	-9.46	108.35	119.70
31	y	1402	C	P-O5'-C5'	-9.20	106.18	120.90
1	w	1743	G	P-O3'-C3'	-9.02	108.88	119.70
1	w	2799	A	O3'-P-O5'	9.00	121.11	104.00
1	w	1448(B)	A	P-O3'-C3'	-8.98	108.92	119.70
31	y	1455	G	OP1-P-O3'	8.80	124.56	105.20
31	y	103(C)	G	P-O3'-C3'	-8.77	109.18	119.70
1	w	2805	G	OP2-P-O3'	8.38	123.62	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	926	A	P-O3'-C3'	-8.35	109.69	119.70
1	w	1577	C	N1-C1'-C2'	-8.29	102.88	112.00
1	w	2795	G	P-O3'-C3'	-8.10	109.97	119.70
1	w	1955	U	N1-C1'-C2'	8.07	124.49	114.00
1	w	1822	G	N9-C1'-C2'	-8.05	103.15	112.00
31	y	99	C	OP2-P-O3'	8.05	122.90	105.20
1	w	2795	G	OP2-P-O3'	7.77	122.29	105.20
1	w	2257	U	N1-C1'-C2'	-7.67	103.57	112.00
1	w	2431	U	N1-C1'-C2'	-7.47	103.78	112.00
1	w	2805	G	OP1-P-O3'	-7.41	88.90	105.20
1	w	1863	G	N9-C1'-C2'	-7.38	103.88	112.00
31	y	1401	G	C3'-C2'-C1'	-7.37	95.60	101.50
1	w	1872	A	P-O3'-C3'	-7.29	110.95	119.70
31	y	82	U	P-O3'-C3'	7.22	128.37	119.70
1	w	366(B)	C	P-O3'-C3'	-7.15	111.12	119.70
1	w	458	G	C1'-O4'-C4'	-7.11	104.21	109.90
1	w	1955	U	O4'-C1'-N1	6.93	113.75	108.20
1	w	1187	G	N9-C1'-C2'	6.92	123.00	114.00
31	y	99	C	O3'-P-O5'	-6.86	90.96	104.00
1	w	1059	G	O4'-C1'-N9	6.86	113.69	108.20
1	w	362	U	C3'-C2'-C1'	-6.85	96.02	101.50
31	y	1401	G	P-O3'-C3'	-6.84	111.49	119.70
1	w	1444(B)	A	P-O3'-C3'	-6.80	111.54	119.70
1	w	1451	C	O3'-P-O5'	-6.77	91.14	104.00
31	y	210	U	P-O3'-C3'	6.69	127.73	119.70
1	w	873	G	N9-C1'-C2'	-6.64	104.70	112.00
1	w	2213	U	P-O3'-C3'	-6.62	111.75	119.70
2	x	21	G	N9-C1'-C2'	-6.58	104.76	112.00
19	Q	51	LEU	CA-CB-CG	6.58	130.43	115.30
1	w	800	A	O4'-C1'-N9	6.53	113.43	108.20
1	w	1171	G	P-O3'-C3'	-6.50	111.90	119.70
31	y	890	G	N9-C1'-C2'	-6.39	104.97	112.00
1	w	1274	A	N9-C1'-C2'	-6.39	104.98	112.00
1	w	1822	G	O4'-C1'-N9	6.38	113.30	108.20
31	y	1498	U	N1-C1'-C2'	6.35	122.26	114.00
31	y	189	U	N1-C1'-C2'	-6.35	105.02	112.00
31	y	93	U	OP2-P-O3'	6.22	118.88	105.20
1	w	1516	U	N1-C1'-C2'	-6.11	105.28	112.00
1	w	458	G	O4'-C1'-N9	6.09	113.07	108.20
31	y	1517	G	C3'-C2'-C1'	-6.07	96.64	101.50
1	w	265	A	N9-C1'-C2'	5.97	121.77	114.00
31	y	99	C	P-O5'-C5'	-5.95	111.39	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	136(B)	C	OP2-P-O3'	5.94	118.28	105.20
31	y	843	U	OP1-P-O3'	5.88	118.13	105.20
1	w	828	U	N1-C1'-C2'	5.87	121.63	114.00
1	w	2885	C	C3'-C2'-C1'	-5.84	96.83	101.50
1	w	1577	C	O4'-C1'-N1	5.80	112.84	108.20
31	y	102(C)	C	OP2-P-O3'	5.78	117.92	105.20
1	w	1221(A)	C	OP2-P-O3'	5.78	117.91	105.20
31	y	102(C)	C	O3'-P-O5'	-5.77	93.04	104.00
1	w	362	U	N1-C1'-C2'	-5.77	105.66	112.00
1	w	2746	U	P-O3'-C3'	-5.74	112.81	119.70
31	y	210	U	OP1-P-O3'	-5.74	92.57	105.20
1	w	227	A	P-O3'-C3'	5.74	126.58	119.70
31	y	1498	U	C5-C4-O4	-5.73	122.46	125.90
1	w	1800	C	O4'-C1'-N1	5.73	112.78	108.20
1	w	1615	C	O4'-C1'-N1	5.69	112.75	108.20
31	y	1105	A	N9-C1'-C2'	-5.65	105.78	112.00
31	y	587	G	O4'-C1'-N9	5.63	112.71	108.20
1	w	241	A	O4'-C1'-N9	5.63	112.70	108.20
1	w	271(D)	U	O4'-C1'-N1	5.62	112.70	108.20
52	t	71	LEU	CA-CB-CG	5.62	128.23	115.30
1	w	15	G	N9-C1'-C2'	-5.61	105.83	112.00
31	y	1455	G	O3'-P-O5'	-5.59	93.38	104.00
1	w	70	G	N9-C1'-C2'	5.57	121.24	114.00
1	w	2393	A	O4'-C1'-N9	5.56	112.65	108.20
1	w	1288	U	P-O3'-C3'	5.55	126.36	119.70
31	y	436	C	N1-C1'-C2'	-5.53	105.92	112.00
1	w	2468	G	N9-C1'-C2'	-5.53	105.92	112.00
1	w	913	U	P-O3'-C3'	5.51	126.32	119.70
31	y	1254	C	N1-C1'-C2'	-5.51	105.94	112.00
1	w	99	U	OP1-P-O3'	5.48	117.25	105.20
1	w	2225	A	P-O3'-C3'	5.48	126.27	119.70
1	w	2171	A	N9-C1'-C2'	5.47	121.12	114.00
31	y	69	G	O3'-P-O5'	-5.46	93.63	104.00
1	w	932	G	N9-C1'-C2'	5.46	121.09	114.00
1	w	1626	G	O4'-C1'-N9	5.43	112.54	108.20
12	J	148	LEU	CA-CB-CG	5.42	127.77	115.30
1	w	1898	U	N1-C1'-C2'	5.41	121.03	114.00
1	w	2497	A	P-O3'-C3'	5.36	126.14	119.70
1	w	2171	A	P-O3'-C3'	5.36	126.13	119.70
31	y	210	U	OP2-P-O3'	5.35	116.97	105.20
31	y	468	A	O3'-P-O5'	5.34	114.14	104.00
7	E	139	LEU	CA-CB-CG	5.33	127.57	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	I	91	LEU	CA-CB-CG	5.32	127.54	115.30
1	w	933	A	O4'-C1'-N9	5.30	112.44	108.20
31	y	250	A	N9-C1'-C2'	-5.30	106.17	112.00
31	y	1521	G	N9-C1'-C2'	-5.28	106.19	112.00
1	w	448	U	C1'-O4'-C4'	-5.28	105.67	109.90
13	K	37	LEU	CA-CB-CG	5.28	127.45	115.30
1	w	270(E)	C	N1-C1'-C2'	5.28	120.86	114.00
1	w	2002	G	O4'-C1'-N9	5.28	112.42	108.20
31	y	1220	G	N9-C1'-C2'	-5.27	106.20	112.00
1	w	2205	C	N1-C1'-C2'	-5.27	106.20	112.00
1	w	739	G	P-O3'-C3'	5.26	126.02	119.70
31	y	1401	G	N9-C1'-C2'	-5.24	106.24	112.00
1	w	1775	U	C3'-C2'-C1'	-5.24	97.31	101.50
31	y	960	U	N1-C1'-C2'	5.24	120.81	114.00
31	y	1498	U	N1-C2-N3	5.21	118.03	114.90
31	y	659	U	C3'-C2'-C1'	-5.21	97.34	101.50
31	y	1498	U	C2-N3-C4	-5.20	123.88	127.00
1	w	1247	A	C1'-O4'-C4'	-5.19	105.75	109.90
1	w	299	A	O4'-C1'-N9	5.18	112.34	108.20
1	w	1266	G	P-O3'-C3'	5.18	125.91	119.70
10	H	38	LEU	CA-CB-CG	5.17	127.20	115.30
37	e	19	LEU	CA-CB-CG	5.15	127.14	115.30
1	w	520	G	C3'-C2'-C1'	-5.15	97.38	101.50
1	w	1426	G	N9-C1'-C2'	5.13	120.68	114.00
1	w	554	U	P-O3'-C3'	-5.13	113.54	119.70
1	w	1812	A	C4'-C3'-C2'	-5.10	97.50	102.60
1	w	204	A	C3'-C2'-C1'	5.09	105.57	101.50
1	w	1356	G	O4'-C1'-N9	5.09	112.27	108.20
31	y	1402	C	C3'-C2'-C1'	5.06	105.55	101.50
1	w	1534	G	C3'-C2'-C1'	-5.04	97.47	101.50
1	w	457	A	N9-C1'-C2'	5.02	120.53	114.00
1	w	2848	G	O4'-C1'-N9	5.01	112.20	108.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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 X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	123/229 (54%)	72 (58%)	31 (25%)	20 (16%)	0	3
4	B	270/276 (98%)	134 (50%)	64 (24%)	72 (27%)	0	0
5	C	199/206 (97%)	99 (50%)	47 (24%)	53 (27%)	0	0
6	D	192/205 (94%)	91 (47%)	45 (23%)	56 (29%)	0	0
7	E	178/182 (98%)	97 (54%)	55 (31%)	26 (15%)	0	4
8	F	171/180 (95%)	90 (53%)	40 (23%)	41 (24%)	0	1
9	G	146/148 (99%)	83 (57%)	35 (24%)	28 (19%)	0	2
10	H	136/140 (97%)	62 (46%)	45 (33%)	29 (21%)	0	1
11	I	120/122 (98%)	62 (52%)	24 (20%)	34 (28%)	0	0
12	J	144/150 (96%)	63 (44%)	46 (32%)	35 (24%)	0	1
13	K	135/141 (96%)	56 (42%)	41 (30%)	38 (28%)	0	0
14	L	116/118 (98%)	64 (55%)	30 (26%)	22 (19%)	0	2
15	M	104/112 (93%)	58 (56%)	22 (21%)	24 (23%)	0	1
16	N	135/146 (92%)	56 (42%)	40 (30%)	39 (29%)	0	0
17	O	115/118 (98%)	66 (57%)	28 (24%)	21 (18%)	0	2
18	P	99/101 (98%)	39 (39%)	28 (28%)	32 (32%)	0	0
19	Q	107/113 (95%)	64 (60%)	23 (22%)	20 (19%)	0	2
20	R	90/96 (94%)	29 (32%)	36 (40%)	25 (28%)	0	0
21	S	101/110 (92%)	28 (28%)	31 (31%)	42 (42%)	0	0
22	T	183/206 (89%)	115 (63%)	45 (25%)	23 (13%)	0	5
23	U	74/85 (87%)	31 (42%)	21 (28%)	22 (30%)	0	0
24	V	86/98 (88%)	41 (48%)	29 (34%)	16 (19%)	0	2
25	W	60/72 (83%)	33 (55%)	11 (18%)	16 (27%)	0	0
26	X	58/60 (97%)	31 (53%)	20 (34%)	7 (12%)	0	6
27	Y	54/60 (90%)	27 (50%)	16 (30%)	11 (20%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Z	46/49 (94%)	31 (67%)	10 (22%)	5 (11%)	0	8
29	a	61/65 (94%)	28 (46%)	20 (33%)	13 (21%)	0	1
30	b	33/37 (89%)	16 (48%)	10 (30%)	7 (21%)	0	2
35	c	232/256 (91%)	142 (61%)	59 (25%)	31 (13%)	0	4
36	d	204/239 (85%)	102 (50%)	60 (29%)	42 (21%)	0	2
37	e	206/209 (99%)	120 (58%)	60 (29%)	26 (13%)	0	5
38	f	148/162 (91%)	102 (69%)	32 (22%)	14 (10%)	0	11
39	g	99/101 (98%)	72 (73%)	19 (19%)	8 (8%)	1	14
40	h	153/156 (98%)	96 (63%)	30 (20%)	27 (18%)	0	3
41	i	136/138 (99%)	84 (62%)	33 (24%)	19 (14%)	0	4
42	j	125/128 (98%)	81 (65%)	29 (23%)	15 (12%)	0	6
43	k	96/105 (91%)	55 (57%)	25 (26%)	16 (17%)	0	3
44	l	114/129 (88%)	74 (65%)	28 (25%)	12 (10%)	0	9
45	m	122/132 (92%)	67 (55%)	35 (29%)	20 (16%)	0	3
46	n	123/126 (98%)	70 (57%)	35 (28%)	18 (15%)	0	4
47	o	58/61 (95%)	30 (52%)	16 (28%)	12 (21%)	0	2
48	p	86/89 (97%)	51 (59%)	24 (28%)	11 (13%)	0	5
49	q	81/88 (92%)	34 (42%)	25 (31%)	22 (27%)	0	0
50	r	102/105 (97%)	54 (53%)	24 (24%)	24 (24%)	0	1
51	s	79/88 (90%)	45 (57%)	21 (27%)	13 (16%)	0	3
52	t	78/93 (84%)	30 (38%)	26 (33%)	22 (28%)	0	0
53	u	97/106 (92%)	47 (48%)	35 (36%)	15 (16%)	0	4
54	v	22/27 (82%)	8 (36%)	6 (27%)	8 (36%)	0	0
All	All	5697/6163 (92%)	3030 (53%)	1515 (27%)	1152 (20%)	0	2

All (1152) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	8	TYR
3	A	16	ASP
3	A	63	VAL
3	A	176	VAL
3	A	179	ALA
3	A	180	SER

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Mol	Chain	Res	Type
3	A	209	PHE
4	B	3	VAL
4	B	6	PHE
4	B	15	PHE
4	B	21	PHE
4	B	36	PRO
4	B	39	LYS
4	B	44	ASN
4	B	59	LYS
4	B	69	ARG
4	B	83	GLU
4	B	91	ARG
4	B	105	ILE
4	B	138	VAL
4	B	149	PRO
4	B	156	ALA
4	B	196	VAL
4	B	206	LEU
4	B	209	ALA
4	B	227	ASN
4	B	228	PRO
4	B	235	GLY
4	B	239	ARG
4	B	259	THR
4	B	262	ARG
4	B	263	ARG
5	C	35	GLN
5	C	51	PHE
5	C	54	GLN
5	C	65	GLY
5	C	67	PHE
5	C	73	GLU
5	C	77	ILE
5	C	82	ARG
5	C	104	VAL
5	C	121	ASN
5	C	122	PHE
5	C	128	SER
5	C	143	ASN
5	C	144	ARG
5	C	149	ARG
5	C	178	GLU

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Mol	Chain	Res	Type
5	C	189	PRO
6	D	17	ALA
6	D	18	ASP
6	D	23	ILE
6	D	38	LYS
6	D	48	THR
6	D	54	TYR
6	D	58	LYS
6	D	59	ILE
6	D	68	ALA
6	D	87	PRO
6	D	120	LEU
6	D	128	ASN
6	D	146	SER
6	D	172	ALA
6	D	176	LEU
6	D	196	VAL
7	E	13	GLU
7	E	26	GLN
7	E	29	TRP
7	E	78	SER
7	E	79	ASN
7	E	82	LEU
7	E	84	LYS
7	E	87	PRO
7	E	88	ILE
7	E	95	ARG
7	E	163	ALA
7	E	181	ARG
8	F	10	PRO
8	F	40	GLU
8	F	52	VAL
8	F	55	PRO
8	F	58	GLU
8	F	71	LEU
8	F	99	VAL
8	F	101	ARG
8	F	109	PHE
8	F	157	TYR
8	F	173	PRO
8	F	178	ALA
9	G	8	PRO

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Mol	Chain	Res	Type
9	G	26	ALA
9	G	29	TYR
9	G	38	LEU
9	G	82	ARG
9	G	94	ALA
9	G	122	GLU
9	G	125	GLU
9	G	132	PRO
9	G	138	ILE
10	H	26	THR
10	H	67	PRO
10	H	102	PRO
10	H	108	ILE
10	H	110	LEU
10	H	146	TYR
10	H	147	ALA
10	H	153	HIS
11	I	5	GLN
11	I	51	ALA
11	I	52	VAL
11	I	54	GLU
11	I	60	ALA
11	I	63	VAL
11	I	75	SER
11	I	85	VAL
11	I	90	GLN
11	I	91	LEU
11	I	115	VAL
12	J	12	ALA
12	J	17	LYS
12	J	33	ARG
12	J	35	HIS
12	J	45	LEU
12	J	52	GLU
12	J	71	VAL
12	J	90	ARG
12	J	106	LEU
12	J	119	GLU
12	J	124	LYS
12	J	148	LEU
13	K	3	MET
13	K	4	PRO

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Mol	Chain	Res	Type
13	K	21	THR
13	K	25	ASP
13	K	27	VAL
13	K	31	ASP
13	K	38	GLU
13	K	68	ILE
13	K	73	PRO
13	K	79	LEU
13	K	80	GLU
13	K	81	VAL
13	K	83	MET
13	K	85	LYS
13	K	108	GLY
13	K	120	ILE
13	K	127	ILE
13	K	133	ARG
14	L	2	ARG
14	L	5	LYS
14	L	12	ARG
14	L	37	THR
14	L	45	ARG
14	L	60	LEU
14	L	62	ALA
14	L	95	THR
14	L	102	GLU
14	L	104	ARG
14	L	117	VAL
15	M	8	GLU
15	M	9	ARG
15	M	10	ARG
15	M	12	PHE
15	M	32	LEU
15	M	35	ILE
16	N	12	SER
16	N	18	ASP
16	N	28	VAL
16	N	30	VAL
16	N	33	LYS
16	N	42	ILE
16	N	45	PHE
16	N	74	ARG
16	N	83	ILE

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Mol	Chain	Res	Type
16	N	96	ARG
16	N	101	PHE
16	N	107	ASP
16	N	135	VAL
17	O	6	THR
17	O	22	LYS
17	O	25	TRP
17	O	76	TYR
17	O	90	VAL
17	O	92	ARG
17	O	104	GLN
17	O	105	VAL
18	P	15	GLU
18	P	22	VAL
18	P	26	ASP
18	P	27	ALA
18	P	29	PRO
18	P	31	ALA
18	P	44	LYS
18	P	50	PRO
18	P	51	VAL
18	P	53	GLU
18	P	68	LYS
18	P	72	VAL
18	P	78	LYS
19	Q	40	ASN
19	Q	67	ASP
19	Q	80	PRO
19	Q	89	ALA
19	Q	90	ARG
19	Q	96	ILE
20	R	6	ASP
20	R	11	PRO
20	R	22	ALA
20	R	30	VAL
20	R	32	PRO
20	R	48	LYS
20	R	49	VAL
20	R	60	ARG
20	R	80	ILE
20	R	81	VAL
20	R	83	VAL

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Mol	Chain	Res	Type
20	R	89	ILE
21	S	7	VAL
21	S	16	ALA
21	S	20	TYR
21	S	21	LYS
21	S	31	LEU
21	S	39	VAL
21	S	46	LYS
21	S	54	LYS
21	S	57	GLN
21	S	61	ILE
21	S	77	PRO
21	S	96	ILE
21	S	100	ALA
22	T	41	LEU
22	T	52	SER
22	T	66	SER
22	T	95	PRO
22	T	146	ILE
23	U	14	ARG
23	U	17	GLN
23	U	18	ALA
23	U	45	PHE
23	U	84	LEU
24	V	11	ARG
24	V	21	ARG
24	V	51	VAL
24	V	52	ARG
24	V	80	LEU
24	V	86	SER
25	W	9	GLN
25	W	13	ALA
25	W	32	LEU
25	W	38	GLN
25	W	39	ALA
25	W	46	GLN
25	W	54	LYS
26	X	8	LEU
26	X	12	PRO
26	X	32	GLN
27	Y	29	ILE
27	Y	34	PRO

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Mol	Chain	Res	Type
27	Y	37	LYS
27	Y	51	TYR
27	Y	52	TYR
28	Z	3	ARG
28	Z	18	PHE
28	Z	22	MET
28	Z	44	PRO
29	a	18	ALA
29	a	19	SER
29	a	26	LYS
29	a	41	ILE
30	b	6	SER
35	c	21	ARG
35	c	91	PRO
35	c	130	ARG
35	c	132	LYS
35	c	165	VAL
35	c	191	ASP
35	c	232	PRO
36	d	24	ALA
36	d	30	ARG
36	d	47	LEU
36	d	49	SER
36	d	62	ASP
36	d	111	LEU
36	d	122	GLU
36	d	127	ARG
36	d	131	ARG
36	d	151	VAL
36	d	152	ILE
36	d	161	GLU
36	d	181	ASN
37	e	5	ILE
37	e	22	LYS
37	e	29	PRO
37	e	32	ALA
37	e	67	ILE
37	e	156	GLU
37	e	172	PRO
37	e	197	PRO
37	e	207	TYR
37	e	208	SER

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Mol	Chain	Res	Type
38	f	44	GLY
38	f	70	PRO
38	f	78	HIS
38	f	101	ILE
38	f	104	ALA
38	f	128	PRO
39	g	35	ALA
39	g	100	ASN
40	h	12	LEU
40	h	20	ASP
40	h	31	MET
40	h	32	ARG
40	h	69	VAL
40	h	133	GLY
40	h	134	ALA
40	h	149	ARG
41	i	27	PRO
41	i	46	LYS
41	i	60	ARG
41	i	76	PRO
41	i	79	VAL
41	i	97	VAL
42	j	37	PHE
42	j	47	LEU
42	j	88	TYR
42	j	110	GLU
42	j	112	LYS
42	j	117	HIS
43	k	59	SER
43	k	60	ARG
43	k	99	LYS
44	l	15	ALA
44	l	50	TYR
44	l	57	THR
45	m	74	HIS
45	m	78	GLU
45	m	97	TYR
45	m	104	TYR
45	m	109	VAL
46	n	17	VAL
46	n	18	ALA
46	n	20	THR

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Mol	Chain	Res	Type
46	n	100	GLY
46	n	116	THR
47	o	3	ARG
47	o	17	LYS
47	o	35	ARG
48	p	28	GLN
48	p	47	LYS
48	p	50	HIS
49	q	3	LYS
49	q	24	ALA
49	q	41	PRO
49	q	47	ASP
50	r	12	SER
50	r	45	HIS
50	r	47	PRO
50	r	68	ARG
50	r	70	ARG
50	r	94	ASN
51	s	15	ARG
51	s	33	ASP
51	s	37	VAL
51	s	59	SER
51	s	83	GLU
52	t	37	ARG
52	t	38	SER
52	t	42	PRO
52	t	65	ASN
52	t	70	LYS
52	t	78	ARG
53	u	10	LEU
53	u	42	GLN
53	u	48	LYS
53	u	71	THR
53	u	73	HIS
53	u	93	GLU
54	v	22	ARG
54	v	23	PRO
3	A	163	GLU
3	A	175	PRO
3	A	223	VAL
4	B	19	ALA
4	B	25	THR

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Mol	Chain	Res	Type
4	B	84	TYR
4	B	113	VAL
4	B	114	GLY
4	B	118	VAL
4	B	174	ILE
4	B	198	ASN
4	B	204	ILE
4	B	223	GLY
4	B	232	PRO
4	B	242	ARG
4	B	272	ALA
5	C	10	GLY
5	C	12	THR
5	C	27	LEU
5	C	46	ALA
5	C	49	LEU
5	C	53	PRO
5	C	64	LYS
5	C	103	ASP
5	C	126	PRO
5	C	151	TYR
5	C	169	ASN
5	C	173	VAL
5	C	177	PRO
5	C	187	ALA
5	C	190	GLY
5	C	195	LEU
5	C	201	THR
6	D	13	ARG
6	D	16	ALA
6	D	56	GLY
6	D	65	THR
6	D	69	ARG
6	D	73	ILE
6	D	82	GLY
6	D	92	TYR
6	D	118	LEU
6	D	129	GLY
6	D	145	GLY
6	D	167	TRP
6	D	173	PRO
6	D	186	ARG

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Mol	Chain	Res	Type
6	D	191	LEU
7	E	8	LYS
7	E	20	ILE
7	E	28	VAL
7	E	46	ALA
7	E	126	ASP
8	F	9	ILE
8	F	13	LYS
8	F	17	VAL
8	F	19	VAL
8	F	21	PRO
8	F	48	GLY
8	F	119	GLU
8	F	136	ILE
8	F	168	PRO
9	G	20	ASP
9	G	23	PRO
9	G	40	THR
9	G	70	GLU
9	G	88	ILE
9	G	89	TYR
9	G	135	GLU
9	G	137	PRO
10	H	30	LYS
10	H	64	ASP
10	H	84	ARG
10	H	85	VAL
10	H	111	GLU
10	H	131	PRO
10	H	148	GLY
10	H	154	GLN
10	H	156	GLN
10	H	158	PRO
11	I	26	LYS
11	I	28	SER
11	I	77	ILE
11	I	89	ASN
11	I	112	MET
11	I	114	ILE
12	J	13	ASN
12	J	21	ARG
12	J	47	ASP

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Mol	Chain	Res	Type
12	J	83	VAL
12	J	89	ALA
12	J	94	GLU
12	J	97	PRO
12	J	115	LEU
12	J	118	GLY
13	K	6	ARG
13	K	20	ALA
13	K	28	ALA
13	K	76	LYS
13	K	119	ARG
14	L	10	LEU
14	L	28	LEU
14	L	74	LYS
15	M	20	ARG
15	M	21	THR
15	M	31	SER
15	M	46	VAL
15	M	91	PRO
15	M	92	TYR
15	M	94	TYR
15	M	96	GLY
15	M	105	ALA
16	N	22	PHE
16	N	29	ARG
16	N	47	GLY
16	N	52	ILE
16	N	68	TYR
16	N	77	PRO
16	N	103	ARG
16	N	116	ALA
17	O	96	ALA
17	O	103	PRO
18	P	2	PHE
18	P	16	PRO
18	P	19	LYS
18	P	36	PRO
18	P	45	THR
18	P	47	VAL
18	P	74	LYS
18	P	86	GLY
18	P	96	ILE

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Mol	Chain	Res	Type
18	P	99	ILE
19	Q	3	ALA
19	Q	6	ILE
19	Q	7	ALA
19	Q	20	VAL
19	Q	41	LYS
19	Q	43	GLY
19	Q	63	ASP
19	Q	92	ARG
20	R	18	TYR
20	R	25	LYS
20	R	69	TYR
20	R	72	LYS
20	R	77	LYS
20	R	93	GLU
21	S	38	ILE
21	S	66	PRO
21	S	68	HIS
21	S	88	LYS
21	S	89	PHE
21	S	91	GLU
21	S	95	LYS
22	T	50	GLN
22	T	51	ALA
22	T	120	ILE
22	T	124	ILE
22	T	152	ALA
22	T	165	VAL
22	T	167	PRO
23	U	13	GLY
23	U	43	THR
23	U	55	ARG
23	U	58	THR
23	U	62	LEU
23	U	63	VAL
23	U	83	PRO
24	V	14	VAL
24	V	18	ILE
24	V	56	GLN
24	V	74	VAL
25	W	42	GLY
25	W	47	ASN

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Mol	Chain	Res	Type
25	W	51	ARG
26	X	50	VAL
27	Y	14	ALA
27	Y	24	ALA
29	a	35	GLN
29	a	39	LYS
29	a	51	ALA
29	a	63	PRO
35	c	9	GLU
35	c	13	ALA
35	c	32	ILE
35	c	74	LYS
35	c	95	GLN
35	c	97	TRP
35	c	131	PRO
35	c	160	ASP
35	c	181	PHE
35	c	229	VAL
36	d	12	LEU
36	d	15	THR
36	d	20	SER
36	d	29	TYR
36	d	45	LYS
36	d	50	ALA
36	d	60	ALA
36	d	63	ASN
36	d	100	ALA
36	d	108	ASN
36	d	109	PRO
36	d	156	ARG
36	d	191	THR
37	e	20	TYR
37	e	39	PRO
37	e	87	GLY
37	e	112	VAL
37	e	190	ASP
38	f	39	GLY
38	f	49	PRO
40	h	8	GLU
40	h	10	ARG
40	h	14	PRO
40	h	16	LEU

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Mol	Chain	Res	Type
40	h	115	ARG
41	i	102	ARG
41	i	131	GLY
42	j	32	ASP
42	j	42	ARG
42	j	68	GLY
43	k	50	ILE
43	k	53	PRO
43	k	58	ASP
43	k	72	VAL
43	k	77	PRO
43	k	93	GLY
44	l	49	GLY
44	l	101	SER
44	l	109	VAL
45	m	7	ASN
45	m	28	GLY
45	m	30	PRO
45	m	62	GLY
45	m	71	GLY
45	m	93	PRO
45	m	106	ALA
45	m	116	ARG
45	m	118	LYS
45	m	124	PRO
46	n	6	GLY
46	n	55	ARG
46	n	64	TRP
46	n	83	ASP
46	n	101	GLN
46	n	106	ASN
47	o	21	TYR
47	o	22	THR
47	o	32	SER
47	o	34	TYR
48	p	27	VAL
48	p	49	ASP
49	q	10	GLY
49	q	12	LYS
49	q	15	PRO
49	q	31	LYS
49	q	36	ILE

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Mol	Chain	Res	Type
49	q	52	ASP
50	r	10	VAL
50	r	17	LYS
50	r	31	LEU
50	r	32	TYR
50	r	33	GLY
50	r	48	GLU
50	r	62	SER
50	r	67	LYS
50	r	75	ARG
51	s	10	LYS
51	s	36	ASN
51	s	47	THR
52	t	7	LYS
52	t	52	TYR
52	t	61	TYR
53	u	41	VAL
53	u	45	GLN
53	u	47	GLY
53	u	74	LYS
53	u	98	PRO
53	u	99	LEU
54	v	15	ARG
54	v	17	THR
3	A	18	ASN
3	A	36	ALA
3	A	206	LYS
3	A	221	PRO
4	B	54	ARG
4	B	75	ILE
4	B	81	ALA
4	B	129	ASN
4	B	139	GLY
4	B	148	GLU
4	B	178	PRO
4	B	201	HIS
4	B	234	GLY
4	B	241	PRO
4	B	260	ARG
5	C	13	ARG
5	C	68	ALA
5	C	76	ARG

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Mol	Chain	Res	Type
5	C	86	PRO
5	C	98	PRO
5	C	152	LYS
5	C	156	MET
6	D	5	PRO
6	D	8	SER
6	D	10	SER
6	D	26	HIS
6	D	40	ARG
6	D	41	ARG
6	D	61	PRO
6	D	90	ARG
6	D	108	ALA
6	D	148	SER
7	E	73	ALA
7	E	117	PHE
7	E	147	ASP
8	F	47	GLU
8	F	59	ARG
8	F	102	ALA
8	F	118	PRO
8	F	135	GLY
8	F	158	HIS
8	F	165	ALA
9	G	7	GLU
9	G	25	TYR
9	G	81	VAL
9	G	86	THR
9	G	91	SER
9	G	95	LYS
9	G	126	TYR
10	H	31	GLN
11	I	30	ALA
11	I	61	VAL
11	I	64	ARG
12	J	72	PRO
12	J	145	PRO
13	K	84	GLY
13	K	91	GLU
13	K	115	MET
14	L	6	SER
14	L	50	HIS

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Mol	Chain	Res	Type
14	L	67	LEU
14	L	94	TYR
14	L	108	GLY
15	M	25	ARG
15	M	28	VAL
15	M	29	PHE
15	M	47	THR
15	M	64	GLU
16	N	2	ASN
16	N	5	ALA
16	N	36	GLU
16	N	93	ARG
16	N	112	ARG
17	O	23	GLY
17	O	24	TYR
17	O	93	LYS
17	O	102	GLU
17	O	116	ALA
18	P	20	LEU
18	P	24	LYS
18	P	59	ALA
18	P	79	VAL
19	Q	42	ARG
19	Q	73	ALA
19	Q	88	ARG
20	R	34	ALA
20	R	59	VAL
20	R	65	ARG
20	R	78	LYS
21	S	9	LYS
21	S	10	GLY
21	S	25	GLY
21	S	29	GLU
21	S	33	LYS
21	S	60	PHE
21	S	65	ALA
21	S	67	LEU
21	S	78	ALA
21	S	101	LYS
22	T	83	PRO
22	T	90	VAL
22	T	122	ARG

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Mol	Chain	Res	Type
23	U	19	LYS
23	U	25	ARG
23	U	70	GLN
24	V	32	LYS
24	V	63	ALA
25	W	14	ARG
25	W	60	LEU
26	X	31	LEU
29	a	31	HIS
29	a	42	ARG
30	b	12	ASP
35	c	54	THR
35	c	60	ASP
35	c	100	GLY
35	c	149	LEU
36	d	43	LEU
36	d	123	GLN
36	d	163	ALA
36	d	178	LEU
37	e	44	GLY
37	e	49	ARG
37	e	147	ALA
38	f	71	LEU
38	f	117	ASP
39	g	81	ILE
39	g	93	SER
40	h	41	ARG
40	h	63	LYS
40	h	73	MET
40	h	90	GLU
40	h	117	ALA
40	h	129	GLU
41	i	20	TYR
41	i	74	PRO
41	i	91	ARG
41	i	107	LEU
41	i	121	ASP
42	j	29	ASN
43	k	12	ASP
43	k	15	THR
44	l	44	SER
44	l	89	ALA

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Mol	Chain	Res	Type
45	m	44	PRO
45	m	103	VAL
46	n	27	LYS
46	n	46	LYS
46	n	67	GLU
47	o	5	ALA
47	o	14	PRO
47	o	18	VAL
48	p	32	LEU
48	p	33	THR
48	p	55	GLY
48	p	56	LEU
48	p	72	ARG
48	p	79	ARG
49	q	13	HIS
49	q	26	ARG
49	q	29	ASP
49	q	30	GLY
49	q	34	GLU
49	q	65	GLN
50	r	83	ASP
51	s	25	THR
51	s	53	ARG
51	s	76	LEU
51	s	82	THR
52	t	5	LEU
52	t	6	LYS
52	t	9	VAL
52	t	28	LYS
52	t	35	SER
52	t	46	GLY
54	v	3	LYS
3	A	19	LYS
3	A	23	ILE
3	A	203	GLU
3	A	207	GLY
4	B	5	LYS
4	B	9	TYR
4	B	35	LYS
4	B	123	ALA
4	B	124	PRO
4	B	159	ALA

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Mol	Chain	Res	Type
4	B	224	ALA
5	C	45	THR
5	C	125	GLY
5	C	153	GLY
5	C	202	LYS
6	D	39	ARG
6	D	70	HIS
6	D	88	LYS
6	D	103	LYS
6	D	179	TYR
6	D	185	GLU
7	E	25	TYR
7	E	76	SER
7	E	122	PRO
8	F	30	LYS
8	F	81	GLU
8	F	126	PRO
8	F	152	ARG
9	G	62	LYS
9	G	74	ASN
10	H	33	GLU
10	H	40	ASP
10	H	42	GLU
10	H	141	LYS
11	I	31	LYS
11	I	49	ARG
11	I	50	GLY
11	I	120	GLU
12	J	23	PRO
12	J	48	PRO
12	J	79	ARG
12	J	108	LYS
12	J	146	VAL
13	K	8	LYS
13	K	23	GLY
13	K	32	PHE
13	K	40	ALA
13	K	125	LEU
13	K	135	ASP
14	L	8	ARG
14	L	46	GLY
15	M	23	ARG

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Mol	Chain	Res	Type
16	N	24	PRO
16	N	32	TYR
16	N	41	ARG
16	N	55	ASN
16	N	131	ALA
16	N	133	GLU
17	O	53	ARG
17	O	77	SER
17	O	91	ASP
19	Q	46	PHE
20	R	7	VAL
20	R	90	GLU
21	S	12	THR
21	S	15	VAL
21	S	18	GLY
21	S	40	GLU
22	T	2	GLU
22	T	39	VAL
22	T	153	SER
23	U	27	GLU
23	U	41	ARG
24	V	62	VAL
24	V	88	LYS
25	W	15	LYS
26	X	9	VAL
35	c	56	ARG
35	c	182	ILE
35	c	209	ARG
35	c	237	ALA
36	d	17	ASP
36	d	129	ALA
36	d	168	ALA
36	d	175	LEU
37	e	101	LEU
38	f	73	ASN
40	h	33	ASP
40	h	36	LYS
40	h	53	LYS
40	h	70	LYS
41	i	52	ASP
42	j	7	THR
42	j	10	ARG

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Mol	Chain	Res	Type
42	j	97	LYS
43	k	71	LEU
44	l	54	ARG
45	m	29	ALA
46	n	105	THR
46	n	117	VAL
47	o	33	VAL
49	q	23	ASP
49	q	28	ARG
49	q	42	ARG
49	q	70	ALA
50	r	50	LYS
50	r	77	VAL
51	s	9	LYS
52	t	20	LEU
52	t	55	LYS
52	t	67	VAL
53	u	43	LEU
54	v	20	LYS
4	B	45	ASN
4	B	47	GLY
4	B	53	PHE
4	B	87	ASN
4	B	116	GLN
4	B	268	ARG
5	C	180	ASN
6	D	12	ARG
6	D	50	GLY
6	D	52	VAL
6	D	83	VAL
6	D	97	PRO
6	D	163	ARG
7	E	107	LEU
7	E	146	TYR
8	F	15	VAL
8	F	38	SER
8	F	170	ARG
10	H	119	GLU
10	H	130	LEU
11	I	24	VAL
11	I	94	ARG
11	I	103	ALA

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Mol	Chain	Res	Type
12	J	61	ARG
12	J	78	PRO
12	J	129	ALA
13	K	2	LEU
13	K	49	ALA
13	K	63	LYS
13	K	121	ALA
13	K	132	VAL
15	M	48	LEU
15	M	56	LEU
16	N	95	ARG
16	N	128	GLU
18	P	23	GLU
18	P	58	VAL
18	P	84	LYS
18	P	90	PRO
19	Q	98	LYS
21	S	3	VAL
21	S	34	LYS
21	S	56	PRO
21	S	86	ARG
22	T	16	SER
22	T	53	ILE
22	T	168	GLU
23	U	20	ARG
23	U	23	VAL
23	U	33	ALA
24	V	68	PRO
25	W	11	GLU
25	W	16	LEU
26	X	18	ASP
29	a	59	LYS
30	b	14	CYS
35	c	19	HIS
35	c	98	LEU
35	c	178	ARG
36	d	9	GLY
36	d	115	LEU
36	d	172	ARG
36	d	204	LEU
37	e	9	CYS
37	e	132	ARG

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Mol	Chain	Res	Type
38	f	143	ARG
39	g	48	LEU
39	g	78	GLU
39	g	88	VAL
40	h	9	VAL
40	h	88	PRO
41	i	24	THR
42	j	54	ASP
43	k	76	ASN
43	k	98	ILE
44	l	39	PRO
45	m	70	PRO
46	n	99	ARG
46	n	119	GLY
49	q	66	PRO
50	r	95	TYR
52	t	8	GLY
54	v	18	TYR
54	v	19	GLY
4	B	251	GLY
5	C	30	PRO
5	C	188	VAL
6	D	89	PRO
8	F	11	VAL
8	F	42	ARG
8	F	82	GLY
8	F	151	ILE
10	H	109	PRO
11	I	22	ILE
11	I	76	ALA
11	I	113	LYS
12	J	8	PRO
13	K	111	GLU
14	L	38	VAL
16	N	20	PRO
16	N	90	GLN
17	O	20	LEU
17	O	88	ILE
19	Q	35	ILE
20	R	88	LYS
21	S	30	VAL
21	S	52	SER

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Mol	Chain	Res	Type
22	T	12	GLY
23	U	57	PHE
25	W	57	ILE
27	Y	55	ARG
29	a	4	MET
29	a	38	GLY
30	b	10	ILE
30	b	30	PRO
35	c	23	ARG
35	c	127	ILE
36	d	61	ALA
36	d	81	GLY
36	d	174	PRO
37	e	51	PRO
40	h	81	GLY
41	i	134	ILE
42	j	53	VAL
45	m	80	SER
50	r	16	GLN
50	r	64	PRO
52	t	76	PRO
3	A	204	GLY
4	B	74	GLY
4	B	125	ILE
6	D	80	GLY
16	N	19	LEU
18	P	65	GLY
27	Y	41	PRO
28	Z	7	PRO
30	b	25	VAL
36	d	116	VAL
37	e	90	GLY
38	f	100	VAL
41	i	6	ILE
43	k	74	ILE
52	t	49	ILE
5	C	139	GLY
7	E	119	GLY
8	F	31	GLY
10	H	77	VAL
10	H	157	ARG
11	I	72	PRO

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Mol	Chain	Res	Type
21	S	45	VAL
21	S	80	GLY
27	Y	33	CYS
38	f	93	PRO
40	h	91	VAL
47	o	56	VAL
49	q	19	ILE
4	B	229	VAL
4	B	246	PRO
5	C	184	VAL
6	D	121	VAL
8	F	121	ILE
9	G	124	GLY
11	I	19	ILE
11	I	101	PRO
12	J	20	GLY
16	N	88	ILE
17	O	82	GLY
22	T	42	VAL
24	V	12	PRO
37	e	37	PRO
37	e	136	PRO
44	l	48	ILE
50	r	46	ASP
52	t	54	GLY
53	u	100	ILE
4	B	92	ILE
4	B	106	ILE
4	B	216	GLY
4	B	244	ARG
5	C	47	VAL
5	C	141	ILE
10	H	149	PRO
11	I	86	ILE
12	J	19	VAL
15	M	85	VAL
16	N	66	VAL
30	b	3	VAL
35	c	164	VAL
37	e	133	VAL
41	i	26	VAL
43	k	41	PRO

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Mol	Chain	Res	Type
50	r	5	VAL
50	r	19	VAL
53	u	97	ALA
3	A	52	PRO
5	C	116	VAL
12	J	62	LEU
23	U	79	VAL
27	Y	6	VAL
39	g	72	VAL
41	i	4	ASP
44	l	21	ILE
4	B	245	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	106/181 (59%)	86 (81%)	20 (19%)	1	10
4	B	214/218 (98%)	179 (84%)	35 (16%)	2	15
5	C	163/166 (98%)	130 (80%)	33 (20%)	1	9
6	D	154/162 (95%)	133 (86%)	21 (14%)	3	21
7	E	154/156 (99%)	130 (84%)	24 (16%)	2	17
8	F	142/148 (96%)	129 (91%)	13 (9%)	9	35
9	G	124/124 (100%)	100 (81%)	24 (19%)	1	9
10	H	117/119 (98%)	96 (82%)	21 (18%)	2	12
11	I	100/100 (100%)	74 (74%)	26 (26%)	0	4
12	J	112/116 (97%)	91 (81%)	21 (19%)	1	10
13	K	108/111 (97%)	84 (78%)	24 (22%)	1	7
14	L	101/101 (100%)	89 (88%)	12 (12%)	5	25
15	M	84/88 (96%)	71 (84%)	13 (16%)	2	17
16	N	121/128 (94%)	101 (84%)	20 (16%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	O	93/94 (99%)	77 (83%)	16 (17%)	2	13
18	P	82/82 (100%)	64 (78%)	18 (22%)	1	7
19	Q	89/92 (97%)	75 (84%)	14 (16%)	2	17
20	R	74/78 (95%)	62 (84%)	12 (16%)	2	15
21	S	86/91 (94%)	73 (85%)	13 (15%)	3	18
22	T	163/179 (91%)	136 (83%)	27 (17%)	2	14
23	U	61/67 (91%)	54 (88%)	7 (12%)	5	27
24	V	73/83 (88%)	61 (84%)	12 (16%)	2	15
25	W	58/67 (87%)	47 (81%)	11 (19%)	1	10
26	X	52/52 (100%)	46 (88%)	6 (12%)	5	27
27	Y	49/52 (94%)	40 (82%)	9 (18%)	1	11
28	Z	41/42 (98%)	34 (83%)	7 (17%)	2	14
29	a	53/55 (96%)	44 (83%)	9 (17%)	2	14
30	b	33/34 (97%)	31 (94%)	2 (6%)	18	50
35	c	202/220 (92%)	169 (84%)	33 (16%)	2	15
36	d	160/188 (85%)	130 (81%)	30 (19%)	1	10
37	e	180/181 (99%)	154 (86%)	26 (14%)	3	19
38	f	115/123 (94%)	102 (89%)	13 (11%)	6	27
39	g	90/90 (100%)	77 (86%)	13 (14%)	3	19
40	h	126/127 (99%)	108 (86%)	18 (14%)	3	20
41	i	119/119 (100%)	96 (81%)	23 (19%)	1	10
42	j	98/99 (99%)	89 (91%)	9 (9%)	9	35
43	k	88/92 (96%)	76 (86%)	12 (14%)	3	21
44	l	88/99 (89%)	78 (89%)	10 (11%)	5	27
45	m	104/109 (95%)	80 (77%)	24 (23%)	1	6
46	n	100/101 (99%)	75 (75%)	25 (25%)	0	4
47	o	49/50 (98%)	37 (76%)	12 (24%)	0	5
48	p	79/80 (99%)	66 (84%)	13 (16%)	2	15
49	q	72/74 (97%)	57 (79%)	15 (21%)	1	8
50	r	96/97 (99%)	79 (82%)	17 (18%)	2	12
51	s	71/77 (92%)	63 (89%)	8 (11%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	t	71/80 (89%)	52 (73%)	19 (27%)	0	3
53	u	76/82 (93%)	66 (87%)	10 (13%)	4	22
54	v	19/22 (86%)	16 (84%)	3 (16%)	2	16
All	All	4810/5096 (94%)	4007 (83%)	803 (17%)	2	14

All (803) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	8	TYR
3	A	12	LEU
3	A	16	ASP
3	A	19	LYS
3	A	20	ILE
3	A	21	TYR
3	A	22	THR
3	A	30	VAL
3	A	32	GLU
3	A	43	GLU
3	A	53	ARG
3	A	163	GLU
3	A	165	ARG
3	A	178	LYS
3	A	189	ASN
3	A	193	PHE
3	A	197	LEU
3	A	198	GLU
3	A	201	LYS
3	A	209	PHE
4	B	10	THR
4	B	13	ARG
4	B	15	PHE
4	B	18	VAL
4	B	24	ILE
4	B	31	LYS
4	B	33	LEU
4	B	37	LEU
4	B	43	ARG
4	B	60	ARG
4	B	61	LEU
4	B	63	ARG
4	B	66	ASP

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Mol	Chain	Res	Type
4	B	67	PHE
4	B	70	TRP
4	B	71	ASP
4	B	79	VAL
4	B	115	GLN
4	B	131	LEU
4	B	150	LYS
4	B	164	GLN
4	B	176	ARG
4	B	177	LEU
4	B	198	ASN
4	B	201	HIS
4	B	213	ARG
4	B	214	TRP
4	B	217	ARG
4	B	229	VAL
4	B	242	ARG
4	B	255	LYS
4	B	257	LEU
4	B	262	ARG
4	B	263	ARG
4	B	271	ILE
5	C	5	LEU
5	C	12	THR
5	C	15	PHE
5	C	19	ARG
5	C	21	VAL
5	C	23	VAL
5	C	24	THR
5	C	27	LEU
5	C	37	ARG
5	C	42	ASP
5	C	44	TYR
5	C	61	ARG
5	C	66	HIS
5	C	67	PHE
5	C	78	LEU
5	C	79	ARG
5	C	84	PHE
5	C	89	ASP
5	C	97	LYS
5	C	107	THR

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Mol	Chain	Res	Type
5	C	117	MET
5	C	119	ARG
5	C	122	PHE
5	C	141	ILE
5	C	156	MET
5	C	173	VAL
5	C	179	GLU
5	C	183	LEU
5	C	188	VAL
5	C	192	ASN
5	C	197	ILE
5	C	201	THR
5	C	203	LYS
6	D	22	GLU
6	D	27	LEU
6	D	77	ILE
6	D	83	VAL
6	D	84	VAL
6	D	92	TYR
6	D	97	PRO
6	D	115	GLU
6	D	117	LYS
6	D	120	LEU
6	D	135	LEU
6	D	137	TRP
6	D	143	LEU
6	D	144	ASP
6	D	149	VAL
6	D	165	LEU
6	D	179	TYR
6	D	180	ASP
6	D	181	ILE
6	D	183	ARG
6	D	196	VAL
7	E	10	LYS
7	E	12	TYR
7	E	19	LEU
7	E	25	TYR
7	E	29	TRP
7	E	31	VAL
7	E	33	ARG
7	E	55	LYS

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Mol	Chain	Res	Type
7	E	72	ARG
7	E	80	PHE
7	E	95	ARG
7	E	99	MET
7	E	115	ARG
7	E	135	LEU
7	E	136	ARG
7	E	138	GLN
7	E	139	LEU
7	E	146	TYR
7	E	148	MET
7	E	155	MET
7	E	165	THR
7	E	173	LEU
7	E	176	LEU
7	E	178	PHE
8	F	65	HIS
8	F	68	THR
8	F	87	LEU
8	F	89	ILE
8	F	90	LYS
8	F	92	ILE
8	F	98	LEU
8	F	110	SER
8	F	139	GLN
8	F	140	LYS
8	F	152	ARG
8	F	162	ILE
8	F	172	LYS
9	G	3	VAL
9	G	20	ASP
9	G	21	VAL
9	G	27	ARG
9	G	31	LEU
9	G	33	ARG
9	G	38	LEU
9	G	41	GLU
9	G	44	LEU
9	G	62	LYS
9	G	76	THR
9	G	77	LEU
9	G	93	THR

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Mol	Chain	Res	Type
9	G	96	ASP
9	G	99	GLU
9	G	103	ARG
9	G	108	THR
9	G	109	ILE
9	G	114	LEU
9	G	118	LYS
9	G	123	LEU
9	G	130	TYR
9	G	136	VAL
9	G	139	GLN
10	H	25	LYS
10	H	33	GLU
10	H	35	ARG
10	H	38	LEU
10	H	60	LYS
10	H	62	ARG
10	H	71	MET
10	H	84	ARG
10	H	86	THR
10	H	92	GLN
10	H	95	TYR
10	H	98	TYR
10	H	129	MET
10	H	132	LYS
10	H	140	PHE
10	H	142	ARG
10	H	143	LEU
10	H	145	VAL
10	H	146	TYR
10	H	159	GLU
10	H	161	LEU
11	I	1	MET
11	I	3	GLN
11	I	9	GLU
11	I	10	VAL
11	I	12	ASP
11	I	21	CYS
11	I	29	ASN
11	I	39	ILE
11	I	45	GLU
11	I	49	ARG

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Mol	Chain	Res	Type
11	I	58	VAL
11	I	59	LYS
11	I	63	VAL
11	I	67	LYS
11	I	68	GLU
11	I	77	ILE
11	I	80	ASP
11	I	91	LEU
11	I	96	THR
11	I	97	ARG
11	I	102	VAL
11	I	104	ARG
11	I	105	GLU
11	I	109	LYS
11	I	114	ILE
11	I	120	GLU
12	J	5	ASP
12	J	13	ASN
12	J	45	LEU
12	J	60	MET
12	J	61	ARG
12	J	62	LEU
12	J	68	GLN
12	J	74	GLU
12	J	77	ARG
12	J	80	TYR
12	J	81	GLN
12	J	84	ASN
12	J	85	LEU
12	J	96	THR
12	J	100	LEU
12	J	110	TYR
12	J	121	LYS
12	J	130	PHE
12	J	145	PRO
12	J	148	LEU
12	J	149	GLU
13	K	3	MET
13	K	8	LYS
13	K	9	TYR
13	K	11	LYS
13	K	14	ARG

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Mol	Chain	Res	Type
13	K	17	LEU
13	K	25	ASP
13	K	29	PHE
13	K	32	PHE
13	K	41	TRP
13	K	42	ILE
13	K	51	ARG
13	K	59	ARG
13	K	64	ILE
13	K	65	PHE
13	K	69	PHE
13	K	82	ARG
13	K	89	ASN
13	K	93	TYR
13	K	103	MET
13	K	111	GLU
13	K	124	LYS
13	K	133	ARG
13	K	134	ARG
14	L	9	LYS
14	L	14	SER
14	L	29	LEU
14	L	31	HIS
14	L	38	VAL
14	L	43	GLU
14	L	59	ASP
14	L	65	LEU
14	L	68	ARG
14	L	88	ARG
14	L	94	TYR
14	L	105	ARG
15	M	7	TYR
15	M	10	ARG
15	M	12	PHE
15	M	14	VAL
15	M	15	ARG
15	M	24	LEU
15	M	39	ILE
15	M	42	ASP
15	M	46	VAL
15	M	54	LEU
15	M	75	GLU

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Mol	Chain	Res	Type
15	M	93	LYS
15	M	94	TYR
16	N	6	LEU
16	N	32	TYR
16	N	35	LYS
16	N	38	ASN
16	N	57	PHE
16	N	61	PHE
16	N	62	THR
16	N	85	LYS
16	N	87	ASP
16	N	88	ILE
16	N	98	LYS
16	N	103	ARG
16	N	107	ASP
16	N	111	ARG
16	N	112	ARG
16	N	113	LYS
16	N	118	ARG
16	N	121	ILE
16	N	123	LYS
16	N	124	ASP
17	O	5	LYS
17	O	14	HIS
17	O	25	TRP
17	O	27	LEU
17	O	51	LYS
17	O	58	ARG
17	O	71	GLN
17	O	74	LEU
17	O	79	PHE
17	O	84	LYS
17	O	85	LYS
17	O	91	ASP
17	O	97	ASP
17	O	106	PHE
17	O	109	LEU
17	O	114	LYS
18	P	13	ARG
18	P	18	LEU
18	P	20	LEU
18	P	23	GLU

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Mol	Chain	Res	Type
18	P	26	ASP
18	P	35	LEU
18	P	39	LEU
18	P	40	LEU
18	P	51	VAL
18	P	58	VAL
18	P	60	GLU
18	P	62	LEU
18	P	80	GLN
18	P	81	TYR
18	P	82	ARG
18	P	89	GLN
18	P	92	THR
18	P	98	GLU
19	Q	6	ILE
19	Q	8	ARG
19	Q	21	VAL
19	Q	23	LEU
19	Q	31	GLU
19	Q	49	LYS
19	Q	51	LEU
19	Q	67	ASP
19	Q	68	ARG
19	Q	70	TYR
19	Q	76	VAL
19	Q	86	LEU
19	Q	88	ARG
19	Q	97	LYS
20	R	3	THR
20	R	13	LEU
20	R	26	TYR
20	R	27	THR
20	R	38	GLU
20	R	49	VAL
20	R	56	THR
20	R	62	LYS
20	R	65	ARG
20	R	76	ARG
20	R	77	LYS
20	R	83	VAL
21	S	9	LYS
21	S	20	TYR

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Mol	Chain	Res	Type
21	S	23	ARG
21	S	28	LYS
21	S	40	GLU
21	S	44	ILE
21	S	50	ARG
21	S	64	GLU
21	S	67	LEU
21	S	71	LYS
21	S	73	ARG
21	S	75	ILE
21	S	97	ARG
22	T	1	MET
22	T	8	TYR
22	T	9	TYR
22	T	19	ARG
22	T	20	ARG
22	T	31	ARG
22	T	41	LEU
22	T	44	PHE
22	T	48	PHE
22	T	50	GLN
22	T	53	ILE
22	T	78	LYS
22	T	80	ARG
22	T	88	PHE
22	T	95	PRO
22	T	104	PHE
22	T	119	GLU
22	T	144	LEU
22	T	145	GLU
22	T	146	ILE
22	T	150	LEU
22	T	151	HIS
22	T	157	LEU
22	T	162	GLU
22	T	163	LEU
22	T	170	THR
22	T	171	ILE
23	U	19	LYS
23	U	20	ARG
23	U	26	TYR
23	U	53	MET

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Mol	Chain	Res	Type
23	U	62	LEU
23	U	64	ASP
23	U	69	PHE
24	V	13	ILE
24	V	18	ILE
24	V	26	ARG
24	V	41	ARG
24	V	43	TYR
24	V	46	LEU
24	V	58	ILE
24	V	60	PHE
24	V	62	VAL
24	V	78	LYS
24	V	85	LEU
24	V	91	LYS
25	W	9	GLN
25	W	12	GLU
25	W	14	ARG
25	W	15	LYS
25	W	27	GLU
25	W	29	LYS
25	W	33	MET
25	W	37	PHE
25	W	47	ASN
25	W	48	HIS
25	W	55	ARG
26	X	8	LEU
26	X	23	LEU
26	X	29	ARG
26	X	30	ARG
26	X	35	ARG
26	X	49	LYS
27	Y	16	ARG
27	Y	25	LEU
27	Y	26	THR
27	Y	29	ILE
27	Y	33	CYS
27	Y	39	MET
27	Y	49	CYS
27	Y	51	TYR
27	Y	56	LYS
28	Z	1	MET

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Mol	Chain	Res	Type
28	Z	2	LYS
28	Z	5	TRP
28	Z	15	THR
28	Z	29	LYS
28	Z	39	ARG
28	Z	44	PRO
29	a	3	LYS
29	a	16	ILE
29	a	17	THR
29	a	25	MET
29	a	34	TRP
29	a	36	LYS
29	a	44	LYS
29	a	48	PHE
29	a	60	LEU
30	b	24	TYR
30	b	25	VAL
35	c	8	LYS
35	c	10	LEU
35	c	17	PHE
35	c	19	HIS
35	c	23	ARG
35	c	42	ILE
35	c	47	THR
35	c	48	MET
35	c	51	LEU
35	c	60	ASP
35	c	67	THR
35	c	71	VAL
35	c	92	TYR
35	c	101	MET
35	c	102	LEU
35	c	118	LEU
35	c	132	LYS
35	c	133	LYS
35	c	136	VAL
35	c	137	ARG
35	c	143	GLU
35	c	146	GLN
35	c	149	LEU
35	c	155	LEU
35	c	156	LYS

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Mol	Chain	Res	Type
35	c	164	VAL
35	c	169	LYS
35	c	172	ILE
35	c	200	ILE
35	c	204	ASN
35	c	209	ARG
35	c	220	ASP
35	c	221	LEU
36	d	3	ASN
36	d	4	LYS
36	d	16	ARG
36	d	27	LYS
36	d	29	TYR
36	d	32	LEU
36	d	33	LEU
36	d	46	GLU
36	d	52	LEU
36	d	56	ASP
36	d	84	ILE
36	d	93	LYS
36	d	94	LEU
36	d	95	THR
36	d	97	LYS
36	d	102	ASN
36	d	107	GLN
36	d	111	LEU
36	d	118	GLN
36	d	123	GLN
36	d	126	ARG
36	d	130	VAL
36	d	131	ARG
36	d	135	LYS
36	d	139	GLN
36	d	175	LEU
36	d	178	LEU
36	d	186	PHE
36	d	193	TYR
36	d	195	VAL
37	e	8	VAL
37	e	14	ARG
37	e	15	GLU
37	e	22	LYS

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Mol	Chain	Res	Type
37	e	29	PRO
37	e	33	MET
37	e	36	ARG
37	e	39	PRO
37	e	59	ARG
37	e	61	LYS
37	e	68	TYR
37	e	72	GLU
37	e	78	LEU
37	e	79	PHE
37	e	94	LEU
37	e	97	LEU
37	e	101	LEU
37	e	104	VAL
37	e	120	LEU
37	e	122	ARG
37	e	134	ASP
37	e	188	LEU
37	e	191	ARG
37	e	199	ASN
37	e	203	VAL
37	e	207	TYR
38	f	6	PHE
38	f	10	MET
38	f	12	LEU
38	f	43	LEU
38	f	57	LYS
38	f	72	GLN
38	f	78	HIS
38	f	105	VAL
38	f	118	ILE
38	f	136	MET
38	f	137	GLU
38	f	143	ARG
38	f	144	THR
39	g	2	ARG
39	g	15	ASP
39	g	17	SER
39	g	27	GLN
39	g	37	VAL
39	g	43	LEU
39	g	55	ASP

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Mol	Chain	Res	Type
39	g	75	LEU
39	g	78	GLU
39	g	83	ASP
39	g	86	ARG
39	g	91	VAL
39	g	100	ASN
40	h	4	ARG
40	h	5	ARG
40	h	16	LEU
40	h	29	LYS
40	h	32	ARG
40	h	35	LYS
40	h	41	ARG
40	h	43	PHE
40	h	59	LEU
40	h	64	GLN
40	h	68	ASN
40	h	84	ASN
40	h	103	TRP
40	h	105	VAL
40	h	113	GLU
40	h	119	ARG
40	h	151	TYR
40	h	155	ARG
41	i	1	MET
41	i	2	LEU
41	i	14	ARG
41	i	17	THR
41	i	21	LYS
41	i	24	THR
41	i	31	PHE
41	i	39	LEU
41	i	45	ILE
41	i	48	TYR
41	i	50	ARG
41	i	52	ASP
41	i	62	TYR
41	i	75	ARG
41	i	85	ARG
41	i	98	LYS
41	i	99	GLU
41	i	103	VAL

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Mol	Chain	Res	Type
41	i	104	ARG
41	i	105	ARG
41	i	107	LEU
41	i	122	ARG
41	i	127	LEU
42	j	5	TYR
42	j	53	VAL
42	j	85	LEU
42	j	89	ASN
42	j	92	TYR
42	j	108	VAL
42	j	114	TYR
42	j	125	TYR
42	j	127	LYS
43	k	8	LEU
43	k	11	PHE
43	k	46	ARG
43	k	47	PHE
43	k	49	VAL
43	k	57	LYS
43	k	61	GLU
43	k	64	GLU
43	k	65	LEU
43	k	71	LEU
43	k	79	ARG
43	k	82	ILE
44	l	20	TYR
44	l	29	ILE
44	l	33	THR
44	l	34	ASP
44	l	41	THR
44	l	51	LYS
44	l	73	MET
44	l	84	VAL
44	l	99	GLN
44	l	104	GLN
45	m	6	ILE
45	m	14	ARG
45	m	17	VAL
45	m	23	VAL
45	m	27	LYS
45	m	40	ARG

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Mol	Chain	Res	Type
45	m	45	LYS
45	m	51	LEU
45	m	52	ARG
45	m	53	LYS
45	m	58	ARG
45	m	64	GLU
45	m	76	LEU
45	m	77	GLN
45	m	81	VAL
45	m	84	ILE
45	m	85	ARG
45	m	101	ARG
45	m	111	ASP
45	m	112	ARG
45	m	114	LYS
45	m	115	SER
45	m	121	THR
45	m	126	GLU
46	n	15	VAL
46	n	16	ASP
46	n	23	TYR
46	n	25	ILE
46	n	59	TYR
46	n	62	ASN
46	n	64	TRP
46	n	66	LEU
46	n	69	GLU
46	n	70	LEU
46	n	73	GLU
46	n	82	MET
46	n	86	CYS
46	n	91	ARG
46	n	92	HIS
46	n	93	ARG
46	n	94	ARG
46	n	98	VAL
46	n	99	ARG
46	n	103	THR
46	n	104	ARG
46	n	105	THR
46	n	108	ARG
46	n	120	LYS

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Mol	Chain	Res	Type
46	n	125	ARG
47	o	8	GLU
47	o	11	LYS
47	o	16	PHE
47	o	21	TYR
47	o	24	CYS
47	o	29	ARG
47	o	33	VAL
47	o	36	PHE
47	o	41	ARG
47	o	42	ILE
47	o	49	HIS
47	o	56	VAL
48	p	6	GLU
48	p	8	LYS
48	p	26	GLU
48	p	32	LEU
48	p	35	ARG
48	p	54	ARG
48	p	56	LEU
48	p	57	LEU
48	p	67	LEU
48	p	69	TYR
48	p	71	GLN
48	p	83	GLU
48	p	84	LYS
49	q	1	MET
49	q	13	HIS
49	q	27	LYS
49	q	32	TYR
49	q	35	LYS
49	q	41	PRO
49	q	43	LYS
49	q	44	THR
49	q	48	TRP
49	q	52	ASP
49	q	58	TYR
49	q	60	LEU
49	q	71	ARG
49	q	74	LEU
49	q	79	VAL
50	r	6	LEU

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Mol	Chain	Res	Type
50	r	14	LYS
50	r	17	LYS
50	r	19	VAL
50	r	36	ILE
50	r	41	LYS
50	r	42	TYR
50	r	43	LEU
50	r	55	ASP
50	r	58	GLU
50	r	69	LYS
50	r	72	ARG
50	r	81	ARG
50	r	84	LEU
50	r	88	TYR
50	r	94	ASN
50	r	100	LYS
51	s	13	GLN
51	s	29	PHE
51	s	31	LEU
51	s	32	ARG
51	s	33	ASP
51	s	34	TYR
51	s	42	ARG
51	s	63	GLN
52	t	6	LYS
52	t	23	ASN
52	t	25	LYS
52	t	29	ARG
52	t	31	ILE
52	t	32	LYS
52	t	33	THR
52	t	34	TRP
52	t	36	ARG
52	t	43	GLU
52	t	44	MET
52	t	49	ILE
52	t	53	ASN
52	t	55	LYS
52	t	60	VAL
52	t	61	TYR
52	t	63	THR
52	t	66	MET

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Mol	Chain	Res	Type
52	t	71	LEU
53	u	10	LEU
53	u	20	LEU
53	u	21	LYS
53	u	23	ARG
53	u	27	LYS
53	u	51	GLU
53	u	53	LEU
53	u	56	MET
53	u	72	LEU
53	u	79	ARG
54	v	6	ARG
54	v	9	ARG
54	v	14	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (134) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	18	ASN
3	A	58	ASN
4	B	46	GLN
4	B	87	ASN
4	B	115	GLN
4	B	129	ASN
4	B	164	GLN
4	B	166	GLN
4	B	198	ASN
4	B	201	HIS
4	B	231	HIS
4	B	253	GLN
5	C	54	GLN
5	C	55	ASN
5	C	66	HIS
5	C	132	HIS
5	C	143	ASN
6	D	35	GLN
6	D	128	ASN
6	D	177	ASN
7	E	40	ASN
7	E	41	GLN
7	E	66	GLN
7	E	79	ASN

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Mol	Chain	Res	Type
7	E	123	ASN
8	F	61	HIS
8	F	65	HIS
8	F	74	ASN
8	F	143	GLN
9	G	28	ASN
9	G	43	ASN
9	G	104	GLN
9	G	147	GLN
10	H	92	GLN
10	H	124	HIS
11	I	3	GLN
11	I	29	ASN
12	J	9	ASN
12	J	38	GLN
12	J	81	GLN
13	K	12	GLN
13	K	45	GLN
13	K	46	GLN
13	K	57	HIS
13	K	123	HIS
14	L	16	HIS
14	L	23	ASN
14	L	71	GLN
15	M	38	GLN
16	N	38	ASN
16	N	90	GLN
17	O	44	ASN
17	O	72	HIS
18	P	64	HIS
18	P	87	HIS
19	Q	57	ASN
20	R	41	ASN
21	S	57	GLN
22	T	34	ASN
22	T	55	HIS
22	T	65	GLN
22	T	73	GLN
22	T	75	ASN
23	U	35	ASN
23	U	40	GLN
23	U	80	HIS

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Mol	Chain	Res	Type
24	V	19	GLN
24	V	45	ASN
25	W	47	ASN
26	X	32	GLN
28	Z	16	HIS
29	a	35	GLN
35	c	25	ASN
35	c	78	GLN
35	c	94	ASN
35	c	135	GLN
35	c	204	ASN
36	d	3	ASN
36	d	6	HIS
36	d	28	GLN
36	d	63	ASN
36	d	102	ASN
36	d	110	ASN
36	d	118	GLN
36	d	136	GLN
36	d	139	GLN
37	e	45	GLN
37	e	74	GLN
37	e	77	ASN
37	e	119	GLN
37	e	129	ASN
37	e	199	ASN
37	e	201	GLN
38	f	20	GLN
38	f	65	ASN
38	f	72	GLN
39	g	18	GLN
39	g	27	GLN
39	g	32	ASN
39	g	94	GLN
40	h	13	GLN
40	h	64	GLN
40	h	68	ASN
40	h	84	ASN
40	h	86	GLN
40	h	97	GLN
40	h	106	GLN
40	h	109	ASN

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Mol	Chain	Res	Type
40	h	110	GLN
40	h	122	HIS
41	i	15	ASN
41	i	70	GLN
42	j	73	GLN
42	j	89	ASN
43	k	56	HIS
43	k	76	ASN
44	l	27	ASN
44	l	38	ASN
45	m	7	ASN
45	m	77	GLN
46	n	40	ASN
46	n	101	GLN
47	o	49	HIS
48	p	13	GLN
48	p	37	ASN
48	p	42	HIS
48	p	62	GLN
49	q	16	HIS
49	q	76	GLN
50	r	26	GLN
51	s	63	GLN
52	t	47	HIS
53	u	26	ASN
53	u	42	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	w	2888/2889 (99%)	983 (34%)	0
2	x	119/120 (99%)	47 (39%)	0
31	y	1511/1522 (99%)	507 (33%)	0
32	z	76/77 (98%)	20 (26%)	0
33	2	75/76 (98%)	22 (29%)	0
34	3	17/18 (94%)	5 (29%)	0
All	All	4686/4702 (99%)	1584 (33%)	0

All (1584) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	w	10	G
1	w	13	A
1	w	15	G
1	w	27	G
1	w	28	A
1	w	29	U
1	w	34	C
1	w	35	G
1	w	37	C
1	w	43	G
1	w	46	C
1	w	49	A
1	w	50	U
1	w	51	G
1	w	52	A
1	w	61	G
1	w	64	A
1	w	69	C
1	w	71	A
1	w	72	U
1	w	73	A
1	w	75	G
1	w	78	A
1	w	83	G
1	w	88	G
1	w	89	G
1	w	90	U
1	w	92	G
1	w	95	G
1	w	96	G
1	w	101	G
1	w	102	G
1	w	103	A
1	w	117	G
1	w	118	A
1	w	119	A
1	w	120	U
1	w	121	G
1	w	125	G
1	w	126	A
1	w	131	G
1	w	137(A)	C
1	w	139	G

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Mol	Chain	Res	Type
1	w	143	C
1	w	144	C
1	w	146	G
1	w	149	A
1	w	151	C
1	w	153	C
1	w	162	U
1	w	163	U
1	w	165	U
1	w	174	C
1	w	175	G
1	w	176	G
1	w	177	G
1	w	182	A
1	w	184	C
1	w	196	A
1	w	199	A
1	w	204	A
1	w	205	G
1	w	206	U
1	w	215	G
1	w	216	A
1	w	221	A
1	w	222	A
1	w	228	A
1	w	229	A
1	w	233	A
1	w	239	U
1	w	241	A
1	w	242	G
1	w	248	G
1	w	249	C
1	w	250	G
1	w	252	G
1	w	265	A
1	w	266	G
1	w	269	U
1	w	270(D)	C
1	w	270(E)	C
1	w	270(F)	G
1	w	270(M)	U
1	w	270(S)	G

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Mol	Chain	Res	Type
1	w	270(T)	G
1	w	271(A)	U
1	w	271(B)	C
1	w	271(C)	G
1	w	271(D)	U
1	w	271	G
1	w	273(C)	C
1	w	273(G)	C
1	w	274	G
1	w	275	G
1	w	278	A
1	w	289	A
1	w	294	A
1	w	296	C
1	w	298	G
1	w	299	A
1	w	301	G
1	w	302	C
1	w	308	G
1	w	310	A
1	w	311	A
1	w	316	C
1	w	317	G
1	w	320	A
1	w	327	G
1	w	329	G
1	w	330	A
1	w	331	A
1	w	332	A
1	w	338	G
1	w	339	U
1	w	341	G
1	w	342	G
1	w	344	G
1	w	347	A
1	w	348	G
1	w	349	G
1	w	355	G
1	w	358	U
1	w	363(A)	G
1	w	363(E)	G
1	w	363(F)	U

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Mol	Chain	Res	Type
1	w	364	C
1	w	366(B)	C
1	w	370	G
1	w	371	A
1	w	372	G
1	w	374	A
1	w	375	C
1	w	380	U
1	w	385	C
1	w	387	U
1	w	388	G
1	w	390	A
1	w	391	G
1	w	392	C
1	w	394	A
1	w	395	U
1	w	396	G
1	w	397	G
1	w	405	U
1	w	408	G
1	w	414	C
1	w	428	A
1	w	438	G
1	w	439	G
1	w	440	G
1	w	444	C
1	w	446	G
1	w	449	A
1	w	450	G
1	w	451	C
1	w	456	C
1	w	457	A
1	w	458	G
1	w	464	U
1	w	469	G
1	w	470	A
1	w	473	G
1	w	475	U
1	w	477	A
1	w	478	A
1	w	480	A
1	w	481	G

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Mol	Chain	Res	Type
1	w	483	A
1	w	488	G
1	w	489	G
1	w	491	G
1	w	492	A
1	w	504	U
1	w	505	A
1	w	508	G
1	w	509	C
1	w	510	C
1	w	517	C
1	w	518	G
1	w	522	G
1	w	527	C
1	w	528	A
1	w	529	A
1	w	531	C
1	w	532	A
1	w	533	G
1	w	537	C
1	w	542	C
1	w	544	C
1	w	549	G
1	w	551	G
1	w	556	G
1	w	559	G
1	w	562	U
1	w	563	G
1	w	567	A
1	w	569	U
1	w	572	A
1	w	573	G
1	w	574	C
1	w	575	A
1	w	583	G
1	w	594	U
1	w	595	C
1	w	598	G
1	w	603	A
1	w	604	G
1	w	610	C
1	w	614	U

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Mol	Chain	Res	Type
1	w	615	G
1	w	616	A
1	w	617	G
1	w	618(B)	C
1	w	620	G
1	w	621	A
1	w	627	A
1	w	628	G
1	w	634	C
1	w	638	G
1	w	640	C
1	w	645	C
1	w	646	A
1	w	647	G
1	w	653	C
1	w	654	U
1	w	656	G
1	w	660	G
1	w	666	G
1	w	669	G
1	w	671	C
1	w	672	C
1	w	674	G
1	w	684	G
1	w	686	G
1	w	701	G
1	w	703	U
1	w	715	G
1	w	716	A
1	w	717	G
1	w	719	C
1	w	722	A
1	w	729	G
1	w	730	C
1	w	739	G
1	w	740	U
1	w	747	U
1	w	748	G
1	w	749	C
1	w	751	A
1	w	753	C
1	w	757	U

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Mol	Chain	Res	Type
1	w	763	G
1	w	764	A
1	w	765	G
1	w	770	G
1	w	775	G
1	w	776	G
1	w	781	A
1	w	782	A
1	w	784	A
1	w	789	A
1	w	790	C
1	w	792	G
1	w	794	G
1	w	796	C
1	w	798	G
1	w	800	A
1	w	805	G
1	w	811	U
1	w	812	C
1	w	817	C
1	w	826	U
1	w	827	U
1	w	828	U
1	w	830	G
1	w	831	G
1	w	835	A
1	w	846	C
1	w	847	U
1	w	848	G
1	w	849	A
1	w	855	G
1	w	856	C
1	w	859	G
1	w	860	U
1	w	861	A
1	w	866	A
1	w	867	C
1	w	870	A
1	w	873	G
1	w	876	C
1	w	885	C
1	w	886	C

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Mol	Chain	Res	Type
1	w	887	A
1	w	888	C
1	w	889	C
1	w	890	A
1	w	897	C
1	w	899	A
1	w	900	A
1	w	902	C
1	w	906	G
1	w	907	U
1	w	909	A
1	w	910	A
1	w	912	C
1	w	914	C
1	w	916	G
1	w	926	A
1	w	928	G
1	w	931	G
1	w	932	G
1	w	933	A
1	w	938	G
1	w	945	A
1	w	946	G
1	w	957	A
1	w	958	U
1	w	959	A
1	w	961	C
1	w	962	G
1	w	963	U
1	w	965	C
1	w	966	G
1	w	972	G
1	w	974(A)	G
1	w	974(B)	C
1	w	975	G
1	w	976	C
1	w	977	G
1	w	980	A
1	w	982	C
1	w	983	A
1	w	989	G
1	w	990	A

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Mol	Chain	Res	Type
1	w	991	C
1	w	992	C
1	w	993	G
1	w	996	A
1	w	997	G
1	w	1006	C
1	w	1008	C
1	w	1009	A
1	w	1011	G
1	w	1012	U
1	w	1013	C
1	w	1015	G
1	w	1016	G
1	w	1017	G
1	w	1020	A
1	w	1021	A
1	w	1022	G
1	w	1023	U
1	w	1025	G
1	w	1026	U
1	w	1033	U
1	w	1034	G
1	w	1042	G
1	w	1043	C
1	w	1045	A
1	w	1046	A
1	w	1047	G
1	w	1054	A
1	w	1059	G
1	w	1060	U
1	w	1061	U
1	w	1062	G
1	w	1070	A
1	w	1071	G
1	w	1072	C
1	w	1079	C
1	w	1080	C
1	w	1083	U
1	w	1087	G
1	w	1088	A
1	w	1089	G
1	w	1111	A

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Mol	Chain	Res	Type
1	w	1112	G
1	w	1126	A
1	w	1129	A
1	w	1130	U
1	w	1131	G
1	w	1132	A
1	w	1135	C
1	w	1136	G
1	w	1139	G
1	w	1141	U
1	w	1142	C
1	w	1142(B)	A
1	w	1143	A
1	w	1144	G
1	w	1148	A
1	w	1152	C
1	w	1155	A
1	w	1157	G
1	w	1161	C
1	w	1166	C
1	w	1170	G
1	w	1175	U
1	w	1177	A
1	w	1179	C
1	w	1180	C
1	w	1182	A
1	w	1183	G
1	w	1186	G
1	w	1187	G
1	w	1188	U
1	w	1191	G
1	w	1194	A
1	w	1195	G
1	w	1197	G
1	w	1199	U
1	w	1200	C
1	w	1201	C
1	w	1202	C
1	w	1204	A
1	w	1205	U
1	w	1208	C
1	w	1210	A

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Mol	Chain	Res	Type
1	w	1211	U
1	w	1212	G
1	w	1220	A
1	w	1221	C
1	w	1224	C
1	w	1227	G
1	w	1229	G
1	w	1237	A
1	w	1238	G
1	w	1240	U
1	w	1244	G
1	w	1247	A
1	w	1248	G
1	w	1250	G
1	w	1251	C
1	w	1252	G
1	w	1253	A
1	w	1256	G
1	w	1265	A
1	w	1266	G
1	w	1267	U
1	w	1271	G
1	w	1272	A
1	w	1273	U
1	w	1274	A
1	w	1275	A
1	w	1276	A
1	w	1278	A
1	w	1280	G
1	w	1289	C
1	w	1295	C
1	w	1296	G
1	w	1298	C
1	w	1300	U
1	w	1301	A
1	w	1302	A
1	w	1305	C
1	w	1310	G
1	w	1313	U
1	w	1320	C
1	w	1321	A
1	w	1325	G

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Mol	Chain	Res	Type
1	w	1326	U
1	w	1329	U
1	w	1339	G
1	w	1341	U
1	w	1343	G
1	w	1347	G
1	w	1359	A
1	w	1360	A
1	w	1362	C
1	w	1365	A
1	w	1366	A
1	w	1368	G
1	w	1378	A
1	w	1379	A
1	w	1384	A
1	w	1385	G
1	w	1395	A
1	w	1398	C
1	w	1416	G
1	w	1419	A
1	w	1420	U
1	w	1426	G
1	w	1427	A
1	w	1428	C
1	w	1434	A
1	w	1436	G
1	w	1438	U
1	w	1444(B)	A
1	w	1445	C
1	w	1448	G
1	w	1448(B)	A
1	w	1449	G
1	w	1451	C
1	w	1453	A
1	w	1454	U
1	w	1455	G
1	w	1458	C
1	w	1459	G
1	w	1460	A
1	w	1461	G
1	w	1467	C
1	w	1471	A

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Mol	Chain	Res	Type
1	w	1472	A
1	w	1478	G
1	w	1479	G
1	w	1481	U
1	w	1483	G
1	w	1485	G
1	w	1487	G
1	w	1488	G
1	w	1490	A
1	w	1491	G
1	w	1497	U
1	w	1498	C
1	w	1502	C
1	w	1506	C
1	w	1508	A
1	w	1509	A
1	w	1510	A
1	w	1517	G
1	w	1519	G
1	w	1520	U
1	w	1521	G
1	w	1522	G
1	w	1535	U
1	w	1536	A
1	w	1537	C
1	w	1538	G
1	w	1540	G
1	w	1543	A
1	w	1544	C
1	w	1545	A
1	w	1546(B)	C
1	w	1547	C
1	w	1555	G
1	w	1558	A
1	w	1559	G
1	w	1560	G
1	w	1567	A
1	w	1569	A
1	w	1570	A
1	w	1576	U
1	w	1577	C
1	w	1578	U

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Mol	Chain	Res	Type
1	w	1579	A
1	w	1581	G
1	w	1585	C
1	w	1586	A
1	w	1595	G
1	w	1596	A
1	w	1603	A
1	w	1607	C
1	w	1608	A
1	w	1609	A
1	w	1610	A
1	w	1613	G
1	w	1616	A
1	w	1617	C
1	w	1618	A
1	w	1619	G
1	w	1626	G
1	w	1628	G
1	w	1634	A
1	w	1635	G
1	w	1639	U
1	w	1640	C
1	w	1642	G
1	w	1646	C
1	w	1647	G
1	w	1648	C
1	w	1654	A
1	w	1664	A
1	w	1669	A
1	w	1670	C
1	w	1672	C
1	w	1674	G
1	w	1682	G
1	w	1688	U
1	w	1693	U
1	w	1694	C
1	w	1699	G
1	w	1700	A
1	w	1703	G
1	w	1707	G
1	w	1717	G
1	w	1718	G

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Mol	Chain	Res	Type
1	w	1731	G
1	w	1733	G
1	w	1742	C
1	w	1743	G
1	w	1747	G
1	w	1748	G
1	w	1754	C
1	w	1756	G
1	w	1758	G
1	w	1759	A
1	w	1763	G
1	w	1764	G
1	w	1773	A
1	w	1777	U
1	w	1780	A
1	w	1781	C
1	w	1782	C
1	w	1785	A
1	w	1787	A
1	w	1792	G
1	w	1800	C
1	w	1801	G
1	w	1802	A
1	w	1806	C
1	w	1810	A
1	w	1815	A
1	w	1816	G
1	w	1817	G
1	w	1818	U
1	w	1819	A
1	w	1820	U
1	w	1821	A
1	w	1823	G
1	w	1824	G
1	w	1825	A
1	w	1829	A
1	w	1836	C
1	w	1838	C
1	w	1839	G
1	w	1843	C
1	w	1847	A
1	w	1858	G

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Mol	Chain	Res	Type
1	w	1859	A
1	w	1863	G
1	w	1864	U
1	w	1869	G
1	w	1878	G
1	w	1879	C
1	w	1885	A
1	w	1886	C
1	w	1888	G
1	w	1889	A
1	w	1900	A
1	w	1903	G
1	w	1906	G
1	w	1912	A
1	w	1913	A
1	w	1914	C
1	w	1915	U
1	w	1916	A
1	w	1929	G
1	w	1930	G
1	w	1935	G
1	w	1936	A
1	w	1937	A
1	w	1938	A
1	w	1939	U
1	w	1944	U
1	w	1955	U
1	w	1956	U
1	w	1960	A
1	w	1963	U
1	w	1964	G
1	w	1965	C
1	w	1966	A
1	w	1967	C
1	w	1968	G
1	w	1969	A
1	w	1971	A
1	w	1972	A
1	w	1982	C
1	w	1987	G
1	w	1991	U
1	w	1992	G

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Mol	Chain	Res	Type
1	w	1993	U
1	w	1997	G
1	w	1998	G
1	w	2001	A
1	w	2010	G
1	w	2013	A
1	w	2014	A
1	w	2020	A
1	w	2023	G
1	w	2026	C
1	w	2031	A
1	w	2033	A
1	w	2035	G
1	w	2040	C
1	w	2041	U
1	w	2043	C
1	w	2050	C
1	w	2051	A
1	w	2052	G
1	w	2055	C
1	w	2056	G
1	w	2057	A
1	w	2059	A
1	w	2060	A
1	w	2061	G
1	w	2062	A
1	w	2063	C
1	w	2066	C
1	w	2067	G
1	w	2068	U
1	w	2069	G
1	w	2076	U
1	w	2077	A
1	w	2080	G
1	w	2087	G
1	w	2092	U
1	w	2093	G
1	w	2096	U
1	w	2099	U
1	w	2100	G
1	w	2110	G
1	w	2111	C

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Mol	Chain	Res	Type
1	w	2112	G
1	w	2116	G
1	w	2118	U
1	w	2119	A
1	w	2120	G
1	w	2122	U
1	w	2124	G
1	w	2126	A
1	w	2127	G
1	w	2128	C
1	w	2129	C
1	w	2130	U
1	w	2131	G
1	w	2132	U
1	w	2133	G
1	w	2136	C
1	w	2138	C
1	w	2157	G
1	w	2158	A
1	w	2160	G
1	w	2169	A
1	w	2171	A
1	w	2172	U
1	w	2173	A
1	w	2174	C
1	w	2176	A
1	w	2177	C
1	w	2179	C
1	w	2181	G
1	w	2188	C
1	w	2190	G
1	w	2191	G
1	w	2192	G
1	w	2194	G
1	w	2195	C
1	w	2205	C
1	w	2211	G
1	w	2213	U
1	w	2215	G
1	w	2217	G
1	w	2225	A
1	w	2226	C

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Mol	Chain	Res	Type
1	w	2238	G
1	w	2239	G
1	w	2243	U
1	w	2251	G
1	w	2257	U
1	w	2264	C
1	w	2269	A
1	w	2275	C
1	w	2276	G
1	w	2283	C
1	w	2287	A
1	w	2288	A
1	w	2290	G
1	w	2294	C
1	w	2297	C
1	w	2304	G
1	w	2305	A
1	w	2307	G
1	w	2308	G
1	w	2309	A
1	w	2310	A
1	w	2319	G
1	w	2320	A
1	w	2321	G
1	w	2323	G
1	w	2325	G
1	w	2327	A
1	w	2333	A
1	w	2334	G
1	w	2336	A
1	w	2344	U
1	w	2345	G
1	w	2346	A
1	w	2347	C
1	w	2350	C
1	w	2354	G
1	w	2356	C
1	w	2361	A
1	w	2365	G
1	w	2368	C
1	w	2376	A
1	w	2377	A

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Mol	Chain	Res	Type
1	w	2379	G
1	w	2382	G
1	w	2383	G
1	w	2385	C
1	w	2388	A
1	w	2391	G
1	w	2394	C
1	w	2398	U
1	w	2399	G
1	w	2400	G
1	w	2402	C
1	w	2406	U
1	w	2407	G
1	w	2422	A
1	w	2423	U
1	w	2425	A
1	w	2427	C
1	w	2428	G
1	w	2429	G
1	w	2430	A
1	w	2431	U
1	w	2432	A
1	w	2434	A
1	w	2435	A
1	w	2439	A
1	w	2441	C
1	w	2442	C
1	w	2447	G
1	w	2448	A
1	w	2449	U
1	w	2450	A
1	w	2452	C
1	w	2455	G
1	w	2469	A
1	w	2472	G
1	w	2478	A
1	w	2480	C
1	w	2483	C
1	w	2484	G
1	w	2487	G
1	w	2491	U
1	w	2498	C

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Mol	Chain	Res	Type
1	w	2501	C
1	w	2502	G
1	w	2503	A
1	w	2504	U
1	w	2505	G
1	w	2506	U
1	w	2513	G
1	w	2514	U
1	w	2515	C
1	w	2516	G
1	w	2518	A
1	w	2519	U
1	w	2523	G
1	w	2529	G
1	w	2542	A
1	w	2543	G
1	w	2549	G
1	w	2551	C
1	w	2554	U
1	w	2555	U
1	w	2560	C
1	w	2563	U
1	w	2566	A
1	w	2567	G
1	w	2569	G
1	w	2572	A
1	w	2573	C
1	w	2574	G
1	w	2576	G
1	w	2578	G
1	w	2581	G
1	w	2582	G
1	w	2584	U
1	w	2588	G
1	w	2589	A
1	w	2590	A
1	w	2602	A
1	w	2606	C
1	w	2609	U
1	w	2611	U
1	w	2612	C
1	w	2615	U

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Mol	Chain	Res	Type
1	w	2616	C
1	w	2618	G
1	w	2619	C
1	w	2621	A
1	w	2622	C
1	w	2628	C
1	w	2629	A
1	w	2630	G
1	w	2635	C
1	w	2637	U
1	w	2639	A
1	w	2642	G
1	w	2643	G
1	w	2645	G
1	w	2646	C
1	w	2647	U
1	w	2653	U
1	w	2654	A
1	w	2655	G
1	w	2656	U
1	w	2658	C
1	w	2665	A
1	w	2674	G
1	w	2681	C
1	w	2682	U
1	w	2691	C
1	w	2694	G
1	w	2695	C
1	w	2702	U
1	w	2712	U
1	w	2712(B)	A
1	w	2713	A
1	w	2714	G
1	w	2718	G
1	w	2719	G
1	w	2720	U
1	w	2721	A
1	w	2722	G
1	w	2735	G
1	w	2739	U
1	w	2744	G
1	w	2746	U

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Mol	Chain	Res	Type
1	w	2747	G
1	w	2750	A
1	w	2752	C
1	w	2754	U
1	w	2755	C
1	w	2757	A
1	w	2758	A
1	w	2759	G
1	w	2762	G
1	w	2763	G
1	w	2765	A
1	w	2766	G
1	w	2768	C
1	w	2772	C
1	w	2775	A
1	w	2778	A
1	w	2779	U
1	w	2781	A
1	w	2785	C
1	w	2791	C
1	w	2792	G
1	w	2795	G
1	w	2797	U
1	w	2798	C
1	w	2799	A
1	w	2802	G
1	w	2804	C
1	w	2807	G
1	w	2808	U
1	w	2809	A
1	w	2820	A
1	w	2827	C
1	w	2830	G
1	w	2833	G
1	w	2834	G
1	w	2835	A
1	w	2836	U
1	w	2844	G
1	w	2845	G
1	w	2849	U
1	w	2858	C
1	w	2865	U

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Mol	Chain	Res	Type
1	w	2866	U
1	w	2867	G
1	w	2868	A
1	w	2872	G
1	w	2873	A
1	w	2875	C
1	w	2876	G
1	w	2880	C
1	w	2883	A
1	w	2884	U
1	w	2887	U
1	w	2889	C
1	w	2892	A
1	w	2895	U
1	w	2896	C
1	w	2901	C
2	x	5	C
2	x	8	U
2	x	9	G
2	x	10	C
2	x	11	C
2	x	13	A
2	x	14	U
2	x	15	A
2	x	16	G
2	x	20	C
2	x	21	G
2	x	25	A
2	x	26	A
2	x	27	C
2	x	29	A
2	x	33	G
2	x	35	U
2	x	39	A
2	x	40	U
2	x	42	C
2	x	43	C
2	x	45	A
2	x	49	C
2	x	50	G
2	x	52	A
2	x	53	A

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Mol	Chain	Res	Type
2	x	54	G
2	x	57	A
2	x	64	C
2	x	66	A
2	x	67	G
2	x	69	G
2	x	74	U
2	x	75	G
2	x	76	G
2	x	79	C
2	x	87	G
2	x	90	C
2	x	98	G
2	x	103	U
2	x	107	U
2	x	108	C
2	x	109	G
2	x	113	C
2	x	114	G
2	x	117	G
2	x	118	G
31	y	6	G
31	y	8	A
31	y	9	G
31	y	13	U
31	y	14	U
31	y	15	G
31	y	21	G
31	y	31	G
31	y	32	A
31	y	37	U
31	y	38	G
31	y	39	G
31	y	44	G
31	y	47	C
31	y	48	C
31	y	50	A
31	y	51	A
31	y	56	U
31	y	61	G
31	y	62	U
31	y	65	U

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Mol	Chain	Res	Type
31	y	69	G
31	y	82	U
31	y	93	U
31	y	95	G
31	y	97	U
31	y	99	C
31	y	104	G
31	y	105	G
31	y	110	C
31	y	112	G
31	y	115	G
31	y	116	A
31	y	120	A
31	y	121	C
31	y	122	G
31	y	129(B)	G
31	y	130	A
31	y	131	C
31	y	133	U
31	y	134	A
31	y	136	C
31	y	139	G
31	y	141	A
31	y	143	A
31	y	145	G
31	y	149	A
31	y	152	A
31	y	157	G
31	y	161	A
31	y	162	A
31	y	163	C
31	y	174	C
31	y	179	A
31	y	189	U
31	y	191(A)	G
31	y	195	A
31	y	196	A
31	y	197	A
31	y	198	G
31	y	208	U
31	y	209	U
31	y	210	U

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Mol	Chain	Res	Type
31	y	216	G
31	y	219	C
31	y	223	U
31	y	234	C
31	y	238	G
31	y	244	U
31	y	247	G
31	y	251	G
31	y	252	U
31	y	253	U
31	y	255	G
31	y	258	G
31	y	259	G
31	y	263	A
31	y	266	G
31	y	267	C
31	y	270	A
31	y	279	A
31	y	280	C
31	y	281	G
31	y	289	G
31	y	295	C
31	y	299	G
31	y	300	A
31	y	312	C
31	y	321	A
31	y	322	C
31	y	327	A
31	y	328	C
31	y	329	A
31	y	330	C
31	y	332	G
31	y	344	A
31	y	345	C
31	y	347	G
31	y	351	G
31	y	352	C
31	y	353	A
31	y	354	G
31	y	357	G
31	y	360	A
31	y	361	G

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Mol	Chain	Res	Type
31	y	363	A
31	y	365	U
31	y	366	C
31	y	368	U
31	y	369	C
31	y	372	C
31	y	373	A
31	y	375	U
31	y	377	G
31	y	378	G
31	y	379	C
31	y	382	A
31	y	388	G
31	y	391	G
31	y	392	G
31	y	395	C
31	y	397	A
31	y	398	C
31	y	406	G
31	y	409	G
31	y	410	G
31	y	412	A
31	y	413	G
31	y	414	A
31	y	421	U
31	y	422	C
31	y	423	G
31	y	428	G
31	y	429	U
31	y	430	A
31	y	436	C
31	y	439	A
31	y	440	A
31	y	445	G
31	y	449	C
31	y	452	A
31	y	466	G
31	y	467	G
31	y	480	U
31	y	484	G
31	y	485	G
31	y	488	C

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Mol	Chain	Res	Type
31	y	491	G
31	y	493	G
31	y	496	A
31	y	497	U
31	y	498	A
31	y	500	G
31	y	506	G
31	y	508	C
31	y	509	A
31	y	511	C
31	y	512	U
31	y	513	C
31	y	516	PSU
31	y	517	G
31	y	518	C
31	y	519	C
31	y	521	G
31	y	523	A
31	y	524	G
31	y	525	C
31	y	527	7MG
31	y	529	G
31	y	531	U
31	y	532	A
31	y	533	A
31	y	543	C
31	y	547	A
31	y	549	C
31	y	552	U
31	y	556	C
31	y	557	G
31	y	560	U
31	y	561	U
31	y	562	C
31	y	563	A
31	y	565	U
31	y	566	G
31	y	570	G
31	y	572	A
31	y	573	A
31	y	575	G
31	y	576	G

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Mol	Chain	Res	Type
31	y	577	G
31	y	585	G
31	y	588	G
31	y	611	A
31	y	616	G
31	y	617	G
31	y	619	U
31	y	623	C
31	y	627	G
31	y	630	G
31	y	631	G
31	y	633	G
31	y	641	U
31	y	643	C
31	y	650	G
31	y	652	U
31	y	653	A
31	y	661	G
31	y	672	U
31	y	673	G
31	y	678	U
31	y	687	A
31	y	688	G
31	y	689	C
31	y	693	G
31	y	697	U
31	y	701	C
31	y	702	A
31	y	703	G
31	y	704	A
31	y	705	U
31	y	718	G
31	y	724	G
31	y	725	G
31	y	733	A
31	y	741	G
31	y	747	C
31	y	748	C
31	y	749	C
31	y	750	G
31	y	752	G
31	y	753	A

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Mol	Chain	Res	Type
31	y	755	G
31	y	759	A
31	y	770	C
31	y	771	G
31	y	772	U
31	y	777	A
31	y	781	A
31	y	792	A
31	y	794	A
31	y	796	C
31	y	800	G
31	y	801	U
31	y	809	G
31	y	813	U
31	y	814	A
31	y	815	A
31	y	816	A
31	y	817	C
31	y	818	G
31	y	820	U
31	y	828	A
31	y	833	U
31	y	841	U
31	y	842	C
31	y	843	U
31	y	848	C
31	y	852	G
31	y	863	U
31	y	870	U
31	y	871	U
31	y	872	A
31	y	873	A
31	y	874	G
31	y	876	G
31	y	885	G
31	y	889	A
31	y	890	G
31	y	900	A
31	y	902	G
31	y	905	U
31	y	910	C
31	y	913	A

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Mol	Chain	Res	Type
31	y	914	A
31	y	916	G
31	y	926	G
31	y	927	G
31	y	928	G
31	y	934	C
31	y	936	C
31	y	939	G
31	y	942	G
31	y	947	G
31	y	948	C
31	y	956	U
31	y	958	A
31	y	960	U
31	y	961	U
31	y	964	A
31	y	965	A
31	y	966	M2G
31	y	967	5MC
31	y	968	A
31	y	969	A
31	y	972	C
31	y	974	A
31	y	975	A
31	y	976	G
31	y	977	A
31	y	978	A
31	y	982	U
31	y	983	A
31	y	991	U
31	y	992	U
31	y	993	G
31	y	995	C
31	y	998(A)	G
31	y	1002	G
31	y	1004	A
31	y	1005	A
31	y	1013	G
31	y	1014	A
31	y	1016	A
31	y	1020	U
31	y	1024	G

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Mol	Chain	Res	Type
31	y	1025	U
31	y	1026	G
31	y	1027	C
31	y	102(A)	C
31	y	102(C)	C
31	y	1029	G
31	y	1030	C
31	y	1042	G
31	y	1050	G
31	y	1053	G
31	y	1054	C
31	y	1055	A
31	y	1062	U
31	y	1064	G
31	y	1065	U
31	y	1066	C
31	y	1068	G
31	y	1070	U
31	y	1078	U
31	y	1079	G
31	y	1080	A
31	y	1081	G
31	y	1085	U
31	y	1086	U
31	y	1089	G
31	y	1090	U
31	y	1094	G
31	y	1095	U
31	y	1101	A
31	y	1102	A
31	y	1104	G
31	y	1108	G
31	y	1109	C
31	y	1114	C
31	y	1118	C
31	y	1126	U
31	y	1127	G
31	y	1130	A
31	y	1136	U
31	y	1137	C
31	y	1139	G
31	y	1140	C

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Mol	Chain	Res	Type
31	y	1142	G
31	y	1143	G
31	y	1144	G
31	y	1146	A
31	y	1152	A
31	y	1154	G
31	y	1157	A
31	y	1158	C
31	y	1159	U
31	y	1162	C
31	y	1167	A
31	y	1175	G
31	y	1176	A
31	y	1178	G
31	y	1179	A
31	y	1184	G
31	y	1188	A
31	y	1190	G
31	y	1196	U
31	y	1197	G
31	y	1198	G
31	y	1200	C
31	y	1202	G
31	y	1203	C
31	y	1207	2MG
31	y	1208	C
31	y	1209	C
31	y	1211	U
31	y	1212	U
31	y	1213	A
31	y	1215	G
31	y	1221	G
31	y	1225	A
31	y	1226	C
31	y	1227	A
31	y	1233	G
31	y	1235	U
31	y	1237	C
31	y	1238	A
31	y	1239	A
31	y	1240	U
31	y	1241	G

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Mol	Chain	Res	Type
31	y	1243	C
31	y	1247	U
31	y	1248	A
31	y	1251	A
31	y	1253	G
31	y	1256	A
31	y	1257	U
31	y	1261	A
31	y	1263	C
31	y	1267	C
31	y	1269	A
31	y	1270	C
31	y	1278	U
31	y	1280	A
31	y	1282	C
31	y	1283	G
31	y	1285	A
31	y	1286	A
31	y	1290	G
31	y	1291	G
31	y	1294	G
31	y	1297	C
31	y	1298	C
31	y	1299	A
31	y	1300	G
31	y	1301	U
31	y	1302	U
31	y	1303	C
31	y	1306	A
31	y	1308	U
31	y	1309	G
31	y	1319	A
31	y	1320	C
31	y	1323	G
31	y	1324	A
31	y	1325	C
31	y	1331	G
31	y	1333	A
31	y	1335	C
31	y	1340	A
31	y	1345	U
31	y	1346	A

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Mol	Chain	Res	Type
31	y	1347	G
31	y	1348	U
31	y	1354	C
31	y	1359	C
31	y	1360	A
31	y	1361	G
31	y	136(B)	C
31	y	1363	A
31	y	1364	U
31	y	1365	G
31	y	1366	C
31	y	1369	C
31	y	1378	C
31	y	1380	U
31	y	1381	U
31	y	1388	C
31	y	1394	A
31	y	1396	A
31	y	1397	C
31	y	1398	A
31	y	1400	5MC
31	y	1401	G
31	y	1402	C
31	y	1404	5MC
31	y	1405	G
31	y	1407	5MC
31	y	1408	A
31	y	1420	C
31	y	1426	C
31	y	1434	A
31	y	1442	G
31	y	1443	G
31	y	1446	A
31	y	1447	G
31	y	1451	A
31	y	1452	C
31	y	1454	G
31	y	1468	A
31	y	1471	G
31	y	1472	U
31	y	1475	G
31	y	1482	G

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Mol	Chain	Res	Type
31	y	1490	C
31	y	1491	G
31	y	1492	A
31	y	1494	G
31	y	1495	U
31	y	1498	U
31	y	1501	C
31	y	1502	A
31	y	1504	G
31	y	1505	G
31	y	1506	U
31	y	1507	A
31	y	1513	A
31	y	1517	G
31	y	1520	G
31	y	1521	G
31	y	1525	G
31	y	1527	C
31	y	1529	G
31	y	1530	G
31	y	1531	A
31	y	1532	U
31	y	1534	A
31	y	1535	C
32	z	9	G
32	z	16	C
32	z	17	C
32	z	17(A)	U
32	z	18	G
32	z	19	G
32	z	20	U
32	z	21	A
32	z	25	C
32	z	26	G
32	z	30	G
32	z	35	A
32	z	46	A
32	z	48	C
32	z	49	G
32	z	59	A
32	z	65	C
32	z	71	C

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Mol	Chain	Res	Type
32	z	73	A
32	z	76	A
33	2	8	U
33	2	9	A
33	2	10	G
33	2	14	A
33	2	15	G
33	2	16	U
33	2	17	U
33	2	18	G
33	2	20	G
33	2	21	A
33	2	22	G
33	2	35	A
33	2	36	A
33	2	40	C
33	2	47	U
33	2	48	C
33	2	55	PSU
33	2	61	C
33	2	67	A
33	2	73	A
33	2	75	C
33	2	76	A
34	3	3	G
34	3	6	G
34	3	12	A
34	3	13	A
34	3	16	A

There are no RNA pucker outliers to report.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

11 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
33	PSU	2	55	33	17,21,22	1.18	2 (11%)	20,30,33	3.58	8 (40%)
31	5MC	y	1400	31	15,22,23	1.13	2 (13%)	19,32,35	1.40	2 (10%)
31	5MC	y	1407	31	15,22,23	1.19	2 (13%)	19,32,35	1.48	2 (10%)
31	2MG	y	1207	31	19,26,27	2.32	5 (26%)	21,38,41	2.82	6 (28%)
31	5MC	y	967	31	15,22,23	1.04	1 (6%)	19,32,35	1.47	2 (10%)
31	PSU	y	516	31	17,21,22	1.29	2 (11%)	20,30,33	3.57	6 (30%)
31	MA6	y	1518	31	19,26,27	1.79	2 (10%)	18,38,41	2.21	6 (33%)
31	7MG	y	527	31	22,26,27	2.18	5 (22%)	28,39,42	2.46	6 (21%)
31	MA6	y	1519	31	19,26,27	2.21	4 (21%)	18,38,41	1.89	5 (27%)
31	5MC	y	1404	31	15,22,23	1.37	2 (13%)	19,32,35	1.48	2 (10%)
31	M2G	y	966	31	20,27,28	2.35	4 (20%)	22,40,43	2.89	7 (31%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	PSU	2	55	33	-	1/7/25/26	0/2/2/2
31	5MC	y	1400	31	-	0/5/25/26	0/2/2/2
31	5MC	y	1407	31	-	0/5/25/26	0/2/2/2
31	2MG	y	1207	31	-	1/5/27/28	0/3/3/3
31	5MC	y	967	31	-	1/5/25/26	0/2/2/2
31	PSU	y	516	31	-	1/7/25/26	0/2/2/2
31	MA6	y	1518	31	-	2/7/29/30	0/3/3/3
31	7MG	y	527	31	-	0/7/37/38	0/3/3/3
31	MA6	y	1519	31	-	3/7/29/30	0/3/3/3
31	5MC	y	1404	31	-	1/5/25/26	0/2/2/2
31	M2G	y	966	31	-	2/7/29/30	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	1207	2MG	C6-N1	6.99	1.45	1.33
31	y	966	M2G	C6-N1	6.48	1.44	1.33
31	y	527	7MG	C6-N1	6.28	1.44	1.33
31	y	1518	MA6	C6-N1	5.46	1.41	1.33
31	y	1519	MA6	O4'-C1'	5.27	1.48	1.41
31	y	966	M2G	C2-N1	5.24	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	1519	MA6	C6-N1	5.10	1.40	1.33
31	y	527	7MG	C6-C5	4.64	1.47	1.41
31	y	966	M2G	C6-C5	4.14	1.48	1.41
31	y	1519	MA6	C10-N6	4.05	1.55	1.45
31	y	1207	2MG	C2-N2	3.84	1.37	1.34
31	y	527	7MG	C2-N1	3.81	1.42	1.35
33	2	55	PSU	C5-C1'	-3.43	1.49	1.52
31	y	527	7MG	C8-N9	-3.35	1.37	1.45
31	y	1207	2MG	C6-C5	3.34	1.47	1.41
31	y	527	7MG	C4-N3	3.10	1.38	1.34
31	y	1404	5MC	O4'-C1'	3.04	1.45	1.41
31	y	516	PSU	C4-N3	2.90	1.38	1.33
31	y	1519	MA6	C9-N6	2.89	1.52	1.45
31	y	1407	5MC	O4'-C1'	2.78	1.45	1.41
31	y	1207	2MG	C2-N1	2.77	1.43	1.34
31	y	516	PSU	C2'-C1'	2.70	1.57	1.54
31	y	1404	5MC	C4-N4	2.66	1.40	1.34
31	y	1207	2MG	CM2-N2	2.63	1.49	1.45
31	y	1407	5MC	C4-N4	2.63	1.40	1.34
31	y	1400	5MC	C4-N4	2.58	1.40	1.34
31	y	966	M2G	C2-N2	2.42	1.38	1.34
31	y	967	5MC	C4-N4	2.36	1.40	1.34
33	2	55	PSU	C4-N3	2.31	1.37	1.33
31	y	1400	5MC	O4'-C1'	2.26	1.44	1.41
31	y	1518	MA6	C2-N3	2.07	1.35	1.32

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	516	PSU	N1-C2-N3	-10.69	119.93	128.43
33	2	55	PSU	N1-C2-N3	-9.91	120.55	128.43
31	y	1207	2MG	C5-C6-N1	-8.76	111.45	123.43
31	y	966	M2G	C5-C6-N1	-8.60	111.67	123.43
33	2	55	PSU	C5-C1'-C2'	-7.21	102.45	115.32
31	y	516	PSU	C4-N3-C2	6.86	120.94	115.14
31	y	516	PSU	C4'-O4'-C1'	-6.73	101.13	109.42
31	y	966	M2G	C6-N1-C2	6.48	123.90	116.18
31	y	527	7MG	N7-C8-N9	6.33	112.42	103.38
31	y	1518	MA6	N1-C6-N6	6.21	123.59	117.06
31	y	527	7MG	C6-C5-C4	6.16	121.82	115.20
33	2	55	PSU	C4-N3-C2	5.98	120.19	115.14
31	y	527	7MG	C5-C6-N1	-5.90	111.01	123.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	1207	2MG	CM2-N2-C2	-5.80	116.59	123.59
31	y	527	7MG	C6-N1-C2	4.90	123.72	115.93
31	y	1207	2MG	C6-N1-C2	4.80	123.78	115.18
33	2	55	PSU	C5-C4-N3	-4.56	119.49	125.36
31	y	966	M2G	CM1-N2-C2	-4.50	117.00	121.29
31	y	1400	5MC	C2-N3-C4	4.44	121.38	116.02
31	y	1519	MA6	C3'-C2'-C1'	4.19	107.28	100.98
31	y	516	PSU	C5-C4-N3	-4.17	119.99	125.36
31	y	1404	5MC	C2-N3-C4	4.13	121.01	116.02
31	y	1407	5MC	C2-N3-C4	4.06	120.92	116.02
31	y	1519	MA6	N1-C6-N6	4.01	121.28	117.06
31	y	1518	MA6	C3'-C2'-C1'	3.94	106.91	100.98
31	y	967	5MC	C2-N3-C4	3.72	120.51	116.02
31	y	967	5MC	C3'-C2'-C1'	3.64	106.45	100.98
33	2	55	PSU	C5-C6-N1	-3.59	120.03	124.44
31	y	1519	MA6	N3-C2-N1	-3.32	123.50	128.68
31	y	1407	5MC	C3'-C2'-C1'	3.25	105.87	100.98
31	y	966	M2G	C3'-C2'-C1'	3.24	105.86	100.98
33	2	55	PSU	C3'-C2'-C1'	3.23	105.65	101.93
31	y	1518	MA6	N3-C2-N1	-2.95	124.06	128.68
31	y	966	M2G	CM2-N2-C2	-2.91	118.52	121.29
31	y	966	M2G	N3-C2-N2	2.89	120.12	117.18
33	2	55	PSU	O4'-C1'-C5	2.83	114.32	109.93
31	y	1519	MA6	C2'-C3'-C4'	2.82	108.11	102.64
31	y	1207	2MG	N2-C2-N3	2.70	119.55	116.96
33	2	55	PSU	C6-N1-C2	2.68	119.78	115.36
31	y	1207	2MG	N3-C2-N1	-2.67	122.00	126.23
31	y	966	M2G	O3'-C3'-C2'	2.66	120.44	111.82
31	y	1518	MA6	O4'-C4'-C5'	2.63	118.04	109.37
31	y	516	PSU	C6-N1-C2	2.62	119.68	115.36
31	y	516	PSU	C5-C6-N1	-2.52	121.34	124.44
31	y	1207	2MG	O4'-C1'-C2'	-2.47	103.31	106.93
31	y	1404	5MC	C3'-C2'-C1'	2.46	104.69	100.98
31	y	527	7MG	C4'-O4'-C1'	-2.32	104.36	109.47
31	y	1519	MA6	C10-N6-C9	2.23	123.31	116.12
31	y	1518	MA6	C1'-N9-C4	2.12	130.36	126.64
31	y	1400	5MC	O3'-C3'-C4'	2.11	117.16	111.05
31	y	527	7MG	N2-C2-N3	2.08	120.49	117.25
31	y	1518	MA6	O4'-C4'-C3'	2.06	109.19	105.11

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	y	967	5MC	O4'-C1'-N1-C6
31	y	1518	MA6	O4'-C4'-C5'-O5'
31	y	1518	MA6	C3'-C4'-C5'-O5'
31	y	1519	MA6	C5-C6-N6-C9
31	y	1404	5MC	C2'-C1'-N1-C6
31	y	1519	MA6	C5-C6-N6-C10
33	2	55	PSU	O4'-C1'-C5-C4
31	y	966	M2G	N1-C2-N2-CM1
31	y	1519	MA6	N1-C6-N6-C9
31	y	1207	2MG	O4'-C4'-C5'-O5'
31	y	966	M2G	N3-C2-N2-CM1
31	y	516	PSU	C2'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	w	35
31	y	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	41:C	O3'	43:G	P	2.13

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	1506:C	O3'	1508:A	P	2.09
1	w	489:G	O3'	491:G	P	2.08
1	w	1448(B):A	O3'	1449:G	P	2.07
1	w	436:C	O3'	438:G	P	2.05
1	w	554:U	O3'	556:G	P	2.05
1	w	1712:C	O3'	1716:U	P	2.04
1	w	1743:G	O3'	1746:G	P	2.04
1	w	366(B):C	O3'	370:G	P	2.03
1	w	890:A	O3'	892:G	P	2.03
1	w	2213:U	O3'	2215:G	P	2.03
1	w	2712(B):A	O3'	2713:A	P	2.03
1	w	155:C	O3'	161:U	P	2.02
1	w	926:A	O3'	928:G	P	2.02
1	w	99:U	O3'	101:G	P	2.01
1	w	1583:A	O3'	1585:C	P	2.01
1	w	1718:G	O3'	1725:G	P	2.01
1	w	1451:C	O3'	1453:A	P	1.99
1	w	1481:U	O3'	1483:G	P	1.99
1	w	1735:U	O3'	1741:C	P	1.99
1	w	537:C	O3'	539:G	P	1.98
1	w	1171:G	O3'	1173:G	P	1.97
1	w	1864:U	O3'	1869:G	P	1.97
1	w	1546(B):C	O3'	1547:C	P	1.96
1	w	1630(B):C	O3'	1631:A	P	1.96
1	w	1142(B):A	O3'	1143:A	P	1.95
1	w	1872:A	O3'	1878:G	P	1.95
1	w	2219:G	O3'	2224:G	P	1.95
1	w	165:U	O3'	171:G	P	1.94
1	w	1221(A):C	O3'	1222:C	P	1.94
1	w	1444(B):A	O3'	1445:C	P	1.93
1	w	1133:U	O3'	1135:C	P	1.91
1	y	201:C	O3'	208:U	P	1.89
1	w	2199:A	O3'	2205:C	P	1.87
1	y	97:U	O3'	99:C	P	1.83
1	w	2799:A	O3'	2801:A	P	1.81
1	w	2795:G	O3'	2797:U	P	1.79
1	y	99:C	O3'	101:A	P	1.79
1	y	103(C):G	O3'	1033:G	P	1.79
1	y	1455:G	O3'	1459:C	P	1.78
1	y	843:U	O3'	848:C	P	1.77
1	y	458:C	O3'	464:G	P	1.76
1	y	102(C):C	O3'	1029:G	P	1.76

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	136(B):C	O3'	1363:A	P	1.76

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	w	2889/2889 (100%)	0.03	107 (3%) 41 33	1, 1, 1, 1	0
2	x	120/120 (100%)	-0.22	0 100 100	1, 1, 1, 1	0
3	A	127/229 (55%)	-0.37	6 (4%) 31 26	1, 1, 1, 1	0
4	B	272/276 (98%)	-0.14	19 (6%) 16 12	1, 1, 1, 1	0
5	C	201/206 (97%)	-0.13	12 (5%) 21 17	1, 1, 1, 1	0
6	D	194/205 (94%)	-0.64	0 100 100	1, 1, 1, 1	0
7	E	180/182 (98%)	-0.30	8 (4%) 34 29	1, 1, 1, 1	0
8	F	173/180 (96%)	-0.46	8 (4%) 32 27	1, 1, 1, 1	0
9	G	148/148 (100%)	-0.21	8 (5%) 25 21	1, 1, 1, 1	0
10	H	138/140 (98%)	-0.43	2 (1%) 75 67	1, 1, 1, 1	0
11	I	122/122 (100%)	-0.17	8 (6%) 18 13	1, 1, 1, 1	0
12	J	146/150 (97%)	-0.51	3 (2%) 63 55	1, 1, 1, 1	0
13	K	137/141 (97%)	-0.08	11 (8%) 12 10	1, 1, 1, 1	0
14	L	118/118 (100%)	-0.24	6 (5%) 28 24	1, 1, 1, 1	0
15	M	106/112 (94%)	-0.16	5 (4%) 31 26	1, 1, 1, 1	0
16	N	137/146 (93%)	-0.24	3 (2%) 62 53	1, 1, 1, 1	0
17	O	117/118 (99%)	-0.40	4 (3%) 45 37	1, 1, 1, 1	0
18	P	101/101 (100%)	0.17	15 (14%) 2 2	1, 1, 1, 1	0
19	Q	109/113 (96%)	0.43	17 (15%) 2 2	1, 1, 1, 1	0
20	R	92/96 (95%)	-0.49	1 (1%) 80 74	1, 1, 1, 1	0
21	S	103/110 (93%)	0.56	22 (21%) 0 1	1, 1, 1, 1	0
22	T	185/206 (89%)	-0.41	5 (2%) 54 45	1, 1, 1, 1	0
23	U	76/85 (89%)	-0.41	1 (1%) 77 70	1, 1, 1, 1	0
24	V	88/98 (89%)	-0.30	2 (2%) 60 52	1, 1, 1, 1	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	W	62/72 (86%)	-0.12	2 (3%) 47 38	1, 1, 1, 1	0
26	X	60/60 (100%)	-0.14	1 (1%) 70 62	1, 1, 1, 1	0
27	Y	56/60 (93%)	-0.72	0 100 100	1, 1, 1, 1	0
28	Z	48/49 (97%)	-0.69	0 100 100	1, 1, 1, 1	0
29	a	63/65 (96%)	-0.07	5 (7%) 12 10	1, 1, 1, 1	0
30	b	35/37 (94%)	0.97	11 (31%) 0 0	1, 1, 1, 1	0
31	y	1504/1522 (98%)	0.04	62 (4%) 37 31	1, 1, 1, 1	0
32	z	77/77 (100%)	0.23	4 (5%) 27 23	1, 1, 1, 1	0
33	2	75/76 (98%)	0.63	7 (9%) 8 7	1, 1, 1, 1	0
34	3	18/18 (100%)	1.14	6 (33%) 0 0	1, 1, 1, 1	0
35	c	234/256 (91%)	-0.28	10 (4%) 35 29	1, 1, 1, 1	0
36	d	206/239 (86%)	-0.50	7 (3%) 45 37	1, 1, 1, 1	0
37	e	208/209 (99%)	-0.40	6 (2%) 51 41	1, 1, 1, 1	0
38	f	150/162 (92%)	-0.49	7 (4%) 31 26	1, 1, 1, 1	0
39	g	101/101 (100%)	-0.56	2 (1%) 65 57	1, 1, 1, 1	0
40	h	155/156 (99%)	-0.37	5 (3%) 47 38	1, 1, 1, 1	0
41	i	138/138 (100%)	-0.04	11 (7%) 12 10	1, 1, 1, 1	0
42	j	127/128 (99%)	-0.03	12 (9%) 8 7	1, 1, 1, 1	0
43	k	98/105 (93%)	-0.32	2 (2%) 65 57	1, 1, 1, 1	0
44	l	116/129 (89%)	0.07	12 (10%) 6 6	1, 1, 1, 1	0
45	m	124/132 (93%)	-0.25	8 (6%) 18 14	1, 1, 1, 1	0
46	n	125/126 (99%)	0.14	16 (12%) 3 4	1, 1, 1, 1	0
47	o	60/61 (98%)	-0.50	2 (3%) 46 37	1, 1, 1, 1	0
48	p	88/89 (98%)	0.18	11 (12%) 3 4	1, 1, 1, 1	0
49	q	83/88 (94%)	1.02	21 (25%) 0 0	1, 1, 1, 1	0
50	r	104/105 (99%)	-0.59	0 100 100	1, 1, 1, 1	0
51	s	81/88 (92%)	-0.65	0 100 100	1, 1, 1, 1	0
52	t	80/93 (86%)	-0.11	6 (7%) 14 11	1, 1, 1, 1	0
53	u	99/106 (93%)	0.44	15 (15%) 2 2	1, 1, 1, 1	0
54	v	24/27 (88%)	-0.51	0 100 100	1, 1, 1, 1	0
All	All	10478/10865 (96%)	-0.11	524 (5%) 28 24	1, 1, 1, 1	0

All (524) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	3	7	G	9.1
31	y	145	G	8.0
41	i	52	ASP	7.4
1	w	2399	G	7.0
44	l	118	GLY	7.0
1	w	1067	A	6.7
1	w	1591	G	6.6
53	u	46	GLU	6.4
1	w	1473	G	6.4
46	n	124	PRO	6.4
41	i	57	PRO	6.3
31	y	144	G	6.2
1	w	1592	C	6.1
31	y	146	G	6.1
41	i	58	TYR	6.0
31	y	416	G	5.9
49	q	70	ALA	5.9
53	u	45	GLN	5.9
46	n	86	CYS	5.8
31	y	865	A	5.8
5	C	167	VAL	5.8
1	w	1983	C	5.7
21	S	34	LYS	5.7
1	w	2400	G	5.6
52	t	56	GLN	5.6
1	w	1679	U	5.6
1	w	1472	A	5.6
13	K	111	GLU	5.5
44	l	119	CYS	5.5
41	i	53	VAL	5.4
45	m	20	LYS	5.3
46	n	85	GLY	5.2
21	S	30	VAL	5.2
31	y	716	A	5.2
33	2	28	C	5.2
42	j	115	GLY	5.2
48	p	15	PHE	5.1
1	w	1116	C	5.1
38	f	13	ILE	5.1
42	j	123	PRO	5.0
41	i	54	ASP	5.0
18	P	87	HIS	5.0

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Mol	Chain	Res	Type	RSRZ
19	Q	85	VAL	5.0
4	B	109	ASP	5.0
42	j	116	LYS	5.0
22	T	154	ASP	4.9
46	n	126	LYS	4.9
19	Q	97	LYS	4.9
30	b	13	LYS	4.8
19	Q	83	LYS	4.8
46	n	125	ARG	4.8
1	w	518	G	4.8
1	w	2398	U	4.8
52	t	57	HIS	4.7
33	2	34	G	4.7
30	b	29	ASN	4.7
25	W	19	VAL	4.7
48	p	16	ALA	4.7
31	y	23	C	4.7
19	Q	82	LEU	4.7
19	Q	95	ILE	4.7
1	w	1460	A	4.7
8	F	166	GLY	4.6
46	n	123	ALA	4.6
1	w	1635	G	4.6
44	l	115	PRO	4.5
46	n	83	ASP	4.5
21	S	5	MET	4.5
15	M	9	ARG	4.5
1	w	989	G	4.5
21	S	29	GLU	4.5
44	l	125	PHE	4.5
31	y	866	C	4.4
42	j	75	ASP	4.4
1	w	134	C	4.4
37	e	44	GLY	4.4
44	l	117	ASN	4.4
31	y	874	G	4.4
21	S	32	PRO	4.4
18	P	57	VAL	4.3
30	b	28	GLU	4.3
46	n	89	GLY	4.3
19	Q	94	ASP	4.3
45	m	19	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
44	l	126	ARG	4.3
31	y	1079	G	4.2
1	w	1405	U	4.2
45	m	21	SER	4.2
49	q	58	TYR	4.2
41	i	51	VAL	4.2
31	y	135	C	4.2
37	e	46	LYS	4.2
33	2	33	U	4.2
18	P	56	SER	4.2
21	S	1	MET	4.2
1	w	1221	C	4.1
53	u	91	LEU	4.1
48	p	3	ILE	4.1
21	S	31	LEU	4.1
4	B	198	ASN	4.1
1	w	270(T)	G	4.1
31	y	731	G	4.0
5	C	104	VAL	4.0
4	B	199	ALA	4.0
7	E	49	ASP	4.0
17	O	14	HIS	4.0
30	b	8	LYS	4.0
1	w	1590	U	4.0
41	i	55	GLY	4.0
1	w	2493	U	3.9
22	T	155	LEU	3.9
31	y	1383	C	3.9
31	y	227	G	3.9
22	T	156	LYS	3.9
30	b	12	ASP	3.9
1	w	364	C	3.9
9	G	16	GLY	3.9
18	P	86	GLY	3.9
45	m	18	ARG	3.8
34	3	6	G	3.8
49	q	65	GLN	3.8
14	L	59	ASP	3.8
21	S	4	LYS	3.8
1	w	1098	A	3.8
19	Q	93	ALA	3.8
38	f	14	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
43	k	18	ALA	3.7
31	y	1535	C	3.7
18	P	74	LYS	3.7
1	w	1680	U	3.7
19	Q	96	ILE	3.7
31	y	715	A	3.7
11	I	9	GLU	3.7
35	c	65	GLY	3.7
31	y	287	U	3.7
31	y	1078	U	3.7
5	C	5	LEU	3.7
1	w	2461	C	3.7
1	w	2600	A	3.7
41	i	56	LYS	3.6
1	w	1808	U	3.6
35	c	157	ARG	3.6
42	j	117	HIS	3.6
49	q	66	PRO	3.6
49	q	61	SER	3.6
31	y	1267	C	3.6
1	w	1764	G	3.6
1	w	1990	C	3.6
4	B	2	ALA	3.6
33	2	29	A	3.6
53	u	47	GLY	3.6
24	V	26	ARG	3.6
13	K	91	GLU	3.6
30	b	14	CYS	3.5
23	U	16	SER	3.5
1	w	1115	G	3.5
31	y	1117	G	3.5
49	q	21	VAL	3.5
1	w	2820	A	3.5
46	n	84	ILE	3.5
1	w	2492	U	3.5
21	S	92	ASN	3.5
34	3	8	U	3.5
32	z	74	C	3.5
37	e	71	SER	3.5
13	K	110	THR	3.5
49	q	69	THR	3.5
18	P	73	SER	3.5

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Mol	Chain	Res	Type	RSRZ
46	n	79	LYS	3.5
46	n	72	ALA	3.4
13	K	32	PHE	3.4
11	I	69	VAL	3.4
13	K	131	ILE	3.4
49	q	24	ALA	3.4
31	y	611	A	3.4
1	w	2161	C	3.4
49	q	62	VAL	3.4
8	F	127	GLU	3.4
18	P	88	ARG	3.4
30	b	7	VAL	3.3
29	a	19	SER	3.3
31	y	864	A	3.3
9	G	59	ALA	3.3
1	w	133	C	3.3
36	d	38	ARG	3.3
43	k	19	SER	3.3
1	w	2274	A	3.3
31	y	134	A	3.3
31	y	1342	C	3.3
11	I	70	LYS	3.3
42	j	105	ASP	3.3
31	y	677	U	3.3
1	w	1348	G	3.3
46	n	76	ALA	3.2
40	h	8	GLU	3.2
1	w	1600	C	3.2
1	w	1099	G	3.2
9	G	63	ALA	3.2
13	K	112	GLU	3.2
35	c	67	THR	3.2
3	A	39	ASP	3.2
4	B	110	GLY	3.2
1	w	270(V)	C	3.2
13	K	80	GLU	3.2
31	y	417	C	3.2
5	C	109	LYS	3.2
21	S	3	VAL	3.2
42	j	76	ALA	3.2
14	L	60	LEU	3.2
31	y	415	A	3.2

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Mol	Chain	Res	Type	RSRZ
38	f	29	GLY	3.2
1	w	888	C	3.2
1	w	34	C	3.1
48	p	11	VAL	3.1
30	b	10	ILE	3.1
31	y	1536	C	3.1
35	c	37	ASN	3.1
49	q	36	ILE	3.1
9	G	60	GLU	3.1
49	q	19	ILE	3.1
13	K	92	GLY	3.1
44	l	121	PRO	3.1
1	w	241	A	3.1
8	F	165	ALA	3.1
1	w	1626	G	3.1
14	L	81	ASP	3.1
31	y	288	A	3.1
49	q	40	ASP	3.1
49	q	54	GLU	3.1
3	A	192	ALA	3.0
4	B	115	GLN	3.0
9	G	65	ALA	3.0
39	g	51	PRO	3.0
1	w	242	G	3.0
11	I	50	GLY	3.0
1	w	1026	U	3.0
4	B	96	HIS	3.0
42	j	13	ALA	3.0
37	e	95	GLY	3.0
48	p	4	THR	3.0
44	l	87	THR	3.0
21	S	27	VAL	3.0
21	S	26	LYS	3.0
38	f	15	ARG	3.0
48	p	80	ALA	3.0
1	w	270(U)	G	3.0
40	h	9	VAL	3.0
4	B	114	GLY	2.9
52	t	58	VAL	2.9
1	w	1369	G	2.9
38	f	12	LEU	2.9
31	y	179	A	2.9

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Mol	Chain	Res	Type	RSRZ
31	y	1252	A	2.9
13	K	78	PRO	2.9
32	z	17(A)	U	2.9
7	E	126	ASP	2.9
1	w	1761	C	2.9
53	u	51	GLU	2.9
31	y	934	C	2.9
44	l	13	GLN	2.9
49	q	37	GLY	2.9
1	w	2145	C	2.9
1	w	2459	A	2.9
19	Q	21	VAL	2.9
4	B	65	ILE	2.9
31	y	861	G	2.9
5	C	168	MET	2.9
30	b	9	ARG	2.9
11	I	10	VAL	2.9
1	w	1989	G	2.9
31	y	714	G	2.9
33	2	65	G	2.9
12	J	93	GLY	2.8
45	m	49	SER	2.8
1	w	1349	A	2.8
1	w	1404	C	2.8
1	w	1068	G	2.8
49	q	59	TRP	2.8
13	K	79	LEU	2.8
1	w	23	G	2.8
30	b	27	CYS	2.8
31	y	262	A	2.8
34	3	18	C	2.8
8	F	129	THR	2.8
8	F	61	HIS	2.8
1	w	615	G	2.8
4	B	112	GLN	2.8
1	w	1498	C	2.8
29	a	27	THR	2.8
1	w	508	G	2.7
31	y	775	G	2.7
53	u	94	ALA	2.7
3	A	176	VAL	2.7
49	q	33	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
38	f	28	PHE	2.7
37	e	45	GLN	2.7
1	w	1678	G	2.7
25	W	18	PRO	2.7
37	e	29	PRO	2.7
8	F	56	SER	2.7
36	d	93	LYS	2.7
1	w	1625	C	2.7
17	O	17	ILE	2.7
29	a	6	THR	2.7
4	B	268	ARG	2.7
22	T	153	SER	2.7
1	w	1474	C	2.7
42	j	72	GLY	2.7
42	j	114	TYR	2.7
1	w	2258	C	2.7
53	u	41	VAL	2.7
31	y	913	A	2.7
31	y	713	G	2.7
46	n	90	LEU	2.6
9	G	64	GLU	2.6
21	S	6	HIS	2.6
48	p	12	ILE	2.6
41	i	25	ASP	2.6
48	p	6	GLU	2.6
40	h	6	ARG	2.6
5	C	166	THR	2.6
7	E	127	GLY	2.6
19	Q	101	SER	2.6
14	L	3	HIS	2.6
21	S	22	GLY	2.6
42	j	122	ALA	2.6
49	q	56	ALA	2.6
9	G	2	LYS	2.6
33	2	36	A	2.6
21	S	37	VAL	2.6
31	y	250	A	2.6
31	y	653	A	2.6
52	t	59	PRO	2.6
13	K	115	MET	2.5
9	G	67	ARG	2.5
21	S	25	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
31	y	1366	C	2.5
18	P	76	LYS	2.5
1	w	2460	U	2.5
1	w	1301	A	2.5
4	B	200	ASP	2.5
26	X	14	GLY	2.5
1	w	1977	A	2.5
3	A	177	GLY	2.5
7	E	119	GLY	2.5
11	I	11	ALA	2.5
48	p	2	PRO	2.5
31	y	828	A	2.5
21	S	2	ARG	2.5
1	w	2599	G	2.5
45	m	27	LYS	2.5
1	w	1578	U	2.5
31	y	863	U	2.5
39	g	32	ASN	2.5
1	w	2248	C	2.5
35	c	66	GLY	2.5
1	w	2162	G	2.5
31	y	818	G	2.5
47	o	16	PHE	2.5
46	n	75	ALA	2.5
19	Q	84	ARG	2.5
1	w	85	G	2.5
1	w	680	G	2.5
35	c	231	GLU	2.5
18	P	95	LEU	2.5
45	m	28	GLY	2.5
1	w	2260	C	2.5
8	F	168	PRO	2.5
49	q	22	THR	2.5
17	O	16	LYS	2.5
21	S	38	ILE	2.5
1	w	2012	G	2.4
4	B	126	GLN	2.4
36	d	189	ALA	2.4
1	w	1266	G	2.4
53	u	44	ALA	2.4
1	w	2730	C	2.4
3	A	195	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
18	P	30	GLY	2.4
5	C	198	VAL	2.4
29	a	26	LYS	2.4
1	w	1807	G	2.4
41	i	50	ARG	2.4
1	w	1117	G	2.4
14	L	82	GLU	2.4
19	Q	13	SER	2.4
53	u	93	GLU	2.4
1	w	436	C	2.4
18	P	29	PRO	2.4
1	w	1097	U	2.4
36	d	192	THR	2.4
21	S	35	TYR	2.4
40	h	94	ARG	2.4
52	t	65	ASN	2.4
3	A	196	ALA	2.4
44	l	114	VAL	2.4
1	w	1496	A	2.4
32	z	17	C	2.4
16	N	66	VAL	2.3
35	c	158	LEU	2.3
47	o	11	LYS	2.3
44	l	12	ARG	2.3
4	B	3	VAL	2.3
5	C	110	GLY	2.3
21	S	90	LEU	2.3
31	y	241	C	2.3
18	P	96	ILE	2.3
42	j	67	GLY	2.3
31	y	935	A	2.3
1	w	1577	C	2.3
49	q	20	VAL	2.3
1	w	1809	A	2.3
1	w	2345	G	2.3
1	w	1417	C	2.3
17	O	13	LYS	2.3
1	w	382	G	2.3
34	3	16	A	2.3
33	2	32	C	2.3
18	P	72	VAL	2.3
1	w	1634	A	2.3

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Mol	Chain	Res	Type	RSRZ
1	w	1636	C	2.3
19	Q	74	ALA	2.3
34	3	17	C	2.3
1	w	2076	U	2.3
48	p	9	GLN	2.3
53	u	90	GLN	2.3
1	w	256	A	2.3
32	z	62	C	2.3
1	w	1593	G	2.3
7	E	50	ALA	2.3
12	J	38	GLN	2.3
21	S	33	LYS	2.3
30	b	11	CYS	2.3
1	w	240	G	2.3
1	w	1692	U	2.3
22	T	63	ASP	2.3
48	p	14	GLU	2.3
53	u	42	GLN	2.3
16	N	67	SER	2.3
20	R	65	ARG	2.3
1	w	1488	G	2.2
31	y	867	G	2.2
36	d	45	LYS	2.2
35	c	131	PRO	2.2
40	h	93	PRO	2.2
31	y	180	U	2.2
7	E	165	THR	2.2
10	H	42	GLU	2.2
19	Q	81	ALA	2.2
1	w	887	A	2.2
31	y	136	C	2.2
52	t	55	LYS	2.2
4	B	34	VAL	2.2
31	y	610	G	2.2
31	y	1187	G	2.2
5	C	197	ILE	2.2
31	y	78	G	2.2
36	d	41	GLY	2.2
1	w	1599	C	2.2
31	y	89	U	2.2
53	u	15	ARG	2.2
38	f	85	GLY	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
11	I	12	ASP	2.2
1	w	1368	G	2.2
1	w	2897	U	2.2
14	L	30	THR	2.1
31	y	676	A	2.1
31	y	79	G	2.1
31	y	1186	G	2.1
31	y	531	U	2.1
1	w	1665	A	2.1
10	H	99	SER	2.1
18	P	65	GLY	2.1
21	S	93	GLY	2.1
4	B	80	ALA	2.1
44	l	124	LYS	2.1
8	F	167	GLU	2.1
35	c	129	GLU	2.1
15	M	29	PHE	2.1
1	w	521	G	2.1
7	E	47	LYS	2.1
46	n	36	LYS	2.1
46	n	122	LYS	2.1
19	Q	44	ALA	2.1
19	Q	86	LEU	2.1
4	B	45	ASN	2.1
4	B	108	PRO	2.1
53	u	49	ALA	2.1
36	d	39	ILE	2.1
31	y	88	C	2.1
45	m	26	LEU	2.1
49	q	1	MET	2.1
41	i	90	GLY	2.1
7	E	51	ARG	2.1
49	q	23	ASP	2.1
31	y	776	G	2.1
1	w	1095	A	2.1
1	w	2755	C	2.1
31	y	240	C	2.1
35	c	240	GLN	2.1
31	y	1166	G	2.1
19	Q	14	PRO	2.1
31	y	136(A)	C	2.1
15	M	83	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
24	V	59	THR	2.0
4	B	95	LEU	2.0
5	C	199	ARG	2.0
53	u	48	LYS	2.0
1	w	1500	G	2.0
1	w	1666	G	2.0
1	w	1763	G	2.0
1	w	2731	G	2.0
5	C	114	ALA	2.0
15	M	37	ALA	2.0
16	N	70	VAL	2.0
12	J	37	GLY	2.0
18	P	31	ALA	2.0
1	w	1633	G	2.0
5	C	196	VAL	2.0
1	w	820	A	2.0
53	u	9	ASN	2.0
15	M	28	VAL	2.0
29	a	5	LYS	2.0
11	I	13	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
33	PSU	2	55	20/21	0.82	0.24	1,1,1,1	0
31	PSU	y	516	20/21	0.92	0.17	1,1,1,1	0
31	M2G	y	966	25/26	0.92	0.14	1,1,1,1	0
31	MA6	y	1518	24/25	0.93	0.17	1,1,1,1	0
31	5MC	y	1407	21/22	0.93	0.16	1,1,1,1	0
31	MA6	y	1519	24/25	0.93	0.16	1,1,1,1	0
31	7MG	y	527	24/25	0.93	0.23	1,1,1,1	0
31	5MC	y	1404	21/22	0.94	0.20	1,1,1,1	0
31	5MC	y	967	21/22	0.94	0.14	1,1,1,1	0
31	2MG	y	1207	24/25	0.95	0.16	1,1,1,1	0
31	5MC	y	1400	21/22	0.97	0.24	1,1,1,1	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.