



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:17 AM BST

PDB ID : 4V4I
Title : Crystal Structure of a 70S Ribosome-tRNA Complex Reveals Functional Interactions and Rearrangements.
Authors : Korostelev, A.; Trakhanov, S.; Laurberg, M.; Noller, H.F.
Deposited on : 2007-02-15
Resolution : 3.71 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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 : 2.13.1
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

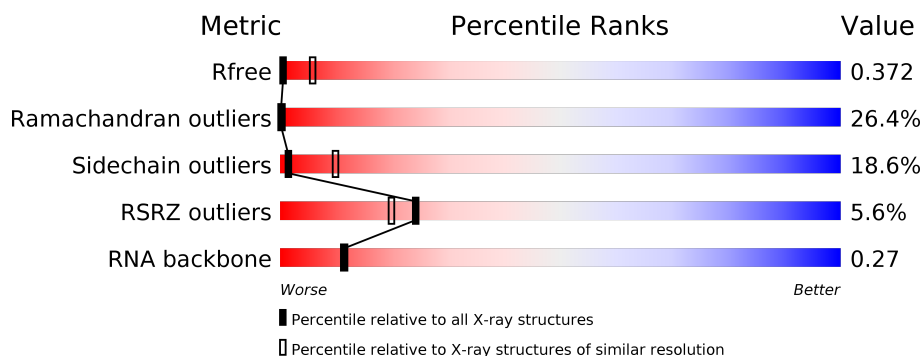
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.71 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	1089 (3.90-3.54)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)
RNA backbone	3102	1027 (4.40-3.00)

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 ≥ 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>3%</div> <div>57%</div> <div>39%</div> <div>.</div> </div>
2	x	121	<div> <div>61%</div> <div>36%</div> <div>..</div> </div>
3	A	229	<div> <div>3%</div> <div>39%</div> <div>14%</div> <div>.</div> <div>45%</div> </div>
4	B	276	<div> <div>5%</div> <div>57%</div> <div>38%</div> <div>..</div> </div>
5	C	206	<div> <div>5%</div> <div>56%</div> <div>34%</div> <div>7%</div> <div>.</div> </div>
6	D	205	<div> <div>4%</div> <div>55%</div> <div>35%</div> <div>5%</div> <div>5%</div> </div>

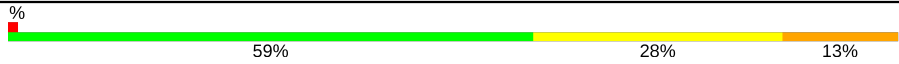

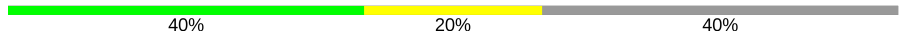

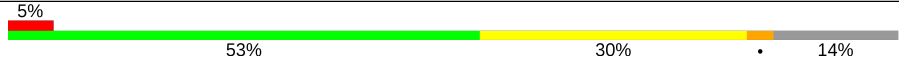
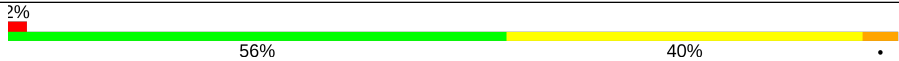
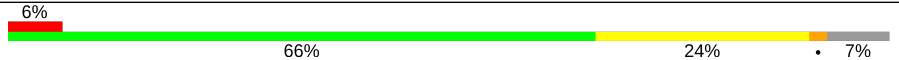
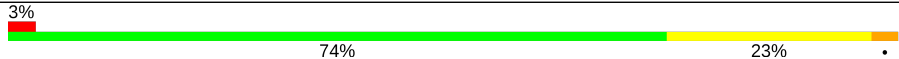
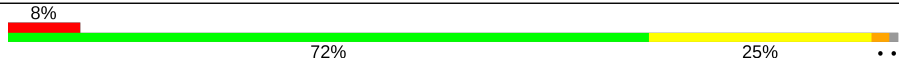
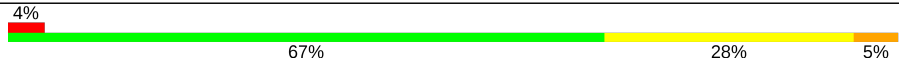
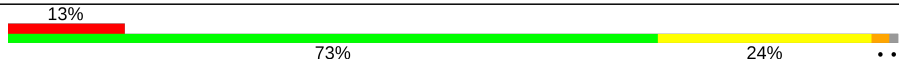
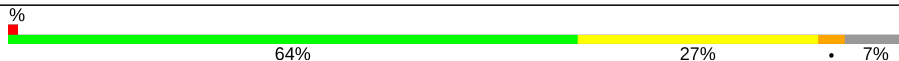
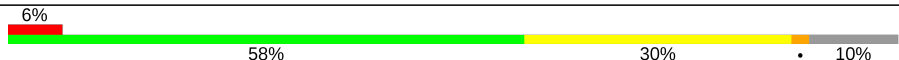



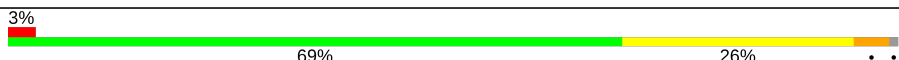
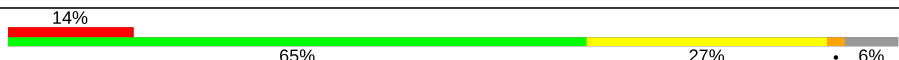
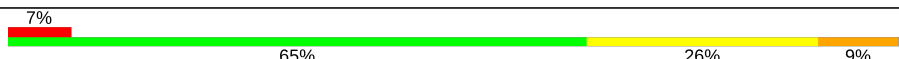
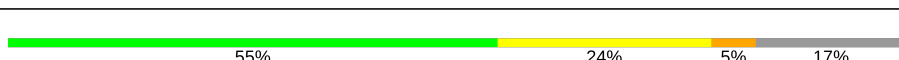

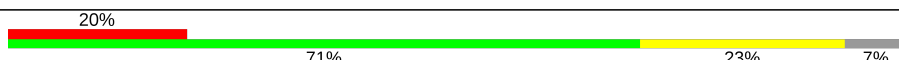
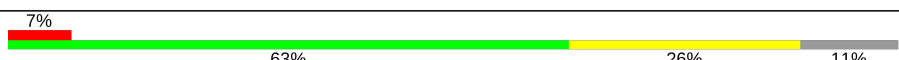
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Mol	Chain	Length	Quality of chain
7	E	182	
8	F	180	
9	G	148	
10	H	163	
11	I	122	
12	J	150	
13	K	141	
14	L	118	
15	M	112	
16	N	146	
17	O	118	
18	P	101	
19	Q	113	
20	R	96	
21	S	110	
22	T	206	
23	U	85	
24	V	98	
25	W	72	
26	X	60	
27	Y	60	
28	Z	49	
29	a	65	
30	b	37	
31	y	1522	

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Mol	Chain	Length	Quality of chain
32	z	76	
33	0	76	
34	l	10	
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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
32	H2U	z	16	-	-	-	X

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 146532 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			

- 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	S	0	0	0
			725	471	131	123				

- 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	0	0	0
			793	510	151	126	6			

- 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	0	0	0
			1475	941	262	269	3			

- 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	0	0	0
			605	376	126	102	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- 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	0	0	0
			520	325	102	91	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

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

- 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 SMALL SUBUNIT RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	y	1502	Total	C	N	O	P	0	0	0
			32302	14386	5984	10431	1501			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	450	G	C	CONFLICT	GB 155076
y	516	PSU	U	MODIFIED RESIDUE	GB 155076
y	527	7MG	G	MODIFIED RESIDUE	GB 155076
y	966	M2G	G	MODIFIED RESIDUE	GB 155076
y	967	5MC	C	MODIFIED RESIDUE	GB 155076
y	1207	2MG	G	MODIFIED RESIDUE	GB 155076
y	1400	5MC	C	MODIFIED RESIDUE	GB 155076
y	1402	4OC	C	MODIFIED RESIDUE	GB 155076
y	1404	5MC	C	MODIFIED RESIDUE	GB 155076
y	1407	5MC	C	MODIFIED RESIDUE	GB 155076
y	1498	UR3	U	MODIFIED RESIDUE	GB 155076
y	1518	MA6	A	MODIFIED RESIDUE	GB 155076
y	1519	MA6	A	MODIFIED RESIDUE	GB 155076

- Molecule 32 is a RNA chain called P-site PHE-tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	z	76	Total	C	N	O	P	S	0	0
			1628	731	290	530	75	2		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	8	4SU	U	MODIFIED RESIDUE	GB 174422
z	16	H2U	U	MODIFIED RESIDUE	GB 174422
z	20	H2U	U	MODIFIED RESIDUE	GB 174422
z	32	PSU	U	MODIFIED RESIDUE	GB 174422
z	37	MIA	A	MODIFIED RESIDUE	GB 174422
z	39	PSU	U	MODIFIED RESIDUE	GB 174422
z	46	7MG	G	MODIFIED RESIDUE	GB 174422
z	54	5MU	U	MODIFIED RESIDUE	GB 174422
z	55	PSU	U	MODIFIED RESIDUE	GB 174422

- Molecule 33 is a RNA chain called E-TRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	0	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	1	6	Total	C	N	O	P	0	0	0
			122	56	19	42	5			

- 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	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.

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	73	Total	C	N	O	0	0	0
			598	381	118	99			

- 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			

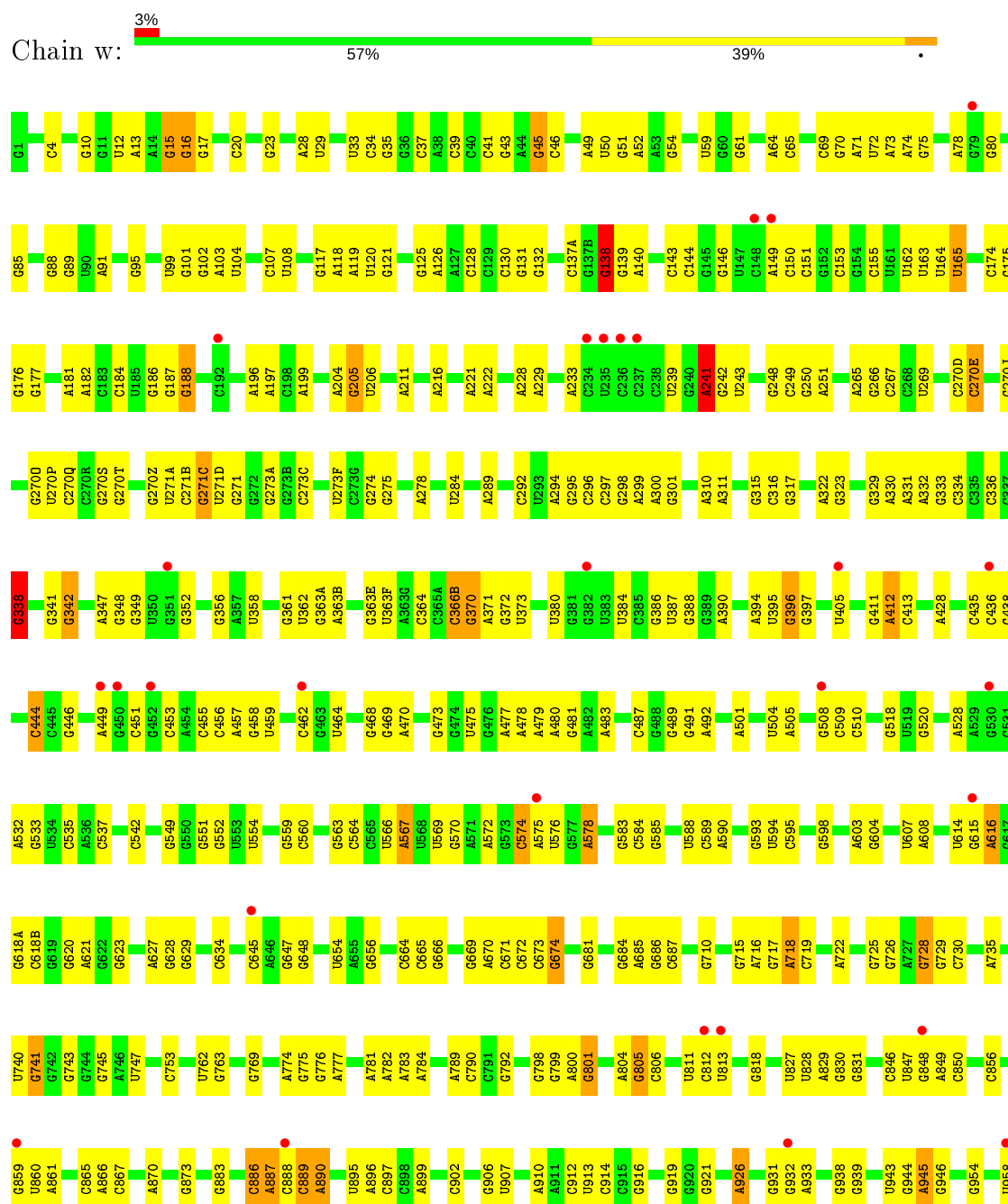
- Molecule 54 is a protein called 30S ribosomal protein Thx.

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

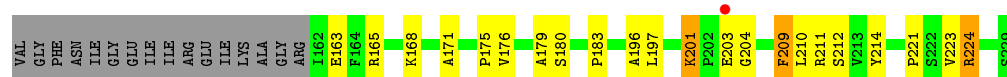
3 Residue-property plots

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.

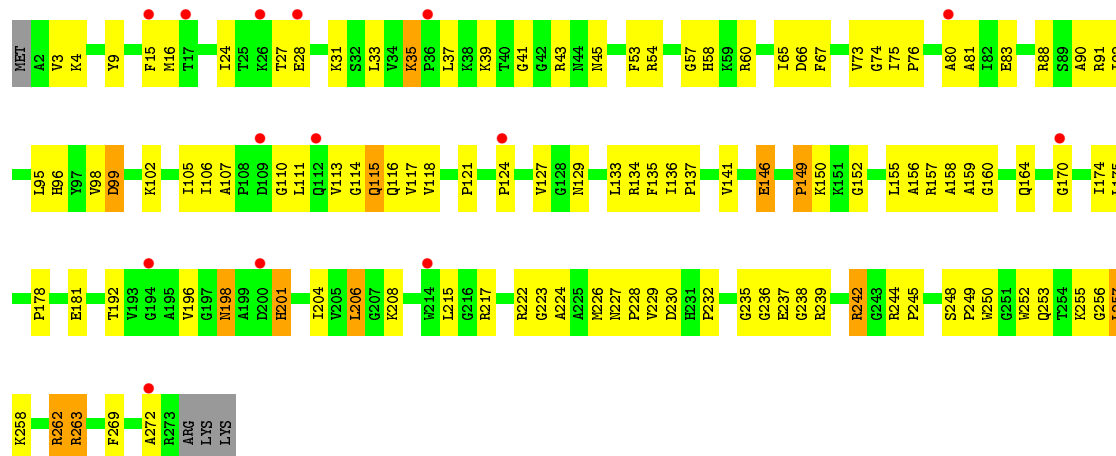
• Molecule 1: 23S LARGE SUBUNIT RIBOSOMAL RNA



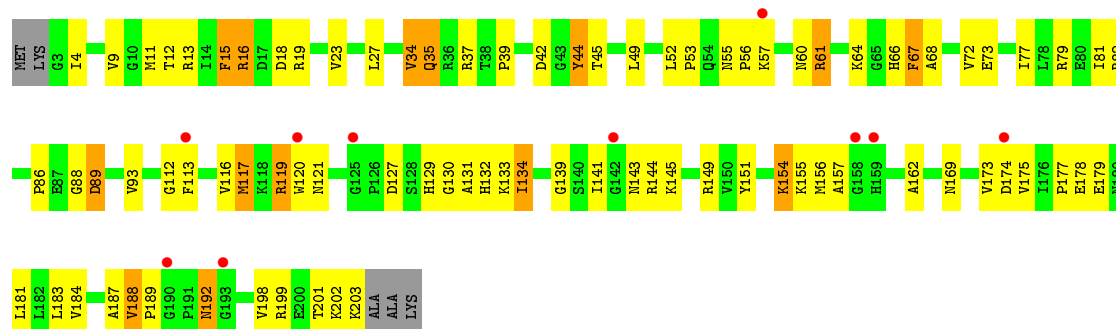
U2130	C2043	A1953	G1568	A1655	G1488	C1399	A1302	G1232	C1152	A1046	A959
G2131	U2047	G1954	A1569	C1662	U1489	G1400	A1305	G1223	C1155	G1047	A960
U2132	G2048	U1955	G1573	C1663	A1490	U1406	G1310	G1224	A1560	A1054	C961
G2133	C2049	G1960	C1574	A1664	G1491	G1413	G1311	G1225	G1160	G1059	U963
C2138	G2050	A1961	C1575	A1665	U1497	G1416	U1312	A1226	G1161	U1060	C964
A2051	A2051	U1963	C1576	G1666	C1498	G1419	U1313	G1227	G1182	U1061	C965
G2052	C2053	G1964	C1577	A1667	C1499	G1419	C1314	G1228	G1183	G1061	G966
C2145	G2054	A1965	C1578	A1668	G1500	U1419	G1319	G1229	G1184	A1070	G972
G2148	A2055	C1967	C1579	A1669	C1501	U1420	G1320	G1230	U1185	G1071	A973
C2153	G2056	A1968	A1580	C1670	C1502	G1421	A1321	G1231	C1166	A1071	A974
A2057	A2057	U1969	C1581	U1671	C1506	G1422	A1322	G1236	U1167	C1079	C974A
G2157	A2060	G1970	C1582	C1672	A1508	G1424	U1323	A1237	A1237	C1080	C974B
A2158	C2061	A1971	A1583	U1673	A1509	G1426	G1324	G1238	G1170	U1081	G975
G2159	A1972	A1784	C1585	G1674	A1510	G1427	U1325	G1239	G1171	G1082	C976
G2160	G1973	A1785	A1586	G1675	A1510	A1428	U1326	U1240	G1173	U1083	G977
C2063	C2063	A1974	G1596	G1682	U1516	G1429	G1329	G1244	A1174	A1087	A980
C2064	C2064	A1786	C1597	C1683	G1517	G1430	U1330	A1245	G1176	G1088	A983
G2168	G2065	A1787	G1601	U1688	C1518	G1436	G1332	A1246	A1177	A1093	A984
A2169	C2066	G1791	U1602	U1689	G1519	C1437	C1333	A1247	C1179	U1094	A988
A2170	A2067	G1792	C1603	U1690	U1520	U1438	G1334	G1248	C1181	A1095	A989
A2171	C2069	C1793	C1604	G1695	G1521	G1439	U1335	G1250	G1182	C991	A990
A2172	A2070	A1794	A1608	A1698	U1522	U1440	A1336	C1251	G1183	A1098	C992
A2173	G2071	U1795	A1609	A1699	U1523	A1441	G1337	G1252	G1184	G1099	G993
C2174	A2071	C1796	A1610	A1700	G1526	C1445	U1341	A1253	G1185	A1103	C994
G2175	C2087	U1796	G1613	A1701	U1527	G1446	A1342	G1256	G1187	G1110	A995
A2176	U2076	U1798	G1615	G1702	A1529	G1448	G1343	U1261	U1188	G1111	G997
C2177	A2077	C1799	A1616	G1703	G1530	A1449	G1344	G1264	G1191	C1116	C1005
C2178	C2078	G1800	A1617	G1706	U1531	C1450	G1345	G1265	A1194	G1112	C1006
C2179	A1900	A1802	A1618	G1707	C1535	C1451	G1346	G1266	G1195	G1122	G1007
U2180	G1903	A1803	G1619	A1707	G1538	G1455	G1347	U1267	G1197	G1125	C1008
G2181	C1906	C1806	G1623	C1712	G1539	A1457	C1350	G1270	U1198	G1126	A1009
C2188	G1906	A1809	U1626	U1712	G1540	C1458	C1351	G1271	U1199	A1127	A1010
C2189	C1909	A1810	C1627	G1716	U1541	G1459	G1358	A1272	C1200	U1012	U1012
G2190	C1996	G1811	G1628	G1717	G1542	A1460	A1359	A1273	C1201	A1128	C1013
G2191	G1997	G1812	U1629	G1718	A1543	G1461	C1362	U1274	A1204	A1129	U1014
C2192	C1998	A1813	G1630	G1719	C1544	G1465	C1363	A1275	U1205	U1130	G1015
G2193	G2000	U1814	C1631	G1720	A1545	G1466	G1364	A1276	A1131	G1016	G1016
C2194	A2013	U1815	C1632	G1721	A1546	C1467	A1365	A1277	U1132	G1017	G1017
C2195	A2014	G1816	U1633	G1722	C1547	G1470	A1366	A1278	C1206	A1133	C1020
A2198	A2014	U1817	C1633B	U1729	A1553	A1471	A1367	G1283	G1209	G1136	A1021
A2199	A2020	A1818	A1641	G1730	U1554	A1471	G1374	G1284	U1211	G1137	A1022
A2205	C2021	U1819	C1644	G1731	A1558	C1474	G1377	U1287	G1212	G1138	U1023
C2206	U2022	U1820	G1645	A1732	C1559	G1478	A1378	C1289	A1213	G1139	G1024
U2208	G2023	A1821	C1646	G1733	G1560	U1481	A1379	G1295	G1216	C1140	G1025
G2211	G2024	G1822	G1647	C1734	A1561	U1481	A1384	G1296	C1217	C1142	U1033
A2212	C2025	G1823	G1648	U1735	A1562	C1483	A1385	G1297	G1218	A1143	G1034
G2213	C2026	A1824	C1649	C1741	U1562	G1484	G1386	U1300	G1219	A1148	C1043
G2215	A2031	A1825	G1650	C1742	A1566	G1485	C1398	A1301	A1221	G1149	A1045
C2216	G2032	G1826	A1652	G1743	A1567	G1487					
A2217	C2033	C1827	C1653	G1746							
G2218	A2033	U1827	C1655	G1747							
G2219	U1938	A1829	G1656	G1748							
G2220	U1939	C1836	G1657	C1751							
G2221	G2035	C1837	G1658	G1752							
G2222	C2036	A1838	G1659	G1753							
G2223	U2041	G1839	A1652	U1757							
G2224	A2042	G1840									
A2225											
C2226											
A2227											
G2228											



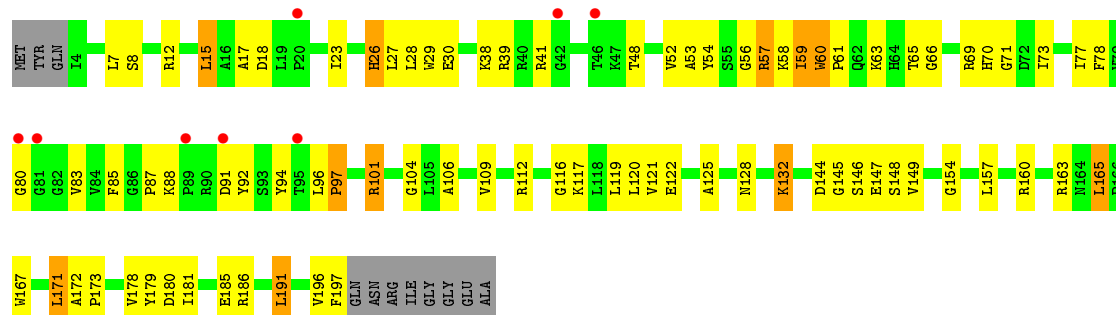
• Molecule 4: 50S ribosomal protein L2



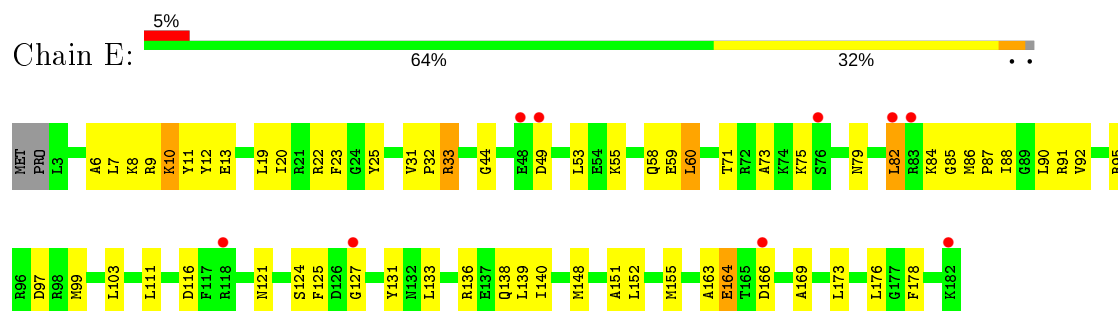
• Molecule 5: 50S ribosomal protein L3



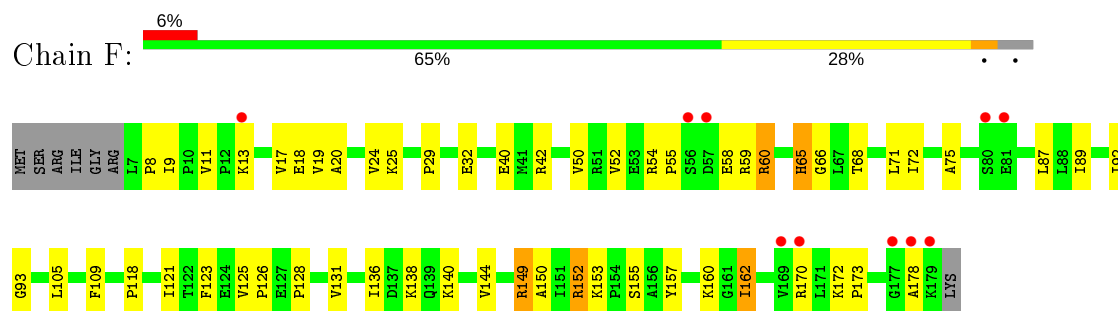
• Molecule 6: 50S ribosomal protein L4



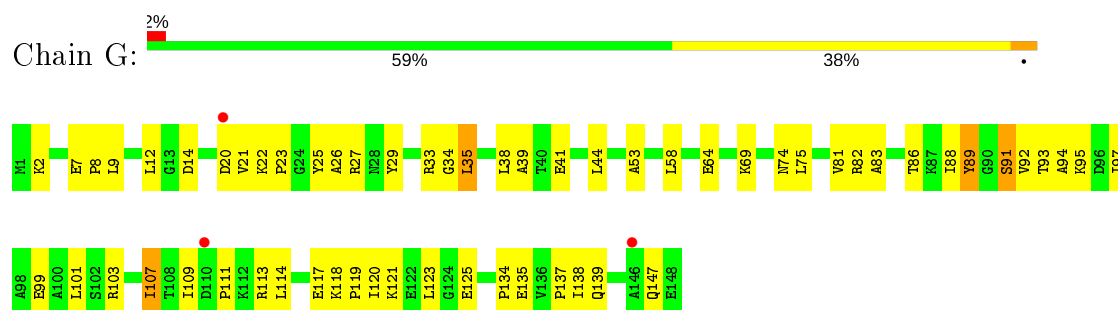
- Molecule 7: 50S ribosomal protein L5



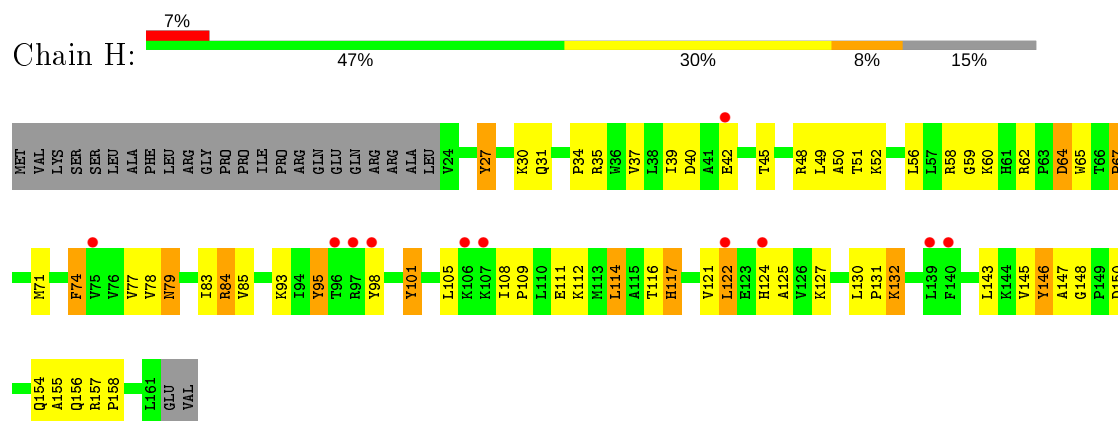
- Molecule 8: 50S ribosomal protein L6



- Molecule 9: 50S ribosomal protein L9

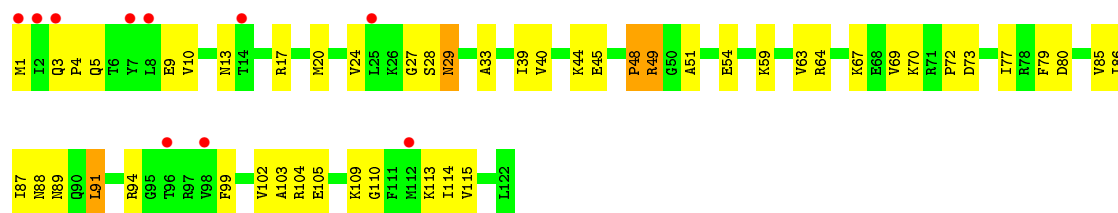


- Molecule 10: 50S ribosomal protein L13

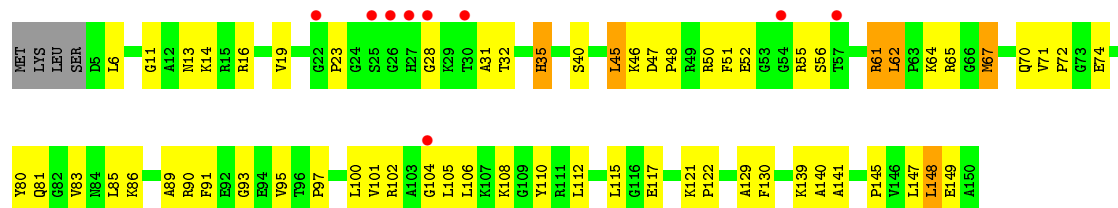


- Molecule 11: 50S ribosomal protein L14

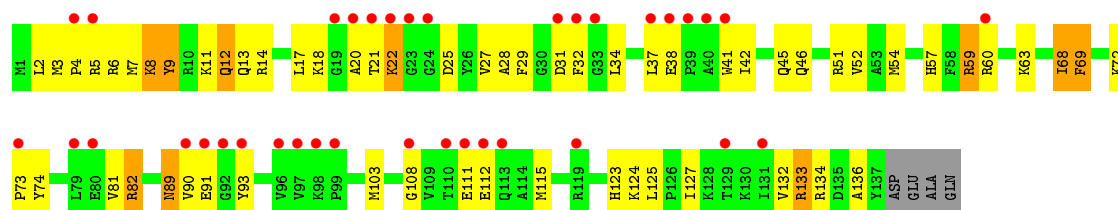




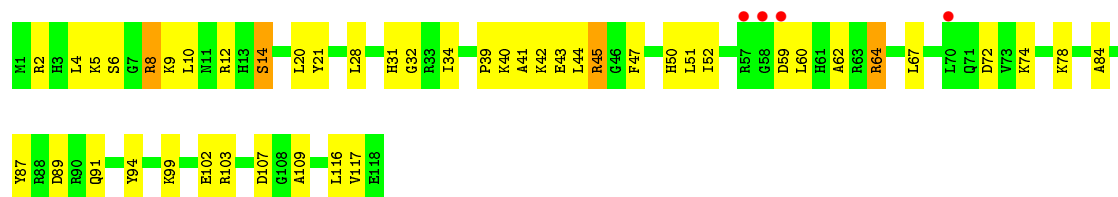
• Molecule 12: 50S ribosomal protein L15



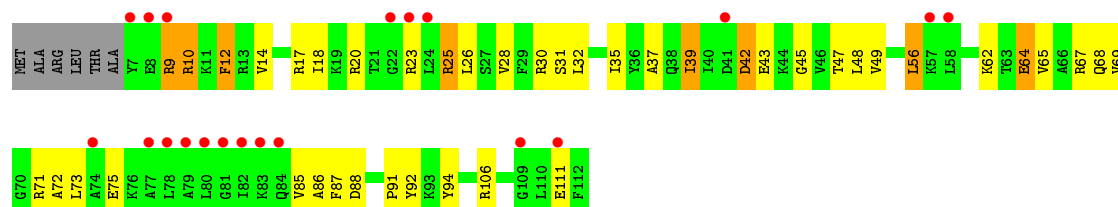
• Molecule 13: 50S ribosomal protein L16



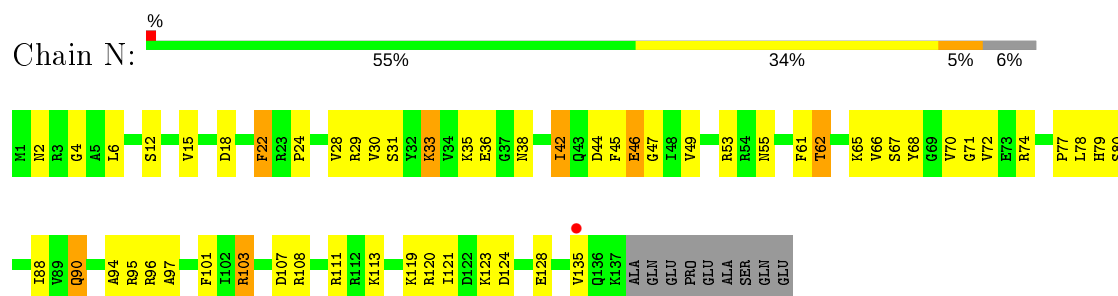
• Molecule 14: 50S ribosomal protein L17



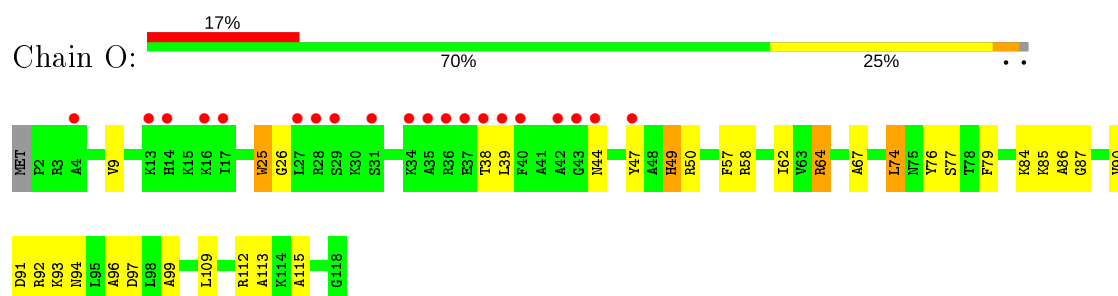
• Molecule 15: 50S ribosomal protein L18



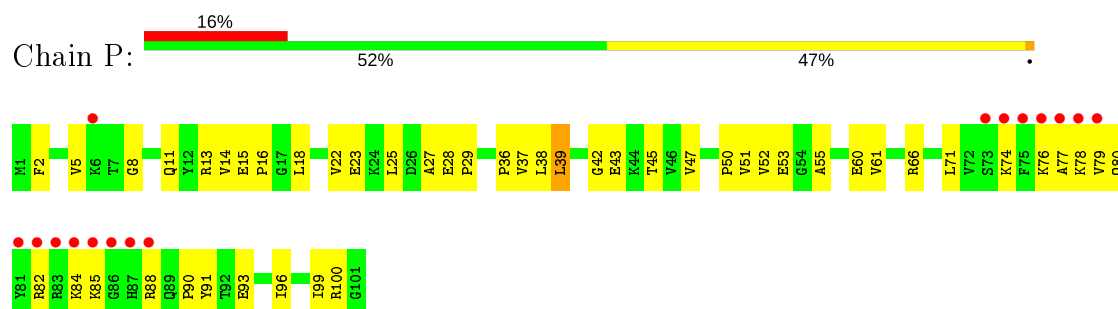
- Molecule 16: 50S ribosomal protein L19



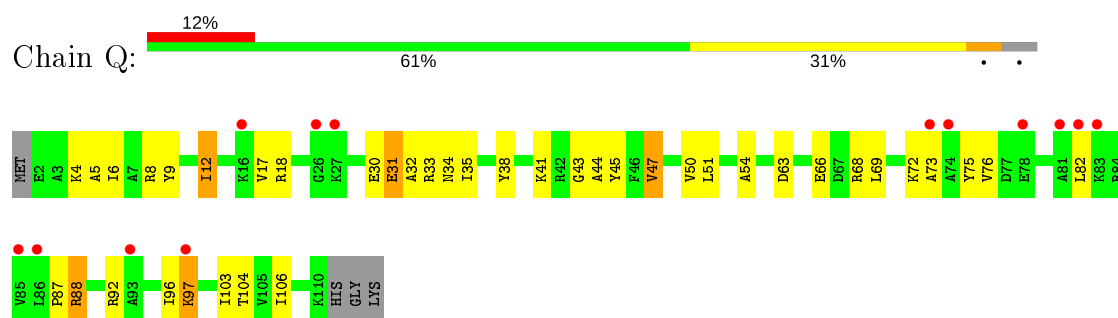
- Molecule 17: 50S ribosomal protein L20



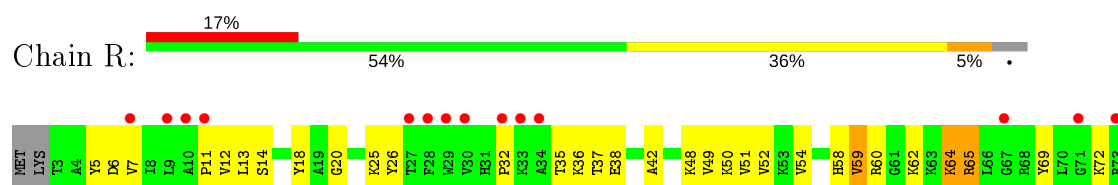
- Molecule 18: 50S ribosomal protein L21

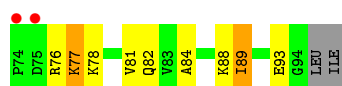


- Molecule 19: 50S ribosomal protein L22

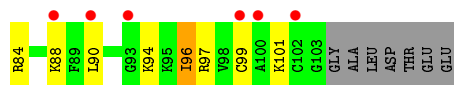
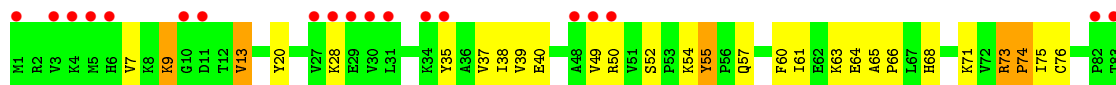


- Molecule 20: 50S ribosomal protein L23

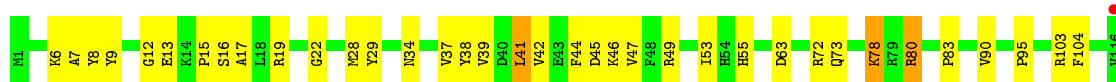




- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L27

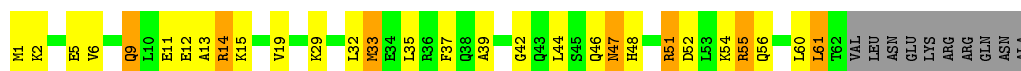


- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29





- Molecule 26: 50S ribosomal protein L30



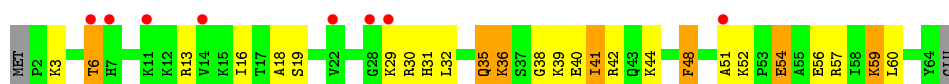
- Molecule 27: 50S ribosomal protein L32



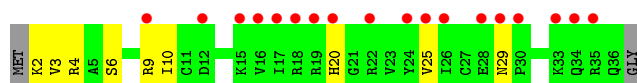
- Molecule 28: 50S ribosomal protein L34



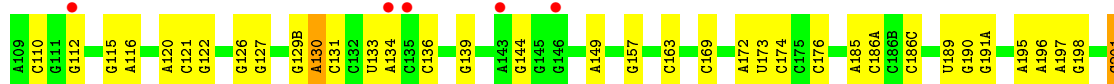
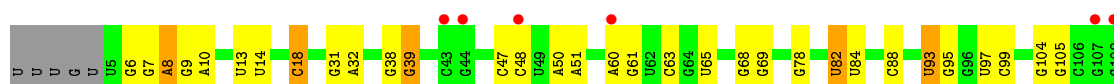
- Molecule 29: 50S ribosomal protein L35



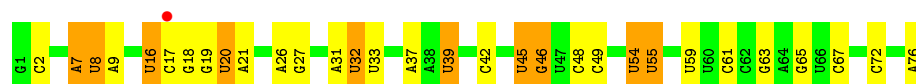
- Molecule 30: 50S ribosomal protein L36



- Molecule 31: 16S SMALL SUBUNIT RIBOSOMAL RNA







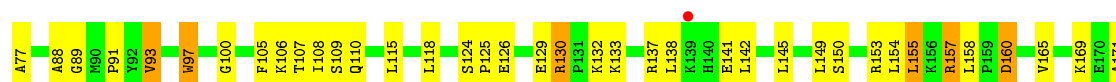
• Molecule 33: E-TRNA



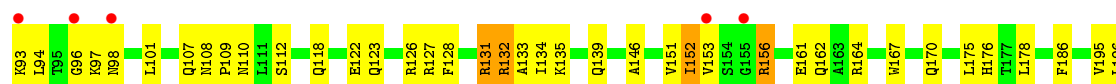
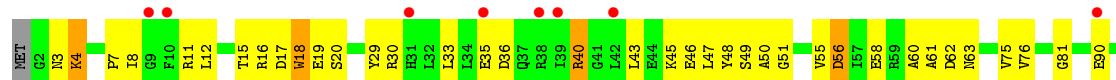
• Molecule 34: MRNA



• Molecule 35: 30S ribosomal protein S2

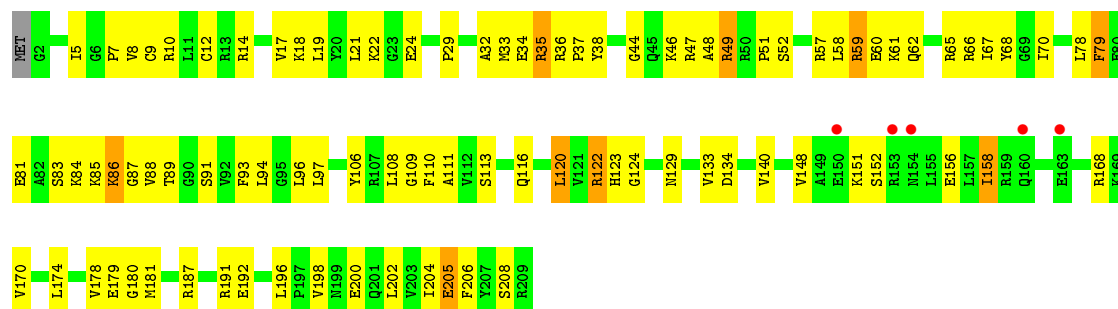


• Molecule 36: 30S ribosomal protein S3

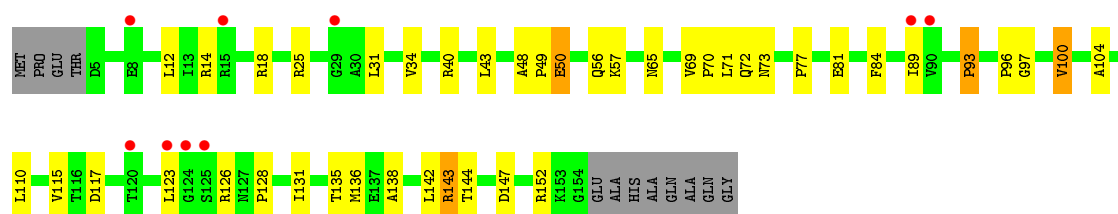


• Molecule 37: 30S ribosomal protein S4

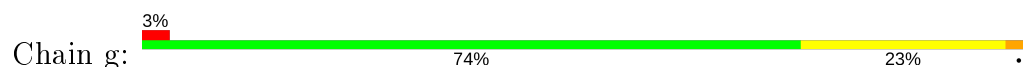




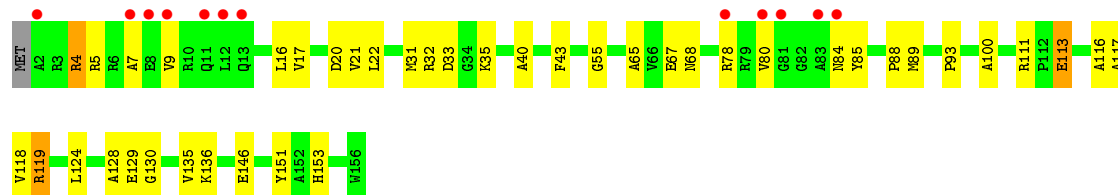
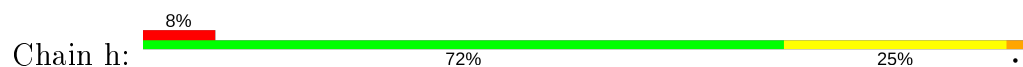
- Molecule 38: 30S ribosomal protein S5



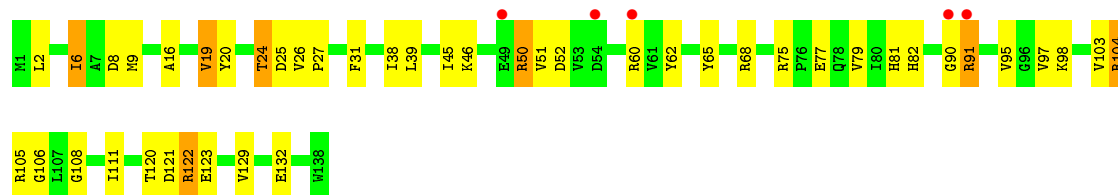
- Molecule 39: 30S ribosomal protein S6



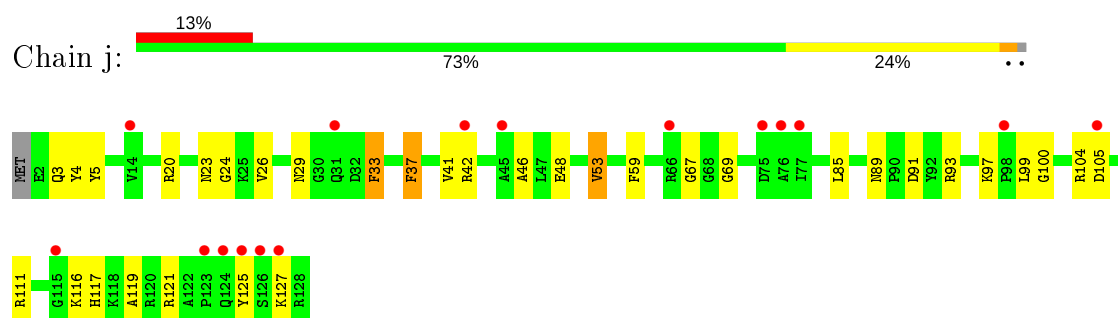
- Molecule 40: 30S ribosomal protein S7



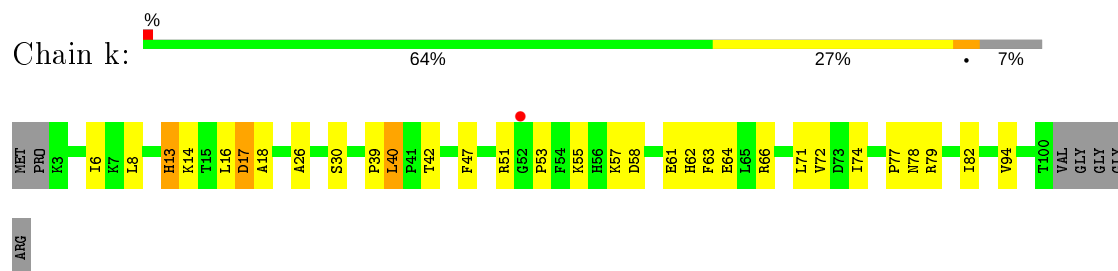
- Molecule 41: 30S ribosomal protein S8



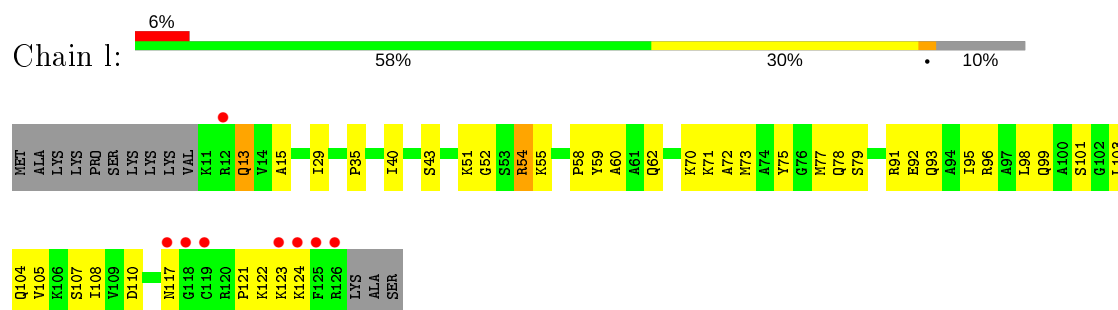
- Molecule 42: 30S ribosomal protein S9



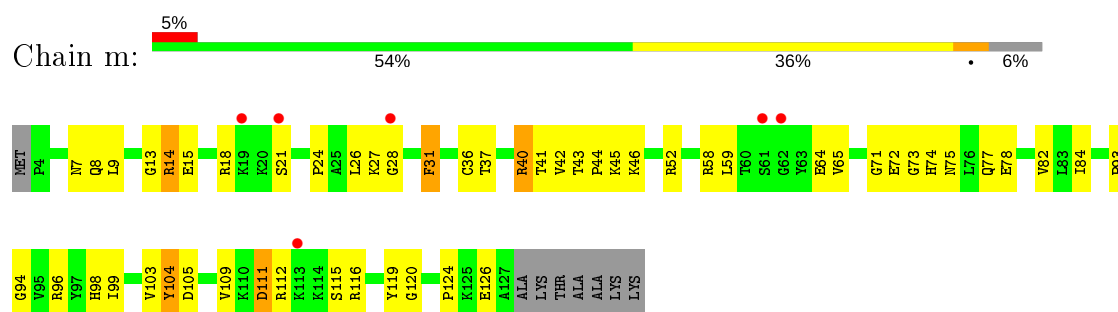
- Molecule 43: 30S ribosomal protein S10



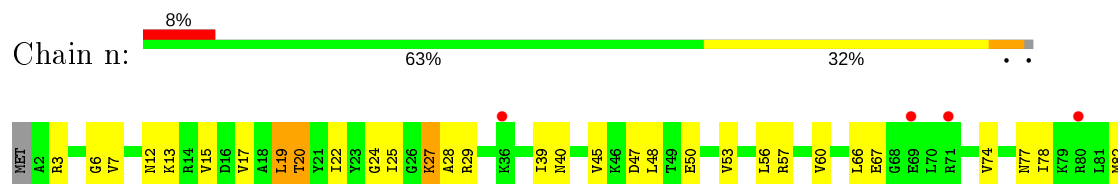
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12

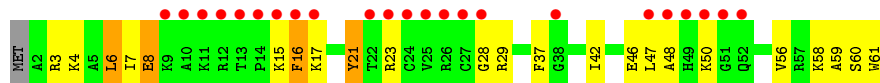


- Molecule 46: 30S ribosomal protein S13

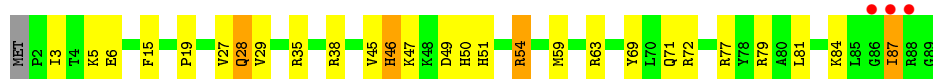




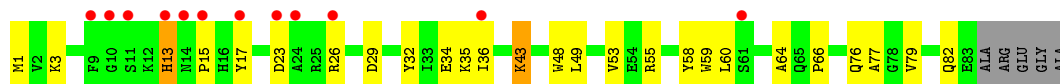
- Molecule 47: 30S ribosomal protein S14



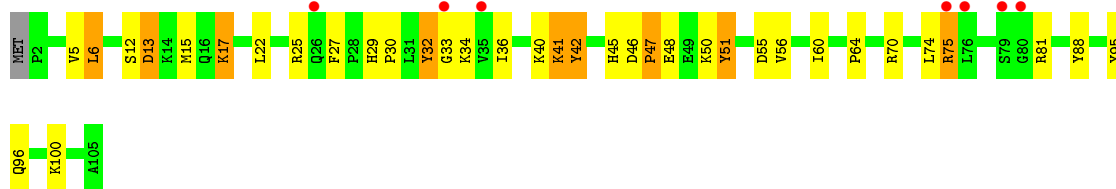
- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16



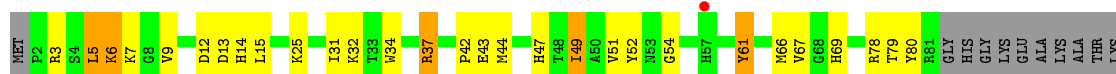
- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



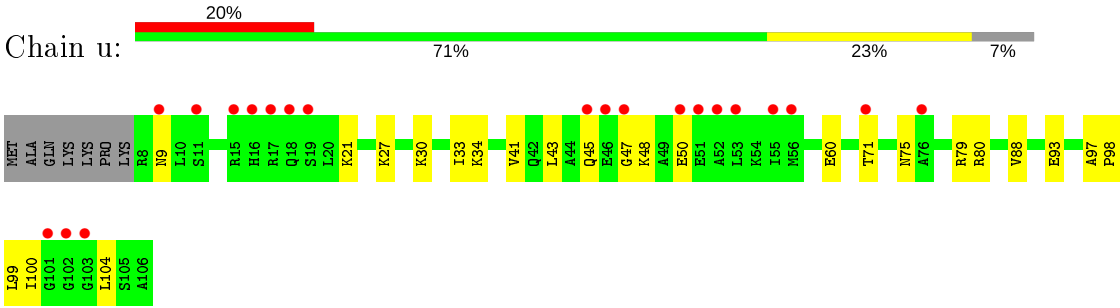
- Molecule 52: 30S ribosomal protein S19



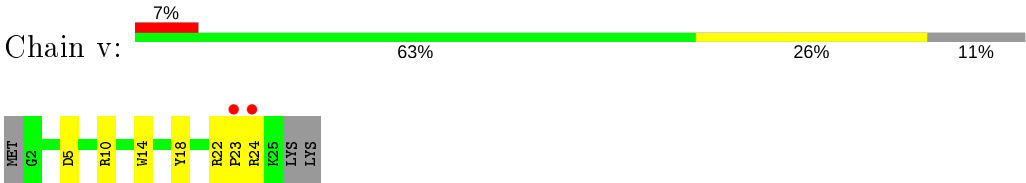
LYS

LYS

● 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, α , β , γ	507.81Å 507.81Å 689.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.71 72.78 – 3.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-3.71) 97.9 (72.78-3.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019, CNS	Depositor
R, R_{free}	0.348 , 0.353 0.367 , 0.372	Depositor DCC
R_{free} test set	11428 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
L-test for twinning ²	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Estimated twinning fraction	0.228 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.219 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	0.76	EDS
Total number of atoms	146532	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 5MU, M2G, MA6, MIA, H2U, 2MG, 5MC, UR3, 4OC, 4SU, 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	1.06	48/69679 (0.1%)	1.11	232/108779 (0.2%)
2	x	0.89	0/2878	1.03	11/4490 (0.2%)
3	A	0.50	0/1015	0.57	0/1369
4	B	0.49	0/2165	0.63	0/2919
5	C	0.57	0/1574	0.68	0/2125
6	D	0.57	0/1551	0.66	0/2101
7	E	0.55	0/1492	0.65	0/2006
8	F	0.55	0/1345	0.66	1/1819 (0.1%)
9	G	0.53	0/1171	0.65	0/1583
10	H	0.47	0/1130	0.59	0/1525
11	I	0.54	0/942	0.66	0/1268
12	J	0.50	0/1131	0.64	0/1504
13	K	0.62	0/1110	0.71	1/1483 (0.1%)
14	L	0.51	0/982	0.65	0/1312
15	M	0.54	0/856	0.63	0/1138
16	N	0.49	0/1157	0.62	0/1544
17	O	0.54	0/982	0.67	0/1306
18	P	0.51	0/790	0.62	0/1057
19	Q	0.56	0/878	0.66	0/1179
20	R	0.59	0/739	0.69	0/993
21	S	0.58	0/806	0.64	0/1074
22	T	0.54	0/1507	0.64	0/2045
23	U	0.57	0/613	0.65	0/816
24	V	0.49	0/701	0.60	0/932
25	W	0.52	0/522	0.65	0/690
26	X	0.56	0/482	0.73	0/646
27	Y	0.45	0/449	0.55	0/606
28	Z	0.80	0/426	0.73	0/561
29	a	0.58	0/515	0.69	0/679
30	b	0.55	0/297	0.61	0/392
31	y	0.97	13/35859 (0.0%)	1.07	96/55966 (0.2%)
32	z	0.98	1/1603 (0.1%)	1.05	3/2497 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	0	0.89	1/1791 (0.1%)	0.97	2/2791 (0.1%)
34	1	0.94	0/135	1.02	0/208
35	c	0.55	0/1935	0.60	0/2609
36	d	0.51	0/1636	0.62	0/2205
37	e	0.53	0/1733	0.62	1/2318 (0.0%)
38	f	0.51	0/1162	0.60	0/1564
39	g	0.56	0/856	0.63	0/1154
40	h	0.53	0/1276	0.57	0/1709
41	i	0.51	0/1136	0.62	0/1527
42	j	0.47	0/1029	0.53	0/1378
43	k	0.52	0/807	0.59	0/1085
44	l	0.49	0/879	0.59	0/1187
45	m	0.57	0/986	0.72	0/1320
46	n	0.52	0/1008	0.61	0/1347
47	o	0.53	0/501	0.57	0/664
48	p	0.49	0/745	0.58	0/992
49	q	0.49	0/716	0.63	0/963
50	r	0.55	0/870	0.63	0/1159
51	s	0.51	0/604	0.63	0/801
52	t	0.54	0/661	0.64	0/890
53	u	0.21	0/764	0.44	0/1006
54	v	0.57	0/212	0.52	0/277
All	All	0.91	63/158789 (0.0%)	0.99	347/237558 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	w	0	24
2	x	2	0
31	y	0	8
All	All	2	32

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	926	A	O3'-P	30.08	1.97	1.61
1	w	1506	C	O3'-P	29.80	1.97	1.61
1	w	1171	G	O3'-P	28.10	1.94	1.61
1	w	890	A	O3'-P	28.02	1.94	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	1481	U	O3'-P	24.13	1.90	1.61
1	w	154(B)	C	O3'-P	24.08	1.90	1.61
1	w	1743	G	O3'-P	23.54	1.89	1.61
31	y	102(C)	C	O3'-P	22.10	1.87	1.61
1	w	41	C	O3'-P	20.99	1.86	1.61
1	w	1133	U	O3'-P	20.84	1.86	1.61
1	w	1712	C	O3'-P	20.82	1.86	1.61
1	w	99	U	O3'-P	20.13	1.85	1.61
1	w	149(B)	A	O3'-P	19.89	1.85	1.61
1	w	1864	U	O3'-P	18.86	1.83	1.61
1	w	2219	G	O3'-P	18.29	1.83	1.61
1	w	2199	A	O3'-P	18.16	1.82	1.61
1	w	155	C	O3'-P	17.94	1.82	1.61
1	w	489	G	O3'-P	17.86	1.82	1.61
1	w	1735	U	O3'-P	17.73	1.82	1.61
31	y	458	C	O3'-P	17.60	1.82	1.61
1	w	114(B)	A	O3'-P	17.30	1.81	1.61
1	w	2213	U	O3'-P	17.17	1.81	1.61
31	y	843	U	O3'-P	16.55	1.81	1.61
1	w	122(A)	C	O3'-P	16.15	1.80	1.61
31	y	210	U	O3'-P	16.06	1.80	1.61
1	w	366(B)	C	O3'-P	16.02	1.80	1.61
1	w	163(B)	C	O3'-P	15.29	1.79	1.61
1	w	1872	A	O3'-P	15.27	1.79	1.61
1	w	165	U	O3'-P	15.22	1.79	1.61
1	w	1451	C	O3'-P	14.26	1.78	1.61
1	w	436	C	O3'-P	13.99	1.77	1.61
1	w	1583	A	O3'-P	13.92	1.77	1.61
1	w	144(B)	A	O3'-P	13.22	1.77	1.61
1	w	537	C	O3'-P	12.96	1.76	1.61
31	y	838	G	O3'-P	12.86	1.76	1.61
31	y	1167	A	O3'-P	-12.34	1.46	1.61
31	y	82	U	O3'-P	-12.18	1.46	1.61
1	w	712(B)	A	O3'-P	12.03	1.75	1.61
1	w	1718	G	O3'-P	10.66	1.74	1.61
1	w	2799	A	O3'-P	10.65	1.74	1.61
31	y	103(C)	G	O3'-P	10.53	1.73	1.61
1	w	2712	U	C4-O4	8.43	1.30	1.23
31	y	1443	G	O3'-P	7.64	1.70	1.61
31	y	440	A	O3'-P	6.99	1.69	1.61
1	w	574	C	N1-C2	6.38	1.46	1.40
31	y	97	U	O3'-P	6.22	1.68	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	w	578	A	C5-C6	6.11	1.46	1.41
1	w	888	C	P-O5'	5.93	1.65	1.59
1	w	1264	G	N9-C4	5.76	1.42	1.38
1	w	990	A	N9-C4	5.53	1.41	1.37
31	y	99	C	O3'-P	5.48	1.67	1.61
1	w	2057	A	N9-C4	-5.33	1.34	1.37
1	w	2877	G	C3'-O3'	5.31	1.49	1.42
1	w	188	G	N7-C5	5.24	1.42	1.39
1	w	16	G	C3'-O3'	5.21	1.49	1.42
32	z	26	A	C5-C6	5.21	1.45	1.41
1	w	973	A	C3'-O3'	5.18	1.49	1.42
1	w	2171	A	C3'-O3'	5.14	1.49	1.42
31	y	1455	G	O3'-P	5.14	1.67	1.61
1	w	2874	C	C3'-O3'	5.06	1.49	1.42
1	w	1826	G	C3'-O3'	5.06	1.49	1.42
33	0	61	C	C3'-O3'	5.05	1.49	1.42
1	w	554	U	O3'-P	5.02	1.67	1.61

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	1822	G	N9-C1'-C2'	-18.71	89.67	114.00
1	w	1577	C	N1-C1'-C2'	-15.42	93.96	114.00
1	w	712(B)	A	P-O3'-C3'	-14.26	102.58	119.70
31	y	93	U	N1-C1'-C2'	-14.11	95.66	114.00
31	y	832	C	N1-C1'-C2'	-13.21	96.82	114.00
1	w	2471	C	N1-C1'-C2'	-13.02	97.08	114.00
1	w	1516	U	N1-C1'-C2'	-12.83	97.32	114.00
1	w	1274	A	N9-C1'-C2'	-12.37	97.92	114.00
1	w	1863	G	N9-C1'-C2'	-12.08	98.30	114.00
31	y	436	C	N1-C1'-C2'	-12.07	98.31	114.00
1	w	1454	U	N1-C1'-C2'	-11.67	98.83	114.00
1	w	489	G	P-O3'-C3'	-11.50	105.90	119.70
1	w	926	A	P-O3'-C3'	-11.21	106.25	119.70
1	w	1627	G	N9-C1'-C2'	-11.15	99.50	114.00
1	w	2393	A	N9-C1'-C2'	-11.13	99.53	114.00
1	w	338	G	N9-C1'-C2'	-11.08	99.59	114.00
1	w	890	A	P-O3'-C3'	-10.90	106.62	119.70
1	w	2848	G	N9-C1'-C2'	-10.89	99.84	114.00
1	w	1506	C	P-O3'-C3'	-10.35	107.29	119.70
1	w	945	A	N9-C1'-C2'	10.30	127.39	114.00
1	w	712(B)	A	N9-C1'-C2'	-10.23	100.70	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	2451	A	N9-C1'-C2'	-10.15	100.81	114.00
1	w	1743	G	P-O3'-C3'	-10.13	107.55	119.70
1	w	873	G	N9-C1'-C2'	-9.85	101.17	112.00
31	y	1230	C	N1-C1'-C2'	-9.80	101.22	112.00
31	y	93	U	P-O3'-C3'	-9.73	108.03	119.70
1	w	1577	C	O4'-C1'-N1	9.66	115.93	108.20
1	w	1171	G	P-O3'-C3'	-9.64	108.13	119.70
31	y	890	G	N9-C1'-C2'	-9.40	101.66	112.00
1	w	1191	G	N9-C1'-C2'	-9.35	101.72	112.00
31	y	280	C	N1-C1'-C2'	-9.29	101.78	112.00
1	w	241	A	N9-C1'-C2'	9.25	126.02	114.00
31	y	189	U	N1-C1'-C2'	-9.20	101.88	112.00
31	y	102(C)	C	P-O3'-C3'	-9.20	108.66	119.70
1	w	1822	G	O4'-C1'-N9	8.90	115.32	108.20
31	y	97	U	P-O3'-C3'	-8.81	109.13	119.70
1	w	2865	U	N1-C1'-C2'	-8.73	102.39	112.00
31	y	210	U	P-O3'-C3'	-8.73	109.22	119.70
1	w	1385	G	N9-C1'-C2'	-8.64	102.49	112.00
1	w	1626	G	N9-C1'-C2'	-8.57	102.57	112.00
1	w	155	C	P-O3'-C3'	-8.53	109.46	119.70
33	0	46	G	N9-C1'-C2'	-8.35	102.81	112.00
31	y	894	G	N9-C1'-C2'	-8.28	102.89	112.00
1	w	537	C	P-O3'-C3'	-8.23	109.82	119.70
1	w	945	A	O4'-C1'-N9	8.23	114.78	108.20
1	w	114(B)	A	P-O3'-C3'	-8.22	109.83	119.70
31	y	748	C	N1-C1'-C2'	-8.20	102.98	112.00
1	w	15	G	N9-C1'-C2'	-8.18	103.00	112.00
31	y	1213	A	N9-C1'-C2'	-8.16	103.02	112.00
31	y	1293	G	N9-C1'-C2'	-8.04	103.16	112.00
31	y	1229	A	N9-C1'-C2'	-7.91	103.30	112.00
1	w	1662	C	N1-C1'-C2'	-7.84	103.38	112.00
31	y	201	C	P-O3'-C3'	-7.81	110.33	119.70
31	y	1455	G	OP2-P-O3'	7.72	122.19	105.20
31	y	773	G	N9-C1'-C2'	-7.72	103.51	112.00
1	w	1163	G	N9-C1'-C2'	-7.68	103.55	112.00
1	w	887	A	C3'-C2'-C1'	-7.66	95.37	101.50
1	w	1059	G	O4'-C1'-N9	7.59	114.28	108.20
1	w	2056	G	C3'-C2'-C1'	-7.58	95.44	101.50
31	y	1455	G	P-O3'-C3'	-7.48	110.72	119.70
31	y	130	A	N9-C1'-C2'	-7.46	103.80	112.00
1	w	2190	G	N9-C1'-C2'	-7.46	103.80	112.00
31	y	1151	A	O4'-C1'-N9	7.44	114.15	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	2243	U	N1-C1'-C2'	-7.43	103.82	112.00
31	y	890	G	O4'-C1'-N9	7.41	114.13	108.20
1	w	99	U	P-O3'-C3'	-7.39	110.84	119.70
1	w	1627	G	O4'-C1'-N9	7.36	114.08	108.20
31	y	1151	A	N9-C1'-C2'	-7.32	103.95	112.00
1	w	1930	G	N9-C1'-C2'	-7.31	103.95	112.00
1	w	2053	G	N9-C1'-C2'	-7.30	103.97	112.00
1	w	1934	C	N1-C1'-C2'	-7.25	104.03	112.00
31	y	403	C	N1-C1'-C2'	-7.23	104.05	112.00
1	w	1626	G	O4'-C1'-N9	7.18	113.95	108.20
1	w	270(E)	C	N1-C1'-C2'	7.16	123.31	114.00
31	y	795	C	N1-C1'-C2'	-7.15	104.13	112.00
2	x	24	G	C4'-C3'-C2'	7.14	109.74	102.60
1	w	1185	C	N1-C1'-C2'	-7.13	104.16	112.00
1	w	205	G	O4'-C1'-N9	7.11	113.89	108.20
2	x	21	G	C2'-C3'-O3'	7.10	125.11	109.50
2	x	14	U	C4'-C3'-C2'	7.09	109.69	102.60
2	x	111	U	C1'-O4'-C4'	-7.09	104.23	109.90
31	y	102(C)	C	OP2-P-O3'	7.06	120.73	105.20
1	w	2263	C	N1-C1'-C2'	-7.04	104.25	112.00
31	y	312	C	N1-C1'-C2'	-7.04	104.26	112.00
1	w	1955	U	N1-C1'-C2'	7.00	123.11	114.00
1	w	1059	G	N9-C1'-C2'	-6.98	104.32	112.00
8	F	149	ARG	N-CA-C	-6.91	92.35	111.00
31	y	1301	U	N1-C1'-C2'	-6.90	104.41	112.00
1	w	1963	U	N1-C1'-C2'	6.88	122.94	114.00
1	w	2484	G	N9-C1'-C2'	-6.86	104.45	112.00
1	w	149(B)	A	P-O3'-C3'	-6.85	111.48	119.70
1	w	1465	G	N9-C1'-C2'	-6.84	104.48	112.00
31	y	650	G	N9-C1'-C2'	-6.81	104.51	112.00
1	w	1247	A	N9-C1'-C2'	6.81	122.85	114.00
31	y	428	G	N9-C1'-C2'	6.80	122.84	114.00
1	w	2431	U	N1-C1'-C2'	-6.79	104.53	112.00
31	y	172	A	N9-C1'-C2'	-6.79	104.53	112.00
1	w	2115	G	N9-C1'-C2'	-6.78	104.54	112.00
1	w	2490	G	N9-C1'-C2'	6.74	122.76	114.00
31	y	1105	A	N9-C1'-C2'	-6.73	104.60	112.00
31	y	1517	G	C4'-C3'-O3'	6.73	126.46	113.00
2	x	21	G	C4'-C3'-C2'	6.72	109.32	102.60
1	w	45	G	N9-C1'-C2'	-6.69	104.64	112.00
1	w	491	G	N9-C1'-C2'	-6.68	104.65	112.00
31	y	241	C	N1-C1'-C2'	-6.67	104.67	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	z	31	A	C3'-C2'-C1'	-6.67	96.17	101.50
31	y	763	G	N9-C1'-C2'	-6.65	104.69	112.00
31	y	752	G	N9-C1'-C2'	-6.64	104.70	112.00
31	y	1517	G	C3'-C2'-C1'	-6.61	96.21	101.50
1	w	674	G	N9-C1'-C2'	-6.61	104.73	112.00
31	y	1517	G	O4'-C4'-C3'	-6.61	97.39	104.00
31	y	1053	G	O4'-C1'-N9	-6.55	102.96	108.20
1	w	1751	C	N1-C1'-C2'	-6.53	104.82	112.00
31	y	303	A	N9-C1'-C2'	-6.53	104.82	112.00
1	w	41	C	P-O3'-C3'	-6.50	111.90	119.70
2	x	24	G	C2'-C3'-O3'	6.48	124.07	113.70
1	w	1577	C	C3'-C2'-C1'	6.46	106.66	101.50
1	w	342	G	N9-C1'-C2'	-6.45	104.90	112.00
1	w	2235	G	N9-C1'-C2'	-6.45	104.91	112.00
31	y	1517	G	N9-C1'-C2'	-6.44	104.91	112.00
1	w	436	C	P-O3'-C3'	-6.41	112.01	119.70
1	w	4	C	O4'-C1'-N1	6.40	113.32	108.20
31	y	1431	C	O4'-C1'-N1	6.40	113.32	108.20
1	w	2481	G	O4'-C1'-N9	6.38	113.31	108.20
31	y	971	G	O4'-C1'-N9	6.37	113.30	108.20
1	w	1245	G	N9-C1'-C2'	-6.37	104.99	112.00
32	z	45	U	C3'-C2'-C1'	-6.35	96.42	101.50
1	w	1735	U	P-O3'-C3'	-6.34	112.09	119.70
31	y	974	A	N9-C1'-C2'	6.31	122.20	114.00
1	w	1278	A	C3'-C2'-C1'	-6.30	96.46	101.50
1	w	2805	G	P-O3'-C3'	-6.29	112.16	119.70
1	w	1131	G	O4'-C1'-N9	6.28	113.22	108.20
1	w	1230	C	N1-C1'-C2'	-6.28	105.09	112.00
1	w	2061	G	N9-C1'-C2'	-6.27	105.11	112.00
31	y	1089	G	N9-C1'-C2'	-6.26	105.11	112.00
31	y	697	U	N1-C1'-C2'	-6.26	105.11	112.00
1	w	54	G	N9-C1'-C2'	-6.25	105.12	112.00
1	w	829	A	N9-C1'-C2'	6.23	122.10	114.00
1	w	1811	G	C3'-C2'-C1'	-6.23	96.52	101.50
1	w	1231	G	N9-C1'-C2'	-6.22	105.16	112.00
1	w	2369	A	N9-C1'-C2'	-6.22	105.16	112.00
1	w	2712	U	N3-C4-C5	6.21	118.33	114.60
1	w	1128	A	N9-C1'-C2'	6.19	122.05	114.00
1	w	436	C	OP1-P-O3'	6.18	118.80	105.20
1	w	1822	G	C3'-C2'-C1'	6.18	106.44	101.50
1	w	681	G	C3'-C2'-C1'	-6.17	96.57	101.50
1	w	23	G	N9-C1'-C2'	-6.15	105.24	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	458	C	P-O3'-C3'	-6.15	112.32	119.70
1	w	728	G	N9-C1'-C2'	6.14	121.98	114.00
1	w	370	G	N9-C1'-C2'	6.14	121.98	114.00
2	x	14	U	C4'-C3'-O3'	6.10	125.20	113.00
2	x	14	U	C2'-C3'-O3'	6.10	123.46	113.70
2	x	12	C	C2'-C3'-O3'	6.09	123.45	113.70
1	w	1218	C	N1-C1'-C2'	-6.09	105.30	112.00
1	w	1650	G	O4'-C1'-N9	6.08	113.07	108.20
31	y	1196	U	N1-C1'-C2'	-6.07	105.32	112.00
1	w	1247	A	O4'-C1'-N9	6.07	113.06	108.20
1	w	990	A	O4'-C1'-N9	6.06	113.05	108.20
2	x	24	G	C4'-C3'-O3'	6.05	125.11	113.00
31	y	1249	C	C3'-C2'-C1'	-6.05	96.66	101.50
1	w	188	G	C3'-C2'-C1'	-6.05	96.66	101.50
1	w	1301	A	N9-C1'-C2'	-6.04	105.36	112.00
1	w	2171	A	N9-C1'-C2'	6.04	121.85	114.00
1	w	718	A	N9-C1'-C2'	-6.00	105.40	112.00
1	w	1218	C	O4'-C1'-N1	6.00	113.00	108.20
1	w	2669	G	N9-C1'-C2'	-5.98	105.42	112.00
1	w	2451	A	C3'-C2'-C1'	-5.96	96.73	101.50
1	w	520	G	C3'-C2'-C1'	-5.95	96.74	101.50
1	w	2765	A	N9-C1'-C2'	5.95	121.73	114.00
1	w	2453	A	O4'-C1'-N9	5.94	112.95	108.20
1	w	889	C	O4'-C1'-N1	5.93	112.94	108.20
1	w	2287	A	O4'-C1'-N9	5.93	112.94	108.20
1	w	187	G	N9-C1'-C2'	-5.92	105.49	112.00
1	w	537	C	OP2-P-O3'	5.91	118.20	105.20
1	w	2262	U	C3'-C2'-C1'	-5.91	96.77	101.50
1	w	567	A	O4'-C1'-N9	5.91	112.93	108.20
32	z	7	A	C2'-C3'-O3'	5.90	123.14	113.70
1	w	1616	A	N9-C1'-C2'	5.90	121.67	114.00
31	y	336	C	N1-C1'-C2'	-5.89	105.52	112.00
1	w	741	G	N9-C1'-C2'	-5.89	105.52	112.00
31	y	1506	U	N1-C1'-C2'	-5.89	105.52	112.00
31	y	749	C	C5'-C4'-C3'	-5.86	106.63	116.00
1	w	1995	U	O4'-C1'-N1	5.85	112.88	108.20
31	y	458	C	OP2-P-O3'	5.85	118.07	105.20
1	w	574	C	N1-C2-O2	5.85	122.41	118.90
31	y	312	C	C3'-C2'-C1'	-5.85	96.82	101.50
1	w	163(B)	C	P-O3'-C3'	-5.84	112.69	119.70
1	w	2395	C	N1-C1'-C2'	-5.83	105.58	112.00
31	y	485	G	N9-C1'-C2'	5.82	121.57	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	1201	A	N9-C1'-C2'	5.82	121.56	114.00
31	y	1406	U	N1-C1'-C2'	-5.79	105.64	112.00
31	y	1484	C	O4'-C1'-N1	5.78	112.82	108.20
1	w	1839	G	N9-C1'-C2'	-5.78	105.65	112.00
31	y	570	G	N9-C1'-C2'	5.77	121.50	114.00
1	w	977	G	N9-C1'-C2'	-5.76	105.67	112.00
1	w	1577	C	C4'-C3'-O3'	5.76	124.52	113.00
1	w	1275	A	O4'-C1'-N9	5.75	112.80	108.20
1	w	1199	U	N1-C1'-C2'	5.74	121.46	114.00
1	w	2595	G	N9-C1'-C2'	-5.73	105.70	112.00
1	w	712(B)	A	OP2-P-O3'	5.73	117.80	105.20
31	y	587	G	O4'-C1'-N9	5.72	112.78	108.20
1	w	412	A	O4'-C1'-N9	5.72	112.78	108.20
31	y	97	U	OP2-P-O3'	5.70	117.74	105.20
1	w	1542	G	C3'-C2'-C1'	-5.70	96.94	101.50
1	w	2257	U	N1-C1'-C2'	-5.69	105.74	112.00
33	0	18	G	N9-C1'-C2'	5.69	121.40	114.00
1	w	1944	U	O4'-C1'-N1	5.69	112.75	108.20
31	y	1497	G	C3'-C2'-C1'	-5.69	96.95	101.50
31	y	276	G	N9-C1'-C2'	-5.68	105.76	112.00
1	w	338	G	C3'-C2'-C1'	5.67	106.04	101.50
1	w	805	G	N9-C1'-C2'	5.66	121.36	114.00
31	y	773	G	C3'-C2'-C1'	-5.66	96.97	101.50
1	w	271(C)	G	N9-C1'-C2'	5.65	121.35	114.00
31	y	879	C	N1-C1'-C2'	-5.65	105.79	112.00
31	y	281	G	N9-C1'-C2'	-5.64	105.80	112.00
31	y	636	U	C1'-O4'-C4'	-5.62	105.40	109.90
31	y	328	C	OP1-P-O3'	5.62	117.56	105.20
1	w	1126	A	N9-C1'-C2'	5.61	121.30	114.00
1	w	1644	C	N1-C1'-C2'	5.61	121.30	114.00
31	y	246	A	O4'-C1'-N9	5.61	112.69	108.20
1	w	1520	U	N1-C1'-C2'	5.60	121.28	114.00
1	w	1497	U	O4'-C1'-N1	-5.60	103.72	108.20
1	w	715	G	N9-C1'-C2'	-5.59	105.85	112.00
1	w	2463	C	O4'-C1'-N1	5.59	112.67	108.20
1	w	1329	U	C5'-C4'-C3'	-5.58	107.07	116.00
1	w	1846	G	C3'-C2'-C1'	-5.57	97.04	101.50
1	w	974(A)	G	O4'-C1'-N9	5.57	112.65	108.20
1	w	2198	A	N9-C1'-C2'	5.56	121.23	114.00
1	w	2866	U	N1-C1'-C2'	5.54	121.20	114.00
1	w	959	A	N9-C1'-C2'	5.54	121.20	114.00
1	w	1610	A	N9-C1'-C2'	5.53	121.19	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	1634	A	O4'-C1'-N9	5.53	112.62	108.20
1	w	1934	C	C2'-C3'-O3'	5.53	122.54	113.70
1	w	2199	A	P-O3'-C3'	-5.53	113.07	119.70
1	w	664	C	O4'-C1'-N1	5.51	112.61	108.20
1	w	1008	C	N1-C1'-C2'	-5.50	105.95	112.00
31	y	1280	A	O4'-C1'-N9	5.50	112.60	108.20
1	w	41	C	N1-C1'-C2'	-5.50	105.95	112.00
1	w	1516	U	O4'-C1'-N1	5.49	112.59	108.20
1	w	2805	G	OP2-P-O3'	5.48	117.26	105.20
1	w	150	C	O4'-C1'-N1	5.47	112.58	108.20
1	w	1460	A	O4'-C1'-N9	5.47	112.57	108.20
1	w	2049	G	N9-C1'-C2'	-5.47	105.99	112.00
1	w	2712	U	C2-N3-C4	-5.46	123.72	127.00
31	y	348	G	N9-C1'-C2'	5.46	121.10	114.00
1	w	1219	G	N9-C1'-C2'	-5.45	106.01	112.00
1	w	585	G	N9-C1'-C2'	5.45	121.08	114.00
1	w	2000	G	N9-C1'-C2'	-5.45	106.01	112.00
1	w	138	G	N9-C1'-C2'	5.44	121.07	114.00
1	w	1237	A	O4'-C1'-N9	5.44	112.55	108.20
1	w	2031	A	O4'-C1'-N9	5.44	112.55	108.20
1	w	1864	U	P-O3'-C3'	-5.43	113.19	119.70
31	y	501	C	N1-C1'-C2'	-5.42	106.04	112.00
1	w	1128	A	C4-N9-C1'	-5.42	116.55	126.30
31	y	189	U	P-O3'-C3'	-5.42	113.20	119.70
1	w	122(A)	C	P-O3'-C3'	-5.40	113.22	119.70
1	w	1332	G	N9-C1'-C2'	5.40	121.02	114.00
1	w	2725	A	N9-C1'-C2'	5.40	121.02	114.00
1	w	886	C	O4'-C1'-N1	5.40	112.52	108.20
1	w	1185	C	C5'-C4'-C3'	-5.40	107.36	116.00
31	y	1064	G	N9-C1'-C2'	5.39	121.01	114.00
1	w	2382	G	N9-C1'-C2'	5.39	121.01	114.00
1	w	673	C	N1-C1'-C2'	-5.38	106.08	112.00
1	w	2262	U	N1-C1'-C2'	-5.38	106.08	112.00
31	y	10	A	N9-C1'-C2'	-5.37	106.09	112.00
1	w	1297	C	O4'-C1'-N1	5.37	112.50	108.20
1	w	1385	G	C3'-C2'-C1'	5.37	105.79	101.50
1	w	1795	C	N1-C1'-C2'	-5.37	106.10	112.00
2	x	16	G	N9-C1'-C2'	-5.36	106.10	112.00
1	w	2754	U	N1-C1'-C2'	-5.36	106.11	112.00
1	w	1837	C	C3'-C2'-C1'	-5.36	97.21	101.50
1	w	273(A)	G	O4'-C1'-N9	5.35	112.48	108.20
1	w	444	C	O4'-C1'-N1	5.35	112.48	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	2819	G	O4'-C1'-N9	5.34	112.48	108.20
1	w	356	G	O4'-C1'-N9	5.34	112.47	108.20
31	y	1053	G	C2'-C3'-O3'	5.34	122.25	113.70
1	w	99	U	OP1-P-O3'	5.34	116.94	105.20
1	w	1601	G	O4'-C1'-N9	5.33	112.47	108.20
37	e	120	LEU	CA-CB-CG	5.33	127.55	115.30
1	w	2315	G	C3'-C2'-C1'	-5.30	97.26	101.50
1	w	1663	C	N1-C1'-C2'	-5.29	106.18	112.00
1	w	2655	G	N9-C1'-C2'	-5.28	106.19	112.00
31	y	297	G	N9-C1'-C2'	-5.28	106.19	112.00
31	y	1188	A	N9-C1'-C2'	-5.28	106.19	112.00
1	w	576	U	O4'-C1'-N1	5.27	112.42	108.20
31	y	301	G	C3'-C2'-C1'	-5.25	97.30	101.50
1	w	1297	C	N1-C1'-C2'	-5.25	106.22	112.00
31	y	522	C	N1-C1'-C2'	-5.24	106.24	112.00
1	w	1934	C	C3'-C2'-C1'	-5.24	97.31	101.50
1	w	2396	G	C3'-C2'-C1'	-5.24	97.31	101.50
1	w	913	U	P-O3'-C3'	5.23	125.98	119.70
1	w	65	C	C3'-C2'-C1'	-5.23	97.32	101.50
1	w	396	G	N9-C1'-C2'	-5.22	106.26	112.00
1	w	1964	G	N9-C1'-C2'	5.22	120.78	114.00
31	y	708	C	N1-C1'-C2'	-5.20	106.28	112.00
31	y	498	A	P-O3'-C3'	5.19	125.93	119.70
1	w	2603	G	N9-C1'-C2'	-5.18	106.30	112.00
1	w	926	A	C3'-C2'-C1'	-5.18	97.36	101.50
1	w	1992	G	O4'-C1'-N9	-5.18	104.06	108.20
1	w	2504	U	O4'-C1'-N1	5.18	112.34	108.20
31	y	1371	G	N9-C1'-C2'	-5.18	106.31	112.00
1	w	2178	C	O4'-C1'-N1	5.16	112.33	108.20
1	w	2885	C	N1-C1'-C2'	-5.16	106.33	112.00
31	y	185	A	O4'-C1'-N9	5.16	112.33	108.20
1	w	144(B)	A	OP2-P-O3'	5.15	116.54	105.20
31	y	39	G	N9-C1'-C2'	-5.15	106.34	112.00
31	y	901	A	O4'-C1'-N9	-5.14	104.09	108.20
1	w	2374	C	N1-C1'-C2'	-5.14	106.34	112.00
1	w	2014	A	O4'-C1'-N9	-5.14	104.09	108.20
1	w	2358	G	N9-C1'-C2'	-5.14	106.35	112.00
31	y	648	A	C3'-C2'-C1'	-5.13	97.39	101.50
1	w	1079	C	N1-C1'-C2'	-5.13	106.36	112.00
31	y	487	A	O4'-C1'-N9	5.13	112.30	108.20
1	w	2262	U	O4'-C1'-N1	5.13	112.30	108.20
1	w	2394	C	O4'-C1'-N1	5.12	112.30	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	w	1516	U	C3'-C2'-C1'	5.10	105.58	101.50
1	w	2483	C	C3'-C2'-C1'	-5.10	97.42	101.50
31	y	538	G	N9-C1'-C2'	-5.09	106.40	112.00
1	w	1566	A	C2'-C3'-O3'	5.09	121.84	113.70
1	w	2848	G	O4'-C1'-N9	5.09	112.27	108.20
31	y	189	U	C3'-C2'-C1'	5.08	105.56	101.50
1	w	1953	A	O4'-C1'-N9	5.08	112.26	108.20
31	y	18	C	N1-C1'-C2'	-5.08	106.42	112.00
1	w	211	A	N9-C1'-C2'	-5.06	106.43	112.00
1	w	479	A	N9-C1'-C2'	5.06	120.58	114.00
1	w	1863	G	C3'-C2'-C1'	5.06	105.55	101.50
1	w	1553	A	O4'-C1'-N9	5.06	112.25	108.20
1	w	2866	U	O4'-C1'-N1	5.06	112.25	108.20
1	w	1149	G	C1'-O4'-C4'	-5.05	105.86	109.90
1	w	150	C	C1'-O4'-C4'	-5.05	105.86	109.90
1	w	2676	C	C3'-C2'-C1'	-5.05	97.46	101.50
31	y	1061	G	O4'-C1'-N9	5.05	112.24	108.20
1	w	2712	U	C5-C4-O4	-5.04	122.87	125.90
31	y	509	A	C3'-C2'-C1'	-5.04	97.47	101.50
1	w	552	G	C8-N9-C4	-5.04	104.38	106.40
31	y	8	A	O4'-C1'-N9	5.04	112.23	108.20
1	w	177	G	N9-C1'-C2'	5.04	120.55	114.00
1	w	2036	C	O4'-C1'-N1	5.04	112.23	108.20
13	K	37	LEU	CA-CB-CG	5.04	126.88	115.30
1	w	2208	U	O4'-C1'-N1	5.03	112.23	108.20
1	w	1128	A	C8-N9-C1'	5.03	136.76	127.70
1	w	616	A	C4'-C3'-C2'	-5.03	97.57	102.60
1	w	33	U	N1-C1'-C2'	-5.02	106.47	112.00
1	w	1748	G	N9-C1'-C2'	-5.02	106.47	112.00
31	y	824	C	N1-C1'-C2'	-5.02	106.48	112.00
1	w	2414	G	C3'-C2'-C1'	-5.00	97.50	101.50
1	w	2471	C	C4'-C3'-C2'	5.00	107.60	102.60

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	x	14	U	C3'
2	x	24	G	C3'

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	w	1191	G	Sidechain
1	w	1231	G	Sidechain
1	w	1247	A	Sidechain
1	w	1274	A	Sidechain
1	w	1323	U	Sidechain
1	w	138	G	Sidechain
1	w	1497	U	Sidechain
1	w	1577	C	Sidechain
1	w	1626	G	Sidechain
1	w	1627	G	Sidechain
1	w	1822	G	Sidechain
1	w	1934	C	Sidechain
1	w	1973	G	Sidechain
1	w	2061	G	Sidechain
1	w	2158	A	Sidechain
1	w	241	A	Sidechain
1	w	2451	A	Sidechain
1	w	2662	A	Sidechain
1	w	2756	U	Sidechain
1	w	338	G	Sidechain
1	w	566	U	Sidechain
1	w	74	A	Sidechain
1	w	801	G	Sidechain
1	w	974(A)	G	Sidechain
31	y	1053	G	Sidechain
31	y	1080	A	Sidechain
31	y	1338	G	Sidechain
31	y	1346	A	Sidechain
31	y	299	G	Sidechain
31	y	832	C	Sidechain
31	y	915	A	Sidechain
31	y	938	A	Sidechain

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%)	54 (44%)	39 (32%)	30 (24%)	0	0
4	B	270/276 (98%)	103 (38%)	84 (31%)	83 (31%)	0	0
5	C	199/206 (97%)	89 (45%)	48 (24%)	62 (31%)	0	0
6	D	192/205 (94%)	76 (40%)	54 (28%)	62 (32%)	0	0
7	E	178/182 (98%)	84 (47%)	53 (30%)	41 (23%)	0	0
8	F	171/180 (95%)	76 (44%)	53 (31%)	42 (25%)	0	0
9	G	146/148 (99%)	75 (51%)	30 (20%)	41 (28%)	0	0
10	H	136/163 (83%)	48 (35%)	40 (29%)	48 (35%)	0	0
11	I	120/122 (98%)	50 (42%)	37 (31%)	33 (28%)	0	0
12	J	144/150 (96%)	59 (41%)	39 (27%)	46 (32%)	0	0
13	K	135/141 (96%)	52 (38%)	44 (33%)	39 (29%)	0	0
14	L	116/118 (98%)	60 (52%)	28 (24%)	28 (24%)	0	0
15	M	104/112 (93%)	40 (38%)	31 (30%)	33 (32%)	0	0
16	N	135/146 (92%)	59 (44%)	36 (27%)	40 (30%)	0	0
17	O	115/118 (98%)	64 (56%)	27 (24%)	24 (21%)	0	1
18	P	99/101 (98%)	30 (30%)	32 (32%)	37 (37%)	0	0
19	Q	107/113 (95%)	49 (46%)	30 (28%)	28 (26%)	0	0
20	R	90/96 (94%)	28 (31%)	29 (32%)	33 (37%)	0	0
21	S	101/110 (92%)	36 (36%)	34 (34%)	31 (31%)	0	0
22	T	183/206 (89%)	104 (57%)	41 (22%)	38 (21%)	0	1
23	U	74/85 (87%)	35 (47%)	23 (31%)	16 (22%)	0	1
24	V	86/98 (88%)	30 (35%)	31 (36%)	25 (29%)	0	0
25	W	60/72 (83%)	28 (47%)	12 (20%)	20 (33%)	0	0
26	X	58/60 (97%)	32 (55%)	15 (26%)	11 (19%)	0	1
27	Y	54/60 (90%)	22 (41%)	12 (22%)	20 (37%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Z	46/49 (94%)	25 (54%)	9 (20%)	12 (26%)	0	0
29	a	61/65 (94%)	20 (33%)	22 (36%)	19 (31%)	0	0
30	b	33/37 (89%)	22 (67%)	5 (15%)	6 (18%)	0	2
35	c	232/256 (91%)	109 (47%)	66 (28%)	57 (25%)	0	0
36	d	204/239 (85%)	98 (48%)	49 (24%)	57 (28%)	0	0
37	e	206/209 (99%)	99 (48%)	44 (21%)	63 (31%)	0	0
38	f	148/162 (91%)	89 (60%)	33 (22%)	26 (18%)	0	2
39	g	99/101 (98%)	61 (62%)	24 (24%)	14 (14%)	0	4
40	h	153/156 (98%)	84 (55%)	40 (26%)	29 (19%)	0	1
41	i	136/138 (99%)	71 (52%)	35 (26%)	30 (22%)	0	1
42	j	125/128 (98%)	73 (58%)	31 (25%)	21 (17%)	0	3
43	k	96/105 (91%)	50 (52%)	24 (25%)	22 (23%)	0	0
44	l	114/129 (88%)	59 (52%)	28 (25%)	27 (24%)	0	0
45	m	122/132 (92%)	51 (42%)	32 (26%)	39 (32%)	0	0
46	n	123/126 (98%)	53 (43%)	35 (28%)	35 (28%)	0	0
47	o	58/61 (95%)	22 (38%)	19 (33%)	17 (29%)	0	0
48	p	86/89 (97%)	46 (54%)	23 (27%)	17 (20%)	0	1
49	q	81/88 (92%)	37 (46%)	28 (35%)	16 (20%)	0	1
50	r	102/105 (97%)	46 (45%)	31 (30%)	25 (24%)	0	0
51	s	71/88 (81%)	42 (59%)	12 (17%)	17 (24%)	0	0
52	t	78/93 (84%)	26 (33%)	31 (40%)	21 (27%)	0	0
53	u	97/106 (92%)	42 (43%)	37 (38%)	18 (19%)	0	1
54	v	22/27 (82%)	11 (50%)	7 (32%)	4 (18%)	0	2
All	All	5689/6186 (92%)	2619 (46%)	1567 (28%)	1503 (26%)	0	0

All (1503) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	63	VAL
3	A	179	ALA
3	A	180	SER
3	A	201	LYS
3	A	203	GLU
3	A	209	PHE

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Mol	Chain	Res	Type
3	A	210	LEU
3	A	224	ARG
4	B	4	LYS
4	B	15	PHE
4	B	28	GLU
4	B	39	LYS
4	B	53	PHE
4	B	58	HIS
4	B	75	ILE
4	B	80	ALA
4	B	81	ALA
4	B	83	GLU
4	B	90	ALA
4	B	99	ASP
4	B	105	ILE
4	B	115	GLN
4	B	124	PRO
4	B	127	VAL
4	B	146	GLU
4	B	149	PRO
4	B	157	ARG
4	B	158	ALA
4	B	178	PRO
4	B	181	GLU
4	B	196	VAL
4	B	198	ASN
4	B	223	GLY
4	B	224	ALA
4	B	227	ASN
4	B	228	PRO
4	B	229	VAL
4	B	244	ARG
4	B	248	SER
4	B	249	PRO
4	B	257	LEU
4	B	262	ARG
4	B	272	ALA
5	C	11	MET
5	C	12	THR
5	C	16	ARG
5	C	37	ARG
5	C	60	ASN

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Mol	Chain	Res	Type
5	C	61	ARG
5	C	64	LYS
5	C	77	ILE
5	C	82	ARG
5	C	89	ASP
5	C	116	VAL
5	C	131	ALA
5	C	134	ILE
5	C	143	ASN
5	C	149	ARG
5	C	154	LYS
5	C	155	LYS
5	C	157	ALA
5	C	178	GLU
5	C	187	ALA
5	C	198	VAL
5	C	201	THR
6	D	15	LEU
6	D	17	ALA
6	D	23	ILE
6	D	26	HIS
6	D	30	GLU
6	D	48	THR
6	D	57	ARG
6	D	58	LYS
6	D	59	ILE
6	D	60	TRP
6	D	65	THR
6	D	87	PRO
6	D	92	TYR
6	D	101	ARG
6	D	119	LEU
6	D	120	LEU
6	D	121	VAL
6	D	122	GLU
6	D	128	ASN
6	D	148	SER
6	D	157	LEU
6	D	165	LEU
6	D	172	ALA
6	D	196	VAL
7	E	6	ALA

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Mol	Chain	Res	Type
7	E	8	LYS
7	E	13	GLU
7	E	20	ILE
7	E	23	PHE
7	E	33	ARG
7	E	49	ASP
7	E	60	LEU
7	E	84	LYS
7	E	86	MET
7	E	88	ILE
7	E	116	ASP
8	F	42	ARG
8	F	55	PRO
8	F	58	GLU
8	F	109	PHE
8	F	118	PRO
8	F	126	PRO
8	F	152	ARG
8	F	153	LYS
8	F	155	SER
8	F	160	LYS
8	F	162	ILE
8	F	178	ALA
9	G	2	LYS
9	G	9	LEU
9	G	14	ASP
9	G	21	VAL
9	G	25	TYR
9	G	35	LEU
9	G	38	LEU
9	G	74	ASN
9	G	82	ARG
9	G	88	ILE
9	G	91	SER
9	G	92	VAL
9	G	93	THR
9	G	120	ILE
9	G	125	GLU
9	G	138	ILE
9	G	147	GLN
10	H	27	TYR
10	H	34	PRO

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Mol	Chain	Res	Type
10	H	40	ASP
10	H	51	THR
10	H	58	ARG
10	H	67	PRO
10	H	74	PHE
10	H	79	ASN
10	H	83	ILE
10	H	85	VAL
10	H	111	GLU
10	H	114	LEU
10	H	121	VAL
10	H	125	ALA
10	H	130	LEU
10	H	146	TYR
10	H	147	ALA
10	H	156	GLN
10	H	157	ARG
11	I	5	GLN
11	I	28	SER
11	I	48	PRO
11	I	51	ALA
11	I	64	ARG
11	I	67	LYS
11	I	70	LYS
11	I	87	ILE
11	I	91	LEU
11	I	102	VAL
11	I	114	ILE
11	I	115	VAL
12	J	14	LYS
12	J	19	VAL
12	J	23	PRO
12	J	35	HIS
12	J	46	LYS
12	J	47	ASP
12	J	51	PHE
12	J	56	SER
12	J	61	ARG
12	J	71	VAL
12	J	83	VAL
12	J	86	LYS
12	J	90	ARG

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Mol	Chain	Res	Type
12	J	97	PRO
12	J	101	VAL
12	J	108	LYS
12	J	115	LEU
12	J	129	ALA
12	J	148	LEU
13	K	4	PRO
13	K	8	LYS
13	K	9	TYR
13	K	12	GLN
13	K	18	LYS
13	K	21	THR
13	K	22	LYS
13	K	27	VAL
13	K	32	PHE
13	K	45	GLN
13	K	52	VAL
13	K	59	ARG
13	K	63	LYS
13	K	68	ILE
13	K	73	PRO
13	K	81	VAL
13	K	82	ARG
13	K	89	ASN
13	K	90	VAL
13	K	111	GLU
13	K	133	ARG
14	L	2	ARG
14	L	4	LEU
14	L	5	LYS
14	L	8	ARG
14	L	10	LEU
14	L	12	ARG
14	L	39	PRO
14	L	43	GLU
14	L	45	ARG
14	L	60	LEU
14	L	62	ALA
14	L	64	ARG
14	L	67	LEU
14	L	72	ASP
14	L	74	LYS

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Mol	Chain	Res	Type
14	L	117	VAL
15	M	9	ARG
15	M	10	ARG
15	M	12	PHE
15	M	14	VAL
15	M	18	ILE
15	M	25	ARG
15	M	35	ILE
15	M	43	GLU
15	M	45	GLY
15	M	48	LEU
15	M	69	VAL
15	M	73	LEU
15	M	85	VAL
15	M	86	ALA
15	M	87	PHE
15	M	92	TYR
16	N	2	ASN
16	N	22	PHE
16	N	24	PRO
16	N	30	VAL
16	N	33	LYS
16	N	36	GLU
16	N	42	ILE
16	N	47	GLY
16	N	49	VAL
16	N	55	ASN
16	N	65	LYS
16	N	66	VAL
16	N	67	SER
16	N	79	HIS
16	N	88	ILE
16	N	90	GLN
16	N	107	ASP
17	O	9	VAL
17	O	26	GLY
17	O	49	HIS
17	O	62	ILE
17	O	64	ARG
17	O	76	TYR
17	O	77	SER
17	O	86	ALA

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Mol	Chain	Res	Type
17	O	91	ASP
17	O	93	LYS
17	O	96	ALA
17	O	112	ARG
18	P	5	VAL
18	P	15	GLU
18	P	16	PRO
18	P	22	VAL
18	P	27	ALA
18	P	28	GLU
18	P	47	VAL
18	P	50	PRO
18	P	51	VAL
18	P	66	ARG
18	P	74	LYS
18	P	77	ALA
18	P	79	VAL
18	P	84	LYS
18	P	90	PRO
18	P	99	ILE
18	P	100	ARG
19	Q	18	ARG
19	Q	30	GLU
19	Q	31	GLU
19	Q	35	ILE
19	Q	43	GLY
19	Q	45	TYR
19	Q	47	VAL
19	Q	63	ASP
19	Q	66	GLU
19	Q	88	ARG
19	Q	96	ILE
19	Q	103	ILE
20	R	5	TYR
20	R	11	PRO
20	R	12	VAL
20	R	14	SER
20	R	35	THR
20	R	37	THR
20	R	42	ALA
20	R	52	VAL
20	R	58	HIS

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Mol	Chain	Res	Type
20	R	59	VAL
20	R	60	ARG
20	R	64	LYS
20	R	65	ARG
20	R	69	TYR
20	R	81	VAL
20	R	82	GLN
20	R	84	ALA
20	R	88	LYS
20	R	89	ILE
21	S	9	LYS
21	S	13	VAL
21	S	37	VAL
21	S	39	VAL
21	S	52	SER
21	S	55	TYR
21	S	60	PHE
21	S	61	ILE
21	S	66	PRO
21	S	68	HIS
21	S	74	PRO
21	S	75	ILE
21	S	88	LYS
21	S	90	LEU
21	S	94	LYS
21	S	99	CYS
21	S	101	LYS
22	T	7	ALA
22	T	13	GLU
22	T	15	PRO
22	T	16	SER
22	T	41	LEU
22	T	42	VAL
22	T	46	LYS
22	T	72	ARG
22	T	73	GLN
22	T	78	LYS
22	T	83	PRO
22	T	95	PRO
22	T	120	ILE
22	T	153	SER
22	T	154	ASP

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Mol	Chain	Res	Type
22	T	155	LEU
22	T	165	VAL
22	T	184	ALA
23	U	20	ARG
23	U	30	VAL
23	U	31	VAL
23	U	47	PRO
23	U	58	THR
23	U	63	VAL
23	U	64	ASP
23	U	81	VAL
24	V	11	ARG
24	V	24	ALA
24	V	33	LYS
24	V	66	HIS
24	V	69	LYS
24	V	70	VAL
24	V	75	GLU
24	V	82	LEU
24	V	83	GLU
24	V	85	LEU
24	V	86	SER
25	W	9	GLN
25	W	13	ALA
25	W	32	LEU
25	W	33	MET
25	W	46	GLN
25	W	54	LYS
26	X	8	LEU
26	X	9	VAL
26	X	12	PRO
26	X	30	ARG
26	X	57	GLU
27	Y	8	LYS
27	Y	35	GLU
27	Y	51	TYR
27	Y	52	TYR
27	Y	55	ARG
28	Z	2	LYS
28	Z	3	ARG
28	Z	9	ARG
28	Z	17	GLY

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Mol	Chain	Res	Type
28	Z	18	PHE
28	Z	22	MET
28	Z	44	PRO
29	a	6	THR
29	a	18	ALA
29	a	19	SER
29	a	29	LYS
29	a	30	ARG
29	a	36	LYS
29	a	40	GLU
29	a	41	ILE
29	a	42	ARG
29	a	51	ALA
29	a	57	ARG
30	b	3	VAL
30	b	10	ILE
35	c	13	ALA
35	c	21	ARG
35	c	24	TRP
35	c	45	GLN
35	c	47	THR
35	c	58	ILE
35	c	107	THR
35	c	109	SER
35	c	130	ARG
35	c	157	ARG
35	c	160	ASP
35	c	172	ILE
35	c	174	VAL
35	c	181	PHE
35	c	190	THR
35	c	195	ASP
35	c	207	ALA
36	d	4	LYS
36	d	12	LEU
36	d	18	TRP
36	d	20	SER
36	d	29	TYR
36	d	30	ARG
36	d	43	LEU
36	d	45	LYS
36	d	47	LEU

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Mol	Chain	Res	Type
36	d	49	SER
36	d	50	ALA
36	d	56	ASP
36	d	61	ALA
36	d	62	ASP
36	d	108	ASN
36	d	127	ARG
36	d	128	PHE
36	d	133	ALA
36	d	146	ALA
36	d	152	ILE
36	d	156	ARG
36	d	161	GLU
36	d	170	GLN
36	d	195	VAL
37	e	22	LYS
37	e	34	GLU
37	e	35	ARG
37	e	52	SER
37	e	59	ARG
37	e	66	ARG
37	e	67	ILE
37	e	79	PHE
37	e	81	GLU
37	e	111	ALA
37	e	113	SER
37	e	140	VAL
37	e	148	VAL
37	e	152	SER
37	e	156	GLU
37	e	178	VAL
37	e	196	LEU
37	e	205	GLU
37	e	206	PHE
38	f	56	GLN
38	f	70	PRO
38	f	73	ASN
38	f	77	PRO
38	f	84	PHE
38	f	144	THR
38	f	152	ARG
39	g	45	LEU

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Mol	Chain	Res	Type
39	g	95	GLU
39	g	99	ALA
40	h	4	ARG
40	h	31	MET
40	h	32	ARG
40	h	65	ALA
40	h	80	VAL
40	h	113	GLU
40	h	117	ALA
40	h	118	VAL
40	h	119	ARG
41	i	19	VAL
41	i	25	ASP
41	i	27	PRO
41	i	50	ARG
41	i	60	ARG
41	i	68	ARG
41	i	79	VAL
41	i	97	VAL
41	i	132	GLU
42	j	3	GLN
42	j	37	PHE
42	j	41	VAL
42	j	91	ASP
42	j	105	ASP
42	j	117	HIS
43	k	18	ALA
43	k	26	ALA
43	k	30	SER
43	k	57	LYS
43	k	58	ASP
43	k	72	VAL
43	k	94	VAL
44	l	54	ARG
44	l	71	LYS
44	l	91	ARG
44	l	123	LYS
45	m	7	ASN
45	m	8	GLN
45	m	24	PRO
45	m	28	GLY
45	m	37	THR

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Mol	Chain	Res	Type
45	m	40	ARG
45	m	46	LYS
45	m	65	VAL
45	m	72	GLU
45	m	73	GLY
45	m	74	HIS
45	m	75	ASN
45	m	78	GLU
45	m	103	VAL
45	m	104	TYR
45	m	109	VAL
45	m	119	TYR
46	n	7	VAL
46	n	12	ASN
46	n	19	LEU
46	n	27	LYS
46	n	57	ARG
46	n	77	ASN
46	n	94	ARG
46	n	98	VAL
46	n	108	ARG
46	n	113	PRO
46	n	122	LYS
46	n	124	PRO
47	o	6	LEU
47	o	8	GLU
47	o	16	PHE
47	o	21	TYR
47	o	50	LYS
47	o	56	VAL
47	o	60	SER
48	p	3	ILE
48	p	6	GLU
48	p	27	VAL
48	p	28	GLN
48	p	29	VAL
48	p	45	VAL
48	p	46	HIS
48	p	49	ASP
49	q	3	LYS
49	q	13	HIS
49	q	17	TYR

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Mol	Chain	Res	Type
49	q	23	ASP
49	q	26	ARG
49	q	34	GLU
49	q	36	ILE
49	q	64	ALA
49	q	66	PRO
49	q	77	ALA
50	r	27	PHE
50	r	33	GLY
50	r	47	PRO
50	r	55	ASP
50	r	74	LEU
50	r	75	ARG
50	r	95	TYR
51	s	17	SER
51	s	48	GLY
51	s	83	GLU
52	t	5	LEU
52	t	6	LYS
52	t	9	VAL
52	t	37	ARG
52	t	43	GLU
52	t	44	MET
52	t	47	HIS
52	t	52	TYR
52	t	61	TYR
52	t	67	VAL
52	t	69	HIS
52	t	79	THR
53	u	48	LYS
53	u	75	ASN
53	u	93	GLU
54	v	22	ARG
54	v	23	PRO
3	A	9	ARG
3	A	15	VAL
3	A	18	ASN
3	A	30	VAL
3	A	163	GLU
3	A	171	ALA
3	A	196	ALA
4	B	41	GLY

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Mol	Chain	Res	Type
4	B	45	ASN
4	B	54	ARG
4	B	65	ILE
4	B	91	ARG
4	B	98	VAL
4	B	113	VAL
4	B	114	GLY
4	B	152	GLY
4	B	156	ALA
4	B	201	HIS
4	B	206	LEU
4	B	222	ARG
4	B	232	PRO
4	B	235	GLY
4	B	237	GLU
4	B	245	PRO
4	B	253	GLN
4	B	258	LYS
4	B	263	ARG
5	C	13	ARG
5	C	35	GLN
5	C	44	TYR
5	C	55	ASN
5	C	68	ALA
5	C	86	PRO
5	C	88	GLY
5	C	112	GLY
5	C	127	ASP
5	C	132	HIS
5	C	133	LYS
5	C	139	GLY
5	C	151	TYR
5	C	184	VAL
6	D	28	LEU
6	D	38	LYS
6	D	53	ALA
6	D	63	LYS
6	D	66	GLY
6	D	71	GLY
6	D	73	ILE
6	D	83	VAL
6	D	97	PRO

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Mol	Chain	Res	Type
6	D	117	LYS
6	D	125	ALA
6	D	145	GLY
6	D	154	GLY
6	D	160	ARG
6	D	185	GLU
6	D	191	LEU
7	E	59	GLU
7	E	75	LYS
7	E	79	ASN
7	E	87	PRO
7	E	151	ALA
7	E	163	ALA
7	E	164	GLU
7	E	173	LEU
8	F	8	PRO
8	F	18	GLU
8	F	24	VAL
8	F	40	GLU
8	F	54	ARG
8	F	65	HIS
8	F	71	LEU
9	G	20	ASP
9	G	22	LYS
9	G	39	ALA
9	G	81	VAL
9	G	83	ALA
9	G	86	THR
9	G	94	ALA
9	G	107	ILE
9	G	113	ARG
9	G	117	GLU
9	G	134	PRO
9	G	137	PRO
10	H	39	ILE
10	H	42	GLU
10	H	50	ALA
10	H	84	ARG
10	H	108	ILE
10	H	122	LEU
10	H	124	HIS
10	H	127	LYS

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Mol	Chain	Res	Type
10	H	148	GLY
11	I	13	ASN
11	I	29	ASN
11	I	49	ARG
11	I	85	VAL
11	I	86	ILE
11	I	88	ASN
11	I	94	ARG
11	I	103	ALA
12	J	11	GLY
12	J	28	GLY
12	J	32	THR
12	J	40	SER
12	J	65	ARG
12	J	67	MET
12	J	70	GLN
12	J	93	GLY
12	J	102	ARG
12	J	104	GLY
12	J	141	ALA
13	K	2	LEU
13	K	20	ALA
13	K	25	ASP
13	K	46	GLN
13	K	115	MET
13	K	136	ALA
14	L	28	LEU
14	L	32	GLY
14	L	102	GLU
15	M	39	ILE
15	M	42	ASP
15	M	67	ARG
15	M	68	GLN
15	M	91	PRO
16	N	4	GLY
16	N	28	VAL
16	N	45	PHE
16	N	46	GLU
16	N	68	TYR
16	N	71	GLY
16	N	77	PRO
16	N	94	ALA

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Mol	Chain	Res	Type
16	N	97	ALA
16	N	120	ARG
17	O	58	ARG
17	O	67	ALA
17	O	92	ARG
17	O	113	ALA
17	O	115	ALA
18	P	8	GLY
18	P	14	VAL
18	P	43	GLU
18	P	45	THR
18	P	76	LYS
18	P	91	TYR
18	P	93	GLU
19	Q	32	ALA
19	Q	41	LYS
20	R	6	ASP
20	R	13	LEU
20	R	20	GLY
20	R	25	LYS
20	R	36	LYS
20	R	93	GLU
21	S	7	VAL
21	S	38	ILE
21	S	50	ARG
21	S	54	LYS
21	S	63	LYS
21	S	65	ALA
21	S	73	ARG
21	S	96	ILE
22	T	12	GLY
22	T	39	VAL
22	T	49	ARG
22	T	63	ASP
22	T	90	VAL
22	T	133	ILE
22	T	182	LYS
23	U	16	SER
23	U	50	ASN
24	V	12	PRO
24	V	23	LYS
24	V	44	PRO

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Mol	Chain	Res	Type
24	V	52	ARG
24	V	56	GLN
24	V	68	PRO
24	V	74	VAL
24	V	78	LYS
24	V	88	LYS
24	V	89	GLU
25	W	11	GLU
25	W	14	ARG
25	W	19	VAL
25	W	39	ALA
25	W	42	GLY
25	W	44	LEU
25	W	47	ASN
25	W	51	ARG
26	X	32	GLN
26	X	53	LEU
26	X	58	VAL
27	Y	18	ALA
27	Y	30	LEU
27	Y	34	PRO
27	Y	42	PRO
27	Y	57	VAL
28	Z	7	PRO
29	a	35	GLN
29	a	38	GLY
29	a	59	LYS
30	b	4	ARG
30	b	9	ARG
30	b	20	HIS
35	c	9	GLU
35	c	15	VAL
35	c	29	ALA
35	c	52	GLU
35	c	62	ALA
35	c	77	ALA
35	c	88	ALA
35	c	93	VAL
35	c	100	GLY
35	c	106	LYS
35	c	115	LEU
35	c	150	SER

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Mol	Chain	Res	Type
35	c	153	ARG
35	c	155	LEU
35	c	165	VAL
35	c	171	ALA
35	c	194	PRO
36	d	8	ILE
36	d	15	THR
36	d	36	ASP
36	d	48	TYR
36	d	51	GLY
36	d	63	ASN
36	d	90	GLU
36	d	98	ASN
36	d	109	PRO
36	d	132	ARG
36	d	164	ARG
36	d	178	LEU
36	d	196	LEU
36	d	200	ALA
37	e	5	ILE
37	e	18	LYS
37	e	19	LEU
37	e	24	GLU
37	e	29	PRO
37	e	85	LYS
37	e	88	VAL
37	e	91	SER
37	e	109	GLY
37	e	134	ASP
37	e	151	LYS
37	e	179	GLU
37	e	181	MET
37	e	204	ILE
38	f	49	PRO
38	f	100	VAL
38	f	104	ALA
38	f	117	ASP
38	f	126	ARG
38	f	131	ILE
39	g	7	ASN
39	g	16	GLN
40	h	7	ALA

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Mol	Chain	Res	Type
40	h	89	MET
40	h	116	ALA
40	h	128	ALA
40	h	153	HIS
41	i	20	TYR
41	i	24	THR
41	i	45	ILE
41	i	46	LYS
41	i	51	VAL
41	i	82	HIS
41	i	91	ARG
41	i	108	GLY
42	j	24	GLY
42	j	46	ALA
42	j	53	VAL
42	j	69	GLY
42	j	100	GLY
42	j	119	ALA
43	k	6	ILE
43	k	14	LYS
43	k	17	ASP
43	k	51	ARG
43	k	55	LYS
43	k	61	GLU
43	k	74	ILE
44	l	13	GLN
44	l	52	GLY
44	l	60	ALA
44	l	78	GLN
44	l	96	ARG
44	l	98	LEU
45	m	9	LEU
45	m	14	ARG
45	m	15	GLU
45	m	21	SER
45	m	36	CYS
45	m	44	PRO
45	m	71	GLY
45	m	99	ILE
45	m	115	SER
45	m	124	PRO
46	n	6	GLY

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Mol	Chain	Res	Type
46	n	20	THR
46	n	22	ILE
46	n	39	ILE
46	n	45	VAL
46	n	48	LEU
46	n	66	LEU
46	n	67	GLU
46	n	74	VAL
46	n	118	ALA
47	o	3	ARG
47	o	42	ILE
48	p	50	HIS
48	p	72	ARG
48	p	81	LEU
49	q	43	LYS
49	q	53	VAL
49	q	76	GLN
50	r	17	LYS
50	r	32	TYR
50	r	34	LYS
50	r	40	LYS
50	r	50	LYS
50	r	56	VAL
50	r	96	GLN
51	s	20	ALA
51	s	42	ARG
51	s	44	LEU
51	s	53	ARG
51	s	58	LEU
51	s	82	THR
51	s	85	LEU
52	t	3	ARG
52	t	51	VAL
52	t	66	MET
52	t	80	TYR
53	u	9	ASN
53	u	50	GLU
53	u	71	THR
53	u	80	ARG
53	u	99	LEU
54	v	18	TYR
3	A	8	TYR

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Mol	Chain	Res	Type
3	A	19	LYS
3	A	29	LEU
3	A	36	ALA
3	A	176	VAL
3	A	211	ARG
3	A	221	PRO
3	A	223	VAL
4	B	3	VAL
4	B	33	LEU
4	B	73	VAL
4	B	107	ALA
4	B	116	GLN
4	B	137	PRO
4	B	170	GLY
4	B	226	MET
4	B	236	GLY
4	B	238	GLY
4	B	239	ARG
4	B	242	ARG
5	C	53	PRO
5	C	56	PRO
5	C	117	MET
5	C	119	ARG
5	C	129	HIS
5	C	169	ASN
6	D	18	ASP
6	D	56	GLY
6	D	70	HIS
6	D	88	LYS
6	D	106	ALA
6	D	132	LYS
6	D	146	SER
6	D	163	ARG
6	D	167	TRP
6	D	173	PRO
6	D	186	ARG
7	E	9	ARG
7	E	82	LEU
7	E	138	GLN
7	E	152	LEU
8	F	9	ILE
8	F	13	LYS

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Mol	Chain	Res	Type
8	F	20	ALA
8	F	32	GLU
8	F	60	ARG
8	F	170	ARG
9	G	8	PRO
9	G	23	PRO
10	H	64	ASP
10	H	65	TRP
10	H	93	LYS
10	H	131	PRO
10	H	132	LYS
10	H	150	ASP
11	I	24	VAL
11	I	33	ALA
11	I	63	VAL
11	I	113	LYS
12	J	16	ARG
12	J	52	GLU
12	J	117	GLU
12	J	122	PRO
12	J	145	PRO
13	K	13	GLN
14	L	6	SER
14	L	42	LYS
15	M	17	ARG
15	M	20	ARG
15	M	56	LEU
15	M	72	ALA
16	N	12	SER
16	N	29	ARG
16	N	62	THR
16	N	96	ARG
16	N	103	ARG
16	N	135	VAL
17	O	25	TRP
17	O	47	TYR
17	O	57	PHE
17	O	87	GLY
17	O	90	VAL
17	O	99	ALA
18	P	29	PRO
19	Q	34	ASN

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Mol	Chain	Res	Type
19	Q	73	ALA
19	Q	87	PRO
19	Q	97	LYS
20	R	32	PRO
20	R	72	LYS
20	R	78	LYS
21	S	20	TYR
21	S	35	TYR
22	T	45	ASP
22	T	80	ARG
22	T	152	ALA
22	T	183	LEU
23	U	44	ARG
24	V	26	ARG
24	V	46	LEU
25	W	2	LYS
27	Y	7	PRO
27	Y	16	ARG
27	Y	24	ALA
27	Y	28	PRO
27	Y	32	PRO
27	Y	39	MET
28	Z	13	ALA
28	Z	31	LEU
28	Z	33	ARG
29	a	48	PHE
29	a	56	GLU
35	c	12	GLU
35	c	26	PRO
35	c	51	LEU
35	c	141	GLU
35	c	142	LEU
35	c	145	LEU
35	c	210	SER
35	c	212	GLN
36	d	17	ASP
36	d	40	ARG
36	d	110	ASN
36	d	122	GLU
37	e	10	ARG
37	e	36	ARG
37	e	37	PRO

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Mol	Chain	Res	Type
37	e	48	ALA
37	e	49	ARG
37	e	51	PRO
37	e	84	LYS
37	e	89	THR
37	e	122	ARG
37	e	168	ARG
37	e	174	LEU
37	e	202	LEU
37	e	208	SER
38	f	48	ALA
38	f	50	GLU
38	f	65	ASN
38	f	71	LEU
38	f	97	GLY
38	f	135	THR
39	g	41	GLU
39	g	82	ARG
40	h	17	VAL
40	h	68	ASN
40	h	93	PRO
40	h	100	ALA
40	h	129	GLU
40	h	130	GLY
41	i	16	ALA
41	i	106	GLY
41	i	121	ASP
42	j	29	ASN
42	j	97	LYS
42	j	111	ARG
43	k	8	LEU
43	k	13	HIS
43	k	39	PRO
43	k	71	LEU
44	l	15	ALA
44	l	59	TYR
44	l	72	ALA
44	l	101	SER
44	l	121	PRO
45	m	26	LEU
45	m	82	VAL
45	m	93	PRO

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Mol	Chain	Res	Type
45	m	111	ASP
45	m	120	GLY
46	n	29	ARG
46	n	105	THR
46	n	106	ASN
46	n	121	LYS
47	o	15	LYS
47	o	59	ALA
48	p	5	LYS
48	p	51	HIS
48	p	54	ARG
48	p	79	ARG
49	q	15	PRO
49	q	55	ARG
49	q	82	GLN
50	r	12	SER
50	r	13	ASP
50	r	30	PRO
50	r	41	LYS
50	r	45	HIS
50	r	46	ASP
51	s	84	LYS
51	s	87	ARG
52	t	42	PRO
52	t	54	GLY
53	u	43	LEU
53	u	98	PRO
54	v	24	ARG
3	A	168	LYS
4	B	57	GLY
4	B	106	ILE
4	B	204	ILE
5	C	18	ASP
5	C	45	THR
5	C	121	ASN
5	C	130	GLY
5	C	145	LYS
5	C	177	PRO
5	C	183	LEU
5	C	188	VAL
5	C	192	ASN
5	C	199	ARG

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Mol	Chain	Res	Type
6	D	39	ARG
6	D	61	PRO
6	D	80	GLY
6	D	91	ASP
6	D	96	LEU
6	D	104	GLY
6	D	116	GLY
7	E	22	ARG
7	E	73	ALA
7	E	124	SER
7	E	127	GLY
7	E	136	ARG
7	E	166	ASP
8	F	25	LYS
8	F	59	ARG
8	F	173	PRO
9	G	7	GLU
9	G	29	TYR
9	G	69	LYS
9	G	75	LEU
9	G	119	PRO
9	G	135	GLU
10	H	101	TYR
11	I	27	GLY
11	I	54	GLU
11	I	89	ASN
12	J	50	ARG
12	J	55	ARG
12	J	89	ALA
12	J	110	TYR
13	K	6	ARG
13	K	31	ASP
13	K	54	MET
13	K	132	VAL
14	L	41	ALA
14	L	50	HIS
14	L	52	ILE
14	L	84	ALA
15	M	37	ALA
15	M	62	LYS
15	M	64	GLU
16	N	31	SER

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Mol	Chain	Res	Type
16	N	80	SER
16	N	128	GLU
18	P	36	PRO
18	P	53	GLU
18	P	55	ALA
19	Q	5	ALA
19	Q	33	ARG
19	Q	44	ALA
19	Q	72	LYS
20	R	7	VAL
20	R	18	TYR
20	R	48	LYS
20	R	77	LYS
21	S	40	GLU
22	T	6	LYS
22	T	29	TYR
22	T	103	ARG
22	T	147	GLY
23	U	41	ARG
23	U	53	MET
23	U	69	PHE
25	W	35	LEU
25	W	56	GLN
26	X	44	ARG
26	X	51	ALA
27	Y	43	HIS
28	Z	20	ALA
29	a	32	LEU
29	a	54	GLU
35	c	46	LYS
35	c	97	TRP
35	c	110	GLN
35	c	216	SER
36	d	19	GLU
36	d	60	ALA
36	d	76	VAL
36	d	131	ARG
36	d	135	LYS
36	d	176	HIS
37	e	32	ALA
37	e	46	LYS
37	e	86	LYS

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Mol	Chain	Res	Type
38	f	40	ARG
38	f	128	PRO
38	f	136	MET
38	f	138	ALA
40	h	9	VAL
40	h	20	ASP
40	h	40	ALA
40	h	78	ARG
40	h	135	VAL
40	h	146	GLU
41	i	81	HIS
41	i	104	ARG
41	i	122	ARG
41	i	123	GLU
42	j	42	ARG
42	j	48	GLU
43	k	42	THR
44	l	35	PRO
44	l	55	LYS
44	l	79	SER
44	l	95	ILE
44	l	104	GLN
44	l	105	VAL
45	m	18	ARG
45	m	45	LYS
45	m	116	ARG
46	n	13	LYS
46	n	24	GLY
46	n	111	LYS
47	o	4	LYS
47	o	28	GLY
47	o	46	GLU
47	o	58	LYS
50	r	42	TYR
51	s	68	LYS
52	t	31	ILE
52	t	78	ARG
53	u	30	LYS
53	u	33	ILE
53	u	97	ALA
3	A	37	LYS
3	A	39	ASP

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Mol	Chain	Res	Type
4	B	35	LYS
4	B	117	VAL
4	B	118	VAL
5	C	67	PHE
5	C	73	GLU
6	D	8	SER
7	E	7	LEU
7	E	19	LEU
7	E	58	GLN
7	E	92	VAL
7	E	111	LEU
7	E	169	ALA
8	F	11	VAL
8	F	19	VAL
8	F	150	ALA
8	F	157	TYR
9	G	26	ALA
9	G	53	ALA
10	H	30	LYS
10	H	31	GLN
10	H	37	VAL
10	H	45	THR
10	H	78	VAL
10	H	145	VAL
10	H	155	ALA
11	I	10	VAL
11	I	69	VAL
11	I	99	PHE
12	J	31	ALA
12	J	45	LEU
12	J	140	ALA
13	K	5	ARG
13	K	7	MET
13	K	28	ALA
13	K	74	TYR
14	L	14	SER
14	L	109	ALA
15	M	30	ARG
15	M	32	LEU
15	M	88	ASP
16	N	6	LEU
16	N	74	ARG

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Mol	Chain	Res	Type
18	P	71	LEU
18	P	78	LYS
19	Q	69	LEU
19	Q	76	VAL
20	R	51	VAL
21	S	57	GLN
21	S	76	CYS
22	T	17	ALA
22	T	22	GLY
23	U	55	ARG
24	V	49	VAL
25	W	6	VAL
29	a	31	HIS
30	b	6	SER
35	c	20	GLU
35	c	67	THR
35	c	89	GLY
35	c	91	PRO
35	c	125	PRO
35	c	154	LEU
35	c	209	ARG
35	c	229	VAL
36	d	151	VAL
36	d	162	GLN
37	e	9	CYS
37	e	78	LEU
37	e	83	SER
37	e	87	GLY
37	e	124	GLY
38	f	93	PRO
38	f	143	ARG
39	g	23	LYS
39	g	61	LEU
39	g	77	ARG
39	g	88	VAL
40	h	33	ASP
42	j	23	ASN
43	k	40	LEU
43	k	77	PRO
44	l	40	ILE
44	l	43	SER
44	l	70	LYS

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Mol	Chain	Res	Type
44	l	117	ASN
45	m	13	GLY
46	n	28	ALA
46	n	40	ASN
46	n	78	ILE
46	n	84	ILE
47	o	37	PHE
50	r	51	TYR
50	r	64	PRO
53	u	45	GLN
53	u	47	GLY
53	u	100	ILE
3	A	58	ASN
3	A	204	GLY
4	B	141	VAL
4	B	159	ALA
5	C	15	PHE
5	C	39	PRO
5	C	52	LEU
5	C	72	VAL
5	C	162	ALA
6	D	52	VAL
6	D	149	VAL
6	D	171	LEU
7	E	10	LYS
7	E	44	GLY
7	E	97	ASP
8	F	66	GLY
8	F	75	ALA
8	F	93	GLY
8	F	121	ILE
10	H	59	GLY
10	H	95	TYR
10	H	109	PRO
12	J	48	PRO
12	J	62	LEU
12	J	72	PRO
12	J	106	LEU
13	K	69	PHE
15	M	28	VAL
15	M	65	VAL
17	O	74	LEU

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Mol	Chain	Res	Type
18	P	39	LEU
18	P	88	ARG
19	Q	9	TYR
19	Q	50	VAL
19	Q	54	ALA
22	T	175	VAL
22	T	177	PRO
23	U	15	ASP
25	W	55	ARG
25	W	61	LEU
26	X	59	VAL
27	Y	9	LYS
35	c	60	ASP
36	d	35	GLU
36	d	75	VAL
36	d	81	GLY
36	d	134	ILE
37	e	70	ILE
37	e	170	VAL
37	e	198	VAL
40	h	88	PRO
41	i	75	ARG
41	i	90	GLY
42	j	33	PHE
42	j	116	LYS
44	l	107	SER
45	m	31	PHE
47	o	48	ALA
48	p	19	PRO
50	r	6	LEU
51	s	66	LEU
51	s	78	LEU
51	s	81	PHE
52	t	49	ILE
3	A	175	PRO
3	A	183	PRO
4	B	74	GLY
4	B	174	ILE
4	B	256	GLY
8	F	17	VAL
9	G	34	GLY
9	G	111	PRO

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Mol	Chain	Res	Type
11	I	4	PRO
11	I	72	PRO
13	K	108	GLY
18	P	42	GLY
18	P	61	VAL
18	P	96	ILE
19	Q	12	ILE
35	c	124	SER
37	e	17	VAL
37	e	133	VAL
37	e	158	ILE
45	m	42	VAL
4	B	24	ILE
5	C	34	VAL
8	F	50	VAL
8	F	52	VAL
8	F	136	ILE
13	K	3	MET
18	P	37	VAL
21	S	49	VAL
24	V	58	ILE
27	Y	29	ILE
36	d	96	GLY
39	g	81	ILE
40	h	55	GLY
41	i	6	ILE
41	i	26	VAL
41	i	38	ILE
41	i	129	VAL
42	j	67	GLY
43	k	53	PRO
45	m	94	GLY
46	n	17	VAL
51	s	52	PRO
4	B	76	PRO
4	B	110	GLY
4	B	121	PRO
10	H	77	VAL
10	H	158	PRO
14	L	34	ILE
22	T	47	VAL
36	d	7	PRO

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Mol	Chain	Res	Type
37	e	7	PRO
37	e	180	GLY
38	f	96	PRO
46	n	53	VAL
53	u	88	VAL
4	B	160	GLY
5	C	189	PRO
7	E	32	PRO
8	F	29	PRO
10	H	117	HIS
16	N	72	VAL
18	P	52	VAL
27	Y	50	GLY
35	c	228	GLY
39	g	6	VAL
39	g	68	PRO
44	l	58	PRO
48	p	87	ILE
50	r	5	VAL
53	u	41	VAL
5	C	173	VAL
7	E	85	GLY
11	I	110	GLY
16	N	70	VAL
36	d	55	VAL
37	e	44	GLY
8	F	128	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%)	91 (86%)	15 (14%)	3	20
4	B	214/218 (98%)	169 (79%)	45 (21%)	1	7
5	C	163/166 (98%)	126 (77%)	37 (23%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	D	154/162 (95%)	123 (80%)	31 (20%)	1	8
7	E	154/156 (99%)	127 (82%)	27 (18%)	2	12
8	F	142/148 (96%)	124 (87%)	18 (13%)	4	23
9	G	124/124 (100%)	103 (83%)	21 (17%)	2	13
10	H	117/139 (84%)	90 (77%)	27 (23%)	1	6
11	I	100/100 (100%)	79 (79%)	21 (21%)	1	7
12	J	112/116 (97%)	89 (80%)	23 (20%)	1	7
13	K	108/111 (97%)	77 (71%)	31 (29%)	0	2
14	L	101/101 (100%)	79 (78%)	22 (22%)	1	6
15	M	84/88 (96%)	66 (79%)	18 (21%)	1	7
16	N	121/128 (94%)	97 (80%)	24 (20%)	1	8
17	O	93/94 (99%)	79 (85%)	14 (15%)	3	18
18	P	82/82 (100%)	70 (85%)	12 (15%)	3	18
19	Q	89/92 (97%)	72 (81%)	17 (19%)	1	9
20	R	74/78 (95%)	62 (84%)	12 (16%)	2	15
21	S	86/91 (94%)	75 (87%)	11 (13%)	4	23
22	T	163/179 (91%)	140 (86%)	23 (14%)	3	20
23	U	61/67 (91%)	47 (77%)	14 (23%)	1	6
24	V	73/83 (88%)	60 (82%)	13 (18%)	2	11
25	W	58/67 (87%)	42 (72%)	16 (28%)	0	3
26	X	52/52 (100%)	41 (79%)	11 (21%)	1	7
27	Y	49/52 (94%)	44 (90%)	5 (10%)	7	31
28	Z	41/42 (98%)	32 (78%)	9 (22%)	1	6
29	a	53/55 (96%)	39 (74%)	14 (26%)	0	3
30	b	33/34 (97%)	30 (91%)	3 (9%)	9	36
35	c	202/220 (92%)	154 (76%)	48 (24%)	0	5
36	d	160/188 (85%)	130 (81%)	30 (19%)	1	10
37	e	180/181 (99%)	143 (79%)	37 (21%)	1	7
38	f	115/123 (94%)	94 (82%)	21 (18%)	1	10
39	g	90/90 (100%)	75 (83%)	15 (17%)	2	14
40	h	126/127 (99%)	110 (87%)	16 (13%)	4	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	i	119/119 (100%)	97 (82%)	22 (18%)	1	10
42	j	98/99 (99%)	82 (84%)	16 (16%)	2	15
43	k	88/92 (96%)	76 (86%)	12 (14%)	3	21
44	l	88/99 (89%)	72 (82%)	16 (18%)	1	10
45	m	104/109 (95%)	85 (82%)	19 (18%)	1	10
46	n	100/101 (99%)	85 (85%)	15 (15%)	3	18
47	o	49/50 (98%)	39 (80%)	10 (20%)	1	7
48	p	79/80 (99%)	65 (82%)	14 (18%)	2	12
49	q	72/74 (97%)	60 (83%)	12 (17%)	2	14
50	r	96/97 (99%)	76 (79%)	20 (21%)	1	7
51	s	64/77 (83%)	52 (81%)	12 (19%)	1	10
52	t	71/80 (89%)	58 (82%)	13 (18%)	1	10
53	u	76/82 (93%)	70 (92%)	6 (8%)	12	42
54	v	19/22 (86%)	16 (84%)	3 (16%)	2	16
All	All	4803/5116 (94%)	3912 (81%)	891 (19%)	1	10

All (891) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	7	ARG
3	A	8	TYR
3	A	9	ARG
3	A	18	ASN
3	A	19	LYS
3	A	23	ILE
3	A	38	PHE
3	A	53	ARG
3	A	165	ARG
3	A	197	LEU
3	A	201	LYS
3	A	209	PHE
3	A	212	SER
3	A	214	TYR
3	A	224	ARG
4	B	9	TYR
4	B	16	MET
4	B	27	THR

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Mol	Chain	Res	Type
4	B	31	LYS
4	B	35	LYS
4	B	37	LEU
4	B	43	ARG
4	B	60	ARG
4	B	66	ASP
4	B	67	PHE
4	B	88	ARG
4	B	92	ILE
4	B	95	LEU
4	B	96	HIS
4	B	99	ASP
4	B	102	LYS
4	B	111	LEU
4	B	115	GLN
4	B	129	ASN
4	B	133	LEU
4	B	134	ARG
4	B	135	PHE
4	B	136	ILE
4	B	146	GLU
4	B	149	PRO
4	B	150	LYS
4	B	155	LEU
4	B	164	GLN
4	B	175	LEU
4	B	192	THR
4	B	198	ASN
4	B	201	HIS
4	B	206	LEU
4	B	208	LYS
4	B	215	LEU
4	B	217	ARG
4	B	230	ASP
4	B	242	ARG
4	B	250	TRP
4	B	252	TRP
4	B	255	LYS
4	B	257	LEU
4	B	262	ARG
4	B	263	ARG
4	B	269	PHE

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Mol	Chain	Res	Type
5	C	4	ILE
5	C	9	VAL
5	C	15	PHE
5	C	16	ARG
5	C	19	ARG
5	C	23	VAL
5	C	27	LEU
5	C	34	VAL
5	C	35	GLN
5	C	42	ASP
5	C	44	TYR
5	C	49	LEU
5	C	57	LYS
5	C	61	ARG
5	C	66	HIS
5	C	67	PHE
5	C	79	ARG
5	C	81	ILE
5	C	89	ASP
5	C	93	VAL
5	C	113	PHE
5	C	117	MET
5	C	119	ARG
5	C	120	TRP
5	C	134	ILE
5	C	141	ILE
5	C	144	ARG
5	C	154	LYS
5	C	156	MET
5	C	174	ASP
5	C	175	VAL
5	C	179	GLU
5	C	181	LEU
5	C	188	VAL
5	C	192	ASN
5	C	202	LYS
5	C	203	LYS
6	D	7	LEU
6	D	12	ARG
6	D	15	LEU
6	D	26	HIS
6	D	27	LEU

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Mol	Chain	Res	Type
6	D	29	TRP
6	D	41	ARG
6	D	54	TYR
6	D	57	ARG
6	D	59	ILE
6	D	60	TRP
6	D	69	ARG
6	D	77	ILE
6	D	78	PHE
6	D	85	PHE
6	D	94	TYR
6	D	97	PRO
6	D	101	ARG
6	D	109	VAL
6	D	112	ARG
6	D	132	LYS
6	D	144	ASP
6	D	147	GLU
6	D	165	LEU
6	D	171	LEU
6	D	178	VAL
6	D	179	TYR
6	D	180	ASP
6	D	181	ILE
6	D	191	LEU
6	D	197	PHE
7	E	10	LYS
7	E	11	TYR
7	E	12	TYR
7	E	25	TYR
7	E	31	VAL
7	E	33	ARG
7	E	53	LEU
7	E	55	LYS
7	E	60	LEU
7	E	71	THR
7	E	82	LEU
7	E	90	LEU
7	E	91	ARG
7	E	95	ARG
7	E	99	MET
7	E	103	LEU

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Mol	Chain	Res	Type
7	E	121	ASN
7	E	125	PHE
7	E	131	TYR
7	E	133	LEU
7	E	139	LEU
7	E	140	ILE
7	E	148	MET
7	E	155	MET
7	E	164	GLU
7	E	176	LEU
7	E	178	PHE
8	F	60	ARG
8	F	65	HIS
8	F	68	THR
8	F	72	ILE
8	F	87	LEU
8	F	89	ILE
8	F	92	ILE
8	F	105	LEU
8	F	123	PHE
8	F	125	VAL
8	F	131	VAL
8	F	138	LYS
8	F	140	LYS
8	F	144	VAL
8	F	149	ARG
8	F	152	ARG
8	F	162	ILE
8	F	172	LYS
9	G	12	LEU
9	G	27	ARG
9	G	33	ARG
9	G	35	LEU
9	G	41	GLU
9	G	44	LEU
9	G	58	LEU
9	G	64	GLU
9	G	89	TYR
9	G	95	LYS
9	G	97	ILE
9	G	99	GLU
9	G	101	LEU

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Mol	Chain	Res	Type
9	G	103	ARG
9	G	107	ILE
9	G	109	ILE
9	G	114	LEU
9	G	118	LYS
9	G	121	LYS
9	G	123	LEU
9	G	139	GLN
10	H	27	TYR
10	H	35	ARG
10	H	48	ARG
10	H	49	LEU
10	H	52	LYS
10	H	56	LEU
10	H	60	LYS
10	H	62	ARG
10	H	64	ASP
10	H	67	PRO
10	H	71	MET
10	H	74	PHE
10	H	79	ASN
10	H	84	ARG
10	H	95	TYR
10	H	98	TYR
10	H	101	TYR
10	H	105	LEU
10	H	112	LYS
10	H	114	LEU
10	H	116	THR
10	H	117	HIS
10	H	122	LEU
10	H	132	LYS
10	H	143	LEU
10	H	146	TYR
10	H	154	GLN
11	I	1	MET
11	I	3	GLN
11	I	9	GLU
11	I	17	ARG
11	I	20	MET
11	I	29	ASN
11	I	39	ILE

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Mol	Chain	Res	Type
11	I	40	VAL
11	I	44	LYS
11	I	45	GLU
11	I	48	PRO
11	I	49	ARG
11	I	59	LYS
11	I	73	ASP
11	I	77	ILE
11	I	79	PHE
11	I	80	ASP
11	I	91	LEU
11	I	104	ARG
11	I	105	GLU
11	I	109	LYS
12	J	6	LEU
12	J	13	ASN
12	J	35	HIS
12	J	45	LEU
12	J	61	ARG
12	J	62	LEU
12	J	64	LYS
12	J	67	MET
12	J	74	GLU
12	J	80	TYR
12	J	81	GLN
12	J	85	LEU
12	J	91	PHE
12	J	95	VAL
12	J	100	LEU
12	J	105	LEU
12	J	112	LEU
12	J	121	LYS
12	J	130	PHE
12	J	139	LYS
12	J	147	LEU
12	J	148	LEU
12	J	149	GLU
13	K	8	LYS
13	K	9	TYR
13	K	11	LYS
13	K	12	GLN
13	K	14	ARG

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Mol	Chain	Res	Type
13	K	17	LEU
13	K	22	LYS
13	K	29	PHE
13	K	34	LEU
13	K	38	GLU
13	K	41	TRP
13	K	42	ILE
13	K	51	ARG
13	K	57	HIS
13	K	59	ARG
13	K	60	ARG
13	K	68	ILE
13	K	69	PHE
13	K	72	LYS
13	K	82	ARG
13	K	89	ASN
13	K	91	GLU
13	K	93	TYR
13	K	103	MET
13	K	112	GLU
13	K	123	HIS
13	K	124	LYS
13	K	125	LEU
13	K	127	ILE
13	K	133	ARG
13	K	134	ARG
14	L	8	ARG
14	L	9	LYS
14	L	14	SER
14	L	20	LEU
14	L	21	TYR
14	L	31	HIS
14	L	40	LYS
14	L	44	LEU
14	L	45	ARG
14	L	47	PHE
14	L	51	LEU
14	L	59	ASP
14	L	64	ARG
14	L	78	LYS
14	L	87	TYR
14	L	89	ASP

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Mol	Chain	Res	Type
14	L	91	GLN
14	L	94	TYR
14	L	99	LYS
14	L	103	ARG
14	L	107	ASP
14	L	116	LEU
15	M	9	ARG
15	M	10	ARG
15	M	12	PHE
15	M	23	ARG
15	M	25	ARG
15	M	26	LEU
15	M	31	SER
15	M	39	ILE
15	M	42	ASP
15	M	47	THR
15	M	49	VAL
15	M	56	LEU
15	M	64	GLU
15	M	71	ARG
15	M	75	GLU
15	M	94	TYR
15	M	106	ARG
15	M	111	GLU
16	N	15	VAL
16	N	18	ASP
16	N	22	PHE
16	N	33	LYS
16	N	35	LYS
16	N	38	ASN
16	N	42	ILE
16	N	44	ASP
16	N	46	GLU
16	N	53	ARG
16	N	61	PHE
16	N	62	THR
16	N	78	LEU
16	N	90	GLN
16	N	95	ARG
16	N	101	PHE
16	N	103	ARG
16	N	108	ARG

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Mol	Chain	Res	Type
16	N	111	ARG
16	N	113	LYS
16	N	119	LYS
16	N	121	ILE
16	N	123	LYS
16	N	124	ASP
17	O	25	TRP
17	O	38	THR
17	O	39	LEU
17	O	44	ASN
17	O	49	HIS
17	O	50	ARG
17	O	64	ARG
17	O	74	LEU
17	O	79	PHE
17	O	84	LYS
17	O	85	LYS
17	O	94	ASN
17	O	97	ASP
17	O	109	LEU
18	P	2	PHE
18	P	11	GLN
18	P	13	ARG
18	P	18	LEU
18	P	23	GLU
18	P	25	LEU
18	P	38	LEU
18	P	39	LEU
18	P	60	GLU
18	P	80	GLN
18	P	82	ARG
18	P	85	LYS
19	Q	4	LYS
19	Q	6	ILE
19	Q	8	ARG
19	Q	12	ILE
19	Q	17	VAL
19	Q	31	GLU
19	Q	38	TYR
19	Q	47	VAL
19	Q	51	LEU
19	Q	68	ARG

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Mol	Chain	Res	Type
19	Q	75	TYR
19	Q	82	LEU
19	Q	88	ARG
19	Q	92	ARG
19	Q	97	LYS
19	Q	104	THR
19	Q	106	ILE
20	R	26	TYR
20	R	38	GLU
20	R	49	VAL
20	R	50	LYS
20	R	54	VAL
20	R	59	VAL
20	R	62	LYS
20	R	64	LYS
20	R	65	ARG
20	R	76	ARG
20	R	77	LYS
20	R	89	ILE
21	S	9	LYS
21	S	13	VAL
21	S	28	LYS
21	S	55	TYR
21	S	64	GLU
21	S	71	LYS
21	S	73	ARG
21	S	74	PRO
21	S	84	ARG
21	S	96	ILE
21	S	97	ARG
22	T	8	TYR
22	T	9	TYR
22	T	19	ARG
22	T	28	MET
22	T	34	ASN
22	T	37	VAL
22	T	38	TYR
22	T	41	LEU
22	T	44	PHE
22	T	53	ILE
22	T	55	HIS
22	T	78	LYS

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Mol	Chain	Res	Type
22	T	80	ARG
22	T	104	PHE
22	T	117	LEU
22	T	119	GLU
22	T	145	GLU
22	T	146	ILE
22	T	155	LEU
22	T	157	LEU
22	T	162	GLU
22	T	165	VAL
22	T	171	ILE
23	U	24	LYS
23	U	31	VAL
23	U	35	ASN
23	U	36	ILE
23	U	40	GLN
23	U	41	ARG
23	U	46	LYS
23	U	53	MET
23	U	56	ASP
23	U	60	PHE
23	U	67	VAL
23	U	69	PHE
23	U	71	ASP
23	U	75	LEU
24	V	11	ARG
24	V	13	ILE
24	V	16	ASN
24	V	18	ILE
24	V	20	ARG
24	V	26	ARG
24	V	33	LYS
24	V	46	LEU
24	V	78	LYS
24	V	82	LEU
24	V	85	LEU
24	V	91	LYS
24	V	94	LEU
25	W	1	MET
25	W	5	GLU
25	W	9	GLN
25	W	12	GLU

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Mol	Chain	Res	Type
25	W	14	ARG
25	W	15	LYS
25	W	29	LYS
25	W	33	MET
25	W	37	PHE
25	W	47	ASN
25	W	48	HIS
25	W	51	ARG
25	W	52	ASP
25	W	55	ARG
25	W	60	LEU
25	W	61	LEU
26	X	8	LEU
26	X	13	ILE
26	X	15	TYR
26	X	17	LYS
26	X	23	LEU
26	X	33	GLN
26	X	43	ILE
26	X	44	ARG
26	X	49	LYS
26	X	53	LEU
26	X	59	VAL
27	Y	15	ARG
27	Y	26	THR
27	Y	29	ILE
27	Y	51	TYR
27	Y	56	LYS
28	Z	2	LYS
28	Z	7	PRO
28	Z	8	ASN
28	Z	15	THR
28	Z	24	THR
28	Z	31	LEU
28	Z	34	ARG
28	Z	39	ARG
28	Z	43	THR
29	a	3	LYS
29	a	6	THR
29	a	13	ARG
29	a	16	ILE
29	a	35	GLN

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Mol	Chain	Res	Type
29	a	36	LYS
29	a	39	LYS
29	a	41	ILE
29	a	44	LYS
29	a	48	PHE
29	a	52	LYS
29	a	54	GLU
29	a	59	LYS
29	a	60	LEU
30	b	2	LYS
30	b	25	VAL
30	b	29	ASN
35	c	8	LYS
35	c	10	LEU
35	c	17	PHE
35	c	19	HIS
35	c	23	ARG
35	c	33	TYR
35	c	40	HIS
35	c	42	ILE
35	c	44	LEU
35	c	46	LYS
35	c	47	THR
35	c	50	GLU
35	c	51	LEU
35	c	53	ARG
35	c	55	PHE
35	c	59	GLU
35	c	63	MET
35	c	70	PHE
35	c	93	VAL
35	c	97	TRP
35	c	105	PHE
35	c	108	ILE
35	c	118	LEU
35	c	126	GLU
35	c	129	GLU
35	c	130	ARG
35	c	132	LYS
35	c	133	LYS
35	c	137	ARG
35	c	138	LEU

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Mol	Chain	Res	Type
35	c	149	LEU
35	c	155	LEU
35	c	157	ARG
35	c	158	LEU
35	c	160	ASP
35	c	169	LYS
35	c	172	ILE
35	c	185	ILE
35	c	191	ASP
35	c	195	ASP
35	c	200	ILE
35	c	204	ASN
35	c	205	ASP
35	c	206	ASP
35	c	209	ARG
35	c	220	ASP
35	c	221	LEU
35	c	222	ILE
36	d	3	ASN
36	d	4	LYS
36	d	11	ARG
36	d	16	ARG
36	d	18	TRP
36	d	33	LEU
36	d	40	ARG
36	d	46	GLU
36	d	56	ASP
36	d	58	GLU
36	d	93	LYS
36	d	94	LEU
36	d	97	LYS
36	d	101	LEU
36	d	107	GLN
36	d	112	SER
36	d	118	GLN
36	d	123	GLN
36	d	126	ARG
36	d	131	ARG
36	d	132	ARG
36	d	139	GLN
36	d	152	ILE
36	d	153	VAL

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Mol	Chain	Res	Type
36	d	156	ARG
36	d	167	TRP
36	d	175	LEU
36	d	186	PHE
36	d	201	TYR
36	d	204	LEU
37	e	8	VAL
37	e	12	CYS
37	e	14	ARG
37	e	21	LEU
37	e	33	MET
37	e	35	ARG
37	e	38	TYR
37	e	47	ARG
37	e	49	ARG
37	e	57	ARG
37	e	58	LEU
37	e	59	ARG
37	e	60	GLU
37	e	61	LYS
37	e	62	GLN
37	e	65	ARG
37	e	68	TYR
37	e	79	PHE
37	e	86	LYS
37	e	93	PHE
37	e	94	LEU
37	e	96	LEU
37	e	97	LEU
37	e	106	TYR
37	e	108	LEU
37	e	110	PHE
37	e	116	GLN
37	e	120	LEU
37	e	122	ARG
37	e	123	HIS
37	e	129	ASN
37	e	158	ILE
37	e	187	ARG
37	e	191	ARG
37	e	192	GLU
37	e	200	GLU

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Mol	Chain	Res	Type
37	e	205	GLU
38	f	12	LEU
38	f	14	ARG
38	f	18	ARG
38	f	25	ARG
38	f	31	LEU
38	f	34	VAL
38	f	43	LEU
38	f	50	GLU
38	f	57	LYS
38	f	69	VAL
38	f	72	GLN
38	f	81	GLU
38	f	89	ILE
38	f	93	PRO
38	f	100	VAL
38	f	110	LEU
38	f	115	VAL
38	f	123	LEU
38	f	142	LEU
38	f	143	ARG
38	f	147	ASP
39	g	6	VAL
39	g	11	ASN
39	g	14	LEU
39	g	28	ARG
39	g	31	GLU
39	g	40	VAL
39	g	45	LEU
39	g	61	LEU
39	g	69	GLU
39	g	71	ARG
39	g	75	LEU
39	g	80	ARG
39	g	85	VAL
39	g	97	PHE
39	g	98	LEU
40	h	4	ARG
40	h	5	ARG
40	h	16	LEU
40	h	21	VAL
40	h	22	LEU

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Mol	Chain	Res	Type
40	h	35	LYS
40	h	43	PHE
40	h	67	GLU
40	h	84	ASN
40	h	85	TYR
40	h	111	ARG
40	h	113	GLU
40	h	119	ARG
40	h	124	LEU
40	h	136	LYS
40	h	151	TYR
41	i	2	LEU
41	i	6	ILE
41	i	8	ASP
41	i	9	MET
41	i	19	VAL
41	i	24	THR
41	i	31	PHE
41	i	39	LEU
41	i	50	ARG
41	i	52	ASP
41	i	62	TYR
41	i	65	TYR
41	i	77	GLU
41	i	91	ARG
41	i	95	VAL
41	i	98	LYS
41	i	103	VAL
41	i	104	ARG
41	i	105	ARG
41	i	111	ILE
41	i	120	THR
41	i	122	ARG
42	j	4	TYR
42	j	5	TYR
42	j	20	ARG
42	j	26	VAL
42	j	33	PHE
42	j	37	PHE
42	j	53	VAL
42	j	59	PHE
42	j	85	LEU

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Mol	Chain	Res	Type
42	j	89	ASN
42	j	93	ARG
42	j	99	LEU
42	j	104	ARG
42	j	121	ARG
42	j	125	TYR
42	j	127	LYS
43	k	13	HIS
43	k	16	LEU
43	k	17	ASP
43	k	40	LEU
43	k	47	PHE
43	k	62	HIS
43	k	63	PHE
43	k	64	GLU
43	k	66	ARG
43	k	78	ASN
43	k	79	ARG
43	k	82	ILE
44	l	13	GLN
44	l	29	ILE
44	l	51	LYS
44	l	54	ARG
44	l	62	GLN
44	l	73	MET
44	l	75	TYR
44	l	77	MET
44	l	92	GLU
44	l	93	GLN
44	l	99	GLN
44	l	103	LEU
44	l	108	ILE
44	l	110	ASP
44	l	122	LYS
44	l	124	LYS
45	m	14	ARG
45	m	27	LYS
45	m	31	PHE
45	m	40	ARG
45	m	41	THR
45	m	43	THR
45	m	52	ARG

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Mol	Chain	Res	Type
45	m	58	ARG
45	m	59	LEU
45	m	64	GLU
45	m	77	GLN
45	m	84	ILE
45	m	96	ARG
45	m	98	HIS
45	m	104	TYR
45	m	105	ASP
45	m	111	ASP
45	m	112	ARG
45	m	126	GLU
46	n	3	ARG
46	n	15	VAL
46	n	19	LEU
46	n	20	THR
46	n	25	ILE
46	n	27	LYS
46	n	47	ASP
46	n	50	GLU
46	n	56	LEU
46	n	60	VAL
46	n	82	MET
46	n	91	ARG
46	n	105	THR
46	n	110	ARG
46	n	113	PRO
47	o	6	LEU
47	o	7	ILE
47	o	8	GLU
47	o	16	PHE
47	o	17	LYS
47	o	21	TYR
47	o	23	ARG
47	o	29	ARG
47	o	47	LEU
47	o	61	TRP
48	p	15	PHE
48	p	28	GLN
48	p	35	ARG
48	p	38	ARG
48	p	46	HIS

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Mol	Chain	Res	Type
48	p	47	LYS
48	p	54	ARG
48	p	59	MET
48	p	63	ARG
48	p	69	TYR
48	p	71	GLN
48	p	77	ARG
48	p	84	LYS
48	p	87	ILE
49	q	1	MET
49	q	13	HIS
49	q	29	ASP
49	q	32	TYR
49	q	35	LYS
49	q	43	LYS
49	q	48	TRP
49	q	49	LEU
49	q	58	TYR
49	q	59	TRP
49	q	60	LEU
49	q	79	VAL
50	r	6	LEU
50	r	13	ASP
50	r	15	MET
50	r	17	LYS
50	r	22	LEU
50	r	25	ARG
50	r	29	HIS
50	r	32	TYR
50	r	36	ILE
50	r	41	LYS
50	r	42	TYR
50	r	47	PRO
50	r	48	GLU
50	r	51	TYR
50	r	60	ILE
50	r	70	ARG
50	r	75	ARG
50	r	81	ARG
50	r	88	TYR
50	r	100	LYS
51	s	19	LYS

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Mol	Chain	Res	Type
51	s	23	LYS
51	s	28	GLU
51	s	31	LEU
51	s	32	ARG
51	s	38	GLU
51	s	41	LYS
51	s	42	ARG
51	s	46	GLU
51	s	66	LEU
51	s	68	LYS
51	s	78	LEU
52	t	5	LEU
52	t	6	LYS
52	t	7	LYS
52	t	12	ASP
52	t	13	ASP
52	t	14	HIS
52	t	15	LEU
52	t	25	LYS
52	t	32	LYS
52	t	34	TRP
52	t	37	ARG
52	t	49	ILE
52	t	61	TYR
53	u	21	LYS
53	u	27	LYS
53	u	34	LYS
53	u	60	GLU
53	u	79	ARG
53	u	104	LEU
54	v	5	ASP
54	v	10	ARG
54	v	14	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (167) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	18	ASN
3	A	45	HIS
3	A	57	GLN
3	A	189	ASN
4	B	44	ASN

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Mol	Chain	Res	Type
4	B	46	GLN
4	B	115	GLN
4	B	116	GLN
4	B	126	GLN
4	B	129	ASN
4	B	164	GLN
4	B	203	ASN
4	B	227	ASN
4	B	253	GLN
5	C	55	ASN
5	C	60	ASN
5	C	66	HIS
5	C	137	HIS
5	C	143	ASN
5	C	159	HIS
6	D	26	HIS
6	D	35	GLN
6	D	70	HIS
6	D	128	ASN
7	E	41	GLN
7	E	123	ASN
8	F	61	HIS
8	F	65	HIS
8	F	74	ASN
8	F	111	HIS
8	F	147	ASN
9	G	17	GLN
9	G	28	ASN
9	G	133	HIS
9	G	147	GLN
10	H	61	HIS
10	H	79	ASN
10	H	154	GLN
11	I	3	GLN
11	I	13	ASN
11	I	29	ASN
11	I	82	ASN
12	J	35	HIS
12	J	81	GLN
12	J	128	HIS
13	K	12	GLN
13	K	46	GLN

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Mol	Chain	Res	Type
14	L	13	HIS
14	L	16	HIS
14	L	50	HIS
14	L	53	HIS
14	L	91	GLN
15	M	68	GLN
15	M	84	GLN
16	N	38	ASN
16	N	55	ASN
16	N	90	GLN
17	O	14	HIS
17	O	72	HIS
17	O	81	HIS
17	O	94	ASN
18	P	64	HIS
18	P	87	HIS
18	P	89	GLN
19	Q	57	ASN
19	Q	61	ASN
19	Q	62	HIS
20	R	31	HIS
20	R	41	ASN
21	S	68	HIS
22	T	34	ASN
22	T	54	HIS
22	T	65	GLN
22	T	73	GLN
22	T	85	HIS
23	U	35	ASN
23	U	40	GLN
23	U	50	ASN
23	U	80	HIS
24	V	19	GLN
24	V	47	GLN
24	V	66	HIS
25	W	47	ASN
27	Y	23	HIS
28	Z	6	GLN
28	Z	36	GLN
29	a	35	GLN
30	b	36	GLN
35	c	16	HIS

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Mol	Chain	Res	Type
35	c	76	GLN
35	c	94	ASN
35	c	95	GLN
35	c	110	GLN
35	c	113	HIS
35	c	135	GLN
35	c	146	GLN
35	c	212	GLN
36	d	3	ASN
36	d	28	GLN
36	d	63	ASN
36	d	69	HIS
36	d	102	ASN
36	d	107	GLN
36	d	108	ASN
36	d	110	ASN
36	d	139	GLN
36	d	162	GLN
36	d	176	HIS
37	e	42	GLN
37	e	62	GLN
37	e	129	ASN
37	e	199	ASN
37	e	201	GLN
38	f	65	ASN
38	f	72	GLN
38	f	73	ASN
39	g	11	ASN
39	g	13	ASN
39	g	16	GLN
39	g	27	GLN
39	g	94	GLN
39	g	100	ASN
40	h	13	GLN
40	h	28	ASN
40	h	64	GLN
40	h	84	ASN
40	h	148	ASN
41	i	15	ASN
41	i	82	HIS
42	j	3	GLN
42	j	73	GLN

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Mol	Chain	Res	Type
42	j	89	ASN
43	k	13	HIS
43	k	69	ASN
43	k	76	ASN
43	k	78	ASN
43	k	84	GLN
44	l	22	HIS
44	l	26	ASN
44	l	38	ASN
44	l	78	GLN
44	l	93	GLN
44	l	99	GLN
44	l	116	HIS
44	l	117	ASN
45	m	74	HIS
45	m	77	GLN
45	m	98	HIS
46	n	77	ASN
47	o	49	HIS
48	p	13	GLN
48	p	42	HIS
48	p	46	HIS
48	p	53	HIS
48	p	71	GLN
49	q	14	ASN
49	q	76	GLN
50	r	26	GLN
50	r	29	HIS
50	r	45	HIS
51	s	63	GLN
52	t	23	ASN
52	t	69	HIS
53	u	16	HIS
53	u	18	GLN
53	u	42	GLN
53	u	75	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	w	2888/2889 (99%)	1138 (39%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	x	119/121 (98%)	42 (35%)	0
31	y	1498/1522 (98%)	502 (33%)	0
32	z	74/76 (97%)	28 (37%)	0
33	0	75/76 (98%)	30 (40%)	5 (6%)
34	1	5/10 (50%)	2 (40%)	0
All	All	4659/4694 (99%)	1742 (37%)	5 (0%)

All (1742) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	w	10	G
1	w	12	U
1	w	13	A
1	w	15	G
1	w	16	G
1	w	17	G
1	w	20	C
1	w	28	A
1	w	29	U
1	w	34	C
1	w	35	G
1	w	37	C
1	w	39	C
1	w	43	G
1	w	45	G
1	w	46	C
1	w	49	A
1	w	50	U
1	w	51	G
1	w	52	A
1	w	59	U
1	w	61	G
1	w	64	A
1	w	69	C
1	w	70	G
1	w	71	A
1	w	72	U
1	w	73	A
1	w	75	G
1	w	78	A
1	w	80	G
1	w	85	G

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Mol	Chain	Res	Type
1	w	88	G
1	w	89	G
1	w	91	A
1	w	95	G
1	w	101	G
1	w	102	G
1	w	103	A
1	w	104	U
1	w	107	C
1	w	108	U
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	128	C
1	w	130	C
1	w	131	G
1	w	132	G
1	w	137(A)	C
1	w	138	G
1	w	139	G
1	w	140	A
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	164	U
1	w	165	U
1	w	174	C
1	w	175	G
1	w	176	G
1	w	181	A
1	w	182	A
1	w	184	C
1	w	186	G

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Mol	Chain	Res	Type
1	w	188	G
1	w	196	A
1	w	197	A
1	w	199	A
1	w	204	A
1	w	205	G
1	w	206	U
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	243	U
1	w	248	G
1	w	249	C
1	w	250	G
1	w	251	A
1	w	265	A
1	w	266	G
1	w	267	C
1	w	269	U
1	w	270(D)	C
1	w	270(E)	C
1	w	270(J)	G
1	w	270(O)	G
1	w	270(P)	U
1	w	270(Q)	C
1	w	270(S)	G
1	w	270(T)	G
1	w	270(Z)	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(F)	U
1	w	274	G

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Mol	Chain	Res	Type
1	w	275	G
1	w	278	A
1	w	284	U
1	w	289	A
1	w	292	C
1	w	294	A
1	w	295	G
1	w	296	C
1	w	297	C
1	w	298	G
1	w	299	A
1	w	300	A
1	w	301	G
1	w	310	A
1	w	311	A
1	w	315	G
1	w	316	C
1	w	317	G
1	w	322	A
1	w	323	G
1	w	329	G
1	w	330	A
1	w	331	A
1	w	332	A
1	w	333	G
1	w	334	C
1	w	336	C
1	w	338	G
1	w	341	G
1	w	342	G
1	w	347	A
1	w	348	G
1	w	349	G
1	w	352	G
1	w	358	U
1	w	361	G
1	w	362	U
1	w	363(A)	G
1	w	363(B)	A
1	w	363(E)	G
1	w	363(F)	U
1	w	364	C

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Mol	Chain	Res	Type
1	w	366(B)	C
1	w	370	G
1	w	371	A
1	w	372	G
1	w	373	U
1	w	380	U
1	w	384	U
1	w	386	G
1	w	387	U
1	w	388	G
1	w	390	A
1	w	394	A
1	w	395	U
1	w	396	G
1	w	397	G
1	w	405	U
1	w	411	G
1	w	412	A
1	w	413	C
1	w	428	A
1	w	435	C
1	w	438	G
1	w	444	C
1	w	446	G
1	w	449	A
1	w	451	C
1	w	453	C
1	w	455	C
1	w	456	C
1	w	457	A
1	w	458	G
1	w	459	U
1	w	462	C
1	w	464	U
1	w	468	G
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

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Mol	Chain	Res	Type
1	w	481	G
1	w	483	A
1	w	487	C
1	w	492	A
1	w	501	A
1	w	504	U
1	w	505	A
1	w	508	G
1	w	509	C
1	w	510	C
1	w	518	G
1	w	528	A
1	w	532	A
1	w	533	G
1	w	535	C
1	w	542	C
1	w	549	G
1	w	551	G
1	w	559	G
1	w	560	C
1	w	563	G
1	w	564	C
1	w	567	A
1	w	569	U
1	w	570	G
1	w	572	A
1	w	574	C
1	w	575	A
1	w	578	A
1	w	583	G
1	w	584	C
1	w	588	U
1	w	589	C
1	w	590	A
1	w	593	G
1	w	594	U
1	w	595	C
1	w	598	G
1	w	603	A
1	w	604	G
1	w	607	U
1	w	608	A

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Mol	Chain	Res	Type
1	w	614	U
1	w	615	G
1	w	616	A
1	w	618(A)	G
1	w	618(B)	C
1	w	620	G
1	w	621	A
1	w	623	G
1	w	627	A
1	w	628	G
1	w	629	G
1	w	634	C
1	w	645	C
1	w	647	G
1	w	648	G
1	w	654	U
1	w	656	G
1	w	665	C
1	w	666	G
1	w	669	G
1	w	670	A
1	w	671	C
1	w	672	C
1	w	674	G
1	w	684	G
1	w	685	A
1	w	686	G
1	w	687	C
1	w	710	G
1	w	716	A
1	w	717	G
1	w	718	A
1	w	719	C
1	w	722	A
1	w	725	G
1	w	726	G
1	w	728	G
1	w	729	G
1	w	730	C
1	w	735	A
1	w	740	U
1	w	741	G

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Mol	Chain	Res	Type
1	w	743	G
1	w	745	G
1	w	747	U
1	w	753	C
1	w	762	U
1	w	763	G
1	w	769	G
1	w	774	A
1	w	775	G
1	w	776	G
1	w	777	A
1	w	781	A
1	w	782	A
1	w	783	A
1	w	784	A
1	w	789	A
1	w	790	C
1	w	792	G
1	w	798	G
1	w	799	G
1	w	800	A
1	w	801	G
1	w	804	A
1	w	805	G
1	w	806	C
1	w	811	U
1	w	812	C
1	w	813	U
1	w	818	G
1	w	827	U
1	w	828	U
1	w	830	G
1	w	831	G
1	w	846	C
1	w	847	U
1	w	848	G
1	w	849	A
1	w	850	C
1	w	856	C
1	w	859	G
1	w	860	U
1	w	861	A

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Mol	Chain	Res	Type
1	w	865	C
1	w	866	A
1	w	867	C
1	w	870	A
1	w	883	G
1	w	886	C
1	w	887	A
1	w	889	C
1	w	890	A
1	w	895	U
1	w	896	A
1	w	897	C
1	w	899	A
1	w	902	C
1	w	906	G
1	w	907	U
1	w	910	A
1	w	912	C
1	w	914	C
1	w	916	G
1	w	919	G
1	w	921	G
1	w	926	A
1	w	931	G
1	w	932	G
1	w	933	A
1	w	938	G
1	w	939	G
1	w	943	U
1	w	944	G
1	w	945	A
1	w	946	G
1	w	954	G
1	w	958	U
1	w	959	A
1	w	960	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

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Mol	Chain	Res	Type
1	w	973	A
1	w	974(A)	G
1	w	974(B)	C
1	w	975	G
1	w	976	C
1	w	980	A
1	w	983	A
1	w	984	A
1	w	988	A
1	w	990	A
1	w	991	C
1	w	992	C
1	w	993	G
1	w	995	C
1	w	996	A
1	w	997	G
1	w	1005	C
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	1022	G
1	w	1023	U
1	w	1024	G
1	w	1025	G
1	w	1033	U
1	w	1034	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	1070	A

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Mol	Chain	Res	Type
1	w	1071	G
1	w	1079	C
1	w	1080	C
1	w	1082	U
1	w	1083	U
1	w	1087	G
1	w	1088	A
1	w	1103	A
1	w	1110	G
1	w	1111	A
1	w	1112	G
1	w	1116	C
1	w	1122	G
1	w	1125	G
1	w	1126	A
1	w	1129	A
1	w	1131	G
1	w	1132	A
1	w	1135	C
1	w	1136	G
1	w	1138	G
1	w	1139	G
1	w	1141	U
1	w	1142	C
1	w	114(B)	A
1	w	1148	A
1	w	1149	G
1	w	1152	C
1	w	1155	A
1	w	1160	G
1	w	1161	C
1	w	1164	G
1	w	1166	C
1	w	1167	U
1	w	1170	G
1	w	1174	A
1	w	1175	U
1	w	1177	A
1	w	1178	C
1	w	1179	C
1	w	1180	C
1	w	1182	A

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Mol	Chain	Res	Type
1	w	1183	G
1	w	1185	C
1	w	1186	G
1	w	1188	U
1	w	1194	A
1	w	1195	G
1	w	1197	G
1	w	1199	U
1	w	1201	C
1	w	1204	A
1	w	1205	U
1	w	1206	G
1	w	1209	G
1	w	1211	U
1	w	1212	G
1	w	1213	A
1	w	1216	G
1	w	1220	A
1	w	1221	C
1	w	1223	G
1	w	1224	C
1	w	1225	G
1	w	1227	G
1	w	1229	G
1	w	1236	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	1254	A
1	w	1256	G
1	w	1261	C
1	w	1265	A
1	w	1266	G
1	w	1267	U
1	w	1270	C

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Mol	Chain	Res	Type
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	1283	G
1	w	1287	A
1	w	1289	C
1	w	1295	C
1	w	1300	U
1	w	1301	A
1	w	1302	A
1	w	1305	C
1	w	1310	G
1	w	1311	G
1	w	1313	U
1	w	1314	C
1	w	1319	G
1	w	1320	C
1	w	1321	A
1	w	1324	G
1	w	1326	U
1	w	1329	U
1	w	1332	G
1	w	1334	G
1	w	1335	U
1	w	1336	A
1	w	1337	G
1	w	1341	U
1	w	1343	G
1	w	1344	G
1	w	1345	C
1	w	1347	G
1	w	1351	C
1	w	1358	G
1	w	1359	A
1	w	1362	C
1	w	1364	G
1	w	1365	A
1	w	1366	A

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Mol	Chain	Res	Type
1	w	1367	A
1	w	1374	G
1	w	1377	G
1	w	1378	A
1	w	1379	A
1	w	1384	A
1	w	1385	G
1	w	1386	C
1	w	1398	C
1	w	1400	G
1	w	1406	U
1	w	1413	G
1	w	1416	G
1	w	1419	A
1	w	1421	G
1	w	1424	G
1	w	1426	G
1	w	1427	A
1	w	1428	C
1	w	1429	G
1	w	1430	C
1	w	1436	G
1	w	1438	U
1	w	144(B)	A
1	w	1445	C
1	w	1448	G
1	w	149(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	1466	G
1	w	1467	C
1	w	1470	G
1	w	1471	A
1	w	1474	C
1	w	1478	G

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Mol	Chain	Res	Type
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	1499	C
1	w	1501	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	1522	G
1	w	1523	U
1	w	1526	G
1	w	1528	A
1	w	1530	G
1	w	1531	C
1	w	1535	U
1	w	1536	A
1	w	1537	C
1	w	1538	G
1	w	1540	G
1	w	1541	U
1	w	1544	C
1	w	1545	A
1	w	1546	A
1	w	154(B)	C
1	w	1547	C
1	w	1553	A
1	w	1558	A
1	w	1559	G
1	w	1560	G
1	w	1562	A
1	w	1565	C
1	w	1567	A

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Mol	Chain	Res	Type
1	w	1569	A
1	w	1574	C
1	w	1576	U
1	w	1577	C
1	w	1578	U
1	w	1579	A
1	w	1581	G
1	w	1585	C
1	w	1586	A
1	w	1596	A
1	w	1603	A
1	w	1604	C
1	w	1608	A
1	w	1609	A
1	w	1613	G
1	w	1616	A
1	w	1617	C
1	w	1618	A
1	w	1619	G
1	w	1623	G
1	w	1627	G
1	w	1628	G
1	w	163(B)	C
1	w	1635	G
1	w	1640	C
1	w	1645	G
1	w	1646	C
1	w	1647	G
1	w	1648	C
1	w	1651	G
1	w	1652	A
1	w	1655	A
1	w	1664	A
1	w	1665	A
1	w	1669	A
1	w	1670	C
1	w	1672	C
1	w	1674	G
1	w	1682	G
1	w	1683	C
1	w	1688	U
1	w	1693	U

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Mol	Chain	Res	Type
1	w	1694	C
1	w	1695	G
1	w	1698	A
1	w	1699	G
1	w	1700	A
1	w	1701	A
1	w	1703	G
1	w	1706	U
1	w	1707	G
1	w	1716	U
1	w	1717	G
1	w	1718	G
1	w	1725	G
1	w	1729	A
1	w	1730	U
1	w	1731	G
1	w	1733	G
1	w	1741	C
1	w	1742	C
1	w	1747	G
1	w	1753	G
1	w	1757	U
1	w	1758	G
1	w	1759	A
1	w	1763	G
1	w	1764	G
1	w	1773	A
1	w	1774	C
1	w	1777	U
1	w	1781	C
1	w	1782	C
1	w	1784	A
1	w	1785	A
1	w	1787	A
1	w	1791	A
1	w	1792	G
1	w	1794	U
1	w	1795	C
1	w	1797	C
1	w	1798	U
1	w	1799	G
1	w	1800	C

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Mol	Chain	Res	Type
1	w	1801	G
1	w	1802	A
1	w	1803	A
1	w	1806	C
1	w	1809	A
1	w	1810	A
1	w	1811	G
1	w	1815	A
1	w	1816	G
1	w	1817	G
1	w	1819	A
1	w	1820	U
1	w	1821	A
1	w	1822	G
1	w	1823	G
1	w	1824	G
1	w	1825	A
1	w	1827	C
1	w	1828	G
1	w	1829	A
1	w	1836	C
1	w	1838	C
1	w	1839	G
1	w	1841	U
1	w	1843	C
1	w	1847	A
1	w	1848	A
1	w	1850	G
1	w	1858	G
1	w	1863	G
1	w	1864	U
1	w	1869	G
1	w	1878	G
1	w	1879	C
1	w	1880	C
1	w	1885	A
1	w	1886	C
1	w	1888	G
1	w	1889	A
1	w	1898	U
1	w	1899	G
1	w	1900	A

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Mol	Chain	Res	Type
1	w	1903	G
1	w	1906	G
1	w	1909	C
1	w	1912	A
1	w	1913	A
1	w	1914	C
1	w	1916	A
1	w	1918	A
1	w	1929	G
1	w	1930	G
1	w	1931	U
1	w	1935	G
1	w	1937	A
1	w	1938	A
1	w	1939	U
1	w	1943	U
1	w	1944	U
1	w	1945	G
1	w	1955	U
1	w	1960	A
1	w	1963	U
1	w	1964	G
1	w	1965	C
1	w	1967	C
1	w	1968	G
1	w	1969	A
1	w	1971	A
1	w	1972	A
1	w	1975	G
1	w	1976	U
1	w	1978	A
1	w	1981	A
1	w	1982	C
1	w	1987	G
1	w	1991	U
1	w	1992	G
1	w	1993	U
1	w	1997	G
1	w	1998	G
1	w	2013	A
1	w	2014	A
1	w	2020	A

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Mol	Chain	Res	Type
1	w	2022	U
1	w	2023	G
1	w	2024	G
1	w	2026	C
1	w	2031	A
1	w	2033	A
1	w	2034	U
1	w	2035	G
1	w	2036	C
1	w	2041	U
1	w	2043	C
1	w	2047	U
1	w	2048	G
1	w	2051	A
1	w	2052	G
1	w	2055	C
1	w	2056	G
1	w	2057	A
1	w	2060	A
1	w	2061	G
1	w	2062	A
1	w	2063	C
1	w	2064	C
1	w	2066	C
1	w	2069	G
1	w	2071	A
1	w	2076	U
1	w	2077	A
1	w	2078	C
1	w	2087	G
1	w	2092	U
1	w	2093	G
1	w	2096	U
1	w	2097	C
1	w	2099	U
1	w	2101	G
1	w	2110	G
1	w	2111	C
1	w	2112	G
1	w	2113	U
1	w	2116	G
1	w	2118	U

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Mol	Chain	Res	Type
1	w	2120	G
1	w	2126	A
1	w	2127	G
1	w	2128	C
1	w	2130	U
1	w	2131	G
1	w	2132	U
1	w	2133	G
1	w	2138	C
1	w	2145	C
1	w	2148	G
1	w	2153	G
1	w	2157	G
1	w	2158	A
1	w	2160	G
1	w	2168	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	2179	C
1	w	2181	G
1	w	2188	C
1	w	2190	G
1	w	2191	G
1	w	2192	G
1	w	2193	G
1	w	2194	G
1	w	2195	C
1	w	2198	A
1	w	2199	A
1	w	2205	C
1	w	2211	G
1	w	2212	A
1	w	2213	U
1	w	2215	G
1	w	2218	G
1	w	2219	G
1	w	2225	A
1	w	2226	C

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Mol	Chain	Res	Type
1	w	2228	G
1	w	2238	G
1	w	2239	G
1	w	2243	U
1	w	2246	G
1	w	2251	G
1	w	2255	G
1	w	2259	G
1	w	2267	A
1	w	2268	A
1	w	2273	A
1	w	2275	C
1	w	2276	G
1	w	2279	G
1	w	2280	G
1	w	2282	G
1	w	2283	C
1	w	2286	A
1	w	2287	A
1	w	2288	A
1	w	2290	G
1	w	2293	C
1	w	2294	C
1	w	2296	U
1	w	2297	C
1	w	2298	A
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	2311	A
1	w	2314	C
1	w	2319	G
1	w	2320	A
1	w	2321	G
1	w	2322	A
1	w	2323	G
1	w	2325	G
1	w	2331	G
1	w	2334	G

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Mol	Chain	Res	Type
1	w	2335	A
1	w	2336	A
1	w	2337	G
1	w	2341	G
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	2357	U
1	w	2359	C
1	w	2361	A
1	w	2363	C
1	w	2365	G
1	w	2367	G
1	w	2368	C
1	w	2374	C
1	w	2378	A
1	w	2379	G
1	w	2383	G
1	w	2385	C
1	w	2390	U
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	2403	C
1	w	2406	U
1	w	2407	G
1	w	2411	A
1	w	2414	G
1	w	2416	C
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	2432	A

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Mol	Chain	Res	Type
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	2457	U
1	w	2463	C
1	w	2469	A
1	w	2471	C
1	w	2478	A
1	w	2480	C
1	w	2491	U
1	w	2492	U
1	w	2495	G
1	w	2498	C
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	2511	U
1	w	2512	C
1	w	2513	G
1	w	2514	U
1	w	2515	C
1	w	2517	C
1	w	2518	A
1	w	2519	U
1	w	2520	C
1	w	2523	G
1	w	2529	G
1	w	2535	G
1	w	2538	C
1	w	2542	A
1	w	2543	G
1	w	2547	U
1	w	2549	G

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Mol	Chain	Res	Type
1	w	2553	G
1	w	2554	U
1	w	2556	C
1	w	2563	U
1	w	2566	A
1	w	2567	G
1	w	2572	A
1	w	2573	C
1	w	2574	G
1	w	2576	G
1	w	2578	G
1	w	2582	G
1	w	2583	G
1	w	2584	U
1	w	2585	U
1	w	2586	C
1	w	2588	G
1	w	2602	A
1	w	2603	G
1	w	2610	C
1	w	2611	U
1	w	2613	U
1	w	2615	U
1	w	2616	C
1	w	2618	G
1	w	2621	A
1	w	2622	C
1	w	2629	A
1	w	2630	G
1	w	2634	G
1	w	2643	G
1	w	2644	G
1	w	2646	C
1	w	2647	U
1	w	2648	C
1	w	2649	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

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Mol	Chain	Res	Type
1	w	2668	G
1	w	2670	A
1	w	2675	A
1	w	2680	C
1	w	2682	U
1	w	2685	G
1	w	2690	C
1	w	2691	C
1	w	2694	G
1	w	2695	C
1	w	2702	U
1	w	2703	C
1	w	2712	U
1	w	712(B)	A
1	w	2713	A
1	w	2714	G
1	w	2718	G
1	w	2720	U
1	w	2721	A
1	w	2723	C
1	w	2724	C
1	w	2726	U
1	w	2727	G
1	w	2732	G
1	w	2734	A
1	w	2736	G
1	w	2744	G
1	w	2745	C
1	w	2751	G
1	w	2752	C
1	w	2754	U
1	w	2755	C
1	w	2756	U
1	w	2757	A
1	w	2759	G
1	w	2761	G
1	w	2762	G
1	w	2763	G
1	w	2766	G
1	w	2768	C
1	w	2771	C
1	w	2775	A

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Mol	Chain	Res	Type
1	w	2777	G
1	w	2778	A
1	w	2779	U
1	w	2781	A
1	w	2785	C
1	w	2787	C
1	w	2789	C
1	w	2791	C
1	w	2792	G
1	w	2793	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	2815	C
1	w	2818	G
1	w	2820	A
1	w	2821	A
1	w	2823	A
1	w	2825	G
1	w	2827	C
1	w	2833	G
1	w	2834	G
1	w	2835	A
1	w	2836	U
1	w	2841	C
1	w	2845	G
1	w	2848	G
1	w	2849	U
1	w	2852	G
1	w	2853	C
1	w	2858	C
1	w	2861	G
1	w	2864	G
1	w	2866	U
1	w	2867	G
1	w	2868	A
1	w	2872	G

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Mol	Chain	Res	Type
1	w	2873	A
1	w	2875	C
1	w	2876	G
1	w	2879	C
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	2894	G
1	w	2895	U
1	w	2896	C
1	w	2901	C
2	x	8	U
2	x	9	G
2	x	10	C
2	x	13	A
2	x	15	A
2	x	21	G
2	x	25	A
2	x	26	A
2	x	27	C
2	x	33	G
2	x	34	U
2	x	35	U
2	x	38	C
2	x	40	U
2	x	42	C
2	x	43	C
2	x	44	G
2	x	45	A
2	x	50	G
2	x	52	A
2	x	53	A
2	x	63	G
2	x	64	C
2	x	65	C
2	x	66	A
2	x	67	G
2	x	75	G
2	x	76	G

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Mol	Chain	Res	Type
2	x	79	C
2	x	83	G
2	x	87	G
2	x	90	C
2	x	98	G
2	x	99	A
2	x	103	U
2	x	108	C
2	x	109	G
2	x	111	U
2	x	113	C
2	x	114	G
2	x	117	G
2	x	118	G
31	y	6	G
31	y	7	G
31	y	8	A
31	y	9	G
31	y	13	U
31	y	14	U
31	y	18	C
31	y	31	G
31	y	32	A
31	y	38	G
31	y	39	G
31	y	47	C
31	y	48	C
31	y	50	A
31	y	51	A
31	y	60	A
31	y	61	G
31	y	63	C
31	y	65	U
31	y	68	G
31	y	69	G
31	y	78	G
31	y	82	U
31	y	84	U
31	y	88	C
31	y	93	U
31	y	95	G
31	y	104	G

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Mol	Chain	Res	Type
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	126	G
31	y	127	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	144	G
31	y	149	A
31	y	157	G
31	y	163	C
31	y	169	C
31	y	173	U
31	y	174	C
31	y	176	C
31	y	186(A)	C
31	y	186(C)	C
31	y	190	G
31	y	191(A)	G
31	y	195	A
31	y	196	A
31	y	197	A
31	y	198	G
31	y	201	C
31	y	208	U
31	y	209	U
31	y	210	U
31	y	223	U
31	y	233	C
31	y	244	U
31	y	245	C
31	y	246	A

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Mol	Chain	Res	Type
31	y	247	G
31	y	251	G
31	y	252	U
31	y	253	U
31	y	263	A
31	y	266	G
31	y	267	C
31	y	275	G
31	y	276	G
31	y	279	A
31	y	280	C
31	y	281	G
31	y	286	G
31	y	289	G
31	y	295	C
31	y	298	A
31	y	299	G
31	y	300	A
31	y	316	G
31	y	320	C
31	y	321	A
31	y	322	C
31	y	328	C
31	y	329	A
31	y	330	C
31	y	332	G
31	y	342	C
31	y	344	A
31	y	345	C
31	y	347	G
31	y	350	G
31	y	351	G
31	y	352	C
31	y	353	A
31	y	354	G
31	y	358	U
31	y	360	A
31	y	361	G
31	y	363	A
31	y	366	C
31	y	367	U
31	y	368	U

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Mol	Chain	Res	Type
31	y	369	C
31	y	372	C
31	y	378	G
31	y	382	A
31	y	383	A
31	y	388	G
31	y	391	G
31	y	392	G
31	y	397	A
31	y	398	C
31	y	406	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	424	G
31	y	428	G
31	y	429	U
31	y	430	A
31	y	436	C
31	y	437	U
31	y	439	A
31	y	440	A
31	y	451	A
31	y	452	A
31	y	455	C
31	y	466	G
31	y	467	G
31	y	468	A
31	y	481	G
31	y	484	G
31	y	485	G
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	508	C
31	y	509	A

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Mol	Chain	Res	Type
31	y	511	C
31	y	512	U
31	y	516	PSU
31	y	517	G
31	y	518	C
31	y	519	C
31	y	520	A
31	y	521	G
31	y	523	A
31	y	524	G
31	y	525	C
31	y	527	7MG
31	y	530	G
31	y	531	U
31	y	532	A
31	y	533	A
31	y	534	U
31	y	535	A
31	y	540	G
31	y	543	C
31	y	547	A
31	y	550	G
31	y	552	U
31	y	556	C
31	y	561	U
31	y	563	A
31	y	564	C
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
31	y	577	G
31	y	580	U
31	y	586	C
31	y	588	G
31	y	596	C
31	y	597	G
31	y	602	A
31	y	612	C

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Mol	Chain	Res	Type
31	y	614	A
31	y	615	C
31	y	618	C
31	y	619	U
31	y	620	C
31	y	622	A
31	y	627	G
31	y	629	G
31	y	631	G
31	y	641	U
31	y	642	A
31	y	652	U
31	y	653	A
31	y	654	G
31	y	661	G
31	y	662	G
31	y	667	G
31	y	674	G
31	y	675	A
31	y	678	U
31	y	687	A
31	y	688	G
31	y	693	G
31	y	695	A
31	y	696	A
31	y	702	A
31	y	703	G
31	y	706	A
31	y	708	C
31	y	713	G
31	y	716	A
31	y	717	C
31	y	718	G
31	y	724	G
31	y	728	A
31	y	732	C
31	y	733	A
31	y	734	G
31	y	741	G
31	y	747	C
31	y	748	C
31	y	749	C

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Mol	Chain	Res	Type
31	y	750	G
31	y	752	G
31	y	753	A
31	y	755	G
31	y	759	A
31	y	765	G
31	y	771	G
31	y	772	U
31	y	776	G
31	y	777	A
31	y	778	G
31	y	779	C
31	y	781	A
31	y	788	U
31	y	792	A
31	y	794	A
31	y	801	U
31	y	812	C
31	y	813	U
31	y	816	A
31	y	817	C
31	y	818	G
31	y	819	A
31	y	820	U
31	y	821	G
31	y	828	A
31	y	832	C
31	y	833	U
31	y	836	G
31	y	841	U
31	y	842	C
31	y	843	U
31	y	855	G
31	y	867	G
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

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Mol	Chain	Res	Type
31	y	890	G
31	y	900	A
31	y	901	A
31	y	902	G
31	y	906	G
31	y	912	C
31	y	913	A
31	y	914	A
31	y	915	A
31	y	916	G
31	y	926	G
31	y	927	G
31	y	931	C
31	y	934	C
31	y	935	A
31	y	936	C
31	y	939	G
31	y	946	A
31	y	956	U
31	y	959	A
31	y	960	U
31	y	961	U
31	y	965	A
31	y	966	M2G
31	y	967	5MC
31	y	968	A
31	y	969	A
31	y	974	A
31	y	976	G
31	y	977	A
31	y	978	A
31	y	981	U
31	y	982	U
31	y	983	A
31	y	991	U
31	y	992	U
31	y	993	G
31	y	1002	G
31	y	1004	A
31	y	1005	A
31	y	1007	C
31	y	1009	G

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Mol	Chain	Res	Type
31	y	1016	A
31	y	1025	U
31	y	1026	G
31	y	1027	C
31	y	102(C)	C
31	y	1030	C
31	y	1037	C
31	y	1042	G
31	y	1050	G
31	y	1052	U
31	y	1053	G
31	y	1054	C
31	y	1055	A
31	y	1056	U
31	y	1064	G
31	y	1065	U
31	y	1066	C
31	y	1068	G
31	y	1080	A
31	y	1085	U
31	y	1086	U
31	y	1089	G
31	y	1094	G
31	y	1095	U
31	y	1101	A
31	y	1102	A
31	y	1104	G
31	y	1109	C
31	y	1111	A
31	y	1118	C
31	y	1126	U
31	y	1130	A
31	y	1131	G
31	y	1136	U
31	y	1137	C
31	y	1139	G
31	y	1140	C
31	y	1142	G
31	y	1146	A
31	y	1151	A
31	y	1152	A
31	y	1154	G

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Mol	Chain	Res	Type
31	y	1158	C
31	y	1159	U
31	y	1160	G
31	y	1176	A
31	y	1177	G
31	y	1178	G
31	y	1179	A
31	y	1181	G
31	y	1184	G
31	y	1186	G
31	y	1187	G
31	y	1189	C
31	y	1190	G
31	y	1193	G
31	y	1196	U
31	y	1197	G
31	y	1200	C
31	y	1201	A
31	y	1202	G
31	y	1207	2MG
31	y	1208	C
31	y	1211	U
31	y	1212	U
31	y	1213	A
31	y	1215	G
31	y	1220	G
31	y	1225	A
31	y	1227	A
31	y	1228	C
31	y	1234	C
31	y	1235	U
31	y	1237	C
31	y	1238	A
31	y	1239	A
31	y	1240	U
31	y	1241	G
31	y	1245	A
31	y	1247	U
31	y	1248	A
31	y	1251	A
31	y	1252	A
31	y	1253	G

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Mol	Chain	Res	Type
31	y	1256	A
31	y	1257	U
31	y	1260	C
31	y	1261	A
31	y	1263	C
31	y	1268	A
31	y	1276	G
31	y	1278	U
31	y	1280	A
31	y	1281	U
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	1293	G
31	y	1296	C
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	1305	G
31	y	1306	A
31	y	1308	U
31	y	1316	G
31	y	1317	C
31	y	1319	A
31	y	1320	C
31	y	1323	G
31	y	1324	A
31	y	1326	C
31	y	1329	A
31	y	1331	G
31	y	1332	A
31	y	1333	A
31	y	1334	G
31	y	1338	G
31	y	1346	A

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Mol	Chain	Res	Type
31	y	1347	G
31	y	1348	U
31	y	1359	C
31	y	1360	A
31	y	1361	G
31	y	136(B)	C
31	y	1364	U
31	y	1365	G
31	y	1373	G
31	y	1375	A
31	y	1378	C
31	y	1380	U
31	y	1381	U
31	y	1388	C
31	y	1393	U
31	y	1395	C
31	y	1397	C
31	y	1398	A
31	y	1399	C
31	y	1400	5MC
31	y	1404	5MC
31	y	1405	G
31	y	1406	U
31	y	1407	5MC
31	y	1409	C
31	y	1417	G
31	y	1424	C
31	y	1428	A
31	y	1429	C
31	y	1431	C
31	y	1433	A
31	y	1443	G
31	y	1446	A
31	y	1447	G
31	y	1452	C
31	y	1461	G
31	y	1469	G
31	y	1471	G
31	y	1473	A
31	y	1483	A
31	y	1484	C
31	y	1492	A

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Mol	Chain	Res	Type
31	y	1494	G
31	y	1495	U
31	y	1498	UR3
31	y	1499	A
31	y	1504	G
31	y	1505	G
31	y	1507	A
31	y	1517	G
31	y	1520	G
31	y	1523	G
31	y	1525	G
31	y	1529	G
32	z	2	C
32	z	7	A
32	z	8	4SU
32	z	9	A
32	z	16	H2U
32	z	17	C
32	z	18	G
32	z	19	G
32	z	20	H2U
32	z	21	A
32	z	27	G
32	z	32	PSU
32	z	33	U
32	z	39	PSU
32	z	42	C
32	z	45	U
32	z	46	7MG
32	z	48	C
32	z	49	C
32	z	54	5MU
32	z	55	PSU
32	z	59	U
32	z	61	C
32	z	63	G
32	z	65	G
32	z	67	C
32	z	72	C
32	z	76	A
33	0	8	U
33	0	14	A

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Mol	Chain	Res	Type
33	0	15	G
33	0	16	U
33	0	17	U
33	0	18	G
33	0	20	G
33	0	21	A
33	0	22	G
33	0	34	G
33	0	35	A
33	0	36	A
33	0	38	A
33	0	39	U
33	0	40	C
33	0	41	U
33	0	45	G
33	0	46	G
33	0	47	U
33	0	48	C
33	0	54	U
33	0	55	PSU
33	0	56	C
33	0	57	G
33	0	59	U
33	0	61	C
33	0	71	G
33	0	72	C
33	0	75	C
33	0	76	A
34	1	-2	U
34	1	1	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	0	7	U
33	0	9	A
33	0	46	G
33	0	48	C
33	0	56	C

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

22 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
31	2MG	y	1207	31	19,26,27	2.06	5 (26%)	21,38,41	2.87	8 (38%)
32	7MG	z	46	32	22,26,27	2.40	5 (22%)	28,39,42	2.26	8 (28%)
31	PSU	y	516	31	17,21,22	1.13	2 (11%)	20,30,33	3.55	8 (40%)
32	H2U	z	20	32	18,21,22	0.76	0	21,30,33	0.89	1 (4%)
33	PSU	0	55	33	17,21,22	2.08	4 (23%)	20,30,33	4.32	9 (45%)
32	MIA	z	37	32	24,31,32	2.36	6 (25%)	26,44,47	2.58	6 (23%)
31	M2G	y	966	31	20,27,28	2.95	6 (30%)	22,40,43	2.78	7 (31%)
31	4OC	y	1402	31	16,23,24	1.68	4 (25%)	17,32,35	1.65	4 (23%)
31	5MC	y	1404	31	15,22,23	1.51	2 (13%)	19,32,35	1.40	2 (10%)
31	UR3	y	1498	31	14,22,23	1.87	3 (21%)	15,32,35	1.36	3 (20%)
32	PSU	z	55	32	17,21,22	2.06	1 (5%)	20,30,33	3.85	9 (45%)
31	5MC	y	1407	31	15,22,23	1.49	3 (20%)	19,32,35	1.46	3 (15%)
32	PSU	z	39	32	17,21,22	1.74	3 (17%)	20,30,33	3.70	9 (45%)
32	H2U	z	16	32	18,21,22	0.97	1 (5%)	21,30,33	0.93	1 (4%)
32	4SU	z	8	32	14,21,22	1.83	4 (28%)	15,30,33	2.33	5 (33%)
31	7MG	y	527	31	22,26,27	2.31	5 (22%)	28,39,42	2.28	6 (21%)
32	5MU	z	54	32	15,22,23	1.80	4 (26%)	16,32,35	2.86	4 (25%)
31	MA6	y	1519	31	19,26,27	2.16	2 (10%)	18,38,41	1.90	4 (22%)
31	5MC	y	1400	31	15,22,23	1.11	1 (6%)	19,32,35	1.77	5 (26%)
31	MA6	y	1518	31	19,26,27	1.80	3 (15%)	18,38,41	2.29	6 (33%)
31	5MC	y	967	31	15,22,23	1.07	1 (6%)	19,32,35	1.46	2 (10%)
32	PSU	z	32	32	17,21,22	1.17	2 (11%)	20,30,33	3.65	9 (45%)

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
31	2MG	y	1207	31	-	0/5/27/28	0/3/3/3
32	7MG	z	46	32	-	0/7/37/38	0/3/3/3
31	PSU	y	516	31	-	2/7/25/26	0/2/2/2
32	H2U	z	20	32	-	2/7/38/39	0/2/2/2
33	PSU	0	55	33	-	1/7/25/26	0/2/2/2
32	MIA	z	37	32	-	5/11/33/34	0/3/3/3
31	M2G	y	966	31	-	0/7/29/30	0/3/3/3
31	4OC	y	1402	31	-	3/9/29/30	0/2/2/2
31	5MC	y	1404	31	-	3/5/25/26	0/2/2/2
31	UR3	y	1498	31	-	4/5/25/26	0/2/2/2
32	PSU	z	55	32	-	3/7/25/26	0/2/2/2
31	5MC	y	1407	31	-	0/5/25/26	0/2/2/2
32	PSU	z	39	32	-	3/7/25/26	0/2/2/2
32	H2U	z	16	32	-	2/7/38/39	0/2/2/2
32	4SU	z	8	32	-	2/5/25/26	0/2/2/2
31	7MG	y	527	31	-	0/7/37/38	0/3/3/3
32	5MU	z	54	32	-	0/5/25/26	0/2/2/2
31	MA6	y	1519	31	-	1/7/29/30	0/3/3/3
31	5MC	y	1400	31	-	0/5/25/26	0/2/2/2
31	MA6	y	1518	31	-	2/7/29/30	0/3/3/3
31	5MC	y	967	31	-	0/5/25/26	0/2/2/2
32	PSU	z	32	32	-	2/7/25/26	0/2/2/2

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	966	M2G	C6-N1	8.38	1.47	1.33
32	z	55	PSU	C5-C1'	-7.33	1.46	1.52
32	z	46	7MG	C6-N1	7.03	1.45	1.33
31	y	1207	2MG	C6-N1	6.48	1.44	1.33
32	z	37	MIA	C13-C14	6.35	1.50	1.32
31	y	1518	MA6	C6-N1	6.32	1.42	1.33
31	y	966	M2G	C2-N1	6.21	1.45	1.34
31	y	527	7MG	C6-N1	6.18	1.43	1.33
33	0	55	PSU	C5-C1'	-6.07	1.47	1.52
31	y	1519	MA6	C6-N1	6.02	1.42	1.33
32	z	37	MIA	C16-C14	5.78	1.66	1.50
31	y	1519	MA6	O4'-C1'	5.69	1.49	1.41
32	z	46	7MG	C6-C5	5.39	1.48	1.41
31	y	527	7MG	C6-C5	4.97	1.48	1.41
31	y	966	M2G	C6-C5	4.85	1.49	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	z	54	5MU	O4-C4	4.81	1.36	1.24
32	z	37	MIA	C6-N1	4.78	1.39	1.32
32	z	39	PSU	C5-C1'	-4.73	1.48	1.52
31	y	527	7MG	C2-N1	4.21	1.42	1.35
31	y	1498	UR3	O4-C4	4.15	1.34	1.24
31	y	1404	5MC	O4'-C1'	4.00	1.46	1.41
32	z	46	7MG	C2-N1	3.97	1.42	1.35
32	z	8	4SU	O4'-C1'	3.94	1.46	1.41
31	y	527	7MG	C8-N9	-3.83	1.36	1.45
31	y	1402	4OC	O2'-CM2	-3.71	1.29	1.42
31	y	966	M2G	O4'-C1'	3.69	1.46	1.41
32	z	39	PSU	C4-N3	3.59	1.39	1.33
32	z	46	7MG	C8-N9	-3.58	1.37	1.45
31	y	1498	UR3	C2'-C1'	3.58	1.59	1.53
32	z	8	4SU	C6-C5	3.48	1.45	1.38
32	z	37	MIA	C2-S10	-3.47	1.72	1.75
31	y	1400	5MC	C4-N4	3.41	1.42	1.34
31	y	1407	5MC	O4'-C1'	3.40	1.45	1.41
31	y	966	M2G	C2-N2	3.22	1.40	1.34
31	y	1207	2MG	C6-C5	3.01	1.46	1.41
33	0	55	PSU	O4'-C1'	2.96	1.49	1.44
32	z	54	5MU	O4'-C1'	2.86	1.45	1.41
31	y	967	5MC	C4-N4	2.86	1.41	1.34
31	y	1404	5MC	C4-N4	2.77	1.41	1.34
31	y	1207	2MG	C2-N1	2.64	1.42	1.34
31	y	1407	5MC	C4-N4	2.61	1.40	1.34
31	y	516	PSU	C4-N3	2.61	1.37	1.33
32	z	37	MIA	C2-N1	2.57	1.37	1.34
31	y	527	7MG	C4-N3	2.52	1.37	1.34
31	y	966	M2G	O5'-C5'	-2.49	1.38	1.44
31	y	1402	4OC	C4-N4	2.44	1.41	1.36
32	z	32	PSU	C4-N3	2.44	1.37	1.33
32	z	37	MIA	O4'-C1'	2.43	1.44	1.41
31	y	516	PSU	C2'-C1'	2.37	1.56	1.54
31	y	1498	UR3	O4'-C1'	2.37	1.44	1.41
33	0	55	PSU	C2-N1	2.36	1.42	1.38
31	y	1402	4OC	CM4-N4	2.32	1.49	1.45
32	z	54	5MU	O5'-C5'	-2.31	1.39	1.44
32	z	8	4SU	C4-S4	2.29	1.71	1.67
31	y	1402	4OC	O3'-C3'	2.26	1.48	1.43
32	z	39	PSU	O4'-C4'	-2.25	1.40	1.45
32	z	46	7MG	C4-N3	2.24	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	z	54	5MU	C4-N3	2.24	1.36	1.33
31	y	1407	5MC	C6-C5	-2.23	1.33	1.40
32	z	16	H2U	C1'-N1	2.19	1.50	1.46
32	z	8	4SU	C5-C4	2.17	1.40	1.38
31	y	1207	2MG	C2-N2	2.09	1.35	1.34
31	y	1207	2MG	C8-N7	-2.07	1.31	1.34
33	0	55	PSU	C2-N3	-2.05	1.34	1.38
32	z	32	PSU	O5'-C5'	-2.02	1.39	1.44
31	y	1518	MA6	C2'-C1'	2.00	1.56	1.53
31	y	1518	MA6	C2-N1	2.00	1.37	1.33

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	0	55	PSU	N1-C2-N3	-11.63	119.19	128.43
32	z	32	PSU	N1-C2-N3	-11.57	119.23	128.43
32	z	39	PSU	N1-C2-N3	-11.38	119.38	128.43
31	y	516	PSU	N1-C2-N3	-11.10	119.61	128.43
32	z	55	PSU	N1-C2-N3	-10.69	119.93	128.43
32	z	54	5MU	C4-N3-C2	10.31	123.85	115.14
33	0	55	PSU	C5-C1'-C2'	-9.36	98.62	115.32
31	y	1207	2MG	C5-C6-N1	-8.86	111.32	123.43
31	y	966	M2G	C5-C6-N1	-8.53	111.77	123.43
32	z	37	MIA	C12-C13-C14	-8.50	110.60	127.14
32	z	55	PSU	C5-C1'-C2'	-8.15	100.78	115.32
32	z	39	PSU	C4-N3-C2	6.80	120.88	115.14
32	z	32	PSU	C4-N3-C2	6.74	120.83	115.14
33	0	55	PSU	C4-N3-C2	6.64	120.75	115.14
31	y	1518	MA6	N1-C6-N6	6.39	123.78	117.06
31	y	1207	2MG	CM2-N2-C2	-6.36	115.92	123.59
31	y	516	PSU	C4-N3-C2	6.35	120.50	115.14
31	y	516	PSU	C4'-O4'-C1'	-6.21	101.76	109.42
32	z	55	PSU	C4-N3-C2	5.97	120.19	115.14
31	y	966	M2G	C6-N1-C2	5.85	123.14	116.18
31	y	527	7MG	N7-C8-N9	5.61	111.41	103.38
31	y	527	7MG	C6-C5-C4	5.50	121.10	115.20
32	z	37	MIA	C12-N6-C6	-5.50	114.41	122.55
33	0	55	PSU	O4'-C1'-C5	5.46	118.39	109.93
32	z	46	7MG	N7-C8-N9	5.45	111.17	103.38
31	y	527	7MG	C5-C6-N1	-5.39	112.07	123.14
32	z	46	7MG	C5-C6-N1	-5.29	112.26	123.14
32	z	39	PSU	C5-C4-N3	-5.09	118.80	125.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	z	8	4SU	C2-N3-C4	5.01	122.42	115.15
33	0	55	PSU	C4'-O4'-C1'	-4.84	103.46	109.42
32	z	39	PSU	C4'-O4'-C1'	-4.82	103.48	109.42
32	z	37	MIA	C11-S10-C2	4.50	105.63	102.27
32	z	46	7MG	O4'-C1'-N9	-4.50	103.27	109.35
32	z	32	PSU	C3'-C2'-C1'	4.44	107.05	101.93
32	z	8	4SU	C5-C4-N3	-4.40	117.94	123.83
32	z	37	MIA	C5-C6-N1	-4.36	117.19	120.81
32	z	46	7MG	C6-N1-C2	4.28	122.73	115.93
31	y	527	7MG	C6-N1-C2	4.27	122.71	115.93
31	y	1519	MA6	N1-C6-N6	4.18	121.46	117.06
31	y	1207	2MG	C6-N1-C2	4.17	122.66	115.18
31	y	1519	MA6	C3'-C2'-C1'	4.06	107.09	100.98
32	z	55	PSU	C5-C4-N3	-4.04	120.15	125.36
31	y	1518	MA6	C3'-C2'-C1'	3.99	106.98	100.98
32	z	55	PSU	C5-C6-N1	-3.92	119.62	124.44
33	0	55	PSU	C3'-C2'-C1'	3.89	106.42	101.93
32	z	46	7MG	C6-C5-C4	3.81	119.29	115.20
31	y	1404	5MC	C2-N3-C4	3.78	120.58	116.02
31	y	967	5MC	C2-N3-C4	3.78	120.58	116.02
31	y	1407	5MC	C2-N3-C4	3.72	120.51	116.02
31	y	516	PSU	C5-C4-N3	-3.72	120.57	125.36
32	z	55	PSU	O4'-C1'-C5	3.68	115.63	109.93
32	z	55	PSU	C4'-O4'-C1'	-3.63	104.94	109.42
32	z	32	PSU	C5-C4-N3	-3.63	120.69	125.36
31	y	1400	5MC	C2-N3-C4	3.62	120.39	116.02
31	y	966	M2G	C3'-C2'-C1'	3.58	106.36	100.98
31	y	1407	5MC	C3'-C2'-C1'	3.57	106.35	100.98
32	z	37	MIA	C16-C14-C13	-3.49	112.56	122.65
31	y	967	5MC	C3'-C2'-C1'	3.43	106.14	100.98
31	y	1519	MA6	N3-C2-N1	-3.39	123.37	128.68
32	z	8	4SU	C5'-C4'-C3'	-3.37	102.55	115.18
31	y	1518	MA6	N3-C2-N1	-3.20	123.67	128.68
33	0	55	PSU	C5-C6-N1	-3.20	120.51	124.44
32	z	8	4SU	C3'-C2'-C1'	3.18	105.77	100.98
32	z	39	PSU	O4'-C1'-C5	-3.17	105.02	109.93
32	z	32	PSU	C5'-C4'-C3'	-3.17	103.31	115.18
31	y	966	M2G	N1-C2-N2	3.15	120.38	117.19
31	y	1519	MA6	C2'-C3'-C4'	3.09	108.65	102.64
32	z	32	PSU	C5-C6-N1	-3.03	120.72	124.44
32	z	55	PSU	C3'-C2'-C1'	3.02	105.41	101.93
31	y	516	PSU	C5-C6-N1	-2.99	120.76	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	z	32	PSU	O4'-C4'-C3'	2.89	110.83	105.11
31	y	1400	5MC	C6-N1-C1'	2.89	125.72	119.24
31	y	1498	UR3	C3'-C2'-C1'	2.87	105.30	100.98
31	y	516	PSU	C6-N1-C2	2.84	120.05	115.36
32	z	54	5MU	C3'-C2'-C1'	2.82	105.23	100.98
31	y	1402	4OC	CM4-N4-C4	2.80	125.37	122.97
32	z	32	PSU	C6-N1-C2	2.79	119.96	115.36
31	y	1207	2MG	O4'-C1'-C2'	-2.79	102.85	106.93
32	z	39	PSU	C6-N1-C2	2.76	119.91	115.36
31	y	1404	5MC	O4'-C4'-C5'	2.76	118.44	109.37
31	y	1518	MA6	O4'-C4'-C3'	2.74	110.54	105.11
31	y	1402	4OC	O4'-C4'-C3'	2.72	110.50	105.11
32	z	55	PSU	C6-N1-C2	2.71	119.84	115.36
33	0	55	PSU	C5-C4-N3	-2.71	121.88	125.36
31	y	966	M2G	C2-N3-C4	2.69	118.33	115.28
31	y	1402	4OC	O4'-C4'-C5'	2.68	118.20	109.37
31	y	1518	MA6	C5'-C4'-C3'	-2.65	105.25	115.18
31	y	966	M2G	O3'-C3'-C2'	2.59	120.21	111.82
32	z	39	PSU	C5-C6-N1	-2.58	121.27	124.44
31	y	1207	2MG	N2-C2-N1	2.58	119.43	116.96
31	y	1400	5MC	O4'-C1'-C2'	2.44	110.49	106.93
32	z	39	PSU	C4-C5-C1'	2.42	125.68	121.12
31	y	1400	5MC	C5-C6-N1	-2.39	119.62	122.19
32	z	16	H2U	C3'-C2'-C1'	2.37	105.93	101.43
32	z	54	5MU	O3'-C3'-C4'	-2.34	104.28	111.05
31	y	1207	2MG	O4'-C4'-C5'	2.34	117.07	109.37
31	y	966	M2G	C5'-C4'-C3'	-2.31	106.53	115.18
31	y	1498	UR3	O3'-C3'-C4'	2.29	117.68	111.05
31	y	516	PSU	C3'-C2'-C1'	2.29	104.58	101.93
31	y	1407	5MC	C2'-C3'-C4'	2.28	107.06	102.64
31	y	1498	UR3	O4'-C4'-C3'	2.27	109.61	105.11
32	z	20	H2U	C3'-C2'-C1'	2.26	105.72	101.43
32	z	8	4SU	O4'-C4'-C3'	2.26	109.58	105.11
32	z	46	7MG	O4'-C4'-C3'	2.23	109.53	105.11
31	y	516	PSU	O4'-C4'-C5'	2.18	116.56	109.37
31	y	527	7MG	N3-C4-N9	2.18	129.71	126.91
31	y	527	7MG	C4'-O4'-C1'	-2.16	104.72	109.47
32	z	46	7MG	C5'-C4'-C3'	-2.16	107.10	115.18
32	z	32	PSU	O4'-C1'-C5	-2.15	106.60	109.93
33	0	55	PSU	C6-N1-C2	2.13	118.88	115.36
31	y	1400	5MC	CM5-C5-C4	-2.12	119.58	121.72
32	z	39	PSU	O3'-C3'-C2'	2.12	118.67	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	y	1207	2MG	O3'-C3'-C2'	2.11	118.63	111.82
32	z	37	MIA	C2-N1-C6	2.07	120.90	117.19
31	y	1402	4OC	O3'-C3'-C4'	2.07	117.03	111.05
31	y	1207	2MG	C2'-C3'-C4'	-2.05	98.66	102.64
32	z	46	7MG	N1-C2-N3	-2.03	122.24	125.42
31	y	1518	MA6	O3'-C3'-C2'	2.01	118.31	111.82
32	z	54	5MU	C2'-C3'-C4'	2.00	106.53	102.64

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	y	516	PSU	C2'-C1'-C5-C4
31	y	516	PSU	C2'-C1'-C5-C6
32	z	37	MIA	O4'-C4'-C5'-O5'
32	z	37	MIA	C3'-C4'-C5'-O5'
32	z	37	MIA	C5-C6-N6-C12
32	z	37	MIA	C12-C13-C14-C16
31	y	1402	4OC	C1'-C2'-O2'-CM2
31	y	1404	5MC	C2'-C1'-N1-C6
31	y	1498	UR3	O4'-C1'-N1-C6
31	y	1498	UR3	C2'-C1'-N1-C6
32	z	55	PSU	O4'-C1'-C5-C6
32	z	16	H2U	O4'-C4'-C5'-O5'
32	z	16	H2U	C3'-C4'-C5'-O5'
31	y	1518	MA6	O4'-C4'-C5'-O5'
31	y	1518	MA6	C3'-C4'-C5'-O5'
31	y	1402	4OC	O4'-C4'-C5'-O5'
32	z	39	PSU	O4'-C4'-C5'-O5'
32	z	20	H2U	O4'-C4'-C5'-O5'
32	z	20	H2U	C3'-C4'-C5'-O5'
31	y	1498	UR3	O4'-C4'-C5'-O5'
32	z	32	PSU	O4'-C4'-C5'-O5'
31	y	1498	UR3	C3'-C4'-C5'-O5'
32	z	32	PSU	C3'-C4'-C5'-O5'
32	z	37	MIA	N1-C6-N6-C12
32	z	39	PSU	C3'-C4'-C5'-O5'
32	z	8	4SU	C3'-C4'-C5'-O5'
32	z	55	PSU	C2'-C1'-C5-C6
32	z	39	PSU	C2'-C1'-C5-C6
31	y	1402	4OC	C3'-C4'-C5'-O5'
32	z	8	4SU	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
31	y	1404	5MC	O4'-C4'-C5'-O5'
33	0	55	PSU	O4'-C1'-C5-C4
32	z	55	PSU	O4'-C1'-C5-C4
31	y	1404	5MC	C3'-C4'-C5'-O5'
31	y	1519	MA6	C3'-C4'-C5'-O5'

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	31
31	y	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	926:A	O3'	928:G	P	1.97
1	w	1506:C	O3'	1508:A	P	1.96
1	w	890:A	O3'	892:G	P	1.94
1	w	1171:G	O3'	1173:G	P	1.94
1	w	1481:U	O3'	1483:G	P	1.90
1	w	154(B):C	O3'	1547:C	P	1.90
1	w	1743:G	O3'	1746:G	P	1.89

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	y	102(C):C	O3'	1029:G	P	1.87
1	w	41:C	O3'	43:G	P	1.86
1	w	1133:U	O3'	1135:C	P	1.86
1	w	1712:C	O3'	1716:U	P	1.86
1	w	99:U	O3'	101:G	P	1.85
1	w	149(B):A	O3'	1449:G	P	1.85
1	w	1864:U	O3'	1869:G	P	1.83
1	w	2219:G	O3'	2224:G	P	1.83
1	w	155:C	O3'	161:U	P	1.82
1	w	489:G	O3'	491:G	P	1.82
1	w	1735:U	O3'	1741:C	P	1.82
1	w	2199:A	O3'	2205:C	P	1.82
1	y	458:C	O3'	464:G	P	1.82
1	w	114(B):A	O3'	1143:A	P	1.81
1	w	2213:U	O3'	2215:G	P	1.81
1	y	843:U	O3'	848:C	P	1.81
1	w	366(B):C	O3'	370:G	P	1.80
1	w	122(A):C	O3'	1222:C	P	1.80
1	y	210:U	O3'	216:G	P	1.80
1	w	165:U	O3'	171:G	P	1.79
1	w	163(B):C	O3'	1631:A	P	1.79
1	w	1872:A	O3'	1878:G	P	1.79
1	w	1451:C	O3'	1453:A	P	1.78
1	w	436:C	O3'	438:G	P	1.77
1	w	144(B):A	O3'	1445:C	P	1.77
1	w	1583:A	O3'	1585:C	P	1.77
1	w	537:C	O3'	539:G	P	1.76
1	y	838:G	O3'	841:U	P	1.76
1	w	712(B):A	O3'	2713:A	P	1.75

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	w	2889/2889 (100%)	0.35	77 (2%) 54 46	5, 5, 117, 159	0
2	x	120/121 (99%)	0.24	0 100 100	5, 13, 95, 127	0
3	A	127/229 (55%)	-0.05	8 (6%) 20 15	5, 50, 148, 151	0
4	B	272/276 (98%)	0.14	14 (5%) 28 24	5, 60, 148, 155	0
5	C	201/206 (97%)	0.09	10 (4%) 28 25	5, 49, 148, 159	0
6	D	194/205 (94%)	-0.19	8 (4%) 37 31	5, 55, 148, 165	0
7	E	180/182 (98%)	-0.39	9 (5%) 28 25	5, 58, 148, 156	0
8	F	173/180 (96%)	-0.29	10 (5%) 23 18	5, 67, 148, 160	0
9	G	148/148 (100%)	-0.33	3 (2%) 65 58	5, 43, 148, 151	0
10	H	138/163 (84%)	0.37	11 (7%) 12 10	5, 52, 147, 152	0
11	I	122/122 (100%)	0.37	10 (8%) 11 10	5, 35, 142, 148	0
12	J	146/150 (97%)	-0.12	9 (6%) 20 16	5, 90, 150, 160	0
13	K	137/141 (97%)	1.03	36 (26%) 0 0	5, 24, 148, 152	0
14	L	118/118 (100%)	-0.11	4 (3%) 45 37	5, 44, 148, 148	0
15	M	106/112 (94%)	0.54	20 (18%) 1 1	5, 48, 148, 160	0
16	N	137/146 (93%)	-0.20	1 (0%) 87 85	5, 74, 150, 167	0
17	O	117/118 (99%)	0.28	20 (17%) 1 1	5, 35, 114, 148	0
18	P	101/101 (100%)	0.23	16 (15%) 2 1	5, 79, 148, 159	0
19	Q	109/113 (96%)	0.34	13 (11%) 4 4	5, 33, 137, 149	0
20	R	92/96 (95%)	0.46	16 (17%) 1 1	5, 73, 148, 161	0
21	S	103/110 (93%)	0.81	25 (24%) 0 0	5, 86, 160, 163	0
22	T	185/206 (89%)	-0.48	2 (1%) 80 76	5, 50, 148, 161	0
23	U	76/85 (89%)	0.35	11 (14%) 2 2	5, 57, 151, 166	0
24	V	88/98 (89%)	0.98	21 (23%) 0 0	5, 91, 148, 154	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	W	62/72 (86%)	-0.38	0 100 100	5, 88, 149, 155	0
26	X	60/60 (100%)	-0.78	0 100 100	5, 36, 148, 150	0
27	Y	56/60 (93%)	0.42	11 (19%) 1 1	7, 77, 164, 168	0
28	Z	48/49 (97%)	0.21	1 (2%) 63 56	5, 5, 42, 126	0
29	a	63/65 (96%)	0.67	8 (12%) 3 4	5, 50, 151, 157	0
30	b	35/37 (94%)	2.44	18 (51%) 0 0	5, 102, 149, 153	0
31	y	1490/1522 (97%)	0.32	27 (1%) 68 62	5, 9, 113, 163	0
32	z	67/76 (88%)	0.24	1 (1%) 73 68	5, 6, 82, 117	0
33	0	75/76 (98%)	0.26	1 (1%) 77 72	5, 37, 129, 148	0
34	l	6/10 (60%)	0.27	0 100 100	5, 5, 54, 67	0
35	c	234/256 (91%)	-0.60	2 (0%) 84 80	5, 50, 151, 165	0
36	d	206/239 (86%)	-0.11	13 (6%) 20 15	5, 57, 148, 151	0
37	e	208/209 (99%)	-0.27	5 (2%) 59 51	5, 50, 148, 157	0
38	f	150/162 (92%)	-0.06	9 (6%) 21 16	5, 62, 148, 154	0
39	g	101/101 (100%)	-0.42	3 (2%) 50 40	5, 72, 148, 156	0
40	h	155/156 (99%)	-0.16	12 (7%) 13 11	5, 73, 155, 163	0
41	i	138/138 (100%)	-0.13	5 (3%) 42 35	5, 43, 148, 149	0
42	j	127/128 (99%)	0.36	16 (12%) 3 4	5, 85, 150, 154	0
43	k	98/105 (93%)	-0.25	1 (1%) 82 78	5, 83, 151, 164	0
44	l	116/129 (89%)	-0.33	8 (6%) 16 12	5, 71, 150, 162	0
45	m	124/132 (93%)	0.02	6 (4%) 30 26	5, 30, 148, 152	0
46	n	125/126 (99%)	-0.22	10 (8%) 12 10	5, 74, 148, 162	0
47	o	60/61 (98%)	1.78	23 (38%) 0 0	5, 66, 151, 161	0
48	p	88/89 (98%)	-0.43	3 (3%) 45 37	5, 57, 148, 163	0
49	q	83/88 (94%)	0.52	12 (14%) 2 2	5, 50, 148, 148	0
50	r	104/105 (99%)	0.11	7 (6%) 17 13	5, 52, 148, 158	0
51	s	73/88 (82%)	-0.75	0 100 100	5, 69, 149, 157	0
52	t	80/93 (86%)	-0.39	1 (1%) 77 72	5, 52, 148, 159	0
53	u	99/106 (93%)	0.90	21 (21%) 0 1	10, 66, 199, 199	0
54	v	24/27 (88%)	0.17	2 (8%) 11 9	5, 47, 139, 142	0
All	All	10434/10880 (95%)	0.17	580 (5%) 24 20	5, 32, 148, 199	0

All (580) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	M	81	GLY	10.0
15	M	82	ILE	8.0
8	F	179	LYS	8.0
44	l	125	PHE	7.7
47	o	13	THR	7.7
7	E	49	ASP	7.3
13	K	23	GLY	7.3
30	b	17	ILE	7.0
47	o	16	PHE	6.8
18	P	77	ALA	6.5
27	Y	55	ARG	6.5
31	y	108	G	6.4
20	R	11	PRO	6.3
15	M	80	LEU	6.3
30	b	24	TYR	6.2
13	K	5	ARG	6.2
30	b	25	VAL	6.2
31	y	107	G	6.1
8	F	56	SER	6.0
42	j	75	ASP	5.9
53	u	51	GLU	5.9
30	b	34	GLN	5.9
7	E	182	LYS	5.9
47	o	12	ARG	5.7
12	J	27	HIS	5.6
1	w	1094	U	5.5
10	H	96	THR	5.5
53	u	16	HIS	5.5
13	K	32	PHE	5.5
53	u	46	GLU	5.4
14	L	58	GLY	5.4
30	b	26	ILE	5.3
53	u	15	ARG	5.3
13	K	39	PRO	5.3
31	y	1492	A	5.2
46	n	124	PRO	5.2
13	K	111	GLU	5.2
1	w	2296	U	5.2
13	K	110	THR	5.1
30	b	28	GLU	5.1
23	U	83	PRO	5.0
6	D	91	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
13	K	31	ASP	4.9
30	b	16	VAL	4.9
47	o	10	ALA	4.9
1	w	1098	A	4.9
12	J	30	THR	4.9
1	w	1573	G	4.8
15	M	83	LYS	4.8
7	E	76	SER	4.8
44	l	126	ARG	4.8
20	R	10	ALA	4.8
30	b	15	LYS	4.8
23	U	85	ALA	4.7
12	J	28	GLY	4.7
47	o	17	LYS	4.7
29	a	28	GLY	4.6
49	q	14	ASN	4.6
24	V	42	GLN	4.6
31	y	723	U	4.6
13	K	112	GLU	4.6
13	K	92	GLY	4.6
15	M	79	ALA	4.6
5	C	57	LYS	4.6
7	E	83	ARG	4.5
1	w	1093	G	4.5
13	K	40	ALA	4.5
44	l	124	LYS	4.4
18	P	76	LYS	4.4
23	U	16	SER	4.4
13	K	24	GLY	4.4
13	K	99	PRO	4.4
46	n	118	ALA	4.4
13	K	21	THR	4.3
24	V	18	ILE	4.3
1	w	405	U	4.3
24	V	43	TYR	4.3
18	P	78	LYS	4.3
53	u	102	GLY	4.2
24	V	17	SER	4.2
13	K	91	GLU	4.2
23	U	84	LEU	4.2
21	S	5	MET	4.2
18	P	73	SER	4.2

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Mol	Chain	Res	Type	RSRZ
47	o	11	LYS	4.2
49	q	23	ASP	4.2
23	U	65	GLY	4.1
18	P	85	LYS	4.1
47	o	23	ARG	4.1
31	y	325	A	4.1
16	N	135	VAL	4.1
15	M	9	ARG	4.1
10	H	75	VAL	4.1
47	o	15	LYS	4.1
24	V	19	GLN	4.1
24	V	35	THR	4.1
21	S	82	PRO	4.0
53	u	50	GLU	4.0
1	w	508	G	4.0
20	R	34	ALA	4.0
21	S	4	LYS	4.0
18	P	83	ARG	4.0
50	r	26	GLN	4.0
53	u	52	ALA	4.0
4	B	170	GLY	4.0
49	q	11	SER	4.0
45	m	28	GLY	3.9
3	A	14	LYS	3.9
1	w	2833	G	3.9
1	w	2087	G	3.9
36	d	31	HIS	3.9
49	q	10	GLY	3.9
37	e	160	GLN	3.9
9	G	20	ASP	3.9
21	S	11	ASP	3.9
47	o	14	PRO	3.8
53	u	11	SER	3.8
30	b	29	ASN	3.8
10	H	122	LEU	3.8
24	V	22	GLY	3.8
15	M	23	ARG	3.8
6	D	81	GLY	3.7
21	S	83	THR	3.7
1	w	449	A	3.7
8	F	80	SER	3.7
19	Q	85	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
20	R	75	ASP	3.7
23	U	15	ASP	3.7
44	l	117	ASN	3.7
1	w	2798	C	3.6
31	y	412	A	3.6
42	j	14	VAL	3.6
40	h	7	ALA	3.6
13	K	90	VAL	3.6
4	B	36	PRO	3.6
39	g	96	PRO	3.6
10	H	106	LYS	3.6
47	o	38	GLY	3.6
18	P	74	LYS	3.6
10	H	42	GLU	3.6
24	V	9	GLY	3.6
18	P	6	LYS	3.6
13	K	38	GLU	3.6
11	I	8	LEU	3.6
12	J	26	GLY	3.6
15	M	24	LEU	3.6
11	I	96	THR	3.5
40	h	8	GLU	3.5
21	S	6	HIS	3.5
40	h	9	VAL	3.5
42	j	31	GLN	3.5
10	H	97	ARG	3.5
31	y	1360	A	3.5
53	u	101	GLY	3.5
20	R	74	PRO	3.5
41	i	90	GLY	3.5
31	y	135	C	3.5
24	V	10	LYS	3.5
3	A	9	ARG	3.5
24	V	15	ALA	3.5
53	u	47	GLY	3.5
53	u	18	GLN	3.5
21	S	35	TYR	3.5
18	P	87	HIS	3.5
27	Y	54	GLY	3.4
27	Y	25	LEU	3.4
10	H	98	TYR	3.4
21	S	29	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
18	P	88	ARG	3.4
36	d	35	GLU	3.4
14	L	57	ARG	3.4
8	F	81	GLU	3.4
15	M	57	LYS	3.4
1	w	2500	U	3.4
36	d	39	ILE	3.4
53	u	55	ILE	3.4
21	S	3	VAL	3.4
21	S	30	VAL	3.4
53	u	71	THR	3.4
42	j	123	PRO	3.3
31	y	731	G	3.3
20	R	33	LYS	3.3
13	K	98	LYS	3.3
49	q	24	ALA	3.3
21	S	28	LYS	3.3
5	C	120	TRP	3.3
23	U	82	ARG	3.3
24	V	24	ALA	3.3
41	i	60	ARG	3.3
29	a	14	VAL	3.3
47	o	48	ALA	3.3
18	P	84	LYS	3.3
47	o	27	CYS	3.3
1	w	2447	G	3.2
37	e	154	ASN	3.2
47	o	49	HIS	3.2
1	w	645	C	3.2
17	O	29	SER	3.2
18	P	75	PHE	3.2
42	j	76	ALA	3.2
47	o	52	GLN	3.2
17	O	36	ARG	3.2
13	K	20	ALA	3.2
53	u	103	GLY	3.2
4	B	194	GLY	3.2
38	f	90	VAL	3.2
39	g	98	LEU	3.2
17	O	40	PHE	3.2
40	h	83	ALA	3.2
17	O	43	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
19	Q	26	GLY	3.2
19	Q	81	ALA	3.2
8	F	178	ALA	3.2
18	P	79	VAL	3.2
12	J	22	GLY	3.1
13	K	97	VAL	3.1
42	j	98	PRO	3.1
21	S	100	ALA	3.1
4	B	109	ASP	3.1
17	O	38	THR	3.1
36	d	90	GLU	3.1
35	c	139	LYS	3.1
38	f	89	ILE	3.1
19	Q	78	GLU	3.1
42	j	126	SER	3.1
36	d	38	ARG	3.1
42	j	105	ASP	3.1
13	K	4	PRO	3.1
20	R	67	GLY	3.1
14	L	59	ASP	3.0
41	i	91	ARG	3.0
47	o	25	VAL	3.0
20	R	27	THR	3.0
11	I	2	ILE	3.0
21	S	48	ALA	3.0
17	O	14	HIS	3.0
21	S	1	MET	3.0
1	w	436	C	3.0
1	w	812	C	3.0
3	A	55	SER	3.0
18	P	86	GLY	3.0
1	w	2323	G	3.0
4	B	80	ALA	3.0
24	V	40	ARG	3.0
38	f	124	GLY	3.0
31	y	44	G	3.0
15	M	8	GLU	3.0
4	B	26	LYS	3.0
17	O	16	LYS	3.0
31	y	1397	C	3.0
5	C	125	GLY	3.0
8	F	13	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
13	K	41	TRP	3.0
1	w	1099	G	3.0
52	t	57	HIS	3.0
24	V	44	PRO	2.9
18	P	82	ARG	2.9
27	Y	56	LYS	2.9
23	U	64	ASP	2.9
47	o	28	GLY	2.9
53	u	45	GLN	2.9
20	R	28	PHE	2.9
41	i	49	GLU	2.9
13	K	131	ILE	2.9
30	b	9	ARG	2.9
29	a	29	LYS	2.9
36	d	10	PHE	2.9
48	p	88	ARG	2.9
47	o	9	LYS	2.9
1	w	79	G	2.9
47	o	22	THR	2.8
31	y	134	A	2.8
24	V	11	ARG	2.8
1	w	2382	G	2.8
17	O	31	SER	2.8
45	m	113	LYS	2.8
47	o	51	GLY	2.8
8	F	177	GLY	2.8
27	Y	53	ALA	2.8
48	p	87	ILE	2.8
15	M	77	ALA	2.8
17	O	28	ARG	2.8
38	f	29	GLY	2.8
9	G	110	ASP	2.8
11	I	14	THR	2.8
27	Y	24	ALA	2.8
44	l	118	GLY	2.8
46	n	71	ARG	2.8
50	r	33	GLY	2.8
23	U	10	THR	2.8
1	w	888	C	2.8
15	M	78	LEU	2.8
46	n	36	LYS	2.8
3	A	13	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
24	V	16	ASN	2.8
22	T	116	VAL	2.8
19	Q	86	LEU	2.8
27	Y	12	SER	2.8
8	F	170	ARG	2.8
29	a	7	HIS	2.7
30	b	33	LYS	2.7
13	K	22	LYS	2.7
31	y	977	A	2.7
13	K	33	GLY	2.7
46	n	125	ARG	2.7
1	w	848	G	2.7
40	h	11	GLN	2.7
36	d	93	LYS	2.7
31	y	1493	A	2.7
24	V	41	ARG	2.7
11	I	7	TYR	2.7
40	h	13	GLN	2.7
27	Y	26	THR	2.7
1	w	2612	C	2.7
12	J	25	SER	2.7
29	a	51	ALA	2.7
36	d	98	ASN	2.7
1	w	2318	G	2.7
23	U	68	GLU	2.7
50	r	75	ARG	2.7
6	D	95	THR	2.7
47	o	24	CYS	2.7
1	w	2322	A	2.7
1	w	2793	G	2.7
5	C	142	GLY	2.7
40	h	84	ASN	2.7
40	h	80	VAL	2.6
4	B	124	PRO	2.6
20	R	32	PRO	2.6
8	F	57	ASP	2.6
21	S	34	LYS	2.6
32	z	17	C	2.6
1	w	2297	C	2.6
29	a	22	VAL	2.6
21	S	90	LEU	2.6
1	w	1817	G	2.6

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Mol	Chain	Res	Type	RSRZ
13	K	119	ARG	2.6
31	y	934	C	2.6
17	O	44	ASN	2.6
41	i	54	ASP	2.6
15	M	111	GLU	2.6
31	y	146	G	2.6
54	v	24	ARG	2.6
46	n	83	ASP	2.6
6	D	46	THR	2.6
49	q	15	PRO	2.6
15	M	109	GLY	2.6
1	w	192	C	2.6
1	w	2446	G	2.6
27	Y	59	GLU	2.6
8	F	169	VAL	2.6
1	w	2499	C	2.5
1	w	2820	A	2.5
15	M	74	ALA	2.5
50	r	80	GLY	2.5
31	y	727	G	2.5
49	q	13	HIS	2.5
7	E	127	GLY	2.5
35	c	36	ARG	2.5
15	M	58	LEU	2.5
13	K	93	TYR	2.5
11	I	1	MET	2.5
1	w	1252	G	2.5
21	S	99	CYS	2.5
1	w	149	A	2.5
38	f	123	LEU	2.5
37	e	153	ARG	2.5
13	K	96	VAL	2.5
1	w	2611	U	2.5
19	Q	16	LYS	2.5
1	w	2317	C	2.5
17	O	13	LYS	2.5
44	l	119	CYS	2.5
53	u	19	SER	2.5
17	O	37	GLU	2.5
36	d	96	GLY	2.5
47	o	47	LEU	2.5
24	V	21	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
6	D	89	PRO	2.5
29	a	6	THR	2.5
9	G	146	ALA	2.4
36	d	9	GLY	2.4
40	h	2	ALA	2.4
10	H	124	HIS	2.4
17	O	17	ILE	2.4
31	y	530	G	2.4
21	S	88	LYS	2.4
6	D	80	GLY	2.4
40	h	81	GLY	2.4
5	C	193	GLY	2.4
1	w	1626	G	2.4
20	R	30	VAL	2.4
21	S	27	VAL	2.4
21	S	93	GLY	2.4
42	j	77	ILE	2.4
49	q	9	PHE	2.4
6	D	20	PRO	2.4
31	y	326	G	2.4
38	f	125	SER	2.4
21	S	49	VAL	2.4
42	j	124	GLN	2.4
1	w	1010	A	2.4
40	h	78	ARG	2.4
13	K	19	GLY	2.4
43	k	52	GLY	2.4
19	Q	74	ALA	2.4
1	w	958	U	2.4
31	y	143	A	2.4
45	m	19	LYS	2.4
3	A	35	THR	2.4
24	V	39	LYS	2.4
19	Q	97	LYS	2.4
5	C	174	ASP	2.4
17	O	42	ALA	2.4
44	l	12	ARG	2.4
53	u	53	LEU	2.4
38	f	120	THR	2.4
42	j	125	TYR	2.4
38	f	15	ARG	2.3
45	m	61	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	w	615	G	2.3
30	b	12	ASP	2.3
30	b	19	ARG	2.3
11	I	25	LEU	2.3
48	p	86	GLY	2.3
31	y	60	A	2.3
7	E	82	LEU	2.3
17	O	27	LEU	2.3
1	w	2387	U	2.3
13	K	129	THR	2.3
1	w	148	C	2.3
7	E	48	GLU	2.3
53	u	9	ASN	2.3
29	a	11	LYS	2.3
3	A	50	ILE	2.3
1	w	530	G	2.3
33	0	53	G	2.3
10	H	107	LYS	2.3
15	M	84	GLN	2.3
5	C	113	PHE	2.3
1	w	2345	G	2.3
42	j	115	GLY	2.3
45	m	62	GLY	2.3
27	Y	11	THR	2.3
5	C	159	HIS	2.3
23	U	80	HIS	2.3
1	w	575	A	2.3
12	J	54	GLY	2.3
49	q	26	ARG	2.3
19	Q	83	LYS	2.3
1	w	813	U	2.2
1	w	1630	G	2.2
30	b	30	PRO	2.2
44	l	123	LYS	2.2
19	Q	82	LEU	2.2
40	h	12	LEU	2.2
46	n	69	GLU	2.2
19	Q	73	ALA	2.2
3	A	56	ASP	2.2
46	n	126	LYS	2.2
36	d	42	LEU	2.2
49	q	36	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	w	1641	A	2.2
4	B	17	THR	2.2
12	J	57	THR	2.2
1	w	1350	C	2.2
7	E	118	ARG	2.2
6	D	42	GLY	2.2
15	M	22	GLY	2.2
50	r	76	LEU	2.2
42	j	42	ARG	2.2
21	S	102	CYS	2.2
5	C	190	GLY	2.2
11	I	98	VAL	2.2
1	w	237	C	2.2
19	Q	93	ALA	2.2
30	b	18	ARG	2.2
50	r	79	SER	2.2
1	w	452	G	2.2
31	y	112	G	2.2
1	w	2020	A	2.2
13	K	79	LEU	2.2
20	R	73	ARG	2.2
21	S	10	GLY	2.2
31	y	48	C	2.2
30	b	20	HIS	2.2
1	w	382	G	2.2
1	w	859	G	2.2
1	w	1095	A	2.2
1	w	2379	G	2.2
3	A	203	GLU	2.2
4	B	15	PHE	2.2
17	O	4	ALA	2.2
18	P	81	TYR	2.2
13	K	80	GLU	2.2
7	E	166	ASP	2.2
19	Q	27	LYS	2.2
24	V	20	ARG	2.2
1	w	351	G	2.2
49	q	61	SER	2.2
1	w	1783	A	2.2
17	O	39	LEU	2.2
1	w	2012	G	2.2
13	K	37	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
31	y	815	A	2.1
1	w	462	C	2.1
13	K	113	GLN	2.1
1	w	2321	G	2.1
1	w	2380	C	2.1
11	I	112	MET	2.1
42	j	127	LYS	2.1
12	J	104	GLY	2.1
1	w	1847	A	2.1
53	u	17	ARG	2.1
1	w	1013	C	2.1
20	R	71	GLY	2.1
13	K	60	ARG	2.1
15	M	41	ASP	2.1
27	Y	27	PRO	2.1
15	M	7	TYR	2.1
1	w	2090	G	2.1
11	I	3	GLN	2.1
42	j	66	ARG	2.1
1	w	1289	C	2.1
47	o	50	LYS	2.1
21	S	31	LEU	2.1
13	K	108	GLY	2.1
24	V	25	LYS	2.1
30	b	22	ARG	2.1
1	w	1554	A	2.1
49	q	17	TYR	2.1
31	y	43	C	2.1
13	K	73	PRO	2.1
17	O	34	LYS	2.1
1	w	1815	A	2.1
4	B	214	TRP	2.1
10	H	139	LEU	2.1
37	e	150	GLU	2.1
46	n	122	LYS	2.1
1	w	1634	A	2.1
1	w	2388	A	2.1
31	y	653	A	2.1
47	o	26	ARG	2.1
39	g	97	PHE	2.1
17	O	47	TYR	2.1
4	B	200	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
10	H	140	PHE	2.1
1	w	1011	G	2.1
20	R	9	LEU	2.1
28	Z	31	LEU	2.1
37	e	163	GLU	2.1
1	w	932	G	2.0
1	w	1667	G	2.0
17	O	35	ALA	2.0
24	V	45	ASN	2.0
50	r	35	VAL	2.0
4	B	272	ALA	2.0
53	u	56	MET	2.0
54	v	23	PRO	2.0
4	B	28	GLU	2.0
31	y	314	C	2.0
36	d	153	VAL	2.0
4	B	112	GLN	2.0
5	C	158	GLY	2.0
42	j	45	ALA	2.0
20	R	7	VAL	2.0
36	d	155	GLY	2.0
38	f	8	GLU	2.0
21	S	50	ARG	2.0
53	u	76	ALA	2.0
14	L	70	LEU	2.0
45	m	21	SER	2.0
30	b	35	ARG	2.0
46	n	80	ARG	2.0
20	R	29	TRP	2.0
22	T	163	LEU	2.0
1	w	234	C	2.0
1	w	235	U	2.0
1	w	236	C	2.0
1	w	450	G	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
32	PSU	z	55	20/21	0.64	0.30	40,50,52,53	0
33	PSU	0	55	20/21	0.75	0.22	36,36,36,36	0
31	4OC	y	1402	22/23	0.80	0.28	10,13,16,16	0
32	H2U	z	16	20/21	0.80	0.55	80,92,93,95	0
32	MIA	z	37	29/30	0.81	0.28	20,26,32,32	0
32	H2U	z	20	20/21	0.81	0.38	124,124,133,133	0
31	5MC	y	967	21/22	0.81	0.39	124,124,133,133	0
31	PSU	y	516	20/21	0.82	0.20	137,138,148,148	0
32	7MG	z	46	24/25	0.82	0.20	5,5,12,12	0
31	MA6	y	1519	24/25	0.84	0.25	5,5,6,8	0
31	M2G	y	966	25/26	0.85	0.28	15,16,20,31	0
31	MA6	y	1518	24/25	0.85	0.20	31,39,52,53	0
32	4SU	z	8	20/21	0.85	0.24	5,5,5,5	0
31	5MC	y	1404	21/22	0.89	0.33	5,6,8,9	0
32	PSU	z	32	20/21	0.89	0.30	42,52,58,59	0
31	2MG	y	1207	24/25	0.90	0.23	21,22,26,26	0
32	PSU	z	39	20/21	0.90	0.22	5,5,5,5	0
31	7MG	y	527	24/25	0.90	0.23	7,10,24,26	0
32	5MU	z	54	21/22	0.90	0.23	5,5,5,5	0
31	5MC	y	1400	21/22	0.93	0.21	5,5,5,5	0
31	UR3	y	1498	21/22	0.94	0.20	5,5,5,5	0
31	5MC	y	1407	21/22	0.95	0.16	25,28,30,30	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.