Full wwPDB X-ray Structure Validation Report (i)

Mar 24, 2024 – 12:07 AM EDT

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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

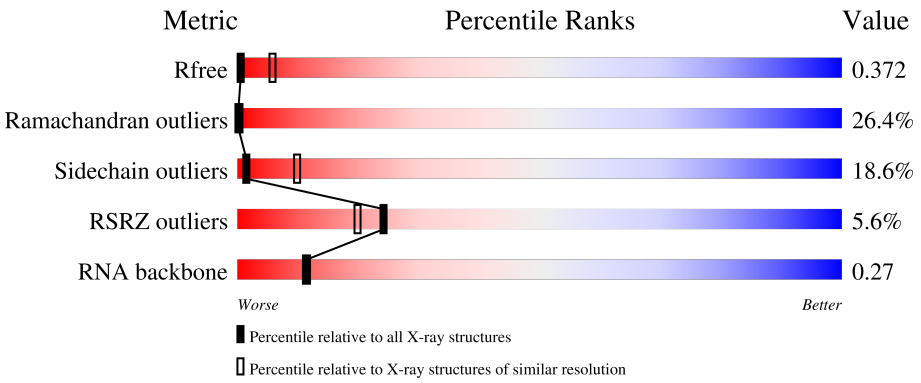
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

1 Overall quality at a glance (i)

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 of 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 <=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	3%, 57%, 39%, •
2	x	121	61%, 36%, • •
3	A	229	3%, 39%, 14%, •, 45%
4	B	276	5%, 57%, 38%, • •
5	C	206	5%, 56%, 34%, 7%, •

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Mol	Chain	Length	Quality of chain
6	D	205	4% 55% 35% 5% 5%
7	E	182	5% 64% 32%
8	F	180	6% 65% 28%
9	G	148	2% 59% 38%
10	H	163	7% 47% 30% 8% 15%
11	I	122	8% 59% 38%
12	J	150	6% 55% 38%
13	K	141	26% 54% 36% 7%
14	L	118	3% 61% 36%
15	M	112	18% 56% 31% 7% 5%
16	N	146	% 55% 34% 5% 6%
17	O	118	17% 70% 25%
18	P	101	16% 52% 47%
19	Q	113	12% 61% 31%
20	R	96	17% 54% 36% 5%
21	S	110	23% 61% 27% 5% 6%
22	T	206	% 63% 25% 10%
23	U	85	13% 59% 26% 5% 11%
24	V	98	21% 58% 24% 7% 10%
25	W	72	46% 31% 10% 14%
26	X	60	70% 23% 7%
27	Y	60	18% 55% 35% 7%
28	Z	49	2% 61% 31% 6%
29	a	65	12% 57% 29% 11%
30	b	37	49% 70% 24% 5%

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Mol	Chain	Length	Quality of chain
31	y	1522	2%, 62%, 32%
32	z	76	%, 59%, 28%, 13%
33	0	76	%, 58%, 37%, 5%
34	1	10	40%, 20%, 40%
35	c	256	%, 55%, 32%, 5%, 9%
36	d	239	5%, 53%, 30%, 14%
37	e	209	2%, 56%, 40%
38	f	162	6%, 66%, 24%, 7%
39	g	101	3%, 74%, 23%
40	h	156	8%, 72%, 25%
41	i	138	4%, 67%, 28%, 5%
42	j	128	12%, 73%, 24%
43	k	105	%, 64%, 27%, 7%
44	l	129	6%, 58%, 30%, 10%
45	m	132	5%, 54%, 36%, 6%
46	n	126	8%, 63%, 32%
47	o	61	38%, 61%, 31%, 7%
48	p	89	3%, 69%, 26%
49	q	88	14%, 65%, 27%, 6%
50	r	105	7%, 65%, 26%, 9%
51	s	88	55%, 24%, 5%, 17%
52	t	93	%, 55%, 26%, 5%, 14%
53	u	106	20%, 71%, 23%, 7%
54	v	27	7%, 63%, 26%, 11%

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 crite-

ria:

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

2 Entry composition (i)

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
			Total	C	N	O	P			
1	w	2889	62213	27690	11624	20011	2888	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 31 is a RNA chain called 16S SMALL SUBUNIT RIBOSOMAL RNA.

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

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
			Total	C	N	O	P	S			
32	z	76	1628	731	290	530	75	2	0	0	0

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
			Total	C	N	O	P			
33	0	76	1621	725	293	528	75	0	0	0

- Molecule 34 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
34	1	6	122	56	19	42	5	0	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
51	s	73	598	381	118	99	0	0	0

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

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

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

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

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

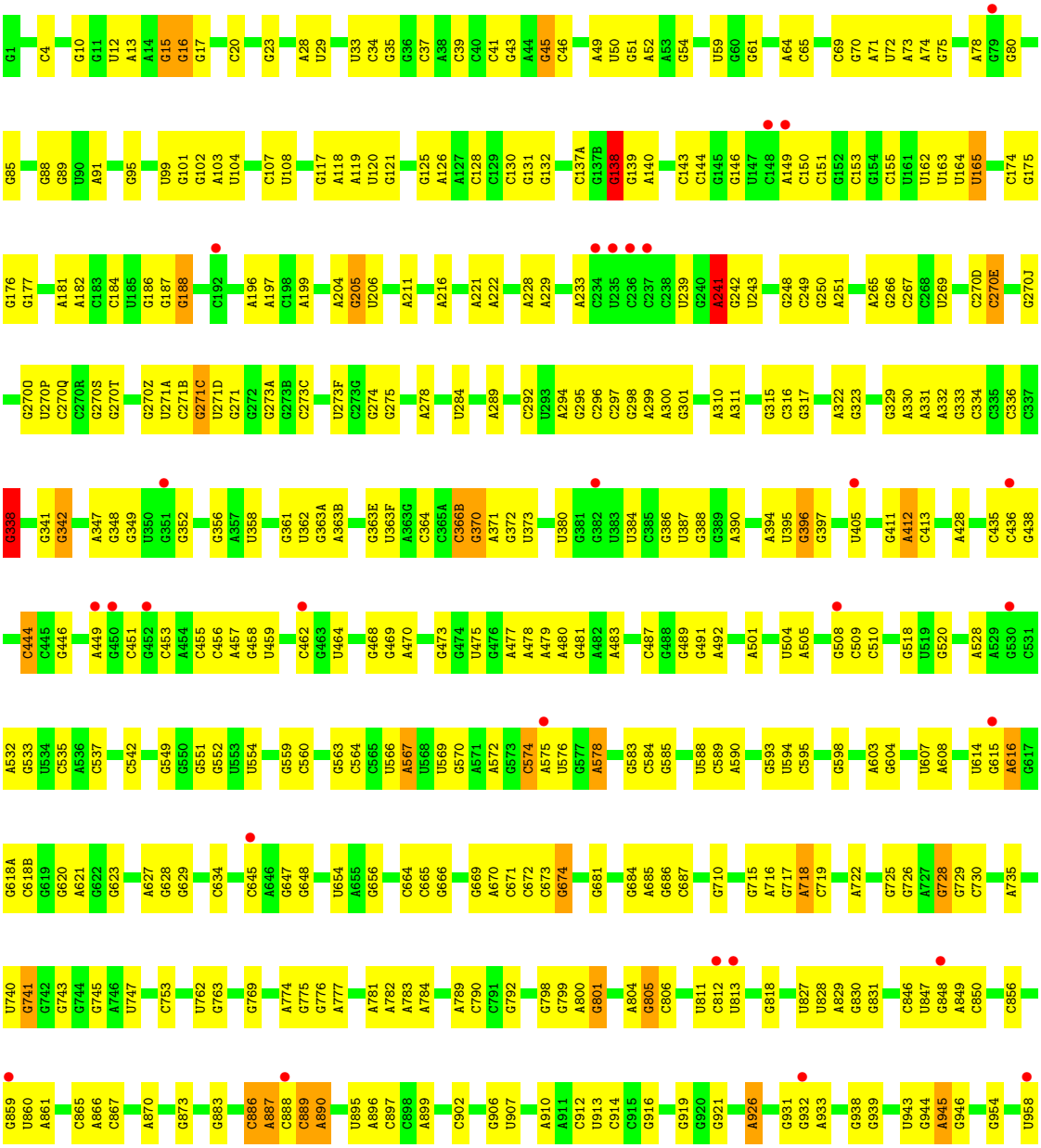
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
54	v	24	208	128	50	30	0	0	0

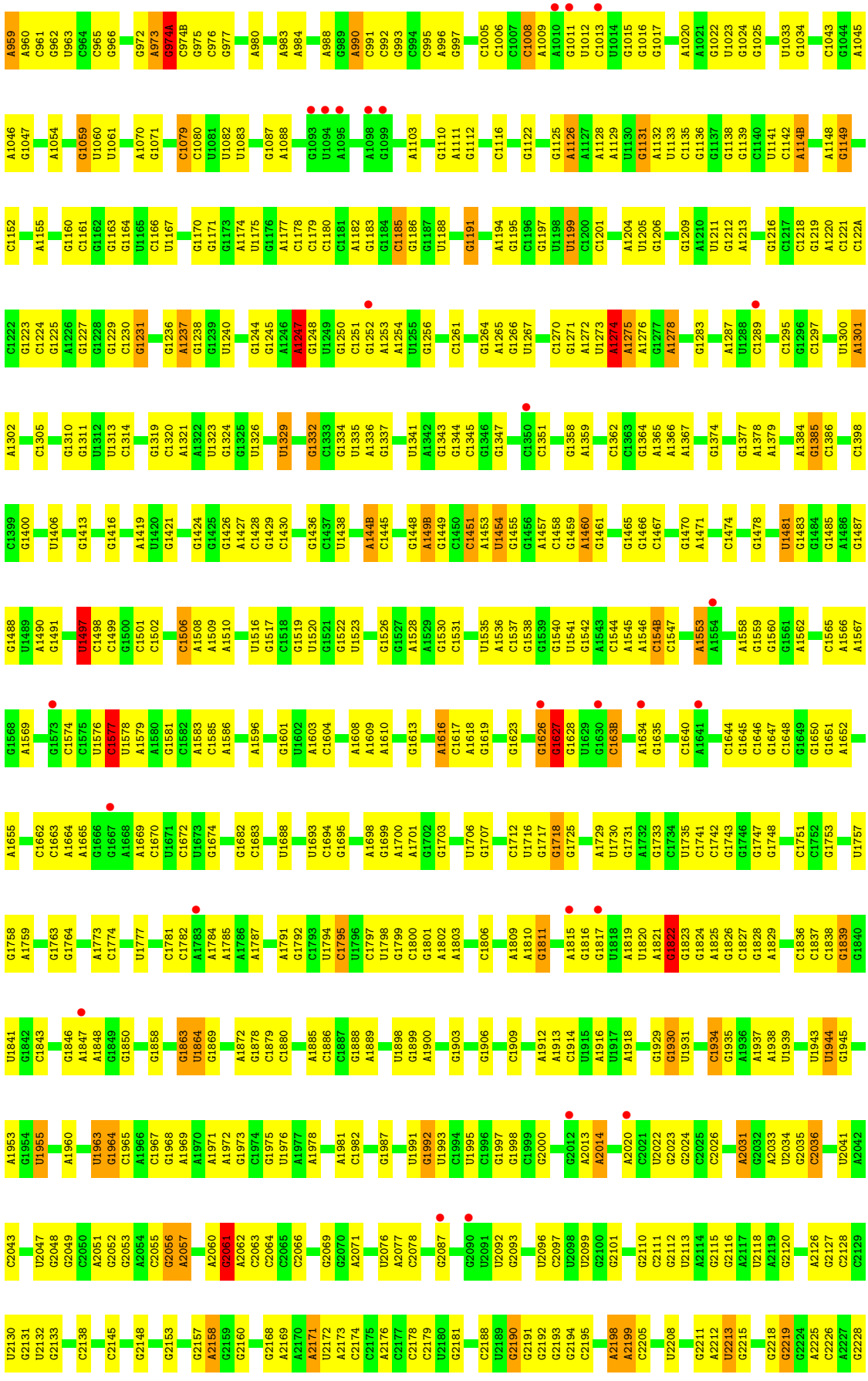
3 Residue-property plots (i)

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

- Molecule 1: 23S LARGE SUBUNIT RIBOSOMAL RNA

Chain w: 3% 57% 39%

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A1046 G1047 A1054 G1059 U1060 U1061 A1070 G1071 C1079 C1080 U1081 U1082 U1083 G1087 A1088 G1093 U1094 A1095 A1098 G1099 A1103 G1110 A1111 G1112 C1116 G1122 G1125 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 C1135 G1136 G1137 G1138 G1139 C1140 U1141 C1142 A114B A1148 G1149
C1152 A1155 G1160 C1161 G1162 G1163 G1164 U1165 C1166 U1167 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186 C1187 U1188 G1191 A1194 G1195 C1196 G1197 U1198 U1199 C1200 C1201 A1204 U1205 G1206 G1209 A1210 U1211 G1212 A1213 G1216 C1217 C1218 G1219 A1220 C1221 C122A
C1222 G1223 C1224 G1225 A1226 G1227 G1228 G1229 C1230 G1231 G1236 A1237 G1238 G1239 U1240 G1244 G1245 A1246 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1261 G1264 A1265 G1266 U1267 C1270 G1271 A1272 U1273 A1274 A1275 A1276 G1277 A1278 G1283 A1287 U1288 C1289 C1295 G1296 C1297 U1300 A1301
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C1399 G1400 U1406 G1413 G1416 A1419 U1420 G1421 G1424 G1425 G1426 A1427 C1428 G1429 C1430 G1436 C1437 U1438 A144B C1445 G1448 A149B G1449 C1450 C1451 A1453 U1454 G1455 G1456 A1457 C1458 G1459 A1460 G1461 G1465 G1466 C1467 G1470 A1471 C1474 G1478 U1481 G1483 G1484 G1485 A1486 G1487
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G1568 A1569 G1573 C1574 C1575 U1576 C1577 U1578 A1579 A1580 G1581 C1582 A1583 C1585 A1586 A1596 G1601 U1602 A1603 C1604 A1608 A1609 A1610 G1613 A1616 C1617 A1618 G1619 G1623 G1626 G1627 G1628 U1629 G1630 C163B A1634 G1635 C1640 A1641 C1644 G1645 C1646 G1647 C1648 G1649 G1650 G1651 A1652
A1655 C1662 C1663 A1664 A1665 G1666 G1667 A1668 A1669 C1670 U1671 C1672 U1673 G1674 G1682 C1683 U1688 U1693 C1694 G1695 A1698 G1699 A1700 A1701 G1702 G1703 U1706 G1707 C1712 U1716 G1717 G1718 G1725 A1729 U1730 G1731 A1732 G1733 C1734 U1735 C1741 C1742 G1743 G1746 G1747 G1748 C1751 C1752 G1753 U1757
G1758 A1759 G1763 G1764 A1773 C1774 U1777 C1781 C1782 A1783 A1784 A1785 A1786 A1787 A1791 G1792 C1793 U1794 C1795 U1796 C1797 U1798 G1799 C1800 G1801 A1802 A1803 C1806 A1809 A1810 G1811 A1815 G1816 G1817 U1818 A1819 U1820 A1821 G1822 G1823 G1824 A1825 G1826 C1827 G1828 A1829 C1836 C1837 C1838 G1839 G1840
U1841 G1842 C1843 G1846 A1847 A1848 G1849 G1850 G1858 G1863 U1864 G1869 A1872 G1878 C1879 C1880 A1885 C1886 C1887 G1888 A1889 U1898 G1899 A1900 G1903 G1906 C1909 A1912 A1913 C1914 U1915 A1916 U1917 A1918 G1929 G1930 U1931 C1934 G1935 A1936 A1937 A1938 U1939 U1943 U1944 G1945
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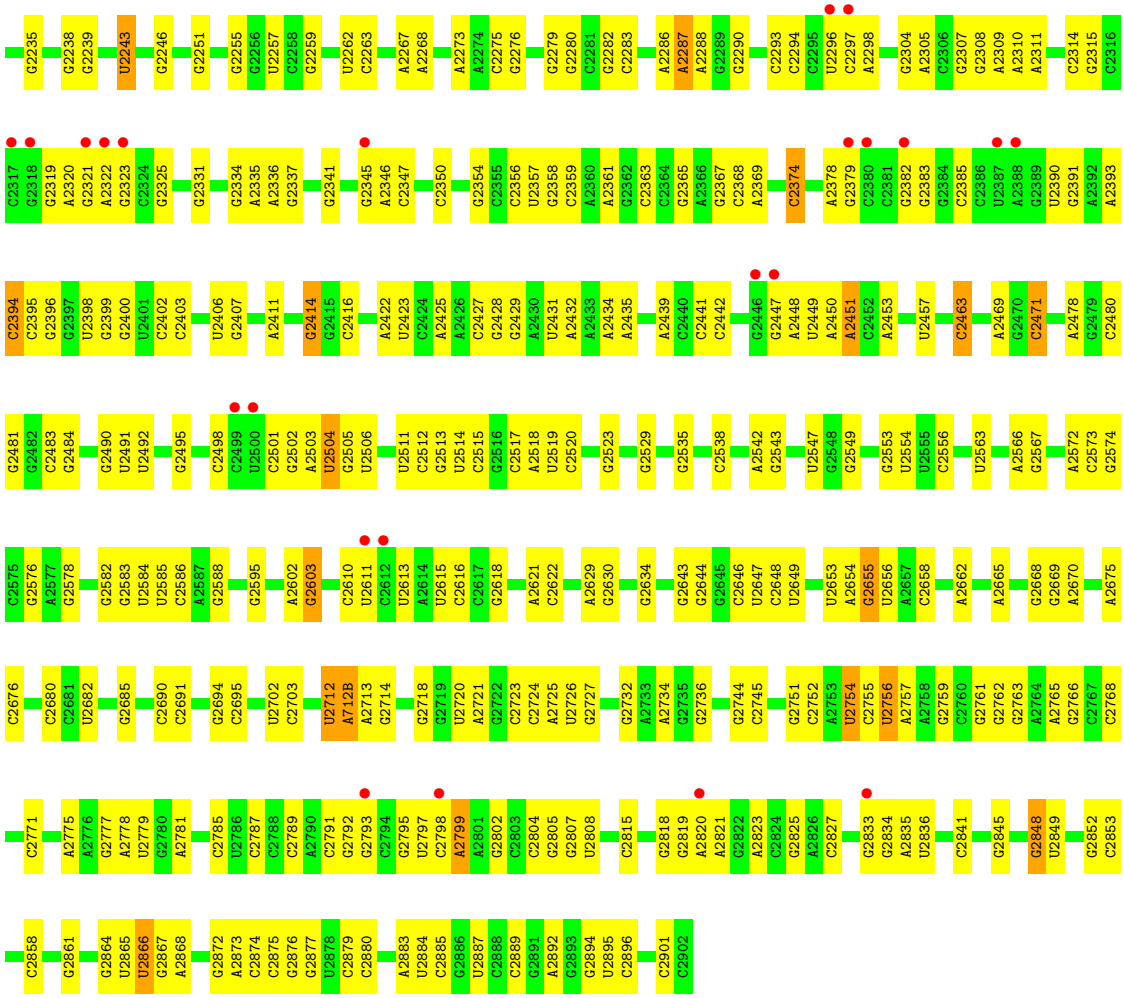
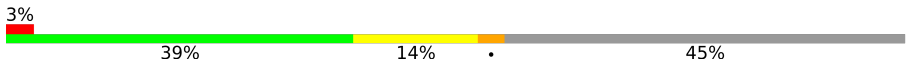


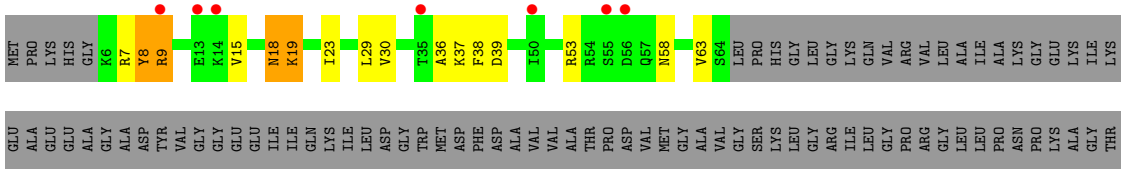
- Molecule 2: 5S LARGE SUBUNIT RIBOSOMAL RNA

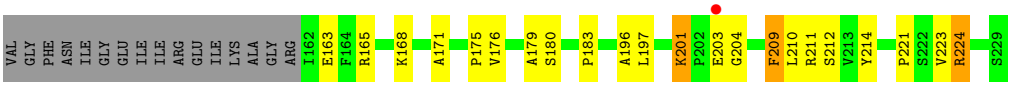
Chain x:

- Molecule 3: 50S ribosomal protein L1

Chain A:

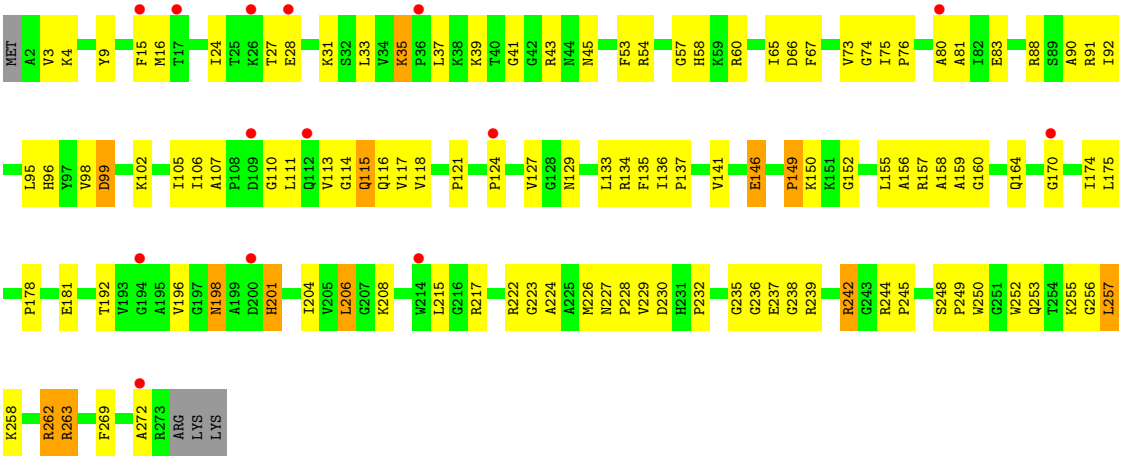






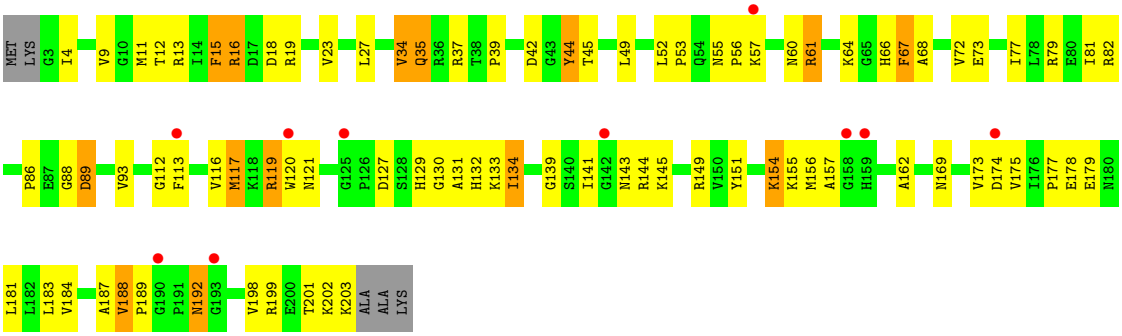
• Molecule 4: 50S ribosomal protein L2

Chain B:



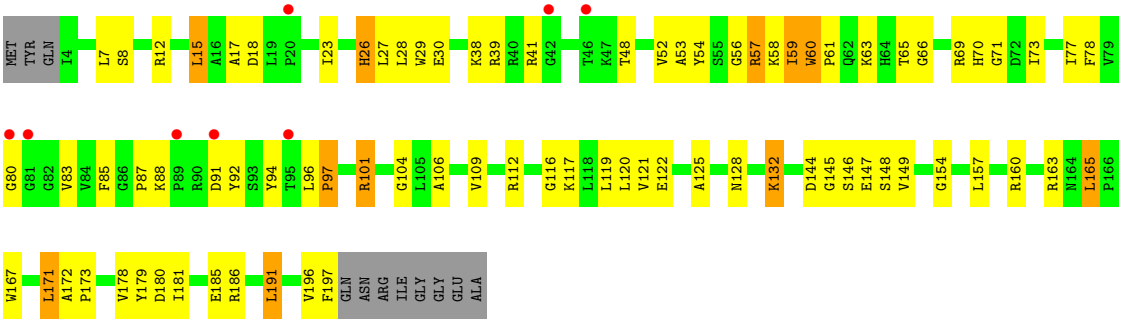
• Molecule 5: 50S ribosomal protein L3

Chain C:



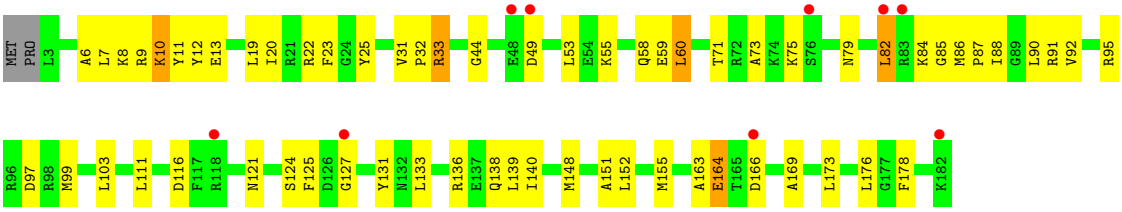
• Molecule 6: 50S ribosomal protein L4

Chain D:



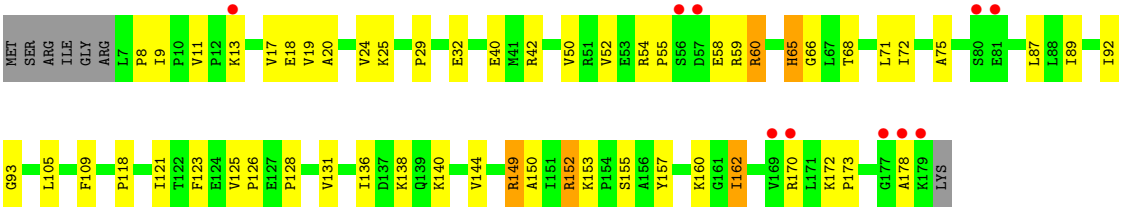
• Molecule 7: 50S ribosomal protein L5

Chain E:



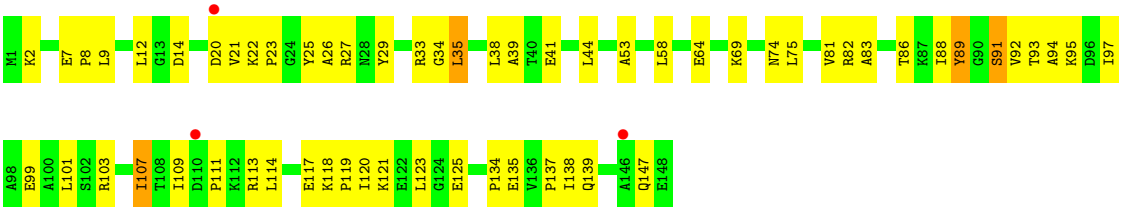
• Molecule 8: 50S ribosomal protein L6

Chain F:



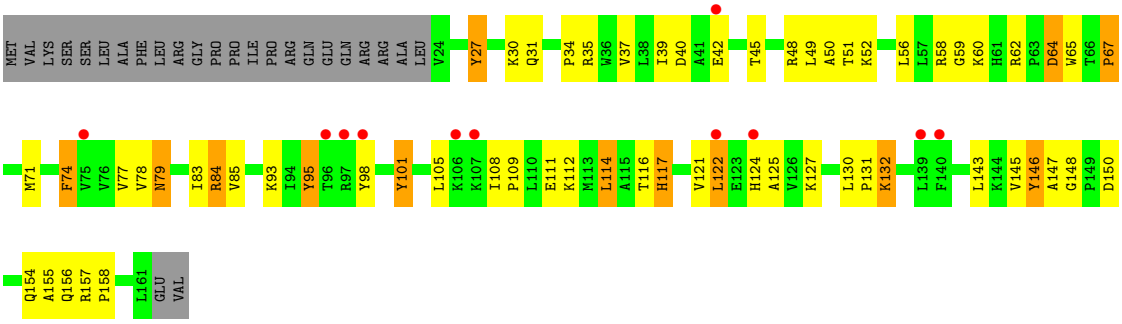
• Molecule 9: 50S ribosomal protein L9

Chain G:



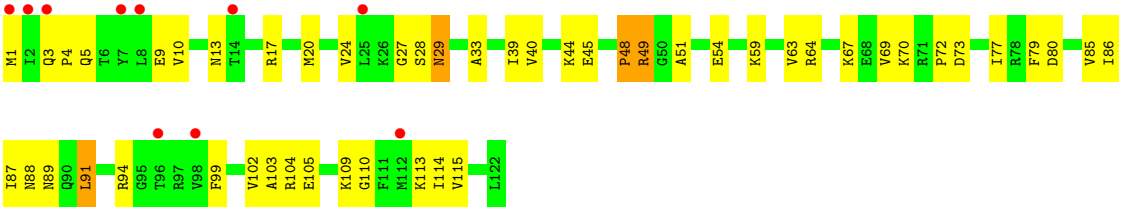
• Molecule 10: 50S ribosomal protein L13

Chain H:



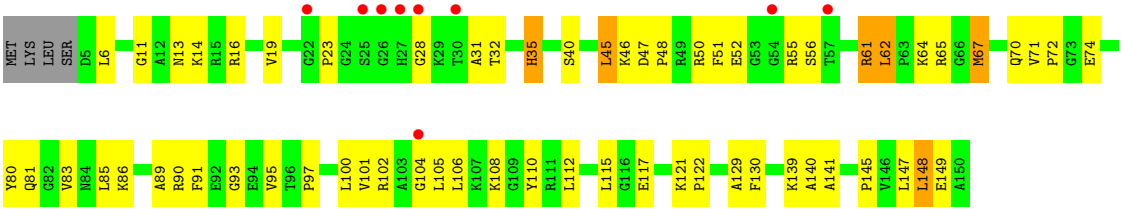
• Molecule 11: 50S ribosomal protein L14

Chain I:



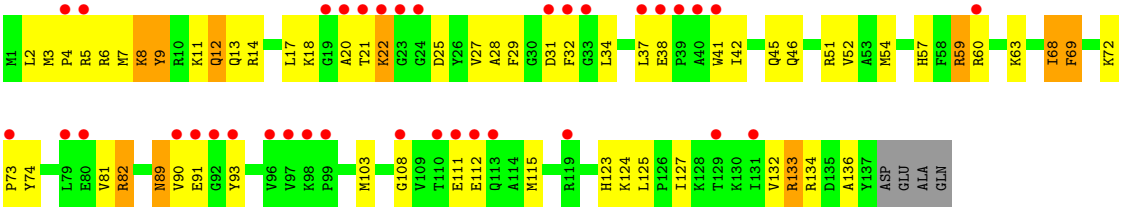
• Molecule 12: 50S ribosomal protein L15

Chain J:



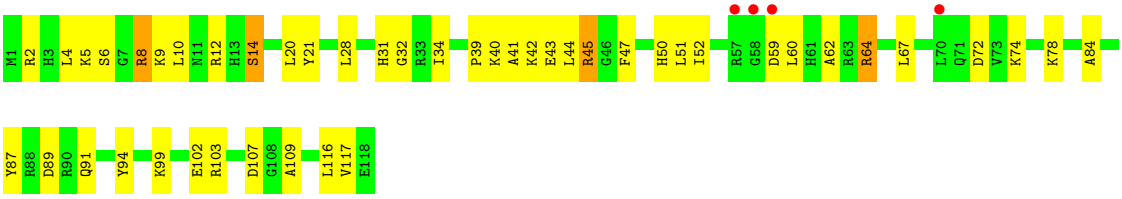
• Molecule 13: 50S ribosomal protein L16

Chain K:



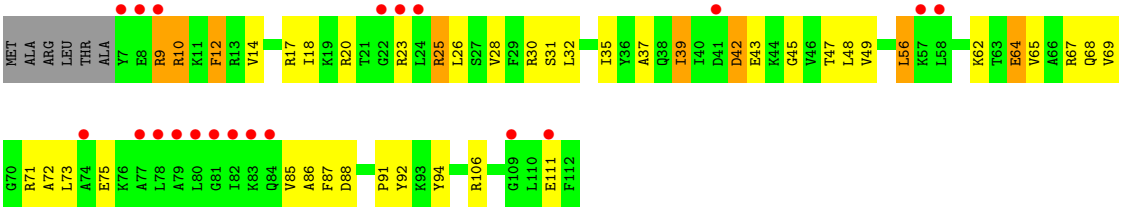
• Molecule 14: 50S ribosomal protein L17

Chain L:



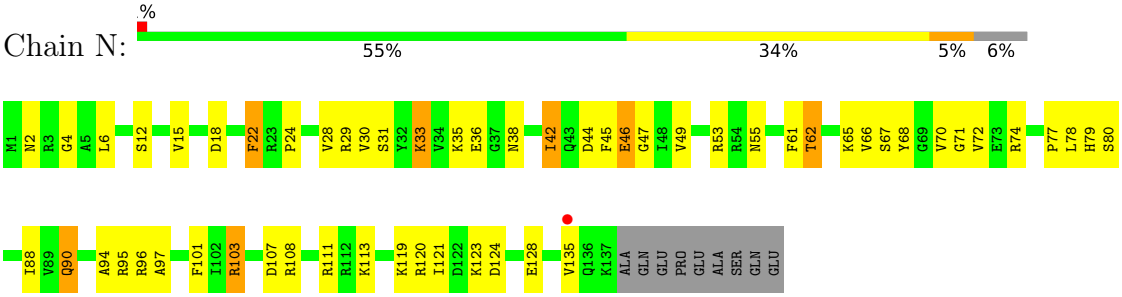
• Molecule 15: 50S ribosomal protein L18

Chain M:



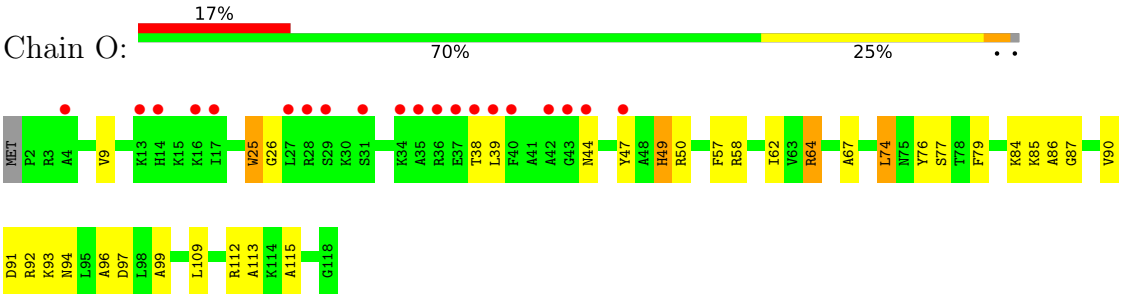
• Molecule 16: 50S ribosomal protein L19

Chain N:



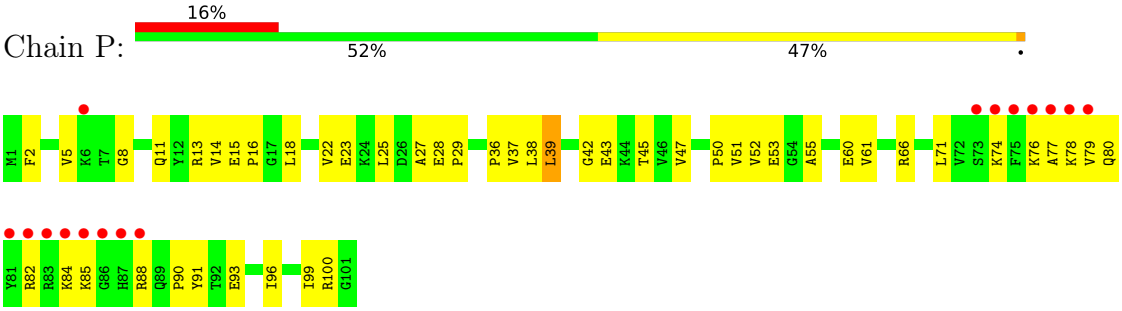
• Molecule 17: 50S ribosomal protein L20

Chain O:



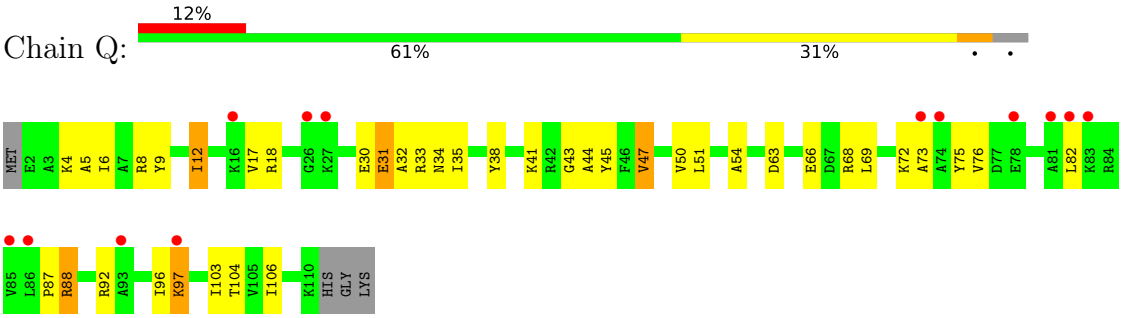
• Molecule 18: 50S ribosomal protein L21

Chain P:



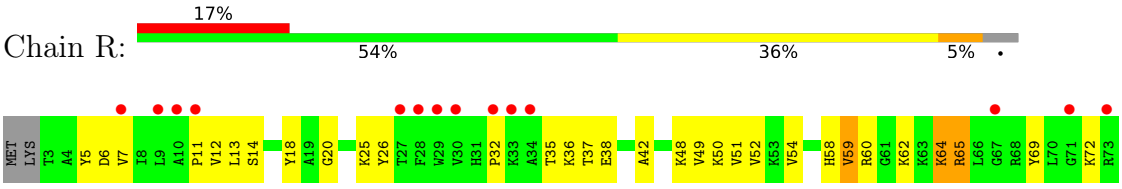
• Molecule 19: 50S ribosomal protein L22

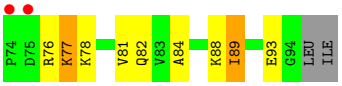
Chain Q:



• Molecule 20: 50S ribosomal protein L23

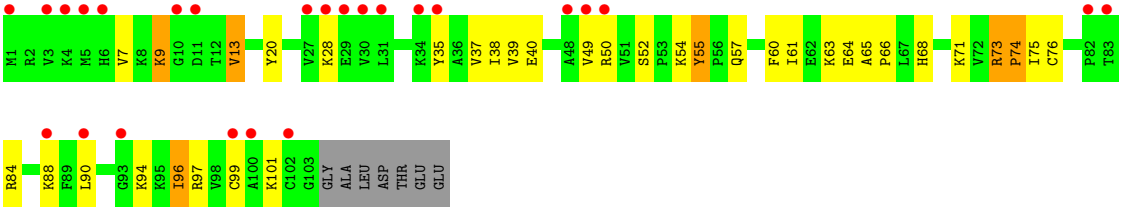
Chain R:





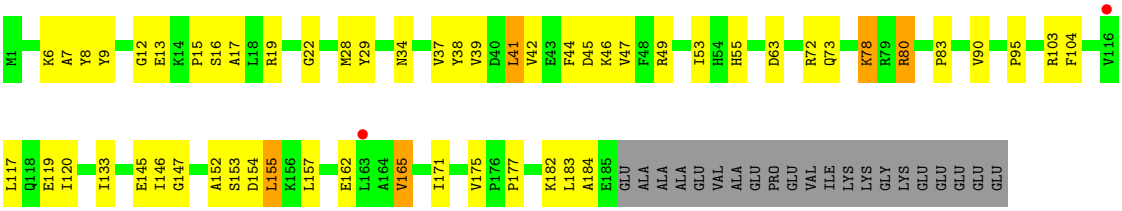
• Molecule 21: 50S ribosomal protein L24

Chain S:



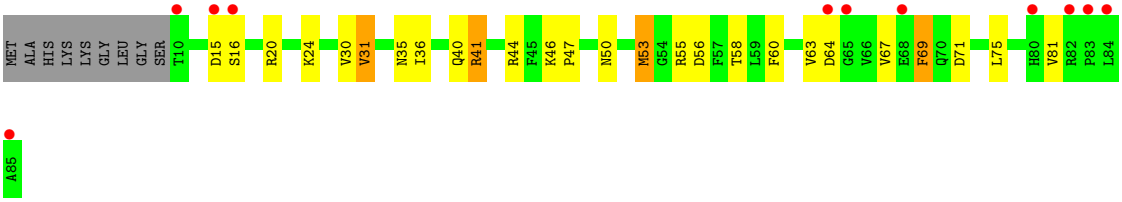
• Molecule 22: 50S ribosomal protein L25

Chain T:



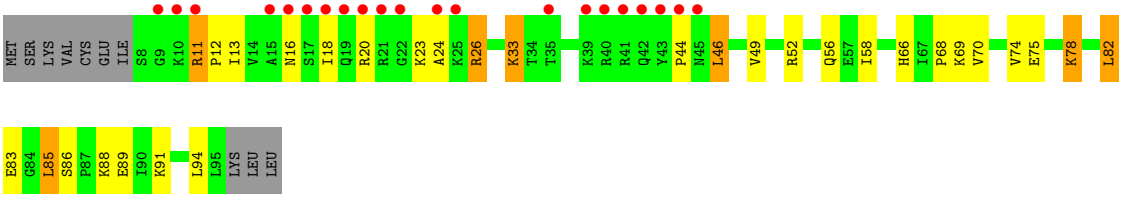
• Molecule 23: 50S ribosomal protein L27

Chain U:



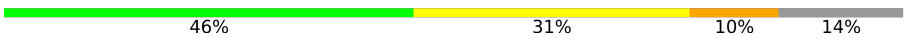
• Molecule 24: 50S ribosomal protein L28

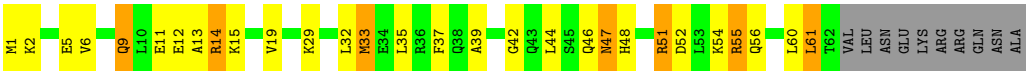
Chain V:



• Molecule 25: 50S ribosomal protein L29

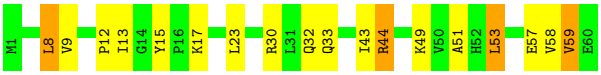
Chain W:





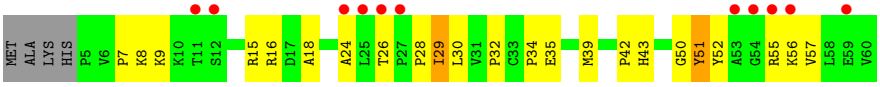
- Molecule 26: 50S ribosomal protein L30

Chain X:



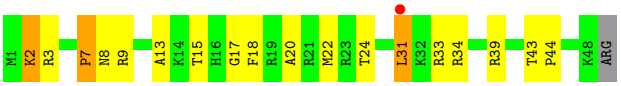
- Molecule 27: 50S ribosomal protein L32

Chain Y:



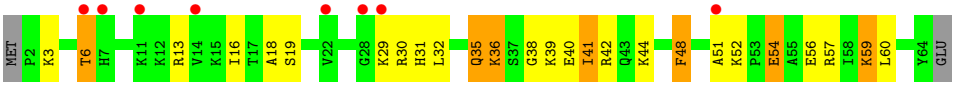
- Molecule 28: 50S ribosomal protein L34

Chain Z:



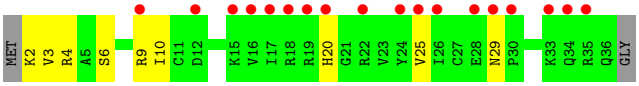
- Molecule 29: 50S ribosomal protein L35

Chain a:



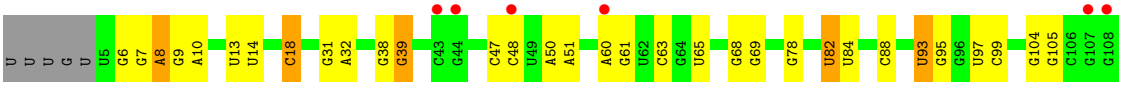
- Molecule 30: 50S ribosomal protein L36

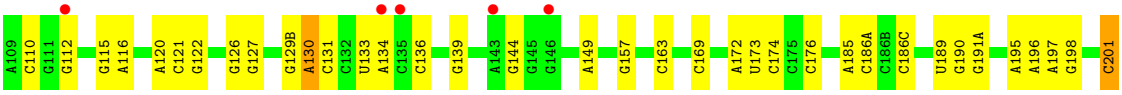
Chain b:

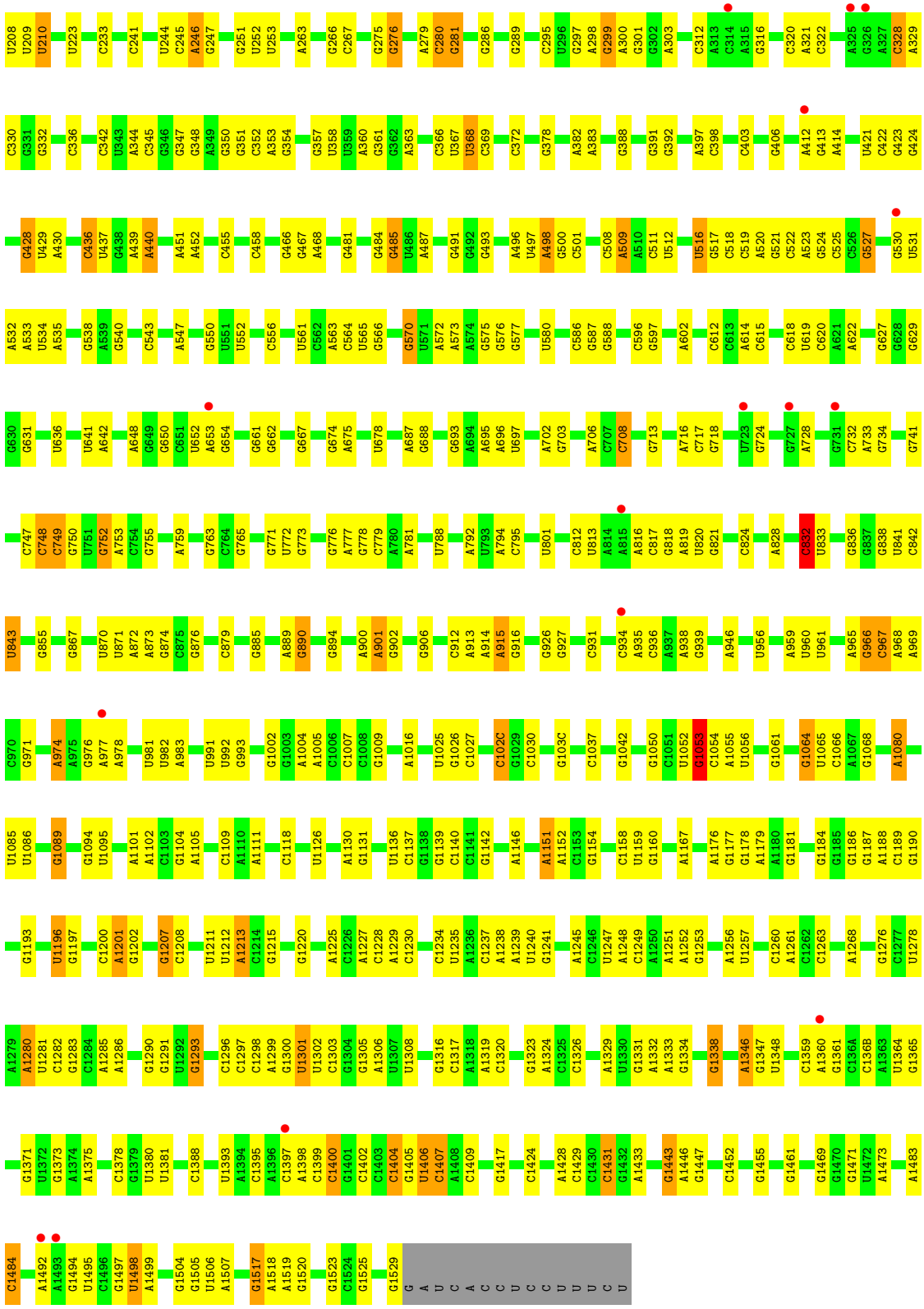


- Molecule 31: 16S SMALL SUBUNIT RIBOSOMAL RNA

Chain y:

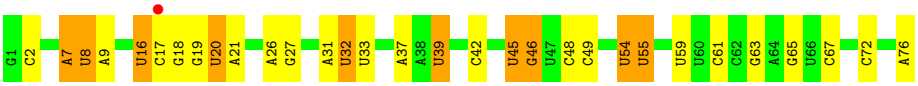






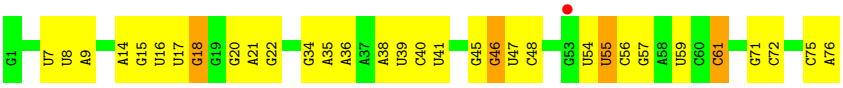
• Molecule 32: P-site PHE-tRNA

Chain z: % 59% 28% 13%



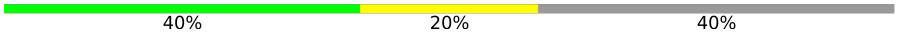
- Molecule 33: E-TRNA

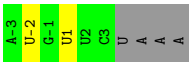
Chain 0:



- Molecule 34: MRNA

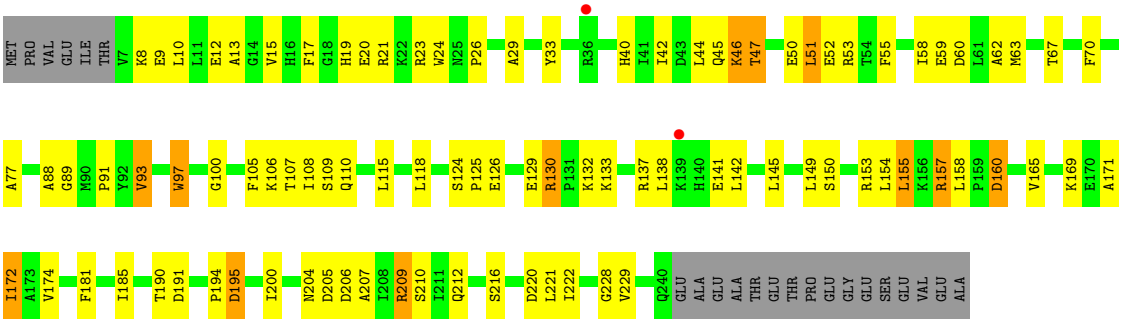
Chain 1:





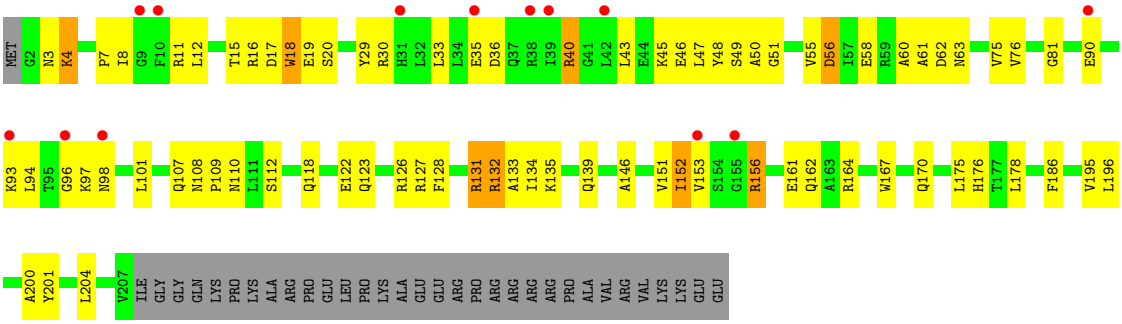
- Molecule 35: 30S ribosomal protein S2

Chain c:



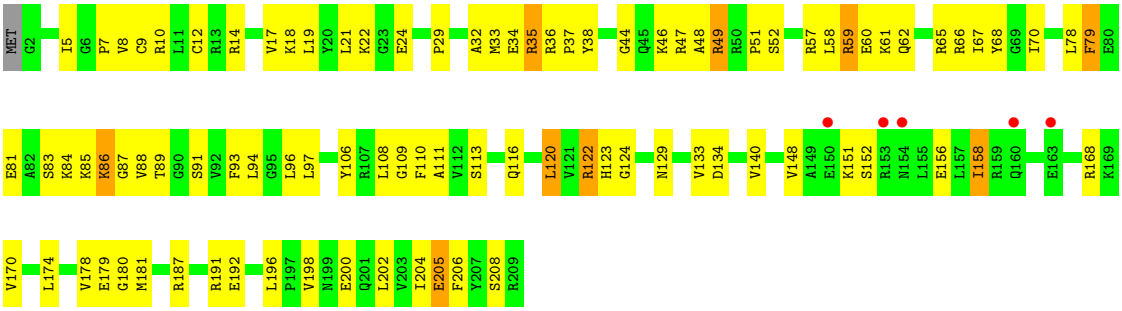
- Molecule 36: 30S ribosomal protein S3

Chain d:



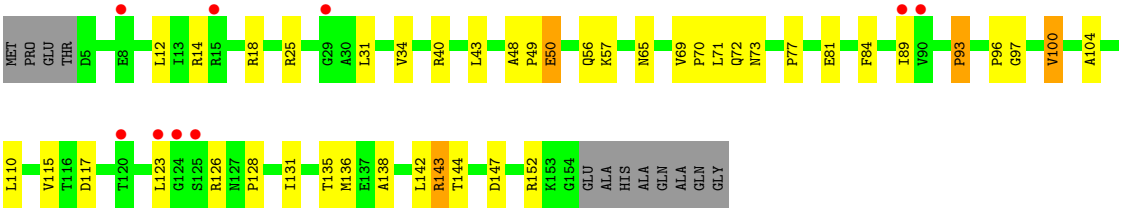
- Molecule 37: 30S ribosomal protein S4

Chain e:



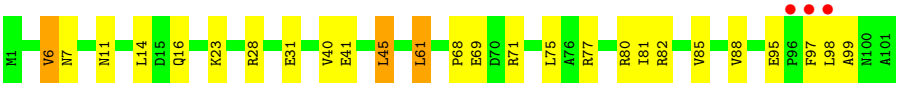
- Molecule 38: 30S ribosomal protein S5

Chain f:



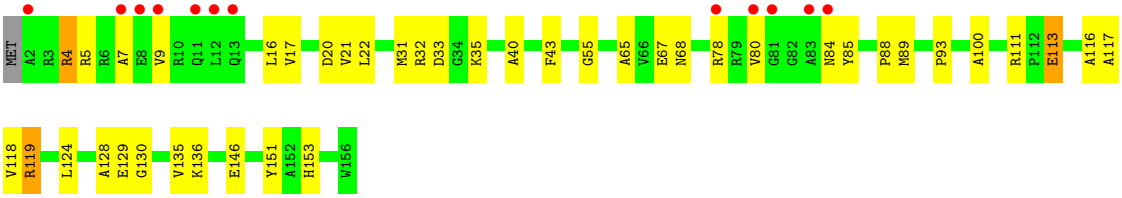
- Molecule 39: 30S ribosomal protein S6

Chain g:



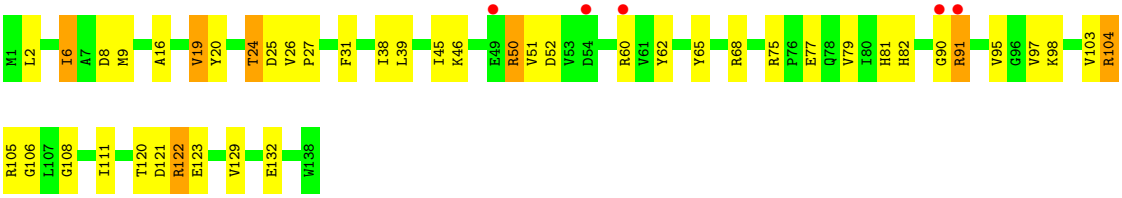
- Molecule 40: 30S ribosomal protein S7

Chain h:



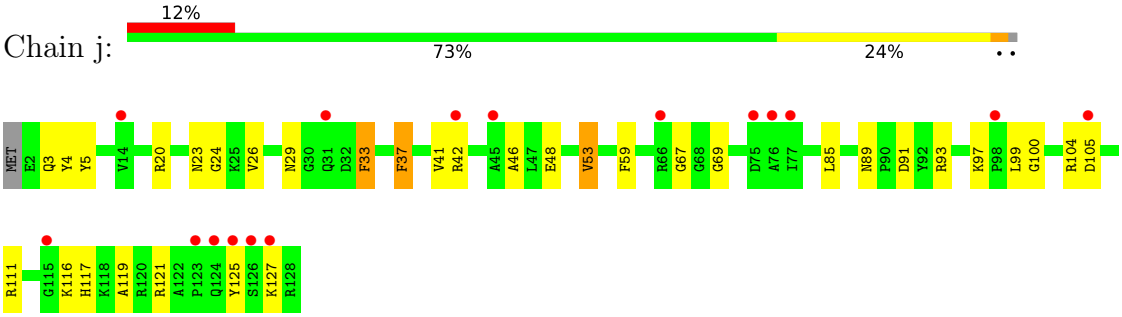
- Molecule 41: 30S ribosomal protein S8

Chain i:



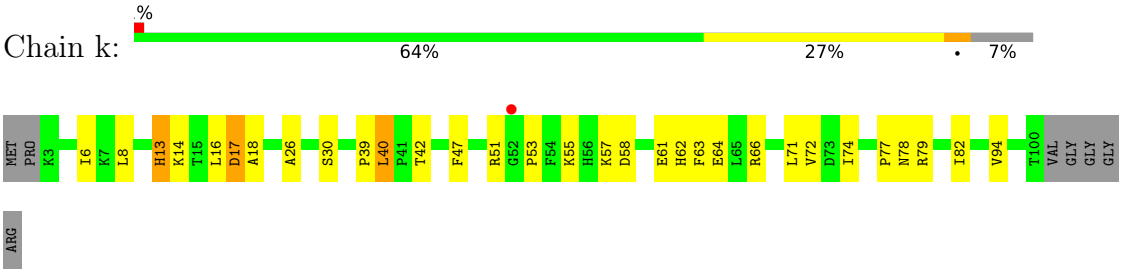
- Molecule 42: 30S ribosomal protein S9

Chain j:



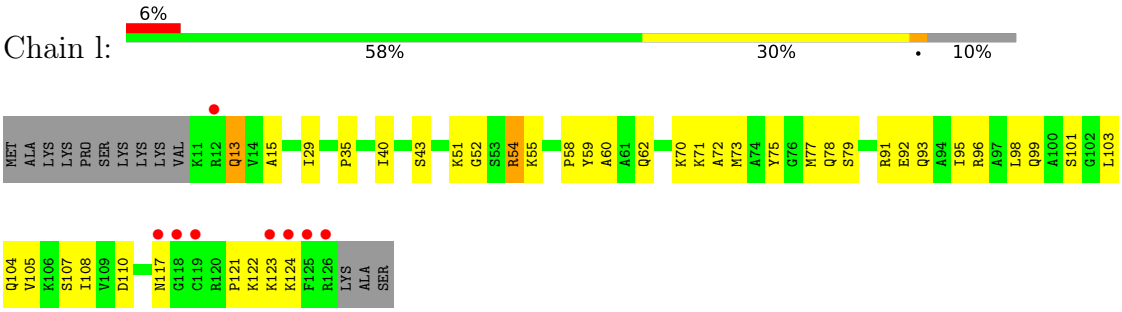
• Molecule 43: 30S ribosomal protein S10

Chain k:



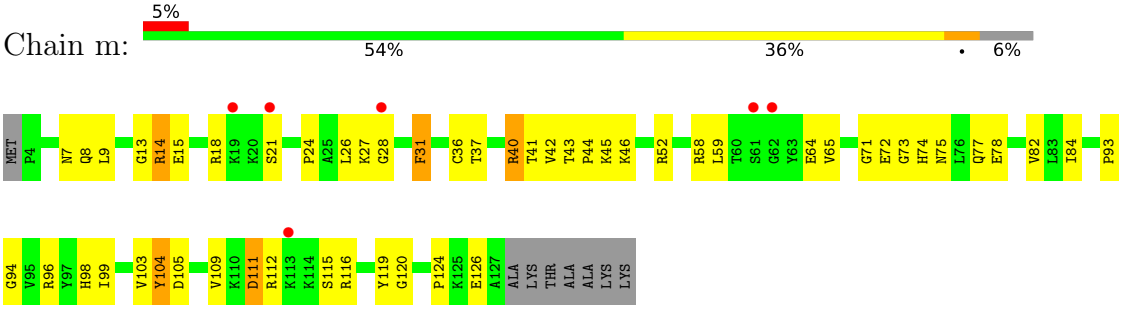
• Molecule 44: 30S ribosomal protein S11

Chain l:



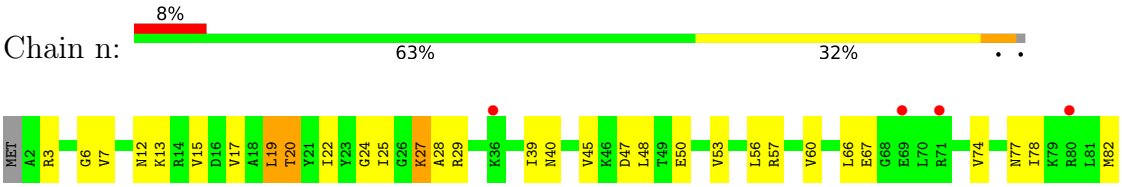
• Molecule 45: 30S ribosomal protein S12

Chain m:



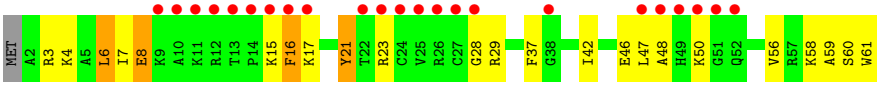
• Molecule 46: 30S ribosomal protein S13

Chain n:



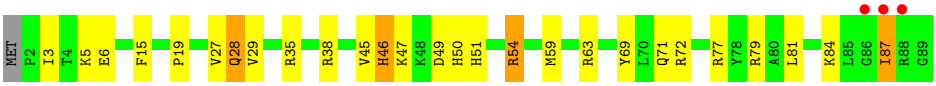
• Molecule 47: 30S ribosomal protein S14

Chain o:



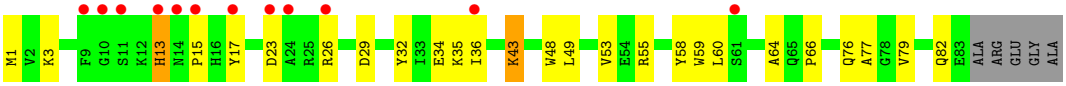
• Molecule 48: 30S ribosomal protein S15

Chain p:



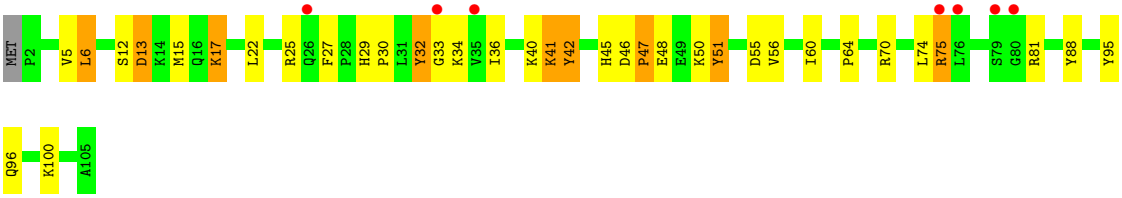
• Molecule 49: 30S ribosomal protein S16

Chain q:



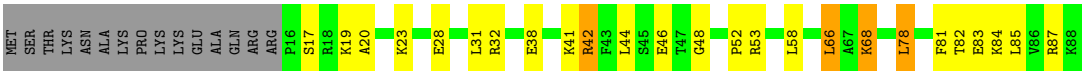
• Molecule 50: 30S ribosomal protein S17

Chain r:



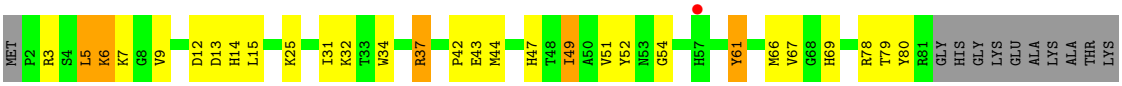
• Molecule 51: 30S ribosomal protein S18

Chain s:



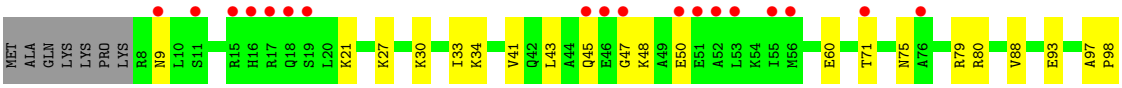
• Molecule 52: 30S ribosomal protein S19

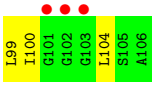
Chain t:



• Molecule 53: 30S ribosomal protein S20

Chain u:





• Molecule 54: 30S ribosomal protein Thx

Chain v:

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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]	$< \|L\| > = 0.26$, $< L^2 > = 0.11$	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.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 4OC, PSU, 7MG, 5MC, M2G, 4SU, H2U, MA6, 5MU, 2MG, UR3

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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

Sometimes 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 (i)

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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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

Continued on next page...

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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 (i)

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	5MC	y	1407	31	18,22,23	0.92	1 (5%)	26,32,35	1.47	5 (19%)
32	MIA	z	37	32	24,31,32	2.36	6 (25%)	26,44,47	2.58	6 (23%)
31	MA6	y	1519	31	19,26,27	2.16	2 (10%)	18,38,41	1.90	4 (22%)
32	PSU	z	39	32	18,21,22	2.29	4 (22%)	22,30,33	1.83	7 (31%)
31	5MC	y	1404	31	18,22,23	1.04	1 (5%)	26,32,35	1.52	5 (19%)
31	5MC	y	1400	31	18,22,23	1.07	2 (11%)	26,32,35	1.46	2 (7%)
32	4SU	z	8	32	18,21,22	1.82	3 (16%)	26,30,33	2.31	9 (34%)
31	2MG	y	1207	31	18,26,27	1.73	3 (16%)	16,38,41	1.70	5 (31%)
32	PSU	z	32	32	18,21,22	2.03	4 (22%)	22,30,33	2.11	6 (27%)
31	MA6	y	1518	31	19,26,27	1.80	3 (15%)	18,38,41	2.29	6 (33%)
32	5MU	z	54	32	19,22,23	1.79	2 (10%)	28,32,35	1.52	7 (25%)
31	4OC	y	1402	31	20,23,24	1.39	3 (15%)	26,32,35	1.55	5 (19%)
31	5MC	y	967	31	18,22,23	0.77	1 (5%)	26,32,35	1.16	3 (11%)
32	PSU	z	55	32	18,21,22	1.96	4 (22%)	22,30,33	1.94	6 (27%)
31	PSU	y	516	31	18,21,22	1.89	4 (22%)	22,30,33	1.87	7 (31%)
31	7MG	y	527	31	22,26,27	3.72	3 (13%)	29,39,42	1.67	6 (20%)
31	UR3	y	1498	31	19,22,23	1.62	1 (5%)	26,32,35	1.52	6 (23%)
31	M2G	y	966	31	20,27,28	2.24	6 (30%)	22,40,43	1.56	4 (18%)
32	H2U	z	20	32	18,21,22	0.76	0	21,30,33	0.89	1 (4%)
32	H2U	z	16	32	18,21,22	0.97	1 (5%)	21,30,33	0.93	1 (4%)
32	7MG	z	46	32	22,26,27	3.56	4 (18%)	29,39,42	1.81	6 (20%)
33	PSU	0	55	33	18,21,22	3.41	5 (27%)	22,30,33	2.05	6 (27%)

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	5MC	y	1407	31	-	0/7/25/26	0/2/2/2
32	MIA	z	37	32	-	5/11/33/34	0/3/3/3
31	MA6	y	1519	31	-	1/7/29/30	0/3/3/3
32	PSU	z	39	32	-	4/7/25/26	0/2/2/2
31	5MC	y	1404	31	-	2/7/25/26	0/2/2/2
31	5MC	y	1400	31	-	0/7/25/26	0/2/2/2
32	4SU	z	8	32	-	2/7/25/26	0/2/2/2
31	2MG	y	1207	31	-	0/5/27/28	0/3/3/3
32	PSU	z	32	32	-	3/7/25/26	0/2/2/2
31	MA6	y	1518	31	-	2/7/29/30	0/3/3/3
32	5MU	z	54	32	-	0/7/25/26	0/2/2/2
31	4OC	y	1402	31	-	3/9/29/30	0/2/2/2
31	5MC	y	967	31	-	0/7/25/26	0/2/2/2
32	PSU	z	55	32	-	1/7/25/26	0/2/2/2
31	PSU	y	516	31	-	4/7/25/26	0/2/2/2
31	7MG	y	527	31	-	0/7/37/38	0/3/3/3
31	UR3	y	1498	31	-	6/7/25/26	0/2/2/2
31	M2G	y	966	31	-	0/7/29/30	0/3/3/3
32	H2U	z	20	32	-	2/7/38/39	0/2/2/2
32	H2U	z	16	32	-	2/7/38/39	0/2/2/2
32	7MG	z	46	32	-	0/7/37/38	0/3/3/3
33	PSU	0	55	33	-	2/7/25/26	0/2/2/2

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	527	7MG	C8-N9	-16.62	1.36	1.46
32	z	46	7MG	C8-N9	-15.58	1.37	1.46
33	0	55	PSU	O2-C2	12.05	1.48	1.23
32	z	39	PSU	O2-C2	6.95	1.38	1.23
32	z	54	5MU	O4-C4	6.87	1.36	1.23
31	y	966	M2G	C6-N1	6.56	1.47	1.37
32	z	37	MIA	C13-C14	6.35	1.50	1.32
31	y	1518	MA6	C6-N1	6.32	1.42	1.33
32	z	32	PSU	O2-C2	6.13	1.36	1.23
31	y	1519	MA6	C6-N1	6.02	1.42	1.33
32	z	55	PSU	O2-C2	5.88	1.35	1.23
32	z	37	MIA	C16-C14	5.78	1.66	1.50
31	y	516	PSU	O2-C2	5.74	1.35	1.23
31	y	1519	MA6	O4'-C1'	5.69	1.49	1.41
31	y	1498	UR3	O4-C4	5.25	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	z	37	MIA	C6-N1	4.78	1.39	1.32
32	z	8	4SU	C6-C5	4.61	1.45	1.35
33	0	55	PSU	C2-N1	4.53	1.42	1.36
31	y	1207	2MG	C6-N1	4.33	1.44	1.37
32	z	39	PSU	C6-C5	3.85	1.39	1.35
33	0	55	PSU	O4'-C1'	3.85	1.49	1.43
32	z	8	4SU	C4-N3	3.82	1.41	1.37
31	y	1207	2MG	C2-N1	3.78	1.42	1.36
32	z	39	PSU	C2-N1	3.76	1.41	1.36
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	32	PSU	C6-C5	3.69	1.39	1.35
31	y	966	M2G	C2-N1	3.49	1.45	1.36
32	z	37	MIA	C2-S10	-3.47	1.72	1.75
32	z	46	7MG	C6-N1	3.47	1.45	1.38
32	z	32	PSU	C2-N1	3.36	1.41	1.36
31	y	1400	5MC	C4-N4	3.31	1.42	1.34
31	y	516	PSU	C6-C5	3.20	1.39	1.35
32	z	55	PSU	C2-N1	3.13	1.41	1.36
32	z	55	PSU	C6-C5	2.84	1.38	1.35
31	y	967	5MC	C4-N4	2.78	1.41	1.34
31	y	1402	4OC	C4-N4	2.71	1.41	1.35
31	y	1404	5MC	C4-N4	2.70	1.41	1.34
31	y	527	7MG	C6-N1	2.68	1.43	1.38
31	y	966	M2G	C2-N2	2.64	1.40	1.35
31	y	966	M2G	C2-N3	2.63	1.33	1.30
31	y	516	PSU	C2-N1	2.62	1.40	1.36
32	z	37	MIA	C2-N1	2.57	1.37	1.34
33	0	55	PSU	C4-N3	-2.54	1.34	1.38
32	z	8	4SU	O2-C2	2.54	1.27	1.23
31	y	1407	5MC	C4-N4	2.54	1.40	1.34
31	y	966	M2G	O5'-C5'	-2.49	1.38	1.44
32	z	37	MIA	O4'-C1'	2.43	1.44	1.41
32	z	46	7MG	C5-N7	2.38	1.38	1.35
31	y	1207	2MG	C8-N7	-2.35	1.31	1.35
32	z	54	5MU	O5'-C5'	-2.31	1.39	1.44
31	y	516	PSU	C2'-C1'	2.30	1.56	1.53
31	y	1402	4OC	O3'-C3'	2.26	1.48	1.43
32	z	39	PSU	O4'-C4'	-2.25	1.40	1.45
33	0	55	PSU	C4-C5	-2.24	1.37	1.44
31	y	1400	5MC	C6-C5	2.21	1.38	1.34
32	z	16	H2U	C1'-N1	2.19	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	527	7MG	C2-N1	2.10	1.42	1.37
32	z	55	PSU	C4-C5	-2.06	1.38	1.44
32	z	46	7MG	C5-C6	2.05	1.48	1.43
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 (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	z	37	MIA	C12-C13-C14	-8.50	110.60	127.14
31	y	1518	MA6	N1-C6-N6	6.39	123.78	117.06
31	y	527	7MG	N9-C8-N7	5.61	111.41	103.38
32	z	37	MIA	C12-N6-C6	-5.50	114.41	122.55
32	z	46	7MG	N9-C8-N7	5.45	111.17	103.38
32	z	8	4SU	C5-C4-S4	-5.08	117.92	124.47
32	z	8	4SU	C4-N3-C2	-5.07	122.42	127.34
32	z	32	PSU	C3'-C2'-C1'	4.65	107.05	101.64
32	z	37	MIA	C11-S10-C2	4.50	105.63	102.27
32	z	46	7MG	O4'-C1'-N9	-4.42	103.27	109.30
32	z	37	MIA	C5-C6-N1	-4.36	117.19	120.81
32	z	55	PSU	C4-N3-C2	-4.27	120.19	126.34
32	z	55	PSU	N1-C2-N3	4.24	119.93	115.13
31	y	1519	MA6	N1-C6-N6	4.18	121.46	117.06
33	0	55	PSU	C3'-C2'-C1'	4.11	106.42	101.64
31	y	1519	MA6	C3'-C2'-C1'	4.06	107.09	100.98
31	y	516	PSU	C4-N3-C2	-4.05	120.50	126.34
31	y	1518	MA6	C3'-C2'-C1'	3.99	106.98	100.98
32	z	8	4SU	S4-C4-N3	3.97	124.12	120.21
31	y	516	PSU	N1-C2-N3	3.95	119.61	115.13
33	0	55	PSU	C4-N3-C2	-3.88	120.75	126.34
32	z	32	PSU	C4-N3-C2	-3.82	120.83	126.34
32	z	39	PSU	C4-N3-C2	-3.79	120.88	126.34
32	z	39	PSU	N1-C2-N3	3.75	119.38	115.13
33	0	55	PSU	C6-N1-C2	-3.72	118.88	122.68
32	z	32	PSU	N1-C2-N3	3.62	119.23	115.13
31	y	1400	5MC	C5-C6-N1	-3.62	119.62	123.34
31	y	1207	2MG	CM2-N2-C2	-3.59	115.92	123.86
31	y	1407	5MC	CM5-C5-C6	-3.59	118.06	122.85
33	0	55	PSU	N1-C2-N3	3.58	119.19	115.13
31	y	966	M2G	C3'-C2'-C1'	3.58	106.36	100.98
32	z	8	4SU	C5-C4-N3	3.51	117.94	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	z	37	MIA	C16-C14-C13	-3.49	112.56	122.65
31	y	1498	UR3	C1'-N1-C2	3.47	122.84	116.99
32	z	8	4SU	N3-C2-N1	3.45	119.47	114.89
32	z	8	4SU	O2-C2-N1	-3.44	118.22	122.79
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
32	z	55	PSU	C3'-C2'-C1'	3.24	105.41	101.64
31	y	1407	5MC	C2'-C1'-N1	-3.22	104.10	113.22
31	y	1518	MA6	N3-C2-N1	-3.20	123.67	128.68
31	y	1404	5MC	C4'-O4'-C1'	-3.18	102.47	109.47
32	z	32	PSU	C5'-C4'-C3'	-3.17	103.31	115.18
31	y	1519	MA6	C2'-C3'-C4'	3.09	108.65	102.64
31	y	1402	4OC	C1'-N1-C2	3.02	125.16	118.42
32	z	46	7MG	C2-N3-C4	3.01	117.66	112.30
32	z	55	PSU	C6-C5-C4	2.95	120.26	118.20
31	y	1404	5MC	CM5-C5-C6	-2.91	118.97	122.85
32	z	54	5MU	N3-C2-N1	2.90	118.74	114.89
32	z	32	PSU	O4'-C4'-C3'	2.89	110.83	105.11
31	y	1404	5MC	C1'-N1-C6	-2.88	116.33	121.12
31	y	1404	5MC	C1'-N1-C2	2.85	124.78	118.42
31	y	527	7MG	N9-C4-N3	2.84	129.71	125.47
31	y	527	7MG	C2-N3-C4	2.83	117.34	112.30
31	y	1498	UR3	C6-N1-C2	-2.80	119.28	121.79
31	y	1207	2MG	O4'-C1'-C2'	-2.79	102.85	106.93
32	z	55	PSU	C6-N1-C2	-2.78	119.84	122.68
31	y	1400	5MC	C1'-N1-C6	2.76	125.72	121.12
31	y	1404	5MC	O4'-C4'-C5'	2.76	118.44	109.37
31	y	966	M2G	N1-C2-N2	2.75	120.38	118.04
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	39	PSU	C6-N1-C2	-2.72	119.91	122.68
32	z	54	5MU	C4-N3-C2	-2.71	123.85	127.35
31	y	516	PSU	C4'-O4'-C1'	-2.70	101.76	108.55
31	y	1402	4OC	O4'-C4'-C5'	2.68	118.20	109.37
32	z	32	PSU	C6-N1-C2	-2.66	119.96	122.68
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
31	y	1407	5MC	C3'-C2'-C1'	2.59	106.35	101.43
31	y	516	PSU	C6-N1-C2	-2.57	120.05	122.68
31	y	967	5MC	C5-C6-N1	-2.57	120.70	123.34
31	y	967	5MC	CM5-C5-C6	-2.55	119.44	122.85
31	y	1402	4OC	C1'-N1-C6	-2.53	115.33	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	516	PSU	C3'-C2'-C1'	2.52	104.58	101.64
32	z	39	PSU	O2-C2-N1	-2.51	120.03	122.79
31	y	967	5MC	C3'-C2'-C1'	2.48	106.14	101.43
31	y	1407	5MC	C5-C6-N1	-2.46	120.81	123.34
31	y	516	PSU	O2-C2-N1	-2.43	120.11	122.79
32	z	46	7MG	C4-C5-N7	2.42	108.89	105.53
31	y	1498	UR3	O4'-C1'-N1	-2.42	102.83	108.36
32	z	54	5MU	C5M-C5-C6	-2.41	119.62	122.85
32	z	55	PSU	O2-C2-N1	-2.41	120.14	122.79
32	z	16	H2U	C3'-C2'-C1'	2.37	105.93	101.43
31	y	527	7MG	C4-C5-N7	2.37	108.81	105.53
33	0	55	PSU	C5-C4-N3	2.34	121.88	116.58
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
32	z	8	4SU	C3'-C2'-C1'	2.28	105.77	101.43
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	39	PSU	C6-C5-C4	2.24	119.76	118.20
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	C4'-O4'-C1'	-2.16	104.72	109.47
32	z	46	7MG	C5'-C4'-C3'	-2.16	107.10	115.18
32	z	39	PSU	O3'-C3'-C2'	2.12	118.67	111.82
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
32	z	54	5MU	C5-C6-N1	-2.07	121.21	123.34
31	y	1207	2MG	C2'-C3'-C4'	-2.05	98.66	102.64
31	y	1498	UR3	C3'-C2'-C1'	2.04	105.30	101.43
31	y	527	7MG	C5-C4-N3	-2.03	124.26	128.13
33	0	55	PSU	C4'-O4'-C1'	-2.03	103.46	108.55
32	z	39	PSU	C4'-O4'-C1'	-2.02	103.48	108.55
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
32	z	54	5MU	C3'-C2'-C1'	2.00	105.23	101.43

There are no chirality outliers.

All (39) 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
31	y	1402	4OC	C1'-C2'-O2'-CM2
31	y	1518	MA6	O4'-C4'-C5'-O5'
31	y	1518	MA6	C3'-C4'-C5'-O5'
32	z	16	H2U	O4'-C4'-C5'-O5'
32	z	16	H2U	C3'-C4'-C5'-O5'
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
32	z	39	PSU	C2'-C1'-C5-C4
32	z	39	PSU	C2'-C1'-C5-C6
33	0	55	PSU	C2'-C1'-C5-C4
31	y	1402	4OC	O4'-C4'-C5'-O5'
32	z	39	PSU	O4'-C4'-C5'-O5'
31	y	1498	UR3	O4'-C4'-C5'-O5'
32	z	20	H2U	O4'-C4'-C5'-O5'
32	z	20	H2U	C3'-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	8	4SU	C3'-C4'-C5'-O5'
32	z	39	PSU	C3'-C4'-C5'-O5'
31	y	1402	4OC	C3'-C4'-C5'-O5'
32	z	8	4SU	O4'-C4'-C5'-O5'
31	y	1404	5MC	O4'-C4'-C5'-O5'
31	y	516	PSU	O4'-C1'-C5-C4
32	z	32	PSU	O4'-C1'-C5-C4
33	0	55	PSU	O4'-C1'-C5-C4
31	y	1498	UR3	O4'-C1'-N1-C6
31	y	1498	UR3	C2'-C1'-N1-C6
31	y	1404	5MC	C3'-C4'-C5'-O5'
31	y	1519	MA6	C3'-C4'-C5'-O5'
31	y	516	PSU	O4'-C1'-C5-C6
32	z	55	PSU	O4'-C1'-C5-C6
31	y	1498	UR3	O4'-C1'-N1-C2
31	y	1498	UR3	C2'-C1'-N1-C2

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
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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 128, 148	0
34	1	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, 164	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å^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
31	5MC	y	967	21/22	0.81	0.39	124,124,133,133	0
32	H2U	z	20	20/21	0.81	0.38	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	MA6	y	1518	24/25	0.85	0.20	31,39,52,53	0
31	M2G	y	966	25/26	0.85	0.28	15,16,20,31	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	5MU	z	54	21/22	0.90	0.23	5,5,5,5	0
31	7MG	y	527	24/25	0.90	0.23	7,10,24,26	0
32	PSU	z	39	20/21	0.90	0.22	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.