Full wwPDB EM Validation Report (i)

Dec 10, 2022 – 09:35 am GMT

PDB ID	:	5AA0
EMDB ID	:	EMD-6397
Title	:	Complex of Thermous thermophilus ribosome (A-and P-site tRNA) bound to BipA-GDPCP
Authors	:	Kumar, V.; Chen, Y.; Ahmed, T.; Tan, J.; Ero, R.; Bhushan, S.; Gao, Y.-G.
Deposited on	:	2015-07-23
Resolution	:	5.00 Å(reported)
Based on initial model	:	4V4Y

This is a Full wwPDB EM 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/EMValidationReportHelp
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 (1)) were used in the production of this report:

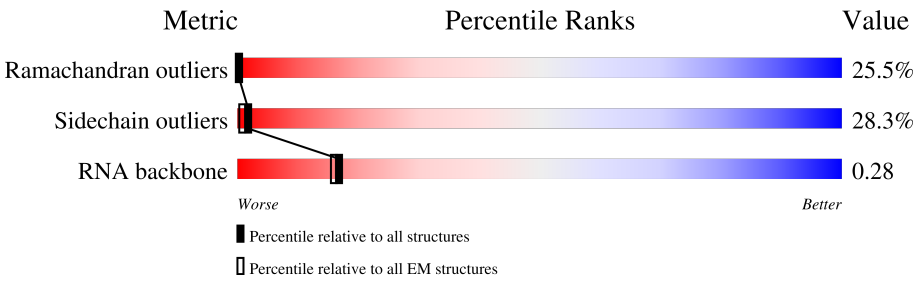
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	2889	44% 44% 9% •
2	AB	123	50% 41% 7% •
3	AC	228	33% 76% 22% •
4	AD	272	53% 36% 11% •
5	AE	206	48% 39% 13%
6	AF	208	6% 54% 37% 9%
7	AG	182	9% 53% 38% 8% •
8	AH	174	7% 59% 34% 6% •

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Mol	Chain	Length	Quality of chain
9	AK	139	41% 50% 9%
10	AL	122	6% 45% 44% 11%
11	AM	145	9% 44% 47% 8%
12	AN	136	38% 50% 11%
13	AO	117	66% 26% 9%
14	AP	110	53% 41% 5%
15	AQ	117	5% 42% 44% 14%
16	AR	117	57% 35% 8%
17	AS	101	50% 39% 11%
18	AT	110	60% 36%
19	AU	94	63% 34%
20	AV	110	15% 53% 45%
21	AW	180	45% 59% 34% 7%
22	AX	85	15% 71% 27%
23	AY	67	64% 31%
24	AZ	59	5% 51% 44% 5%
25	Aa	71	37% 46% 15%
26	Ab	57	5% 37% 49% 12%
27	Ac	49	24% 53% 22%
28	Ad	49	53% 37% 10%
29	Ae	64	50% 42% 8%
30	Af	37	62% 32% 5%
31	AI	153	45% 80% 20%
32	AJ	134	16% 59% 30% 11%
33	Ag	128	96% 100%

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Mol	Chain	Length	Quality of chain
34	BA	1515	56% 37% 6%
35	BF	234	9% 51% 37% 12%
36	BG	206	60% 35%
37	BH	208	10% 56% 38% 6%
38	BI	150	65% 33%
39	BJ	101	13% 55% 38% 7%
40	BK	155	63% 29% 8%
41	BL	138	58% 34% 8%
42	BM	127	62% 32% 6%
43	BN	98	7% 57% 39%
44	BO	119	8% 71% 24% 5%
45	BP	124	17% 52% 40% 7%
46	BQ	114	5% 66% 27% 7%
47	BR	60	58% 30% 10%
48	BS	88	5% 68% 30%
49	BT	83	59% 35% 6%
50	BU	104	8% 59% 36% 6%
51	BV	73	14% 62% 27% 11%
52	BW	80	11% 51% 42% 6%
53	BX	99	12% 58% 38%
54	BY	24	71% 21% 8%
55	BC	76	66% 34%
56	BD	75	16% 57% 43%
56	BE	75	11% 68% 32%
57	BZ	605	8% 59% 34% 6%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 155482 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	AA	2889	62218	27691	11629	20009	2889	0	0

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	A	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	G	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	?	-	C	deletion	GB 37223181
AA	1134	G	UNK	conflict	GB 37223181

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	AB	123	2641	1175	488	855	123	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	AC	228	1742	1102	318	319	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	AD	272	2124	1339	424	358	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	206	1578	997	302	273	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	AF	208	1625	1034	303	286	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AG	182	1482	947	269	261	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	AH	174	1328	844	248	235	1	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	AK	139	1113	717	207	186	3	0	0

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AL	122	932	587	171	170	4	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	AM	145	1106	688	226	190	2	0	0

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AN	136	1080	688	204	183	5	0	0

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
13	AO	117	960	599	202	159	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
14	AP	110	877	553	175	149	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	AQ	117	976	614	197	164	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	AS	101	779	501	142	135	1	0	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	AT	110	876	552	171	151	2	0	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	AU	94	742	483	133	126	0	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AV	110	844	539	158	141	6	0	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	AW	180	1435	916	256	260	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	AX	85	670	415	141	112	2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	AY	67	567	350	116	99	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	AZ	59	469	298	90	81	0	0

- Molecule 25 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Aa	71	581	364	108	104	5	0	0

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	Ab	57	445	279	87	74	5	0	0

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Ac	49	426	265	87	70	4	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	Ad	49	430	263	108	57	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Ae	64	515	331	102	79	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Af	37	307	188	68	47	4	0	0

- Molecule 31 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
31	AI	153	752	446	153	153	0	0

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	AJ	134	993	632	175	181	5	0	0

- Molecule 33 is a protein called Unknown peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Ag	128	620	369	128	123	0	5

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
34	BA	1515	32554	14490	6022	10527	1515	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	BM	127	1010	639	197	174	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	BO	119	885	549	168	165	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	BQ	114	914	565	189	158	2	0	0

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	96	GLN	GLU	conflict	UNP Q5SHP7

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	BV	73	597	380	118	99	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	BX	99	763	470	162	129	2	0	0

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

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

- Molecule 55 is a RNA chain called tRNA chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	BC	76	1619	723	290	531	75	0	0

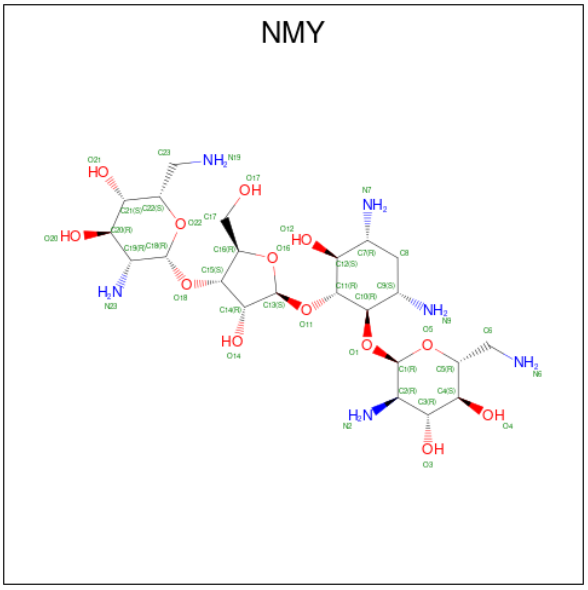
- Molecule 56 is a RNA chain called tRNA chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	BD	75	1597	713	285	525	74	0	0
56	BE	75	1597	713	285	525	74	0	0

- Molecule 57 is a protein called GTP-binding protein.

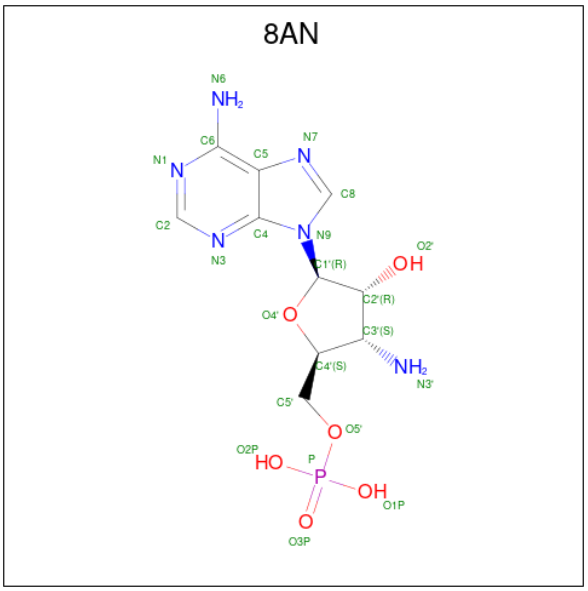
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	BZ	605	4610	2902	807	883	18	0	0

- Molecule 58 is NEOMYCIN (three-letter code: NMY) (formula: $C_{23}H_{46}N_6O_{13}$).



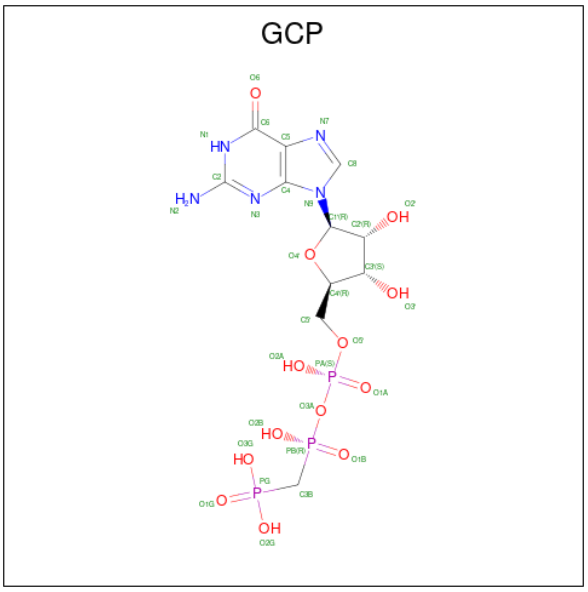
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
58	AA	1	42	23	6	13	0
			Total	C	N	O	
58	BA	1	42	23	6	13	0

- Molecule 59 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
59	AA	1	44	20	12	10	2	0
			Total	C	N	O	P	
59	AA	1	44	20	12	10	2	0

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



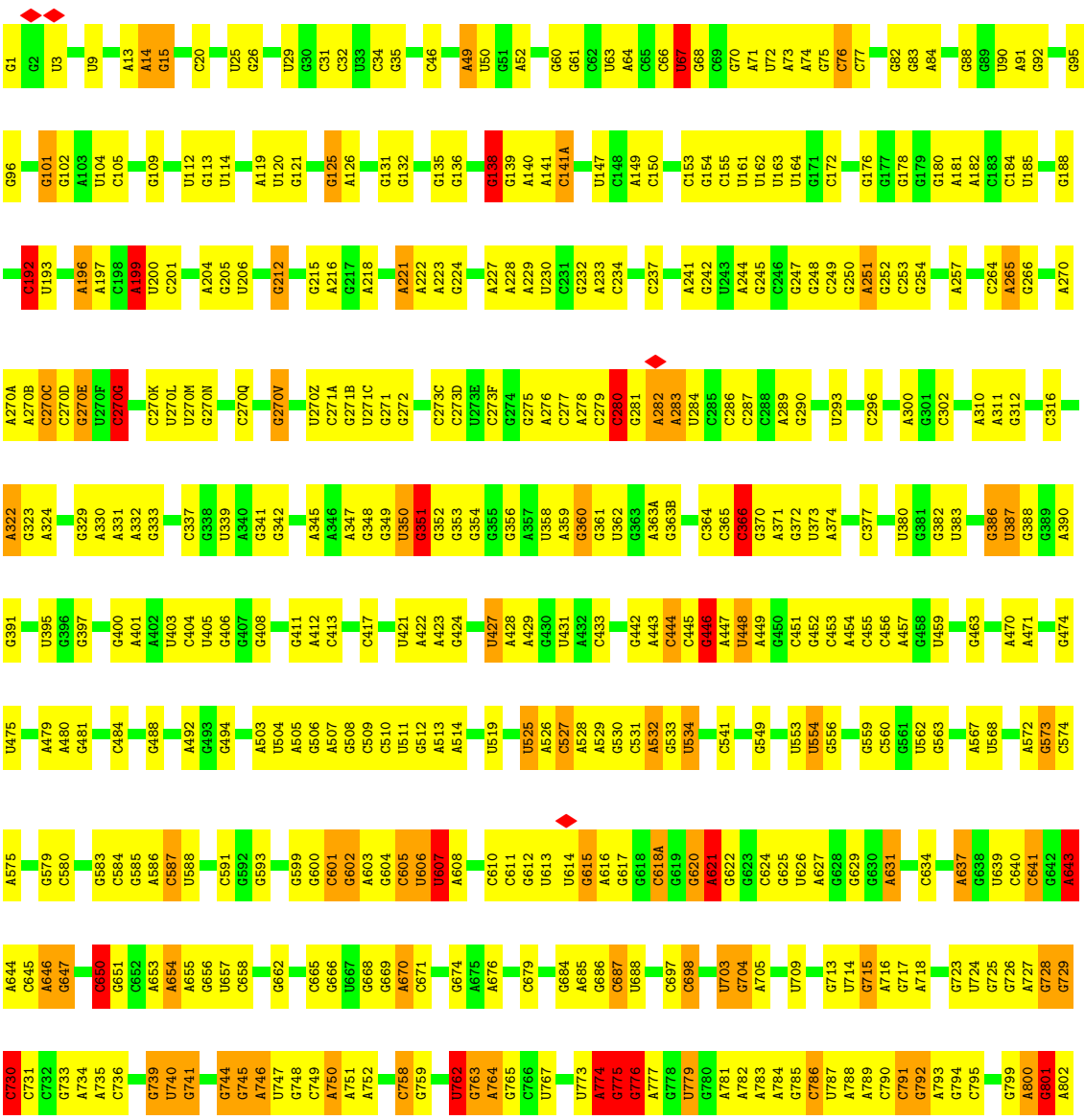
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	BZ	1	32	11	5	13	3	0

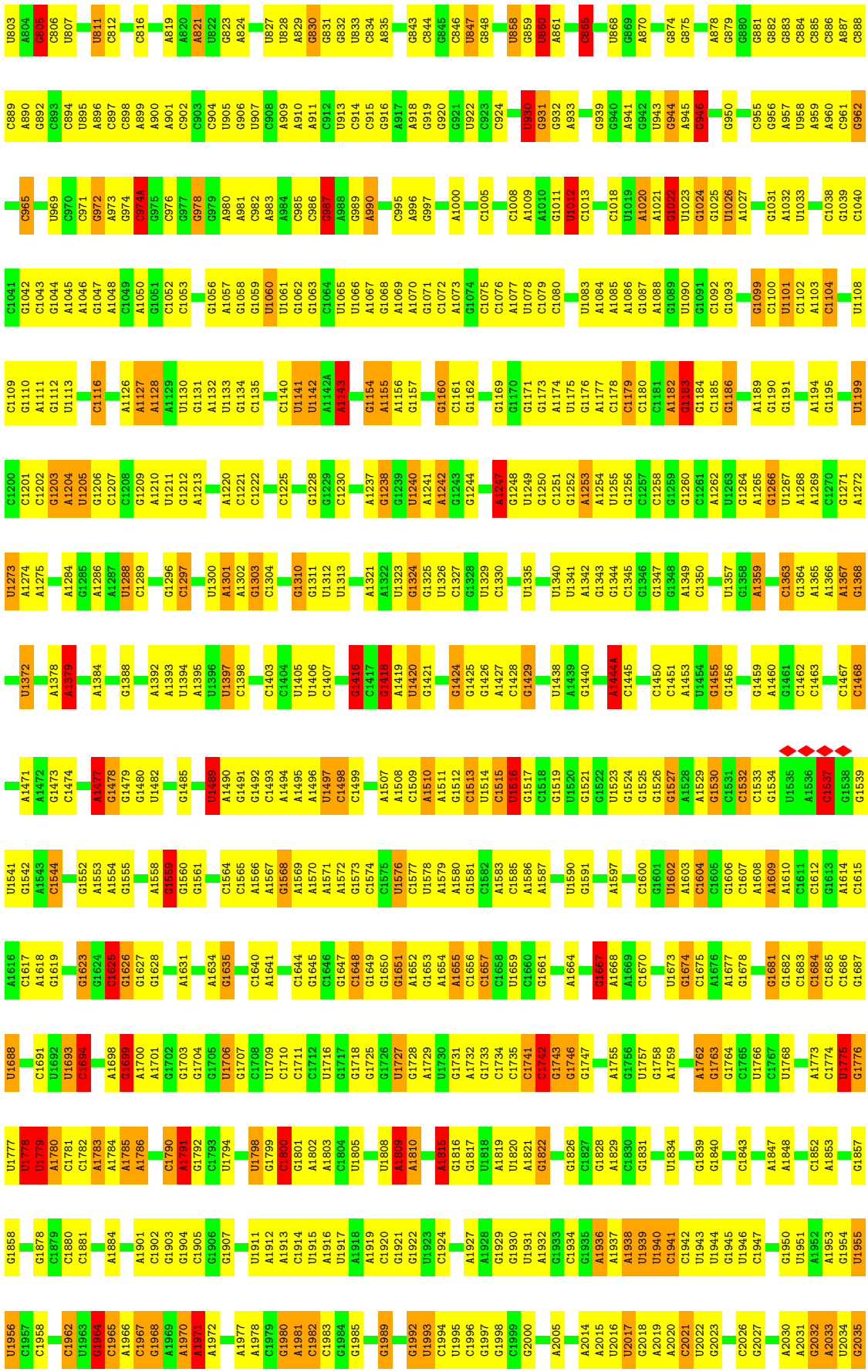
3 Residue-property plots (i)

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 atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 23S ribosomal RNA

Chain AA: 44% 44% 9%

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C889 A890 G892 C893 C894 U895 A896 C897 C898 A899 A900 A901 C902 C903 C904 U905 G906 U907 C908 A909 A910 A911 C912 U913 C914 C915 G916 A917 A918 G919 G920 G921 U922 C923 C924 U930 U931 G932 A933 G939 G940 A941 G942 U943 G944 A945 G946 G950 C955 G956 A957 U958 A959 A960 C961 G962
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C1041 G1042 C1043 G1044 A1045 A1046 G1047 A1048 C1049 A1050 G1051 C1052 C1053 G1056 A1057 G1058 G1059 U1060 U1061 G1062 G1063 C1064 U1065 U1066 A1067 G1068 A1069 A1070 G1071 C1072 A1073 G1074 C1075 C1076 A1077 U1078 C1079 C1080 U1083 A1084 A1085 A1086 G1087 A1088 G1089 U1090 G1091 C1092 G1093 G1099 C1100 U1101 C1102 A1103 C1104 U1108
C1109 G1110 A1111 G1112 U1113 C1116 A1126 A1127 A1128 A1129 U1130 G1131 A1132 U1133 G1134 C1135 C1140 U1141 U1142 A1142A A1143 G1154 A1155 A1156 G1157 G1160 C1161 G1162 G1169 G1170 G1171 G1173 A1174 U1175 G1176 A1177 C1178 C1179 C1180 C1181 A1182 G1183 G1184 C1185 G1186 A1189 G1190 G1191 A1194 G1195 U1199
C1200 C1201 C1202 G1203 A1204 U1205 G1206 C1207 C1208 G1209 A1210 U1211 G1212 A1213 A1220 C1221 C1222 C1225 G1228 G1229 C1230 A1237 G1238 G1239 U1240 A1241 A1242 G1243 G1244 A1247 G1248 U1249 G1250 C1251 G1252 A1253 A1254 U1255 G1256 C1257 C1258 G1259 G1260 C1261 A1262 U1263 G1264 A1265 G1266 U1267 A1268 A1269 C1270 G1271 A1272
U1273 A1274 A1275 A1284 G1285 A1286 A1287 U1288 C1289 G1296 C1297 U1300 A1301 A1302 G1303 C1304 G1310 G1311 U1312 U1313 A1321 A1322 U1323 G1324 G1325 U1326 C1327 G1328 U1329 C1330 U1335 U1340 U1341 A1342 G1343 G1344 C1345 G1346 G1347 G1348 A1349 C1350 U1357 G1358 A1359 C1363 G1364 A1365 A1366 A1367 G1368
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A1471 A1472 G1473 C1474 A1477 G1478 G1479 G1480 U1482 G1485 U1489 A1490 G1491 G1492 C1493 A1494 A1495 A1496 U1497 C1498 C1499 A1507 A1508 C1509 A1510 A1511 G1512 C1513 U1514 C1515 U1516 G1517 C1518 G1519 U1520 G1521 G1522 U1523 G1524 G1525 G1526 G1527 A1528 A1529 G1530 C1531 C1532 C1533 G1534 U1535 A1536 C1537 G1538 G1539 G1540
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U1688 C1691 U1692 U1693 C1694 A1698 G1699 A1700 A1701 G1702 G1703 G1704 G1705 U1706 G1707 C1708 U1709 C1710 C1711 C1712 U1716 G1717 G1718 G1725 G1726 U1727 G1728 A1729 U1730 G1731 A1732 G1733 C1734 C1735 C1741 C1742 G1743 G1746 G1747 A1755 G1756 U1757 G1758 A1759 A1762 G1763 G1764 C1765 U1766 C1767 U1768 A1773 C1774 U1775 G1776
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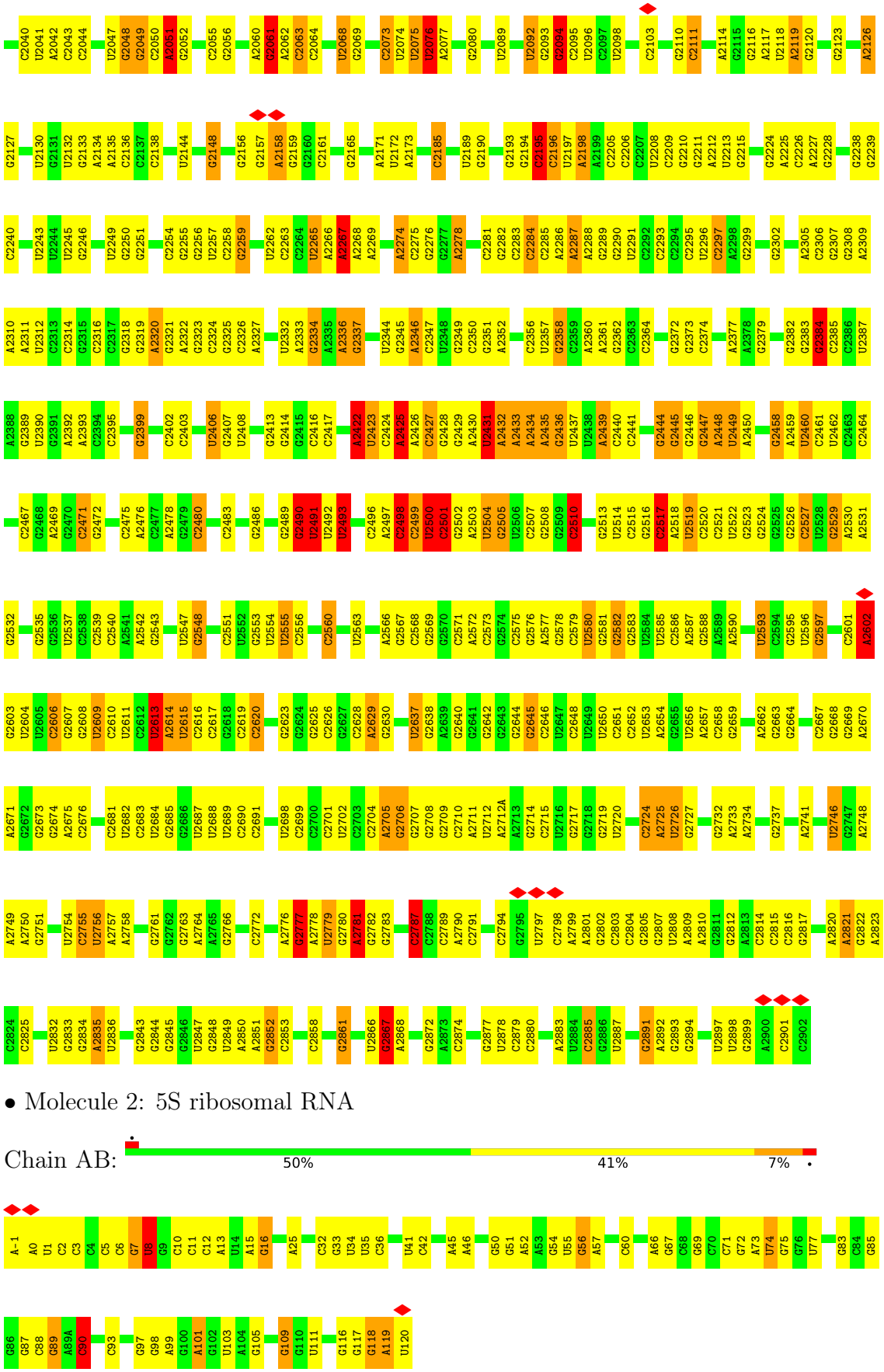
U1956 C1957 C1958 C1962 U1963 G1964 C1965 A1966 C1967 G1968 A1969 A1970 A1971 A1972 A1977 A1978 C1979 G1980 A1981 C1982 C1983 G1984 G1985 G1989 G1992 U1993 C1994 U1995 C1996 G1997 G1998 C1999 G2000 A2005 A2014 A2015 U2016 U2017 G2018 A2019 A2020 C2021 U2022 G2023 C2026 G2027 A2030 A2031 G2032 A2033 U2034 G2035

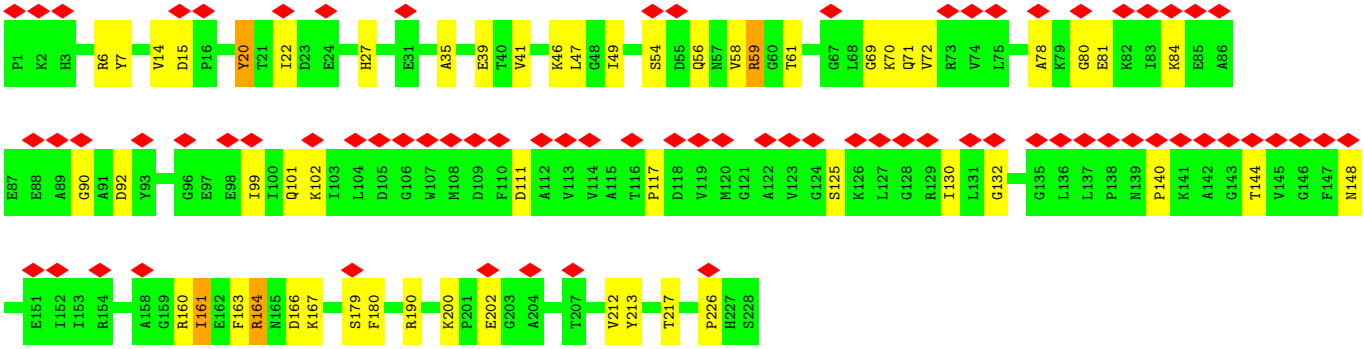


• Molecule 2: 5S ribosomal RNA

Chain AB:

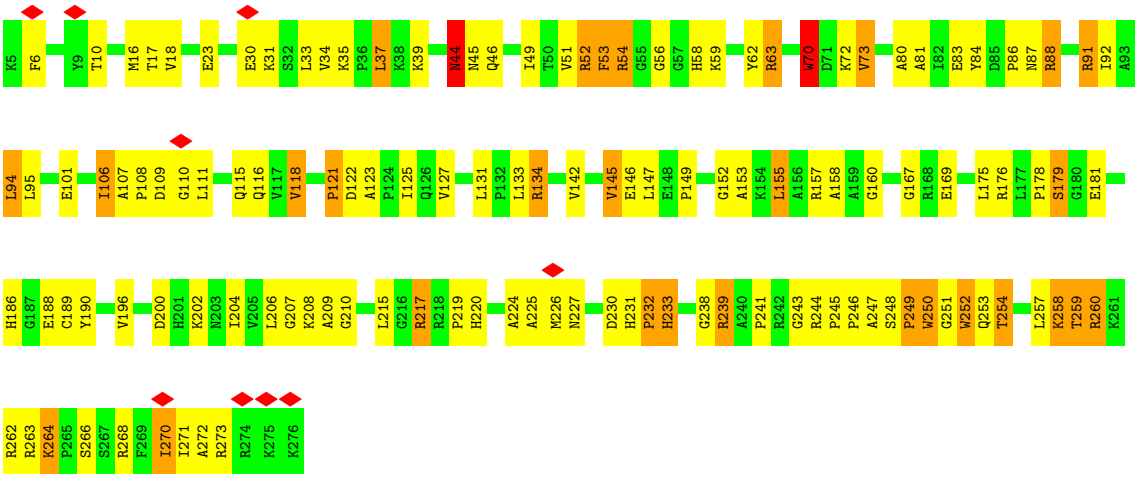
- Molecule 3: 50S ribosomal protein L1

Chain AC:



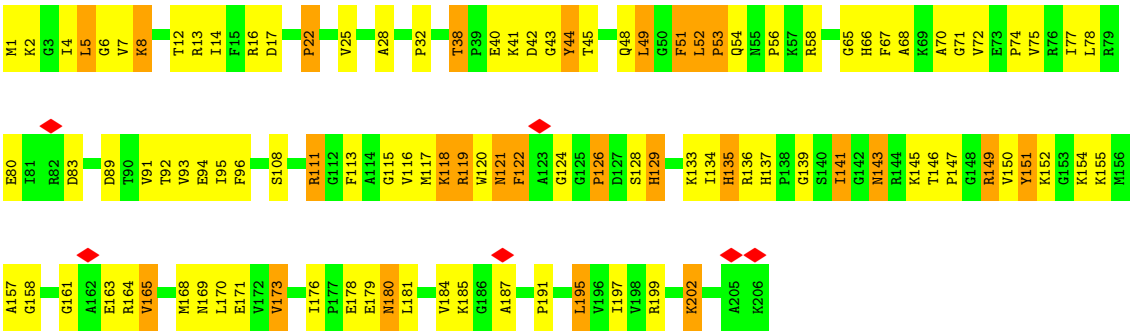
- Molecule 4: 50S ribosomal protein L2

Chain AD:



- Molecule 5: 50S ribosomal protein L3

Chain AE:



- Molecule 6: 50S ribosomal protein L4

Chain AF: 6% 54% 37% 9%

E3 V4 A5 V6 Y7 Q8 S13 P14 R17 R18 E19 L20 A21 A22 D23 L24 E27 I28 N29 P30 H31 L32 L33 W34 E35 W39 R45 R46 G47 K52 T53 R54 V57 A58 Y59 S60 G61 R62 K63 I64 Q67 K68 H69 R72 A73 R74 H75 G76 D77 I78 G79

A80 P81 I82 F83 V84 G85 V89 F90 G91 R95 S98 Y99 T100 L101 P102 K103 K104 V105 R106 K107 K108 A111 R117 A118 R119 E120 G121 K122 V126 E127 V132 N133 G134 K135 T136 K137 E138 F139 L140 S151 E152 L155 L156 V157 T158 G159 A167 R168 N169 L170

P171 W172 T175 L176 A177 P178 L181 N182 V183 Y184 D185 I186 V187 R188 T189 E190 R191 L192 L196 D197 A198 W199 E200 V201 F202 Q203 N204 E209 A210

- Molecule 7: 50S ribosomal protein L5

Chain AG: 9% 53% 38% 8%

M1 L7 K8 Y12 R16 P17 E18 L19 I20 R21 R22 F23 G24 Y25 Q26 N27 E30 V31 P32 R33 L34 E35 K36 I39 N40 Q41 G42 L43 G44 E48 R51 I52 L53 E54 K55 A56 A57 A61 Q66 K67 P68 T71 R72 A73 S76 I77 S78 N79 F80

K81 L82 M86 P87 I88 R91 L94 R95 R96 D97 I101 F102 L103 E104 K105 L106 L111 P112 R113 I114 R115 D116 F117 L120 N123 S124 F125 D126 G127 R128 Y131 N132 L133 G134 L135 Q138 L139 I140 E143 I144 T145 Y146 D147 M148 V149 D150 A151 L152 R153 G154

M155 A163 E164 T165 D166 E167 R170 A171 L172 L173 E174 F178 P179 F180 R181 K182

- Molecule 8: 50S ribosomal protein L6

Chain AH: 7% 59% 34% 6%

I4 G5 R6 L7 V11 P12 K13 G14 V15 E18 V19 A20 R23 V24 K25 K30 G31 E32 L33 E34 V35 P36 E40 M41 R42 E46 E47 G48 V49 V50 R51 V52 P55 S56 D57 E58 L67 T68 R69 N74 A75 V76 Y83 K90 Y94 R95 V99

L103 E104 L105 T106 V107 G108 F109 S110 H111 V114 V115 E116 P117 P118 E119 G120 V125 P126 E127 R130 V131 R132 I136 D137 K138 I151 R152 K153 P154 S155 A156 Y157 H158 E159 K160 Y164 A165 G166 E167 P168 V169 R170 L171 K172 P173 G174 K175 A176 G177

- Molecule 9: 50S ribosomal protein L13

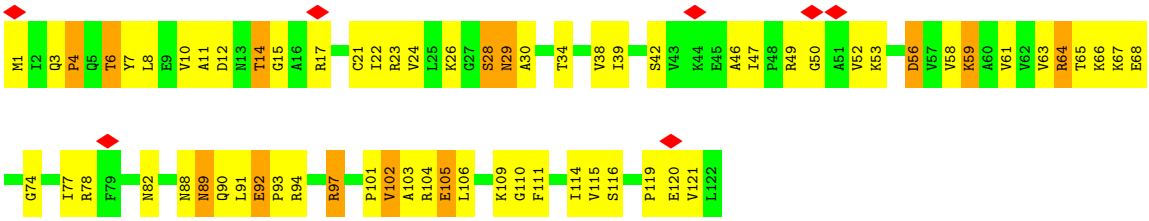
Chain AK: 41% 50% 9%

K2 T3 Y4 K7 Q8 V9 R12 W13 V14 L15 I16 D17 A18 E19 T22 L23 G24 R25 T28 K29 I30 A31 T32 L33 L34 R35 G36 K37 H38 R39 P40 D41 W42 T43 P44 N45 V46 A47 M48 G49 D50 F51 V52 V55 D58 K59 T63 K66 L67 E68 Q69

Y72 Y75 S76 G77 Y78 P79 G80 G81 L82 K83 K84 I85 P86 L87 E88 K89 M90 L91 A92 V98 H101 K104 G105 P108 K109 G110 P111 L112 G113 R114 R115 L116 R119 V122 G125 P126 D127 Q131 R134 P135 E136 K137 L138 E139 V140

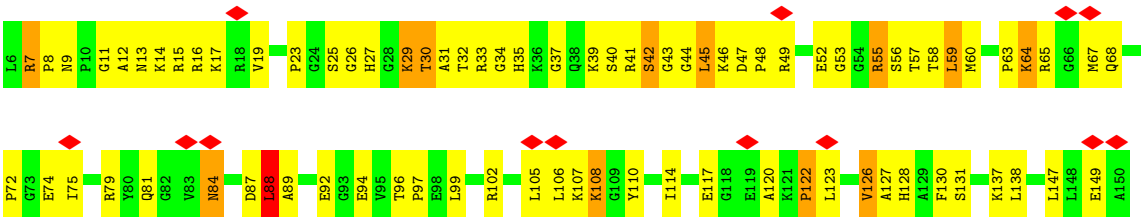
- Molecule 10: 50S ribosomal protein L14

Chain AL:



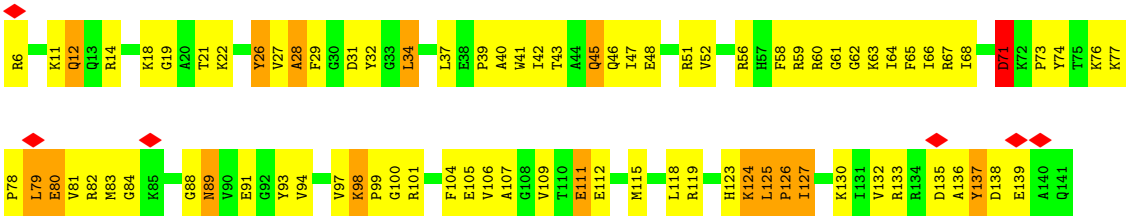
- Molecule 11: 50S ribosomal protein L15

Chain AM:



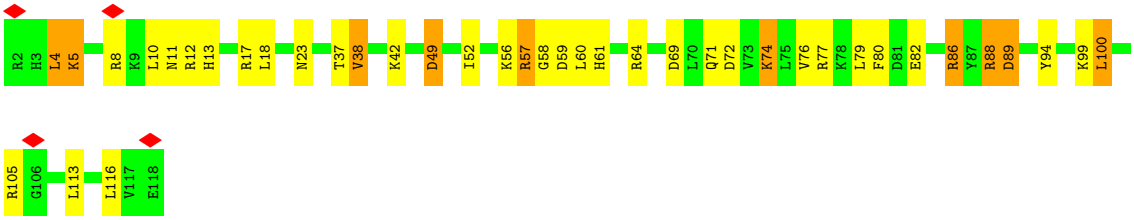
- Molecule 12: 50S ribosomal protein L16

Chain AN:



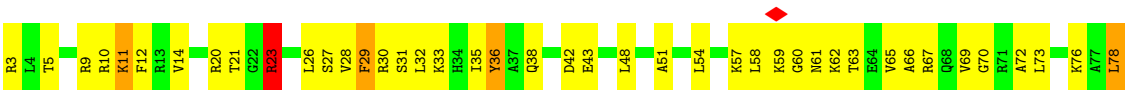
- Molecule 13: 50S ribosomal protein L17

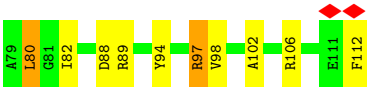
Chain AO:



- Molecule 14: 50S ribosomal protein L18

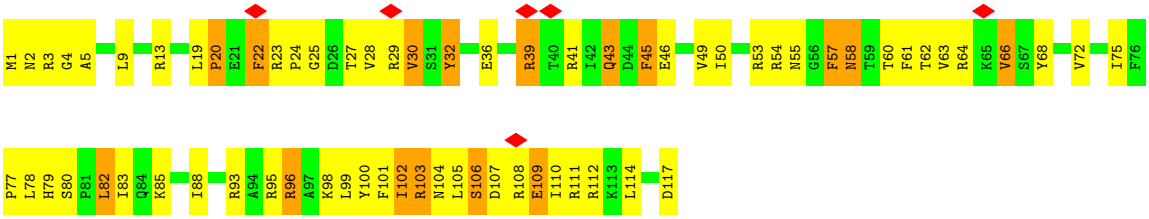
Chain AP:





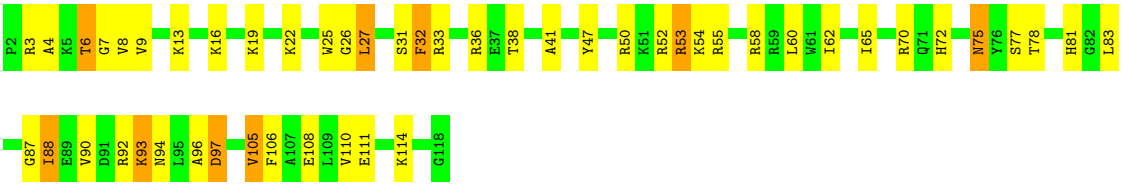
• Molecule 15: 50S ribosomal protein L19

Chain AQ:



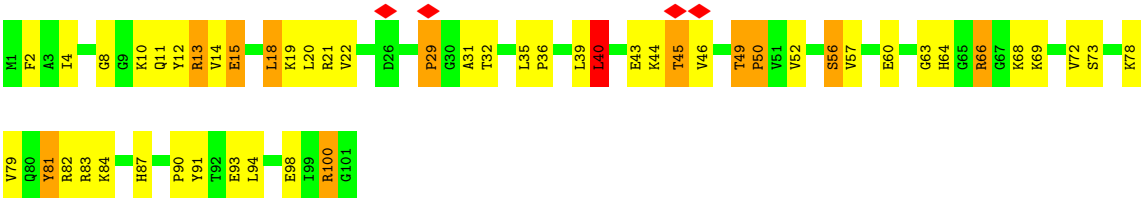
• Molecule 16: 50S ribosomal protein L20

Chain AR:



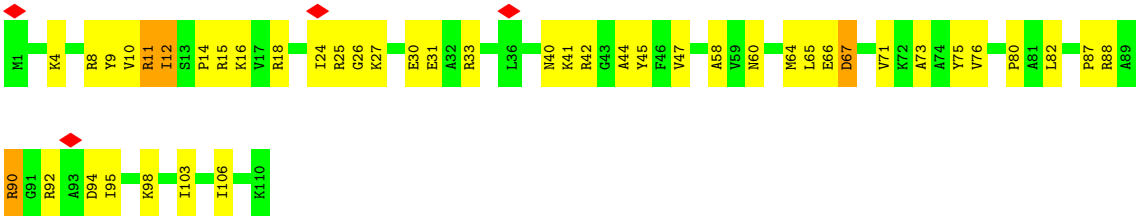
• Molecule 17: 50S ribosomal protein L21

Chain AS:



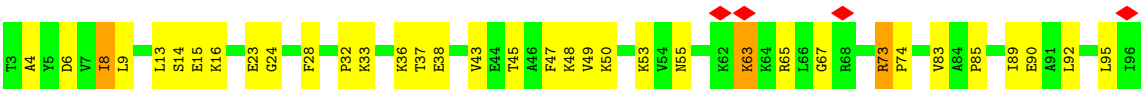
• Molecule 18: 50S ribosomal protein L22

Chain AT:



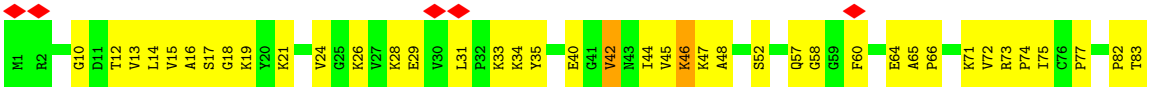
• Molecule 19: 50S ribosomal protein L23

Chain AU:



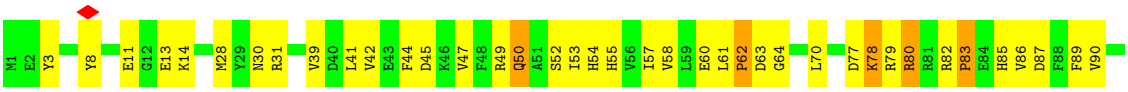
• Molecule 20: 50S ribosomal protein L24

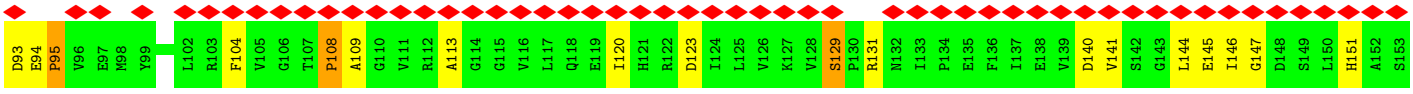
Chain AV:

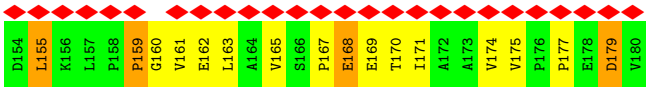


• Molecule 21: 50S ribosomal protein L25

Chain AW:

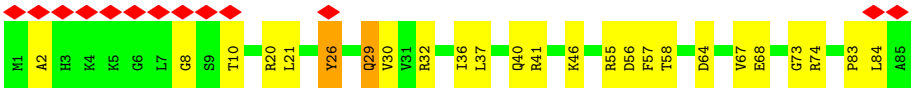






• Molecule 22: 50S ribosomal protein L27

Chain AX:



• Molecule 23: 50S ribosomal protein L29

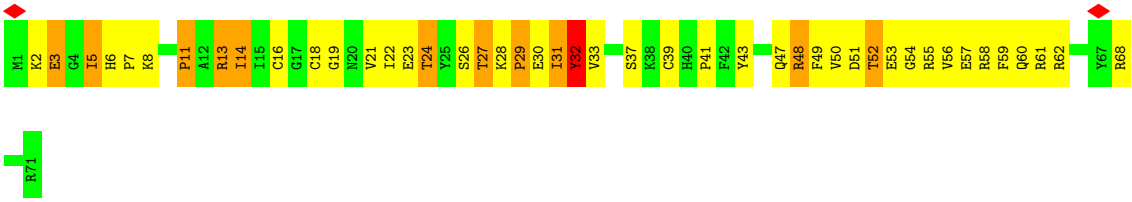
Chain AY:

• Molecule 24: 50S ribosomal protein L30

Chain AZ:

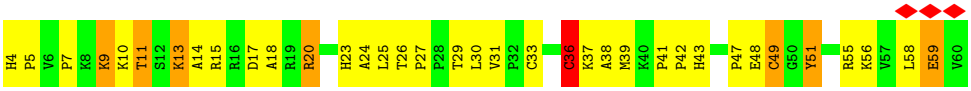
• Molecule 25: 50S ribosomal protein L31

Chain Aa:



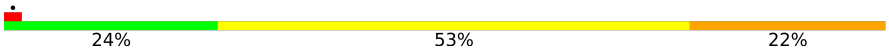
• Molecule 26: 50S ribosomal protein L32

Chain Ab:



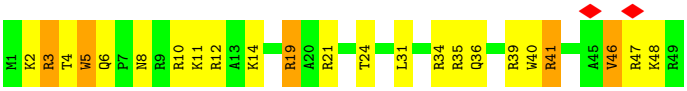
• Molecule 27: 50S ribosomal protein L33

Chain Ac:



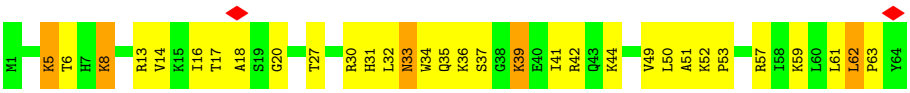
• Molecule 28: 50S ribosomal protein L34

Chain Ad:



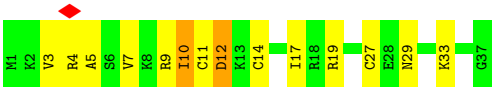
• Molecule 29: 50S ribosomal protein L35

Chain Ae:



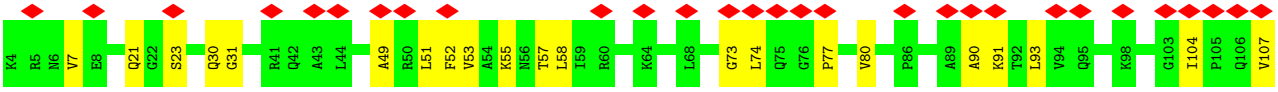
• Molecule 30: 50S ribosomal protein L36

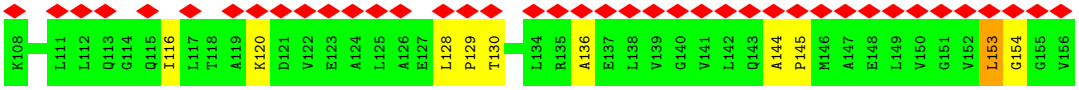
Chain Af:



• Molecule 31: 50S ribosomal protein L10

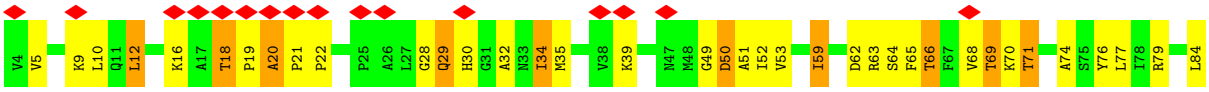
Chain AI:

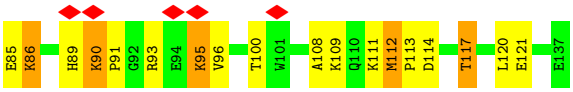




• Molecule 32: 50S ribosomal protein L11

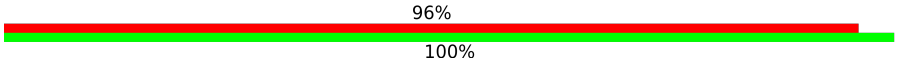
Chain AJ:

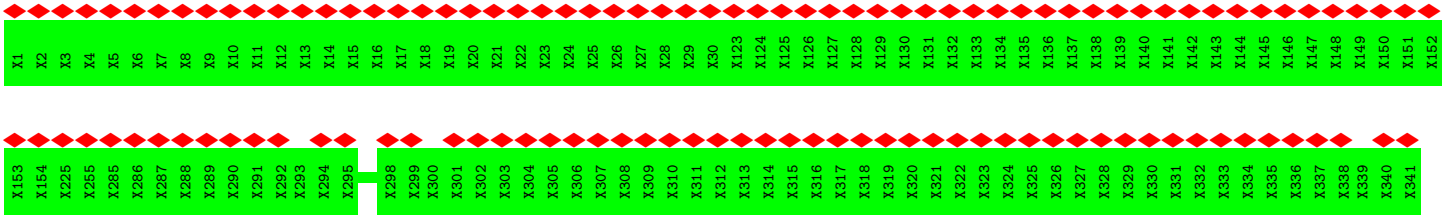


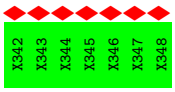


• Molecule 33: Unknown peptide

Chain Ag:

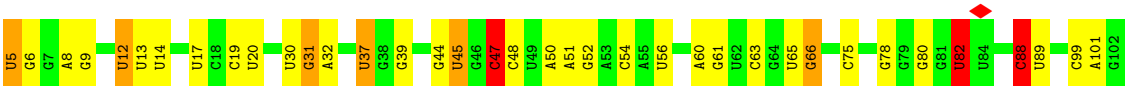


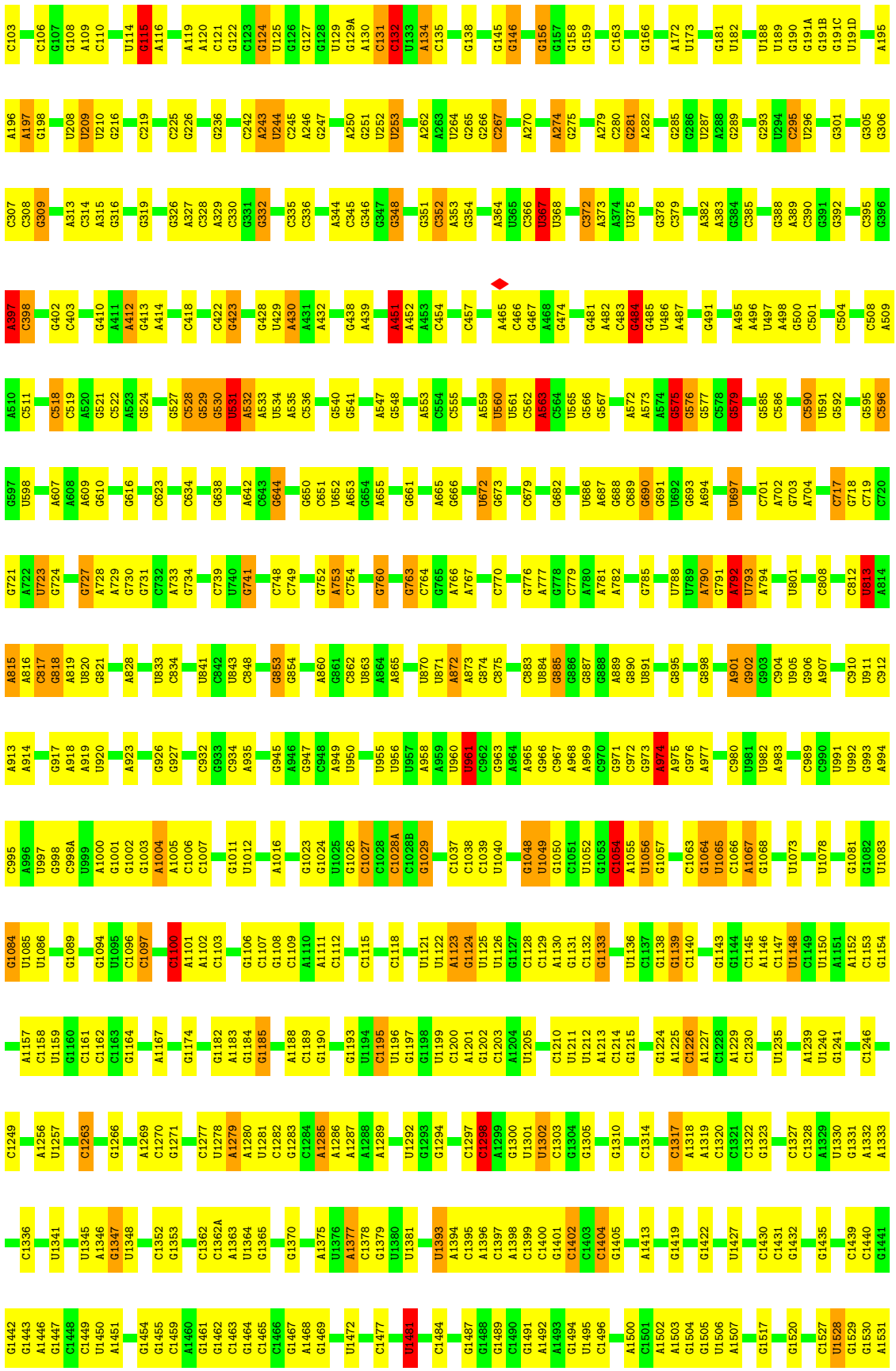


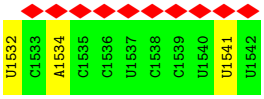


• Molecule 34: 16S ribosomal RNA

Chain BA:

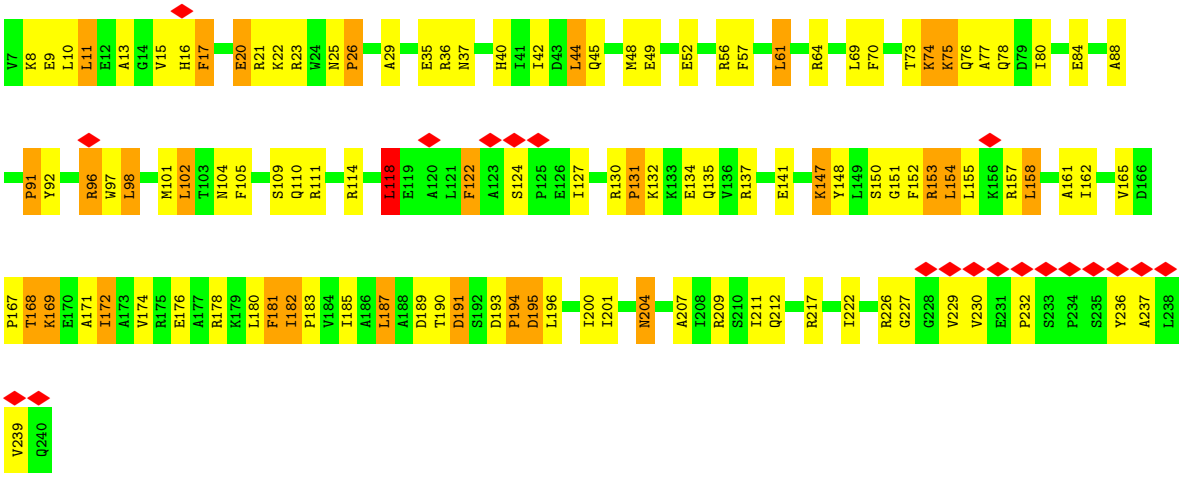



C103 C106 G107 G108 A109 C110 U114 G115 A116 A119 A120 C121 G122 C123 G124 U125 G126 G127 G128 U129 G129A A130 C131 G132 U133 A134 C135 G138 G145 G146 G156 G157 G158 G159 C163 G166 A172 U173 G181 U182 U188 U189 G190 G191A G191B G191C U191D A195
A196 A197 G198 U208 U209 U210 G216 C219 C225 G226 G236 C242 A243 U244 C245 A246 G247 A250 G251 U252 U253 A262 A263 U264 G265 G266 C267 A270 A274 G275 A279 C280 G281 A282 G285 G286 U287 A288 G289 G293 U294 C295 U296 G301 G305 G306
C307 C308 G309 A313 C314 A315 G316 G319 G326 A327 C328 A329 C330 G331 G332 C335 C336 A344 C345 G346 G347 G348 G351 C352 A353 G354 A364 U365 C366 U367 U368 C372 A373 A374 U375 G378 C379 A382 A383 G384 C385 G388 A389 C390 G391 G392 C395 G396
A397 C398 G402 C403 G410 A411 A412 G413 A414 C418 C422 G423 G428 U429 A430 A431 A432 G438 A439 A451 A452 A453 C454 C457 A465 C466 G467 A468 G474 G481 A482 C483 G484 G485 U486 A487 G491 A495 A496 U497 A498 G500 C501 C504 C508 A509
A510 C511 C518 C519 A520 G521 C522 A523 G524 G527 C528 G529 G530 U531 A532 A533 U534 A535 C536 G540 G541 A547 G548 A553 C554 C555 A559 U560 U561 C562 A563 C564 U565 G566 G567 A572 A573 A574 G575 G576 G577 C578 G579 G585 C586 C590 U591 G592 G595 C596
G597 U598 A607 A608 A609 G610 G616 C623 C634 G638 A642 G643 G644 G650 C651 U652 A653 G654 A655 G661 A665 G666 U672 G673 C679 G682 U686 A687 G688 G689 G690 G691 U692 G693 A694 U697 C701 A702 G703 A704 G717 G718 C719 G720
G721 A722 U723 G724 G727 A728 A729 G730 G731 C732 A733 G734 C739 U740 G741 C748 C749 G752 A753 C754 G760 G763 C764 G765 A766 A767 C770 G776 A777 G778 C779 A780 A781 A782 G785 U788 U789 A790 G791 A792 U793 A794 U801 C808 C812 U813 A814
A815 A816 C817 G818 A819 U820 G821 A828 U833 C834 U841 C842 U843 C848 G853 G854 A860 G861 C862 U863 A864 A865 U870 U871 A872 A873 G874 C875 C883 U884 G885 G886 G887 G888 A889 G890 U891 G895 G898 A901 G902 G903 C904 U905 G906 A907 C910 U911 C912
A913 A914 G917 A918 A919 U920 A923 G926 G927 C932 G933 C934 A935 G945 A946 G947 C948 A949 U950 U955 U956 U957 A958 A959 U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 C980 U981 U982 A983 C989 C990 U991 U992 G993 A994
C995 A996 U997 G998 C998A U999 A1000 G1001 G1002 G1003 A1004 A1005 C1006 C1007 G1011 U1012 A1016 G1023 G1024 U1025 G1026 C1027 C1028 C1028A C1028B G1029 C1037 C1038 C1039 U1040 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 C1063 G1064 U1065 C1066 A1067 G1068 U1073 U1078 G1081 G1082 U1083
G1084 U1085 U1086 G1089 G1094 U1095 C1096 C1097 C1100 A1101 A1102 C1103 G1106 C1107 G1108 C1109 A1110 A1111 C1112 C1115 C1118 U1121 U1122 A1123 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 U1136 C1137 G1138 G1139 C1140 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 G1154
A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1164 A1167 G1174 G1182 A1183 G1184 G1185 A1188 C1189 G1190 G1193 U1194 C1195 U1196 G1197 G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 C1210 U1211 U1212 A1213 C1214 G1215 G1224 A1225 C1226 A1227 C1228 A1229 C1230 U1235 A1239 U1240 G1241 C1246
C1249 A1256 U1257 C1263 G1266 A1269 C1270 G1271 C1277 U1278 A1279 A1280 U1281 C1282 G1283 C1284 A1285 A1286 A1287 A1288 A1289 U1292 G1293 G1294 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 G1310 C1314 C1317 A1318 A1319 C1320 C1321 C1322 G1323 C1327 C1328 A1329 U1330 G1331 A1332 A1333
C1336 U1341 U1345 A1346 G1347 U1348 C1352 G1353 C1362 C1362A A1363 U1364 G1365 G1370 A1375 U1376 A1377 C1378 G1379 U1380 U1381 U1393 A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 A1413 G1419 G1422 U1427 C1430 C1431 G1432 G1435 C1439 C1440 G1441
G1442 G1443 A1446 G1447 C1448 C1449 U1450 A1451 G1454 G1455 C1459 A1460 G1461 G1462 C1463 G1464 C1465 C1466 G1467 A1468 G1469 U1472 C1477 U1481 C1484 G1487 G1488 G1489 C1490 G1491 A1492 A1493 G1494 U1495 C1496 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1507 G1517 G1520 C1527 U1528 G1529 G1530 A1531



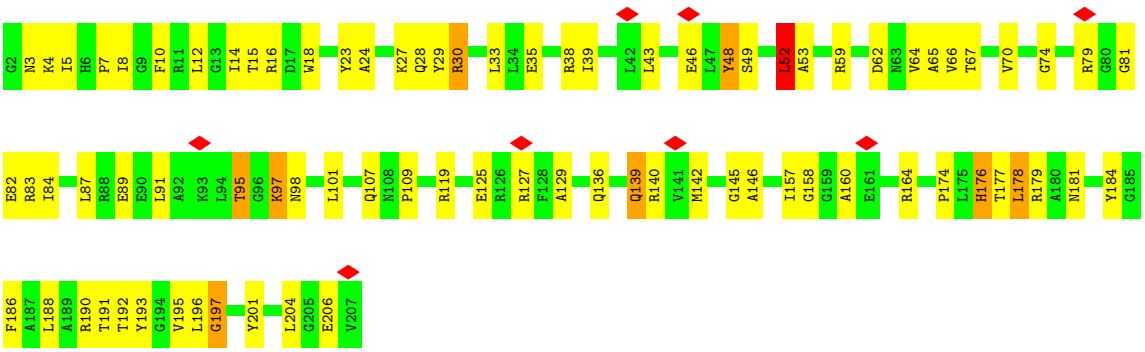
• Molecule 35: 30S ribosomal protein S2

Chain BF:



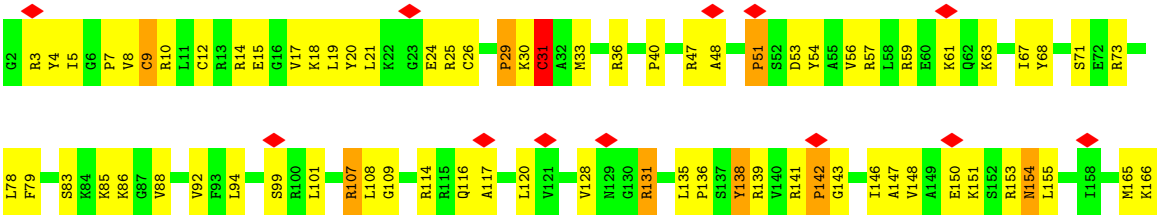
• Molecule 36: 30S ribosomal protein S3

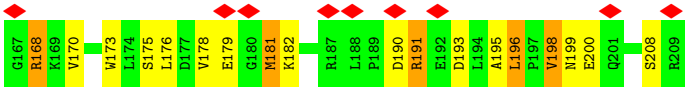
Chain BG:



• Molecule 37: 30S ribosomal protein S4

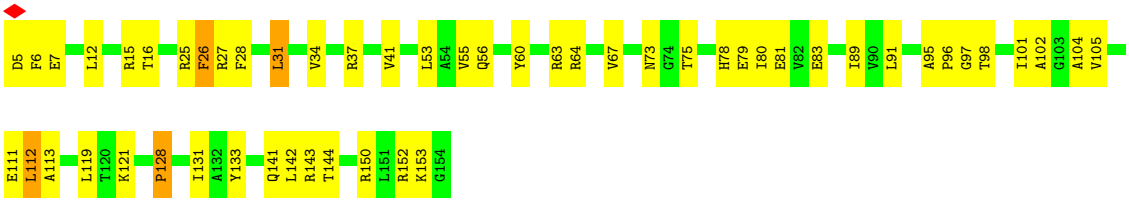
Chain BH:





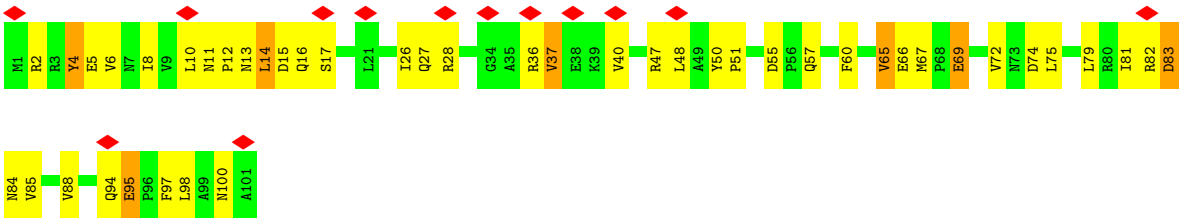
• Molecule 38: 30S ribosomal protein S5

Chain BI:



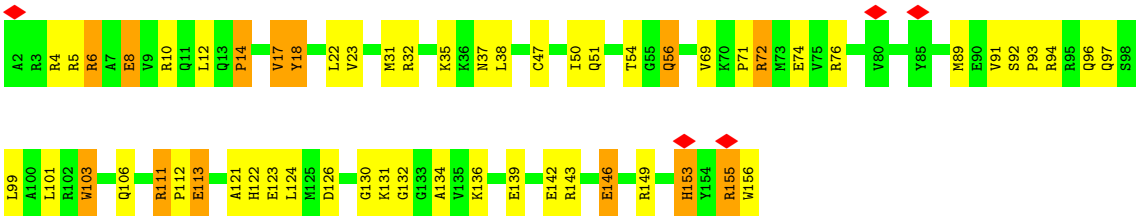
• Molecule 39: 30S ribosomal protein S6

Chain BJ:



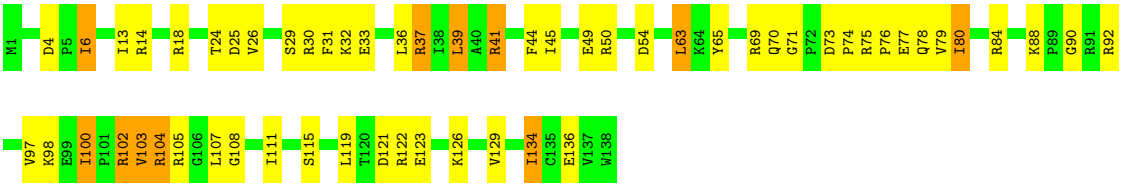
• Molecule 40: 30S ribosomal protein S7

Chain BK:



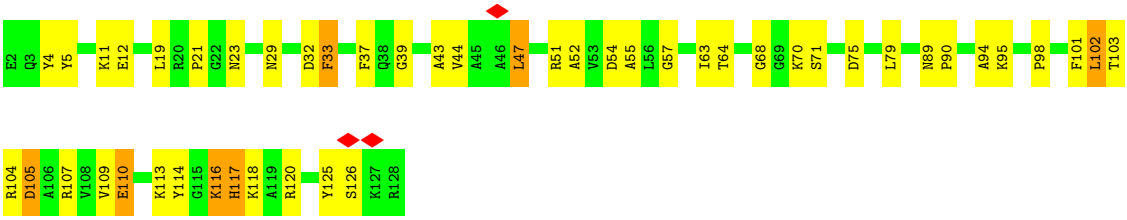
• Molecule 41: 30S ribosomal protein S8

Chain BL:



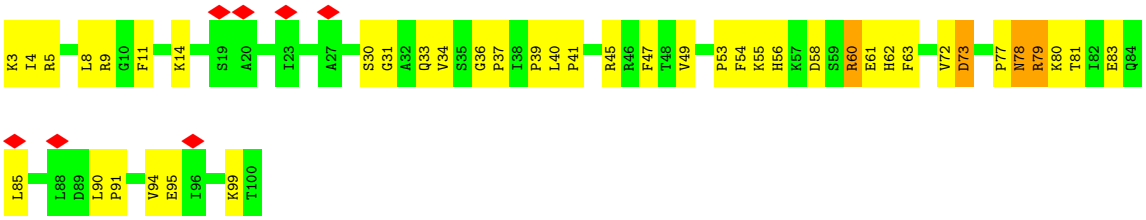
• Molecule 42: 30S ribosomal protein S9

Chain BM:



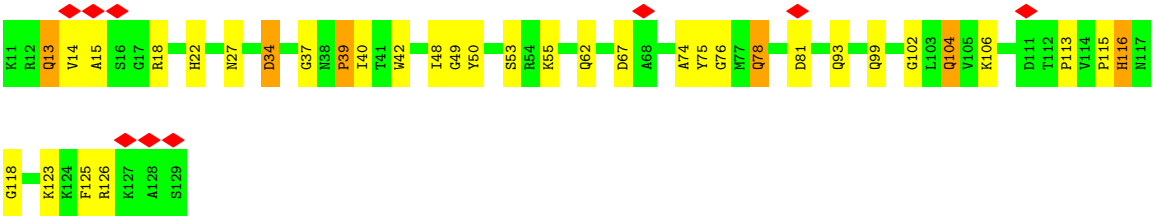
• Molecule 43: 30S ribosomal protein S10

Chain BN:



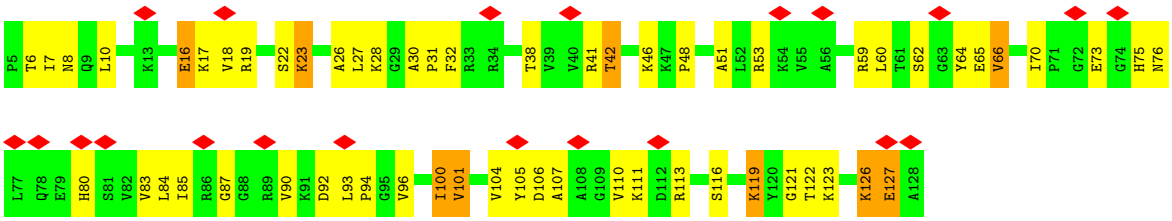
• Molecule 44: 30S ribosomal protein S11

Chain BO:



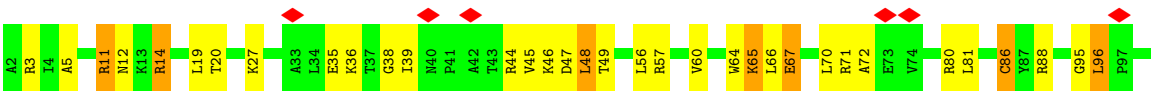
• Molecule 45: 30S ribosomal protein S12

Chain BP:



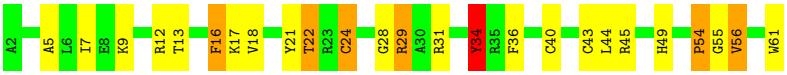
• Molecule 46: 30S ribosomal protein S13

Chain BQ:



• Molecule 47: 30S ribosomal protein S14 type Z

Chain BR:

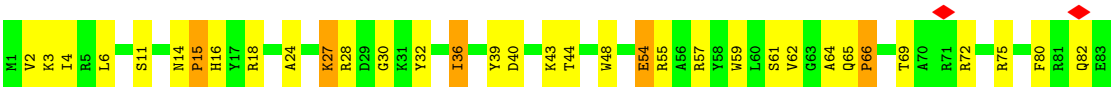


• Molecule 48: 30S ribosomal protein S15

Chain BS:

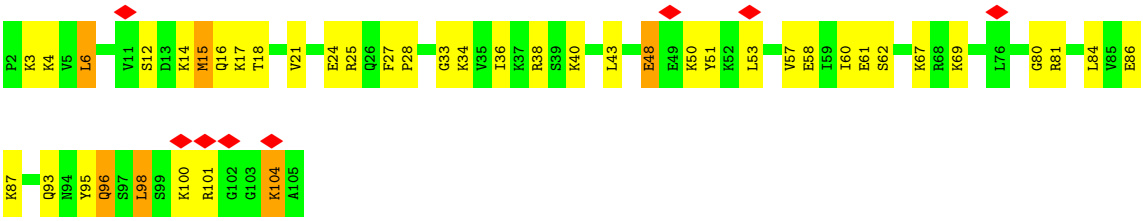
• Molecule 49: 30S ribosomal protein S16

Chain BT:



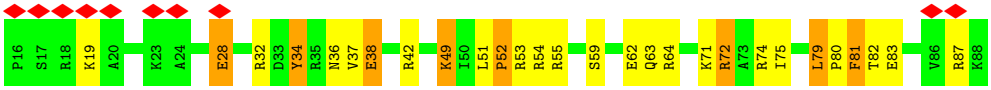
• Molecule 50: 30S ribosomal protein S17

Chain BU:



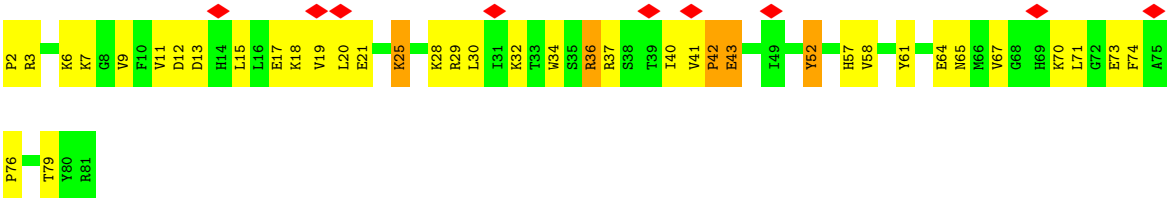
• Molecule 51: 30S ribosomal protein S18

Chain BV:



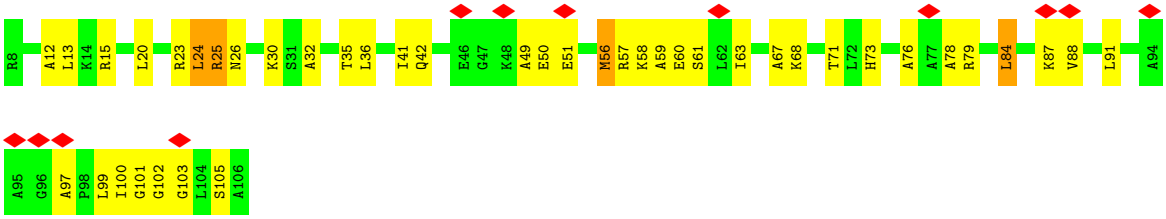
• Molecule 52: 30S ribosomal protein S19

Chain BW:



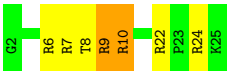
• Molecule 53: 30S ribosomal protein S20

Chain BX:



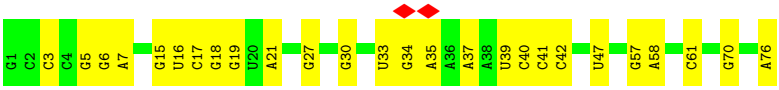
• Molecule 54: 30S ribosomal protein Thx

Chain BY:



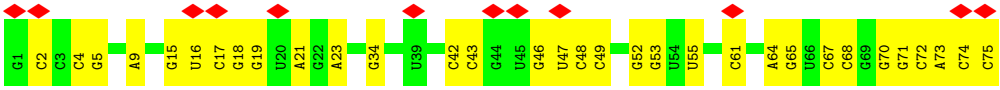
• Molecule 55: tRNA chain 1

Chain BC:



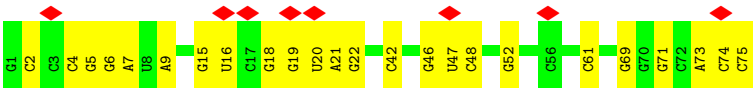
• Molecule 56: tRNA chain 2

Chain BD:



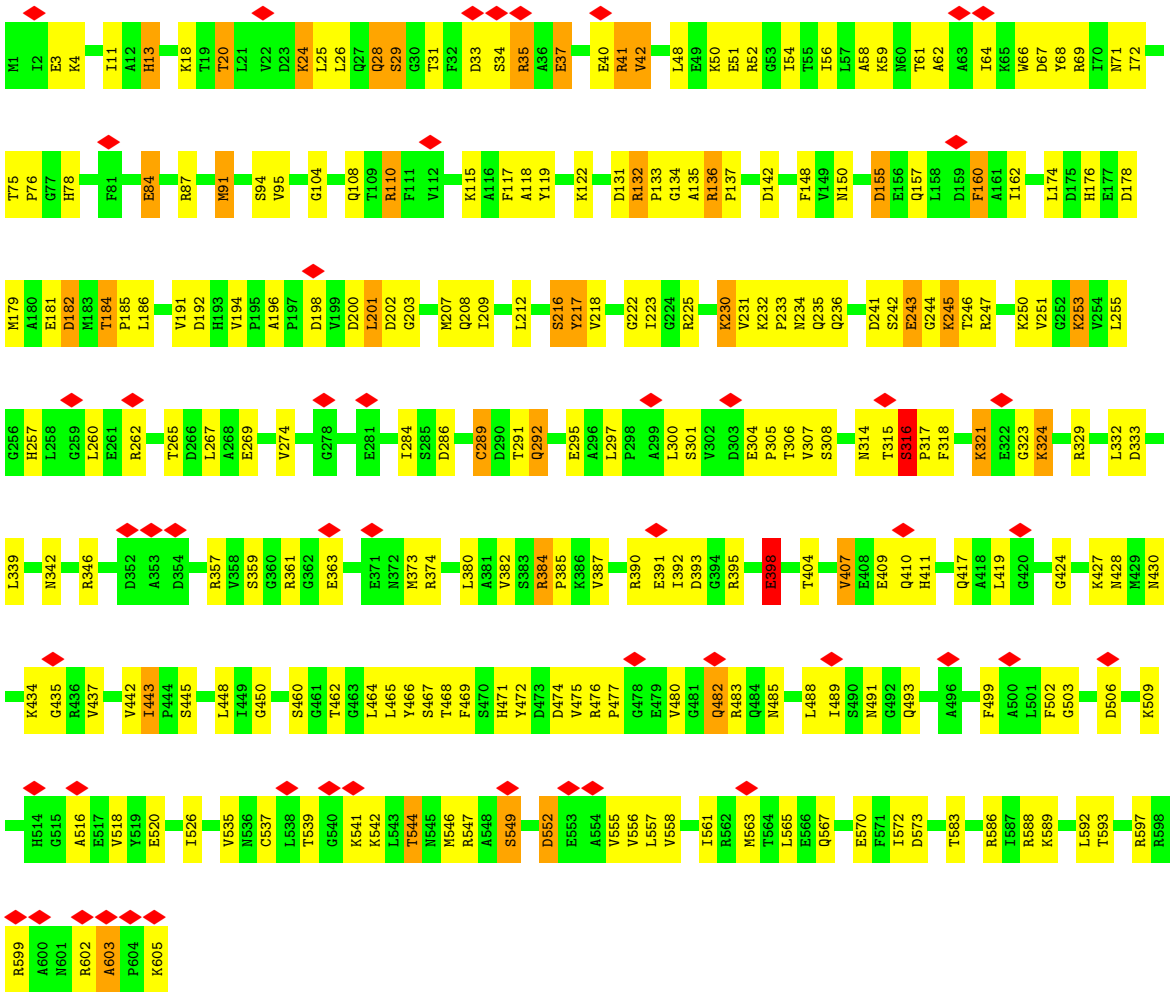
• Molecule 56: tRNA chain 2

Chain BE:



• Molecule 57: GTP-binding protein

Chain BZ:


M1 I2 E3 K4 I11 A12 H13 K18 T19 T20 L21 V22 D23 K24 L25 L26 Q27 Q28 S29 G30 T31 F32 D33 S34 R35 A36 E37 E40 R41 V42 L48 E49 K50 E51 R52 G53 I54 T55 I56 L57 A58 K59 N60 T61 A62 A63 I64 K65 W66 D67 Y68 R69 I70 N71 I72
T75 P76 G77 H78 F81 E84 R87 M91 S94 V95 G104 Q108 T109 R110 F111 V112 K115 A116 F117 A118 Y119 K122 D131 R132 P133 G134 A135 R136 P137 D142 F148 V149 N150 D155 E156 Q157 L158 D159 F160 A161 I162 L174 D175 H176 E177 D178
M179 A180 E181 D182 M183 T184 P185 L186 V191 D192 H193 V194 P195 A196 P197 D198 V199 D200 L201 D202 G203 M207 Q208 I209 L212 S216 Y217 V218 G222 I223 G224 R225 K230 V231 K232 P233 N234 Q235 Q236 D241 S242 E243 G244 K245 T246 R247 K250 V251 G252 K253 V254 L255
G256 H257 L258 G259 L260 E261 R262 T265 D266 L267 A268 E269 V274 G278 E281 I284 S285 D286 C289 D290 T291 Q292 E295 A296 L297 P298 A299 L300 S301 V302 D303 E304 P305 T306 V307 S308 N314 T315 S316 P317 F318 K321 E322 G323 K324 R329 L332 D333
L339 N342 R346 D352 A353 D354 R357 V358 S359 G360 R361 G362 E363 E371 N372 M373 R374 L380 A381 V382 S383 R384 P385 K386 V387 R390 E391 I392 D393 G394 R395 E398 T404 V407 E408 E409 Q410 H411 Q417 A418 L419 G420 G424 K427 N428 M429 N430
K434 G435 R436 V437 V442 I443 P444 S445 L448 I449 G450 S460 G461 T462 G463 L464 L465 Y466 S467 T468 F469 S470 H471 Y472 D473 D474 V475 R476 P477 G478 E479 Y480 G481 Q482 R483 Q484 N485 L488 I489 S490 N491 G492 Q493 A496 F499 A500 L501 F502 G503 D506 K509
H514 G515 A516 E517 V518 Y519 E520 I526 V535 N536 C537 L538 T539 G540 K541 K542 L543 T544 N545 M546 R547 A548 S549 D552 E553 A554 V555 V556 L557 V558 I561 R562 M563 T564 L565 E566 Q567 E570 F571 I572 D573 T583 R586 I587 R588 K589 L592 T593 R597 R598
R599 A600 N601 R602 A603 P604 K605

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	77127	Depositor
Resolution determination method	Not provided	
CTF correction method	CTFFIND3	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	73684	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.359	Depositor
Minimum map value	-0.095	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.0392	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.28, 1.28, 1.28	Depositor

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: GCP, 8AN, NMY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	AA	1.00	107/69678 (0.2%)	1.08	348/108758 (0.3%)
2	AB	0.83	4/2954 (0.1%)	0.99	7/4606 (0.2%)
3	AC	0.54	0/1772	0.87	0/2383
4	AD	0.72	2/2174 (0.1%)	1.19	13/2927 (0.4%)
5	AE	0.75	0/1611	1.16	13/2171 (0.6%)
6	AF	0.64	0/1660	1.03	4/2247 (0.2%)
7	AG	0.62	0/1507	1.06	4/2027 (0.2%)
8	AH	0.59	0/1354	0.98	4/1831 (0.2%)
9	AK	0.78	1/1140 (0.1%)	1.16	8/1537 (0.5%)
10	AL	0.92	1/942 (0.1%)	1.31	10/1268 (0.8%)
11	AM	0.71	0/1123	1.12	5/1493 (0.3%)
12	AN	0.72	0/1100	1.19	8/1470 (0.5%)
13	AO	0.70	0/974	1.06	2/1302 (0.2%)
14	AP	0.72	0/887	1.06	4/1180 (0.3%)
15	AQ	0.85	0/990	1.31	9/1325 (0.7%)
16	AR	0.76	0/982	1.08	0/1306
17	AS	0.87	1/790 (0.1%)	1.28	9/1057 (0.9%)
18	AT	0.66	0/886	1.04	1/1189 (0.1%)
19	AU	0.57	0/756	0.93	0/1015
20	AV	0.54	0/857	1.05	2/1142 (0.2%)
21	AW	0.66	0/1467	1.11	7/1992 (0.4%)
22	AX	0.65	0/679	1.04	1/902 (0.1%)
23	AY	0.59	0/569	0.88	0/751
24	AZ	0.59	0/474	1.10	2/635 (0.3%)
25	Aa	0.84	1/594 (0.2%)	1.31	8/795 (1.0%)
26	Ab	0.72	0/459	1.16	3/621 (0.5%)
27	Ac	0.85	1/433 (0.2%)	1.36	5/576 (0.9%)
28	Ad	0.73	0/438	1.01	0/575
29	Ae	0.59	0/523	1.14	5/690 (0.7%)
30	Af	0.59	0/310	1.08	1/407 (0.2%)
31	AI	0.50	1/751 (0.1%)	0.82	4/1042 (0.4%)
32	AJ	0.52	0/1012	0.64	8/1373 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
34	BA	0.92	26/36437 (0.1%)	1.10	139/56865 (0.2%)
35	BF	0.65	0/1935	1.00	4/2609 (0.2%)
36	BG	0.55	0/1636	0.92	4/2205 (0.2%)
37	BH	0.64	1/1733 (0.1%)	0.98	3/2318 (0.1%)
38	BI	0.63	0/1162	1.01	3/1564 (0.2%)
39	BJ	0.60	0/856	0.95	0/1154
40	BK	0.57	0/1276	0.90	3/1709 (0.2%)
41	BL	0.62	0/1136	1.01	3/1527 (0.2%)
42	BM	0.54	0/1029	0.83	0/1379
43	BN	0.48	0/807	0.89	1/1085 (0.1%)
44	BO	0.62	0/900	0.98	0/1213
45	BP	0.60	0/986	1.00	3/1320 (0.2%)
46	BQ	0.33	0/924	0.45	2/1238 (0.2%)
47	BR	0.55	0/501	0.97	1/664 (0.2%)
48	BS	0.62	0/745	0.95	0/992
49	BT	0.62	0/716	0.95	1/963 (0.1%)
50	BU	0.68	1/870 (0.1%)	0.99	2/1159 (0.2%)
51	BV	0.59	0/603	1.01	1/799 (0.1%)
52	BW	0.53	1/661 (0.2%)	1.34	5/890 (0.6%)
53	BX	0.65	0/765	1.00	2/1007 (0.2%)
54	BY	0.45	0/212	0.80	0/277
55	BC	0.36	0/1809	0.67	0/2819
56	BD	0.37	0/1784	0.68	0/2780
56	BE	0.35	0/1784	0.70	0/2780
57	BZ	0.37	0/4678	0.50	16/6310 (0.3%)
All	All	0.86	148/167791 (0.1%)	1.05	688/250219 (0.3%)

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	AA	0	432
2	AB	0	17
3	AC	0	1
5	AE	0	1
6	AF	0	1
9	AK	0	1
12	AN	0	1
15	AQ	0	1
17	AS	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	Aa	0	1
26	Ab	0	1
31	AI	0	2
34	BA	0	170
37	BH	0	1
39	BJ	0	1
44	BO	0	1
47	BR	0	1
All	All	0	634

All (148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1060	U	O3'-P	-80.27	0.64	1.61
34	BA	1317	C	O3'-P	-70.10	0.77	1.61
1	AA	1203	G	O3'-P	-34.75	1.19	1.61
34	BA	1167	A	O3'-P	20.86	1.86	1.61
1	AA	2500	U	C4-O4	18.56	1.38	1.23
1	AA	2500	U	O3'-P	-15.05	1.43	1.61
1	AA	2448	A	O3'-P	-14.41	1.43	1.61
1	AA	607	U	N3-C4	-14.40	1.25	1.38
1	AA	621	A	C6-N6	14.15	1.45	1.33
1	AA	1240	U	O3'-P	-13.46	1.45	1.61
1	AA	2756	U	O3'-P	13.37	1.77	1.61
1	AA	607	U	C2-N3	-13.22	1.28	1.37
31	AI	153	LEU	C-N	-12.16	1.11	1.33
1	AA	1993	U	N1-C2	11.37	1.48	1.38
1	AA	2491	U	N1-C2	10.60	1.48	1.38
1	AA	607	U	C5-C6	-10.59	1.24	1.34
1	AA	1202	C	O3'-P	-9.79	1.49	1.61
34	BA	1064	G	C5-C6	-9.65	1.32	1.42
34	BA	530	G	N9-C4	-9.60	1.30	1.38
1	AA	2499	C	O3'-P	9.41	1.72	1.61
1	AA	2755	C	O3'-P	8.91	1.71	1.61
1	AA	607	U	C4-O4	-8.66	1.16	1.23
1	AA	2460	U	N1-C2	8.57	1.46	1.38
1	AA	1956	U	N1-C2	8.39	1.46	1.38
1	AA	2035	G	N9-C4	7.93	1.44	1.38
34	BA	1064	G	C2-N3	7.84	1.39	1.32
1	AA	2447	G	O3'-P	-7.82	1.51	1.61
9	AK	42	TRP	CB-CG	7.79	1.64	1.50
1	AA	1	G	OP3-P	-7.76	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	687	C	N1-C2	7.68	1.47	1.40
17	AS	81	TYR	CB-CG	7.59	1.63	1.51
1	AA	1204	A	O3'-P	7.51	1.70	1.61
1	AA	775	G	N9-C4	7.44	1.43	1.38
1	AA	607	U	N1-C6	7.42	1.44	1.38
2	AB	-1	A	OP3-P	-7.38	1.52	1.61
34	BA	974	A	C2-N3	7.34	1.40	1.33
34	BA	974	A	C6-N1	7.20	1.40	1.35
1	AA	1763	G	C6-O6	7.00	1.30	1.24
1	AA	607	U	C2-O2	-6.99	1.16	1.22
1	AA	2448	A	C5'-C4'	6.98	1.59	1.51
1	AA	1313	U	N1-C2	6.97	1.44	1.38
1	AA	621	A	N7-C5	-6.78	1.35	1.39
1	AA	1956	U	N3-C4	6.72	1.44	1.38
1	AA	2491	U	C2-N3	6.69	1.42	1.37
1	AA	688	U	N1-C2	6.64	1.44	1.38
1	AA	726	G	N9-C4	6.62	1.43	1.38
34	BA	37	U	C4-O4	-6.56	1.18	1.23
1	AA	640	C	N1-C2	-6.51	1.33	1.40
1	AA	2522	U	N1-C2	6.49	1.44	1.38
34	BA	132	C	N1-C2	-6.42	1.33	1.40
1	AA	1240	U	N3-C4	-6.38	1.32	1.38
1	AA	1785	A	C6-N1	-6.29	1.31	1.35
34	BA	1064	G	N1-C2	6.26	1.42	1.37
1	AA	2460	U	C4-O4	6.21	1.28	1.23
34	BA	397	A	C5-C6	-6.19	1.35	1.41
34	BA	1064	G	C5-C4	-6.18	1.34	1.38
1	AA	1674	G	N9-C4	-6.16	1.33	1.38
1	AA	2588	G	C6-N1	-6.13	1.35	1.39
1	AA	930	U	N1-C2	-6.13	1.33	1.38
1	AA	1775	U	C5-C6	-6.10	1.28	1.34
34	BA	974	A	N9-C4	6.09	1.41	1.37
1	AA	1994	C	C2-N3	-6.02	1.30	1.35
1	AA	1303	G	C5-C6	5.97	1.48	1.42
1	AA	1786	A	N9-C4	5.95	1.41	1.37
52	BW	2	PRO	CA-C	5.91	1.64	1.52
34	BA	579	G	C3'-O3'	5.88	1.50	1.42
1	AA	1993	U	C2-N3	5.88	1.41	1.37
2	AB	16	G	N9-C4	-5.84	1.33	1.38
34	BA	196	A	O3'-P	-5.84	1.54	1.61
1	AA	1626	G	C5'-C4'	5.81	1.58	1.51
1	AA	621	A	C5-C4	5.80	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	2195	C	C3'-O3'	5.79	1.50	1.42
1	AA	2073	C	C2-O2	-5.76	1.19	1.24
2	AB	72	G	N9-C4	5.75	1.42	1.38
1	AA	2460	U	N3-C4	5.73	1.43	1.38
50	BU	21	VAL	CA-CB	-5.70	1.42	1.54
1	AA	1786	A	C2-N3	5.69	1.38	1.33
1	AA	2548	G	C2-N2	-5.67	1.28	1.34
1	AA	2445	G	C6-O6	-5.66	1.19	1.24
34	BA	579	G	O3'-P	5.66	1.68	1.61
34	BA	309	G	N9-C4	-5.62	1.33	1.38
1	AA	1775	U	N1-C6	-5.61	1.32	1.38
34	BA	37	U	C5-C6	-5.61	1.29	1.34
34	BA	697	U	C2-N3	5.57	1.41	1.37
1	AA	717	G	N9-C4	-5.57	1.33	1.38
34	BA	173	U	O3'-P	5.57	1.67	1.61
1	AA	860	U	C5-C6	-5.56	1.29	1.34
1	AA	2491	U	N3-C4	5.55	1.43	1.38
1	AA	2255	G	N1-C2	5.53	1.42	1.37
34	BA	651	C	N1-C2	5.50	1.45	1.40
1	AA	270(V)	G	N9-C4	-5.49	1.33	1.38
1	AA	775	G	C2-N3	5.48	1.37	1.32
1	AA	2063	C	N1-C2	5.46	1.45	1.40
1	AA	1468	C	N1-C2	-5.45	1.34	1.40
1	AA	2489	G	C6-O6	-5.45	1.19	1.24
1	AA	916	G	N9-C4	5.44	1.42	1.38
34	BA	697	U	N3-C4	5.44	1.43	1.38
1	AA	2460	U	C2-N3	5.43	1.41	1.37
1	AA	2852	G	N1-C2	-5.42	1.33	1.37
1	AA	2358	G	N9-C4	-5.39	1.33	1.38
1	AA	1524	G	C2-N3	-5.38	1.28	1.32
1	AA	1426	G	N9-C4	-5.37	1.33	1.38
1	AA	1938	A	O3'-P	5.36	1.67	1.61
1	AA	1359	A	C5-C6	-5.35	1.36	1.41
1	AA	2604	U	N3-C4	-5.35	1.33	1.38
1	AA	1994	C	C5-C6	-5.35	1.30	1.34
1	AA	2620	C	C2-O2	-5.33	1.19	1.24
4	AD	54	ARG	CG-CD	5.33	1.65	1.51
1	AA	1778	U	N1-C2	5.32	1.43	1.38
10	AL	105	GLU	CB-CG	5.31	1.62	1.52
1	AA	2334	G	N9-C4	5.29	1.42	1.38
1	AA	860	U	N1-C6	-5.25	1.33	1.38
1	AA	1372	U	C5-C6	-5.25	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	592	G	N9-C4	5.23	1.42	1.38
1	AA	1524	G	N9-C4	-5.23	1.33	1.38
1	AA	950	G	N9-C4	-5.21	1.33	1.38
1	AA	1950	G	N1-C2	-5.21	1.33	1.37
1	AA	1778	U	C4-O4	-5.20	1.19	1.23
1	AA	2548	G	C6-N1	-5.18	1.35	1.39
1	AA	1956	U	C2-N3	5.18	1.41	1.37
2	AB	8	U	N1-C2	-5.17	1.33	1.38
1	AA	1785	A	C6-N6	-5.17	1.29	1.33
1	AA	978	G	C2-N3	-5.17	1.28	1.32
1	AA	1776	G	C6-O6	-5.17	1.19	1.24
1	AA	985	C	C2-O2	-5.16	1.19	1.24
27	Ac	43	CYS	CB-SG	-5.16	1.73	1.81
1	AA	2604	U	N1-C2	-5.16	1.33	1.38
1	AA	1951	U	N1-C2	5.14	1.43	1.38
34	BA	697	U	N1-C2	5.14	1.43	1.38
1	AA	2560	C	C2-O2	-5.13	1.19	1.24
1	AA	2462	U	C4-O4	-5.12	1.19	1.23
1	AA	2491	U	O4'-C1'	5.12	1.48	1.41
37	BH	12	CYS	CA-CB	5.12	1.65	1.53
34	BA	114	U	N3-C4	-5.11	1.33	1.38
1	AA	2459	A	N9-C4	5.11	1.41	1.37
1	AA	1742	C	N1-C2	-5.10	1.35	1.40
1	AA	1628	G	N9-C4	-5.07	1.33	1.38
1	AA	1778	U	C2-N3	5.07	1.41	1.37
1	AA	2593	U	N1-C2	-5.05	1.34	1.38
25	Aa	48	ARG	CG-CD	5.05	1.64	1.51
1	AA	1516	U	N1-C2	-5.03	1.34	1.38
1	AA	1524	G	C6-N1	-5.03	1.36	1.39
1	AA	764	A	C5-C6	-5.03	1.36	1.41
34	BA	540	G	C2-N3	-5.03	1.28	1.32
1	AA	2553	G	C2-N2	-5.02	1.29	1.34
4	AD	250	TRP	CB-CG	-5.01	1.41	1.50
1	AA	1994	C	C2-O2	-5.01	1.20	1.24
1	AA	2461	C	C2-N3	-5.01	1.31	1.35

All (688) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	1064	G	N1-C2-N2	-71.66	51.71	116.20
34	BA	1064	G	N3-C2-N2	57.63	160.24	119.90
34	BA	1317	C	P-O3'-C3'	-48.78	61.17	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	1317	C	O3'-P-O5'	30.58	162.11	104.00
1	AA	1060	U	O3'-P-O5'	28.68	158.49	104.00
1	AA	1203	G	P-O3'-C3'	27.68	152.91	119.70
1	AA	2448	A	C5'-C4'-O4'	-27.30	76.34	109.10
34	BA	1064	G	N1-C2-N3	-25.61	108.54	123.90
34	BA	1317	C	OP2-P-O3'	-23.50	53.51	105.20
1	AA	1060	U	OP1-P-O3'	-23.00	54.60	105.20
52	BW	2	PRO	CA-C-N	-19.27	74.82	117.20
52	BW	2	PRO	CA-C-O	-18.94	74.74	120.20
52	BW	2	PRO	O-C-N	16.79	149.56	122.70
31	AI	153	LEU	O-C-N	-15.12	97.50	123.20
34	BA	1064	G	C2-N3-C4	14.67	119.24	111.90
1	AA	1204	A	N9-C1'-C2'	14.59	132.97	114.00
1	AA	1060	U	OP2-P-O3'	-13.66	75.14	105.20
1	AA	607	U	C5-C6-N1	-12.60	116.40	122.70
34	BA	172	A	OP1-P-O3'	12.60	132.92	105.20
1	AA	2384	G	N9-C1'-C2'	12.16	129.81	114.00
31	AI	153	LEU	C-N-CA	12.00	147.50	122.30
34	BA	973	G	O3'-P-O5'	11.52	125.89	104.00
34	BA	1317	C	OP1-P-O3'	-11.50	79.90	105.20
34	BA	1064	G	C6-N1-C2	11.40	131.94	125.10
1	AA	2459	A	N9-C1'-C2'	11.31	128.71	114.00
1	AA	2500	U	N3-C4-O4	11.18	127.22	119.40
34	BA	173	U	P-O3'-C3'	11.03	132.93	119.70
31	AI	153	LEU	CA-C-N	10.79	137.78	116.20
1	AA	2500	U	C5-C4-O4	-10.74	119.45	125.90
1	AA	2446	G	P-O3'-C3'	10.71	132.55	119.70
1	AA	1800	C	N1-C1'-C2'	-10.69	100.11	114.00
1	AA	2490	G	N9-C1'-C2'	10.66	127.86	114.00
15	AQ	66	VAL	N-CA-C	-10.58	82.43	111.00
1	AA	1938	A	N9-C1'-C2'	10.41	127.54	114.00
1	AA	1203	G	O3'-P-O5'	10.04	123.08	104.00
1	AA	607	U	N3-C4-O4	-9.98	112.42	119.40
1	AA	1992	G	N9-C1'-C2'	9.86	126.82	114.00
1	AA	1240	U	P-O3'-C3'	9.86	131.53	119.70
1	AA	2501	C	P-O3'-C3'	-9.83	107.91	119.70
34	BA	88	C	O4'-C1'-N1	9.78	116.02	108.20
34	BA	974	A	N9-C1'-C2'	9.74	126.67	114.00
1	AA	1809	A	O4'-C1'-N9	9.74	115.99	108.20
1	AA	1205	U	O4'-C1'-N1	9.68	115.94	108.20
1	AA	2779	U	N1-C1'-C2'	-9.65	101.39	112.00
1	AA	2460	U	N1-C1'-C2'	9.63	126.53	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2522	U	N1-C1'-C2'	9.63	126.52	114.00
1	AA	2581	G	N9-C1'-C2'	9.61	126.50	114.00
1	AA	1625	C	N1-C1'-C2'	9.47	126.31	114.00
34	BA	727	G	N9-C1'-C2'	-9.45	101.61	112.00
1	AA	2032	G	N9-C1'-C2'	9.45	126.28	114.00
1	AA	801	G	N9-C1'-C2'	9.44	126.27	114.00
34	BA	37	U	C5-C4-O4	-9.42	120.25	125.90
1	AA	2755	C	OP1-P-O3'	-9.38	84.57	105.20
34	BA	793	U	N1-C1'-C2'	9.37	126.18	114.00
15	AQ	29	ARG	N-CA-C	-9.35	85.76	111.00
27	Ac	24	GLU	N-CA-C	9.32	136.18	111.00
1	AA	138	G	N9-C1'-C2'	-9.30	101.77	112.00
1	AA	974(A)	C	N1-C1'-C2'	9.29	126.07	114.00
1	AA	776	G	N9-C1'-C2'	9.27	126.06	114.00
34	BA	1528	U	N1-C1'-C2'	9.22	125.98	114.00
36	BG	48	TYR	N-CA-C	-9.21	86.12	111.00
2	AB	119	A	N9-C1'-C2'	-9.12	101.97	112.00
1	AA	1363	C	N1-C1'-C2'	-9.09	102.00	112.00
1	AA	2756	U	P-O3'-C3'	9.04	130.55	119.70
1	AA	2459	A	C4-N9-C1'	9.00	142.49	126.30
1	AA	978	G	O4'-C1'-N9	8.96	115.37	108.20
1	AA	199	A	N9-C1'-C2'	8.95	125.64	114.00
1	AA	607	U	N3-C2-O2	-8.88	115.98	122.20
1	AA	280	C	N1-C1'-C2'	8.87	125.53	114.00
34	BA	397	A	C4-N9-C1'	8.86	142.25	126.30
1	AA	1951	U	N1-C1'-C2'	8.84	125.49	114.00
34	BA	1133	G	N9-C1'-C2'	-8.76	102.37	112.00
1	AA	2756	U	N1-C1'-C2'	8.69	125.30	114.00
1	AA	1313	U	N1-C1'-C2'	8.65	125.25	114.00
1	AA	1786	A	C5-C6-N6	-8.65	116.78	123.70
34	BA	397	A	C8-N9-C1'	-8.65	112.12	127.70
1	AA	1939	U	O5'-P-OP1	-8.65	97.92	105.70
1	AA	2459	A	C8-N9-C1'	-8.56	112.30	127.70
1	AA	1240	U	O3'-P-O5'	8.47	120.09	104.00
27	Ac	39	TYR	N-CA-C	8.45	133.82	111.00
1	AA	621	A	N9-C1'-C2'	-8.45	102.71	112.00
1	AA	2755	C	OP2-P-O3'	8.45	123.78	105.20
1	AA	2501	C	O3'-P-O5'	8.43	120.01	104.00
10	AL	74	GLY	N-CA-C	-8.38	92.15	113.10
34	BA	974	A	O3'-P-O5'	8.36	119.89	104.00
34	BA	451	A	N9-C1'-C2'	8.36	124.86	114.00
1	AA	1970	A	O4'-C1'-N9	8.27	114.81	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	1489	U	O4'-C1'-N1	8.21	114.77	108.20
4	AD	63	ARG	N-CA-C	8.18	133.09	111.00
1	AA	1455	G	N9-C1'-C2'	-8.18	103.01	112.00
34	BA	530	G	C4-N9-C1'	-8.09	115.98	126.50
1	AA	1498	C	N1-C1'-C2'	8.07	124.50	114.00
1	AA	775	G	N9-C1'-C2'	8.02	124.43	114.00
1	AA	730	C	N1-C1'-C2'	7.97	124.37	114.00
1	AA	2051	A	N9-C1'-C2'	7.96	124.35	114.00
1	AA	2491	U	C2'-C3'-O3'	7.89	126.86	109.50
1	AA	2491	U	C5-C4-O4	-7.83	121.20	125.90
1	AA	2491	U	O4'-C4'-C3'	-7.83	96.17	104.00
34	BA	792	A	N9-C1'-C2'	7.81	124.16	114.00
1	AA	1778	U	C5-C4-O4	-7.79	121.22	125.90
34	BA	974	A	C5-C6-N6	-7.74	117.51	123.70
34	BA	1167	A	P-O3'-C3'	7.74	128.99	119.70
11	AM	45	LEU	CA-CB-CG	-7.74	97.50	115.30
1	AA	2076	U	N1-C1'-C2'	7.70	124.01	114.00
1	AA	2491	U	O4'-C1'-C2'	-7.67	98.13	105.80
1	AA	196	A	N9-C1'-C2'	7.65	123.94	114.00
10	AL	15	GLY	N-CA-C	-7.64	93.99	113.10
6	AF	79	GLY	N-CA-C	-7.64	93.99	113.10
4	AD	251	GLY	N-CA-C	-7.61	94.07	113.10
1	AA	2035	G	N9-C1'-C2'	7.60	123.88	114.00
1	AA	1667	G	O4'-C1'-N9	7.60	114.28	108.20
34	BA	1054	C	N1-C1'-C2'	-7.53	103.72	112.00
1	AA	1786	A	C6-N1-C2	-7.52	114.09	118.60
7	AG	95	ARG	N-CA-C	7.50	131.25	111.00
1	AA	1189	A	N9-C1'-C2'	-7.49	103.77	112.00
26	Ab	36	CYS	CA-CB-SG	7.47	127.45	114.00
1	AA	2587	A	N9-C1'-C2'	7.42	123.65	114.00
1	AA	607	U	C5-C4-O4	-7.41	121.45	125.90
34	BA	974	A	C6-N1-C2	-7.38	114.17	118.60
34	BA	457	C	N1-C1'-C2'	-7.36	103.91	112.00
1	AA	1203	G	OP2-P-O3'	-7.35	89.03	105.20
4	AD	49	ILE	N-CA-C	-7.35	91.16	111.00
21	AW	77	ASP	N-CA-C	7.34	130.83	111.00
17	AS	50	PRO	N-CA-C	7.34	131.19	112.10
57	BZ	196	ALA	C-N-CD	-7.32	104.49	120.60
1	AA	2510	C	N1-C1'-C2'	-7.32	103.95	112.00
34	BA	563	A	N9-C1'-C2'	7.31	123.51	114.00
1	AA	1786	A	C4-N9-C1'	7.30	139.45	126.30
1	AA	2422	A	N9-C1'-C2'	7.30	123.50	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	184	C	N1-C1'-C2'	7.28	123.46	114.00
1	AA	1537	C	N1-C1'-C2'	-7.28	103.99	112.00
34	BA	397	A	C5-C6-N6	-7.26	117.89	123.70
4	AD	45	ASN	N-CA-C	-7.25	91.41	111.00
34	BA	790	A	N9-C1'-C2'	-7.23	104.05	112.00
1	AA	1778	U	C2-N3-C4	-7.18	122.69	127.00
53	BX	36	LEU	CA-CB-CG	-7.18	98.79	115.30
27	Ac	26	ASN	N-CA-C	7.16	130.34	111.00
1	AA	265	A	N1-C6-N6	7.16	122.89	118.60
1	AA	2259	G	N9-C1'-C2'	-7.15	104.14	112.00
1	AA	2582	G	O4'-C1'-N9	-7.14	102.49	108.20
1	AA	1604	C	N1-C1'-C2'	7.10	123.23	114.00
1	AA	2491	U	C3'-C2'-C1'	-7.06	95.85	101.50
1	AA	2448	A	O5'-C5'-C4'	-7.06	98.29	111.70
34	BA	367	U	N1-C1'-C2'	7.06	123.18	114.00
1	AA	1372	U	C5-C4-O4	-7.04	121.68	125.90
1	AA	654	A	N9-C1'-C2'	-7.00	104.29	112.00
1	AA	1786	A	C8-N9-C1'	-7.00	115.10	127.70
1	AA	1792	G	N9-C1'-C2'	-6.99	104.31	112.00
1	AA	2602	A	N9-C1'-C2'	6.99	123.09	114.00
34	BA	530	G	C5'-C4'-O4'	-6.99	100.72	109.10
1	AA	282	A	N9-C1'-C2'	-6.98	104.33	112.00
1	AA	1205	U	C5'-C4'-O4'	6.97	117.47	109.10
4	AD	16	MET	N-CA-C	-6.97	92.19	111.00
1	AA	1205	U	C1'-O4'-C4'	-6.95	104.34	109.90
1	AA	1699	G	N9-C1'-C2'	6.95	123.04	114.00
9	AK	36	GLY	N-CA-C	-6.94	95.74	113.10
1	AA	620	G	N9-C1'-C2'	6.93	123.01	114.00
1	AA	554	U	N1-C1'-C2'	6.92	123.00	114.00
1	AA	1971	A	N9-C1'-C2'	-6.92	104.39	112.00
1	AA	1359	A	N9-C1'-C2'	-6.91	104.40	112.00
1	AA	1694	C	N1-C1'-C2'	6.91	122.98	114.00
53	BX	24	LEU	CA-CB-CG	6.90	131.18	115.30
1	AA	1240	U	OP2-P-O3'	-6.89	90.04	105.20
1	AA	2346	A	O4'-C1'-N9	6.89	113.71	108.20
17	AS	63	GLY	N-CA-C	-6.89	95.88	113.10
1	AA	911	A	N9-C1'-C2'	6.88	122.95	114.00
17	AS	94	LEU	N-CA-C	-6.87	92.45	111.00
5	AE	6	GLY	N-CA-C	-6.87	95.92	113.10
1	AA	2596	U	N1-C1'-C2'	-6.87	104.45	112.00
1	AA	527	C	N1-C1'-C2'	6.85	122.91	114.00
26	Ab	13	LYS	N-CA-C	-6.85	92.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	1402	C	N1-C1'-C2'	-6.84	104.48	112.00
1	AA	2459	A	C6-N1-C2	-6.83	114.50	118.60
1	AA	607	U	N1-C2-O2	6.83	127.58	122.80
34	BA	1393	U	N1-C1'-C2'	-6.82	104.50	112.00
1	AA	607	U	N3-C4-C5	6.80	118.68	114.60
1	AA	2501	C	OP2-P-O3'	-6.79	90.26	105.20
34	BA	197	A	P-O3'-C3'	-6.79	111.56	119.70
1	AA	865	C	N1-C1'-C2'	6.76	122.79	114.00
1	AA	387	U	N1-C1'-C2'	6.75	122.78	114.00
34	BA	530	G	C8-N9-C1'	6.74	135.76	127.00
34	BA	885	G	N9-C1'-C2'	-6.73	104.60	112.00
1	AA	534	U	O4'-C1'-N1	6.71	113.57	108.20
1	AA	2447	G	N9-C1'-C2'	6.71	122.72	114.00
1	AA	762	U	N1-C1'-C2'	6.70	122.71	114.00
1	AA	615	G	N9-C1'-C2'	6.68	122.69	114.00
34	BA	1123	A	N9-C1'-C2'	6.67	122.67	114.00
34	BA	397	A	O4'-C1'-N9	-6.66	102.87	108.20
34	BA	813	U	N1-C1'-C2'	6.66	122.66	114.00
1	AA	1775	U	C5-C4-O4	-6.66	121.90	125.90
1	AA	2073	C	O4'-C1'-N1	-6.66	102.87	108.20
1	AA	2498	C	C5'-C4'-C3'	-6.65	105.37	116.00
25	Aa	32	TYR	N-CA-C	6.64	128.93	111.00
1	AA	1635	G	C5'-C4'-C3'	-6.64	105.38	116.00
34	BA	1279	A	N9-C1'-C2'	6.63	122.62	114.00
14	AP	63	THR	N-CA-C	-6.63	93.09	111.00
34	BA	47	C	N1-C1'-C2'	6.63	122.62	114.00
34	BA	531	U	N1-C1'-C2'	6.63	122.62	114.00
34	BA	12	U	O4'-C1'-N1	6.62	113.50	108.20
1	AA	1938	A	C4-N9-C1'	6.62	138.21	126.30
1	AA	1626	G	C5'-C4'-O4'	6.60	117.02	109.10
1	AA	1444(A)	A	N9-C1'-C2'	6.60	122.58	114.00
21	AW	52	SER	N-CA-C	-6.60	93.18	111.00
29	Ae	6	THR	N-CA-C	-6.59	93.20	111.00
11	AM	30	THR	N-CA-C	6.59	128.78	111.00
34	BA	397	A	N9-C1'-C2'	6.58	122.56	114.00
1	AA	650	C	O4'-C1'-N1	6.58	113.46	108.20
1	AA	1822	G	N9-C1'-C2'	-6.56	104.79	112.00
1	AA	270(G)	C	O4'-C1'-N1	6.56	113.44	108.20
1	AA	1786	A	N1-C6-N6	6.55	122.53	118.60
1	AA	1247	A	N9-C1'-C2'	6.55	122.52	114.00
34	BA	644	G	N9-C1'-C2'	-6.55	104.79	112.00
1	AA	1667	G	C5'-C4'-C3'	6.55	126.48	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AD	250	TRP	N-CA-C	6.55	128.68	111.00
1	AA	1143	A	N9-C1'-C2'	6.54	122.50	114.00
2	AB	118	G	N9-C1'-C2'	-6.54	104.81	112.00
1	AA	431	U	N1-C1'-C2'	-6.54	104.81	112.00
1	AA	703	U	O4'-C1'-N1	6.52	113.42	108.20
1	AA	2447	G	OP2-P-O3'	6.52	119.55	105.20
1	AA	2336	A	N9-C1'-C2'	6.52	122.48	114.00
1	AA	1955	U	N1-C1'-C2'	6.52	122.47	114.00
34	BA	974	A	N1-C6-N6	6.51	122.51	118.60
4	AD	215	LEU	CA-CB-CG	-6.50	100.36	115.30
34	BA	172	A	O3'-P-O5'	-6.49	91.67	104.00
1	AA	2320	A	N9-C1'-C2'	6.48	122.43	114.00
1	AA	1815	A	N9-C1'-C2'	6.46	122.40	114.00
1	AA	2726	U	N1-C1'-C2'	6.45	122.38	114.00
12	AN	82	ARG	N-CA-C	-6.44	93.61	111.00
1	AA	1604	C	O4'-C1'-N1	6.44	113.35	108.20
1	AA	725	G	N9-C1'-C2'	6.43	122.36	114.00
34	BA	1341	U	N1-C1'-C2'	-6.41	104.95	112.00
34	BA	1193	G	N9-C1'-C2'	-6.40	104.96	112.00
1	AA	2196	C	N1-C1'-C2'	6.40	122.32	114.00
34	BA	37	U	N3-C4-O4	-6.40	114.92	119.40
15	AQ	60	THR	N-CA-C	-6.39	93.75	111.00
34	BA	397	A	N1-C6-N6	6.38	122.42	118.60
34	BA	818	G	N9-C1'-C2'	6.37	122.28	114.00
34	BA	172	A	OP2-P-O3'	-6.36	91.21	105.20
7	AG	42	GLY	N-CA-C	6.35	128.97	113.10
1	AA	1367	A	N9-C1'-C2'	-6.33	105.03	112.00
1	AA	265	A	C5-C6-N6	-6.33	118.64	123.70
1	AA	2522	U	C2-N1-C1'	6.33	125.29	117.70
1	AA	828	U	N1-C1'-C2'	6.32	122.21	114.00
34	BA	1100	C	N1-C1'-C2'	6.32	122.21	114.00
27	Ac	37	ARG	N-CA-C	6.31	128.04	111.00
34	BA	974	A	C4-N9-C1'	6.31	137.66	126.30
34	BA	1049	U	C2'-C3'-O3'	6.31	123.80	113.70
17	AS	98	GLU	N-CA-C	6.31	128.03	111.00
34	BA	82	U	N3-C4-O4	-6.31	114.98	119.40
9	AK	51	PHE	N-CA-C	-6.31	93.97	111.00
1	AA	1204	A	C4-N9-C1'	6.30	137.65	126.30
1	AA	607	U	C2-N1-C1'	-6.30	110.14	117.70
1	AA	2448	A	P-O3'-C3'	-6.29	112.16	119.70
8	AH	111	HIS	N-CA-C	6.28	127.96	111.00
1	AA	101	G	N9-C1'-C2'	6.28	122.17	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	BH	19	LEU	N-CA-C	-6.28	94.04	111.00
1	AA	488	G	N9-C1'-C2'	-6.28	105.09	112.00
34	BA	760	G	N9-C1'-C2'	-6.27	105.10	112.00
1	AA	2460	U	C2-N1-C1'	6.27	125.22	117.70
1	AA	265	A	C4-N9-C1'	6.26	137.58	126.30
1	AA	1956	U	C2-N1-C1'	6.26	125.21	117.70
15	AQ	43	GLN	N-CA-C	-6.26	94.11	111.00
4	AD	94	LEU	N-CA-C	-6.25	94.14	111.00
34	BA	1298	C	N1-C1'-C2'	6.25	122.12	114.00
1	AA	1169	G	N9-C1'-C2'	-6.24	105.14	112.00
9	AK	125	GLY	N-CA-C	-6.24	97.50	113.10
11	AM	59	LEU	CA-CB-CG	6.24	129.64	115.30
1	AA	1060	U	P-O3'-C3'	-6.23	112.22	119.70
34	BA	372	C	N1-C1'-C2'	6.23	122.10	114.00
1	AA	745	G	N9-C1'-C2'	6.23	122.09	114.00
12	AN	125	LEU	CA-CB-CG	-6.23	100.98	115.30
1	AA	1559	G	O4'-C1'-N9	-6.22	103.23	108.20
1	AA	1941	C	O4'-C4'-C3'	-6.20	97.80	104.00
1	AA	1950	G	O4'-C1'-N9	6.20	113.16	108.20
1	AA	676	A	N9-C1'-C2'	6.17	122.02	114.00
52	BW	2	PRO	N-CA-C	6.17	128.15	112.10
12	AN	28	ALA	N-CA-C	-6.17	94.34	111.00
34	BA	1054	C	O4'-C4'-C3'	-6.17	97.83	104.00
1	AA	2835	A	N9-C1'-C2'	6.16	122.01	114.00
34	BA	88	C	C1'-O4'-C4'	-6.16	104.97	109.90
29	Ae	35	GLN	N-CA-C	-6.15	94.40	111.00
34	BA	1167	A	OP1-P-O3'	6.15	118.73	105.20
4	AD	272	ALA	N-CA-C	6.14	127.58	111.00
1	AA	2198	A	N9-C1'-C2'	6.14	121.98	114.00
34	BA	528	C	N1-C1'-C2'	-6.14	105.25	112.00
1	AA	739	G	O4'-C1'-N9	6.13	113.10	108.20
34	BA	530	G	N3-C4-N9	-6.12	122.33	126.00
1	AA	741	G	C5'-C4'-C3'	6.12	125.79	116.00
1	AA	562	U	N1-C1'-C2'	6.11	121.95	114.00
34	BA	961	U	C5-C4-O4	-6.11	122.23	125.90
1	AA	67	U	N1-C2-O2	6.11	127.08	122.80
1	AA	494	G	N9-C1'-C2'	-6.10	105.29	112.00
34	BA	974	A	C8-N9-C1'	-6.10	116.72	127.70
5	AE	141	ILE	N-CA-C	6.10	127.46	111.00
1	AA	2447	G	P-O3'-C3'	6.10	127.02	119.70
34	BA	173	U	O3'-P-O5'	-6.09	92.43	104.00
5	AE	5	LEU	N-CA-C	6.09	127.44	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	191(B)	G	N9-C1'-C2'	-6.08	105.31	112.00
1	AA	1418	G	N9-C1'-C2'	-6.08	105.31	112.00
1	AA	1626	G	O4'-C1'-N9	6.08	113.06	108.20
1	AA	1324	G	N9-C1'-C2'	6.08	121.90	114.00
1	AA	1022	G	N9-C1'-C2'	6.07	121.89	114.00
38	BI	83	GLU	N-CA-C	-6.07	94.62	111.00
34	BA	319	G	N9-C1'-C2'	-6.05	105.34	112.00
1	AA	1786	A	C4-C5-C6	6.05	120.02	117.00
1	AA	1941	C	O4'-C1'-N1	6.04	113.04	108.20
1	AA	1161	C	N1-C1'-C2'	-6.04	105.35	112.00
1	AA	621	A	C5-C6-N1	-6.04	114.68	117.70
34	BA	1481	U	O4'-C1'-N1	6.04	113.03	108.20
34	BA	853	G	O4'-C1'-N9	6.03	113.02	108.20
1	AA	2478	A	N9-C1'-C2'	-6.03	105.37	112.00
21	AW	147	GLY	N-CA-C	-6.02	98.06	113.10
1	AA	1938	A	C8-N9-C1'	-6.01	116.87	127.70
1	AA	787	U	C5'-C4'-O4'	6.01	116.31	109.10
1	AA	2092	U	N1-C1'-C2'	6.01	121.81	114.00
1	AA	1809	A	C1'-O4'-C4'	-6.00	105.10	109.90
34	BA	973	G	OP1-P-O3'	-6.00	92.00	105.20
1	AA	1626	G	N9-C1'-C2'	6.00	121.80	114.00
1	AA	1746	G	N9-C1'-C2'	-6.00	105.41	112.00
1	AA	1936	A	N9-C1'-C2'	6.00	121.79	114.00
1	AA	265	A	C8-N9-C1'	-5.98	116.93	127.70
5	AE	49	LEU	CA-CB-CG	5.98	129.06	115.30
34	BA	397	A	C5'-C4'-C3'	-5.98	106.43	116.00
1	AA	746	A	N9-C1'-C2'	-5.98	105.43	112.00
1	AA	1602	U	N1-C1'-C2'	-5.97	105.43	112.00
1	AA	637	A	N9-C1'-C2'	5.95	121.74	114.00
1	AA	2597	G	N9-C1'-C2'	5.95	121.74	114.00
1	AA	2471	C	N1-C1'-C2'	-5.95	105.46	112.00
1	AA	607	U	C6-N1-C1'	5.94	129.52	121.20
1	AA	1310	G	C5'-C4'-O4'	5.94	116.23	109.10
1	AA	730	C	C5'-C4'-O4'	5.94	116.22	109.10
1	AA	2431	U	O4'-C1'-N1	5.93	112.95	108.20
31	AI	145	PRO	N-CA-CB	5.93	110.42	103.30
35	BF	98	LEU	CA-CB-CG	5.93	128.94	115.30
1	AA	1533	C	N1-C1'-C2'	-5.92	105.49	112.00
1	AA	49	A	N9-C1'-C2'	-5.92	105.49	112.00
1	AA	791	C	O4'-C1'-N1	5.92	112.94	108.20
34	BA	402	G	N9-C1'-C2'	-5.92	105.49	112.00
1	AA	1947	C	C5'-C4'-C3'	-5.92	106.54	116.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	301	G	N9-C1'-C2'	-5.91	105.50	112.00
1	AA	2821	A	N9-C1'-C2'	-5.90	105.51	112.00
34	BA	484	G	C2'-C3'-O3'	5.89	123.13	113.70
1	AA	1128	A	C5'-C4'-C3'	5.89	125.43	116.00
1	AA	1791	A	N9-C1'-C2'	5.89	121.65	114.00
5	AE	146	THR	N-CA-C	-5.88	95.13	111.00
35	BF	118	LEU	CA-CB-CG	5.87	128.80	115.30
1	AA	1379	A	N9-C1'-C2'	5.87	121.63	114.00
1	AA	427	U	C5-C4-O4	-5.87	122.38	125.90
1	AA	2681	C	N1-C1'-C2'	5.86	121.62	114.00
5	AE	195	LEU	N-CA-C	5.86	126.82	111.00
1	AA	1786	A	C6-C5-N7	-5.86	128.20	132.30
1	AA	2781	A	N9-C1'-C2'	-5.86	105.56	112.00
2	AB	50	G	N9-C1'-C2'	-5.85	105.57	112.00
5	AE	158	GLY	N-CA-C	5.84	127.69	113.10
36	BG	188	LEU	CA-CB-CG	5.84	128.73	115.30
43	BN	8	LEU	CA-CB-CG	5.84	128.73	115.30
1	AA	2614	A	N9-C1'-C2'	5.83	121.58	114.00
41	BL	134	ILE	CB-CA-C	-5.83	99.94	111.60
1	AA	1625	C	C2-N1-C1'	5.83	125.21	118.80
1	AA	196	A	O4'-C1'-N9	5.82	112.85	108.20
1	AA	2255	G	C5'-C4'-O4'	5.82	116.08	109.10
6	AF	60	SER	N-CA-C	-5.82	95.30	111.00
34	BA	590	C	N1-C1'-C2'	-5.82	105.60	112.00
34	BA	1294	G	N9-C1'-C2'	-5.81	105.61	112.00
14	AP	65	VAL	N-CA-C	-5.81	95.31	111.00
9	AK	77	GLY	N-CA-C	-5.81	98.58	113.10
5	AE	25	VAL	CB-CA-C	-5.81	100.37	111.40
1	AA	650	C	N1-C1'-C2'	5.80	121.55	114.00
1	AA	2613	U	N1-C1'-C2'	5.80	121.54	114.00
34	BA	80	G	N9-C1'-C2'	5.79	121.53	114.00
10	AL	4	PRO	N-CA-C	-5.79	97.03	112.10
34	BA	872	A	O4'-C1'-N9	5.79	112.83	108.20
34	BA	1029	G	N9-C1'-C2'	-5.78	105.64	112.00
1	AA	1530	G	C5-C6-O6	5.78	132.06	128.60
34	BA	397	A	C6-N1-C2	-5.77	115.14	118.60
21	AW	144	LEU	CA-CB-CG	5.76	128.56	115.30
24	AZ	27	GLY	N-CA-C	-5.76	98.69	113.10
1	AA	1313	U	C2-N1-C1'	5.75	124.61	117.70
1	AA	1440	G	N9-C1'-C2'	-5.75	105.68	112.00
21	AW	39	VAL	N-CA-C	5.73	126.48	111.00
29	Ae	49	VAL	CB-CA-C	-5.73	100.51	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2491	U	C4'-C3'-O3'	5.73	124.46	113.00
1	AA	2746	U	N1-C1'-C2'	-5.73	105.70	112.00
1	AA	446	G	N9-C1'-C2'	5.73	121.44	114.00
1	AA	1359	A	C5-C6-N6	-5.72	119.12	123.70
34	BA	1336	C	O4'-C1'-N1	5.72	112.78	108.20
34	BA	115	G	N9-C1'-C2'	5.72	121.44	114.00
5	AE	195	LEU	CA-CB-CG	-5.72	102.15	115.30
1	AA	662	G	N9-C1'-C2'	-5.70	105.73	112.00
41	BL	100	ILE	N-CA-C	-5.70	95.61	111.00
1	AA	1980	G	N9-C1'-C2'	5.70	121.41	114.00
1	AA	687	C	N1-C2-O2	5.70	122.32	118.90
1	AA	1204	A	C8-N9-C1'	-5.69	117.45	127.70
1	AA	946	G	N9-C1'-C2'	-5.69	105.74	112.00
1	AA	1489	U	C5'-C4'-O4'	5.69	115.93	109.10
34	BA	372	C	C2'-C3'-O3'	5.69	122.80	113.70
1	AA	1786	A	C5-C6-N1	5.67	120.54	117.70
1	AA	687	C	N1-C1'-C2'	5.67	121.37	114.00
34	BA	1139	G	N9-C1'-C2'	5.67	121.37	114.00
38	BI	31	LEU	CA-CB-CG	5.67	128.34	115.30
1	AA	2267	A	O4'-C1'-N9	5.67	112.73	108.20
34	BA	638	G	N9-C1'-C2'	-5.66	105.77	112.00
34	BA	146	G	N9-C1'-C2'	-5.66	105.78	112.00
1	AA	1420	U	N1-C1'-C2'	5.66	121.35	114.00
12	AN	111	GLU	N-CA-C	5.66	126.27	111.00
34	BA	833	U	C2-N3-C4	-5.65	123.61	127.00
12	AN	71	ASP	N-CA-C	5.65	126.25	111.00
1	AA	2517	C	N1-C1'-C2'	5.64	121.34	114.00
15	AQ	57	PHE	N-CA-C	5.64	126.23	111.00
1	AA	740	U	O5'-P-OP1	-5.62	100.64	105.70
1	AA	2761	G	C5'-C4'-C3'	5.62	124.99	116.00
34	BA	1185	G	N9-C1'-C2'	-5.62	105.82	112.00
1	AA	1625	C	O4'-C1'-N1	-5.61	103.71	108.20
1	AA	2256	G	O4'-C1'-N9	-5.61	103.71	108.20
9	AK	49	GLY	N-CA-C	-5.61	99.08	113.10
34	BA	209	U	N1-C1'-C2'	5.61	121.29	114.00
1	AA	2861	G	O4'-C1'-N9	5.60	112.68	108.20
34	BA	13	U	C5'-C4'-O4'	5.60	115.82	109.10
1	AA	1183	G	N9-C1'-C2'	5.60	121.28	114.00
8	AH	165	ALA	N-CA-C	-5.60	95.88	111.00
1	AA	2472	G	C5'-C4'-C3'	-5.59	107.05	116.00
1	AA	1786	A	N3-C4-N9	5.59	131.87	127.40
34	BA	853	G	C5-C6-O6	5.59	131.95	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	1004	A	C2'-C3'-O3'	5.58	122.63	113.70
1	AA	1424	G	N9-C1'-C2'	-5.58	105.86	112.00
6	AF	13	SER	N-CA-C	-5.58	95.95	111.00
14	AP	62	LYS	N-CA-C	5.58	126.06	111.00
34	BA	767	A	N9-C1'-C2'	-5.57	105.87	112.00
5	AE	52	LEU	CA-CB-CG	5.57	128.12	115.30
40	BK	132	GLY	N-CA-C	5.57	127.02	113.10
1	AA	587	C	N1-C1'-C2'	5.57	121.23	114.00
1	AA	602	G	N9-C1'-C2'	5.57	121.23	114.00
1	AA	2111	C	N1-C1'-C2'	5.57	121.24	114.00
1	AA	978	G	C8-N9-C1'	5.56	134.23	127.00
1	AA	2414	G	N9-C1'-C2'	-5.56	105.88	112.00
17	AS	56	SER	N-CA-C	5.55	126.00	111.00
1	AA	444	C	N1-C1'-C2'	-5.55	105.89	112.00
1	AA	2458	G	N9-C1'-C2'	5.55	121.21	114.00
17	AS	49	THR	C-N-CD	-5.55	108.40	120.60
1	AA	791	C	N1-C1'-C2'	5.54	121.21	114.00
1	AA	2491	U	C2-N3-C4	-5.54	123.67	127.00
34	BA	833	U	N1-C2-O2	-5.54	118.92	122.80
1	AA	1191	G	N9-C1'-C2'	-5.54	105.91	112.00
1	AA	1667	G	C1'-O4'-C4'	-5.54	105.47	109.90
6	AF	47	GLY	N-CA-C	5.54	126.94	113.10
25	Aa	5	ILE	CB-CA-C	-5.53	100.53	111.60
29	Ae	17	THR	N-CA-C	-5.53	96.06	111.00
1	AA	606	U	C5-C4-O4	-5.53	122.58	125.90
27	Ac	22	ALA	N-CA-C	5.53	125.93	111.00
34	BA	242	C	N1-C1'-C2'	-5.53	105.92	112.00
51	BV	52	PRO	N-CA-C	5.53	126.47	112.10
34	BA	1028(A)	C	N1-C1'-C2'	-5.52	105.92	112.00
1	AA	631	A	N9-C1'-C2'	-5.52	105.93	112.00
1	AA	1253	A	N9-C1'-C2'	5.52	121.18	114.00
34	BA	723	U	N1-C1'-C2'	5.52	121.18	114.00
1	AA	834	C	N1-C1'-C2'	-5.51	105.94	112.00
1	AA	1559	G	N9-C1'-C2'	-5.51	105.94	112.00
34	BA	156	G	N9-C1'-C2'	-5.51	105.94	112.00
15	AQ	72	VAL	N-CA-C	-5.51	96.13	111.00
34	BA	1124	G	N9-C1'-C2'	5.51	121.16	114.00
10	AL	6	THR	N-CA-C	5.50	125.85	111.00
1	AA	141	A	N9-C1'-C2'	-5.50	105.95	112.00
1	AA	805	G	N9-C1'-C2'	-5.50	105.95	112.00
1	AA	1800	C	O4'-C4'-C3'	-5.50	98.50	104.00
1	AA	1785	A	N9-C1'-C2'	5.50	121.14	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	AD	44	ASN	N-CA-C	-5.49	96.17	111.00
1	AA	2491	U	C2-N1-C1'	5.48	124.28	117.70
45	BP	119	LYS	N-CA-C	-5.48	96.21	111.00
25	Aa	52	THR	N-CA-C	5.47	125.78	111.00
35	BF	61	LEU	CA-CB-CG	5.47	127.89	115.30
34	BA	1084	G	N9-C1'-C2'	5.47	121.11	114.00
37	BH	9	CYS	CA-CB-SG	5.46	123.83	114.00
1	AA	2158	A	N9-C1'-C2'	5.46	121.10	114.00
1	AA	2285	C	N1-C1'-C2'	-5.46	105.99	112.00
14	AP	23	ARG	N-CA-C	5.46	125.74	111.00
34	BA	243	A	N9-C1'-C2'	5.46	121.10	114.00
1	AA	763	G	O4'-C4'-C3'	-5.45	98.55	104.00
34	BA	106	C	N1-C1'-C2'	-5.45	106.01	112.00
1	AA	1970	A	C5'-C4'-O4'	5.44	115.63	109.10
20	AV	52	SER	N-CA-C	-5.44	96.32	111.00
1	AA	192	C	O4'-C1'-N1	5.43	112.55	108.20
13	AO	38	VAL	C-N-CD	5.43	139.81	128.40
34	BA	682	G	N9-C1'-C2'	-5.43	106.03	112.00
41	BL	80	ILE	N-CA-C	-5.43	96.34	111.00
1	AA	2040	C	N1-C1'-C2'	-5.42	106.03	112.00
1	AA	2867	G	N9-C1'-C2'	5.42	121.04	114.00
25	Aa	19	GLY	N-CA-C	-5.41	99.57	113.10
1	AA	2885	C	N1-C1'-C2'	-5.41	106.05	112.00
1	AA	1600	C	N1-C1'-C2'	-5.40	106.06	112.00
11	AM	88	LEU	N-CA-C	5.40	125.58	111.00
1	AA	1544	C	N1-C1'-C2'	5.39	121.01	114.00
1	AA	1416	G	N9-C1'-C2'	5.39	121.01	114.00
25	Aa	13	ARG	N-CA-C	5.39	125.56	111.00
1	AA	1956	U	C5-C4-O4	-5.39	122.67	125.90
34	BA	753	A	N9-C1'-C2'	5.39	121.01	114.00
8	AH	111	HIS	C-N-CD	5.39	139.71	128.40
1	AA	1142	U	O4'-C1'-N1	5.38	112.50	108.20
34	BA	13	U	O4'-C1'-N1	-5.38	103.90	108.20
34	BA	88	C	C2-N1-C1'	-5.37	112.89	118.80
1	AA	2399	G	N9-C1'-C2'	-5.36	106.11	112.00
40	BK	76	ARG	N-CA-C	-5.36	96.53	111.00
1	AA	2705	A	N9-C1'-C2'	-5.35	106.11	112.00
1	AA	688	U	C2-N3-C4	-5.35	123.79	127.00
1	AA	1186	G	O4'-C1'-N9	-5.35	103.92	108.20
1	AA	1359	A	N1-C6-N6	5.34	121.81	118.60
15	AQ	45	PHE	N-CA-C	-5.34	96.58	111.00
1	AA	2777	G	O4'-C1'-N9	-5.33	103.93	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	AS	66	ARG	N-CA-C	5.33	125.40	111.00
5	AE	43	GLY	N-CA-C	-5.33	99.77	113.10
10	AL	68	GLU	N-CA-C	-5.33	96.61	111.00
1	AA	987	G	N9-C1'-C2'	-5.33	106.14	112.00
1	AA	15	G	N9-C1'-C2'	-5.33	106.14	112.00
1	AA	1968	G	N9-C1'-C2'	-5.33	106.14	112.00
1	AA	366	C	N1-C1'-C2'	-5.32	106.15	112.00
50	BU	61	GLU	N-CA-C	-5.32	96.63	111.00
1	AA	400	G	N9-C1'-C2'	-5.32	106.15	112.00
1	AA	2500	U	P-O3'-C3'	5.32	126.08	119.70
1	AA	532	A	N9-C1'-C2'	5.31	120.91	114.00
34	BA	529	G	N9-C1'-C2'	-5.31	106.16	112.00
34	BA	1011	G	N9-C1'-C2'	-5.31	106.16	112.00
34	BA	88	C	N1-C1'-C2'	5.31	120.90	114.00
4	AD	70	TRP	N-CA-C	-5.31	96.67	111.00
1	AA	1534	G	N9-C1'-C2'	-5.30	106.17	112.00
1	AA	2787	C	O4'-C1'-N1	5.30	112.44	108.20
1	AA	774	A	N9-C1'-C2'	5.30	120.89	114.00
1	AA	1020	A	N9-C1'-C2'	-5.30	106.17	112.00
24	AZ	38	GLU	N-CA-C	-5.29	96.70	111.00
1	AA	1762	A	N9-C1'-C2'	-5.29	106.18	112.00
1	AA	698	C	N1-C1'-C2'	5.28	120.87	114.00
34	BA	815	A	C1'-O4'-C4'	-5.28	105.67	109.90
34	BA	575	G	N9-C1'-C2'	5.27	120.86	114.00
36	BG	52	LEU	CA-CB-CG	5.27	127.43	115.30
1	AA	1230	C	N1-C1'-C2'	-5.27	106.20	112.00
10	AL	120	GLU	N-CA-C	5.27	125.22	111.00
1	AA	2358	G	N9-C1'-C2'	-5.27	106.21	112.00
1	AA	1005	C	N1-C1'-C2'	5.26	120.84	114.00
1	AA	1127	A	N9-C1'-C2'	-5.26	106.22	112.00
1	AA	2249	U	N1-C1'-C2'	5.26	120.84	114.00
30	Af	14	CYS	CA-CB-SG	-5.26	104.53	114.00
34	BA	37	U	N1-C1'-C2'	-5.26	106.21	112.00
1	AA	351	G	N9-C1'-C2'	5.25	120.83	114.00
1	AA	1964	G	N9-C1'-C2'	5.25	120.83	114.00
1	AA	2094	G	O4'-C1'-N9	5.25	112.40	108.20
1	AA	2448	A	OP1-P-O3'	5.25	116.75	105.20
9	AK	116	LEU	CA-CB-CG	-5.25	103.23	115.30
12	AN	125	LEU	C-N-CA	-5.24	100.00	122.00
34	BA	226	G	C1'-O4'-C4'	-5.24	105.71	109.90
50	BU	104	LYS	N-CA-C	5.24	125.14	111.00
9	AK	80	GLY	N-CA-C	-5.24	100.01	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	2724	C	O4'-C1'-N1	5.23	112.39	108.20
32	AJ	21	PRO	C-N-CD	5.23	139.39	128.40
49	BT	16	HIS	N-CA-C	-5.23	96.88	111.00
13	AO	69	ASP	N-CA-C	5.23	125.11	111.00
45	BP	59	ARG	N-CA-C	-5.23	96.89	111.00
1	AA	2461	C	N1-C2-O2	5.22	122.03	118.90
10	AL	102	VAL	N-CA-C	5.22	125.09	111.00
20	AV	46	LYS	N-CA-C	5.21	125.08	111.00
1	AA	1993	U	C2-N1-C1'	5.21	123.95	117.70
1	AA	2493	U	N1-C1'-C2'	-5.21	106.27	112.00
10	AL	61	VAL	N-CA-C	5.21	125.06	111.00
1	AA	2243	U	N1-C1'-C2'	5.21	120.77	114.00
1	AA	2491	U	C6-N1-C2	-5.21	117.88	121.00
34	BA	1271	G	N9-C1'-C2'	-5.21	106.27	112.00
25	Aa	43	TYR	CA-CB-CG	5.21	123.29	113.40
1	AA	1635	G	C2'-C3'-O3'	5.20	122.02	113.70
1	AA	1956	U	C6-N1-C1'	-5.20	113.92	121.20
1	AA	463	G	N9-C1'-C2'	-5.19	106.29	112.00
2	AB	90	C	C5'-C4'-O4'	5.19	115.33	109.10
26	Ab	41	PRO	N-CA-C	-5.19	98.61	112.10
1	AA	2431	U	O4'-C4'-C3'	-5.19	98.81	104.00
1	AA	1510	A	N9-C1'-C2'	5.19	120.74	114.00
4	AD	260	ARG	N-CA-C	-5.19	97.00	111.00
1	AA	2464	C	N1-C1'-C2'	-5.18	106.30	112.00
1	AA	2195	C	N1-C1'-C2'	5.18	120.73	114.00
34	BA	5	U	OP1-P-OP2	-5.18	111.83	119.60
8	AH	130	ARG	N-CA-C	-5.17	97.03	111.00
1	AA	1694	C	O4'-C1'-N1	5.17	112.34	108.20
34	BA	1210	C	O4'-C1'-N1	5.17	112.34	108.20
25	Aa	31	ILE	N-CA-C	5.17	124.96	111.00
1	AA	860	U	C5-C4-O4	-5.17	122.80	125.90
29	Ae	51	ALA	N-CA-C	-5.17	97.05	111.00
34	BA	173	U	OP1-P-O3'	5.17	116.56	105.20
7	AG	48	GLU	N-CA-C	-5.16	97.06	111.00
1	AA	2027	G	C5'-C4'-C3'	5.16	124.26	116.00
17	AS	12	TYR	N-CA-C	5.16	124.93	111.00
15	AQ	49	VAL	N-CA-C	-5.15	97.09	111.00
15	AQ	63	VAL	N-CA-C	-5.15	97.09	111.00
1	AA	212	G	N9-C1'-C2'	-5.15	106.34	112.00
12	AN	34	LEU	CA-CB-CG	-5.15	103.47	115.30
34	BA	1148	U	N1-C1'-C2'	5.15	120.69	114.00
34	BA	1310	G	N9-C1'-C2'	-5.14	106.34	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	BA	586	C	N1-C1'-C2'	-5.14	106.35	112.00
22	AX	26	TYR	N-CA-C	5.14	124.87	111.00
1	AA	775	G	C4-N9-C1'	5.14	133.18	126.50
10	AL	22	ILE	N-CA-C	-5.14	97.13	111.00
1	AA	643	A	N9-C1'-C2'	5.13	120.67	114.00
21	AW	179	ASP	N-CA-C	5.13	124.86	111.00
25	Aa	30	GLU	N-CA-C	-5.13	97.16	111.00
5	AE	147	PRO	N-CA-C	-5.12	98.77	112.10
34	BA	307	C	O4'-C1'-N1	-5.12	104.10	108.20
1	AA	1477	A	N9-C1'-C2'	5.12	120.66	114.00
34	BA	423	G	N9-C1'-C2'	5.12	120.66	114.00
10	AL	56	ASP	N-CA-CB	-5.12	101.39	110.60
18	AT	76	VAL	N-CA-C	5.12	124.82	111.00
7	AG	68	PRO	N-CA-C	5.12	125.40	112.10
32	AJ	53	VAL	C-N-CD	5.12	139.14	128.40
40	BK	8	GLU	N-CA-C	5.11	124.81	111.00
1	AA	2510	C	C5'-C4'-O4'	5.11	115.23	109.10
1	AA	930	U	C5'-C4'-O4'	-5.11	102.97	109.10
1	AA	265	A	C4-C5-C6	5.10	119.55	117.00
1	AA	1012	U	O4'-C4'-C3'	-5.10	98.90	104.00
1	AA	1746	G	O4'-C4'-C3'	-5.10	98.90	104.00
32	AJ	12	LEU	C-N-CD	5.10	139.11	128.40
5	AE	65	GLY	N-CA-C	-5.10	100.35	113.10
9	AK	104	LYS	N-CA-C	-5.10	97.23	111.00
1	AA	1706	U	N1-C1'-C2'	5.10	120.63	114.00
35	BF	187	LEU	N-CA-C	-5.10	97.24	111.00
1	AA	647	G	N9-C1'-C2'	5.10	120.62	114.00
2	AB	56	G	C2'-C3'-O3'	5.09	121.85	113.70
1	AA	283	A	O4'-C1'-N9	-5.09	104.13	108.20
1	AA	1956	U	C5'-C4'-C3'	-5.09	107.85	116.00
1	AA	2894	G	N9-C1'-C2'	5.09	120.62	114.00
2	AB	-1	A	OP1-P-OP2	-5.09	111.97	119.60
1	AA	2302	G	N9-C1'-C2'	-5.09	106.41	112.00
17	AS	40	LEU	N-CA-C	-5.09	97.27	111.00
34	BA	906	G	N9-C1'-C2'	-5.09	106.40	112.00
1	AA	1516	U	N3-C4-O4	-5.08	115.84	119.40
1	AA	2061	G	N9-C1'-C2'	5.08	120.60	114.00
1	AA	728	G	N9-C1'-C2'	5.08	120.60	114.00
1	AA	573	G	N9-C1'-C2'	5.08	120.60	114.00
1	AA	1240	U	N3-C4-O4	-5.08	115.85	119.40
47	BR	24	CYS	CA-CB-SG	5.08	123.14	114.00
38	BI	97	GLY	N-CA-C	-5.07	100.42	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	BQ	112	GLY	C-N-CD	5.07	139.05	128.40
57	BZ	132	ARG	C-N-CD	5.07	139.05	128.40
52	BW	58	VAL	C-N-CD	5.07	139.05	128.40
1	AA	1266	G	C5'-C4'-C3'	5.07	124.11	116.00
57	BZ	136	ARG	C-N-CD	5.07	139.05	128.40
1	AA	270(E)	G	O4'-C1'-N9	5.07	112.25	108.20
1	AA	66	C	N1-C1'-C2'	-5.07	106.43	112.00
57	BZ	104	GLY	C-N-CD	5.07	139.04	128.40
37	BH	31	CYS	CA-CB-SG	5.06	123.11	114.00
46	BQ	96	LEU	C-N-CD	5.06	139.03	128.40
32	AJ	71	THR	C-N-CD	5.06	139.03	128.40
34	BA	1230	C	N1-C1'-C2'	-5.06	106.43	112.00
57	BZ	194	VAL	C-N-CD	5.06	139.03	128.40
57	BZ	603	ALA	C-N-CD	5.06	139.03	128.40
12	AN	123	HIS	N-CA-C	-5.06	97.34	111.00
57	BZ	316	SER	C-N-CD	5.06	139.02	128.40
34	BA	13	U	N1-C1'-C2'	5.06	120.57	114.00
57	BZ	398	GLU	C-N-CD	5.06	139.02	128.40
57	BZ	443	ILE	C-N-CD	5.06	139.02	128.40
57	BZ	558	VAL	C-N-CD	5.06	139.02	128.40
32	AJ	90	LYS	C-N-CD	5.05	139.02	128.40
57	BZ	184	THR	C-N-CD	5.05	139.01	128.40
57	BZ	203	GLY	C-N-CD	5.05	139.01	128.40
21	AW	61	LEU	C-N-CD	-5.05	109.48	120.60
1	AA	2448	A	C5'-C4'-C3'	-5.05	107.92	116.00
45	BP	27	LEU	CA-CB-CG	5.05	126.91	115.30
57	BZ	304	GLU	C-N-CD	5.05	139.00	128.40
34	BA	491	G	N9-C1'-C2'	-5.05	106.45	112.00
11	AM	42	SER	N-CA-C	5.05	124.63	111.00
34	BA	741	G	N9-C1'-C2'	-5.05	106.45	112.00
1	AA	150	C	N1-C1'-C2'	5.04	120.56	114.00
1	AA	2425	A	O4'-C1'-N9	5.04	112.23	108.20
2	AB	74	U	N1-C1'-C2'	-5.04	106.45	112.00
32	AJ	18	THR	C-N-CD	5.04	138.99	128.40
34	BA	166	G	N9-C1'-C2'	-5.04	106.45	112.00
57	BZ	430	ASN	C-N-CD	5.04	138.99	128.40
1	AA	1429	G	N9-C1'-C2'	5.04	120.55	114.00
32	AJ	20	ALA	C-N-CD	5.04	138.99	128.40
36	BG	197	GLY	N-CA-C	5.04	125.69	113.10
57	BZ	75	THR	C-N-CD	5.04	138.98	128.40
34	BA	1205	U	O4'-C1'-N1	5.03	112.22	108.20
57	BZ	384	ARG	C-N-CD	5.03	138.96	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AA	95	G	N9-C1'-C2'	-5.03	106.47	112.00
32	AJ	112	MET	C-N-CD	5.03	138.96	128.40
1	AA	2447	G	O5'-P-OP1	-5.03	101.18	105.70
1	AA	125	G	N9-C1'-C2'	5.02	120.53	114.00
34	BA	226	G	N9-C1'-C2'	-5.02	106.48	112.00
34	BA	13	U	C2-N1-C1'	5.02	123.72	117.70
1	AA	1199	U	N1-C1'-C2'	5.01	120.52	114.00
1	AA	1778	U	C2'-C3'-O3'	5.01	121.72	113.70
1	AA	1559	G	C3'-C2'-C1'	-5.01	97.49	101.50
1	AA	1779	U	C6-N1-C2	-5.00	118.00	121.00
34	BA	1048	G	N9-C1'-C2'	-5.00	106.50	112.00
4	AD	80	ALA	N-CA-C	-5.00	97.49	111.00
1	AA	962	G	N9-C1'-C2'	5.00	120.50	114.00

There are no chirality outliers.

All (634) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	1000	A	Sidechain
1	AA	1012	U	Sidechain
1	AA	1018	C	Sidechain
1	AA	1020	A	Sidechain
1	AA	1022	G	Sidechain
1	AA	1024	G	Sidechain
1	AA	1026	U	Sidechain
1	AA	1092	C	Sidechain
1	AA	1099	G	Sidechain
1	AA	1101	U	Sidechain
1	AA	1102	C	Sidechain
1	AA	1104	C	Sidechain
1	AA	1113	U	Sidechain
1	AA	1116	C	Sidechain
1	AA	1133	U	Sidechain
1	AA	114	U	Sidechain
1	AA	1141	U	Sidechain
1	AA	1142	U	Sidechain
1	AA	1143	A	Sidechain
1	AA	1154	G	Sidechain
1	AA	1155	A	Sidechain
1	AA	1160	G	Sidechain
1	AA	1179	C	Sidechain
1	AA	1182	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1183	G	Sidechain
1	AA	1194	A	Sidechain
1	AA	1195	G	Sidechain
1	AA	1206	G	Sidechain
1	AA	1238	G	Sidechain
1	AA	1240	U	Sidechain
1	AA	1242	A	Sidechain
1	AA	1247	A	Sidechain
1	AA	1262	A	Sidechain
1	AA	1269	A	Sidechain
1	AA	1273	U	Sidechain
1	AA	1284	A	Sidechain
1	AA	1288	U	Sidechain
1	AA	1297	C	Sidechain
1	AA	1301	A	Sidechain
1	AA	1310	G	Sidechain
1	AA	135	G	Sidechain
1	AA	1357	U	Sidechain
1	AA	1359	A	Sidechain
1	AA	1363	C	Sidechain
1	AA	1367	A	Sidechain
1	AA	1368	G	Sidechain
1	AA	1372	U	Sidechain
1	AA	1379	A	Sidechain
1	AA	138	G	Sidechain
1	AA	1384	A	Sidechain
1	AA	1392	A	Sidechain
1	AA	1393	A	Sidechain
1	AA	1397	U	Sidechain
1	AA	14	A	Sidechain
1	AA	1405	U	Sidechain
1	AA	141(A)	C	Sidechain
1	AA	1416	G	Sidechain
1	AA	1418	G	Sidechain
1	AA	1444(A)	A	Sidechain
1	AA	1450	C	Sidechain
1	AA	1473	G	Sidechain
1	AA	1474	C	Sidechain
1	AA	1477	A	Sidechain
1	AA	1478	G	Sidechain
1	AA	1479	G	Sidechain
1	AA	1489	U	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1497	U	Sidechain
1	AA	1513	C	Sidechain
1	AA	1515	C	Sidechain
1	AA	1516	U	Sidechain
1	AA	1523	U	Sidechain
1	AA	1525	G	Sidechain
1	AA	1527	G	Sidechain
1	AA	1532	C	Sidechain
1	AA	1537	C	Sidechain
1	AA	1539	G	Sidechain
1	AA	1541	U	Sidechain
1	AA	1559	G	Sidechain
1	AA	1564	C	Sidechain
1	AA	1565	C	Sidechain
1	AA	1568	G	Sidechain
1	AA	1574	C	Sidechain
1	AA	1576	U	Sidechain
1	AA	1590	U	Sidechain
1	AA	1597	A	Sidechain
1	AA	1604	C	Sidechain
1	AA	1606	G	Sidechain
1	AA	1609	A	Sidechain
1	AA	1623	G	Sidechain
1	AA	1625	C	Sidechain
1	AA	1648	C	Sidechain
1	AA	1651	G	Sidechain
1	AA	1655	A	Sidechain
1	AA	1657	C	Sidechain
1	AA	1659	U	Sidechain
1	AA	1661	G	Sidechain
1	AA	1667	G	Sidechain
1	AA	1677	A	Sidechain
1	AA	1681	G	Sidechain
1	AA	1684	C	Sidechain
1	AA	1685	C	Sidechain
1	AA	1686	C	Sidechain
1	AA	1687	G	Sidechain
1	AA	1688	U	Sidechain
1	AA	1691	C	Sidechain
1	AA	1693	U	Sidechain
1	AA	1694	C	Sidechain
1	AA	1699	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1704	G	Sidechain
1	AA	1711	C	Sidechain
1	AA	1716	U	Sidechain
1	AA	1718	G	Sidechain
1	AA	1727	U	Sidechain
1	AA	1735	C	Sidechain
1	AA	1741	C	Sidechain
1	AA	1742	C	Sidechain
1	AA	1743	G	Sidechain
1	AA	176	G	Sidechain
1	AA	1766	U	Sidechain
1	AA	1768	U	Sidechain
1	AA	1774	C	Sidechain
1	AA	1775	U	Sidechain
1	AA	1776	G	Sidechain
1	AA	1777	U	Sidechain
1	AA	1778	U	Sidechain
1	AA	1779	U	Sidechain
1	AA	1780	A	Sidechain
1	AA	1783	A	Sidechain
1	AA	1786	A	Sidechain
1	AA	1790	C	Sidechain
1	AA	1791	A	Sidechain
1	AA	1794	U	Sidechain
1	AA	1798	U	Sidechain
1	AA	1800	C	Sidechain
1	AA	1808	U	Sidechain
1	AA	1809	A	Sidechain
1	AA	1810	A	Sidechain
1	AA	1815	A	Sidechain
1	AA	1822	G	Sidechain
1	AA	1831	G	Sidechain
1	AA	1843	C	Sidechain
1	AA	185	U	Sidechain
1	AA	188	G	Sidechain
1	AA	1902	C	Sidechain
1	AA	192	C	Sidechain
1	AA	1940	U	Sidechain
1	AA	1962	C	Sidechain
1	AA	1964	G	Sidechain
1	AA	1965	C	Sidechain
1	AA	1967	C	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	1971	A	Sidechain
1	AA	1981	A	Sidechain
1	AA	1982	C	Sidechain
1	AA	1983	C	Sidechain
1	AA	1985	G	Sidechain
1	AA	1989	G	Sidechain
1	AA	199	A	Sidechain
1	AA	1998	G	Sidechain
1	AA	2017	U	Sidechain
1	AA	2021	C	Sidechain
1	AA	2026	C	Sidechain
1	AA	2033	A	Sidechain
1	AA	2042	A	Sidechain
1	AA	2048	G	Sidechain
1	AA	2049	G	Sidechain
1	AA	2051	A	Sidechain
1	AA	2061	G	Sidechain
1	AA	2068	U	Sidechain
1	AA	2075	U	Sidechain
1	AA	2076	U	Sidechain
1	AA	2089	U	Sidechain
1	AA	2094	G	Sidechain
1	AA	2095	C	Sidechain
1	AA	2096	U	Sidechain
1	AA	2098	U	Sidechain
1	AA	2103	C	Sidechain
1	AA	2119	A	Sidechain
1	AA	212	G	Sidechain
1	AA	2126	A	Sidechain
1	AA	2130	U	Sidechain
1	AA	2138	C	Sidechain
1	AA	2148	G	Sidechain
1	AA	2161	C	Sidechain
1	AA	2185	C	Sidechain
1	AA	2189	U	Sidechain
1	AA	2190	G	Sidechain
1	AA	2193	G	Sidechain
1	AA	2195	C	Sidechain
1	AA	221	A	Sidechain
1	AA	2215	G	Sidechain
1	AA	224	G	Sidechain
1	AA	2246	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2259	G	Sidechain
1	AA	2262	U	Sidechain
1	AA	2263	C	Sidechain
1	AA	2265	U	Sidechain
1	AA	2267	A	Sidechain
1	AA	2274	A	Sidechain
1	AA	2278	A	Sidechain
1	AA	2284	C	Sidechain
1	AA	2287	A	Sidechain
1	AA	2293	C	Sidechain
1	AA	2295	C	Sidechain
1	AA	2296	U	Sidechain
1	AA	2297	C	Sidechain
1	AA	2299	G	Sidechain
1	AA	2314	C	Sidechain
1	AA	2326	C	Sidechain
1	AA	2332	U	Sidechain
1	AA	2336	A	Sidechain
1	AA	2337	G	Sidechain
1	AA	2352	A	Sidechain
1	AA	2364	C	Sidechain
1	AA	237	C	Sidechain
1	AA	2384	G	Sidechain
1	AA	2395	C	Sidechain
1	AA	2399	G	Sidechain
1	AA	2406	U	Sidechain
1	AA	2408	U	Sidechain
1	AA	2413	G	Sidechain
1	AA	2422	A	Sidechain
1	AA	2423	U	Sidechain
1	AA	2425	A	Sidechain
1	AA	2427	C	Sidechain
1	AA	2431	U	Sidechain
1	AA	2432	A	Sidechain
1	AA	2433	A	Sidechain
1	AA	2434	A	Sidechain
1	AA	2435	A	Sidechain
1	AA	2436	G	Sidechain
1	AA	2439	A	Sidechain
1	AA	2444	G	Sidechain
1	AA	2449	U	Sidechain
1	AA	2450	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2458	G	Sidechain
1	AA	2467	C	Sidechain
1	AA	2471	C	Sidechain
1	AA	2480	C	Sidechain
1	AA	2483	C	Sidechain
1	AA	2486	G	Sidechain
1	AA	2490	G	Sidechain
1	AA	2491	U	Sidechain
1	AA	2493	U	Sidechain
1	AA	2498	C	Sidechain
1	AA	25	U	Sidechain
1	AA	2500	U	Sidechain
1	AA	2501	C	Sidechain
1	AA	2504	U	Sidechain
1	AA	2505	G	Sidechain
1	AA	2507	C	Sidechain
1	AA	2508	G	Sidechain
1	AA	251	A	Sidechain
1	AA	2510	C	Sidechain
1	AA	2514	U	Sidechain
1	AA	2515	C	Sidechain
1	AA	2516	G	Sidechain
1	AA	2517	C	Sidechain
1	AA	2519	U	Sidechain
1	AA	2521	C	Sidechain
1	AA	2524	G	Sidechain
1	AA	2527	C	Sidechain
1	AA	2529	G	Sidechain
1	AA	253	C	Sidechain
1	AA	2530	A	Sidechain
1	AA	2537	U	Sidechain
1	AA	2540	C	Sidechain
1	AA	2555	U	Sidechain
1	AA	2560	C	Sidechain
1	AA	2568	C	Sidechain
1	AA	2569	G	Sidechain
1	AA	257	A	Sidechain
1	AA	2579	C	Sidechain
1	AA	2580	U	Sidechain
1	AA	2583	G	Sidechain
1	AA	2590	A	Sidechain
1	AA	2595	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2597	G	Sidechain
1	AA	2601	C	Sidechain
1	AA	2602	A	Sidechain
1	AA	2606	C	Sidechain
1	AA	2607	G	Sidechain
1	AA	2608	G	Sidechain
1	AA	2609	U	Sidechain
1	AA	2613	U	Sidechain
1	AA	2615	U	Sidechain
1	AA	2619	C	Sidechain
1	AA	2623	G	Sidechain
1	AA	2629	A	Sidechain
1	AA	2637	U	Sidechain
1	AA	2642	G	Sidechain
1	AA	2645	G	Sidechain
1	AA	2684	U	Sidechain
1	AA	2687	U	Sidechain
1	AA	2698	U	Sidechain
1	AA	270(C)	C	Sidechain
1	AA	270(D)	C	Sidechain
1	AA	270(G)	C	Sidechain
1	AA	270(Q)	C	Sidechain
1	AA	2706	G	Sidechain
1	AA	2724	C	Sidechain
1	AA	2725	A	Sidechain
1	AA	273(C)	C	Sidechain
1	AA	273(D)	C	Sidechain
1	AA	2737	G	Sidechain
1	AA	2741	A	Sidechain
1	AA	2746	U	Sidechain
1	AA	2763	G	Sidechain
1	AA	2764	A	Sidechain
1	AA	2777	G	Sidechain
1	AA	2781	A	Sidechain
1	AA	2787	C	Sidechain
1	AA	280	C	Sidechain
1	AA	2816	C	Sidechain
1	AA	2817	G	Sidechain
1	AA	2825	C	Sidechain
1	AA	2853	C	Sidechain
1	AA	2867	G	Sidechain
1	AA	2885	C	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	2887	U	Sidechain
1	AA	2891	G	Sidechain
1	AA	2897	U	Sidechain
1	AA	2898	U	Sidechain
1	AA	2901	C	Sidechain
1	AA	296	C	Sidechain
1	AA	3	U	Sidechain
1	AA	31	C	Sidechain
1	AA	32	C	Sidechain
1	AA	322	A	Sidechain
1	AA	337	C	Sidechain
1	AA	350	U	Sidechain
1	AA	351	G	Sidechain
1	AA	353	G	Sidechain
1	AA	358	U	Sidechain
1	AA	360	G	Sidechain
1	AA	362	U	Sidechain
1	AA	366	C	Sidechain
1	AA	380	U	Sidechain
1	AA	383	U	Sidechain
1	AA	386	G	Sidechain
1	AA	417	C	Sidechain
1	AA	427	U	Sidechain
1	AA	433	C	Sidechain
1	AA	445	C	Sidechain
1	AA	446	G	Sidechain
1	AA	448	U	Sidechain
1	AA	459	U	Sidechain
1	AA	474	G	Sidechain
1	AA	511	U	Sidechain
1	AA	513	A	Sidechain
1	AA	514	A	Sidechain
1	AA	525	U	Sidechain
1	AA	534	U	Sidechain
1	AA	553	U	Sidechain
1	AA	584	C	Sidechain
1	AA	585	G	Sidechain
1	AA	601	C	Sidechain
1	AA	605	C	Sidechain
1	AA	606	U	Sidechain
1	AA	607	U	Sidechain
1	AA	608	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	610	C	Sidechain
1	AA	611	C	Sidechain
1	AA	618(A)	C	Sidechain
1	AA	621	A	Sidechain
1	AA	639	U	Sidechain
1	AA	641	C	Sidechain
1	AA	643	A	Sidechain
1	AA	646	A	Sidechain
1	AA	647	G	Sidechain
1	AA	650	C	Sidechain
1	AA	658	C	Sidechain
1	AA	67	U	Sidechain
1	AA	670	A	Sidechain
1	AA	679	C	Sidechain
1	AA	697	C	Sidechain
1	AA	703	U	Sidechain
1	AA	704	G	Sidechain
1	AA	709	U	Sidechain
1	AA	715	G	Sidechain
1	AA	724	U	Sidechain
1	AA	729	G	Sidechain
1	AA	730	C	Sidechain
1	AA	733	G	Sidechain
1	AA	744	G	Sidechain
1	AA	750	A	Sidechain
1	AA	758	C	Sidechain
1	AA	76	C	Sidechain
1	AA	762	U	Sidechain
1	AA	767	U	Sidechain
1	AA	774	A	Sidechain
1	AA	775	G	Sidechain
1	AA	776	G	Sidechain
1	AA	779	U	Sidechain
1	AA	786	C	Sidechain
1	AA	792	G	Sidechain
1	AA	795	C	Sidechain
1	AA	800	A	Sidechain
1	AA	801	G	Sidechain
1	AA	805	G	Sidechain
1	AA	807	U	Sidechain
1	AA	811	U	Sidechain
1	AA	821	A	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	830	G	Sidechain
1	AA	832	G	Sidechain
1	AA	835	A	Sidechain
1	AA	843	G	Sidechain
1	AA	847	U	Sidechain
1	AA	848	G	Sidechain
1	AA	858	U	Sidechain
1	AA	860	U	Sidechain
1	AA	865	C	Sidechain
1	AA	9	U	Sidechain
1	AA	913	U	Sidechain
1	AA	915	C	Sidechain
1	AA	922	U	Sidechain
1	AA	924	C	Sidechain
1	AA	930	U	Sidechain
1	AA	931	G	Sidechain
1	AA	944	G	Sidechain
1	AA	946	G	Sidechain
1	AA	955	C	Sidechain
1	AA	965	C	Sidechain
1	AA	969	U	Sidechain
1	AA	971	C	Sidechain
1	AA	972	G	Sidechain
1	AA	974(A)	C	Sidechain
1	AA	978	G	Sidechain
1	AA	980	A	Sidechain
1	AA	981	A	Sidechain
1	AA	986	C	Sidechain
1	AA	987	G	Sidechain
1	AA	990	A	Sidechain
2	AB	10	C	Sidechain
2	AB	101	A	Sidechain
2	AB	109	G	Sidechain
2	AB	11	C	Sidechain
2	AB	33	G	Sidechain
2	AB	34	U	Sidechain
2	AB	55	U	Sidechain
2	AB	60	C	Sidechain
2	AB	7	G	Sidechain
2	AB	71	C	Sidechain
2	AB	77	U	Sidechain
2	AB	8	U	Sidechain

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Mol	Chain	Res	Type	Group
2	AB	89	G	Sidechain
2	AB	90	C	Sidechain
2	AB	93	C	Sidechain
2	AB	97	G	Sidechain
2	AB	98	G	Sidechain
3	AC	179	SER	Mainchain
5	AE	151	TYR	Sidechain
6	AF	7	TYR	Sidechain
31	AI	153	LEU	Mainchain,Peptide
9	AK	4	TYR	Sidechain
12	AN	93	TYR	Sidechain
15	AQ	32	TYR	Sidechain
17	AS	91	TYR	Sidechain
25	Aa	32	TYR	Sidechain
26	Ab	29	THR	Mainchain
34	BA	1012	U	Sidechain
34	BA	1027	C	Sidechain
34	BA	1028(A)	C	Sidechain
34	BA	1037	C	Sidechain
34	BA	1038	C	Sidechain
34	BA	1039	C	Sidechain
34	BA	1040	U	Sidechain
34	BA	1048	G	Sidechain
34	BA	1052	U	Sidechain
34	BA	1054	C	Sidechain
34	BA	1056	U	Sidechain
34	BA	1065	U	Sidechain
34	BA	1067	A	Sidechain
34	BA	1073	U	Sidechain
34	BA	1078	U	Sidechain
34	BA	1083	U	Sidechain
34	BA	1097	C	Sidechain
34	BA	1100	C	Sidechain
34	BA	1121	U	Sidechain
34	BA	1122	U	Sidechain
34	BA	1124	G	Sidechain
34	BA	1128	C	Sidechain
34	BA	1133	G	Sidechain
34	BA	1143	G	Sidechain
34	BA	115	G	Sidechain
34	BA	1150	U	Sidechain
34	BA	1195	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	1199	U	Sidechain
34	BA	12	U	Sidechain
34	BA	1226	C	Sidechain
34	BA	1235	U	Sidechain
34	BA	124	G	Sidechain
34	BA	1246	C	Sidechain
34	BA	125	U	Sidechain
34	BA	1263	C	Sidechain
34	BA	1266	G	Sidechain
34	BA	1277	C	Sidechain
34	BA	1285	A	Sidechain
34	BA	129	U	Sidechain
34	BA	1298	C	Sidechain
34	BA	1302	U	Sidechain
34	BA	131	C	Sidechain
34	BA	1314	C	Sidechain
34	BA	132	C	Sidechain
34	BA	1327	C	Sidechain
34	BA	1328	C	Sidechain
34	BA	1330	U	Sidechain
34	BA	134	A	Sidechain
34	BA	1347	G	Sidechain
34	BA	135	C	Sidechain
34	BA	1352	C	Sidechain
34	BA	1362	C	Sidechain
34	BA	1370	G	Sidechain
34	BA	1377	A	Sidechain
34	BA	138	G	Sidechain
34	BA	1402	C	Sidechain
34	BA	1404	C	Sidechain
34	BA	1405	G	Sidechain
34	BA	1422	G	Sidechain
34	BA	1427	U	Sidechain
34	BA	145	G	Sidechain
34	BA	146	G	Sidechain
34	BA	1472	U	Sidechain
34	BA	1477	C	Sidechain
34	BA	1481	U	Sidechain
34	BA	1541	U	Sidechain
34	BA	156	G	Sidechain
34	BA	158	G	Sidechain
34	BA	159	G	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	17	U	Sidechain
34	BA	191(C)	G	Sidechain
34	BA	191(D)	U	Sidechain
34	BA	219	C	Sidechain
34	BA	225	C	Sidechain
34	BA	244	U	Sidechain
34	BA	253	U	Sidechain
34	BA	267	C	Sidechain
34	BA	274	A	Sidechain
34	BA	281	G	Sidechain
34	BA	285	G	Sidechain
34	BA	287	U	Sidechain
34	BA	295	C	Sidechain
34	BA	31	G	Sidechain
34	BA	332	G	Sidechain
34	BA	335	C	Sidechain
34	BA	348	G	Sidechain
34	BA	352	C	Sidechain
34	BA	367	U	Sidechain
34	BA	37	U	Sidechain
34	BA	375	U	Sidechain
34	BA	385	C	Sidechain
34	BA	395	C	Sidechain
34	BA	397	A	Sidechain
34	BA	398	C	Sidechain
34	BA	403	C	Sidechain
34	BA	412	A	Sidechain
34	BA	418	C	Sidechain
34	BA	430	A	Sidechain
34	BA	432	A	Sidechain
34	BA	45	U	Sidechain
34	BA	451	A	Sidechain
34	BA	47	C	Sidechain
34	BA	484	G	Sidechain
34	BA	501	C	Sidechain
34	BA	504	C	Sidechain
34	BA	518	C	Sidechain
34	BA	529	G	Sidechain
34	BA	531	U	Sidechain
34	BA	532	A	Sidechain
34	BA	54	C	Sidechain
34	BA	56	U	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	560	U	Sidechain
34	BA	563	A	Sidechain
34	BA	575	G	Sidechain
34	BA	576	G	Sidechain
34	BA	579	G	Sidechain
34	BA	590	C	Sidechain
34	BA	591	U	Sidechain
34	BA	596	C	Sidechain
34	BA	610	G	Sidechain
34	BA	616	G	Sidechain
34	BA	63	C	Sidechain
34	BA	634	C	Sidechain
34	BA	644	G	Sidechain
34	BA	66	G	Sidechain
34	BA	661	G	Sidechain
34	BA	666	G	Sidechain
34	BA	672	U	Sidechain
34	BA	689	C	Sidechain
34	BA	690	G	Sidechain
34	BA	717	C	Sidechain
34	BA	727	G	Sidechain
34	BA	729	A	Sidechain
34	BA	734	G	Sidechain
34	BA	739	C	Sidechain
34	BA	741	G	Sidechain
34	BA	75	C	Sidechain
34	BA	760	G	Sidechain
34	BA	763	G	Sidechain
34	BA	770	C	Sidechain
34	BA	779	C	Sidechain
34	BA	792	A	Sidechain
34	BA	808	C	Sidechain
34	BA	813	U	Sidechain
34	BA	817	C	Sidechain
34	BA	82	U	Sidechain
34	BA	834	C	Sidechain
34	BA	853	G	Sidechain
34	BA	862	C	Sidechain
34	BA	863	U	Sidechain
34	BA	875	C	Sidechain
34	BA	88	C	Sidechain
34	BA	883	C	Sidechain

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Mol	Chain	Res	Type	Group
34	BA	887	G	Sidechain
34	BA	895	G	Sidechain
34	BA	898	G	Sidechain
34	BA	901	A	Sidechain
34	BA	902	G	Sidechain
34	BA	904	C	Sidechain
34	BA	905	U	Sidechain
34	BA	911	U	Sidechain
34	BA	912	C	Sidechain
34	BA	923	A	Sidechain
34	BA	947	G	Sidechain
34	BA	955	U	Sidechain
34	BA	961	U	Sidechain
34	BA	974	A	Sidechain
34	BA	983	A	Sidechain
34	BA	989	C	Sidechain
34	BA	998(A)	C	Sidechain
37	BH	54	TYR	Sidechain
39	BJ	4	TYR	Sidechain
44	BO	75	TYR	Sidechain
47	BR	34	TYR	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	AC	220/228 (96%)	153 (70%)	39 (18%)	28 (13%)	0 5
4	AD	270/272 (99%)	125 (46%)	59 (22%)	86 (32%)	0 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	204/206 (99%)	117 (57%)	31 (15%)	56 (28%)	0	0
6	AF	206/208 (99%)	109 (53%)	46 (22%)	51 (25%)	0	1
7	AG	180/182 (99%)	79 (44%)	47 (26%)	54 (30%)	0	0
8	AH	172/174 (99%)	80 (46%)	46 (27%)	46 (27%)	0	0
9	AK	137/139 (99%)	64 (47%)	28 (20%)	45 (33%)	0	0
10	AL	120/122 (98%)	59 (49%)	23 (19%)	38 (32%)	0	0
11	AM	143/145 (99%)	57 (40%)	36 (25%)	50 (35%)	0	0
12	AN	134/136 (98%)	49 (37%)	33 (25%)	52 (39%)	0	0
13	AO	115/117 (98%)	57 (50%)	39 (34%)	19 (16%)	0	3
14	AP	108/110 (98%)	48 (44%)	28 (26%)	32 (30%)	0	0
15	AQ	115/117 (98%)	52 (45%)	26 (23%)	37 (32%)	0	0
16	AR	115/117 (98%)	35 (30%)	50 (44%)	30 (26%)	0	1
17	AS	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	0
18	AT	108/110 (98%)	63 (58%)	24 (22%)	21 (19%)	0	2
19	AU	92/94 (98%)	57 (62%)	16 (17%)	19 (21%)	0	2
20	AV	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	0
21	AW	178/180 (99%)	96 (54%)	43 (24%)	39 (22%)	0	1
22	AX	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	6
23	AY	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	4
24	AZ	57/59 (97%)	34 (60%)	8 (14%)	15 (26%)	0	1
25	Aa	69/71 (97%)	23 (33%)	15 (22%)	31 (45%)	0	0
26	Ab	55/57 (96%)	14 (26%)	19 (34%)	22 (40%)	0	0
27	Ac	47/49 (96%)	14 (30%)	7 (15%)	26 (55%)	0	0
28	Ad	47/49 (96%)	20 (43%)	12 (26%)	15 (32%)	0	0
29	Ae	62/64 (97%)	23 (37%)	17 (27%)	22 (36%)	0	0
30	Af	35/37 (95%)	20 (57%)	5 (14%)	10 (29%)	0	0
31	AI	151/153 (99%)	89 (59%)	33 (22%)	29 (19%)	0	2
32	AJ	132/134 (98%)	56 (42%)	44 (33%)	32 (24%)	0	1
35	BF	232/234 (99%)	114 (49%)	41 (18%)	77 (33%)	0	0
36	BG	204/206 (99%)	107 (52%)	46 (22%)	51 (25%)	0	1
37	BH	206/208 (99%)	95 (46%)	58 (28%)	53 (26%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BI	148/150 (99%)	93 (63%)	38 (26%)	17 (12%)	0	6
39	BJ	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
40	BK	153/155 (99%)	73 (48%)	45 (29%)	35 (23%)	0	1
41	BL	136/138 (99%)	68 (50%)	35 (26%)	33 (24%)	0	1
42	BM	125/127 (98%)	62 (50%)	33 (26%)	30 (24%)	0	1
43	BN	96/98 (98%)	52 (54%)	20 (21%)	24 (25%)	0	1
44	BO	117/119 (98%)	65 (56%)	29 (25%)	23 (20%)	0	2
45	BP	122/124 (98%)	50 (41%)	30 (25%)	42 (34%)	0	0
46	BQ	112/114 (98%)	64 (57%)	28 (25%)	20 (18%)	0	3
47	BR	58/60 (97%)	24 (41%)	16 (28%)	18 (31%)	0	0
48	BS	86/88 (98%)	36 (42%)	35 (41%)	15 (17%)	0	3
49	BT	81/83 (98%)	42 (52%)	24 (30%)	15 (18%)	0	2
50	BU	102/104 (98%)	62 (61%)	23 (22%)	17 (17%)	0	3
51	BV	71/73 (97%)	26 (37%)	26 (37%)	19 (27%)	0	0
52	BW	78/80 (98%)	30 (38%)	25 (32%)	23 (30%)	0	0
53	BX	97/99 (98%)	38 (39%)	32 (33%)	27 (28%)	0	0
54	BY	22/24 (92%)	9 (41%)	6 (27%)	7 (32%)	0	0
57	BZ	603/605 (100%)	280 (46%)	200 (33%)	123 (20%)	0	2
All	All	6575/6683 (98%)	3224 (49%)	1675 (26%)	1676 (26%)	0	1

All (1676) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	35	ALA
3	AC	39	GLU
3	AC	54	SER
3	AC	61	THR
3	AC	72	VAL
3	AC	217	THR
4	AD	6	PHE
4	AD	10	THR
4	AD	17	THR
4	AD	18	VAL
4	AD	30	GLU
4	AD	33	LEU
4	AD	35	LYS

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Mol	Chain	Res	Type
4	AD	44	ASN
4	AD	53	PHE
4	AD	54	ARG
4	AD	58	HIS
4	AD	70	TRP
4	AD	72	LYS
4	AD	73	VAL
4	AD	81	ALA
4	AD	91	ARG
4	AD	106	ILE
4	AD	107	ALA
4	AD	108	PRO
4	AD	118	VAL
4	AD	121	PRO
4	AD	122	ASP
4	AD	125	ILE
4	AD	133	LEU
4	AD	134	ARG
4	AD	145	VAL
4	AD	153	ALA
4	AD	155	LEU
4	AD	157	ARG
4	AD	158	ALA
4	AD	160	GLY
4	AD	167	GLY
4	AD	178	PRO
4	AD	179	SER
4	AD	219	PRO
4	AD	224	ALA
4	AD	225	ALA
4	AD	232	PRO
4	AD	239	ARG
4	AD	241	PRO
4	AD	244	ARG
4	AD	247	ALA
4	AD	249	PRO
4	AD	252	TRP
4	AD	258	LYS
4	AD	264	LYS
4	AD	268	ARG
4	AD	270	ILE
4	AD	271	ILE

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Mol	Chain	Res	Type
5	AE	16	ARG
5	AE	38	THR
5	AE	42	ASP
5	AE	54	GLN
5	AE	68	ALA
5	AE	70	ALA
5	AE	74	PRO
5	AE	92	THR
5	AE	111	ARG
5	AE	117	MET
5	AE	122	PHE
5	AE	128	SER
5	AE	133	LYS
5	AE	134	ILE
5	AE	145	LYS
5	AE	149	ARG
5	AE	151	TYR
5	AE	157	ALA
5	AE	168	MET
5	AE	173	VAL
5	AE	180	ASN
5	AE	191	PRO
5	AE	202	LYS
6	AF	13	SER
6	AF	14	PRO
6	AF	30	PRO
6	AF	45	ARG
6	AF	52	LYS
6	AF	53	THR
6	AF	57	VAL
6	AF	58	ALA
6	AF	62	ARG
6	AF	67	GLN
6	AF	68	LYS
6	AF	69	HIS
6	AF	75	HIS
6	AF	82	ILE
6	AF	84	VAL
6	AF	85	GLY
6	AF	89	VAL
6	AF	91	GLY
6	AF	99	TYR

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Mol	Chain	Res	Type
6	AF	100	THR
6	AF	104	LYS
6	AF	132	VAL
6	AF	151	SER
6	AF	169	ASN
6	AF	172	TRP
6	AF	186	ILE
6	AF	196	LEU
7	AG	16	ARG
7	AG	18	GLU
7	AG	27	ASN
7	AG	32	PRO
7	AG	36	LYS
7	AG	42	GLY
7	AG	43	LEU
7	AG	51	ARG
7	AG	66	GLN
7	AG	68	PRO
7	AG	73	ALA
7	AG	76	SER
7	AG	78	SER
7	AG	86	MET
7	AG	104	GLU
7	AG	111	LEU
7	AG	114	ILE
7	AG	115	ARG
7	AG	116	ASP
7	AG	117	PHE
7	AG	123	ASN
7	AG	124	SER
7	AG	128	ARG
7	AG	131	TYR
7	AG	132	ASN
7	AG	133	LEU
7	AG	138	GLN
7	AG	140	ILE
7	AG	143	GLU
7	AG	144	ILE
7	AG	148	MET
7	AG	164	GLU
7	AG	172	LEU
7	AG	181	ARG

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Mol	Chain	Res	Type
8	AH	6	ARG
8	AH	7	LEU
8	AH	12	PRO
8	AH	15	VAL
8	AH	20	ALA
8	AH	30	LYS
8	AH	56	SER
8	AH	99	VAL
8	AH	104	GLU
8	AH	107	VAL
8	AH	111	HIS
8	AH	127	GLU
8	AH	136	ILE
8	AH	152	ARG
8	AH	153	LYS
8	AH	155	SER
8	AH	157	TYR
8	AH	160	LYS
8	AH	164	TYR
8	AH	168	PRO
9	AK	3	THR
9	AK	4	TYR
9	AK	7	LYS
9	AK	9	VAL
9	AK	23	LEU
9	AK	31	ALA
9	AK	35	ARG
9	AK	43	THR
9	AK	46	VAL
9	AK	48	MET
9	AK	50	ASP
9	AK	58	ASP
9	AK	59	LYS
9	AK	66	LYS
9	AK	68	GLU
9	AK	76	SER
9	AK	79	PRO
9	AK	83	LYS
9	AK	127	ASP
9	AK	135	PRO
9	AK	136	GLU
10	AL	4	PRO

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Mol	Chain	Res	Type
10	AL	11	ALA
10	AL	14	THR
10	AL	17	ARG
10	AL	26	LYS
10	AL	28	SER
10	AL	29	ASN
10	AL	30	ALA
10	AL	46	ALA
10	AL	53	LYS
10	AL	63	VAL
10	AL	64	ARG
10	AL	66	LYS
10	AL	89	ASN
10	AL	93	PRO
10	AL	97	ARG
10	AL	101	PRO
10	AL	103	ALA
10	AL	105	GLU
10	AL	110	GLY
10	AL	111	PHE
10	AL	119	PRO
11	AM	8	PRO
11	AM	12	ALA
11	AM	14	LYS
11	AM	27	HIS
11	AM	29	LYS
11	AM	42	SER
11	AM	44	GLY
11	AM	47	ASP
11	AM	55	ARG
11	AM	56	SER
11	AM	57	THR
11	AM	58	THR
11	AM	64	LYS
11	AM	72	PRO
11	AM	88	LEU
11	AM	96	THR
11	AM	102	ARG
11	AM	106	LEU
11	AM	107	LYS
11	AM	122	PRO
11	AM	127	ALA

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Mol	Chain	Res	Type
12	AN	11	LYS
12	AN	21	THR
12	AN	27	VAL
12	AN	29	PHE
12	AN	39	PRO
12	AN	40	ALA
12	AN	58	PHE
12	AN	59	ARG
12	AN	66	ILE
12	AN	67	ARG
12	AN	68	ILE
12	AN	71	ASP
12	AN	77	LYS
12	AN	78	PRO
12	AN	80	GLU
12	AN	81	VAL
12	AN	111	GLU
12	AN	124	LYS
12	AN	125	LEU
12	AN	126	PRO
12	AN	132	VAL
12	AN	138	ASP
13	AO	4	LEU
13	AO	38	VAL
13	AO	57	ARG
13	AO	72	ASP
13	AO	76	VAL
13	AO	88	ARG
13	AO	89	ASP
14	AP	5	THR
14	AP	14	VAL
14	AP	28	VAL
14	AP	29	PHE
14	AP	30	ARG
14	AP	31	SER
14	AP	32	LEU
14	AP	35	ILE
14	AP	36	TYR
14	AP	48	LEU
14	AP	51	ALA
14	AP	54	LEU
14	AP	58	LEU

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Mol	Chain	Res	Type
14	AP	61	ASN
15	AQ	2	ASN
15	AQ	3	ARG
15	AQ	5	ALA
15	AQ	19	LEU
15	AQ	20	PRO
15	AQ	22	PHE
15	AQ	25	GLY
15	AQ	27	THR
15	AQ	39	ARG
15	AQ	45	PHE
15	AQ	58	ASN
15	AQ	83	ILE
15	AQ	98	LYS
15	AQ	100	TYR
15	AQ	103	ARG
15	AQ	105	LEU
15	AQ	106	SER
15	AQ	109	GLU
16	AR	3	ARG
16	AR	4	ALA
16	AR	8	VAL
16	AR	22	LYS
16	AR	31	SER
16	AR	32	PHE
16	AR	33	ARG
16	AR	62	ILE
16	AR	75	ASN
16	AR	94	ASN
17	AS	10	LYS
17	AS	11	GLN
17	AS	13	ARG
17	AS	15	GLU
17	AS	19	LYS
17	AS	22	VAL
17	AS	31	ALA
17	AS	32	THR
17	AS	39	LEU
17	AS	40	LEU
17	AS	46	VAL
17	AS	50	PRO
17	AS	57	VAL

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Mol	Chain	Res	Type
17	AS	68	LYS
17	AS	69	LYS
17	AS	73	SER
17	AS	82	ARG
17	AS	100	ARG
18	AT	9	TYR
18	AT	11	ARG
18	AT	12	ILE
18	AT	14	PRO
18	AT	25	ARG
18	AT	27	LYS
18	AT	41	LYS
18	AT	44	ALA
18	AT	58	ALA
18	AT	64	MET
18	AT	65	LEU
18	AT	73	ALA
18	AT	92	ARG
19	AU	4	ALA
19	AU	6	ASP
19	AU	63	LYS
19	AU	73	ARG
19	AU	89	ILE
19	AU	90	GLU
19	AU	95	LEU
20	AV	10	GLY
20	AV	15	VAL
20	AV	31	LEU
20	AV	40	GLU
20	AV	42	VAL
20	AV	45	VAL
20	AV	46	LYS
20	AV	47	LYS
20	AV	57	GLN
20	AV	58	GLY
20	AV	65	ALA
20	AV	71	LYS
20	AV	72	VAL
20	AV	77	PRO
20	AV	82	PRO
20	AV	108	THR
21	AW	41	LEU

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Mol	Chain	Res	Type
21	AW	42	VAL
21	AW	57	ILE
21	AW	62	PRO
21	AW	78	LYS
21	AW	79	ARG
21	AW	83	PRO
21	AW	93	ASP
21	AW	94	GLU
21	AW	108	PRO
21	AW	109	ALA
21	AW	146	ILE
21	AW	155	LEU
21	AW	159	PRO
21	AW	161	VAL
21	AW	162	GLU
21	AW	165	VAL
22	AX	2	ALA
22	AX	29	GLN
22	AX	55	ARG
22	AX	84	LEU
23	AY	12	SER
23	AY	13	PRO
23	AY	15	GLU
23	AY	34	ALA
23	AY	35	SER
23	AY	42	ASN
24	AZ	9	VAL
24	AZ	11	SER
24	AZ	13	ILE
24	AZ	28	LEU
24	AZ	29	ARG
24	AZ	30	ARG
24	AZ	31	LEU
24	AZ	52	HIS
25	Aa	6	HIS
25	Aa	8	LYS
25	Aa	11	PRO
25	Aa	13	ARG
25	Aa	14	ILE
25	Aa	18	CYS
25	Aa	32	TYR
25	Aa	33	VAL

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Mol	Chain	Res	Type
25	Aa	39	CYS
25	Aa	53	GLU
25	Aa	55	ARG
26	Ab	7	PRO
26	Ab	10	LYS
26	Ab	11	THR
26	Ab	18	ALA
26	Ab	23	HIS
26	Ab	36	CYS
26	Ab	38	ALA
26	Ab	42	PRO
27	Ac	8	LYS
27	Ac	17	LYS
27	Ac	20	ASN
27	Ac	23	THR
27	Ac	26	ASN
27	Ac	27	LYS
27	Ac	29	ASN
27	Ac	30	THR
27	Ac	36	LEU
27	Ac	37	ARG
27	Ac	38	LYS
27	Ac	46	HIS
27	Ac	49	HIS
27	Ac	50	ARG
27	Ac	51	GLU
27	Ac	53	LYS
28	Ad	2	LYS
28	Ad	10	ARG
28	Ad	41	ARG
28	Ad	47	ARG
29	Ae	5	LYS
29	Ae	27	THR
29	Ae	30	ARG
29	Ae	36	LYS
29	Ae	37	SER
29	Ae	39	LYS
29	Ae	62	LEU
29	Ae	63	PRO
30	Af	5	ALA
30	Af	9	ARG
30	Af	10	ILE

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Mol	Chain	Res	Type
30	Af	11	CYS
31	AI	7	VAL
31	AI	30	GLN
31	AI	52	PHE
31	AI	53	VAL
31	AI	57	THR
31	AI	58	LEU
31	AI	74	LEU
31	AI	77	PRO
31	AI	80	VAL
31	AI	90	ALA
31	AI	93	LEU
31	AI	107	VAL
32	AJ	20	ALA
32	AJ	29	GLN
32	AJ	34	ILE
32	AJ	50	ASP
32	AJ	51	ALA
32	AJ	68	VAL
32	AJ	71	THR
32	AJ	84	LEU
32	AJ	93	ARG
32	AJ	108	ALA
32	AJ	111	LYS
32	AJ	113	PRO
35	BF	8	LYS
35	BF	11	LEU
35	BF	13	ALA
35	BF	15	VAL
35	BF	16	HIS
35	BF	17	PHE
35	BF	22	LYS
35	BF	26	PRO
35	BF	37	ASN
35	BF	42	ILE
35	BF	44	LEU
35	BF	45	GLN
35	BF	76	GLN
35	BF	77	ALA
35	BF	78	GLN
35	BF	97	TRP
35	BF	104	ASN

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Mol	Chain	Res	Type
35	BF	109	SER
35	BF	122	PHE
35	BF	124	SER
35	BF	127	ILE
35	BF	131	PRO
35	BF	147	LYS
35	BF	153	ARG
35	BF	154	LEU
35	BF	155	LEU
35	BF	161	ALA
35	BF	165	VAL
35	BF	168	THR
35	BF	169	LYS
35	BF	171	ALA
35	BF	172	ILE
35	BF	181	PHE
35	BF	191	ASP
35	BF	194	PRO
35	BF	195	ASP
35	BF	200	ILE
35	BF	201	ILE
35	BF	204	ASN
35	BF	207	ALA
35	BF	211	ILE
35	BF	226	ARG
35	BF	230	VAL
35	BF	232	PRO
35	BF	236	TYR
36	BG	4	LYS
36	BG	12	LEU
36	BG	14	ILE
36	BG	18	TRP
36	BG	24	ALA
36	BG	28	GLN
36	BG	39	ILE
36	BG	43	LEU
36	BG	52	LEU
36	BG	53	ALA
36	BG	64	VAL
36	BG	65	ALA
36	BG	79	ARG
36	BG	83	ARG

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Mol	Chain	Res	Type
36	BG	84	ILE
36	BG	95	THR
36	BG	97	LYS
36	BG	98	ASN
36	BG	119	ARG
36	BG	129	ALA
36	BG	157	ILE
36	BG	160	ALA
36	BG	176	HIS
36	BG	177	THR
36	BG	179	ARG
36	BG	191	THR
36	BG	192	THR
37	BH	3	ARG
37	BH	17	VAL
37	BH	18	LYS
37	BH	21	LEU
37	BH	29	PRO
37	BH	30	LYS
37	BH	31	CYS
37	BH	48	ALA
37	BH	56	VAL
37	BH	71	SER
37	BH	86	LYS
37	BH	88	VAL
37	BH	99	SER
37	BH	109	GLY
37	BH	131	ARG
37	BH	142	PRO
37	BH	148	VAL
37	BH	150	GLU
37	BH	151	LYS
37	BH	154	ASN
37	BH	166	LYS
37	BH	168	ARG
37	BH	170	VAL
37	BH	179	GLU
37	BH	191	ARG
37	BH	195	ALA
37	BH	198	VAL
37	BH	199	ASN
38	BI	12	LEU

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Mol	Chain	Res	Type
38	BI	55	VAL
38	BI	75	THR
38	BI	128	PRO
38	BI	144	THR
39	BJ	11	ASN
39	BJ	16	GLN
39	BJ	27	GLN
39	BJ	72	VAL
39	BJ	81	ILE
39	BJ	82	ARG
39	BJ	84	ASN
39	BJ	85	VAL
39	BJ	95	GLU
39	BJ	97	PHE
40	BK	4	ARG
40	BK	8	GLU
40	BK	14	PRO
40	BK	17	VAL
40	BK	31	MET
40	BK	35	LYS
40	BK	37	ASN
40	BK	71	PRO
40	BK	91	VAL
40	BK	111	ARG
40	BK	134	ALA
40	BK	142	GLU
41	BL	6	ILE
41	BL	13	ILE
41	BL	29	SER
41	BL	30	ARG
41	BL	63	LEU
41	BL	74	PRO
41	BL	75	ARG
41	BL	76	PRO
41	BL	77	GLU
41	BL	79	VAL
41	BL	103	VAL
41	BL	105	ARG
41	BL	115	SER
41	BL	121	ASP
41	BL	129	VAL
42	BM	29	ASN

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Mol	Chain	Res	Type
42	BM	33	PHE
42	BM	44	VAL
42	BM	70	LYS
42	BM	98	PRO
42	BM	109	VAL
42	BM	116	LYS
42	BM	118	LYS
43	BN	34	VAL
43	BN	36	GLY
43	BN	39	PRO
43	BN	40	LEU
43	BN	55	LYS
43	BN	56	HIS
43	BN	60	ARG
43	BN	72	VAL
43	BN	79	ARG
43	BN	80	LYS
43	BN	90	LEU
44	BO	14	VAL
44	BO	15	ALA
44	BO	27	ASN
44	BO	39	PRO
44	BO	74	ALA
44	BO	78	GLN
44	BO	106	LYS
44	BO	113	PRO
44	BO	116	HIS
45	BP	6	THR
45	BP	7	ILE
45	BP	18	VAL
45	BP	19	ARG
45	BP	22	SER
45	BP	28	LYS
45	BP	30	ALA
45	BP	46	LYS
45	BP	48	PRO
45	BP	51	ALA
45	BP	62	SER
45	BP	66	VAL
45	BP	83	VAL
45	BP	92	ASP
45	BP	101	VAL

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Mol	Chain	Res	Type
45	BP	110	VAL
45	BP	116	SER
45	BP	127	GLU
46	BQ	12	ASN
46	BQ	47	ASP
46	BQ	48	LEU
46	BQ	102	ARG
46	BQ	107	ALA
47	BR	12	ARG
47	BR	18	VAL
47	BR	29	ARG
47	BR	31	ARG
47	BR	34	TYR
47	BR	36	PHE
47	BR	44	LEU
47	BR	54	PRO
47	BR	55	GLY
48	BS	3	ILE
48	BS	16	ALA
49	BT	11	SER
49	BT	15	PRO
49	BT	24	ALA
49	BT	27	LYS
49	BT	61	SER
50	BU	3	LYS
50	BU	4	LYS
50	BU	15	MET
50	BU	34	LYS
50	BU	48	GLU
50	BU	50	LYS
50	BU	81	ARG
50	BU	104	LYS
51	BV	42	ARG
51	BV	49	LYS
51	BV	52	PRO
51	BV	59	SER
51	BV	75	ILE
51	BV	79	LEU
51	BV	82	THR
51	BV	87	ARG
52	BW	9	VAL
52	BW	21	GLU

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Mol	Chain	Res	Type
52	BW	28	LYS
52	BW	32	LYS
52	BW	40	ILE
52	BW	42	PRO
52	BW	43	GLU
52	BW	64	GLU
52	BW	70	LYS
52	BW	79	THR
53	BX	12	ALA
53	BX	99	LEU
53	BX	105	SER
54	BY	6	ARG
54	BY	9	ARG
57	BZ	11	ILE
57	BZ	18	LYS
57	BZ	28	GLN
57	BZ	42	VAL
57	BZ	56	ILE
57	BZ	58	ALA
57	BZ	71	ASN
57	BZ	133	PRO
57	BZ	135	ALA
57	BZ	179	MET
57	BZ	182	ASP
57	BZ	184	THR
57	BZ	209	ILE
57	BZ	231	VAL
57	BZ	253	LYS
57	BZ	284	ILE
57	BZ	289	CYS
57	BZ	305	PRO
57	BZ	307	VAL
57	BZ	314	ASN
57	BZ	321	LYS
57	BZ	395	ARG
57	BZ	424	GLY
57	BZ	437	VAL
57	BZ	442	VAL
57	BZ	475	VAL
57	BZ	476	ARG
57	BZ	477	PRO
57	BZ	557	LEU

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Mol	Chain	Res	Type
57	BZ	561	ILE
57	BZ	567	GLN
57	BZ	583	THR
57	BZ	603	ALA
3	AC	22	ILE
3	AC	80	GLY
3	AC	132	GLY
3	AC	140	PRO
3	AC	161	ILE
3	AC	164	ARG
4	AD	52	ARG
4	AD	62	TYR
4	AD	110	GLY
4	AD	111	LEU
4	AD	123	ALA
4	AD	149	PRO
4	AD	152	GLY
4	AD	189	CYS
4	AD	196	VAL
4	AD	204	ILE
4	AD	207	GLY
4	AD	217	ARG
4	AD	243	GLY
4	AD	262	ARG
4	AD	263	ARG
4	AD	266	SER
5	AE	22	PRO
5	AE	44	TYR
5	AE	72	VAL
5	AE	93	VAL
5	AE	95	ILE
5	AE	115	GLY
5	AE	118	LYS
5	AE	121	ASN
5	AE	124	GLY
5	AE	139	GLY
5	AE	155	LYS
5	AE	178	GLU
5	AE	187	ALA
6	AF	54	ARG
6	AF	81	PRO
6	AF	98	SER

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Mol	Chain	Res	Type
6	AF	102	PRO
6	AF	126	VAL
6	AF	136	THR
6	AF	158	THR
6	AF	167	ALA
6	AF	177	ALA
6	AF	184	TYR
6	AF	190	GLU
7	AG	20	ILE
7	AG	24	GLY
7	AG	61	ALA
7	AG	88	ILE
7	AG	151	ALA
7	AG	154	GLY
7	AG	163	ALA
8	AH	31	GLY
8	AH	33	LEU
8	AH	42	ARG
8	AH	57	ASP
8	AH	105	LEU
8	AH	110	SER
8	AH	118	PRO
8	AH	120	GLY
8	AH	151	ILE
8	AH	156	ALA
8	AH	169	VAL
9	AK	19	GLU
9	AK	30	ILE
9	AK	34	LEU
9	AK	38	HIS
9	AK	40	PRO
9	AK	47	ALA
9	AK	63	THR
9	AK	67	LEU
9	AK	88	GLU
9	AK	92	ALA
9	AK	105	GLY
9	AK	110	GLY
9	AK	114	ARG
10	AL	49	ARG
10	AL	50	GLY
10	AL	52	VAL

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Mol	Chain	Res	Type
10	AL	88	ASN
10	AL	90	GLN
10	AL	102	VAL
10	AL	104	ARG
10	AL	121	VAL
11	AM	7	ARG
11	AM	11	GLY
11	AM	23	PRO
11	AM	32	THR
11	AM	34	GLY
11	AM	39	LYS
11	AM	43	GLY
11	AM	67	MET
11	AM	84	ASN
11	AM	87	ASP
11	AM	92	GLU
12	AN	12	GLN
12	AN	45	GLN
12	AN	88	GLY
12	AN	94	VAL
12	AN	100	GLY
12	AN	107	ALA
12	AN	127	ILE
12	AN	136	ALA
12	AN	137	TYR
13	AO	8	ARG
13	AO	71	GLN
13	AO	86	ARG
13	AO	94	TYR
14	AP	11	LYS
14	AP	23	ARG
14	AP	33	LYS
14	AP	43	GLU
14	AP	67	ARG
14	AP	78	LEU
14	AP	82	ILE
14	AP	97	ARG
15	AQ	24	PRO
15	AQ	30	VAL
15	AQ	36	GLU
15	AQ	41	ARG
15	AQ	82	LEU

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Mol	Chain	Res	Type
15	AQ	99	LEU
15	AQ	104	ASN
15	AQ	114	LEU
16	AR	26	GLY
16	AR	27	LEU
16	AR	47	TYR
16	AR	53	ARG
16	AR	78	THR
16	AR	88	ILE
16	AR	90	VAL
16	AR	93	LYS
16	AR	110	VAL
17	AS	8	GLY
17	AS	14	VAL
17	AS	18	LEU
17	AS	45	THR
17	AS	72	VAL
17	AS	81	TYR
18	AT	15	ARG
18	AT	26	GLY
18	AT	30	GLU
18	AT	75	TYR
18	AT	90	ARG
19	AU	8	ILE
19	AU	15	GLU
19	AU	33	LYS
19	AU	49	VAL
19	AU	53	LYS
19	AU	67	GLY
19	AU	74	PRO
19	AU	85	PRO
20	AV	21	LYS
20	AV	29	GLU
20	AV	33	LYS
20	AV	34	LYS
20	AV	48	ALA
20	AV	66	PRO
20	AV	83	THR
20	AV	86	ARG
20	AV	95	LYS
20	AV	106	LEU
21	AW	11	GLU

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Mol	Chain	Res	Type
21	AW	31	ARG
21	AW	50	GLN
21	AW	54	HIS
21	AW	123	ASP
21	AW	169	GLU
21	AW	170	THR
22	AX	21	LEU
22	AX	67	VAL
23	AY	17	GLU
23	AY	66	ASN
24	AZ	39	ASP
24	AZ	53	LEU
25	Aa	3	GLU
25	Aa	7	PRO
25	Aa	21	VAL
25	Aa	48	ARG
25	Aa	50	VAL
25	Aa	51	ASP
25	Aa	56	VAL
26	Ab	20	ARG
27	Ac	18	ARG
27	Ac	28	ARG
27	Ac	31	PRO
27	Ac	32	ASN
27	Ac	48	VAL
27	Ac	52	VAL
28	Ad	3	ARG
28	Ad	5	TRP
28	Ad	14	LYS
28	Ad	19	ARG
29	Ae	32	LEU
29	Ae	34	TRP
29	Ae	52	LYS
30	Af	3	VAL
30	Af	7	VAL
30	Af	33	LYS
31	AI	23	SER
31	AI	55	LYS
31	AI	73	GLY
31	AI	91	LYS
31	AI	116	ILE
31	AI	136	ALA

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Mol	Chain	Res	Type
31	AI	154	GLY
32	AJ	66	THR
32	AJ	69	THR
32	AJ	74	ALA
32	AJ	86	LYS
32	AJ	90	LYS
35	BF	9	GLU
35	BF	29	ALA
35	BF	73	THR
35	BF	102	LEU
35	BF	151	GLY
35	BF	178	ARG
35	BF	190	THR
35	BF	227	GLY
36	BG	27	LYS
36	BG	30	ARG
36	BG	66	VAL
36	BG	74	GLY
36	BG	101	LEU
36	BG	158	GLY
36	BG	206	GLU
37	BH	4	TYR
37	BH	67	ILE
37	BH	73	ARG
37	BH	101	LEU
37	BH	107	ARG
37	BH	138	TYR
37	BH	139	ARG
37	BH	165	MET
37	BH	181	MET
37	BH	200	GLU
37	BH	208	SER
38	BI	37	ARG
38	BI	98	THR
38	BI	102	ALA
38	BI	104	ALA
39	BJ	13	ASN
39	BJ	14	LEU
39	BJ	51	PRO
39	BJ	83	ASP
40	BK	23	VAL
40	BK	56	GLN

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Mol	Chain	Res	Type
40	BK	72	ARG
40	BK	92	SER
40	BK	94	ARG
40	BK	112	PRO
40	BK	113	GLU
40	BK	146	GLU
40	BK	153	HIS
41	BL	37	ARG
41	BL	78	GLN
41	BL	97	VAL
41	BL	102	ARG
41	BL	108	GLY
41	BL	123	GLU
41	BL	134	ILE
42	BM	39	GLY
42	BM	68	GLY
42	BM	71	SER
42	BM	94	ALA
42	BM	104	ARG
42	BM	114	TYR
42	BM	120	ARG
42	BM	125	TYR
43	BN	31	GLY
43	BN	58	ASP
43	BN	61	GLU
43	BN	78	ASN
43	BN	94	VAL
44	BO	13	GLN
44	BO	55	LYS
44	BO	76	GLY
44	BO	102	GLY
44	BO	104	GLN
44	BO	115	PRO
45	BP	31	PRO
45	BP	41	ARG
45	BP	42	THR
45	BP	76	ASN
45	BP	87	GLY
45	BP	94	PRO
45	BP	126	LYS
46	BQ	46	LYS
46	BQ	64	TRP

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Mol	Chain	Res	Type
46	BQ	65	LYS
46	BQ	86	CYS
47	BR	5	ALA
47	BR	9	LYS
47	BR	17	LYS
47	BR	22	THR
47	BR	28	GLY
47	BR	56	VAL
48	BS	6	GLU
48	BS	46	HIS
48	BS	76	GLU
48	BS	83	GLU
48	BS	87	ILE
49	BT	30	GLY
49	BT	43	LYS
49	BT	82	GLN
50	BU	16	GLN
50	BU	33	GLY
50	BU	96	GLN
50	BU	98	LEU
51	BV	28	GLU
51	BV	34	TYR
51	BV	37	VAL
51	BV	38	GLU
51	BV	54	ARG
51	BV	64	ARG
52	BW	13	ASP
52	BW	20	LEU
52	BW	36	ARG
52	BW	65	ASN
52	BW	71	LEU
53	BX	49	ALA
53	BX	56	MET
53	BX	68	LYS
53	BX	101	GLY
53	BX	102	GLY
53	BX	103	GLY
54	BY	7	ARG
57	BZ	13	HIS
57	BZ	54	ILE
57	BZ	62	ALA
57	BZ	84	GLU

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Mol	Chain	Res	Type
57	BZ	91	MET
57	BZ	155	ASP
57	BZ	160	PHE
57	BZ	181	GLU
57	BZ	216	SER
57	BZ	217	TYR
57	BZ	218	VAL
57	BZ	236	GLN
57	BZ	246	THR
57	BZ	306	THR
57	BZ	316	SER
57	BZ	323	GLY
57	BZ	392	ILE
57	BZ	462	THR
57	BZ	468	THR
57	BZ	503	GLY
57	BZ	516	ALA
57	BZ	535	VAL
57	BZ	565	LEU
57	BZ	572	ILE
57	BZ	573	ASP
3	AC	59	ARG
3	AC	69	GLY
3	AC	78	ALA
3	AC	90	GLY
3	AC	167	LYS
3	AC	226	PRO
4	AD	56	GLY
4	AD	86	PRO
4	AD	226	MET
4	AD	227	ASN
4	AD	233	HIS
4	AD	245	PRO
4	AD	246	PRO
4	AD	259	THR
5	AE	51	PHE
5	AE	67	PHE
5	AE	75	VAL
5	AE	126	PRO
6	AF	21	ALA
6	AF	24	LEU
6	AF	72	ARG

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Mol	Chain	Res	Type
6	AF	159	GLY
7	AG	30	GLU
7	AG	57	ALA
7	AG	81	LYS
7	AG	106	LEU
7	AG	125	PHE
7	AG	167	GLU
7	AG	178	PHE
8	AH	67	LEU
8	AH	94	TYR
8	AH	114	VAL
9	AK	18	ALA
9	AK	29	LYS
9	AK	109	LYS
9	AK	138	LEU
10	AL	10	VAL
10	AL	59	LYS
10	AL	91	LEU
10	AL	92	GLU
10	AL	109	LYS
11	AM	16	ARG
11	AM	26	GLY
11	AM	37	GLY
11	AM	81	GLN
12	AN	26	TYR
12	AN	31	ASP
12	AN	46	GLN
12	AN	73	PRO
12	AN	115	MET
13	AO	5	LYS
13	AO	49	ASP
13	AO	58	GLY
13	AO	100	LEU
14	AP	10	ARG
14	AP	60	GLY
14	AP	66	ALA
14	AP	72	ALA
14	AP	102	ALA
15	AQ	4	GLY
15	AQ	28	VAL
15	AQ	102	ILE
16	AR	6	THR

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Mol	Chain	Res	Type
16	AR	96	ALA
16	AR	97	ASP
17	AS	29	PRO
18	AT	66	GLU
18	AT	67	ASP
19	AU	48	LYS
20	AV	16	ALA
20	AV	74	PRO
21	AW	64	GLY
21	AW	80	ARG
21	AW	82	ARG
21	AW	95	PRO
21	AW	131	ARG
21	AW	145	GLU
21	AW	160	GLY
22	AX	56	ASP
22	AX	83	PRO
25	Aa	27	THR
25	Aa	58	ARG
25	Aa	61	ARG
26	Ab	5	PRO
26	Ab	9	LYS
26	Ab	14	ALA
26	Ab	47	PRO
26	Ab	59	GLU
27	Ac	25	LYS
27	Ac	34	LEU
28	Ad	4	THR
28	Ad	11	LYS
28	Ad	31	LEU
28	Ad	39	ARG
28	Ad	40	TRP
28	Ad	46	VAL
29	Ae	13	ARG
29	Ae	18	ALA
29	Ae	41	ILE
29	Ae	53	PRO
29	Ae	57	ARG
29	Ae	61	LEU
31	AI	49	ALA
31	AI	104	ILE
32	AJ	22	PRO

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Mol	Chain	Res	Type
32	AJ	32	ALA
32	AJ	117	THR
35	BF	88	ALA
35	BF	96	ARG
35	BF	110	GLN
35	BF	141	GLU
35	BF	157	ARG
35	BF	180	LEU
35	BF	183	PRO
35	BF	237	ALA
36	BG	7	PRO
36	BG	49	SER
36	BG	62	ASP
36	BG	81	GLY
36	BG	127	ARG
36	BG	139	GLN
36	BG	145	GLY
36	BG	178	LEU
36	BG	181	ASN
37	BH	7	PRO
37	BH	40	PRO
37	BH	51	PRO
37	BH	53	ASP
37	BH	153	ARG
38	BI	26	PHE
38	BI	96	PRO
38	BI	112	LEU
39	BJ	12	PRO
39	BJ	15	ASP
39	BJ	17	SER
39	BJ	69	GLU
40	BK	6	ARG
40	BK	38	LEU
40	BK	103	TRP
40	BK	121	ALA
41	BL	24	THR
41	BL	39	LEU
41	BL	41	ARG
41	BL	44	PHE
41	BL	69	ARG
41	BL	73	ASP
41	BL	90	GLY

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Mol	Chain	Res	Type
42	BM	43	ALA
42	BM	47	LEU
42	BM	102	LEU
42	BM	103	THR
42	BM	105	ASP
42	BM	117	HIS
43	BN	77	PRO
44	BO	37	GLY
44	BO	53	SER
44	BO	93	GLN
44	BO	123	LYS
45	BP	23	LYS
45	BP	26	ALA
45	BP	80	HIS
45	BP	100	ILE
45	BP	105	TYR
45	BP	106	ASP
45	BP	107	ALA
45	BP	121	GLY
45	BP	122	THR
46	BQ	11	ARG
46	BQ	14	ARG
46	BQ	38	GLY
46	BQ	67	GLU
46	BQ	72	ALA
46	BQ	96	LEU
48	BS	19	PRO
48	BS	33	THR
48	BS	88	ARG
49	BT	28	ARG
49	BT	44	THR
49	BT	66	PRO
50	BU	14	LYS
51	BV	71	LYS
51	BV	72	ARG
51	BV	81	PHE
52	BW	25	LYS
52	BW	30	LEU
52	BW	52	TYR
53	BX	15	ARG
53	BX	24	LEU
53	BX	32	ALA

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Mol	Chain	Res	Type
53	BX	50	GLU
53	BX	57	ARG
53	BX	59	ALA
53	BX	76	ALA
53	BX	84	LEU
57	BZ	37	GLU
57	BZ	64	ILE
57	BZ	110	ARG
57	BZ	118	ALA
57	BZ	178	ASP
57	BZ	185	PRO
57	BZ	230	LYS
57	BZ	243	GLU
57	BZ	244	GLY
57	BZ	245	LYS
57	BZ	257	HIS
57	BZ	267	LEU
57	BZ	292	GLN
57	BZ	315	THR
57	BZ	317	PRO
57	BZ	324	LYS
57	BZ	409	GLU
57	BZ	428	ASN
57	BZ	434	LYS
57	BZ	471	HIS
57	BZ	485	ASN
57	BZ	539	THR
57	BZ	552	ASP
3	AC	56	GLN
3	AC	71	GLN
3	AC	148	ASN
4	AD	37	LEU
4	AD	209	ALA
4	AD	248	SER
4	AD	257	LEU
5	AE	28	ALA
5	AE	32	PRO
5	AE	53	PRO
5	AE	89	ASP
5	AE	94	GLU
5	AE	119	ARG
5	AE	135	HIS

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Mol	Chain	Res	Type
5	AE	143	ASN
5	AE	165	VAL
6	AF	64	ILE
6	AF	111	ALA
6	AF	137	LYS
6	AF	168	ARG
6	AF	183	VAL
7	AG	153	ARG
7	AG	166	ASP
8	AH	58	GLU
8	AH	138	LYS
8	AH	154	PRO
9	AK	28	THR
9	AK	90	MET
9	AK	108	PRO
10	AL	106	LEU
11	AM	9	ASN
11	AM	15	ARG
11	AM	25	SER
11	AM	35	HIS
11	AM	63	PRO
11	AM	89	ALA
11	AM	108	LYS
12	AN	22	LYS
12	AN	37	LEU
12	AN	79	LEU
12	AN	84	GLY
12	AN	89	ASN
12	AN	98	LYS
13	AO	12	ARG
13	AO	42	LYS
14	AP	59	LYS
14	AP	80	LEU
14	AP	89	ARG
15	AQ	9	LEU
15	AQ	77	PRO
15	AQ	96	ARG
15	AQ	110	ILE
15	AQ	111	ARG
15	AQ	112	ARG
16	AR	41	ALA
16	AR	60	LEU

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Mol	Chain	Res	Type
16	AR	72	HIS
16	AR	111	GLU
17	AS	2	PHE
19	AU	32	PRO
20	AV	85	VAL
21	AW	47	VAL
21	AW	113	ALA
23	AY	36	ILE
24	AZ	23	LEU
24	AZ	42	ALA
25	Aa	26	SER
25	Aa	41	PRO
25	Aa	52	THR
26	Ab	24	ALA
26	Ab	48	GLU
26	Ab	56	LYS
26	Ab	58	LEU
27	Ac	40	CYS
27	Ac	47	THR
28	Ad	35	ARG
30	Af	4	ARG
30	Af	12	ASP
30	Af	29	ASN
31	AI	21	GLN
31	AI	129	PRO
31	AI	144	ALA
32	AJ	28	GLY
32	AJ	95	LYS
35	BF	74	LYS
35	BF	91	PRO
35	BF	98	LEU
35	BF	150	SER
35	BF	158	LEU
35	BF	167	PRO
35	BF	174	VAL
35	BF	193	ASP
35	BF	229	VAL
36	BG	3	ASN
36	BG	16	ARG
36	BG	109	PRO
37	BH	36	ARG
37	BH	147	ALA

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Mol	Chain	Res	Type
37	BH	196	LEU
38	BI	53	LEU
38	BI	153	LYS
40	BK	32	ARG
40	BK	93	PRO
40	BK	97	GLN
40	BK	131	LYS
40	BK	155	ARG
41	BL	71	GLY
42	BM	55	ALA
42	BM	95	LYS
42	BM	110	GLU
42	BM	126	SER
43	BN	30	SER
43	BN	53	PRO
43	BN	54	PHE
44	BO	118	GLY
45	BP	16	GLU
45	BP	17	LYS
45	BP	70	ILE
46	BQ	5	ALA
47	BR	16	PHE
48	BS	5	LYS
48	BS	44	LYS
49	BT	54	GLU
49	BT	57	ARG
49	BT	64	ALA
50	BU	6	LEU
50	BU	53	LEU
52	BW	76	PRO
53	BX	58	LYS
53	BX	61	SER
53	BX	78	ALA
53	BX	97	ALA
54	BY	8	THR
54	BY	24	ARG
57	BZ	20	THR
57	BZ	24	LYS
57	BZ	51	GLU
57	BZ	76	PRO
57	BZ	269	GLU
57	BZ	286	ASP

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Mol	Chain	Res	Type
57	BZ	427	LYS
57	BZ	544	THR
57	BZ	592	LEU
3	AC	20	TYR
3	AC	84	LYS
3	AC	117	PRO
3	AC	200	LYS
4	AD	88	ARG
4	AD	208	LYS
4	AD	210	GLY
4	AD	231	HIS
5	AE	8	LYS
5	AE	58	ARG
5	AE	129	HIS
5	AE	179	GLU
6	AF	178	PRO
6	AF	182	ASN
6	AF	185	ASP
7	AG	7	LEU
7	AG	113	ARG
7	AG	135	LEU
8	AH	75	ALA
8	AH	175	LYS
9	AK	78	TYR
9	AK	87	LEU
9	AK	112	LEU
10	AL	67	LYS
11	AM	19	VAL
11	AM	31	ALA
11	AM	120	ALA
11	AM	131	SER
12	AN	62	GLY
12	AN	119	ARG
13	AO	74	LYS
15	AQ	13	ARG
16	AR	9	VAL
17	AS	66	ARG
19	AU	24	GLY
20	AV	17	SER
21	AW	85	HIS
21	AW	168	GLU
24	AZ	17	LYS

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Mol	Chain	Res	Type
25	Aa	24	THR
26	Ab	51	TYR
31	AI	51	LEU
31	AI	120	LYS
31	AI	128	LEU
31	AI	130	THR
32	AJ	12	LEU
32	AJ	100	THR
35	BF	75	LYS
36	BG	146	ALA
36	BG	174	PRO
38	BI	95	ALA
38	BI	113	ALA
39	BJ	36	ARG
40	BK	122	HIS
41	BL	65	TYR
41	BL	104	ARG
42	BM	52	ALA
42	BM	107	ARG
43	BN	73	ASP
45	BP	111	LYS
45	BP	123	LYS
46	BQ	45	VAL
47	BR	13	THR
48	BS	29	VAL
49	BT	36	ILE
51	BV	19	LYS
52	BW	11	VAL
52	BW	29	ARG
52	BW	67	VAL
52	BW	73	GLU
53	BX	25	ARG
53	BX	60	GLU
54	BY	10	ARG
54	BY	22	ARG
57	BZ	25	LEU
57	BZ	29	SER
57	BZ	35	ARG
57	BZ	69	ARG
57	BZ	132	ARG
57	BZ	137	PRO
57	BZ	157	GLN

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Mol	Chain	Res	Type
57	BZ	201	LEU
57	BZ	212	LEU
57	BZ	223	ILE
57	BZ	339	LEU
57	BZ	398	GLU
57	BZ	407	VAL
57	BZ	467	SER
57	BZ	469	PHE
57	BZ	482	GLN
57	BZ	518	VAL
57	BZ	537	CYS
57	BZ	549	SER
57	BZ	556	VAL
3	AC	49	ILE
4	AD	83	GLU
4	AD	238	GLY
4	AD	254	THR
6	AF	134	GLY
7	AG	44	GLY
8	AH	125	VAL
8	AH	131	VAL
8	AH	173	PRO
10	AL	115	VAL
12	AN	28	ALA
12	AN	47	ILE
12	AN	91	GLU
13	AO	61	HIS
15	AQ	80	SER
16	AR	7	GLY
25	Aa	2	LYS
25	Aa	22	ILE
25	Aa	29	PRO
26	Ab	27	PRO
26	Ab	31	VAL
26	Ab	49	CYS
29	Ae	8	LYS
29	Ae	14	VAL
29	Ae	20	GLY
29	Ae	31	HIS
29	Ae	33	ASN
32	AJ	19	PRO
32	AJ	52	ILE

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Mol	Chain	Res	Type
32	AJ	89	HIS
32	AJ	91	PRO
35	BF	20	GLU
35	BF	118	LEU
35	BF	176	GLU
36	BG	87	LEU
37	BH	94	LEU
37	BH	117	ALA
38	BI	142	LEU
39	BJ	37	VAL
40	BK	18	TYR
40	BK	50	ILE
40	BK	96	GLN
40	BK	130	GLY
41	BL	80	ILE
42	BM	57	GLY
43	BN	37	PRO
43	BN	41	PRO
44	BO	34	ASP
45	BP	90	VAL
46	BQ	20	THR
50	BU	17	LYS
50	BU	80	GLY
53	BX	20	LEU
53	BX	67	ALA
57	BZ	41	ARG
57	BZ	66	TRP
57	BZ	198	ASP
57	BZ	251	VAL
3	AC	41	VAL
4	AD	127	VAL
11	AM	53	GLY
12	AN	19	GLY
12	AN	61	GLY
16	AR	87	GLY
16	AR	105	VAL
20	AV	24	VAL
21	AW	141	VAL
24	AZ	43	ILE
31	AI	31	GLY
32	AJ	96	VAL
35	BF	130	ARG

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Mol	Chain	Res	Type
36	BG	70	VAL
37	BH	92	VAL
44	BO	49	GLY
46	BQ	60	VAL
47	BR	7	ILE
48	BS	82	ILE
57	BZ	162	ILE
57	BZ	222	GLY
57	BZ	435	GLY
5	AE	71	GLY
5	AE	116	VAL
5	AE	161	GLY
8	AH	76	VAL
9	AK	44	PRO
11	AM	97	PRO
12	AN	99	PRO
19	AU	43	VAL
22	AX	8	GLY
22	AX	73	GLY
24	AZ	45	GLY
32	AJ	49	GLY
37	BH	128	VAL
37	BH	143	GLY
39	BJ	26	ILE
46	BQ	95	GLY
48	BS	45	VAL
51	BV	51	LEU
53	BX	100	ILE
57	BZ	385	PRO
4	AD	142	VAL
8	AH	55	PRO
8	AH	126	PRO
12	AN	106	VAL
21	AW	167	PRO
36	BG	197	GLY
37	BH	136	PRO
45	BP	104	VAL
57	BZ	191	VAL
57	BZ	450	GLY
57	BZ	480	VAL
3	AC	14	VAL
8	AH	115	VAL

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Mol	Chain	Res	Type
12	AN	52	VAL
14	AP	69	VAL
17	AS	90	PRO
20	AV	44	ILE
21	AW	129	SER
21	AW	177	PRO
25	Aa	5	ILE
25	Aa	28	LYS
25	Aa	54	GLY
32	AJ	59	ILE
32	AJ	112	MET
35	BF	239	VAL
39	BJ	65	VAL
43	BN	91	PRO
45	BP	96	VAL
53	BX	41	ILE
57	BZ	134	GLY
57	BZ	233	PRO
11	AM	126	VAL
14	AP	70	GLY
18	AT	80	PRO
20	AV	18	GLY
35	BF	182	ILE
42	BM	90	PRO
44	BO	48	ILE

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	AC	180/180 (100%)	151 (84%)	29 (16%)	2 14
4	AD	215/215 (100%)	153 (71%)	62 (29%)	0 3
5	AE	166/166 (100%)	102 (61%)	64 (39%)	0 0
6	AF	164/164 (100%)	105 (64%)	59 (36%)	0 1
7	AG	156/156 (100%)	112 (72%)	44 (28%)	0 3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	143/143 (100%)	108 (76%)	35 (24%)	0	4
9	AK	118/118 (100%)	79 (67%)	39 (33%)	0	2
10	AL	100/100 (100%)	69 (69%)	31 (31%)	0	2
11	AM	111/111 (100%)	71 (64%)	40 (36%)	0	1
12	AN	106/106 (100%)	65 (61%)	41 (39%)	0	0
13	AO	100/100 (100%)	71 (71%)	29 (29%)	0	3
14	AP	87/87 (100%)	63 (72%)	24 (28%)	0	3
15	AQ	105/105 (100%)	68 (65%)	37 (35%)	0	1
16	AR	93/93 (100%)	64 (69%)	29 (31%)	0	2
17	AS	82/82 (100%)	57 (70%)	25 (30%)	0	2
18	AT	90/90 (100%)	64 (71%)	26 (29%)	0	2
19	AU	76/76 (100%)	57 (75%)	19 (25%)	0	4
20	AV	91/91 (100%)	72 (79%)	19 (21%)	1	7
21	AW	159/159 (100%)	120 (76%)	39 (24%)	0	4
22	AX	67/67 (100%)	51 (76%)	16 (24%)	0	5
23	AY	62/62 (100%)	44 (71%)	18 (29%)	0	3
24	AZ	51/51 (100%)	36 (71%)	15 (29%)	0	2
25	Aa	63/63 (100%)	45 (71%)	18 (29%)	0	3
26	Ab	50/50 (100%)	31 (62%)	19 (38%)	0	1
27	Ac	48/48 (100%)	32 (67%)	16 (33%)	0	2
28	Ad	42/42 (100%)	29 (69%)	13 (31%)	0	2
29	Ae	54/54 (100%)	44 (82%)	10 (18%)	1	10
30	Af	34/34 (100%)	29 (85%)	5 (15%)	3	16
32	AJ	101/101 (100%)	71 (70%)	30 (30%)	0	2
35	BF	202/202 (100%)	138 (68%)	64 (32%)	0	2
36	BG	160/160 (100%)	123 (77%)	37 (23%)	1	5
37	BH	180/180 (100%)	131 (73%)	49 (27%)	0	3
38	BI	115/115 (100%)	78 (68%)	37 (32%)	0	2
39	BJ	90/90 (100%)	61 (68%)	29 (32%)	0	2
40	BK	126/126 (100%)	93 (74%)	33 (26%)	0	4
41	BL	119/119 (100%)	86 (72%)	33 (28%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BM	98/98 (100%)	73 (74%)	25 (26%)	0	4
43	BN	88/88 (100%)	67 (76%)	21 (24%)	0	5
44	BO	90/90 (100%)	73 (81%)	17 (19%)	1	9
45	BP	104/104 (100%)	81 (78%)	23 (22%)	1	6
46	BQ	92/92 (100%)	67 (73%)	25 (27%)	0	3
47	BR	49/49 (100%)	36 (74%)	13 (26%)	0	4
48	BS	79/79 (100%)	64 (81%)	15 (19%)	1	9
49	BT	72/72 (100%)	49 (68%)	23 (32%)	0	2
50	BU	96/96 (100%)	67 (70%)	29 (30%)	0	2
51	BV	64/64 (100%)	48 (75%)	16 (25%)	0	4
52	BW	71/71 (100%)	52 (73%)	19 (27%)	0	3
53	BX	76/76 (100%)	59 (78%)	17 (22%)	1	6
54	BY	19/19 (100%)	17 (90%)	2 (10%)	7	26
57	BZ	486/514 (95%)	338 (70%)	148 (30%)	0	2
All	All	5390/5418 (100%)	3864 (72%)	1526 (28%)	2	3

All (1526) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	AC	6	ARG
3	AC	7	TYR
3	AC	15	ASP
3	AC	20	TYR
3	AC	27	HIS
3	AC	46	LYS
3	AC	47	LEU
3	AC	58	VAL
3	AC	59	ARG
3	AC	70	LYS
3	AC	81	GLU
3	AC	92	ASP
3	AC	99	ILE
3	AC	101	GLN
3	AC	102	LYS
3	AC	111	ASP
3	AC	125	SER
3	AC	130	ILE

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Mol	Chain	Res	Type
3	AC	144	THR
3	AC	160	ARG
3	AC	161	ILE
3	AC	163	PHE
3	AC	164	ARG
3	AC	166	ASP
3	AC	180	PHE
3	AC	190	ARG
3	AC	202	GLU
3	AC	212	VAL
3	AC	213	TYR
4	AD	23	GLU
4	AD	31	LYS
4	AD	34	VAL
4	AD	37	LEU
4	AD	39	LYS
4	AD	44	ASN
4	AD	46	GLN
4	AD	51	VAL
4	AD	52	ARG
4	AD	53	PHE
4	AD	59	LYS
4	AD	63	ARG
4	AD	70	TRP
4	AD	73	VAL
4	AD	84	TYR
4	AD	87	ASN
4	AD	88	ARG
4	AD	91	ARG
4	AD	92	ILE
4	AD	94	LEU
4	AD	95	LEU
4	AD	101	GLU
4	AD	106	ILE
4	AD	109	ASP
4	AD	115	GLN
4	AD	116	GLN
4	AD	118	VAL
4	AD	121	PRO
4	AD	131	LEU
4	AD	134	ARG
4	AD	145	VAL

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Mol	Chain	Res	Type
4	AD	146	GLU
4	AD	147	LEU
4	AD	155	LEU
4	AD	169	GLU
4	AD	175	LEU
4	AD	176	ARG
4	AD	179	SER
4	AD	181	GLU
4	AD	186	HIS
4	AD	188	GLU
4	AD	190	TYR
4	AD	200	ASP
4	AD	202	LYS
4	AD	206	LEU
4	AD	217	ARG
4	AD	220	HIS
4	AD	230	ASP
4	AD	232	PRO
4	AD	233	HIS
4	AD	239	ARG
4	AD	249	PRO
4	AD	250	TRP
4	AD	252	TRP
4	AD	253	GLN
4	AD	254	THR
4	AD	258	LYS
4	AD	259	THR
4	AD	260	ARG
4	AD	264	LYS
4	AD	270	ILE
4	AD	273	ARG
5	AE	1	MET
5	AE	2	LYS
5	AE	4	ILE
5	AE	5	LEU
5	AE	7	VAL
5	AE	8	LYS
5	AE	12	THR
5	AE	13	ARG
5	AE	14	ILE
5	AE	17	ASP
5	AE	22	PRO

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Mol	Chain	Res	Type
5	AE	38	THR
5	AE	40	GLU
5	AE	41	LYS
5	AE	44	TYR
5	AE	45	THR
5	AE	48	GLN
5	AE	49	LEU
5	AE	51	PHE
5	AE	52	LEU
5	AE	53	PRO
5	AE	56	PRO
5	AE	66	HIS
5	AE	77	ILE
5	AE	78	LEU
5	AE	80	GLU
5	AE	83	ASP
5	AE	91	VAL
5	AE	96	PHE
5	AE	108	SER
5	AE	111	ARG
5	AE	113	PHE
5	AE	118	LYS
5	AE	119	ARG
5	AE	120	TRP
5	AE	121	ASN
5	AE	122	PHE
5	AE	126	PRO
5	AE	129	HIS
5	AE	135	HIS
5	AE	136	ARG
5	AE	137	HIS
5	AE	141	ILE
5	AE	143	ASN
5	AE	149	ARG
5	AE	150	VAL
5	AE	152	LYS
5	AE	154	LYS
5	AE	163	GLU
5	AE	164	ARG
5	AE	165	VAL
5	AE	169	ASN
5	AE	170	LEU

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Mol	Chain	Res	Type
5	AE	171	GLU
5	AE	173	VAL
5	AE	176	ILE
5	AE	180	ASN
5	AE	181	LEU
5	AE	184	VAL
5	AE	185	LYS
5	AE	195	LEU
5	AE	197	ILE
5	AE	199	ARG
5	AE	202	LYS
6	AF	8	GLN
6	AF	14	PRO
6	AF	17	ARG
6	AF	19	GLU
6	AF	23	ASP
6	AF	27	GLU
6	AF	29	ASN
6	AF	30	PRO
6	AF	31	HIS
6	AF	33	LEU
6	AF	34	TRP
6	AF	35	GLU
6	AF	39	TRP
6	AF	46	ARG
6	AF	60	SER
6	AF	64	ILE
6	AF	67	GLN
6	AF	69	HIS
6	AF	74	ARG
6	AF	75	HIS
6	AF	77	ASP
6	AF	78	ILE
6	AF	82	ILE
6	AF	83	PHE
6	AF	95	ARG
6	AF	99	TYR
6	AF	102	PRO
6	AF	105	VAL
6	AF	106	ARG
6	AF	108	LYS
6	AF	117	ARG

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Mol	Chain	Res	Type
6	AF	119	ARG
6	AF	120	GLU
6	AF	122	LYS
6	AF	126	VAL
6	AF	127	GLU
6	AF	133	ASN
6	AF	137	LYS
6	AF	138	GLU
6	AF	140	LEU
6	AF	152	GLU
6	AF	155	LEU
6	AF	157	VAL
6	AF	158	THR
6	AF	168	ARG
6	AF	170	LEU
6	AF	172	TRP
6	AF	175	THR
6	AF	178	PRO
6	AF	181	LEU
6	AF	184	TYR
6	AF	185	ASP
6	AF	188	ARG
6	AF	192	LEU
6	AF	197	ASP
6	AF	200	GLU
6	AF	202	PHE
6	AF	203	GLN
6	AF	204	ASN
7	AG	8	LYS
7	AG	12	TYR
7	AG	16	ARG
7	AG	20	ILE
7	AG	21	ARG
7	AG	22	ARG
7	AG	25	TYR
7	AG	32	PRO
7	AG	33	ARG
7	AG	34	LEU
7	AG	36	LYS
7	AG	39	ILE
7	AG	41	GLN
7	AG	51	ARG

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Mol	Chain	Res	Type
7	AG	54	GLU
7	AG	68	PRO
7	AG	77	ILE
7	AG	82	LEU
7	AG	91	ARG
7	AG	94	LEU
7	AG	96	ARG
7	AG	97	ASP
7	AG	101	ILE
7	AG	102	PHE
7	AG	103	LEU
7	AG	117	PHE
7	AG	120	LEU
7	AG	126	ASP
7	AG	128	ARG
7	AG	131	TYR
7	AG	133	LEU
7	AG	135	LEU
7	AG	139	LEU
7	AG	143	GLU
7	AG	146	TYR
7	AG	148	MET
7	AG	150	ASP
7	AG	152	LEU
7	AG	153	ARG
7	AG	155	MET
7	AG	170	ARG
7	AG	174	GLU
7	AG	180	PHE
7	AG	181	ARG
8	AH	7	LEU
8	AH	11	VAL
8	AH	13	LYS
8	AH	18	GLU
8	AH	23	ARG
8	AH	25	LYS
8	AH	32	GLU
8	AH	35	VAL
8	AH	40	GLU
8	AH	46	GLU
8	AH	50	VAL
8	AH	52	VAL

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Mol	Chain	Res	Type
8	AH	68	THR
8	AH	69	ARG
8	AH	74	ASN
8	AH	83	TYR
8	AH	90	LYS
8	AH	94	TYR
8	AH	95	ARG
8	AH	103	LEU
8	AH	105	LEU
8	AH	111	HIS
8	AH	115	VAL
8	AH	116	GLU
8	AH	131	VAL
8	AH	132	ARG
8	AH	136	ILE
8	AH	153	LYS
8	AH	157	TYR
8	AH	158	HIS
8	AH	164	TYR
8	AH	167	GLU
8	AH	168	PRO
8	AH	172	LYS
8	AH	175	LYS
9	AK	7	LYS
9	AK	8	GLN
9	AK	12	ARG
9	AK	13	TRP
9	AK	15	LEU
9	AK	16	ILE
9	AK	17	ASP
9	AK	22	THR
9	AK	25	ARG
9	AK	28	THR
9	AK	32	THR
9	AK	33	LEU
9	AK	37	LYS
9	AK	38	HIS
9	AK	39	ARG
9	AK	42	TRP
9	AK	43	THR
9	AK	45	ASN
9	AK	52	VAL

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Mol	Chain	Res	Type
9	AK	55	VAL
9	AK	69	GLN
9	AK	72	TYR
9	AK	75	TYR
9	AK	78	TYR
9	AK	79	PRO
9	AK	82	LEU
9	AK	85	ILE
9	AK	89	LYS
9	AK	90	MET
9	AK	91	LEU
9	AK	98	VAL
9	AK	101	HIS
9	AK	109	LYS
9	AK	119	ARG
9	AK	122	VAL
9	AK	127	ASP
9	AK	131	GLN
9	AK	134	ARG
9	AK	136	GLU
10	AL	1	MET
10	AL	3	GLN
10	AL	6	THR
10	AL	7	TYR
10	AL	8	LEU
10	AL	12	ASP
10	AL	14	THR
10	AL	21	CYS
10	AL	23	ARG
10	AL	24	VAL
10	AL	28	SER
10	AL	29	ASN
10	AL	34	THR
10	AL	38	VAL
10	AL	39	ILE
10	AL	42	SER
10	AL	47	ILE
10	AL	56	ASP
10	AL	58	VAL
10	AL	59	LYS
10	AL	64	ARG
10	AL	65	THR

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Mol	Chain	Res	Type
10	AL	77	ILE
10	AL	78	ARG
10	AL	82	ASN
10	AL	89	ASN
10	AL	92	GLU
10	AL	94	ARG
10	AL	97	ARG
10	AL	114	ILE
10	AL	116	SER
11	AM	7	ARG
11	AM	13	ASN
11	AM	17	LYS
11	AM	29	LYS
11	AM	30	THR
11	AM	33	ARG
11	AM	40	SER
11	AM	41	ARG
11	AM	45	LEU
11	AM	46	LYS
11	AM	48	PRO
11	AM	49	ARG
11	AM	52	GLU
11	AM	55	ARG
11	AM	59	LEU
11	AM	60	MET
11	AM	64	LYS
11	AM	65	ARG
11	AM	68	GLN
11	AM	74	GLU
11	AM	75	ILE
11	AM	79	ARG
11	AM	84	ASN
11	AM	88	LEU
11	AM	94	GLU
11	AM	99	LEU
11	AM	105	LEU
11	AM	108	LYS
11	AM	110	TYR
11	AM	114	ILE
11	AM	117	GLU
11	AM	122	PRO
11	AM	123	LEU

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Mol	Chain	Res	Type
11	AM	126	VAL
11	AM	128	HIS
11	AM	130	PHE
11	AM	137	LYS
11	AM	138	LEU
11	AM	147	LEU
11	AM	149	GLU
12	AN	6	ARG
12	AN	12	GLN
12	AN	14	ARG
12	AN	18	LYS
12	AN	26	TYR
12	AN	32	TYR
12	AN	34	LEU
12	AN	41	TRP
12	AN	42	ILE
12	AN	43	THR
12	AN	45	GLN
12	AN	48	GLU
12	AN	51	ARG
12	AN	56	ARG
12	AN	60	ARG
12	AN	63	LYS
12	AN	64	ILE
12	AN	65	PHE
12	AN	71	ASP
12	AN	74	TYR
12	AN	76	LYS
12	AN	79	LEU
12	AN	80	GLU
12	AN	83	MET
12	AN	89	ASN
12	AN	97	VAL
12	AN	98	LYS
12	AN	101	ARG
12	AN	104	PHE
12	AN	105	GLU
12	AN	109	VAL
12	AN	112	GLU
12	AN	118	LEU
12	AN	124	LYS
12	AN	126	PRO

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Mol	Chain	Res	Type
12	AN	127	ILE
12	AN	130	LYS
12	AN	133	ARG
12	AN	135	ASP
12	AN	137	TYR
12	AN	139	GLU
13	AO	4	LEU
13	AO	5	LYS
13	AO	10	LEU
13	AO	11	ASN
13	AO	13	HIS
13	AO	17	ARG
13	AO	18	LEU
13	AO	23	ASN
13	AO	37	THR
13	AO	49	ASP
13	AO	52	ILE
13	AO	56	LYS
13	AO	57	ARG
13	AO	59	ASP
13	AO	60	LEU
13	AO	64	ARG
13	AO	74	LYS
13	AO	77	ARG
13	AO	79	LEU
13	AO	80	PHE
13	AO	82	GLU
13	AO	86	ARG
13	AO	88	ARG
13	AO	89	ASP
13	AO	99	LYS
13	AO	100	LEU
13	AO	105	ARG
13	AO	113	LEU
13	AO	116	LEU
14	AP	3	ARG
14	AP	9	ARG
14	AP	11	LYS
14	AP	12	PHE
14	AP	20	ARG
14	AP	21	THR
14	AP	23	ARG

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Mol	Chain	Res	Type
14	AP	26	LEU
14	AP	27	SER
14	AP	29	PHE
14	AP	36	TYR
14	AP	38	GLN
14	AP	42	ASP
14	AP	57	LYS
14	AP	73	LEU
14	AP	76	LYS
14	AP	78	LEU
14	AP	80	LEU
14	AP	88	ASP
14	AP	94	TYR
14	AP	97	ARG
14	AP	98	VAL
14	AP	106	ARG
14	AP	112	PHE
15	AQ	1	MET
15	AQ	20	PRO
15	AQ	22	PHE
15	AQ	23	ARG
15	AQ	30	VAL
15	AQ	32	TYR
15	AQ	39	ARG
15	AQ	43	GLN
15	AQ	46	GLU
15	AQ	50	ILE
15	AQ	53	ARG
15	AQ	54	ARG
15	AQ	55	ASN
15	AQ	57	PHE
15	AQ	58	ASN
15	AQ	61	PHE
15	AQ	62	THR
15	AQ	64	ARG
15	AQ	66	VAL
15	AQ	68	TYR
15	AQ	75	ILE
15	AQ	78	LEU
15	AQ	79	HIS
15	AQ	82	LEU
15	AQ	85	LYS

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Mol	Chain	Res	Type
15	AQ	88	ILE
15	AQ	93	ARG
15	AQ	95	ARG
15	AQ	96	ARG
15	AQ	101	PHE
15	AQ	102	ILE
15	AQ	103	ARG
15	AQ	106	SER
15	AQ	107	ASP
15	AQ	108	ARG
15	AQ	109	GLU
15	AQ	117	ASP
16	AR	6	THR
16	AR	13	LYS
16	AR	16	LYS
16	AR	19	LYS
16	AR	25	TRP
16	AR	27	LEU
16	AR	32	PHE
16	AR	36	ARG
16	AR	38	THR
16	AR	50	ARG
16	AR	52	ARG
16	AR	53	ARG
16	AR	54	LYS
16	AR	55	ARG
16	AR	58	ARG
16	AR	65	ILE
16	AR	70	ARG
16	AR	75	ASN
16	AR	77	SER
16	AR	81	HIS
16	AR	83	LEU
16	AR	88	ILE
16	AR	92	ARG
16	AR	93	LYS
16	AR	97	ASP
16	AR	105	VAL
16	AR	106	PHE
16	AR	108	GLU
16	AR	114	LYS
17	AS	4	ILE

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Mol	Chain	Res	Type
17	AS	13	ARG
17	AS	15	GLU
17	AS	18	LEU
17	AS	20	LEU
17	AS	21	ARG
17	AS	29	PRO
17	AS	35	LEU
17	AS	36	PRO
17	AS	40	LEU
17	AS	43	GLU
17	AS	44	LYS
17	AS	45	THR
17	AS	49	THR
17	AS	52	VAL
17	AS	56	SER
17	AS	60	GLU
17	AS	64	HIS
17	AS	78	LYS
17	AS	79	VAL
17	AS	83	ARG
17	AS	84	LYS
17	AS	87	HIS
17	AS	93	GLU
17	AS	100	ARG
18	AT	4	LYS
18	AT	8	ARG
18	AT	10	VAL
18	AT	11	ARG
18	AT	12	ILE
18	AT	16	LYS
18	AT	18	ARG
18	AT	24	ILE
18	AT	31	GLU
18	AT	33	ARG
18	AT	40	ASN
18	AT	42	ARG
18	AT	45	TYR
18	AT	47	VAL
18	AT	60	ASN
18	AT	67	ASP
18	AT	71	VAL
18	AT	82	LEU

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Mol	Chain	Res	Type
18	AT	87	PRO
18	AT	88	ARG
18	AT	90	ARG
18	AT	94	ASP
18	AT	95	ILE
18	AT	98	LYS
18	AT	103	ILE
18	AT	106	ILE
19	AU	8	ILE
19	AU	9	LEU
19	AU	13	LEU
19	AU	14	SER
19	AU	16	LYS
19	AU	23	GLU
19	AU	28	PHE
19	AU	36	LYS
19	AU	37	THR
19	AU	38	GLU
19	AU	45	THR
19	AU	47	PHE
19	AU	50	LYS
19	AU	55	ASN
19	AU	63	LYS
19	AU	65	ARG
19	AU	73	ARG
19	AU	83	VAL
19	AU	92	LEU
20	AV	12	THR
20	AV	13	VAL
20	AV	14	LEU
20	AV	19	LYS
20	AV	26	LYS
20	AV	28	LYS
20	AV	35	TYR
20	AV	42	VAL
20	AV	60	PHE
20	AV	64	GLU
20	AV	73	ARG
20	AV	75	ILE
20	AV	84	ARG
20	AV	89	PHE
20	AV	90	LEU

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Mol	Chain	Res	Type
20	AV	91	GLU
20	AV	102	CYS
20	AV	107	ASP
20	AV	109	GLU
21	AW	3	TYR
21	AW	8	TYR
21	AW	13	GLU
21	AW	14	LYS
21	AW	28	MET
21	AW	30	ASN
21	AW	44	PHE
21	AW	45	ASP
21	AW	49	ARG
21	AW	50	GLN
21	AW	53	ILE
21	AW	55	HIS
21	AW	58	VAL
21	AW	60	GLU
21	AW	62	PRO
21	AW	63	ASP
21	AW	70	LEU
21	AW	78	LYS
21	AW	80	ARG
21	AW	83	PRO
21	AW	86	VAL
21	AW	87	ASP
21	AW	89	PHE
21	AW	90	VAL
21	AW	95	PRO
21	AW	104	PHE
21	AW	108	PRO
21	AW	120	ILE
21	AW	129	SER
21	AW	140	ASP
21	AW	151	HIS
21	AW	155	LEU
21	AW	159	PRO
21	AW	163	LEU
21	AW	168	GLU
21	AW	171	ILE
21	AW	174	VAL
21	AW	175	VAL

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Mol	Chain	Res	Type
21	AW	179	ASP
22	AX	10	THR
22	AX	20	ARG
22	AX	26	TYR
22	AX	29	GLN
22	AX	30	VAL
22	AX	32	ARG
22	AX	36	ILE
22	AX	37	LEU
22	AX	40	GLN
22	AX	41	ARG
22	AX	46	LYS
22	AX	57	PHE
22	AX	58	THR
22	AX	64	ASP
22	AX	68	GLU
22	AX	74	ARG
23	AY	1	MET
23	AY	2	ARG
23	AY	6	GLU
23	AY	12	SER
23	AY	19	LEU
23	AY	22	GLU
23	AY	25	ARG
23	AY	30	LEU
23	AY	32	PHE
23	AY	33	GLN
23	AY	35	SER
23	AY	45	ILE
23	AY	50	ARG
23	AY	56	LEU
23	AY	58	VAL
23	AY	64	ARG
23	AY	65	GLN
23	AY	66	ASN
24	AZ	3	ARG
24	AZ	5	LYS
24	AZ	6	VAL
24	AZ	12	PRO
24	AZ	15	TYR
24	AZ	26	LEU
24	AZ	28	LEU

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Mol	Chain	Res	Type
24	AZ	30	ARG
24	AZ	31	LEU
24	AZ	32	GLN
24	AZ	35	ARG
24	AZ	37	LEU
24	AZ	41	PRO
24	AZ	55	ARG
24	AZ	59	VAL
25	Aa	3	GLU
25	Aa	11	PRO
25	Aa	14	ILE
25	Aa	16	CYS
25	Aa	23	GLU
25	Aa	24	THR
25	Aa	27	THR
25	Aa	29	PRO
25	Aa	31	ILE
25	Aa	32	TYR
25	Aa	37	SER
25	Aa	47	GLN
25	Aa	49	PHE
25	Aa	57	GLU
25	Aa	59	PHE
25	Aa	60	GLN
25	Aa	62	ARG
25	Aa	68	ARG
26	Ab	4	HIS
26	Ab	9	LYS
26	Ab	11	THR
26	Ab	13	LYS
26	Ab	15	ARG
26	Ab	17	ASP
26	Ab	20	ARG
26	Ab	25	LEU
26	Ab	26	THR
26	Ab	30	LEU
26	Ab	33	CYS
26	Ab	36	CYS
26	Ab	37	LYS
26	Ab	39	MET
26	Ab	43	HIS
26	Ab	49	CYS

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Mol	Chain	Res	Type
26	Ab	51	TYR
26	Ab	55	ARG
26	Ab	59	GLU
27	Ac	11	LEU
27	Ac	13	CYS
27	Ac	19	ARG
27	Ac	21	TYR
27	Ac	29	ASN
27	Ac	30	THR
27	Ac	31	PRO
27	Ac	32	ASN
27	Ac	33	LYS
27	Ac	38	LYS
27	Ac	40	CYS
27	Ac	42	TRP
27	Ac	43	CYS
27	Ac	46	HIS
27	Ac	51	GLU
27	Ac	54	ILE
28	Ad	3	ARG
28	Ad	5	TRP
28	Ad	6	GLN
28	Ad	8	ASN
28	Ad	12	ARG
28	Ad	19	ARG
28	Ad	21	ARG
28	Ad	24	THR
28	Ad	34	ARG
28	Ad	36	GLN
28	Ad	41	ARG
28	Ad	46	VAL
28	Ad	48	LYS
29	Ae	5	LYS
29	Ae	8	LYS
29	Ae	16	ILE
29	Ae	33	ASN
29	Ae	39	LYS
29	Ae	42	ARG
29	Ae	44	LYS
29	Ae	50	LEU
29	Ae	59	LYS
29	Ae	62	LEU

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Mol	Chain	Res	Type
30	Af	10	ILE
30	Af	12	ASP
30	Af	17	ILE
30	Af	19	ARG
30	Af	27	CYS
32	AJ	5	VAL
32	AJ	9	LYS
32	AJ	10	LEU
32	AJ	16	LYS
32	AJ	18	THR
32	AJ	29	GLN
32	AJ	30	HIS
32	AJ	34	ILE
32	AJ	35	MET
32	AJ	39	LYS
32	AJ	50	ASP
32	AJ	59	ILE
32	AJ	62	ASP
32	AJ	63	ARG
32	AJ	64	SER
32	AJ	65	PHE
32	AJ	66	THR
32	AJ	69	THR
32	AJ	70	LYS
32	AJ	76	TYR
32	AJ	77	LEU
32	AJ	79	ARG
32	AJ	85	GLU
32	AJ	86	LYS
32	AJ	95	LYS
32	AJ	109	LYS
32	AJ	114	ASP
32	AJ	117	THR
32	AJ	120	LEU
32	AJ	121	GLU
35	BF	10	LEU
35	BF	11	LEU
35	BF	17	PHE
35	BF	20	GLU
35	BF	21	ARG
35	BF	23	ARG
35	BF	25	ASN

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Mol	Chain	Res	Type
35	BF	26	PRO
35	BF	35	GLU
35	BF	36	ARG
35	BF	40	HIS
35	BF	44	LEU
35	BF	48	MET
35	BF	49	GLU
35	BF	52	GLU
35	BF	56	ARG
35	BF	57	PHE
35	BF	61	LEU
35	BF	64	ARG
35	BF	69	LEU
35	BF	70	PHE
35	BF	74	LYS
35	BF	75	LYS
35	BF	80	ILE
35	BF	84	GLU
35	BF	91	PRO
35	BF	92	TYR
35	BF	96	ARG
35	BF	101	MET
35	BF	102	LEU
35	BF	105	PHE
35	BF	111	ARG
35	BF	114	ARG
35	BF	118	LEU
35	BF	122	PHE
35	BF	131	PRO
35	BF	132	LYS
35	BF	134	GLU
35	BF	135	GLN
35	BF	137	ARG
35	BF	147	LYS
35	BF	148	TYR
35	BF	152	PHE
35	BF	153	ARG
35	BF	154	LEU
35	BF	158	LEU
35	BF	162	ILE
35	BF	168	THR
35	BF	169	LYS

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Mol	Chain	Res	Type
35	BF	172	ILE
35	BF	181	PHE
35	BF	182	ILE
35	BF	185	ILE
35	BF	187	LEU
35	BF	189	ASP
35	BF	191	ASP
35	BF	194	PRO
35	BF	195	ASP
35	BF	196	LEU
35	BF	204	ASN
35	BF	209	ARG
35	BF	212	GLN
35	BF	217	ARG
35	BF	222	ILE
36	BG	5	ILE
36	BG	8	ILE
36	BG	10	PHE
36	BG	15	THR
36	BG	23	TYR
36	BG	29	TYR
36	BG	30	ARG
36	BG	33	LEU
36	BG	35	GLU
36	BG	38	ARG
36	BG	46	GLU
36	BG	48	TYR
36	BG	52	LEU
36	BG	59	ARG
36	BG	67	THR
36	BG	82	GLU
36	BG	89	GLU
36	BG	91	LEU
36	BG	95	THR
36	BG	97	LYS
36	BG	107	GLN
36	BG	125	GLU
36	BG	136	GLN
36	BG	139	GLN
36	BG	140	ARG
36	BG	142	MET
36	BG	164	ARG

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Mol	Chain	Res	Type
36	BG	176	HIS
36	BG	178	LEU
36	BG	184	TYR
36	BG	186	PHE
36	BG	190	ARG
36	BG	193	TYR
36	BG	195	VAL
36	BG	196	LEU
36	BG	201	TYR
36	BG	204	LEU
37	BH	5	ILE
37	BH	8	VAL
37	BH	9	CYS
37	BH	10	ARG
37	BH	14	ARG
37	BH	15	GLU
37	BH	20	TYR
37	BH	24	GLU
37	BH	25	ARG
37	BH	26	CYS
37	BH	29	PRO
37	BH	31	CYS
37	BH	33	MET
37	BH	47	ARG
37	BH	51	PRO
37	BH	57	ARG
37	BH	59	ARG
37	BH	61	LYS
37	BH	63	LYS
37	BH	68	TYR
37	BH	78	LEU
37	BH	79	PHE
37	BH	83	SER
37	BH	85	LYS
37	BH	107	ARG
37	BH	108	LEU
37	BH	114	ARG
37	BH	116	GLN
37	BH	120	LEU
37	BH	131	ARG
37	BH	135	LEU
37	BH	138	TYR

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Mol	Chain	Res	Type
37	BH	141	ARG
37	BH	142	PRO
37	BH	146	ILE
37	BH	154	ASN
37	BH	155	LEU
37	BH	168	ARG
37	BH	173	TRP
37	BH	175	SER
37	BH	176	LEU
37	BH	178	VAL
37	BH	181	MET
37	BH	182	LYS
37	BH	190	ASP
37	BH	191	ARG
37	BH	193	ASP
37	BH	196	LEU
37	BH	198	VAL
38	BI	5	ASP
38	BI	6	PHE
38	BI	7	GLU
38	BI	15	ARG
38	BI	16	THR
38	BI	25	ARG
38	BI	26	PHE
38	BI	27	ARG
38	BI	28	PHE
38	BI	31	LEU
38	BI	34	VAL
38	BI	41	VAL
38	BI	56	GLN
38	BI	60	TYR
38	BI	63	ARG
38	BI	64	ARG
38	BI	67	VAL
38	BI	73	ASN
38	BI	78	HIS
38	BI	79	GLU
38	BI	80	ILE
38	BI	81	GLU
38	BI	89	ILE
38	BI	91	LEU
38	BI	101	ILE

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Mol	Chain	Res	Type
38	BI	105	VAL
38	BI	111	GLU
38	BI	112	LEU
38	BI	119	LEU
38	BI	121	LYS
38	BI	128	PRO
38	BI	131	ILE
38	BI	133	TYR
38	BI	141	GLN
38	BI	143	ARG
38	BI	150	ARG
38	BI	152	ARG
39	BJ	2	ARG
39	BJ	4	TYR
39	BJ	5	GLU
39	BJ	6	VAL
39	BJ	8	ILE
39	BJ	10	LEU
39	BJ	14	LEU
39	BJ	28	ARG
39	BJ	37	VAL
39	BJ	40	VAL
39	BJ	47	ARG
39	BJ	48	LEU
39	BJ	50	TYR
39	BJ	55	ASP
39	BJ	57	GLN
39	BJ	60	PHE
39	BJ	65	VAL
39	BJ	66	GLU
39	BJ	67	MET
39	BJ	69	GLU
39	BJ	74	ASP
39	BJ	75	LEU
39	BJ	79	LEU
39	BJ	83	ASP
39	BJ	88	VAL
39	BJ	94	GLN
39	BJ	95	GLU
39	BJ	98	LEU
39	BJ	100	ASN
40	BK	5	ARG

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Mol	Chain	Res	Type
40	BK	6	ARG
40	BK	10	ARG
40	BK	12	LEU
40	BK	14	PRO
40	BK	17	VAL
40	BK	18	TYR
40	BK	22	LEU
40	BK	47	CYS
40	BK	51	GLN
40	BK	54	THR
40	BK	56	GLN
40	BK	69	VAL
40	BK	72	ARG
40	BK	74	GLU
40	BK	89	MET
40	BK	99	LEU
40	BK	101	LEU
40	BK	103	TRP
40	BK	106	GLN
40	BK	111	ARG
40	BK	113	GLU
40	BK	123	GLU
40	BK	124	LEU
40	BK	126	ASP
40	BK	136	LYS
40	BK	139	GLU
40	BK	143	ARG
40	BK	146	GLU
40	BK	149	ARG
40	BK	153	HIS
40	BK	155	ARG
40	BK	156	TRP
41	BL	4	ASP
41	BL	6	ILE
41	BL	14	ARG
41	BL	18	ARG
41	BL	25	ASP
41	BL	26	VAL
41	BL	31	PHE
41	BL	32	LYS
41	BL	33	GLU
41	BL	36	LEU

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Mol	Chain	Res	Type
41	BL	37	ARG
41	BL	39	LEU
41	BL	41	ARG
41	BL	45	ILE
41	BL	49	GLU
41	BL	50	ARG
41	BL	54	ASP
41	BL	63	LEU
41	BL	70	GLN
41	BL	84	ARG
41	BL	88	LYS
41	BL	92	ARG
41	BL	98	LYS
41	BL	100	ILE
41	BL	102	ARG
41	BL	103	VAL
41	BL	104	ARG
41	BL	107	LEU
41	BL	111	ILE
41	BL	119	LEU
41	BL	122	ARG
41	BL	126	LYS
41	BL	136	GLU
42	BM	4	TYR
42	BM	5	TYR
42	BM	11	LYS
42	BM	12	GLU
42	BM	19	LEU
42	BM	21	PRO
42	BM	23	ASN
42	BM	32	ASP
42	BM	33	PHE
42	BM	37	PHE
42	BM	47	LEU
42	BM	51	ARG
42	BM	54	ASP
42	BM	63	ILE
42	BM	64	THR
42	BM	75	ASP
42	BM	79	LEU
42	BM	89	ASN
42	BM	101	PHE

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Mol	Chain	Res	Type
42	BM	102	LEU
42	BM	105	ASP
42	BM	110	GLU
42	BM	113	LYS
42	BM	116	LYS
42	BM	117	HIS
43	BN	3	LYS
43	BN	4	ILE
43	BN	5	ARG
43	BN	9	ARG
43	BN	11	PHE
43	BN	14	LYS
43	BN	33	GLN
43	BN	45	ARG
43	BN	47	PHE
43	BN	49	VAL
43	BN	60	ARG
43	BN	62	HIS
43	BN	63	PHE
43	BN	73	ASP
43	BN	78	ASN
43	BN	79	ARG
43	BN	81	THR
43	BN	83	GLU
43	BN	85	LEU
43	BN	95	GLU
43	BN	99	LYS
44	BO	13	GLN
44	BO	18	ARG
44	BO	22	HIS
44	BO	34	ASP
44	BO	39	PRO
44	BO	40	ILE
44	BO	42	TRP
44	BO	50	TYR
44	BO	62	GLN
44	BO	67	ASP
44	BO	78	GLN
44	BO	81	ASP
44	BO	99	GLN
44	BO	104	GLN
44	BO	116	HIS

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Mol	Chain	Res	Type
44	BO	125	PHE
44	BO	126	ARG
45	BP	8	ASN
45	BP	10	LEU
45	BP	16	GLU
45	BP	23	LYS
45	BP	32	PHE
45	BP	38	THR
45	BP	42	THR
45	BP	53	ARG
45	BP	60	LEU
45	BP	64	TYR
45	BP	65	GLU
45	BP	66	VAL
45	BP	73	GLU
45	BP	75	HIS
45	BP	84	LEU
45	BP	85	ILE
45	BP	93	LEU
45	BP	100	ILE
45	BP	101	VAL
45	BP	113	ARG
45	BP	119	LYS
45	BP	126	LYS
45	BP	127	GLU
46	BQ	3	ARG
46	BQ	11	ARG
46	BQ	14	ARG
46	BQ	19	LEU
46	BQ	27	LYS
46	BQ	35	GLU
46	BQ	36	LYS
46	BQ	39	ILE
46	BQ	44	ARG
46	BQ	48	LEU
46	BQ	49	THR
46	BQ	56	LEU
46	BQ	57	ARG
46	BQ	65	LYS
46	BQ	66	LEU
46	BQ	67	GLU
46	BQ	70	LEU

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Mol	Chain	Res	Type
46	BQ	71	ARG
46	BQ	80	ARG
46	BQ	81	LEU
46	BQ	86	CYS
46	BQ	88	ARG
46	BQ	102	ARG
46	BQ	108	ARG
46	BQ	110	ARG
47	BR	16	PHE
47	BR	21	TYR
47	BR	22	THR
47	BR	24	CYS
47	BR	29	ARG
47	BR	34	TYR
47	BR	40	CYS
47	BR	43	CYS
47	BR	45	ARG
47	BR	49	HIS
47	BR	54	PRO
47	BR	56	VAL
47	BR	61	TRP
48	BS	3	ILE
48	BS	4	THR
48	BS	5	LYS
48	BS	13	GLN
48	BS	38	ARG
48	BS	41	GLU
48	BS	42	HIS
48	BS	49	ASP
48	BS	54	ARG
48	BS	64	ARG
48	BS	66	LEU
48	BS	73	GLU
48	BS	77	ARG
48	BS	78	TYR
48	BS	79	ARG
49	BT	2	VAL
49	BT	3	LYS
49	BT	4	ILE
49	BT	6	LEU
49	BT	14	ASN
49	BT	15	PRO

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Mol	Chain	Res	Type
49	BT	18	ARG
49	BT	27	LYS
49	BT	32	TYR
49	BT	36	ILE
49	BT	39	TYR
49	BT	40	ASP
49	BT	48	TRP
49	BT	54	GLU
49	BT	55	ARG
49	BT	59	TRP
49	BT	62	VAL
49	BT	65	GLN
49	BT	66	PRO
49	BT	69	THR
49	BT	72	ARG
49	BT	75	ARG
49	BT	80	PHE
50	BU	6	LEU
50	BU	12	SER
50	BU	15	MET
50	BU	18	THR
50	BU	24	GLU
50	BU	25	ARG
50	BU	27	PHE
50	BU	28	PRO
50	BU	36	ILE
50	BU	38	ARG
50	BU	40	LYS
50	BU	43	LEU
50	BU	48	GLU
50	BU	51	TYR
50	BU	57	VAL
50	BU	58	GLU
50	BU	60	ILE
50	BU	62	SER
50	BU	67	LYS
50	BU	69	LYS
50	BU	84	LEU
50	BU	86	GLU
50	BU	87	LYS
50	BU	93	GLN
50	BU	95	TYR

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Mol	Chain	Res	Type
50	BU	96	GLN
50	BU	98	LEU
50	BU	100	LYS
50	BU	101	ARG
51	BV	28	GLU
51	BV	32	ARG
51	BV	34	TYR
51	BV	36	ASN
51	BV	38	GLU
51	BV	49	LYS
51	BV	53	ARG
51	BV	55	ARG
51	BV	62	GLU
51	BV	63	GLN
51	BV	72	ARG
51	BV	74	ARG
51	BV	79	LEU
51	BV	80	PRO
51	BV	81	PHE
51	BV	83	GLU
52	BW	3	ARG
52	BW	6	LYS
52	BW	7	LYS
52	BW	12	ASP
52	BW	15	LEU
52	BW	17	GLU
52	BW	18	LYS
52	BW	19	VAL
52	BW	25	LYS
52	BW	34	TRP
52	BW	36	ARG
52	BW	37	ARG
52	BW	41	VAL
52	BW	42	PRO
52	BW	43	GLU
52	BW	52	TYR
52	BW	57	HIS
52	BW	61	TYR
52	BW	74	PHE
53	BX	13	LEU
53	BX	23	ARG
53	BX	25	ARG

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Mol	Chain	Res	Type
53	BX	26	ASN
53	BX	30	LYS
53	BX	35	THR
53	BX	42	GLN
53	BX	51	GLU
53	BX	56	MET
53	BX	63	ILE
53	BX	71	THR
53	BX	73	HIS
53	BX	79	ARG
53	BX	84	LEU
53	BX	87	LYS
53	BX	88	VAL
53	BX	91	LEU
54	BY	9	ARG
54	BY	10	ARG
57	BZ	3	GLU
57	BZ	4	LYS
57	BZ	13	HIS
57	BZ	20	THR
57	BZ	24	LYS
57	BZ	26	LEU
57	BZ	28	GLN
57	BZ	29	SER
57	BZ	31	THR
57	BZ	33	ASP
57	BZ	34	SER
57	BZ	35	ARG
57	BZ	37	GLU
57	BZ	40	GLU
57	BZ	41	ARG
57	BZ	42	VAL
57	BZ	48	LEU
57	BZ	50	LYS
57	BZ	52	ARG
57	BZ	59	LYS
57	BZ	61	THR
57	BZ	67	ASP
57	BZ	68	TYR
57	BZ	72	ILE
57	BZ	78	HIS
57	BZ	84	GLU

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Mol	Chain	Res	Type
57	BZ	87	ARG
57	BZ	91	MET
57	BZ	94	SER
57	BZ	95	VAL
57	BZ	108	GLN
57	BZ	110	ARG
57	BZ	115	LYS
57	BZ	117	PHE
57	BZ	119	TYR
57	BZ	122	LYS
57	BZ	131	ASP
57	BZ	136	ARG
57	BZ	142	ASP
57	BZ	148	PHE
57	BZ	150	ASN
57	BZ	155	ASP
57	BZ	160	PHE
57	BZ	174	LEU
57	BZ	176	HIS
57	BZ	182	ASP
57	BZ	186	LEU
57	BZ	192	ASP
57	BZ	200	ASP
57	BZ	201	LEU
57	BZ	202	ASP
57	BZ	207	MET
57	BZ	208	GLN
57	BZ	216	SER
57	BZ	217	TYR
57	BZ	225	ARG
57	BZ	230	LYS
57	BZ	232	LYS
57	BZ	234	ASN
57	BZ	235	GLN
57	BZ	241	ASP
57	BZ	242	SER
57	BZ	243	GLU
57	BZ	245	LYS
57	BZ	247	ARG
57	BZ	250	LYS
57	BZ	253	LYS
57	BZ	255	LEU

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Mol	Chain	Res	Type
57	BZ	260	LEU
57	BZ	262	ARG
57	BZ	265	THR
57	BZ	274	VAL
57	BZ	289	CYS
57	BZ	291	THR
57	BZ	292	GLN
57	BZ	295	GLU
57	BZ	297	LEU
57	BZ	300	LEU
57	BZ	301	SER
57	BZ	308	SER
57	BZ	316	SER
57	BZ	318	PHE
57	BZ	321	LYS
57	BZ	324	LYS
57	BZ	329	ARG
57	BZ	332	LEU
57	BZ	333	ASP
57	BZ	342	ASN
57	BZ	346	ARG
57	BZ	357	ARG
57	BZ	359	SER
57	BZ	361	ARG
57	BZ	363	GLU
57	BZ	373	MET
57	BZ	374	ARG
57	BZ	380	LEU
57	BZ	382	VAL
57	BZ	384	ARG
57	BZ	387	VAL
57	BZ	390	ARG
57	BZ	391	GLU
57	BZ	393	ASP
57	BZ	398	GLU
57	BZ	404	THR
57	BZ	407	VAL
57	BZ	410	GLN
57	BZ	411	HIS
57	BZ	417	GLN
57	BZ	419	LEU
57	BZ	443	ILE

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Mol	Chain	Res	Type
57	BZ	445	SER
57	BZ	448	LEU
57	BZ	460	SER
57	BZ	464	LEU
57	BZ	465	LEU
57	BZ	466	TYR
57	BZ	472	TYR
57	BZ	474	ASP
57	BZ	482	GLN
57	BZ	483	ARG
57	BZ	488	LEU
57	BZ	489	ILE
57	BZ	491	ASN
57	BZ	493	GLN
57	BZ	499	PHE
57	BZ	502	PHE
57	BZ	506	ASP
57	BZ	509	LYS
57	BZ	520	GLU
57	BZ	526	ILE
57	BZ	541	LYS
57	BZ	542	LYS
57	BZ	544	THR
57	BZ	546	MET
57	BZ	547	ARG
57	BZ	549	SER
57	BZ	552	ASP
57	BZ	555	VAL
57	BZ	563	MET
57	BZ	570	GLU
57	BZ	586	ARG
57	BZ	588	ARG
57	BZ	589	LYS
57	BZ	593	THR
57	BZ	597	ARG
57	BZ	599	ARG
57	BZ	602	ARG
57	BZ	605	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (192) such sidechains are listed below:

Mol	Chain	Res	Type
3	AC	56	GLN
3	AC	71	GLN
3	AC	148	ASN
3	AC	165	ASN
3	AC	172	HIS
3	AC	188	ASN
3	AC	225	ASN
4	AD	45	ASN
4	AD	87	ASN
4	AD	115	GLN
4	AD	166	GLN
4	AD	198	ASN
4	AD	201	HIS
4	AD	203	ASN
5	AE	35	GLN
5	AE	85	ASN
5	AE	121	ASN
5	AE	129	HIS
6	AF	67	GLN
6	AF	133	ASN
6	AF	169	ASN
7	AG	26	GLN
7	AG	40	ASN
7	AG	41	GLN
7	AG	130	ASN
8	AH	74	ASN
8	AH	143	GLN
9	AK	38	HIS
9	AK	94	HIS
10	AL	5	GLN
10	AL	89	ASN
10	AL	90	GLN
11	AM	13	ASN
11	AM	35	HIS
11	AM	38	GLN
11	AM	68	GLN
11	AM	81	GLN
11	AM	84	ASN
12	AN	12	GLN
12	AN	57	HIS
12	AN	89	ASN
13	AO	24	GLN
13	AO	31	HIS

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Mol	Chain	Res	Type
14	AP	38	GLN
14	AP	84	GLN
15	AQ	55	ASN
15	AQ	58	ASN
16	AR	44	ASN
16	AR	71	GLN
16	AR	94	ASN
16	AR	117	GLN
17	AS	11	GLN
17	AS	87	HIS
17	AS	89	GLN
18	AT	34	ASN
18	AT	61	ASN
18	AT	62	HIS
18	AT	102	HIS
19	AU	31	HIS
19	AU	55	ASN
19	AU	82	GLN
19	AU	87	GLN
20	AV	6	HIS
20	AV	43	ASN
21	AW	32	HIS
21	AW	34	ASN
21	AW	75	ASN
21	AW	118	GLN
22	AX	35	ASN
22	AX	80	HIS
23	AY	33	GLN
23	AY	41	GLN
23	AY	51	GLN
23	AY	65	GLN
24	AZ	32	GLN
25	Aa	46	GLN
26	Ab	23	HIS
27	Ac	20	ASN
27	Ac	29	ASN
27	Ac	32	ASN
28	Ad	6	GLN
28	Ad	8	ASN
28	Ad	16	HIS
28	Ad	36	GLN
29	Ae	31	HIS

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Mol	Chain	Res	Type
29	Ae	33	ASN
29	Ae	35	GLN
29	Ae	43	GLN
30	Af	32	HIS
30	Af	36	GLN
32	AJ	11	GLN
32	AJ	33	ASN
32	AJ	116	ASN
35	BF	40	HIS
35	BF	78	GLN
35	BF	94	ASN
35	BF	135	GLN
35	BF	204	ASN
35	BF	224	GLN
36	BG	3	ASN
36	BG	6	HIS
36	BG	28	GLN
36	BG	102	ASN
36	BG	108	ASN
36	BG	110	ASN
36	BG	136	GLN
36	BG	139	GLN
36	BG	170	GLN
37	BH	42	GLN
37	BH	62	GLN
37	BH	74	GLN
37	BH	77	ASN
37	BH	154	ASN
37	BH	161	ASN
37	BH	201	GLN
38	BI	56	GLN
38	BI	65	ASN
38	BI	72	GLN
39	BJ	7	ASN
39	BJ	13	ASN
39	BJ	18	GLN
39	BJ	32	ASN
39	BJ	64	GLN
39	BJ	84	ASN
39	BJ	94	GLN
39	BJ	100	ASN
40	BK	56	GLN

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Mol	Chain	Res	Type
40	BK	68	ASN
40	BK	96	GLN
40	BK	97	GLN
40	BK	106	GLN
40	BK	109	ASN
40	BK	110	GLN
40	BK	148	ASN
40	BK	153	HIS
41	BL	15	ASN
41	BL	70	GLN
42	BM	23	ASN
42	BM	58	HIS
42	BM	73	GLN
42	BM	87	GLN
42	BM	89	ASN
42	BM	117	HIS
43	BN	56	HIS
43	BN	62	HIS
43	BN	68	HIS
43	BN	76	ASN
43	BN	78	ASN
44	BO	26	ASN
44	BO	27	ASN
44	BO	38	ASN
44	BO	104	GLN
44	BO	117	ASN
45	BP	8	ASN
45	BP	49	ASN
45	BP	99	HIS
46	BQ	40	ASN
46	BQ	101	GLN
47	BR	52	GLN
48	BS	9	GLN
48	BS	13	GLN
48	BS	37	ASN
48	BS	62	GLN
49	BT	82	GLN
50	BU	93	GLN
52	BW	53	ASN
52	BW	65	ASN
52	BW	69	HIS
53	BX	16	HIS

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Mol	Chain	Res	Type
53	BX	42	GLN
53	BX	45	GLN
53	BX	73	HIS
53	BX	75	ASN
57	BZ	16	HIS
57	BZ	28	GLN
57	BZ	78	HIS
57	BZ	128	ASN
57	BZ	150	ASN
57	BZ	157	GLN
57	BZ	193	HIS
57	BZ	206	GLN
57	BZ	211	GLN
57	BZ	215	ASN
57	BZ	257	HIS
57	BZ	283	ASN
57	BZ	292	GLN
57	BZ	314	ASN
57	BZ	365	HIS
57	BZ	410	GLN
57	BZ	412	GLN
57	BZ	417	GLN
57	BZ	527	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2881/2889 (99%)	1265 (43%)	253 (8%)
2	AB	122/123 (99%)	46 (37%)	3 (2%)
34	BA	1514/1515 (99%)	484 (31%)	140 (9%)
55	BC	75/76 (98%)	26 (34%)	0
56	BD	74/75 (98%)	31 (41%)	2 (2%)
56	BE	74/75 (98%)	23 (31%)	1 (1%)
All	All	4740/4753 (99%)	1875 (39%)	399 (8%)

All (1875) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	13	A
1	AA	14	A
1	AA	15	G

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Mol	Chain	Res	Type
1	AA	20	C
1	AA	26	G
1	AA	29	U
1	AA	34	C
1	AA	35	G
1	AA	46	C
1	AA	49	A
1	AA	50	U
1	AA	52	A
1	AA	60	G
1	AA	61	G
1	AA	63	U
1	AA	64	A
1	AA	68	G
1	AA	71	A
1	AA	72	U
1	AA	73	A
1	AA	74	A
1	AA	75	G
1	AA	76	C
1	AA	77	C
1	AA	82	G
1	AA	84	A
1	AA	88	G
1	AA	90	U
1	AA	91	A
1	AA	92	G
1	AA	96	G
1	AA	101	G
1	AA	102	G
1	AA	104	U
1	AA	105	C
1	AA	109	G
1	AA	112	U
1	AA	113	G
1	AA	119	A
1	AA	120	U
1	AA	121	G
1	AA	125	G
1	AA	126	A
1	AA	131	G
1	AA	132	G

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Mol	Chain	Res	Type
1	AA	136	G
1	AA	138	G
1	AA	139	G
1	AA	140	A
1	AA	141(A)	C
1	AA	147	U
1	AA	149	A
1	AA	153	C
1	AA	154	G
1	AA	155	C
1	AA	161	U
1	AA	162	U
1	AA	163	U
1	AA	164	U
1	AA	172	C
1	AA	178	G
1	AA	180	G
1	AA	181	A
1	AA	182	A
1	AA	192	C
1	AA	193	U
1	AA	196	A
1	AA	197	A
1	AA	199	A
1	AA	200	U
1	AA	201	C
1	AA	204	A
1	AA	205	G
1	AA	206	U
1	AA	216	A
1	AA	218	A
1	AA	221	A
1	AA	222	A
1	AA	223	A
1	AA	228	A
1	AA	229	A
1	AA	230	U
1	AA	232	G
1	AA	233	A
1	AA	234	C
1	AA	241	A
1	AA	242	G

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Mol	Chain	Res	Type
1	AA	244	A
1	AA	245	G
1	AA	247	G
1	AA	248	G
1	AA	249	C
1	AA	250	G
1	AA	251	A
1	AA	252	G
1	AA	254	G
1	AA	264	C
1	AA	265	A
1	AA	266	G
1	AA	270	A
1	AA	270(A)	A
1	AA	270(B)	A
1	AA	270(C)	C
1	AA	270(E)	G
1	AA	270(G)	C
1	AA	270(K)	C
1	AA	270(L)	U
1	AA	270(M)	U
1	AA	270(N)	G
1	AA	270(V)	G
1	AA	270(Z)	U
1	AA	271(A)	C
1	AA	271(B)	G
1	AA	271(C)	U
1	AA	271	G
1	AA	272	G
1	AA	273(F)	C
1	AA	275	G
1	AA	276	A
1	AA	277	C
1	AA	278	A
1	AA	279	C
1	AA	280	C
1	AA	281	G
1	AA	282	A
1	AA	283	A
1	AA	284	U
1	AA	286	C
1	AA	287	C

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Mol	Chain	Res	Type
1	AA	289	A
1	AA	290	G
1	AA	293	U
1	AA	300	A
1	AA	302	C
1	AA	310	A
1	AA	311	A
1	AA	312	G
1	AA	316	C
1	AA	322	A
1	AA	323	G
1	AA	324	A
1	AA	329	G
1	AA	330	A
1	AA	332	A
1	AA	333	G
1	AA	339	U
1	AA	341	G
1	AA	342	G
1	AA	345	A
1	AA	347	A
1	AA	348	G
1	AA	349	G
1	AA	350	U
1	AA	351	G
1	AA	352	G
1	AA	354	G
1	AA	356	G
1	AA	359	A
1	AA	360	G
1	AA	361	G
1	AA	363(A)	A
1	AA	363(B)	G
1	AA	364	C
1	AA	365	C
1	AA	366	C
1	AA	370	G
1	AA	372	G
1	AA	373	U
1	AA	374	A
1	AA	377	C
1	AA	382	G

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Mol	Chain	Res	Type
1	AA	386	G
1	AA	387	U
1	AA	388	G
1	AA	390	A
1	AA	391	G
1	AA	395	U
1	AA	397	G
1	AA	401	A
1	AA	404	C
1	AA	405	U
1	AA	406	G
1	AA	408	G
1	AA	411	G
1	AA	412	A
1	AA	413	C
1	AA	421	U
1	AA	422	A
1	AA	423	A
1	AA	424	G
1	AA	428	A
1	AA	429	A
1	AA	443	A
1	AA	444	C
1	AA	446	G
1	AA	447	A
1	AA	448	U
1	AA	449	A
1	AA	451	C
1	AA	452	G
1	AA	453	C
1	AA	454	A
1	AA	455	C
1	AA	456	C
1	AA	457	A
1	AA	470	A
1	AA	471	A
1	AA	475	U
1	AA	479	A
1	AA	480	A
1	AA	481	G
1	AA	484	C
1	AA	492	A

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Mol	Chain	Res	Type
1	AA	503	A
1	AA	504	U
1	AA	505	A
1	AA	506	G
1	AA	507	A
1	AA	508	G
1	AA	509	C
1	AA	510	C
1	AA	512	G
1	AA	519	U
1	AA	525	U
1	AA	527	C
1	AA	528	A
1	AA	529	A
1	AA	530	G
1	AA	531	C
1	AA	532	A
1	AA	533	G
1	AA	541	C
1	AA	549	G
1	AA	554	U
1	AA	556	G
1	AA	559	G
1	AA	560	C
1	AA	563	G
1	AA	567	A
1	AA	568	U
1	AA	572	A
1	AA	573	G
1	AA	574	C
1	AA	575	A
1	AA	579	G
1	AA	580	C
1	AA	583	G
1	AA	586	A
1	AA	588	U
1	AA	591	C
1	AA	593	G
1	AA	599	G
1	AA	600	G
1	AA	601	C
1	AA	603	A

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Mol	Chain	Res	Type
1	AA	604	G
1	AA	605	C
1	AA	607	U
1	AA	612	G
1	AA	613	U
1	AA	614	U
1	AA	615	G
1	AA	616	A
1	AA	617	G
1	AA	618(A)	C
1	AA	620	G
1	AA	621	A
1	AA	622	G
1	AA	624	C
1	AA	625	G
1	AA	626	U
1	AA	627	A
1	AA	629	G
1	AA	631	A
1	AA	634	C
1	AA	637	A
1	AA	641	C
1	AA	643	A
1	AA	644	A
1	AA	646	A
1	AA	650	C
1	AA	651	G
1	AA	653	A
1	AA	654	A
1	AA	655	A
1	AA	656	G
1	AA	657	U
1	AA	665	C
1	AA	666	G
1	AA	668	G
1	AA	669	G
1	AA	670	A
1	AA	671	C
1	AA	674	G
1	AA	684	G
1	AA	686	G
1	AA	687	C

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Mol	Chain	Res	Type
1	AA	698	C
1	AA	704	G
1	AA	705	A
1	AA	713	G
1	AA	714	U
1	AA	715	G
1	AA	716	A
1	AA	718	A
1	AA	723	G
1	AA	727	A
1	AA	728	G
1	AA	729	G
1	AA	730	C
1	AA	731	C
1	AA	734	A
1	AA	735	A
1	AA	736	C
1	AA	739	G
1	AA	740	U
1	AA	741	G
1	AA	744	G
1	AA	745	G
1	AA	746	A
1	AA	747	U
1	AA	748	G
1	AA	749	C
1	AA	750	A
1	AA	751	A
1	AA	752	A
1	AA	758	C
1	AA	759	G
1	AA	762	U
1	AA	763	G
1	AA	764	A
1	AA	765	G
1	AA	774	A
1	AA	775	G
1	AA	776	G
1	AA	777	A
1	AA	779	U
1	AA	781	A
1	AA	782	A

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Mol	Chain	Res	Type
1	AA	783	A
1	AA	784	A
1	AA	785	G
1	AA	786	C
1	AA	789	A
1	AA	790	C
1	AA	791	C
1	AA	792	G
1	AA	793	A
1	AA	794	G
1	AA	799	G
1	AA	800	A
1	AA	801	G
1	AA	802	A
1	AA	803	U
1	AA	805	G
1	AA	806	C
1	AA	812	C
1	AA	816	C
1	AA	819	A
1	AA	821	A
1	AA	823	G
1	AA	824	A
1	AA	827	U
1	AA	829	A
1	AA	830	G
1	AA	831	G
1	AA	833	U
1	AA	844	C
1	AA	846	C
1	AA	847	U
1	AA	858	U
1	AA	859	G
1	AA	860	U
1	AA	861	A
1	AA	865	C
1	AA	868	U
1	AA	870	A
1	AA	874	G
1	AA	875	G
1	AA	878	A
1	AA	879	G

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Mol	Chain	Res	Type
1	AA	881	G
1	AA	882	G
1	AA	883	G
1	AA	884	C
1	AA	885	C
1	AA	886	C
1	AA	887	A
1	AA	888	C
1	AA	889	C
1	AA	890	A
1	AA	892	G
1	AA	894	C
1	AA	895	U
1	AA	896	A
1	AA	897	C
1	AA	898	C
1	AA	899	A
1	AA	900	A
1	AA	901	A
1	AA	902	C
1	AA	904	C
1	AA	905	U
1	AA	906	G
1	AA	907	U
1	AA	909	A
1	AA	910	A
1	AA	914	C
1	AA	918	A
1	AA	919	G
1	AA	920	G
1	AA	930	U
1	AA	931	G
1	AA	932	G
1	AA	933	A
1	AA	939	G
1	AA	941	A
1	AA	943	U
1	AA	944	G
1	AA	945	A
1	AA	946	G
1	AA	956	G
1	AA	957	A

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Mol	Chain	Res	Type
1	AA	958	U
1	AA	959	A
1	AA	961	C
1	AA	962	G
1	AA	965	C
1	AA	972	G
1	AA	973	A
1	AA	974	G
1	AA	974(A)	C
1	AA	976	C
1	AA	982	C
1	AA	983	A
1	AA	987	G
1	AA	990	A
1	AA	995	C
1	AA	996	A
1	AA	997	G
1	AA	1008	C
1	AA	1009	A
1	AA	1011	G
1	AA	1012	U
1	AA	1013	C
1	AA	1021	A
1	AA	1022	G
1	AA	1023	U
1	AA	1024	G
1	AA	1025	G
1	AA	1026	U
1	AA	1027	A
1	AA	1031	G
1	AA	1032	A
1	AA	1033	U
1	AA	1039	G
1	AA	1040	C
1	AA	1042	G
1	AA	1043	C
1	AA	1044	G
1	AA	1045	A
1	AA	1046	A
1	AA	1047	G
1	AA	1048	A
1	AA	1050	A

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Mol	Chain	Res	Type
1	AA	1052	C
1	AA	1053	C
1	AA	1056	G
1	AA	1057	A
1	AA	1058	G
1	AA	1059	G
1	AA	1060	U
1	AA	1061	U
1	AA	1062	G
1	AA	1063	G
1	AA	1065	U
1	AA	1066	U
1	AA	1067	A
1	AA	1068	G
1	AA	1069	A
1	AA	1070	A
1	AA	1071	G
1	AA	1072	C
1	AA	1073	A
1	AA	1075	C
1	AA	1076	C
1	AA	1077	A
1	AA	1078	U
1	AA	1079	C
1	AA	1080	C
1	AA	1083	U
1	AA	1084	A
1	AA	1085	A
1	AA	1086	A
1	AA	1087	G
1	AA	1088	A
1	AA	1090	U
1	AA	1093	G
1	AA	1099	G
1	AA	1101	U
1	AA	1103	A
1	AA	1104	C
1	AA	1108	U
1	AA	1109	C
1	AA	1110	G
1	AA	1111	A
1	AA	1112	G

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Mol	Chain	Res	Type
1	AA	1116	C
1	AA	1126	A
1	AA	1127	A
1	AA	1128	A
1	AA	1130	U
1	AA	1131	G
1	AA	1132	A
1	AA	1134	G
1	AA	1135	C
1	AA	1140	C
1	AA	1141	U
1	AA	1143	A
1	AA	1154	G
1	AA	1155	A
1	AA	1156	A
1	AA	1157	G
1	AA	1160	G
1	AA	1162	G
1	AA	1171	G
1	AA	1173	G
1	AA	1174	A
1	AA	1175	U
1	AA	1176	G
1	AA	1177	A
1	AA	1179	C
1	AA	1180	C
1	AA	1182	A
1	AA	1183	G
1	AA	1184	G
1	AA	1185	C
1	AA	1186	G
1	AA	1190	G
1	AA	1199	U
1	AA	1201	C
1	AA	1203	G
1	AA	1204	A
1	AA	1205	U
1	AA	1207	C
1	AA	1209	G
1	AA	1211	U
1	AA	1212	G
1	AA	1213	A

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Mol	Chain	Res	Type
1	AA	1220	A
1	AA	1221	C
1	AA	1222	C
1	AA	1225	C
1	AA	1228	G
1	AA	1238	G
1	AA	1241	A
1	AA	1242	A
1	AA	1244	G
1	AA	1247	A
1	AA	1248	G
1	AA	1249	U
1	AA	1251	C
1	AA	1252	G
1	AA	1253	A
1	AA	1254	A
1	AA	1255	U
1	AA	1256	G
1	AA	1258	C
1	AA	1260	G
1	AA	1264	G
1	AA	1265	A
1	AA	1266	G
1	AA	1267	U
1	AA	1268	A
1	AA	1271	G
1	AA	1272	A
1	AA	1273	U
1	AA	1274	A
1	AA	1275	A
1	AA	1286	A
1	AA	1289	C
1	AA	1296	G
1	AA	1297	C
1	AA	1301	A
1	AA	1302	A
1	AA	1303	G
1	AA	1304	C
1	AA	1311	G
1	AA	1312	U
1	AA	1321	A
1	AA	1324	G

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Mol	Chain	Res	Type
1	AA	1325	G
1	AA	1326	U
1	AA	1327	C
1	AA	1329	U
1	AA	1330	C
1	AA	1335	U
1	AA	1340	U
1	AA	1341	U
1	AA	1342	A
1	AA	1343	G
1	AA	1344	G
1	AA	1345	C
1	AA	1347	G
1	AA	1350	C
1	AA	1364	G
1	AA	1365	A
1	AA	1366	A
1	AA	1368	G
1	AA	1378	A
1	AA	1379	A
1	AA	1388	G
1	AA	1394	U
1	AA	1395	A
1	AA	1397	U
1	AA	1398	C
1	AA	1403	C
1	AA	1407	C
1	AA	1416	G
1	AA	1418	G
1	AA	1419	A
1	AA	1420	U
1	AA	1421	G
1	AA	1424	G
1	AA	1425	G
1	AA	1427	A
1	AA	1428	C
1	AA	1429	G
1	AA	1438	U
1	AA	1444(A)	A
1	AA	1445	C
1	AA	1451	C
1	AA	1453	A

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Mol	Chain	Res	Type
1	AA	1455	G
1	AA	1456	G
1	AA	1459	G
1	AA	1460	A
1	AA	1462	C
1	AA	1463	C
1	AA	1467	C
1	AA	1468	C
1	AA	1471	A
1	AA	1477	A
1	AA	1478	G
1	AA	1480	G
1	AA	1482	U
1	AA	1485	G
1	AA	1489	U
1	AA	1490	A
1	AA	1491	G
1	AA	1492	G
1	AA	1493	C
1	AA	1494	A
1	AA	1495	A
1	AA	1496	A
1	AA	1497	U
1	AA	1498	C
1	AA	1499	C
1	AA	1507	A
1	AA	1508	A
1	AA	1509	C
1	AA	1510	A
1	AA	1511	A
1	AA	1512	G
1	AA	1513	C
1	AA	1514	U
1	AA	1515	C
1	AA	1516	U
1	AA	1517	G
1	AA	1519	G
1	AA	1521	G
1	AA	1526	G
1	AA	1527	G
1	AA	1529	A
1	AA	1530	G

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Mol	Chain	Res	Type
1	AA	1532	C
1	AA	1537	C
1	AA	1540	G
1	AA	1542	G
1	AA	1544	C
1	AA	1552	G
1	AA	1553	A
1	AA	1554	A
1	AA	1555	G
1	AA	1558	A
1	AA	1559	G
1	AA	1560	G
1	AA	1561	G
1	AA	1566	A
1	AA	1567	A
1	AA	1569	A
1	AA	1570	A
1	AA	1571	A
1	AA	1572	A
1	AA	1573	G
1	AA	1576	U
1	AA	1577	C
1	AA	1578	U
1	AA	1579	A
1	AA	1580	A
1	AA	1581	G
1	AA	1583	A
1	AA	1585	C
1	AA	1586	A
1	AA	1587	A
1	AA	1591	G
1	AA	1602	U
1	AA	1603	A
1	AA	1607	C
1	AA	1608	A
1	AA	1609	A
1	AA	1610	A
1	AA	1612	C
1	AA	1614	A
1	AA	1615	C
1	AA	1617	C
1	AA	1618	A

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Mol	Chain	Res	Type
1	AA	1619	G
1	AA	1623	G
1	AA	1625	C
1	AA	1626	G
1	AA	1627	G
1	AA	1631	A
1	AA	1634	A
1	AA	1635	G
1	AA	1640	C
1	AA	1641	A
1	AA	1644	C
1	AA	1645	G
1	AA	1647	G
1	AA	1648	C
1	AA	1649	G
1	AA	1651	G
1	AA	1652	A
1	AA	1653	G
1	AA	1654	A
1	AA	1655	A
1	AA	1656	C
1	AA	1657	C
1	AA	1664	A
1	AA	1667	G
1	AA	1668	A
1	AA	1670	C
1	AA	1673	U
1	AA	1674	G
1	AA	1675	C
1	AA	1678	G
1	AA	1681	G
1	AA	1682	G
1	AA	1683	C
1	AA	1684	C
1	AA	1688	U
1	AA	1694	C
1	AA	1698	A
1	AA	1699	G
1	AA	1700	A
1	AA	1701	A
1	AA	1703	G
1	AA	1706	U

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Mol	Chain	Res	Type
1	AA	1707	G
1	AA	1709	U
1	AA	1710	C
1	AA	1725	G
1	AA	1728	G
1	AA	1729	A
1	AA	1731	G
1	AA	1732	A
1	AA	1733	G
1	AA	1734	C
1	AA	1741	C
1	AA	1742	C
1	AA	1743	G
1	AA	1746	G
1	AA	1747	G
1	AA	1755	A
1	AA	1757	U
1	AA	1758	G
1	AA	1759	A
1	AA	1762	A
1	AA	1763	G
1	AA	1764	G
1	AA	1773	A
1	AA	1775	U
1	AA	1779	U
1	AA	1780	A
1	AA	1781	C
1	AA	1782	C
1	AA	1783	A
1	AA	1784	A
1	AA	1785	A
1	AA	1790	C
1	AA	1791	A
1	AA	1798	U
1	AA	1799	G
1	AA	1800	C
1	AA	1801	G
1	AA	1802	A
1	AA	1803	A
1	AA	1805	U
1	AA	1809	A
1	AA	1810	A

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Mol	Chain	Res	Type
1	AA	1815	A
1	AA	1816	G
1	AA	1817	G
1	AA	1819	A
1	AA	1820	U
1	AA	1821	A
1	AA	1826	G
1	AA	1828	G
1	AA	1829	A
1	AA	1834	U
1	AA	1839	G
1	AA	1840	G
1	AA	1847	A
1	AA	1848	A
1	AA	1852	C
1	AA	1853	A
1	AA	1857	G
1	AA	1858	G
1	AA	1878	G
1	AA	1880	C
1	AA	1881	C
1	AA	1884	A
1	AA	1901	A
1	AA	1903	G
1	AA	1904	G
1	AA	1905	C
1	AA	1907	G
1	AA	1911	U
1	AA	1912	A
1	AA	1913	A
1	AA	1914	C
1	AA	1915	U
1	AA	1916	A
1	AA	1917	U
1	AA	1919	A
1	AA	1920	C
1	AA	1921	G
1	AA	1922	G
1	AA	1924	C
1	AA	1927	A
1	AA	1929	G
1	AA	1930	G

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Mol	Chain	Res	Type
1	AA	1931	U
1	AA	1932	A
1	AA	1934	C
1	AA	1936	A
1	AA	1937	A
1	AA	1938	A
1	AA	1939	U
1	AA	1940	U
1	AA	1941	C
1	AA	1942	C
1	AA	1943	U
1	AA	1944	U
1	AA	1945	G
1	AA	1946	U
1	AA	1953	A
1	AA	1954	G
1	AA	1955	U
1	AA	1956	U
1	AA	1958	C
1	AA	1962	C
1	AA	1964	G
1	AA	1965	C
1	AA	1966	A
1	AA	1967	C
1	AA	1968	G
1	AA	1970	A
1	AA	1971	A
1	AA	1972	A
1	AA	1977	A
1	AA	1978	A
1	AA	1981	A
1	AA	1982	C
1	AA	1989	G
1	AA	1992	G
1	AA	1993	U
1	AA	1995	U
1	AA	1996	C
1	AA	1997	G
1	AA	2000	G
1	AA	2005	A
1	AA	2014	A
1	AA	2015	A

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Mol	Chain	Res	Type
1	AA	2016	U
1	AA	2018	G
1	AA	2019	A
1	AA	2020	A
1	AA	2021	C
1	AA	2022	U
1	AA	2023	G
1	AA	2030	A
1	AA	2031	A
1	AA	2032	G
1	AA	2033	A
1	AA	2034	U
1	AA	2035	G
1	AA	2041	U
1	AA	2043	C
1	AA	2044	C
1	AA	2048	G
1	AA	2050	C
1	AA	2051	A
1	AA	2052	G
1	AA	2055	C
1	AA	2056	G
1	AA	2060	A
1	AA	2061	G
1	AA	2062	A
1	AA	2063	C
1	AA	2064	C
1	AA	2068	U
1	AA	2069	G
1	AA	2073	C
1	AA	2074	U
1	AA	2075	U
1	AA	2076	U
1	AA	2077	A
1	AA	2080	G
1	AA	2092	U
1	AA	2093	G
1	AA	2094	G
1	AA	2110	G
1	AA	2111	C
1	AA	2114	A
1	AA	2116	G

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Mol	Chain	Res	Type
1	AA	2117	A
1	AA	2119	A
1	AA	2120	G
1	AA	2123	G
1	AA	2126	A
1	AA	2127	G
1	AA	2132	U
1	AA	2133	G
1	AA	2134	A
1	AA	2135	A
1	AA	2136	C
1	AA	2144	U
1	AA	2148	G
1	AA	2156	G
1	AA	2157	G
1	AA	2158	A
1	AA	2159	G
1	AA	2165	G
1	AA	2172	U
1	AA	2173	A
1	AA	2185	C
1	AA	2194	G
1	AA	2195	C
1	AA	2196	C
1	AA	2197	U
1	AA	2198	A
1	AA	2205	C
1	AA	2206	C
1	AA	2208	U
1	AA	2209	C
1	AA	2210	G
1	AA	2211	G
1	AA	2212	A
1	AA	2213	U
1	AA	2224	G
1	AA	2225	A
1	AA	2226	C
1	AA	2227	A
1	AA	2228	G
1	AA	2238	G
1	AA	2239	G
1	AA	2240	C

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Mol	Chain	Res	Type
1	AA	2245	U
1	AA	2250	G
1	AA	2251	G
1	AA	2254	C
1	AA	2257	U
1	AA	2258	C
1	AA	2265	U
1	AA	2266	A
1	AA	2267	A
1	AA	2268	A
1	AA	2269	A
1	AA	2274	A
1	AA	2275	C
1	AA	2276	G
1	AA	2278	A
1	AA	2281	C
1	AA	2283	C
1	AA	2284	C
1	AA	2286	A
1	AA	2287	A
1	AA	2288	A
1	AA	2289	G
1	AA	2290	G
1	AA	2291	U
1	AA	2297	C
1	AA	2305	A
1	AA	2306	C
1	AA	2307	G
1	AA	2308	G
1	AA	2309	A
1	AA	2310	A
1	AA	2311	A
1	AA	2312	U
1	AA	2316	C
1	AA	2318	G
1	AA	2319	G
1	AA	2320	A
1	AA	2321	G
1	AA	2322	A
1	AA	2323	G
1	AA	2325	G
1	AA	2327	A

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Mol	Chain	Res	Type
1	AA	2333	A
1	AA	2334	G
1	AA	2337	G
1	AA	2344	U
1	AA	2345	G
1	AA	2346	A
1	AA	2347	C
1	AA	2349	G
1	AA	2350	C
1	AA	2351	G
1	AA	2356	C
1	AA	2357	U
1	AA	2358	G
1	AA	2360	A
1	AA	2361	A
1	AA	2362	G
1	AA	2372	G
1	AA	2373	G
1	AA	2374	C
1	AA	2377	A
1	AA	2379	G
1	AA	2382	G
1	AA	2383	G
1	AA	2384	G
1	AA	2385	C
1	AA	2387	U
1	AA	2389	G
1	AA	2390	U
1	AA	2393	A
1	AA	2402	C
1	AA	2403	C
1	AA	2406	U
1	AA	2407	G
1	AA	2416	C
1	AA	2417	C
1	AA	2423	U
1	AA	2424	C
1	AA	2425	A
1	AA	2426	A
1	AA	2427	C
1	AA	2428	G
1	AA	2429	G

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Mol	Chain	Res	Type
1	AA	2430	A
1	AA	2431	U
1	AA	2432	A
1	AA	2433	A
1	AA	2434	A
1	AA	2435	A
1	AA	2437	U
1	AA	2439	A
1	AA	2440	C
1	AA	2441	C
1	AA	2444	G
1	AA	2445	G
1	AA	2447	G
1	AA	2448	A
1	AA	2449	U
1	AA	2460	U
1	AA	2469	A
1	AA	2475	C
1	AA	2476	A
1	AA	2480	C
1	AA	2490	G
1	AA	2491	U
1	AA	2492	U
1	AA	2493	U
1	AA	2496	C
1	AA	2497	A
1	AA	2498	C
1	AA	2499	C
1	AA	2500	U
1	AA	2501	C
1	AA	2502	G
1	AA	2503	A
1	AA	2504	U
1	AA	2505	G
1	AA	2510	C
1	AA	2513	G
1	AA	2518	A
1	AA	2519	U
1	AA	2520	C
1	AA	2523	G
1	AA	2526	G
1	AA	2527	C

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Mol	Chain	Res	Type
1	AA	2529	G
1	AA	2531	A
1	AA	2532	G
1	AA	2535	G
1	AA	2539	C
1	AA	2542	A
1	AA	2543	G
1	AA	2547	U
1	AA	2548	G
1	AA	2551	C
1	AA	2554	U
1	AA	2555	U
1	AA	2556	C
1	AA	2563	U
1	AA	2566	A
1	AA	2567	G
1	AA	2572	A
1	AA	2573	C
1	AA	2575	C
1	AA	2576	G
1	AA	2577	A
1	AA	2578	G
1	AA	2580	U
1	AA	2582	G
1	AA	2585	U
1	AA	2586	C
1	AA	2593	U
1	AA	2602	A
1	AA	2603	G
1	AA	2606	C
1	AA	2609	U
1	AA	2610	C
1	AA	2611	U
1	AA	2613	U
1	AA	2614	A
1	AA	2615	U
1	AA	2616	C
1	AA	2617	C
1	AA	2620	C
1	AA	2625	G
1	AA	2626	C
1	AA	2628	C

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Mol	Chain	Res	Type
1	AA	2629	A
1	AA	2630	G
1	AA	2637	U
1	AA	2638	G
1	AA	2640	G
1	AA	2644	G
1	AA	2645	G
1	AA	2646	C
1	AA	2648	C
1	AA	2650	U
1	AA	2651	C
1	AA	2652	C
1	AA	2653	U
1	AA	2654	A
1	AA	2656	U
1	AA	2657	A
1	AA	2658	C
1	AA	2659	G
1	AA	2662	A
1	AA	2663	G
1	AA	2664	G
1	AA	2667	C
1	AA	2668	G
1	AA	2669	G
1	AA	2670	A
1	AA	2671	A
1	AA	2673	G
1	AA	2674	G
1	AA	2675	A
1	AA	2676	C
1	AA	2682	U
1	AA	2683	C
1	AA	2685	G
1	AA	2689	U
1	AA	2690	C
1	AA	2691	C
1	AA	2699	C
1	AA	2701	C
1	AA	2702	U
1	AA	2704	C
1	AA	2706	G
1	AA	2708	G

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Mol	Chain	Res	Type
1	AA	2709	G
1	AA	2710	C
1	AA	2711	A
1	AA	2712	U
1	AA	2712(A)	A
1	AA	2714	G
1	AA	2715	C
1	AA	2717	G
1	AA	2719	G
1	AA	2720	U
1	AA	2725	A
1	AA	2726	U
1	AA	2727	G
1	AA	2732	G
1	AA	2733	A
1	AA	2734	A
1	AA	2748	A
1	AA	2749	A
1	AA	2750	A
1	AA	2751	G
1	AA	2754	U
1	AA	2756	U
1	AA	2757	A
1	AA	2758	A
1	AA	2766	G
1	AA	2772	C
1	AA	2777	G
1	AA	2778	A
1	AA	2779	U
1	AA	2780	G
1	AA	2781	A
1	AA	2782	G
1	AA	2783	G
1	AA	2787	C
1	AA	2789	C
1	AA	2790	A
1	AA	2791	C
1	AA	2794	C
1	AA	2797	U
1	AA	2798	C
1	AA	2799	A
1	AA	2801	A

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Mol	Chain	Res	Type
1	AA	2802	G
1	AA	2803	C
1	AA	2804	C
1	AA	2805	G
1	AA	2807	G
1	AA	2808	U
1	AA	2809	A
1	AA	2810	A
1	AA	2812	G
1	AA	2814	C
1	AA	2815	C
1	AA	2820	A
1	AA	2821	A
1	AA	2822	G
1	AA	2823	A
1	AA	2832	U
1	AA	2833	G
1	AA	2834	G
1	AA	2835	A
1	AA	2836	U
1	AA	2843	G
1	AA	2844	G
1	AA	2845	G
1	AA	2847	U
1	AA	2849	U
1	AA	2850	A
1	AA	2851	A
1	AA	2852	G
1	AA	2858	C
1	AA	2861	G
1	AA	2866	U
1	AA	2867	G
1	AA	2868	A
1	AA	2872	G
1	AA	2874	C
1	AA	2877	G
1	AA	2878	U
1	AA	2879	C
1	AA	2880	C
1	AA	2883	A
1	AA	2891	G
1	AA	2892	A

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Mol	Chain	Res	Type
1	AA	2893	G
1	AA	2899	G
2	AB	0	A
2	AB	1	U
2	AB	2	C
2	AB	3	C
2	AB	5	C
2	AB	6	C
2	AB	8	U
2	AB	12	C
2	AB	13	A
2	AB	15	A
2	AB	16	G
2	AB	25	A
2	AB	32	C
2	AB	35	U
2	AB	36	C
2	AB	41	U
2	AB	42	C
2	AB	45	A
2	AB	46	A
2	AB	51	G
2	AB	52	A
2	AB	54	G
2	AB	57	A
2	AB	66	A
2	AB	67	G
2	AB	69	G
2	AB	73	A
2	AB	74	U
2	AB	75	G
2	AB	83	G
2	AB	85	G
2	AB	87	G
2	AB	88	C
2	AB	89	G
2	AB	90	C
2	AB	99	A
2	AB	101	A
2	AB	103	U
2	AB	105	G
2	AB	109	G

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Mol	Chain	Res	Type
2	AB	111	U
2	AB	116	G
2	AB	117	G
2	AB	118	G
2	AB	119	A
2	AB	120	U
34	BA	6	G
34	BA	8	A
34	BA	9	G
34	BA	14	U
34	BA	19	C
34	BA	20	U
34	BA	31	G
34	BA	32	A
34	BA	39	G
34	BA	44	G
34	BA	45	U
34	BA	48	C
34	BA	50	A
34	BA	51	A
34	BA	52	G
34	BA	61	G
34	BA	65	U
34	BA	66	G
34	BA	78	G
34	BA	82	U
34	BA	89	U
34	BA	101	A
34	BA	103	C
34	BA	108	G
34	BA	110	C
34	BA	115	G
34	BA	116	A
34	BA	120	A
34	BA	121	C
34	BA	122	G
34	BA	124	G
34	BA	127	G
34	BA	129(A)	G
34	BA	130	A
34	BA	131	C
34	BA	132	C

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Mol	Chain	Res	Type
34	BA	134	A
34	BA	163	C
34	BA	182	U
34	BA	188	U
34	BA	189	U
34	BA	190	G
34	BA	191(A)	G
34	BA	195	A
34	BA	197	A
34	BA	198	G
34	BA	209	U
34	BA	210	U
34	BA	216	G
34	BA	236	G
34	BA	243	A
34	BA	244	U
34	BA	245	C
34	BA	247	G
34	BA	251	G
34	BA	252	U
34	BA	253	U
34	BA	262	A
34	BA	264	U
34	BA	265	G
34	BA	266	G
34	BA	267	C
34	BA	270	A
34	BA	275	G
34	BA	279	A
34	BA	280	C
34	BA	281	G
34	BA	282	A
34	BA	289	G
34	BA	293	G
34	BA	295	C
34	BA	296	U
34	BA	306	G
34	BA	308	C
34	BA	309	G
34	BA	313	A
34	BA	314	C
34	BA	315	A

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Mol	Chain	Res	Type
34	BA	316	G
34	BA	326	G
34	BA	328	C
34	BA	329	A
34	BA	330	C
34	BA	332	G
34	BA	336	C
34	BA	345	C
34	BA	346	G
34	BA	348	G
34	BA	351	G
34	BA	352	C
34	BA	353	A
34	BA	354	G
34	BA	364	A
34	BA	367	U
34	BA	368	U
34	BA	372	C
34	BA	373	A
34	BA	378	G
34	BA	379	C
34	BA	382	A
34	BA	383	A
34	BA	388	G
34	BA	389	A
34	BA	390	C
34	BA	392	G
34	BA	397	A
34	BA	398	C
34	BA	410	G
34	BA	412	A
34	BA	413	G
34	BA	414	A
34	BA	422	C
34	BA	423	G
34	BA	428	G
34	BA	429	U
34	BA	430	A
34	BA	438	G
34	BA	439	A
34	BA	451	A
34	BA	452	A

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Mol	Chain	Res	Type
34	BA	454	C
34	BA	465	A
34	BA	466	C
34	BA	467	G
34	BA	474	G
34	BA	481	G
34	BA	482	A
34	BA	483	C
34	BA	484	G
34	BA	485	G
34	BA	486	U
34	BA	487	A
34	BA	496	A
34	BA	497	U
34	BA	500	G
34	BA	508	C
34	BA	509	A
34	BA	511	C
34	BA	518	C
34	BA	519	C
34	BA	521	G
34	BA	522	C
34	BA	524	G
34	BA	527	G
34	BA	528	C
34	BA	530	G
34	BA	531	U
34	BA	532	A
34	BA	533	A
34	BA	534	U
34	BA	535	A
34	BA	536	C
34	BA	541	G
34	BA	548	G
34	BA	553	A
34	BA	555	C
34	BA	559	A
34	BA	560	U
34	BA	561	U
34	BA	563	A
34	BA	565	U
34	BA	566	G

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Mol	Chain	Res	Type
34	BA	567	G
34	BA	572	A
34	BA	573	A
34	BA	575	G
34	BA	577	G
34	BA	579	G
34	BA	585	G
34	BA	595	G
34	BA	596	C
34	BA	598	U
34	BA	607	A
34	BA	609	A
34	BA	623	C
34	BA	642	A
34	BA	650	G
34	BA	653	A
34	BA	655	A
34	BA	665	A
34	BA	672	U
34	BA	673	G
34	BA	679	C
34	BA	687	A
34	BA	688	G
34	BA	690	G
34	BA	691	G
34	BA	693	G
34	BA	694	A
34	BA	697	U
34	BA	702	A
34	BA	703	G
34	BA	704	A
34	BA	718	G
34	BA	719	C
34	BA	721	G
34	BA	723	U
34	BA	724	G
34	BA	728	A
34	BA	730	G
34	BA	731	G
34	BA	733	A
34	BA	749	C
34	BA	752	G

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Mol	Chain	Res	Type
34	BA	753	A
34	BA	754	C
34	BA	763	G
34	BA	764	C
34	BA	766	A
34	BA	776	G
34	BA	777	A
34	BA	781	A
34	BA	782	A
34	BA	785	G
34	BA	788	U
34	BA	790	A
34	BA	791	G
34	BA	793	U
34	BA	794	A
34	BA	801	U
34	BA	812	C
34	BA	813	U
34	BA	815	A
34	BA	816	A
34	BA	817	C
34	BA	818	G
34	BA	819	A
34	BA	820	U
34	BA	821	G
34	BA	828	A
34	BA	841	U
34	BA	843	U
34	BA	848	C
34	BA	854	G
34	BA	860	A
34	BA	865	A
34	BA	870	U
34	BA	871	U
34	BA	872	A
34	BA	873	A
34	BA	874	G
34	BA	884	U
34	BA	885	G
34	BA	889	A
34	BA	890	G
34	BA	891	U

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Mol	Chain	Res	Type
34	BA	901	A
34	BA	902	G
34	BA	907	A
34	BA	910	C
34	BA	913	A
34	BA	914	A
34	BA	917	G
34	BA	919	A
34	BA	920	U
34	BA	926	G
34	BA	927	G
34	BA	932	C
34	BA	934	C
34	BA	935	A
34	BA	945	G
34	BA	949	A
34	BA	950	U
34	BA	956	U
34	BA	958	A
34	BA	960	U
34	BA	961	U
34	BA	963	G
34	BA	965	A
34	BA	966	G
34	BA	967	C
34	BA	968	A
34	BA	969	A
34	BA	971	G
34	BA	972	C
34	BA	974	A
34	BA	975	A
34	BA	976	G
34	BA	977	A
34	BA	980	C
34	BA	982	U
34	BA	991	U
34	BA	993	G
34	BA	994	A
34	BA	995	C
34	BA	997	U
34	BA	998	G
34	BA	1000	A

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Mol	Chain	Res	Type
34	BA	1001	G
34	BA	1002	G
34	BA	1003	G
34	BA	1004	A
34	BA	1005	A
34	BA	1006	C
34	BA	1007	C
34	BA	1016	A
34	BA	1023	G
34	BA	1024	G
34	BA	1026	G
34	BA	1027	C
34	BA	1029	G
34	BA	1049	U
34	BA	1050	G
34	BA	1054	C
34	BA	1056	U
34	BA	1057	G
34	BA	1063	C
34	BA	1064	G
34	BA	1065	U
34	BA	1066	C
34	BA	1067	A
34	BA	1068	G
34	BA	1081	G
34	BA	1084	G
34	BA	1085	U
34	BA	1086	U
34	BA	1089	G
34	BA	1094	G
34	BA	1096	C
34	BA	1097	C
34	BA	1100	C
34	BA	1101	A
34	BA	1102	A
34	BA	1103	C
34	BA	1106	G
34	BA	1107	C
34	BA	1108	G
34	BA	1109	C
34	BA	1111	A
34	BA	1112	C

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Mol	Chain	Res	Type
34	BA	1115	C
34	BA	1118	C
34	BA	1123	A
34	BA	1125	U
34	BA	1126	U
34	BA	1129	C
34	BA	1130	A
34	BA	1131	G
34	BA	1132	C
34	BA	1136	U
34	BA	1138	G
34	BA	1139	G
34	BA	1140	C
34	BA	1145	C
34	BA	1146	A
34	BA	1147	C
34	BA	1148	U
34	BA	1152	A
34	BA	1153	C
34	BA	1154	G
34	BA	1157	A
34	BA	1158	C
34	BA	1159	U
34	BA	1161	C
34	BA	1162	C
34	BA	1164	G
34	BA	1174	G
34	BA	1182	G
34	BA	1183	A
34	BA	1184	G
34	BA	1185	G
34	BA	1188	A
34	BA	1189	C
34	BA	1190	G
34	BA	1195	C
34	BA	1196	U
34	BA	1197	G
34	BA	1200	C
34	BA	1201	A
34	BA	1202	G
34	BA	1203	C
34	BA	1211	U

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Mol	Chain	Res	Type
34	BA	1212	U
34	BA	1213	A
34	BA	1215	G
34	BA	1225	A
34	BA	1226	C
34	BA	1227	A
34	BA	1229	A
34	BA	1240	U
34	BA	1241	G
34	BA	1249	C
34	BA	1256	A
34	BA	1257	U
34	BA	1263	C
34	BA	1269	A
34	BA	1270	C
34	BA	1278	U
34	BA	1279	A
34	BA	1280	A
34	BA	1281	U
34	BA	1282	C
34	BA	1283	G
34	BA	1285	A
34	BA	1286	A
34	BA	1287	A
34	BA	1289	A
34	BA	1292	U
34	BA	1297	C
34	BA	1298	C
34	BA	1301	U
34	BA	1302	U
34	BA	1303	C
34	BA	1305	G
34	BA	1317	C
34	BA	1318	A
34	BA	1319	A
34	BA	1320	C
34	BA	1322	C
34	BA	1323	G
34	BA	1331	G
34	BA	1332	A
34	BA	1333	A
34	BA	1345	U

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Mol	Chain	Res	Type
34	BA	1346	A
34	BA	1347	G
34	BA	1348	U
34	BA	1353	G
34	BA	1362(A)	C
34	BA	1363	A
34	BA	1364	U
34	BA	1365	G
34	BA	1375	A
34	BA	1378	C
34	BA	1379	G
34	BA	1381	U
34	BA	1393	U
34	BA	1394	A
34	BA	1395	C
34	BA	1396	A
34	BA	1397	C
34	BA	1398	A
34	BA	1399	C
34	BA	1400	C
34	BA	1401	G
34	BA	1404	C
34	BA	1413	A
34	BA	1419	G
34	BA	1430	C
34	BA	1431	C
34	BA	1432	G
34	BA	1435	G
34	BA	1439	C
34	BA	1440	C
34	BA	1442	G
34	BA	1443	G
34	BA	1446	A
34	BA	1447	G
34	BA	1449	C
34	BA	1450	U
34	BA	1451	A
34	BA	1454	G
34	BA	1455	G
34	BA	1459	C
34	BA	1461	G
34	BA	1462	G

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Mol	Chain	Res	Type
34	BA	1463	C
34	BA	1464	G
34	BA	1465	C
34	BA	1467	G
34	BA	1469	G
34	BA	1481	U
34	BA	1484	C
34	BA	1487	G
34	BA	1489	G
34	BA	1491	G
34	BA	1492	A
34	BA	1494	G
34	BA	1495	U
34	BA	1496	C
34	BA	1500	A
34	BA	1502	A
34	BA	1503	A
34	BA	1504	G
34	BA	1505	G
34	BA	1506	U
34	BA	1507	A
34	BA	1517	G
34	BA	1520	G
34	BA	1527	C
34	BA	1530	G
34	BA	1531	A
34	BA	1532	U
34	BA	1534	A
55	BC	3	C
55	BC	5	G
55	BC	6	G
55	BC	7	A
55	BC	15	G
55	BC	16	U
55	BC	17	C
55	BC	18	G
55	BC	19	G
55	BC	21	A
55	BC	27	G
55	BC	30	G
55	BC	33	U
55	BC	34	G

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Mol	Chain	Res	Type
55	BC	35	A
55	BC	37	A
55	BC	39	U
55	BC	40	C
55	BC	41	C
55	BC	42	C
55	BC	47	U
55	BC	57	G
55	BC	58	A
55	BC	61	C
55	BC	70	G
55	BC	76	A
56	BD	2	C
56	BD	4	C
56	BD	5	G
56	BD	9	A
56	BD	16	U
56	BD	17	C
56	BD	18	G
56	BD	19	G
56	BD	21	A
56	BD	23	A
56	BD	34	G
56	BD	42	C
56	BD	43	C
56	BD	46	G
56	BD	47	U
56	BD	48	C
56	BD	49	C
56	BD	52	G
56	BD	53	G
56	BD	55	U
56	BD	61	C
56	BD	64	A
56	BD	65	G
56	BD	67	C
56	BD	68	C
56	BD	70	G
56	BD	71	G
56	BD	72	C
56	BD	73	A
56	BD	74	C

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Mol	Chain	Res	Type
56	BD	75	C
56	BE	2	C
56	BE	4	C
56	BE	6	G
56	BE	7	A
56	BE	9	A
56	BE	15	G
56	BE	16	U
56	BE	18	G
56	BE	19	G
56	BE	20	U
56	BE	21	A
56	BE	22	G
56	BE	42	C
56	BE	46	G
56	BE	47	U
56	BE	48	C
56	BE	52	G
56	BE	61	C
56	BE	69	G
56	BE	71	G
56	BE	73	A
56	BE	74	C
56	BE	75	C

All (399) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	13	A
1	AA	60	G
1	AA	67	U
1	AA	70	G
1	AA	71	A
1	AA	83	G
1	AA	90	U
1	AA	119	A
1	AA	125	G
1	AA	196	A
1	AA	199	A
1	AA	204	A
1	AA	205	G
1	AA	215	G

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Mol	Chain	Res	Type
1	AA	221	A
1	AA	227	A
1	AA	251	A
1	AA	270(B)	A
1	AA	270(L)	U
1	AA	270(M)	U
1	AA	270(Z)	U
1	AA	271(B)	G
1	AA	280	C
1	AA	283	A
1	AA	311	A
1	AA	323	G
1	AA	329	G
1	AA	331	A
1	AA	332	A
1	AA	351	G
1	AA	371	A
1	AA	403	U
1	AA	442	G
1	AA	455	C
1	AA	470	A
1	AA	503	A
1	AA	504	U
1	AA	506	G
1	AA	508	G
1	AA	526	A
1	AA	530	G
1	AA	559	G
1	AA	573	G
1	AA	574	C
1	AA	587	C
1	AA	602	G
1	AA	616	A
1	AA	620	G
1	AA	637	A
1	AA	643	A
1	AA	645	C
1	AA	669	G
1	AA	670	A
1	AA	685	A
1	AA	686	G
1	AA	730	C

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Mol	Chain	Res	Type
1	AA	740	U
1	AA	745	G
1	AA	746	A
1	AA	747	U
1	AA	750	A
1	AA	762	U
1	AA	773	U
1	AA	774	A
1	AA	776	G
1	AA	782	A
1	AA	783	A
1	AA	785	G
1	AA	788	A
1	AA	789	A
1	AA	800	A
1	AA	801	G
1	AA	811	U
1	AA	829	A
1	AA	830	G
1	AA	846	C
1	AA	858	U
1	AA	884	C
1	AA	897	C
1	AA	930	U
1	AA	944	G
1	AA	945	A
1	AA	957	A
1	AA	958	U
1	AA	960	A
1	AA	961	C
1	AA	973	A
1	AA	974(A)	C
1	AA	989	G
1	AA	1008	C
1	AA	1011	G
1	AA	1022	G
1	AA	1024	G
1	AA	1038	C
1	AA	1047	G
1	AA	1062	G
1	AA	1069	A
1	AA	1085	A

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Mol	Chain	Res	Type
1	AA	1100	C
1	AA	1126	A
1	AA	1130	U
1	AA	1131	G
1	AA	1154	G
1	AA	1178	C
1	AA	1179	C
1	AA	1183	G
1	AA	1204	A
1	AA	1210	A
1	AA	1212	G
1	AA	1221	C
1	AA	1237	A
1	AA	1241	A
1	AA	1247	A
1	AA	1248	G
1	AA	1250	G
1	AA	1253	A
1	AA	1267	U
1	AA	1272	A
1	AA	1288	U
1	AA	1300	U
1	AA	1302	A
1	AA	1323	U
1	AA	1342	A
1	AA	1349	A
1	AA	1378	A
1	AA	1379	A
1	AA	1406	U
1	AA	1420	U
1	AA	1427	A
1	AA	1428	C
1	AA	1444(A)	A
1	AA	1477	A
1	AA	1489	U
1	AA	1515	C
1	AA	1554	A
1	AA	1558	A
1	AA	1566	A
1	AA	1568	G
1	AA	1572	A
1	AA	1585	C

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Mol	Chain	Res	Type
1	AA	1603	A
1	AA	1608	A
1	AA	1610	A
1	AA	1625	C
1	AA	1626	G
1	AA	1634	A
1	AA	1647	G
1	AA	1650	G
1	AA	1693	U
1	AA	1694	C
1	AA	1698	A
1	AA	1699	G
1	AA	1727	U
1	AA	1758	G
1	AA	1778	U
1	AA	1780	A
1	AA	1784	A
1	AA	1791	A
1	AA	1800	C
1	AA	1801	G
1	AA	1819	A
1	AA	1820	U
1	AA	1828	G
1	AA	1919	A
1	AA	1920	C
1	AA	1936	A
1	AA	1937	A
1	AA	1938	A
1	AA	1940	U
1	AA	1943	U
1	AA	1962	C
1	AA	1964	G
1	AA	1966	A
1	AA	1970	A
1	AA	1977	A
1	AA	1980	G
1	AA	1981	A
1	AA	1992	G
1	AA	1996	C
1	AA	2017	U
1	AA	2021	C
1	AA	2022	U

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Mol	Chain	Res	Type
1	AA	2030	A
1	AA	2032	G
1	AA	2033	A
1	AA	2047	U
1	AA	2049	G
1	AA	2051	A
1	AA	2055	C
1	AA	2073	C
1	AA	2076	U
1	AA	2110	G
1	AA	2111	C
1	AA	2118	U
1	AA	2126	A
1	AA	2157	G
1	AA	2158	A
1	AA	2171	A
1	AA	2172	U
1	AA	2210	G
1	AA	2213	U
1	AA	2225	A
1	AA	2240	C
1	AA	2275	C
1	AA	2282	G
1	AA	2319	G
1	AA	2324	C
1	AA	2345	G
1	AA	2350	C
1	AA	2384	G
1	AA	2392	A
1	AA	2416	C
1	AA	2422	A
1	AA	2427	C
1	AA	2428	G
1	AA	2436	G
1	AA	2439	A
1	AA	2447	G
1	AA	2490	G
1	AA	2491	U
1	AA	2497	A
1	AA	2500	U
1	AA	2501	C
1	AA	2503	A

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Mol	Chain	Res	Type
1	AA	2517	C
1	AA	2519	U
1	AA	2542	A
1	AA	2571	C
1	AA	2572	A
1	AA	2602	A
1	AA	2609	U
1	AA	2610	C
1	AA	2613	U
1	AA	2615	U
1	AA	2637	U
1	AA	2652	C
1	AA	2688	U
1	AA	2689	U
1	AA	2690	C
1	AA	2705	A
1	AA	2707	G
1	AA	2726	U
1	AA	2755	C
1	AA	2756	U
1	AA	2776	A
1	AA	2777	G
1	AA	2778	A
1	AA	2790	A
1	AA	2835	A
1	AA	2848	G
1	AA	2849	U
1	AA	2866	U
1	AA	2879	C
2	AB	7	G
2	AB	15	A
2	AB	56	G
34	BA	5	U
34	BA	8	A
34	BA	30	U
34	BA	31	G
34	BA	47	C
34	BA	51	A
34	BA	60	A
34	BA	65	U
34	BA	88	C
34	BA	99	C

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Mol	Chain	Res	Type
34	BA	109	A
34	BA	115	G
34	BA	119	A
34	BA	129(A)	G
34	BA	181	G
34	BA	190	G
34	BA	208	U
34	BA	210	U
34	BA	243	A
34	BA	244	U
34	BA	246	A
34	BA	250	A
34	BA	251	G
34	BA	266	G
34	BA	274	A
34	BA	279	A
34	BA	280	C
34	BA	281	G
34	BA	305	G
34	BA	308	C
34	BA	327	A
34	BA	328	C
34	BA	329	A
34	BA	344	A
34	BA	345	C
34	BA	351	G
34	BA	366	C
34	BA	367	U
34	BA	372	C
34	BA	413	G
34	BA	428	G
34	BA	429	U
34	BA	451	A
34	BA	484	G
34	BA	495	A
34	BA	496	A
34	BA	498	A
34	BA	508	C
34	BA	518	C
34	BA	531	U
34	BA	535	A
34	BA	547	A

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Mol	Chain	Res	Type
34	BA	559	A
34	BA	560	U
34	BA	562	C
34	BA	563	A
34	BA	566	G
34	BA	576	G
34	BA	652	U
34	BA	686	U
34	BA	687	A
34	BA	701	C
34	BA	702	A
34	BA	703	G
34	BA	717	C
34	BA	721	G
34	BA	723	U
34	BA	748	C
34	BA	753	A
34	BA	781	A
34	BA	792	A
34	BA	793	U
34	BA	812	C
34	BA	815	A
34	BA	816	A
34	BA	817	C
34	BA	818	G
34	BA	819	A
34	BA	820	U
34	BA	871	U
34	BA	872	A
34	BA	873	A
34	BA	889	A
34	BA	890	G
34	BA	901	A
34	BA	913	A
34	BA	918	A
34	BA	960	U
34	BA	965	A
34	BA	968	A
34	BA	974	A
34	BA	975	A
34	BA	992	U
34	BA	993	G

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Mol	Chain	Res	Type
34	BA	1004	A
34	BA	1049	U
34	BA	1055	A
34	BA	1065	U
34	BA	1067	A
34	BA	1084	G
34	BA	1085	U
34	BA	1101	A
34	BA	1129	C
34	BA	1145	C
34	BA	1157	A
34	BA	1182	G
34	BA	1183	A
34	BA	1196	U
34	BA	1212	U
34	BA	1214	C
34	BA	1224	G
34	BA	1226	C
34	BA	1239	A
34	BA	1240	U
34	BA	1285	A
34	BA	1297	C
34	BA	1300	G
34	BA	1302	U
34	BA	1317	C
34	BA	1322	C
34	BA	1331	G
34	BA	1345	U
34	BA	1346	A
34	BA	1347	G
34	BA	1363	A
34	BA	1364	U
34	BA	1377	A
34	BA	1394	A
34	BA	1399	C
34	BA	1400	C
34	BA	1442	G
34	BA	1443	G
34	BA	1446	A
34	BA	1468	A
34	BA	1494	G
34	BA	1504	G

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Mol	Chain	Res	Type
34	BA	1506	U
34	BA	1528	U
34	BA	1529	G
34	BA	1531	A
56	BD	15	G
56	BD	74	C
56	BE	5	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands 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	$\#\|Z\| > 2$
60	GCP	BZ	701	-	27,34,34	1.84	7 (25%)	34,54,54	1.99	8 (23%)
58	NMY	AA	3001	-	45,45,45	0.51	0	63,67,67	1.19	7 (11%)
59	8AN	AA	3002	-	19,24,25	1.10	1 (5%)	13,35,38	1.70	4 (30%)
58	NMY	BA	1601	-	45,45,45	0.51	0	63,67,67	1.06	6 (9%)
59	8AN	AA	3003	56	19,24,25	1.09	1 (5%)	13,35,38	1.70	4 (30%)

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
60	GCP	BZ	701	-	-	5/15/38/38	0/3/3/3
58	NMY	AA	3001	-	-	4/18/94/94	1/4/4/4
59	8AN	AA	3002	-	-	2/3/25/26	0/3/3/3
58	NMY	BA	1601	-	-	5/18/94/94	0/4/4/4
59	8AN	AA	3003	56	-	3/3/25/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BZ	701	GCP	PG-O1G	5.39	1.61	1.50
60	BZ	701	GCP	C5-C6	4.19	1.48	1.41
60	BZ	701	GCP	PG-O2G	-2.85	1.48	1.54
60	BZ	701	GCP	PG-O3G	2.85	1.61	1.54
60	BZ	701	GCP	PB-O3A	2.72	1.61	1.58
60	BZ	701	GCP	C5-C4	2.52	1.47	1.40
59	AA	3003	8AN	C5-C4	2.50	1.47	1.40
59	AA	3002	8AN	C5-C4	2.46	1.47	1.40
60	BZ	701	GCP	PB-O2B	2.17	1.61	1.56

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	BZ	701	GCP	C2-N3-C4	5.02	121.09	115.36
60	BZ	701	GCP	C2-N1-C6	3.99	122.27	115.93
60	BZ	701	GCP	C5-C6-N1	-3.93	118.06	123.43
60	BZ	701	GCP	PB-O3A-PA	-3.80	120.51	132.56
60	BZ	701	GCP	C4-C5-C6	-3.75	117.22	120.80
58	BA	1601	NMY	C13-C14-C15	3.50	106.31	102.10
60	BZ	701	GCP	C3'-C2'-C1'	3.49	106.23	100.98
58	AA	3001	NMY	C13-C14-C15	3.49	106.30	102.10
60	BZ	701	GCP	N3-C2-N1	-3.28	122.84	127.22
59	AA	3003	8AN	N3-C2-N1	-3.19	123.69	128.68
59	AA	3002	8AN	N3-C2-N1	-3.17	123.73	128.68
60	BZ	701	GCP	C4-C5-N7	-2.73	106.55	109.40
59	AA	3003	8AN	C4-C5-N7	-2.68	106.61	109.40
59	AA	3002	8AN	C4-C5-N7	-2.66	106.62	109.40
59	AA	3003	8AN	O4'-C4'-C3'	2.58	107.85	104.15
59	AA	3002	8AN	C2'-C3'-C4'	2.58	106.29	102.68
59	AA	3003	8AN	C2'-C3'-C4'	2.58	106.28	102.68
59	AA	3002	8AN	O4'-C4'-C3'	2.56	107.82	104.15
58	AA	3001	NMY	C13-O11-C11	-2.50	111.77	117.96
58	BA	1601	NMY	C13-O11-C11	-2.49	111.79	117.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	AA	3001	NMY	O22-C22-C23	2.49	110.65	106.01
58	AA	3001	NMY	C1-O1-C10	-2.49	111.81	117.96
58	AA	3001	NMY	C18-O18-C15	-2.49	111.81	117.96
58	BA	1601	NMY	C18-O18-C15	-2.49	111.81	117.96
58	BA	1601	NMY	O22-C22-C23	2.49	110.64	106.01
58	BA	1601	NMY	C1-O1-C10	-2.48	111.82	117.96
58	AA	3001	NMY	O16-C13-C14	2.22	107.84	104.98
58	BA	1601	NMY	O16-C13-C14	2.21	107.83	104.98
58	AA	3001	NMY	C3-C4-C5	2.01	113.83	110.24

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	3001	NMY	C19-C18-O18-C15
58	BA	1601	NMY	O5-C5-C6-N6
58	BA	1601	NMY	C14-C13-O11-C11
59	AA	3003	8AN	C4'-C5'-O5'-P
59	AA	3003	8AN	O4'-C4'-C5'-O5'
59	AA	3003	8AN	C3'-C4'-C5'-O5'
60	BZ	701	GCP	PG-C3B-PB-O1B
60	BZ	701	GCP	PG-C3B-PB-O2B
60	BZ	701	GCP	PG-C3B-PB-O3A
58	BA	1601	NMY	O16-C16-C17-O17
58	BA	1601	NMY	C15-C16-C17-O17
59	AA	3002	8AN	C3'-C4'-C5'-O5'
58	AA	3001	NMY	O22-C18-O18-C15
59	AA	3002	8AN	O4'-C4'-C5'-O5'
58	BA	1601	NMY	O16-C13-O11-C11
60	BZ	701	GCP	C5'-O5'-PA-O3A
58	AA	3001	NMY	O22-C22-C23-N19
60	BZ	701	GCP	C5'-O5'-PA-O1A
58	AA	3001	NMY	C2-C1-O1-C10

All (1) ring outliers are listed below:

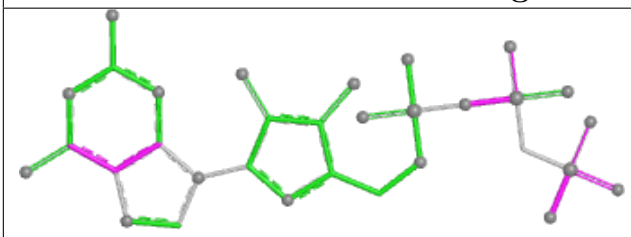
Mol	Chain	Res	Type	Atoms
58	AA	3001	NMY	C10-C11-C12-C7-C8-C9

No monomer is involved in short contacts.

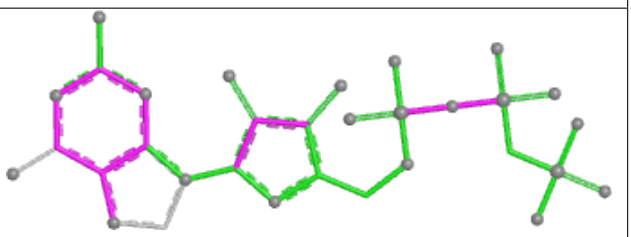
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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

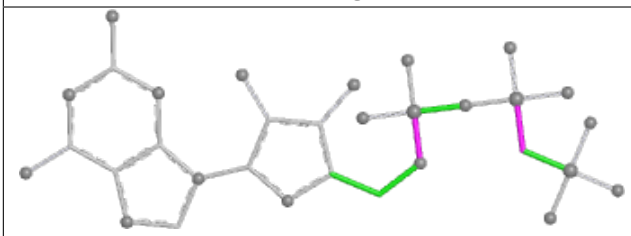
Ligand GCP BZ 701



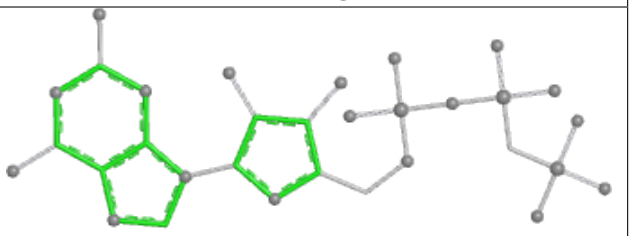
Bond lengths



Bond angles

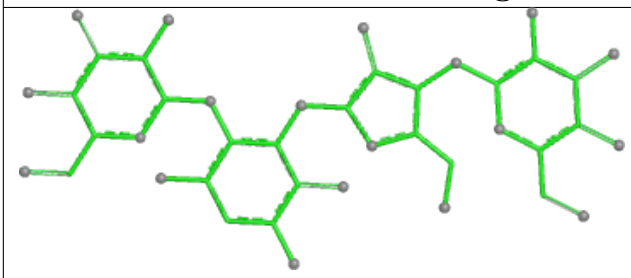


Torsions

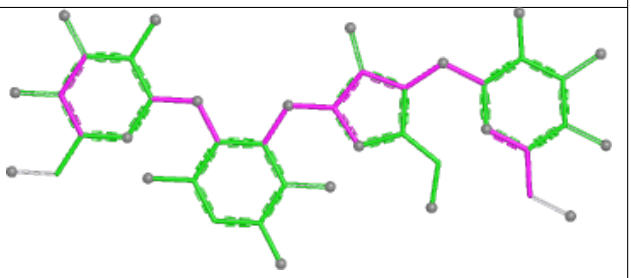


Rings

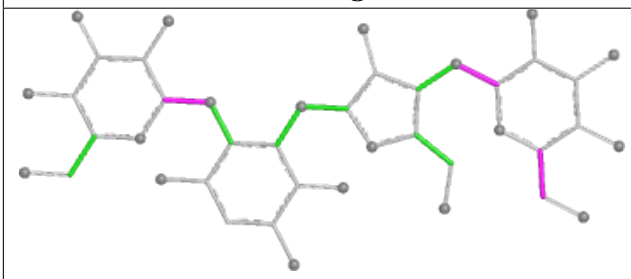
Ligand NMY AA 3001



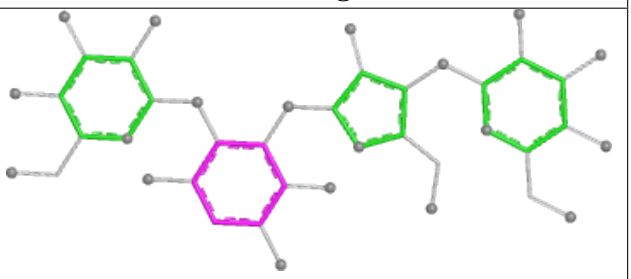
Bond lengths



Bond angles

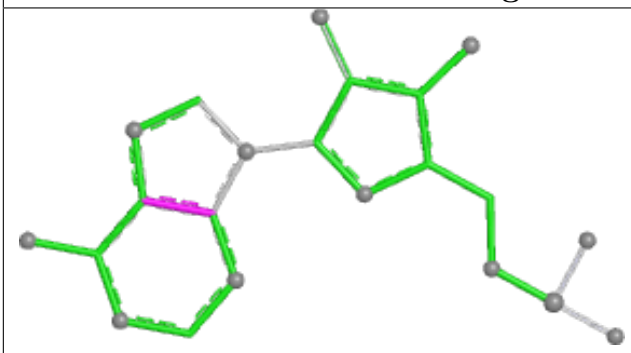


Torsions

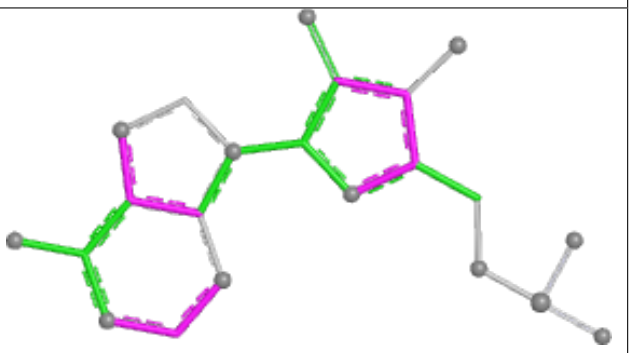


Rings

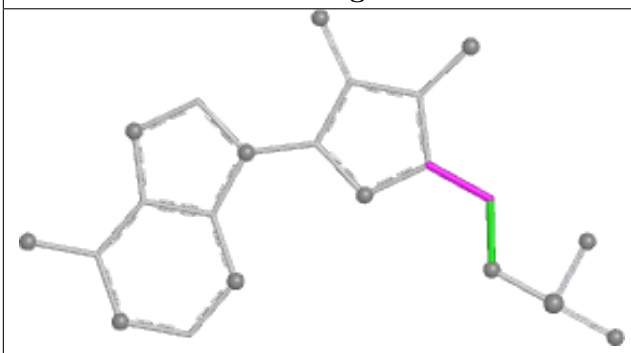
Ligand 8AN AA 3002



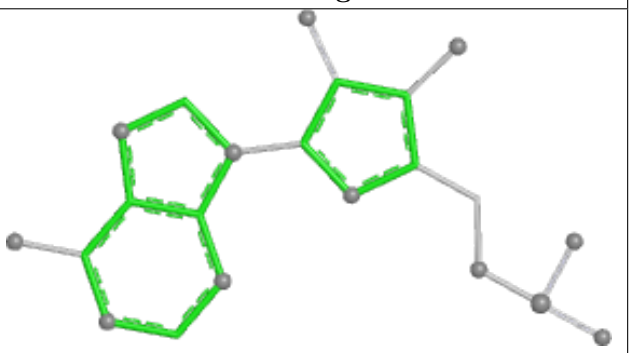
Bond lengths



Bond angles

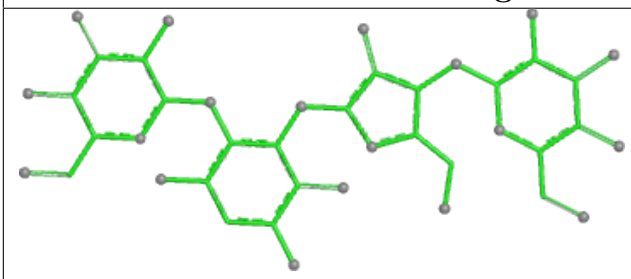


Torsions

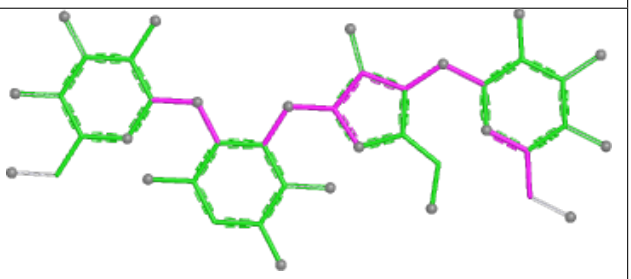


Rings

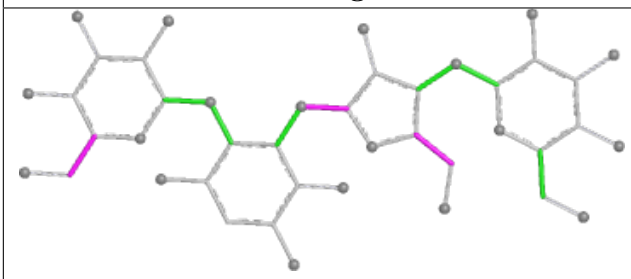
Ligand NMY BA 1601



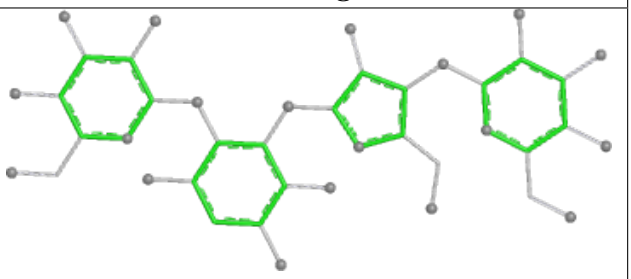
Bond lengths



Bond angles

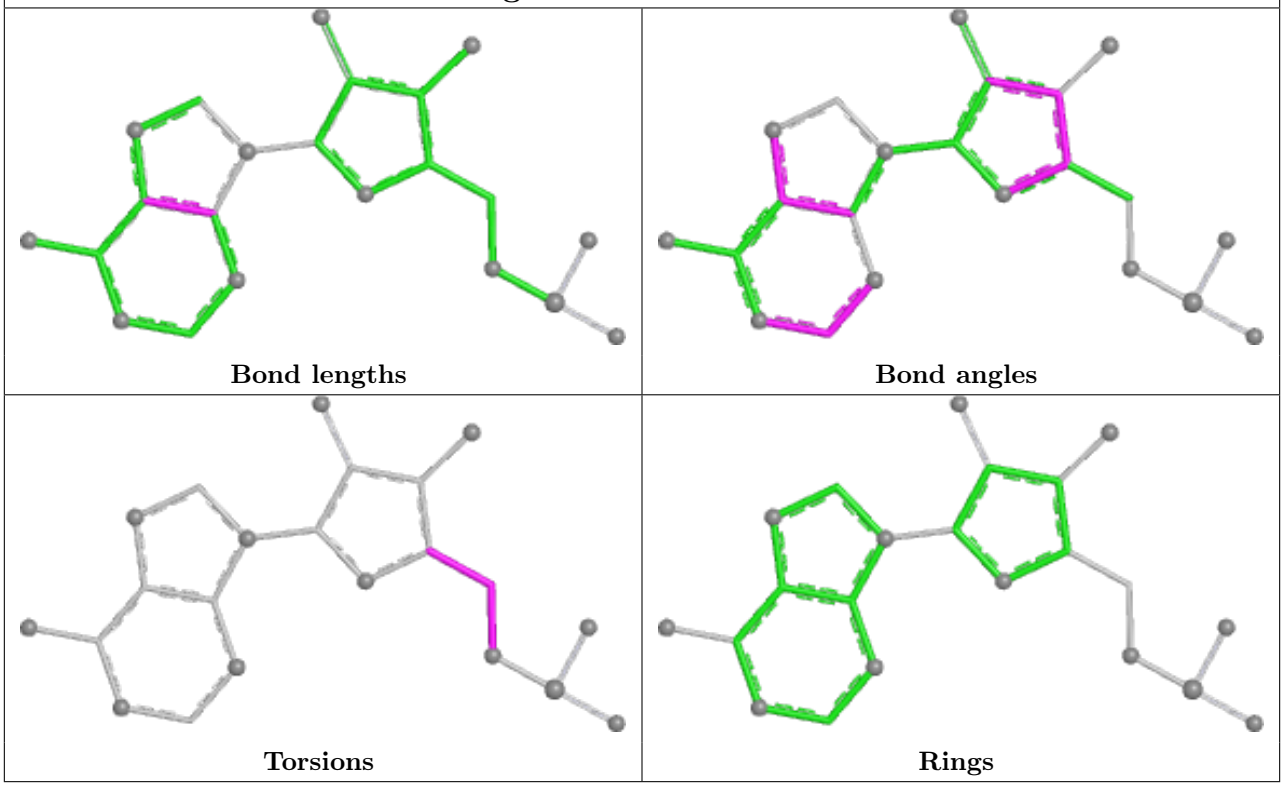


Torsions



Rings

Ligand 8AN AA 3003



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	AA	10
3	AC	3
34	BA	3
33	Ag	2
31	AI	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Ag	30:UNK	C	123:UNK	N	31.39
1	AA	164:U	O3'	171:G	P	7.68
1	AA	2893:G	O3'	2894:G	P	5.34
1	AA	2107:C	O3'	2108:C	P	4.97

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AC	180:PHE	C	181:PRO	N	4.62
1	AA	1105:U	O3'	1106:G	P	4.46
1	AA	2181:G	O3'	2182:G	P	4.08
1	BA	1308:U	O3'	1309:G	P	3.99
1	Ag	153:UNK	C	154:UNK	N	3.23
1	AC	158:ALA	C	159:GLY	N	3.01
1	AC	66:HIS	C	67:GLY	N	2.81
1	AA	1073:A	O3'	1074:G	P	2.79
1	AA	1033:U	O3'	1034:G	P	2.34
1	BA	1167:A	O3'	1169:A	P	1.86
1	AA	2756:U	O3'	2757:A	P	1.77
1	AA	1203:G	O3'	1204:A	P	1.19
1	AI	153:LEU	C	154:GLY	N	1.11
1	BA	1317:C	O3'	1318:A	P	0.77
1	AA	1060:U	O3'	1061:U	P	0.64

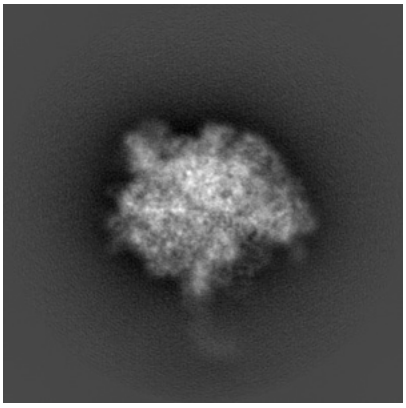
6 Map visualisation (i)

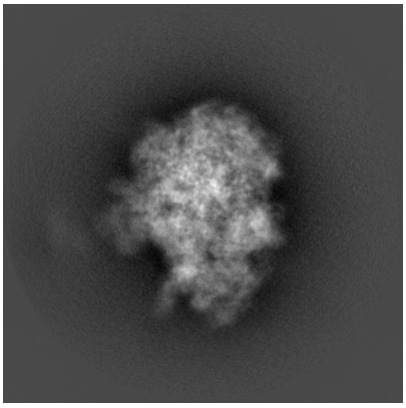
This section contains visualisations of the EMDB entry EMD-6397. These allow visual inspection of the internal detail of the map and identification of artifacts.

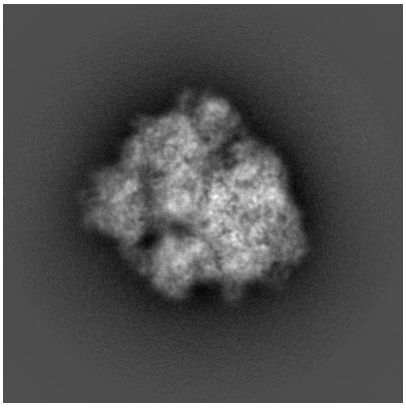
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

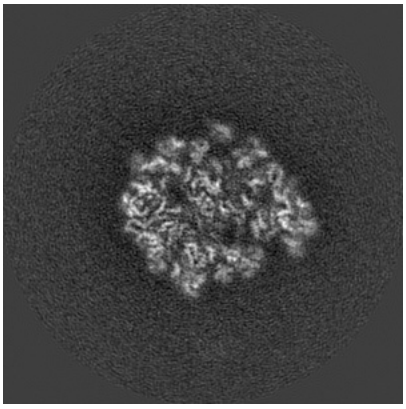

Y

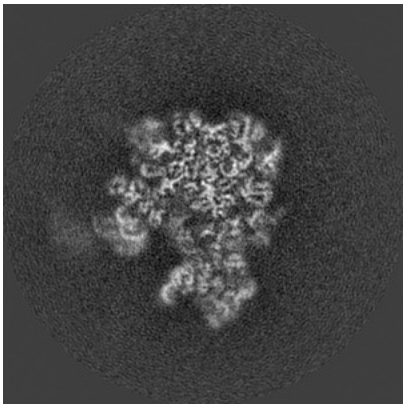

Z

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

6.2 Central slices (i)

6.2.1 Primary map


X Index: 180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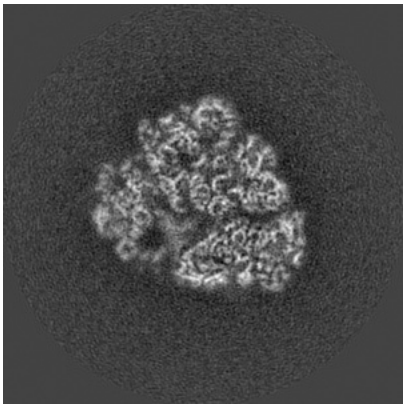
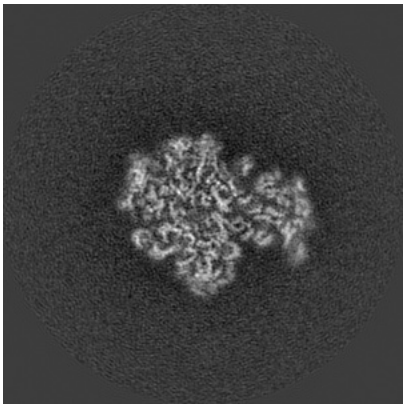

Z Index: 180

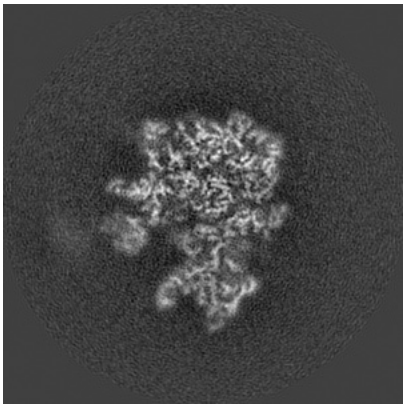
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

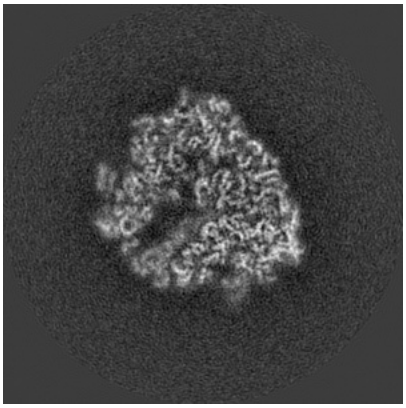
6.3.1 Primary map



X Index: 189



Y Index: 185



Z Index: 173

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0392. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

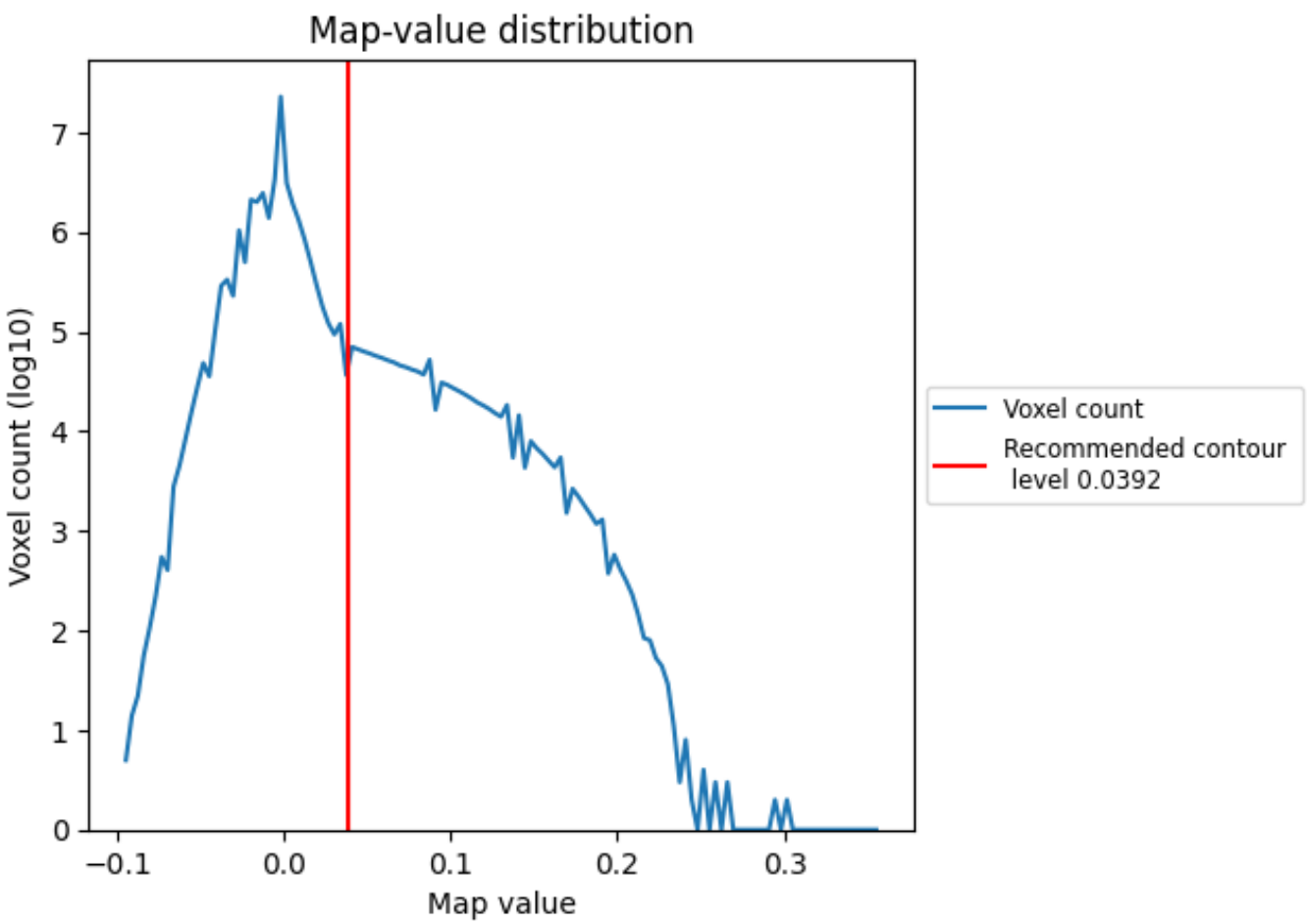
6.5 Mask visualisation (i)

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

7 Map analysis (i)

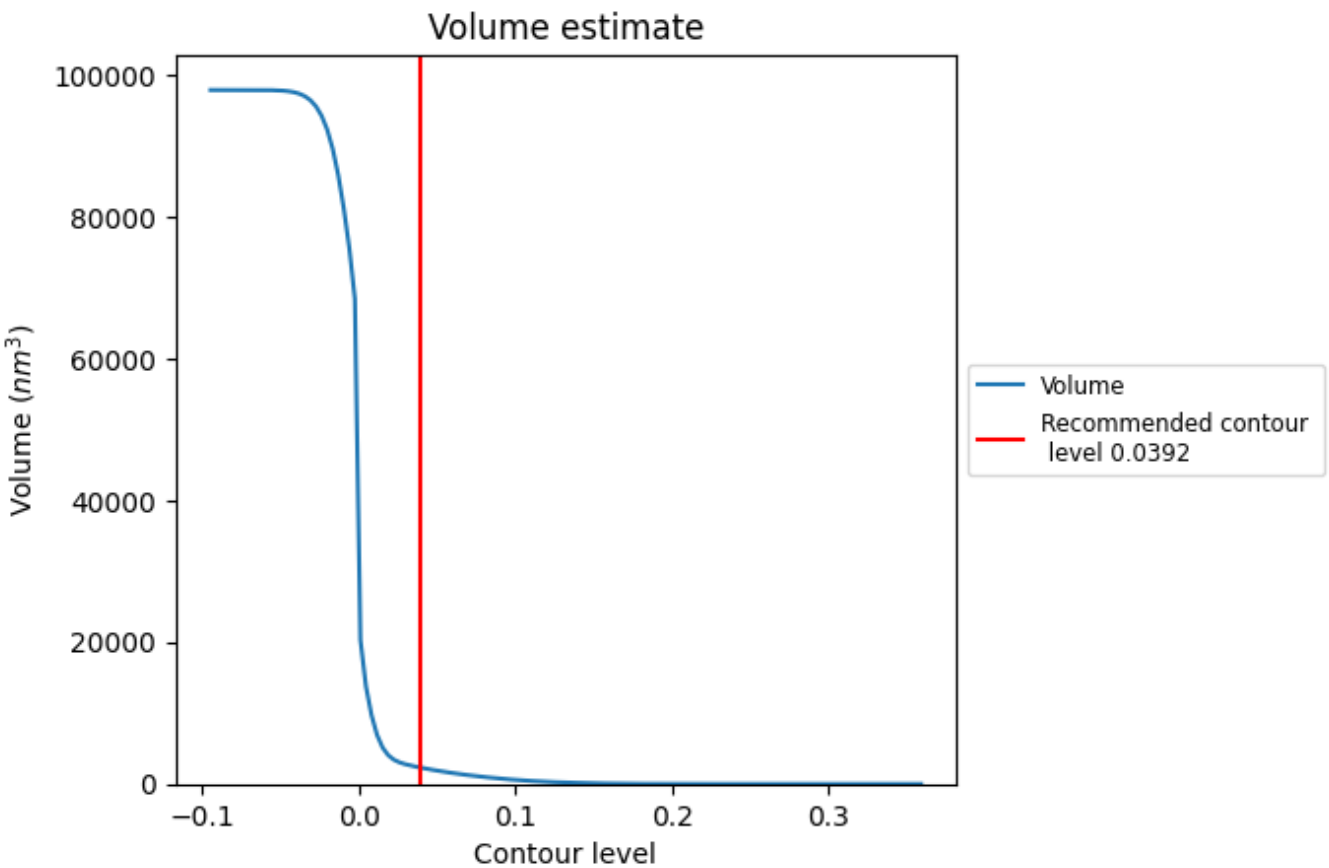
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

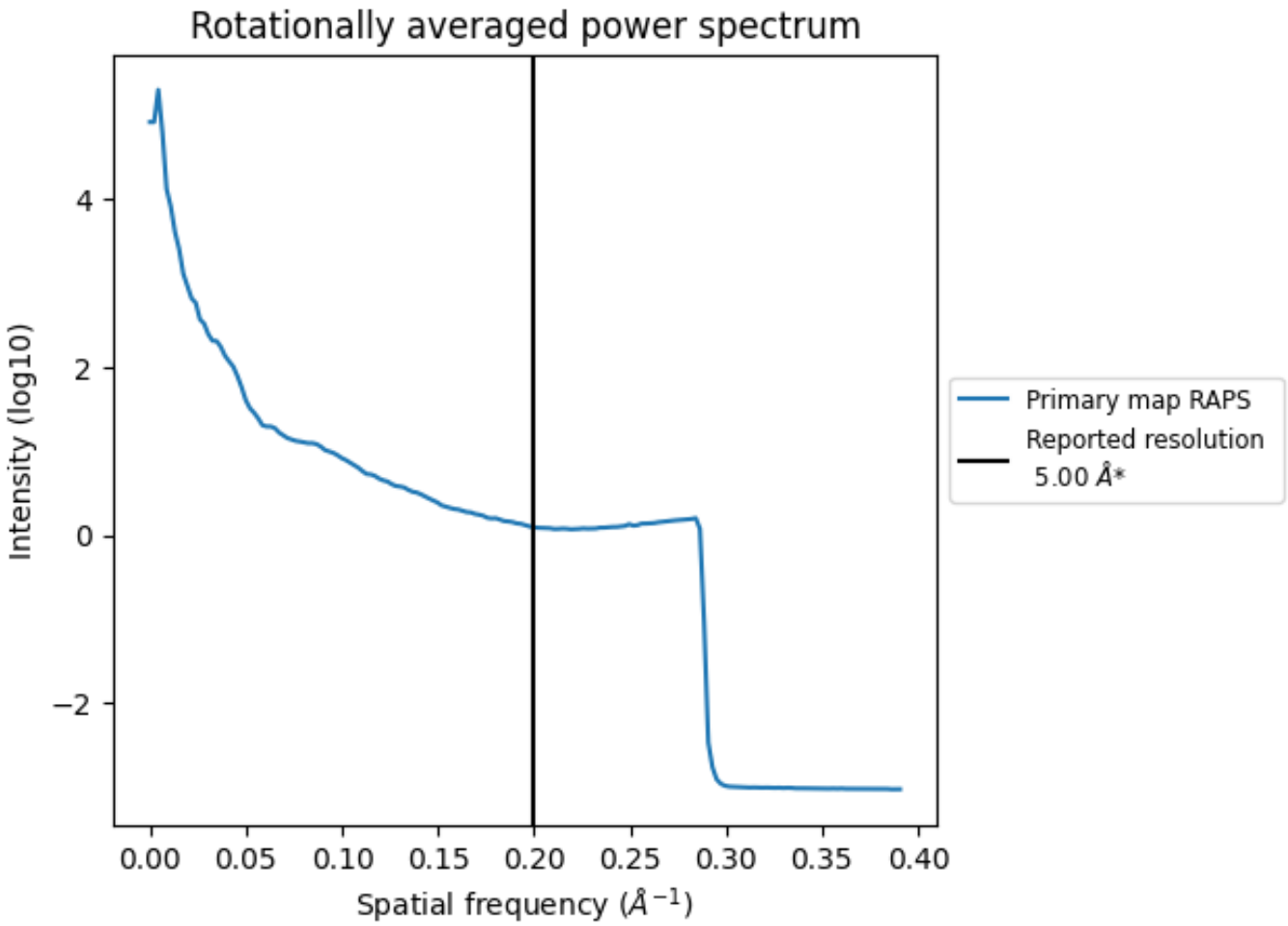
7.2 Volume estimate (i)



The volume at the recommended contour level is 2310 nm^3; this corresponds to an approximate mass of 2087 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.200 Å^{-1}

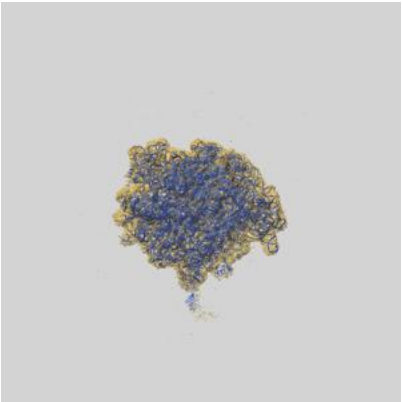
8 Fourier-Shell correlation (i)

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

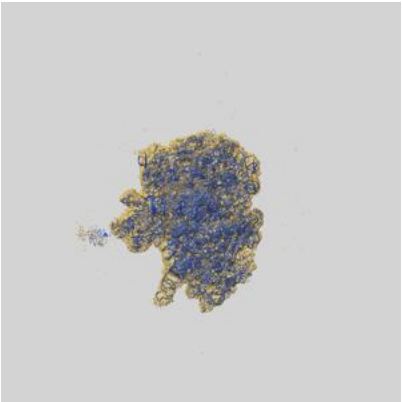
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-6397 and PDB model 5AA0. Per-residue inclusion information can be found in section 3 on page 16.

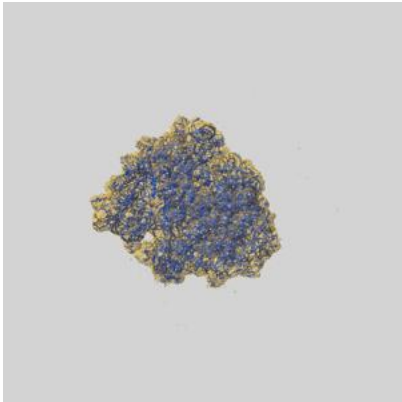
9.1 Map-model overlay (i)



X



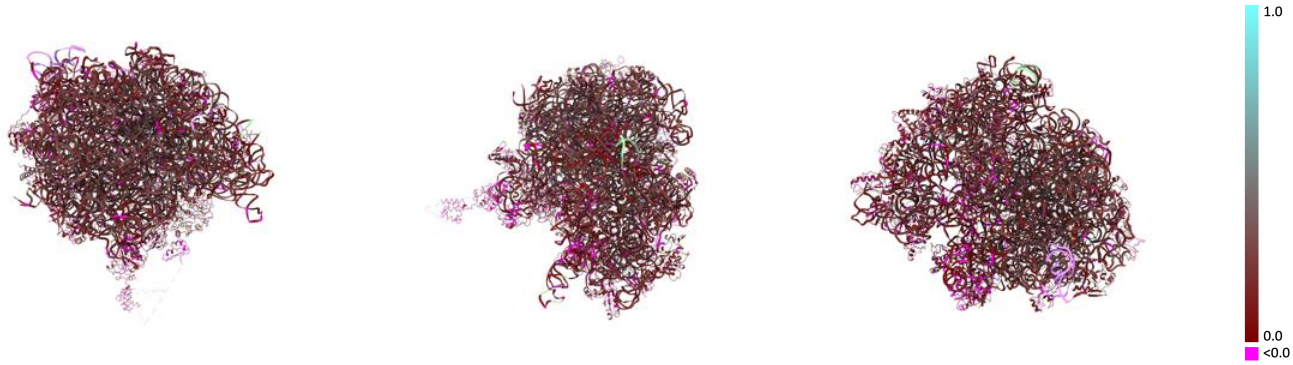
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0392 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

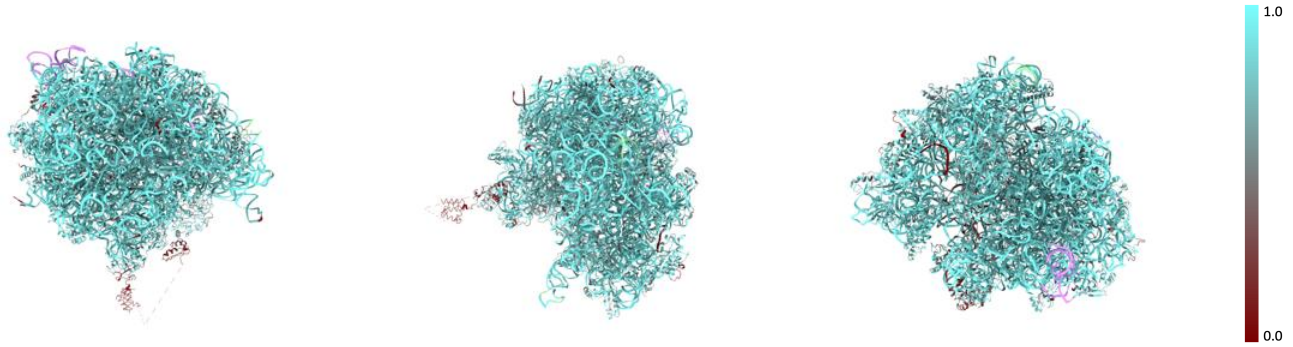
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

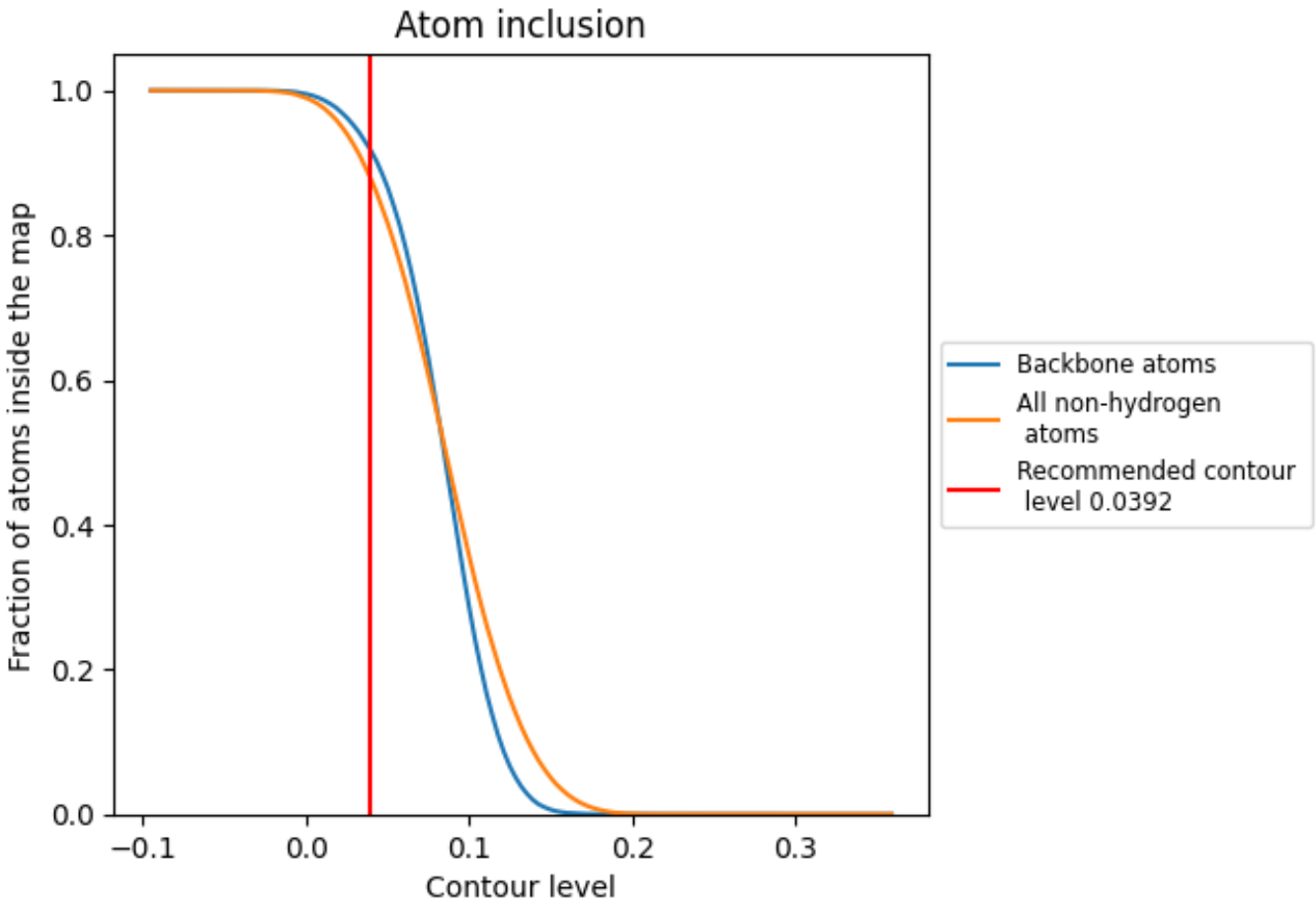
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0392).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0392) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8821	0.2090
AA	0.9585	0.2510
AB	0.9652	0.2250
AC	0.6046	0.0530
AD	0.7908	0.2240
AE	0.8381	0.2250
AF	0.7986	0.2090
AG	0.7882	0.1390
AH	0.8149	0.1570
AI	0.5160	0.0600
AJ	0.7137	0.0610
AK	0.8201	0.2220
AL	0.7495	0.2390
AM	0.7589	0.1540
AN	0.7684	0.2120
AO	0.8096	0.2250
AP	0.8553	0.1900
AQ	0.7720	0.2120
AR	0.8438	0.2120
AS	0.8241	0.1840
AT	0.7995	0.2290
AU	0.8033	0.2180
AV	0.7231	0.1390
AW	0.5104	0.1160
AX	0.7601	0.1740
AY	0.7971	0.1880
AZ	0.7917	0.1800
Aa	0.7625	0.1890
Ab	0.8037	0.2150
Ac	0.8117	0.1740
Ad	0.7663	0.2270
Ae	0.7356	0.2190
Af	0.7891	0.2040
Ag	0.0774	-0.0030
BA	0.9479	0.2080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BC	0.8672	0.1270
BD	0.6450	0.1440
BE	0.7038	0.1190
BF	0.7673	0.1800
BG	0.8073	0.1710
BH	0.7465	0.1310
BI	0.7930	0.2130
BJ	0.7454	0.1320
BK	0.8071	0.1720
BL	0.8662	0.2100
BM	0.8416	0.1450
BN	0.7662	0.1360
BO	0.7995	0.1660
BP	0.6724	0.1320
BQ	0.7865	0.1020
BR	0.8287	0.1150
BS	0.8051	0.1600
BT	0.8486	0.1850
BU	0.7349	0.1380
BV	0.7334	0.1350
BW	0.7639	0.0140
BX	0.7226	0.1530
BY	0.9110	0.1500
BZ	0.7425	0.1900