



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 02:32 AM EDT

PDB ID : 4V4P
Title : Crystal structure of 70S ribosome with thrS operator and tRNAs.
Authors : Jenner, L.; Romby, P.; Rees, B.; Schulze-Briese, C.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.; Yusupova, G.; Yusupov, M.
Deposited on : 2005-01-19
Resolution : 5.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

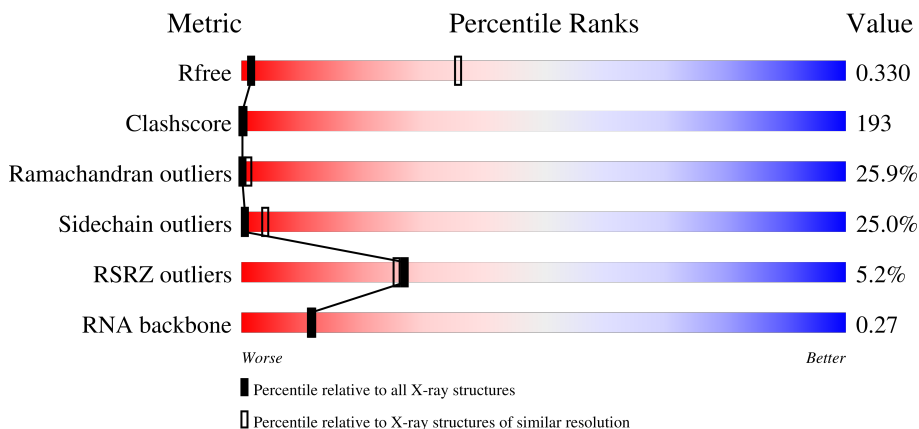
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1019 (7.12-3.82)
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)
RNA backbone	3102	1074 (7.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	AB	123	 52% 41% 7%
2	AA	2915	 2% 41% 39% 18%
3	AC	228	 2% 9% 64% 19%
4	AD	178	 6% 39% 40% 16%

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Mol	Chain	Length	Quality of chain
5	AE	338	
6	AF	246	
7	AG	176	
8	AH	177	
9	AI	128	
9	AJ	128	
10	AK	149	
11	AL	141	
12	AM	145	
13	AN	122	
14	AO	164	
15	AP	138	
16	AQ	186	
17	AR	66	
18	AS	113	
19	AT	84	
20	AU	119	
21	AV	253	
22	AW	70	
23	AX	60	
24	A0	118	
25	A1	118	
26	A2	100	
27	A3	91	
28	A4	73	



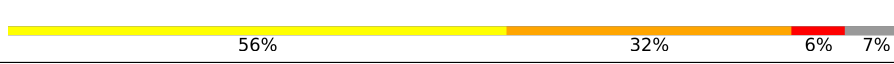
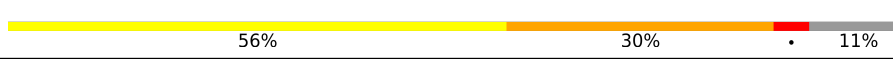
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Mol	Chain	Length	Quality of chain
29	A5	60	
30	A6	82	
31	A7	47	
32	A8	64	
33	A9	36	
34	BA	1522	
35	BB	76	
35	BC	76	
36	B1	78	
37	BE	256	
38	BF	239	
39	BG	209	
40	BH	162	
41	BI	101	
42	BJ	156	
43	BK	138	
44	BL	128	
45	BM	105	
46	BN	129	
47	BO	135	
48	BP	126	
49	BQ	61	
50	BR	89	
51	BS	88	
52	BT	105	

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Mol	Chain	Length	Quality of chain
53	BU	88	
54	BV	93	
55	BW	106	
56	BX	27	

2 Entry composition [i](#)

There are 56 unique types of molecules in this entry. The entry contains 148539 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S ribosomal RNA.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	-1	A	-	insertion	GB 48271
AB	120	U	-	insertion	GB 48271

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	AA	2872	61847	27526	11556	19893	2872	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	494	G	-	insertion	GB 48268

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	AC	221	1687	1066	306	312	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	AD	173	1308	820	246	236	6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	AE	191	1507	940	290	273	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	AF	189	1430	872	255	302	1	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	AG	122	957	597	176	180	4	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	AH	164	1251	787	225	237	2	0	0	0

- Molecule 9 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	AI	128	945	599	152	193	1	0	0	0
9	AJ	128	945	599	152	193	1	0	0	0

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	AK	148	1145	727	205	212	1	0	0	0

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	AL	133	999	642	169	182	6	0	0	0

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	AM	117	917	570	164	180	3	0	0	0

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	AN	122	937	585	180	169	3	0	0	0

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	AO	84	639	391	109	139	0	0	0

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AP	138	1081	678	208	192	3	0	0	0

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
16	AQ	113	866	536	165	164	1	0	0	0

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
17	AR	52	406	242	74	85	5	0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
18	AS	108	860	542	169	149	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AT	76	602	366	102	131	3	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
20	AU	110	879	531	166	182		0	0	0

- Molecule 21 is a protein called 50S general stress protein CTC (L25).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
21	AV	177	1360	859	238	257	6	0	0	0

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
22	AW	64	494	301	93	99	1	0	0	0

- Molecule 23 is a protein called 50S ribosomal protein L30.

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

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
24	A0	105	855	536	174	145		0	0	0

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
25	A1	117	978	608	210	159	1	0	0	0

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
26	A2	100	787	495	146	145	1	0	0	0

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
27	A3	86	641	402	124	114	1	0	0	0

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
28	A4	73	604	382	110	108	4	0	0	0

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
29	A5	58	457	281	94	77	5	0	0	0

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	A6	53	431	274	80	76	1	0	0	0

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
31	A7	46	383	230	91	60	2	0	0	0

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
32	A8	63	496	312	101	78	5	0	0	0

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
33	A9	35	285	172	64	45	4	0	0	0

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

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

- Molecule 35 is a RNA chain called tRNA Phe (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
35	BB	76	1626	725	293	532	76	0	0	0
35	BC	76	1626	725	293	532	76	0	0	0

- Molecule 36 is a RNA chain called thrS mRNA operator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
36	B1	66	1405	629	247	463	66	0	0	0

- Molecule 37 is a protein called 30S ribosomal protein S2.

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

- Molecule 38 is a protein called 30S ribosomal protein S3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	25	ASP	GLU	conflict	UNP Q5SHQ2
BK	37	ARG	LYS	conflict	UNP Q5SHQ2
BK	52	ASP	GLU	conflict	UNP Q5SHQ2
BK	61	VAL	ILE	conflict	UNP Q5SHQ2
BK	62	TYR	HIS	conflict	UNP Q5SHQ2
BK	81	HIS	LYS	conflict	UNP Q5SHQ2
BK	88	LYS	ARG	conflict	UNP Q5SHQ2
BK	115	SER	PRO	conflict	UNP Q5SHQ2

- Molecule 44 is a protein called 30S ribosomal protein S9.

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

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
46	BN	119	885	549	168	165	3	0	0	0

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
53	BU	73	597	380	118	99	0	0	0

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	41	VAL	ILE	conflict	UNP Q5SIH2

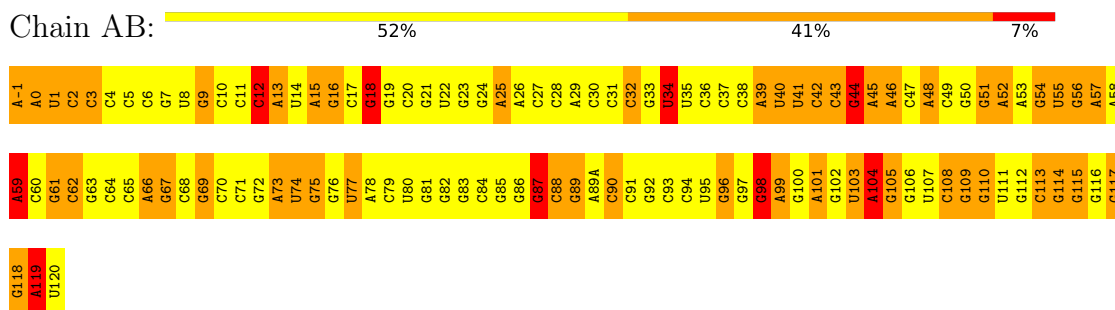
- Molecule 56 is a protein called 30S ribosomal protein Thx.

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

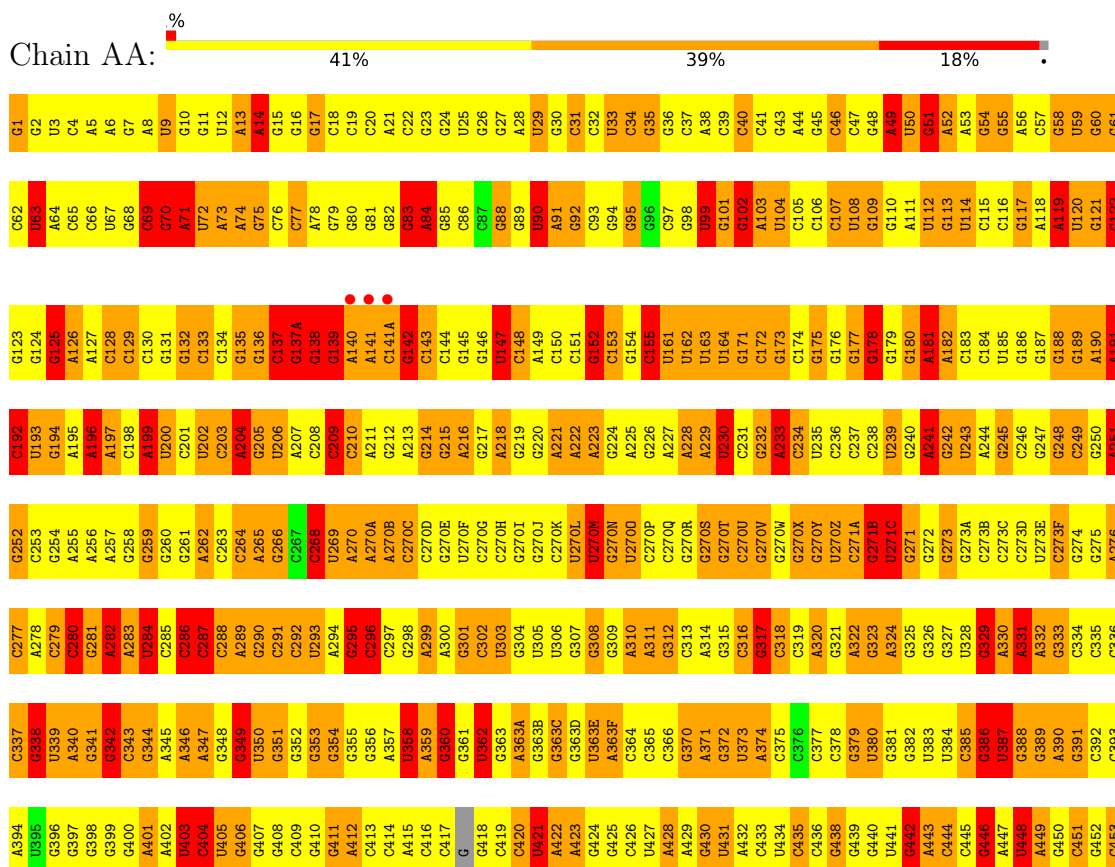
3 Residue-property plots

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

- Molecule 1: 5S ribosomal RNA



- Molecule 2: 23S ribosomal RNA

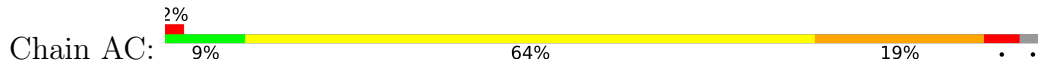


A1395	A1396	A1397	A1398	A1399	A1400	A1401	A1402	A1403	A1404	A1405	A1406	A1407	A1408	A1409	A1410	A1411	A1412	A1413	A1414	A1415	G1416	G1417	G1418	G1419	A1420	A1421	A1422	A1423	A1424	A1425	A1426	A1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	A1435	A1436	A1437	A1438	A1439	G1440	G1441	G1442	G1443	G1444	A4444	C1445	C1446	C1447	C1448	A1449	C1450	A1451	A1453	A1453				
U1335	A1336	G1337	G1338	G1339	U1340	U1341	A1342	G1343	G1344	G1345	G1346	G1347	G1348	C1349	C1350	C1351	U1352	A1353	A1354	G1355	G1356	U1357	G1358	A1359	A1360	G1361	G1362	G1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	U1372	A1373	G1374	C1375	C1376	G1377	A1378	A1379	G1380	G1381	G1382	C1383	A1384	G1385	C1386	C1387	G1388	G1389	U1390	U1391	A1392	A1393	U1394				
A1275	A1276	G1277	A1278	G1279	G1280	G1281	A1282	G1283	A1284	G1285	A1286	A1287	U1288	C1289	C1290	C1291	U1292	C1293	U1294	G1295	G1296	C1297	G1298	U1299	U1300	A1301	A1302	G1303	G1304	C1305	C1306	A1247	G1248	G1249	G1310	G1311	U1312	U1313	C1314	C1315	U1316	C1317	C1318	G1319	C1320	A1321	A1322	U1323	G1324	G1325	U1326	G1327	C1328	A1269	U1329	U1330	A1331	A1272	C1332	G1334			
G1215	G1216	C1217	G1218	G1219	A1220	G1221	C1222	G1223	G1224	C1225	G1226	A1227	G1228	G1229	C1230	G1231	G1232	C1233	U1234	G1235	G1236	A1237	G1238	G1239	U1240	A1241	A1242	G1243	G1244	G1245	A1246	A1247	G1248	G1249	G1250	G1251	G1252	A1253	A1254	U1255	U1256	G1257	C1258	G1259	G1260	C1261	A1262	U1263	G1264	A1265	G1266	U1267	A1268	A1269	U1270	C1271	A1272	C1273	A1274				
G1154	A1155	A1156	U1157	C1158	U1159	G1160	C1161	G1162	G1163	U1164	C1165	U1167	G1168	G1169	C1170	G1171	G1172	G1173	A1174	U1175	G1176	A1177	C1178	C1179	C1180	C1181	A1182	G1183	G1184	C1185	G1186	G1187	U1188	A1189	U1190	G1191	G1192	U1193	A1194	U1195	C1196	U1197	U1198	U1199	C1200	C1201	C1202	G1203	A1204	U1205	G1206	U1207	C1208	G1209	U1210	U1211	A1212	C1213	A1214				
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G2454	U2574	G2634	C2695	U2754	G2817	G2877	U2754	G2817	G2877
G2455	C2575	C2635	C2696	C2755	G2818	U2778	C2755	G2818	U2778
C2456	G2576	U2636	U2697	U2756	G2819	C2879	U2756	G2819	C2879
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G2458	C2578	G2638	C2699	G2758	A2821	C2881	G2758	A2821	C2881
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U2519	U2520	U2640	C2701	C2760	A2823	A2883	U2519	U2520	U2640
U2460	C2521	C2461	U2702	G2761	C2824	U2884	U2460	C2521	C2461
U2462	U2522	G2582	C2703	G2762	C2825	C2885	U2462	U2522	G2582
C2463	G2523	U2583	C2704	G2763	A2826	G2886	C2463	G2523	U2583
C2464	G2524	U2584	A2705	G2764	C2827	U2887	C2464	G2524	U2584
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C2466	G2526	C2586	G2707	G2766	C2829	C2889	C2466	G2526	C2586
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G2468	U2528	G2588	G2709	C2768	G2831	A2892	G2468	U2528	G2588
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G2472	G2532	U2592	A712A	C2772	A2835	C2896	G2472	G2532	U2592
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C2475	G2535	U2595	C2715	A2775	C2838	G2899	C2475	G2535	U2595
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C2477	C2537	G2597	A2717	G2777	C2840	C2901	C2477	C2537	G2597
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G2481	A2541	G2601	A2721	A2781	G2844	C	G2481	A2541	G2601
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C2483	G2543	G2603	C2723	G2783	U2846		C2483	G2543	G2603
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G2487	U2547	G2607	G2727	C2787	A2850		G2487	U2547	G2607
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G2489	G2549	U2609	G2729	C2789	G2852		G2489	G2549	U2609
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C2502	U2562	C2622	C2742	C2804	U2865		C2502	U2562	C2622
A2503	U2563	G2623	C2743	G2805	G2866		A2503	U2563	G2623
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G2505	A2565	G2625	C2745	U2808	A2868		G2505	A2565	G2625
U2506	A2566	C2626	U2746	A2809	G2869		U2506	A2566	C2626
C2507	G2567	U2627	G2747	A2810	C2870		C2507	G2567	U2627
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• Molecule 3: 50S ribosomal protein L1

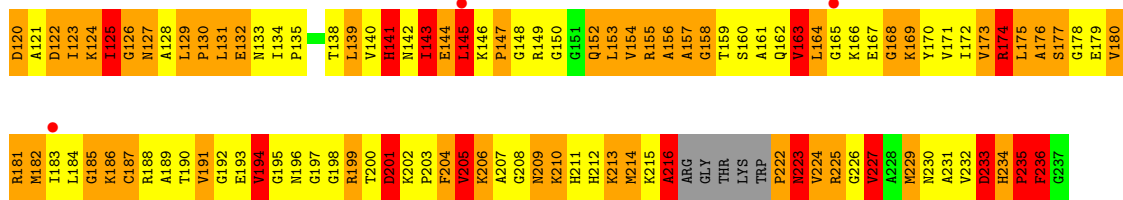


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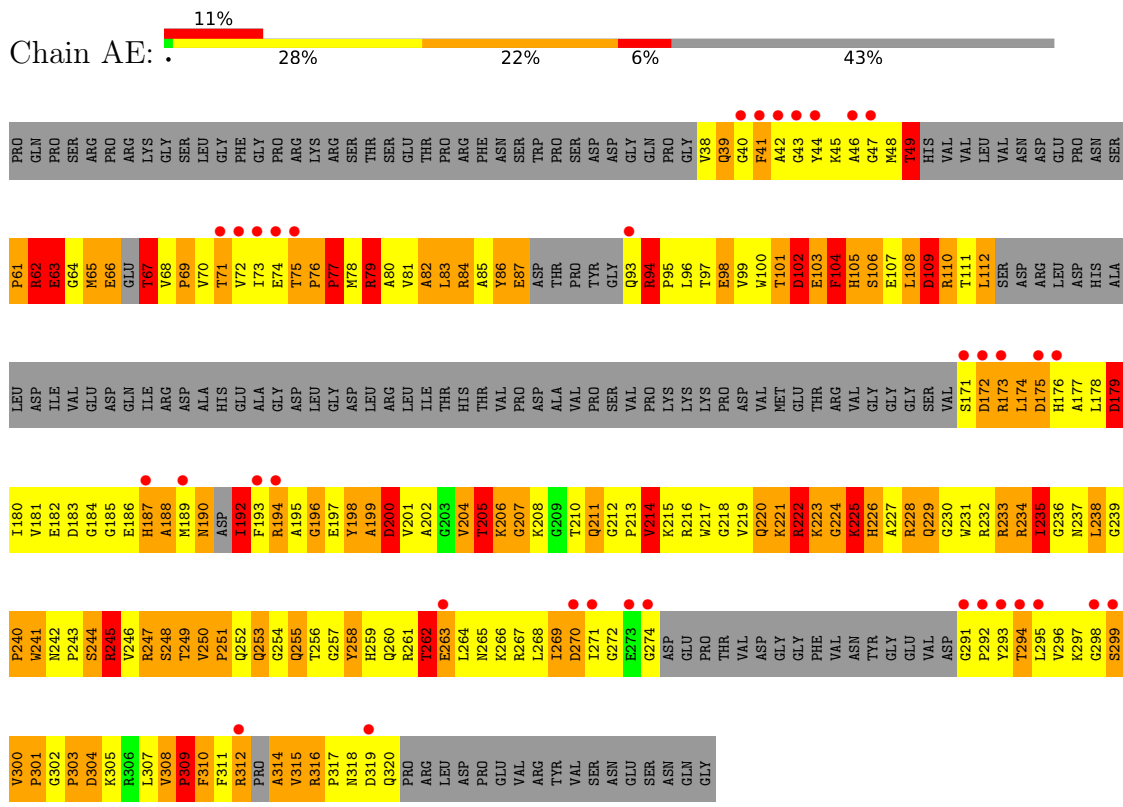
• Molecule 4: 50S ribosomal protein L2



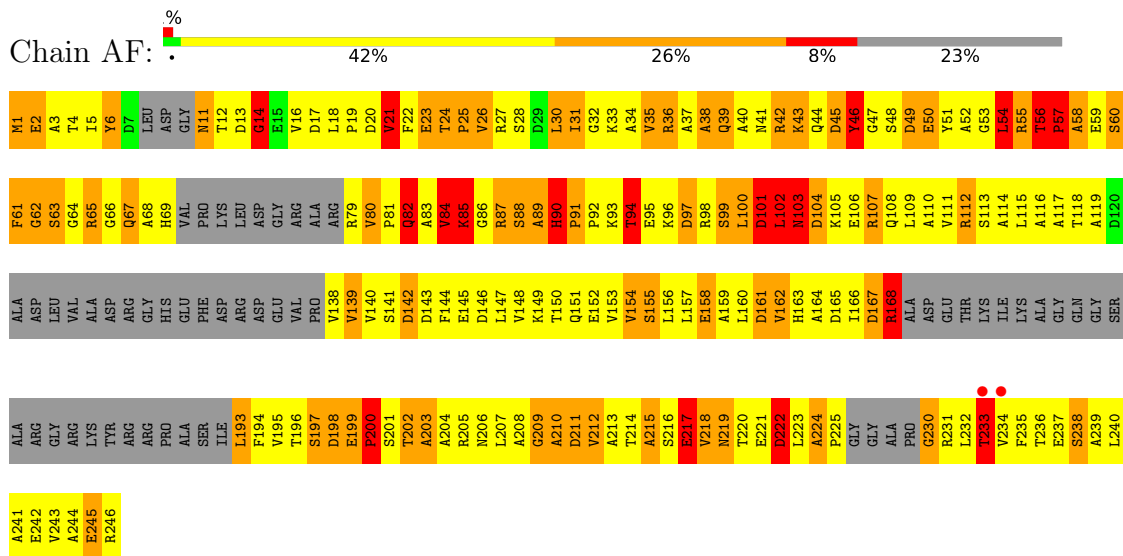
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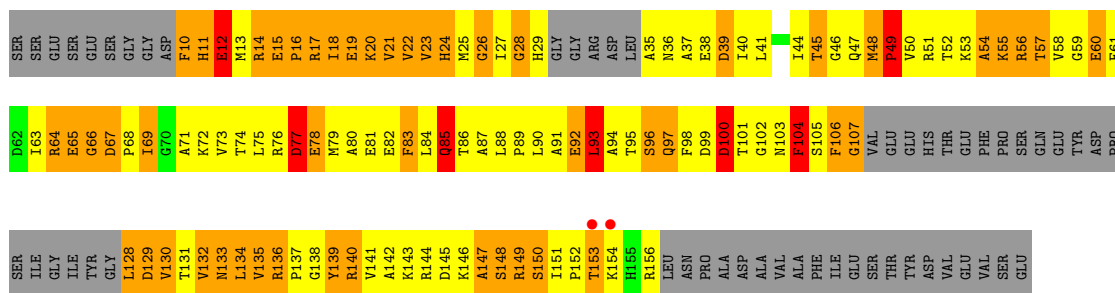
• Molecule 5: 50S ribosomal protein L3



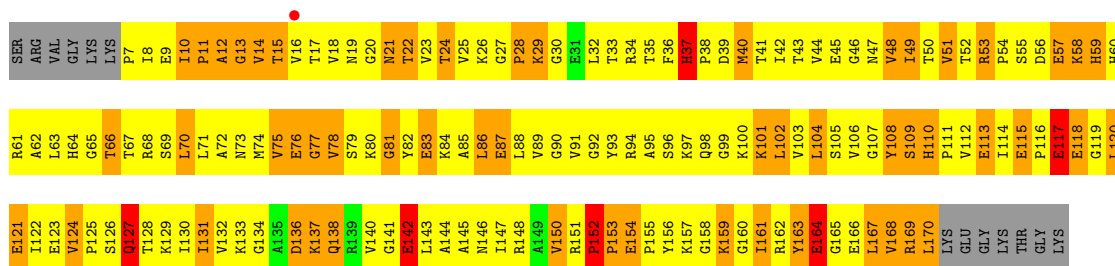
• Molecule 6: 50S ribosomal protein L4



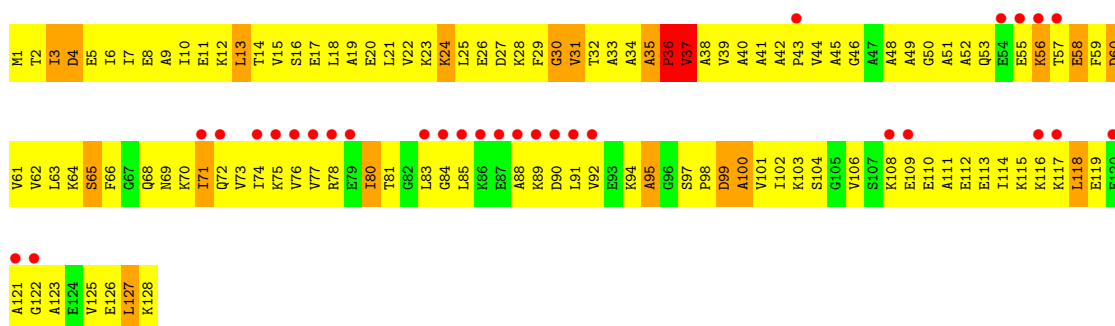
• Molecule 7: 50S ribosomal protein L5



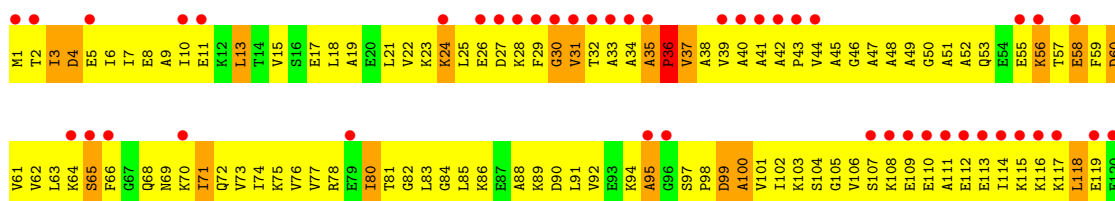
- Molecule 8: 50S ribosomal protein L6

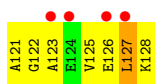


- Molecule 9: 50S ribosomal protein L7/L12

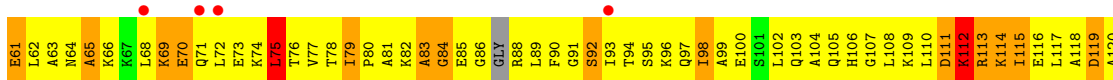


- Molecule 9: 50S ribosomal protein L7/L12

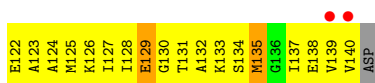




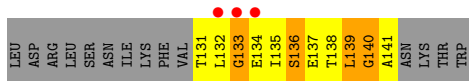
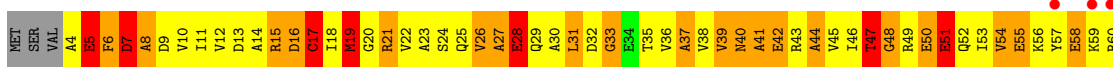
- Molecule 10: 50S ribosomal protein L9



- Molecule 11: 50S ribosomal protein L11

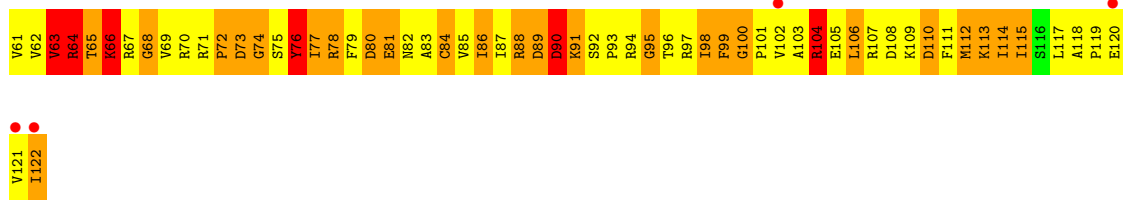


- Molecule 12: 50S ribosomal protein L13

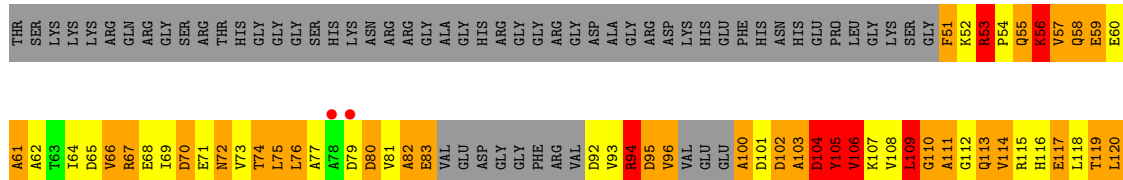
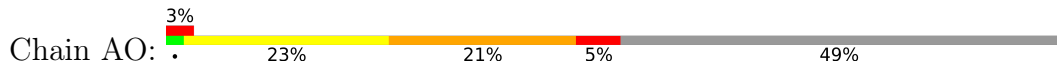


- Molecule 13: 50S ribosomal protein L14

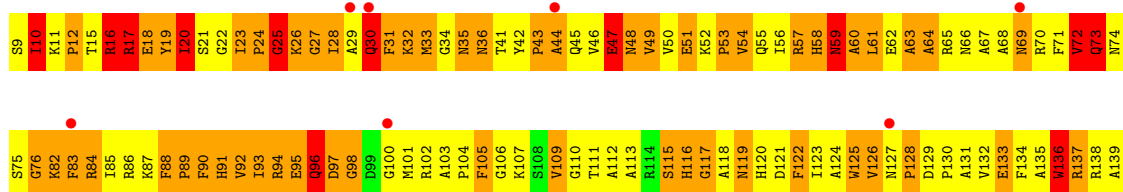




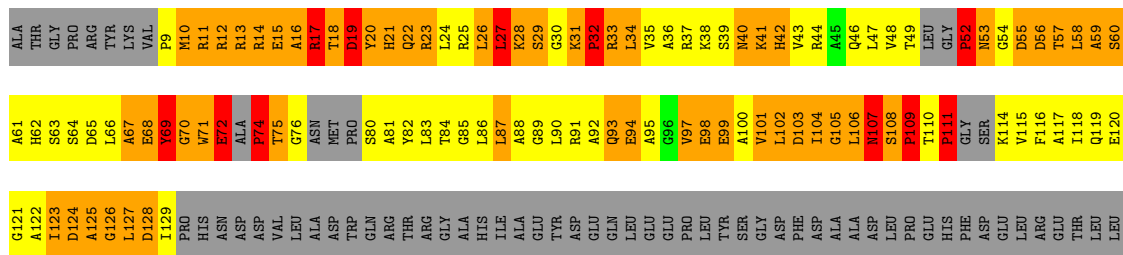
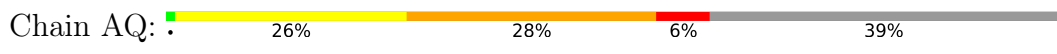
• Molecule 14: 50S ribosomal protein L15



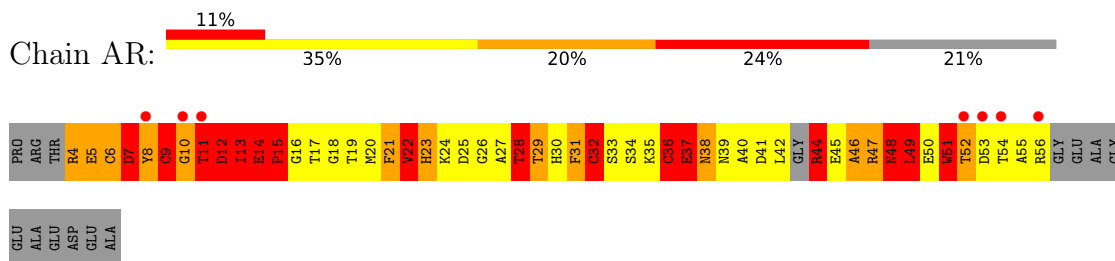
• Molecule 15: 50S ribosomal protein L16



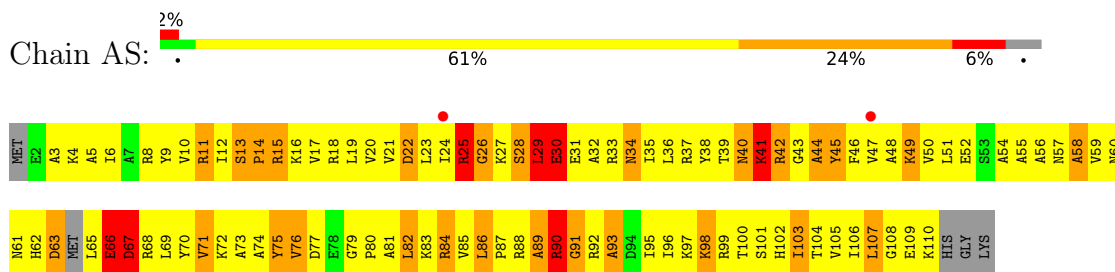
• Molecule 16: 50S ribosomal protein L18



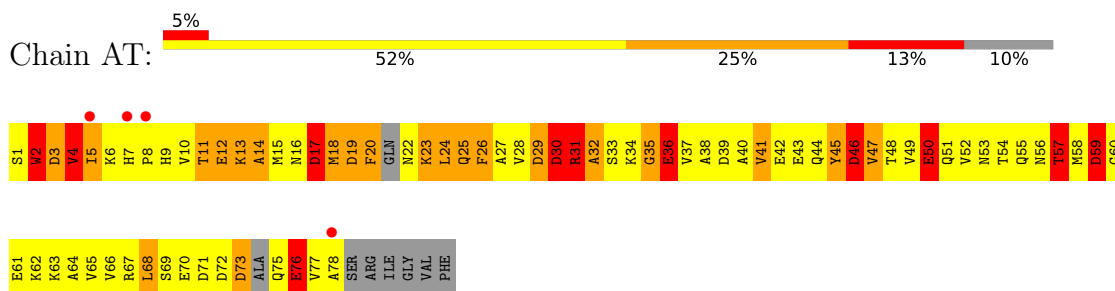
• Molecule 17: 50S ribosomal protein L19



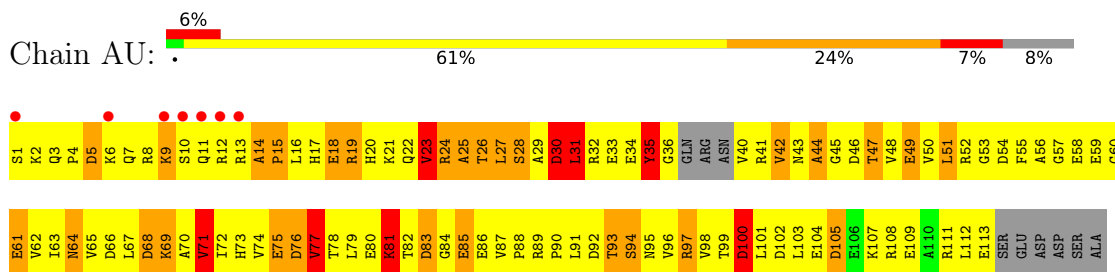
• Molecule 18: 50S ribosomal protein L22



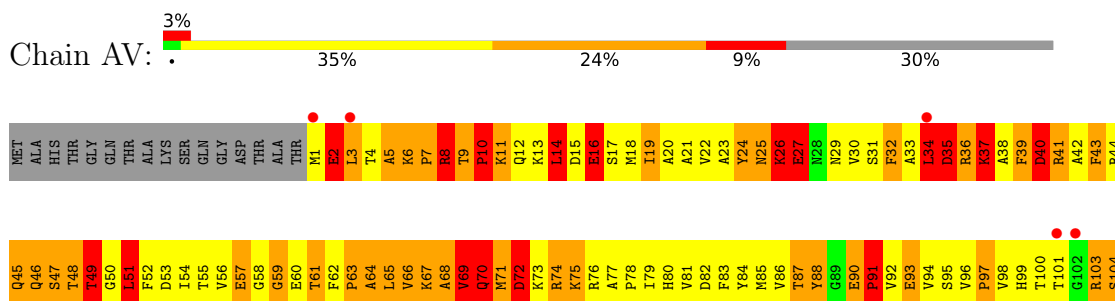
• Molecule 19: 50S ribosomal protein L23

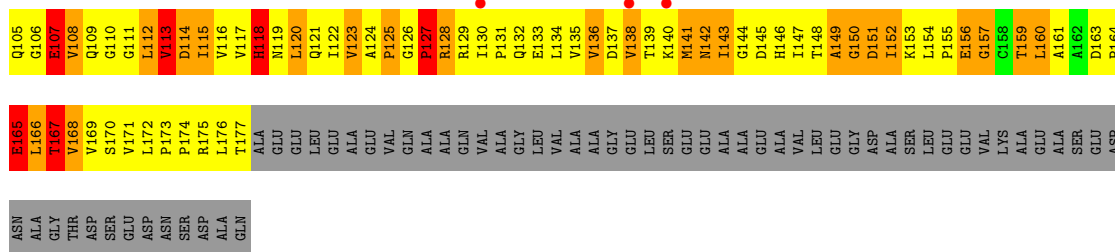


• Molecule 20: 50S ribosomal protein L24

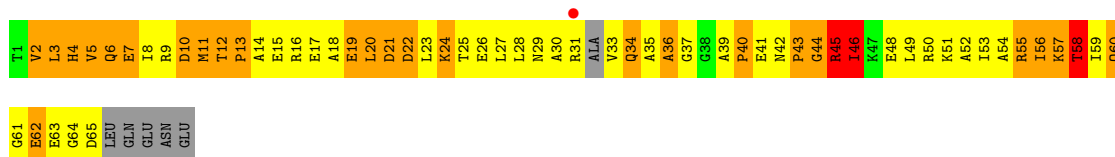


• Molecule 21: 50S general stress protein CTC (L25)

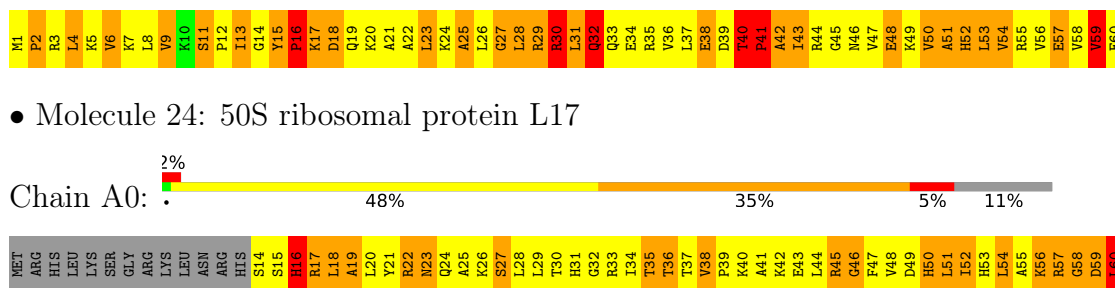




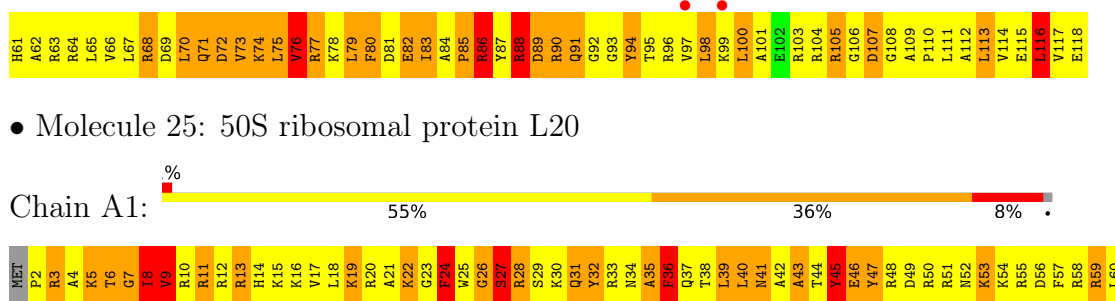
• Molecule 22: 50S ribosomal protein L29



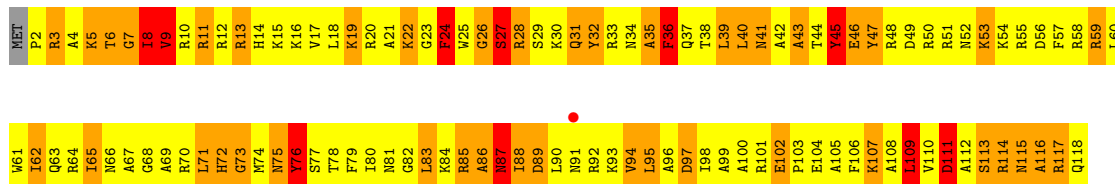
• Molecule 23: 50S ribosomal protein L30



• Molecule 24: 50S ribosomal protein L17

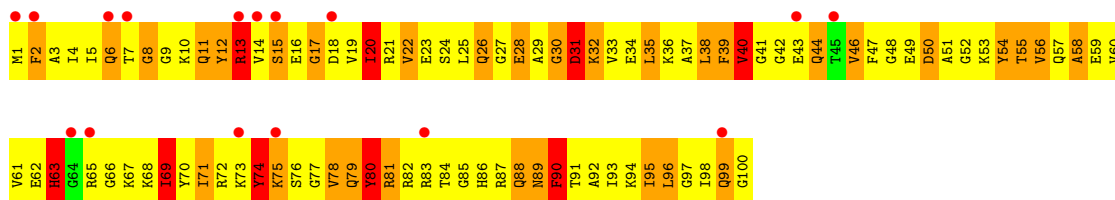


• Molecule 25: 50S ribosomal protein L20

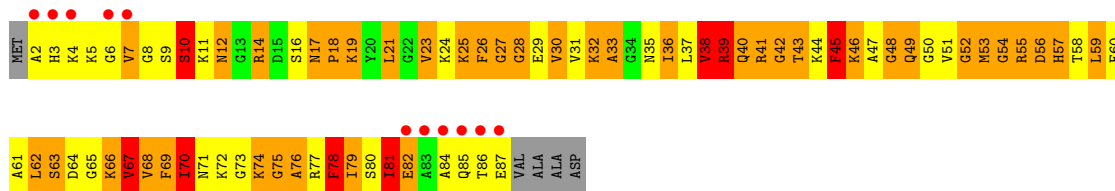


• Molecule 26: 50S ribosomal protein L21





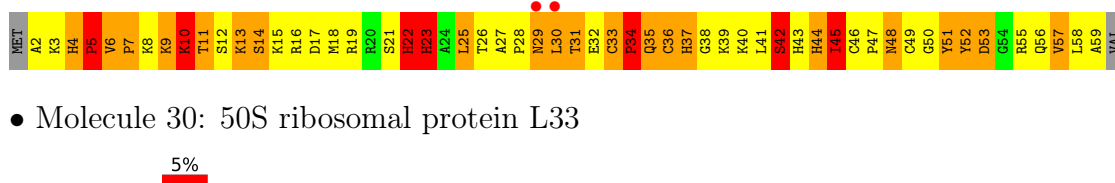
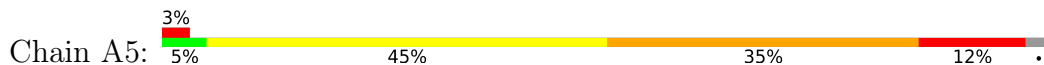
• Molecule 27: 50S ribosomal protein L27



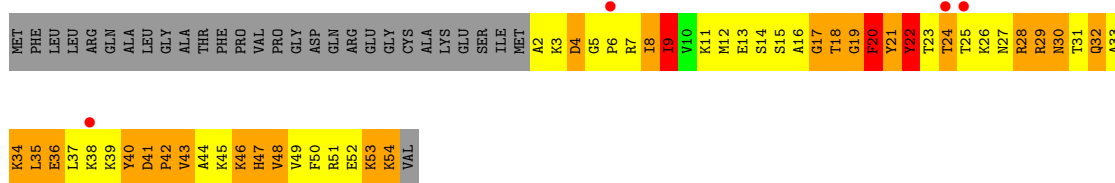
• Molecule 28: 50S ribosomal protein L31



• Molecule 29: 50S ribosomal protein L32



• Molecule 30: 50S ribosomal protein L33

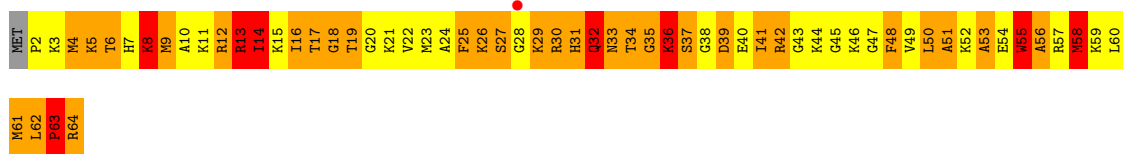


• Molecule 31: 50S ribosomal protein L34

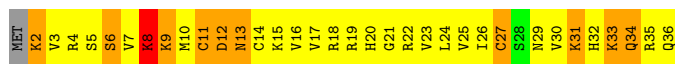
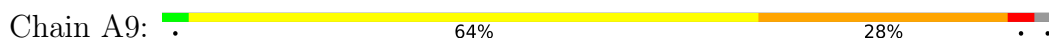




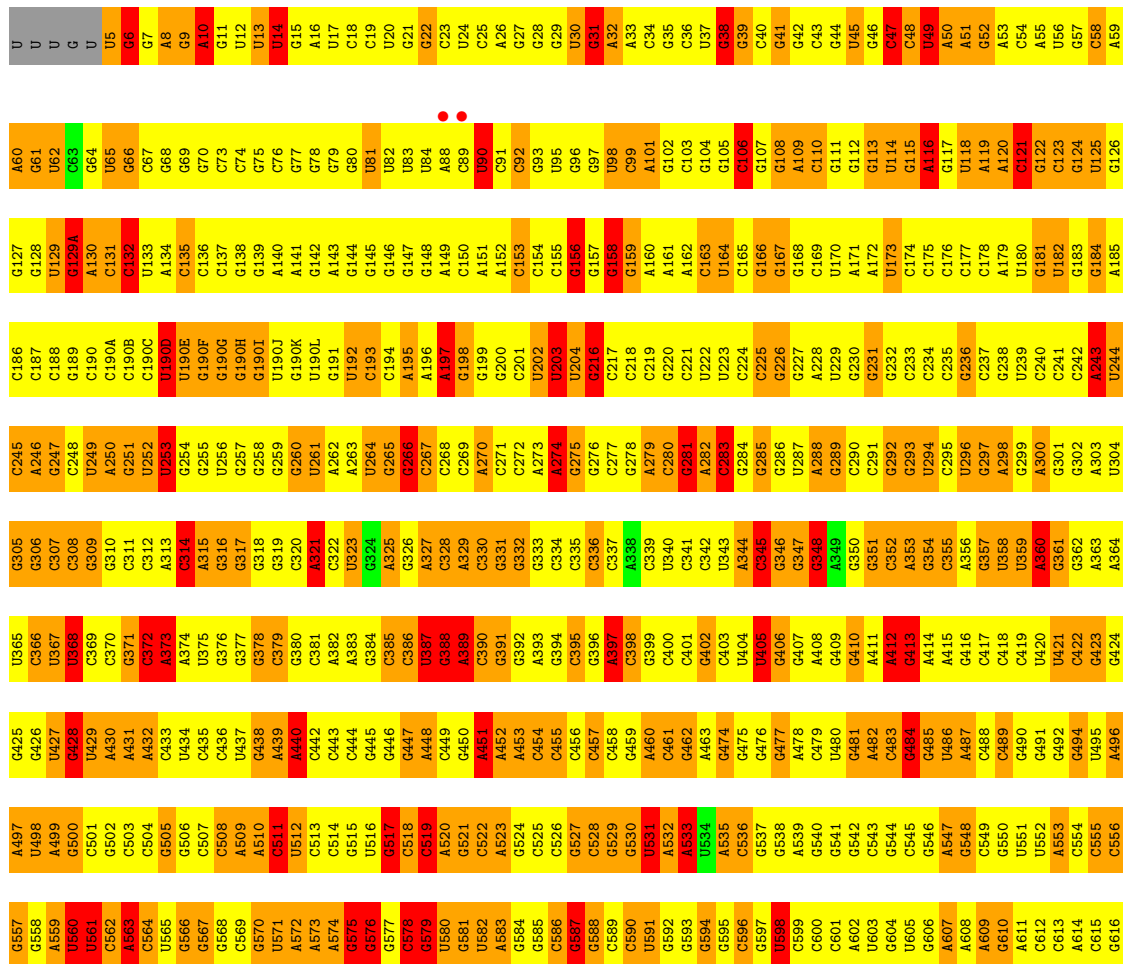
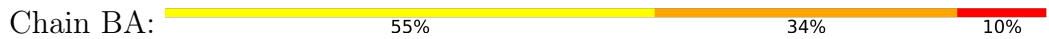
• Molecule 32: 50S ribosomal protein L35



• Molecule 33: 50S ribosomal protein L36

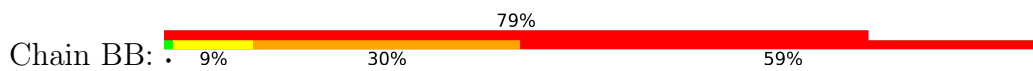


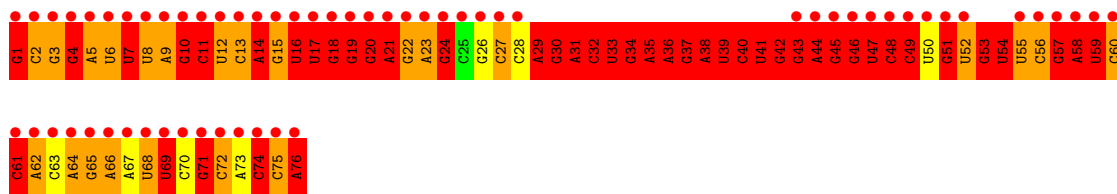
• Molecule 34: 16S rRNA



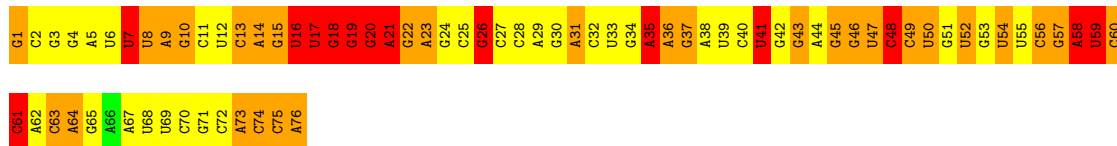
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G1398	G1399	G1400	G1401	G1402	G1403	G1404	G1405	G1406	G1407	G1408	G1409	G1410	G1411	G1412	G1413	G1414	G1415	G1416	G1417	G1418	G1419	G1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	G1430	G1431	G1432	G1433	G1434	G1435	G1436	G1437	G1438	G1439	G1440	G1441	G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
A1339	A1340	U1341	C1342	G1343	C1344	U1345	A1346	G1347	U1348	A1349	U1350	A1351	C1352	G1353	C1354	G1355	G1356	A1357	U1358	C1359	A1360	G1361	C361A	C1362	A1363	U1364	G1365	C1366	C1367	A1368	C1369	G1370	G1371	U1372	G1373	A1374	A1375	U1376	A1377	G1378	G1379	U1380	U1381	C1382	C1383	C1384	G1385	G1386	G1387	C1388	C1389	U1390	U1391	C1392	U1393	A1394	C1395	A1396	U1397	G1398																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
U1219	G1220	G1221	G1222	C1223	G1224	A1225	C1226	A1227	G1228	A1229	U1230	G1231	U1232	G1233	C1234	U1235	A1236	G1237	A1238	A1239	U1240	G1241	G1242	C1243	G1244	A1245	G1246	U1247	A1248	G1249	A1250	A1251	G1252	G1253	C1254	A1255	G1256	U1257	G1258	C1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	C1267	A1268	A1269	C1270	G1271	G1272	G1273	A1274	A1275	G1276	C1277	U1278																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
A1279	A1280	U1281	C1282	G1283	C1284	A1285	A1286	A1287	A1288	A1289	G1290	U1291	U1292	G1293	C1294	G1295	U1296	C1297	C1298	A1299	U1300	U1301	C1302	G1303	G1304	G1305	A1306	C1307	U1308	G1309	A1310	G1311	G1312	G1313	G1314	C1315	G1316	C1317	A1318	A1319	C1320	C1321	G1322	G1323	A1324	C1325	G1326	C1327	C1328	A1329	U1330	G1331	A1332	C1333	G1334	C1335	A1336	C1337	G1338																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C1463	G1464	C1465	G1466	G1467	C1468	G1469	G1470	G1471	G1472	A1473	G1474	G1475	G1476	C1477	G1478	G1479	G1480	U1481	A1482	A1483	A1418	A1419	C1420	G1421	G1422	G1423	G1424	U1425	G1426	A1427	A1428	C1429	U1430	C1431	A1432	A1433	A1434	G1435	U1436	U1437	G1438	C1439	C1440	G1441	G1442	A1443	A1444	G1445	G1446	G1447	C1448	C1449	U1450	C1451	G1452	C1453	G1454	G1455	A1456	G1457	G1458	G1459	G1460	G1461	G1462																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																	
G1617	C618	U619	C620	A621	G622	C623	G624	C625	U626	G627	G628	G629	C630	G631	C632	G633	C634	G635	G636	G637	G638	G639	A640	U641	A642	C643	G644	C645	U646	G647	A648	G649	G650	C651	U652	A653	G654	A655	C656	G657	U658	G659	G660	C661	A662	G663	U664	G665	G666	G667	U668	G669	G670	G671	U672	C673	G674	A675	C676																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
U677	U678	C679	C680	U681	G682	C683	A684	G685	U686	G687	G688	G689	C690	G691	U692	G693	A694	G695	A696	U697	G698	G699	G700	C701	A702	G703	A704	U705	U706	G707	A708	G709	C710	G711	U712	G713	G714	A715	C716	G717	G718	U719	C720	G721	A722	U723	G724	G725	C726	G727	A728	U729	G730	G731	U732	A733	G734	C735	A736	C737																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
A737	C738	C739	U740	G741	G742	U743	C744	C745	U746	G747	G748	G749	C750	U751	C752	A753	C754	G755	A756	U757	G758	C759	G760	G761	C762	G763	C764	G765	U766	G767	A768	G769	C770	G771	U772	G773	G774	C775	A776	G777	G778	U779	A780	C781	A782	C783	U784	G785	C786	A787	U788	G789	A790	G791	U792	U793	A794	C795	C796	A797	C798	U799	G800	C801	G802	C803	U804	C805	A806	U807	C808	A809	U810	C811	U812	U813	A814	A815	C816	U817	C818	A819	U820	G821	C822	G823	C824	G825	U826	C827	C828	A829	G830	U831	C832	U833	C834	U835	A836	G837	C838	U839	A840	C841	U842	A843	C844	U845	C846	U847	A848	U849	C850	U851	C852	A853	C854	U855	C856	G857	U858	A859	U860	C861	G862	U863	C864	U865	C866	U867	A868	U869	C870	G871	C872	A873	U874	C875	A876	U877	C878	U879	C880	A881	C882	U883	G884	C885	A886	U887	C888	U889	A890	C891	U892	C893	A894	U895	C896	U897	A898	C899	U900	A901	C902	G903	C904	U905	A906	C907	U908	A909	C910	U911	C912	A913	U914	C915	U916	A917	C918	U919	A920	C921	U922	A923	C924	U925	G926	C927	U928	A929	C930	U931	C932	A933	U934	C935	A936	U937	C938	U939	A940	C941	U942	C943	A944	U945	C946	U947	A948	C949	U950	C951	U952	A953	C954	U955	C956	A957	C958	U959	A960	C961	U962	A963	C964	U965	C966	U967	A968	C969	U970	A971	C972	A973	U974	C975	A976	C977	U978	A979	C980	U981	C982	U983	A984	C985	U986	A987	C988	U989	A990	C991	U992	C993	A994	U995	C996	U997	A998	C999	U1000	A1001	G1002	C1003	U1004	G1005	C1006	C1007	U1008	A1009	G1010	C1011	U1012	A1013	C1014	U1015	G1016	C1017	U1018	C1019	U1020	C1021	G1022	A1023	U1024	C1025	G1026	C1027	U1028	C1029	U1030	G30A	C30B	G30C	A30D	U1031	A1032	C1033	U1034	G1035	U1036	C1037	U1038	A1039	U1040	C1041	U1042	A1043	U1044	C1045	U1046	A1047	C1048	U1049	A1050	C1051	U1052	G1053	C1054	A1055	U1056	C1057	U1058	G1059	C1060	A1061	U1062	C1063	U1064	C1065	A1066	C1067	U1068	C1069	U1070	C1071	G1072	U1073	C1074	U1075	C1076	U1077	G1078	C1079	A1080	U1081	C1082	U1083	G1084	C1085	U1086	G1087	C1088	U1089	C1090	U1091	A1092	C1093	U1094	G1095	U1096	C1097	A1098	U1099	C1099	U1100	G1101	C1102	U1103	A1104	C1105	U1106	G1107	C1108	U1109	A1110	C1111	U1112	G1113	C1114	A1115	U1116	G1117	C1118	U1119	G1120	C1121	U1122	A1123	G1124	U1125	C1126	U1127	A1128	C1129	A1130	G1131	C1132	U1133	A1134	U1135	C1136	U1137	G1138	C1139	A1140	C1141	G1142	U1143	C1144	U1145	A1146	C1147	U1148	C1149	U1150	A1151	C1152	U1153	A1154	G1155	U1156	C1157	A1158	U1159	C1160	U1161	A1162	C1163	U1164	G1165	U1166	C1167	A1168	U1169	C1170	G1171	C1172	U1173	G1174	C1175	U1176	A1177	C1178	U1179	G1180	C1181	U1182	A1183	G1184	U1185	C1186	U1187	A1188	C1189	U1190	A1191	C1192	U1193	A1194	C1195	U1196	U1197	G1198	U1199	C1200	A1201	C1202	U1203	G1204	C1205	A1206	U1207	C1208	C1209	G1210	U1211	C1212	A1213	C1214	G1215	U1216	C1217	A1218	U1219	C1220	U1221	A1222	C1223	U1224	G1225	A1226	C1227	U1228	A1229	C1230	U1231	C1232	A1233	G1234	U1235	A1236	C1237	U1238	A1239	U1240	C1241	G1242	U1243	C1244	A1245	U1246	C1247	A1248	U1249	C1250	A1251	U1252	C1253	U1254	A1255	C1256	U1257	A1258	C1259	C1260	A1261	C1262	C1263	C1264	G1265	G1266	C1267	A1268	A1269	C1270	G1271	G1272	G1273	A1274	A1275	G1276	C1277	U1278

• Molecule 35: tRNA Phe (unmodified bases)

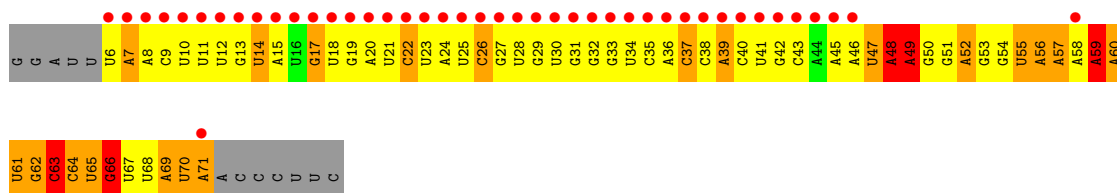




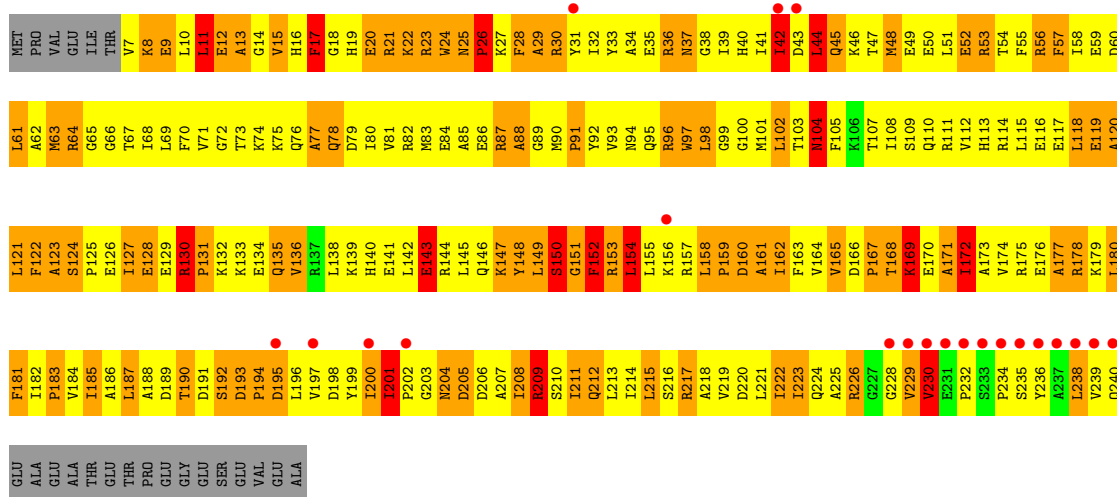
• Molecule 35: tRNA Phe (unmodified bases)



• Molecule 36: thrS mRNA operator

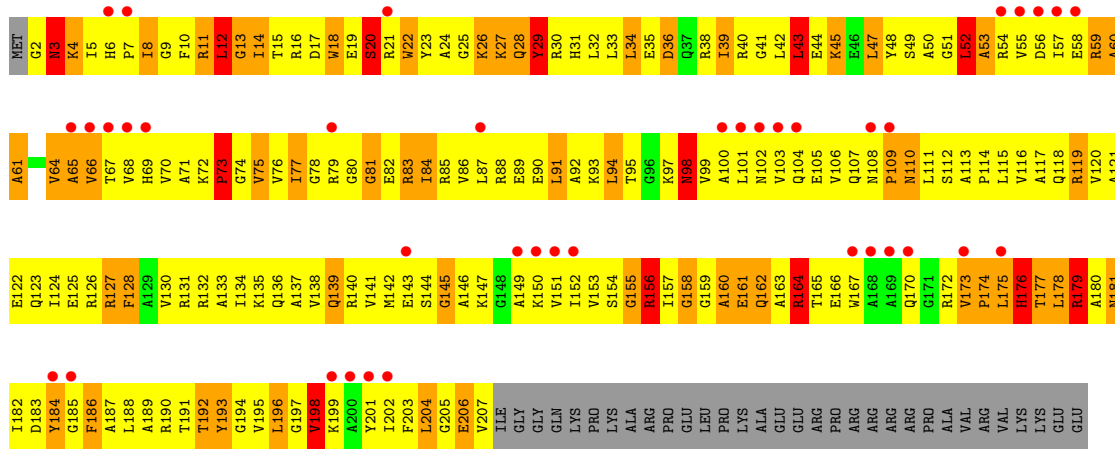


• Molecule 37: 30S ribosomal protein S2

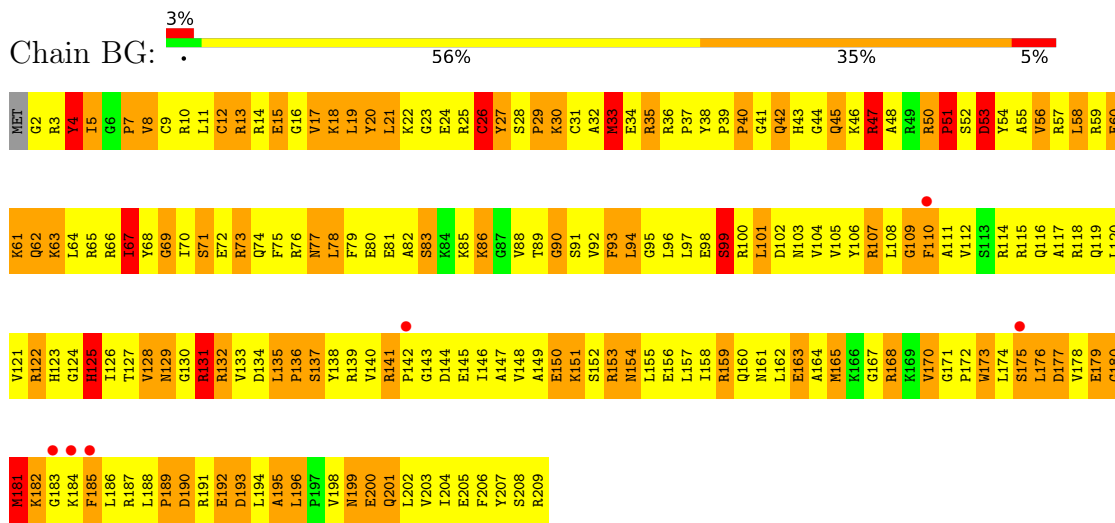


• Molecule 38: 30S ribosomal protein S3

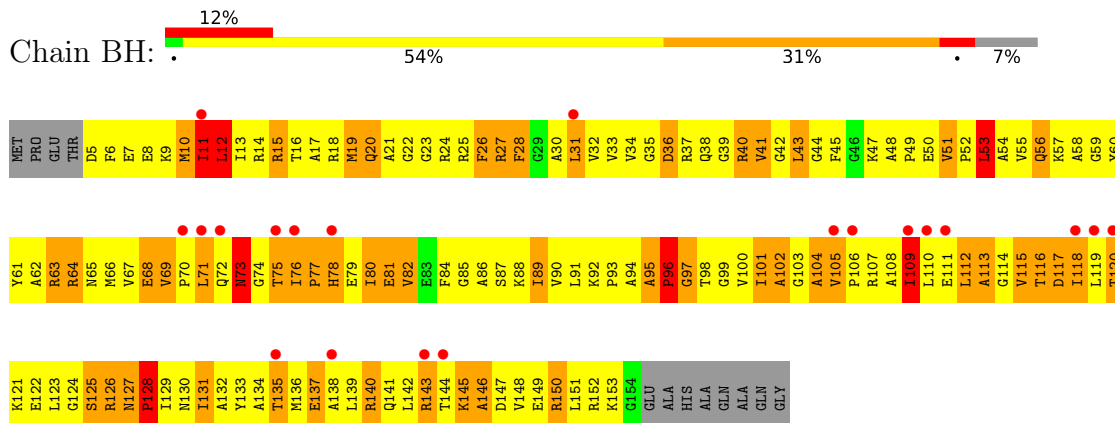




• Molecule 39: 30S ribosomal protein S4

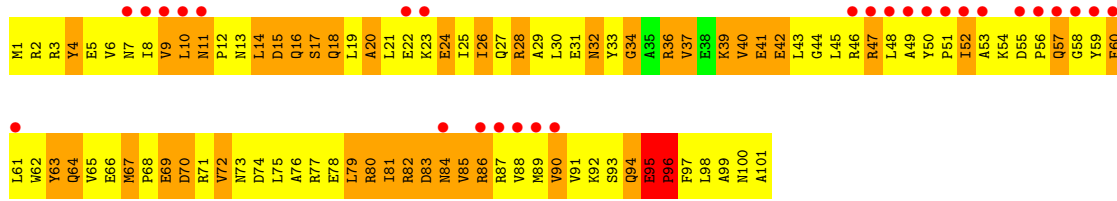


• Molecule 40: 30S ribosomal protein S5

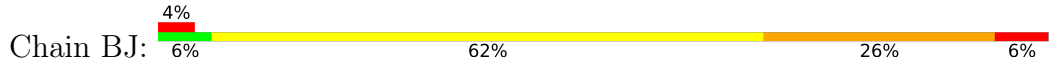


• Molecule 41: 30S ribosomal protein S6

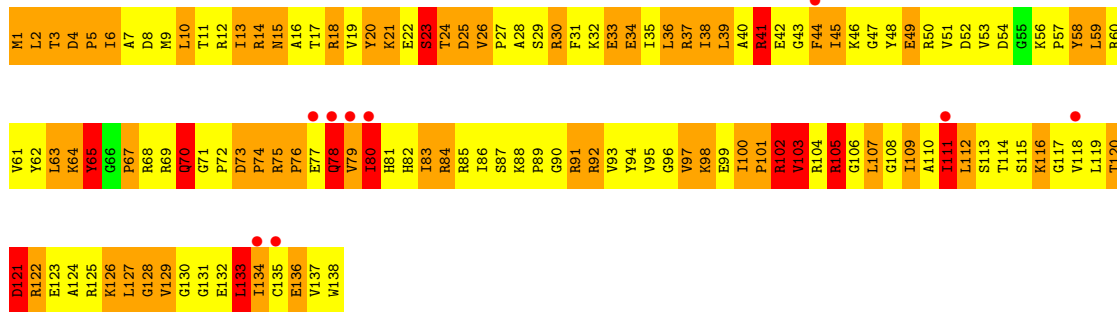




• Molecule 42: 30S ribosomal protein S7



• Molecule 43: 30S ribosomal protein S8

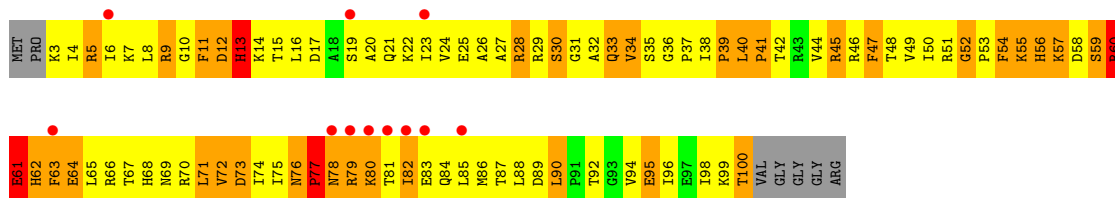


• Molecule 44: 30S ribosomal protein S9

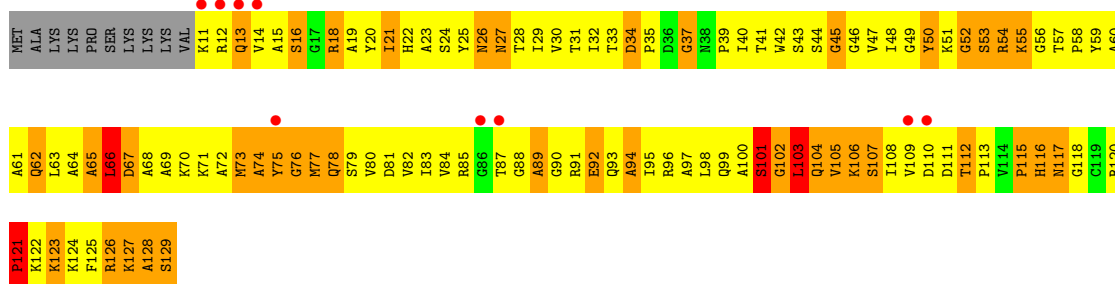


• Molecule 45: 30S ribosomal protein S10

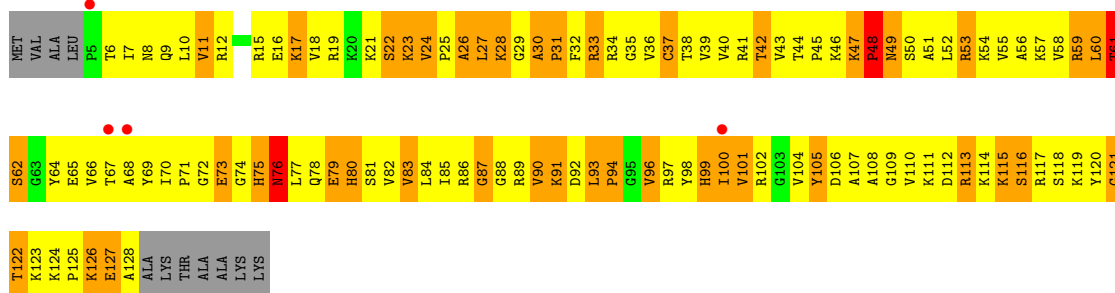




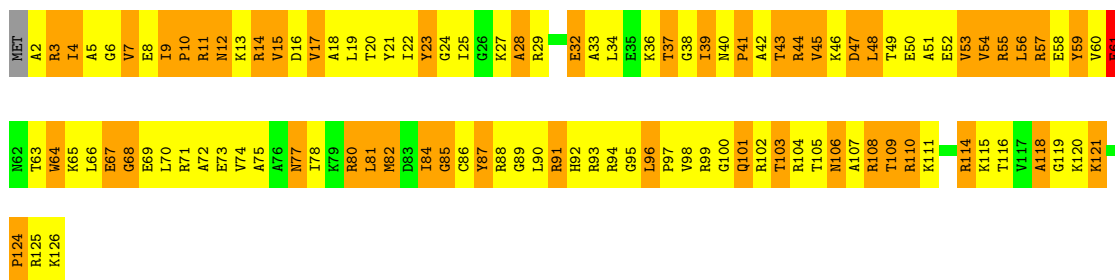
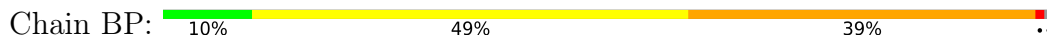
- Molecule 46: 30S ribosomal protein S11



- Molecule 47: 30S ribosomal protein S12



- Molecule 48: 30S ribosomal protein S13



- Molecule 49: 30S ribosomal protein S14





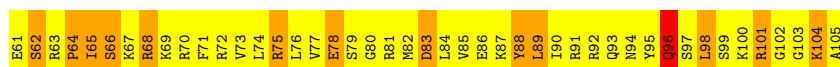
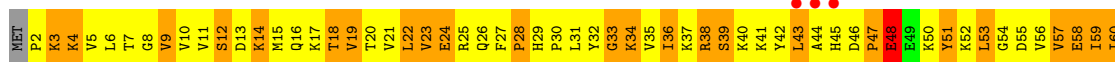
- Molecule 50: 30S ribosomal protein S15



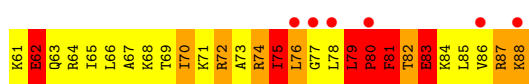
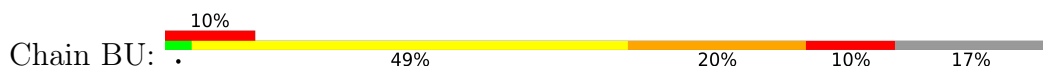
- Molecule 51: 30S ribosomal protein S16



- Molecule 52: 30S ribosomal protein S17



- Molecule 53: 30S ribosomal protein S18



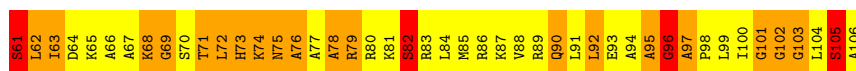
- Molecule 54: 30S ribosomal protein S19





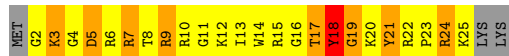
- Molecule 55: 30S ribosomal protein S20

Chain BW: 56% 32% 6% 7%



- Molecule 56: 30S ribosomal protein Thx

Chain BX: 56% 30% 1% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.64Å 508.64Å 806.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 268.38 – 5.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (300.00-5.50) 97.5 (268.38-5.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 5.42Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.307 , 0.356 0.288 , 0.330	Depositor DCC
R_{free} test set	7724 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	206.2	Xtrriage
Anisotropy	0.054	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.11 , 178.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	148539	wwPDB-VP
Average B, all atoms (Å ²)	338.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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	AB	0.95	1/2954 (0.0%)	1.06	7/4606 (0.2%)
2	AA	1.16	181/69267 (0.3%)	1.22	549/108130 (0.5%)
3	AC	0.62	0/1715	0.94	2/2310 (0.1%)
4	AD	1.11	6/1329 (0.5%)	1.52	22/1787 (1.2%)
5	AE	1.04	3/1542 (0.2%)	1.41	21/2084 (1.0%)
6	AF	0.82	0/1446	1.26	14/1960 (0.7%)
7	AG	0.83	0/972	1.20	6/1307 (0.5%)
8	AH	0.76	0/1272	1.13	1/1721 (0.1%)
9	AI	0.48	0/950	0.72	0/1275
9	AJ	0.43	0/950	0.68	0/1275
10	AK	0.73	0/1157	1.17	8/1547 (0.5%)
11	AL	0.48	0/1015	0.91	4/1366 (0.3%)
12	AM	1.04	2/928 (0.2%)	1.23	2/1248 (0.2%)
13	AN	1.06	2/946 (0.2%)	1.43	14/1269 (1.1%)
14	AO	0.67	0/643	1.30	9/870 (1.0%)
15	AP	1.04	1/1109 (0.1%)	1.43	16/1499 (1.1%)
16	AQ	0.71	0/880	1.23	5/1189 (0.4%)
17	AR	1.37	4/413 (1.0%)	2.01	18/557 (3.2%)
18	AS	0.81	0/869	1.19	3/1166 (0.3%)
19	AT	0.76	0/609	1.05	0/823
20	AU	0.46	0/887	0.89	0/1195
21	AV	0.71	0/1385	1.10	7/1883 (0.4%)
22	AW	0.73	0/497	1.05	1/668 (0.1%)
23	AX	0.81	0/482	1.18	2/646 (0.3%)
24	A0	0.86	0/867	1.24	3/1162 (0.3%)
25	A1	1.03	0/994	1.33	6/1323 (0.5%)
26	A2	0.71	0/797	1.14	4/1061 (0.4%)
27	A3	0.72	0/649	1.14	3/860 (0.3%)
28	A4	0.97	1/620 (0.2%)	1.18	4/831 (0.5%)
29	A5	0.79	0/469	1.41	5/629 (0.8%)
30	A6	0.93	0/438	1.25	4/583 (0.7%)
31	A7	0.78	0/387	1.05	0/509
32	A8	0.98	2/503 (0.4%)	1.48	8/657 (1.2%)
33	A9	1.36	1/286 (0.3%)	1.44	4/375 (1.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BA	1.03	30/36438 (0.1%)	1.17	167/56869 (0.3%)
35	BB	2.33	76/1818 (4.2%)	2.48	157/2831 (5.5%)
35	BC	1.09	5/1818 (0.3%)	1.11	7/2831 (0.2%)
36	B1	1.14	7/1571 (0.4%)	0.96	7/2445 (0.3%)
37	BE	0.75	0/1935	1.06	3/2609 (0.1%)
38	BF	0.62	0/1636	0.99	5/2205 (0.2%)
39	BG	0.86	2/1733 (0.1%)	1.16	4/2318 (0.2%)
40	BH	0.85	0/1162	1.12	1/1564 (0.1%)
41	BI	0.78	0/856	1.06	1/1154 (0.1%)
42	BJ	0.70	1/1276 (0.1%)	1.00	6/1709 (0.4%)
43	BK	0.81	0/1136	1.18	5/1527 (0.3%)
44	BL	0.52	0/1029	0.86	1/1378 (0.1%)
45	BM	0.58	0/807	0.94	2/1085 (0.2%)
46	BN	0.75	0/900	1.04	0/1213
47	BO	0.78	0/986	1.22	3/1320 (0.2%)
48	BP	0.59	0/1008	0.98	0/1347
49	BQ	0.83	1/501 (0.2%)	1.09	2/664 (0.3%)
50	BR	0.74	0/745	1.05	2/992 (0.2%)
51	BS	0.81	0/716	1.10	3/963 (0.3%)
52	BT	0.82	0/870	1.11	2/1159 (0.2%)
53	BU	0.72	0/603	1.18	2/799 (0.3%)
54	BV	0.59	0/661	0.98	1/890 (0.1%)
55	BW	0.84	0/764	1.12	2/1006 (0.2%)
56	BX	0.45	0/212	0.81	0/277
All	All	1.05	326/161408 (0.2%)	1.21	1135/241526 (0.5%)

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	AB	0	14
2	AA	0	527
4	AD	0	1
5	AE	0	1
6	AF	0	1
7	AG	0	2
12	AM	0	2
13	AN	0	2
14	AO	0	2
16	AQ	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
23	AX	0	1
25	A1	0	3
26	A2	0	1
28	A4	0	1
30	A6	0	1
34	BA	0	220
35	BB	0	35
35	BC	0	12
36	B1	0	4
38	BF	0	1
39	BG	0	1
41	BI	0	1
43	BK	0	1
48	BP	0	1
51	BS	0	2
All	All	0	838

The worst 5 of 326 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	142	G	C5-C6	27.73	1.70	1.42
36	B1	48	A	C5-C6	27.45	1.65	1.41
35	BB	37	G	C2-N2	18.34	1.52	1.34
34	BA	1541	U	C4-C5	17.23	1.59	1.43
2	AA	142	G	C2-N3	16.69	1.46	1.32

The worst 5 of 1135 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1064	G	N1-C2-N2	-65.61	57.15	116.20
34	BA	1064	G	N3-C2-N2	63.69	164.48	119.90
34	BA	1064	G	N1-C2-N3	-27.38	107.47	123.90
2	AA	1084	A	O5'-P-OP2	-26.59	78.79	110.70
35	BB	36	A	OP1-P-O3'	-18.47	64.57	105.20

There are no chirality outliers.

5 of 838 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	12	C	Sidechain
1	AB	18	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AB	34	U	Sidechain
1	AB	39	A	Sidechain
1	AB	44	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	2641	0	1337	635	1
2	AA	61847	0	31165	17729	1
3	AC	1687	0	1737	723	0
4	AD	1308	0	1355	898	0
5	AE	1507	0	1494	986	0
6	AF	1430	0	1386	832	0
7	AG	957	0	959	519	0
8	AH	1251	0	1298	612	0
9	AI	945	0	999	497	0
9	AJ	945	0	999	362	0
10	AK	1145	0	1227	630	0
11	AL	999	0	1071	497	0
12	AM	917	0	904	616	0
13	AN	937	0	1000	549	0
14	AO	639	0	615	373	0
15	AP	1081	0	1062	743	0
16	AQ	866	0	875	512	0
17	AR	406	0	361	160	0
18	AS	860	0	919	442	0
19	AT	602	0	563	332	0
20	AU	879	0	868	477	0
21	AV	1360	0	1390	788	0
22	AW	494	0	506	240	0
23	AX	477	0	529	309	0
24	A0	855	0	906	492	0
25	A1	978	0	1020	685	0
26	A2	787	0	804	571	0
27	A3	641	0	668	421	0
28	A4	604	0	595	365	0
29	A5	457	0	462	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A6	431	0	456	224	0
31	A7	383	0	414	260	0
32	A8	496	0	549	296	0
33	A9	285	0	312	125	0
34	BA	32554	0	16429	7563	1
35	BB	1626	0	817	629	0
35	BC	1626	0	820	429	0
36	B1	1405	0	706	258	1
37	BE	1900	0	1951	930	0
38	BF	1612	0	1677	662	0
39	BG	1703	0	1763	719	0
40	BH	1146	0	1207	489	1
41	BI	843	0	857	398	0
42	BJ	1257	0	1296	527	0
43	BK	1116	0	1177	677	0
44	BL	1011	0	1043	442	0
45	BM	794	0	840	332	0
46	BN	885	0	904	409	0
47	BO	970	0	1057	459	0
48	BP	997	0	1072	493	0
49	BQ	492	0	529	258	0
50	BR	734	0	771	330	0
51	BS	700	0	720	318	0
52	BT	857	0	930	423	0
53	BU	597	0	668	334	0
54	BV	647	0	673	254	0
55	BW	762	0	859	366	0
56	BX	208	0	221	103	0
All	All	148539	0	99792	47710	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 193.

The worst 5 of 47710 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AA:2515:C:N4	2:AA:2569:G:H1	1.08	1.45
34:BA:144:G:H1	34:BA:178:C:N4	1.13	1.45
34:BA:292:G:H1	34:BA:308:C:N4	1.08	1.45
2:AA:447:A:H1'	2:AA:449:A:N6	1.28	1.44
33:A9:11:CYS:SG	33:A9:11:CYS:CB	2.06	1.44

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AB:-1:A:O2'	1:AB:-1:A:O2'[15_545]	1.59	0.61
2:AA:2153:G:O2'	34:BA:423:G:OP2[3_655]	2.16	0.04
36:B1:29:G:O3'	40:BH:5:ASP:OD2[3_655]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AC	217/228 (95%)	143 (66%)	36 (17%)	38 (18%)	0	3
4	AD	171/178 (96%)	71 (42%)	38 (22%)	62 (36%)	0	0
5	AE	187/338 (55%)	89 (48%)	41 (22%)	57 (30%)	0	0
6	AF	183/246 (74%)	83 (45%)	40 (22%)	60 (33%)	0	0
7	AG	118/176 (67%)	57 (48%)	29 (25%)	32 (27%)	0	0
8	AH	162/177 (92%)	89 (55%)	39 (24%)	34 (21%)	0	2
9	AI	126/128 (98%)	87 (69%)	24 (19%)	15 (12%)	0	6
9	AJ	126/128 (98%)	86 (68%)	25 (20%)	15 (12%)	0	6
10	AK	146/149 (98%)	83 (57%)	34 (23%)	29 (20%)	0	2
11	AL	131/141 (93%)	66 (50%)	33 (25%)	32 (24%)	0	1
12	AM	113/145 (78%)	48 (42%)	26 (23%)	39 (34%)	0	0
13	AN	120/122 (98%)	60 (50%)	33 (28%)	27 (22%)	0	1
14	AO	82/164 (50%)	40 (49%)	17 (21%)	25 (30%)	0	0
15	AP	136/138 (99%)	50 (37%)	43 (32%)	43 (32%)	0	0
16	AQ	111/186 (60%)	41 (37%)	32 (29%)	38 (34%)	0	0
17	AR	50/66 (76%)	19 (38%)	17 (34%)	14 (28%)	0	0
18	AS	104/113 (92%)	70 (67%)	18 (17%)	16 (15%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	74/84 (88%)	33 (45%)	17 (23%)	24 (32%)	0	0
20	AU	108/119 (91%)	60 (56%)	25 (23%)	23 (21%)	0	2
21	AV	175/253 (69%)	69 (39%)	46 (26%)	60 (34%)	0	0
22	AW	62/70 (89%)	21 (34%)	25 (40%)	16 (26%)	0	1
23	AX	58/60 (97%)	29 (50%)	13 (22%)	16 (28%)	0	0
24	A0	103/118 (87%)	50 (48%)	33 (32%)	20 (19%)	0	2
25	A1	115/118 (98%)	48 (42%)	40 (35%)	27 (24%)	0	1
26	A2	98/100 (98%)	54 (55%)	18 (18%)	26 (26%)	0	0
27	A3	84/91 (92%)	32 (38%)	16 (19%)	36 (43%)	0	0
28	A4	71/73 (97%)	21 (30%)	19 (27%)	31 (44%)	0	0
29	A5	56/60 (93%)	25 (45%)	11 (20%)	20 (36%)	0	0
30	A6	51/82 (62%)	26 (51%)	8 (16%)	17 (33%)	0	0
31	A7	44/47 (94%)	14 (32%)	12 (27%)	18 (41%)	0	0
32	A8	61/64 (95%)	24 (39%)	16 (26%)	21 (34%)	0	0
33	A9	33/36 (92%)	19 (58%)	8 (24%)	6 (18%)	0	3
37	BE	232/256 (91%)	107 (46%)	58 (25%)	67 (29%)	0	0
38	BF	204/239 (85%)	113 (55%)	46 (22%)	45 (22%)	0	1
39	BG	206/209 (99%)	97 (47%)	63 (31%)	46 (22%)	0	1
40	BH	148/162 (91%)	90 (61%)	38 (26%)	20 (14%)	0	4
41	BI	99/101 (98%)	55 (56%)	24 (24%)	20 (20%)	0	2
42	BJ	153/156 (98%)	63 (41%)	49 (32%)	41 (27%)	0	0
43	BK	136/138 (99%)	67 (49%)	39 (29%)	30 (22%)	0	1
44	BL	125/128 (98%)	64 (51%)	27 (22%)	34 (27%)	0	0
45	BM	96/105 (91%)	54 (56%)	19 (20%)	23 (24%)	0	1
46	BN	117/129 (91%)	54 (46%)	33 (28%)	30 (26%)	0	1
47	BO	122/135 (90%)	65 (53%)	28 (23%)	29 (24%)	0	1
48	BP	123/126 (98%)	59 (48%)	30 (24%)	34 (28%)	0	0
49	BQ	58/61 (95%)	22 (38%)	10 (17%)	26 (45%)	0	0
50	BR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	3
51	BS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	2
52	BT	102/105 (97%)	62 (61%)	20 (20%)	20 (20%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BU	71/88 (81%)	29 (41%)	24 (34%)	18 (25%)	0	1
54	BV	78/93 (84%)	35 (45%)	17 (22%)	26 (33%)	0	0
55	BW	97/106 (92%)	27 (28%)	46 (47%)	24 (25%)	0	1
56	BX	22/27 (82%)	9 (41%)	5 (23%)	8 (36%)	0	0
All	All	5832/6739 (86%)	2857 (49%)	1467 (25%)	1508 (26%)	0	1

5 of 1508 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	ASN
3	AC	35	ALA
3	AC	54	SER
3	AC	68	LEU
3	AC	87	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	174/180 (97%)	144 (83%)	30 (17%)	2	12
4	AD	135/139 (97%)	90 (67%)	45 (33%)	0	2
5	AE	156/284 (55%)	114 (73%)	42 (27%)	0	3
6	AF	152/193 (79%)	121 (80%)	31 (20%)	1	7
7	AG	102/147 (69%)	74 (72%)	28 (28%)	0	3
8	AH	137/147 (93%)	99 (72%)	38 (28%)	0	3
9	AI	98/98 (100%)	89 (91%)	9 (9%)	9	30
9	AJ	98/98 (100%)	89 (91%)	9 (9%)	9	30
10	AK	119/119 (100%)	96 (81%)	23 (19%)	1	9
11	AL	108/113 (96%)	91 (84%)	17 (16%)	2	14
12	AM	95/121 (78%)	71 (75%)	24 (25%)	0	4
13	AN	101/101 (100%)	74 (73%)	27 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	67/126 (53%)	51 (76%)	16 (24%)	0	4
15	AP	110/110 (100%)	73 (66%)	37 (34%)	0	2
16	AQ	89/149 (60%)	58 (65%)	31 (35%)	0	1
17	AR	44/52 (85%)	24 (54%)	20 (46%)	0	0
18	AS	88/92 (96%)	65 (74%)	23 (26%)	0	3
19	AT	67/73 (92%)	48 (72%)	19 (28%)	0	2
20	AU	97/105 (92%)	75 (77%)	22 (23%)	1	5
21	AV	151/203 (74%)	109 (72%)	42 (28%)	0	3
22	AW	51/56 (91%)	36 (71%)	15 (29%)	0	2
23	AX	52/52 (100%)	34 (65%)	18 (35%)	0	1
24	A0	89/101 (88%)	59 (66%)	30 (34%)	0	2
25	A1	96/97 (99%)	67 (70%)	29 (30%)	0	2
26	A2	79/79 (100%)	60 (76%)	19 (24%)	0	4
27	A3	64/67 (96%)	46 (72%)	18 (28%)	0	3
28	A4	66/66 (100%)	50 (76%)	16 (24%)	0	4
29	A5	51/53 (96%)	38 (74%)	13 (26%)	0	4
30	A6	46/69 (67%)	35 (76%)	11 (24%)	0	4
31	A7	39/40 (98%)	30 (77%)	9 (23%)	1	5
32	A8	50/51 (98%)	33 (66%)	17 (34%)	0	1
33	A9	34/35 (97%)	30 (88%)	4 (12%)	5	21
37	BE	202/220 (92%)	152 (75%)	50 (25%)	0	4
38	BF	160/188 (85%)	127 (79%)	33 (21%)	1	7
39	BG	180/181 (99%)	136 (76%)	44 (24%)	0	4
40	BH	115/123 (94%)	66 (57%)	49 (43%)	0	0
41	BI	90/90 (100%)	64 (71%)	26 (29%)	0	2
42	BJ	126/127 (99%)	106 (84%)	20 (16%)	2	14
43	BK	119/119 (100%)	73 (61%)	46 (39%)	0	0
44	BL	98/99 (99%)	81 (83%)	17 (17%)	2	12
45	BM	88/92 (96%)	70 (80%)	18 (20%)	1	7
46	BN	90/99 (91%)	70 (78%)	20 (22%)	1	6
47	BO	104/111 (94%)	85 (82%)	19 (18%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BP	100/101 (99%)	80 (80%)	20 (20%)	1	8
49	BQ	49/50 (98%)	41 (84%)	8 (16%)	2	13
50	BR	79/80 (99%)	59 (75%)	20 (25%)	0	4
51	BS	72/74 (97%)	44 (61%)	28 (39%)	0	0
52	BT	96/97 (99%)	74 (77%)	22 (23%)	1	5
53	BU	64/77 (83%)	47 (73%)	17 (27%)	0	3
54	BV	71/80 (89%)	59 (83%)	12 (17%)	2	12
55	BW	76/82 (93%)	53 (70%)	23 (30%)	0	2
56	BX	19/22 (86%)	17 (90%)	2 (10%)	7	26
All	All	4903/5528 (89%)	3677 (75%)	1226 (25%)	0	4

5 of 1226 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	BI	70	ASP
51	BS	69	THR
42	BJ	155	ARG
41	BI	67	MET
46	BN	50	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
37	BE	240	GLN
42	BJ	68	ASN
38	BF	107	GLN
40	BH	65	ASN
44	BL	3	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	122/123 (99%)	47 (38%)	5 (4%)
2	AA	2870/2915 (98%)	1226 (42%)	290 (10%)
34	BA	1515/1522 (99%)	452 (29%)	161 (10%)
35	BB	76/76 (100%)	34 (44%)	16 (21%)
35	BC	75/76 (98%)	31 (41%)	9 (12%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	B1	65/78 (83%)	24 (36%)	4 (6%)
All	All	4723/4790 (98%)	1814 (38%)	485 (10%)

5 of 1814 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	0	A
1	AB	1	U
1	AB	2	C
1	AB	3	C
1	AB	9	G

5 of 485 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AA	2067	G
34	BA	1399	C
2	AA	2781	A
34	BA	1362	C
35	BC	9	A

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	123/123 (100%)	-0.47	0 100 100	308, 357, 402, 412	0
2	AA	2872/2915 (98%)	-0.48	15 (0%) 91 85	232, 307, 404, 474	0
3	AC	221/228 (96%)	-0.06	4 (1%) 68 60	384, 428, 464, 467	0
4	AD	173/178 (97%)	0.47	11 (6%) 19 17	243, 279, 292, 298	0
5	AE	191/338 (56%)	0.54	36 (18%) 1 3	258, 311, 397, 403	0
6	AF	189/246 (76%)	-0.37	2 (1%) 80 73	233, 399, 427, 434	0
7	AG	122/176 (69%)	-0.35	2 (1%) 72 63	350, 366, 443, 447	0
8	AH	164/177 (92%)	-0.37	1 (0%) 89 84	320, 351, 366, 370	0
9	AI	128/128 (100%)	1.33	30 (23%) 0 2	580, 591, 602, 603	0
9	AJ	128/128 (100%)	1.93	49 (38%) 0 1	569, 582, 594, 596	0
10	AK	148/149 (99%)	-0.12	4 (2%) 54 46	305, 329, 353, 361	0
11	AL	133/141 (94%)	0.11	7 (5%) 26 25	455, 504, 541, 543	0
12	AM	117/145 (80%)	0.25	12 (10%) 6 8	286, 310, 364, 368	0
13	AN	122/122 (100%)	0.29	10 (8%) 11 12	245, 262, 277, 293	0
14	AO	84/164 (51%)	0.22	5 (5%) 21 20	330, 452, 471, 473	0
15	AP	138/138 (100%)	0.42	9 (6%) 18 17	283, 324, 364, 379	0
16	AQ	113/186 (60%)	-0.77	0 100 100	317, 367, 386, 390	0
17	AR	52/66 (78%)	0.62	7 (13%) 3 5	251, 267, 285, 288	0
18	AS	108/113 (95%)	0.15	2 (1%) 66 58	280, 311, 324, 332	0
19	AT	76/84 (90%)	-0.09	4 (5%) 26 25	329, 344, 360, 363	0
20	AU	110/119 (92%)	-0.08	7 (6%) 19 17	647, 661, 722, 724	0
21	AV	177/253 (69%)	-0.07	8 (4%) 33 29	295, 365, 416, 424	0
22	AW	64/70 (91%)	0.11	1 (1%) 72 63	346, 364, 373, 375	0
23	AX	60/60 (100%)	-0.22	0 100 100	291, 306, 315, 316	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
24	A0	105/118 (88%)	-0.16	2 (1%) 66 58	263, 281, 304, 308	0
25	A1	117/118 (99%)	-0.52	1 (0%) 84 77	267, 297, 311, 317	0
26	A2	100/100 (100%)	0.72	16 (16%) 1 4	416, 430, 462, 470	0
27	A3	86/91 (94%)	0.53	11 (12%) 3 6	359, 389, 475, 486	0
28	A4	73/73 (100%)	-0.00	6 (8%) 11 12	319, 354, 373, 378	0
29	A5	58/60 (96%)	0.04	2 (3%) 45 38	259, 314, 361, 373	0
30	A6	53/82 (64%)	0.17	4 (7%) 14 14	287, 316, 332, 340	0
31	A7	46/47 (97%)	0.19	1 (2%) 62 53	316, 339, 352, 357	0
32	A8	63/64 (98%)	-0.02	1 (1%) 72 63	262, 282, 294, 306	0
33	A9	35/36 (97%)	-0.58	0 100 100	281, 303, 316, 319	0
34	BA	1515/1522 (99%)	-0.49	4 (0%) 94 90	251, 312, 419, 609	0
35	BB	76/76 (100%)	7.38	60 (78%) 0 0	631, 651, 667, 669	0
35	BC	76/76 (100%)	-0.66	0 100 100	273, 310, 328, 337	0
36	B1	66/78 (84%)	5.89	43 (65%) 0 0	337, 829, 918, 922	0
37	BE	234/256 (91%)	0.16	21 (8%) 9 10	293, 321, 364, 385	0
38	BF	206/239 (86%)	0.73	39 (18%) 1 3	301, 349, 377, 382	0
39	BG	208/209 (99%)	0.05	6 (2%) 51 43	276, 299, 318, 329	0
40	BH	150/162 (92%)	0.64	20 (13%) 3 5	277, 295, 315, 324	0
41	BI	101/101 (100%)	1.10	28 (27%) 0 2	299, 318, 330, 336	0
42	BJ	155/156 (99%)	0.02	6 (3%) 39 33	326, 357, 370, 373	0
43	BK	138/138 (100%)	0.17	9 (6%) 18 17	266, 284, 297, 306	0
44	BL	127/128 (99%)	-0.37	0 100 100	385, 487, 499, 500	0
45	BM	98/105 (93%)	0.83	11 (11%) 5 8	337, 394, 423, 424	0
46	BN	119/129 (92%)	0.20	9 (7%) 13 14	288, 307, 330, 334	0
47	BO	124/135 (91%)	0.20	4 (3%) 47 39	265, 282, 319, 328	0
48	BP	125/126 (99%)	-0.90	0 100 100	350, 370, 412, 415	0
49	BQ	60/61 (98%)	-0.09	2 (3%) 46 39	322, 352, 360, 365	0
50	BR	88/89 (98%)	-0.39	3 (3%) 45 38	277, 288, 315, 318	0
51	BS	83/88 (94%)	-0.41	1 (1%) 79 70	271, 284, 303, 316	0
52	BT	104/105 (99%)	-0.21	3 (2%) 51 43	249, 268, 323, 344	0
53	BU	73/88 (82%)	0.27	9 (12%) 4 7	259, 296, 323, 348	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	BV	80/93 (86%)	0.17	5 (6%) 20 17	353, 369, 395, 399	0
55	BW	99/106 (93%)	-0.54	0 100 100	264, 281, 292, 300	0
56	BX	24/27 (88%)	-1.09	0 100 100	475, 489, 493, 496	0
All	All	10678/11529 (92%)	-0.05	553 (5%) 27 26	232, 322, 533, 922	0

The worst 5 of 553 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	B1	15	A	20.7
35	BB	4	G	18.9
36	B1	42	G	18.3
36	B1	17	G	17.4
35	BB	5	A	17.2

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.