



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:03 PM BST

PDB ID : 4V6K
EMDB ID: : EMD-1849
Title : Structural insights into cognate vs. near-cognate discrimination during decoding.
Authors : Agirrezabala, X.; Schreiner, E.; Trabuco, L.G.; Lei, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-01-07
Resolution : 8.25 Å(reported)
Based on PDB ID : 2I2V

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

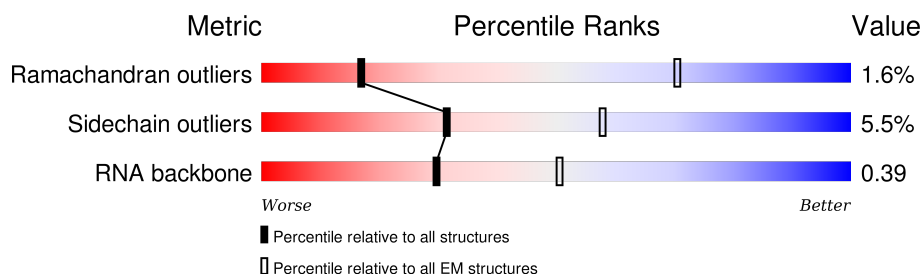
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.25 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.



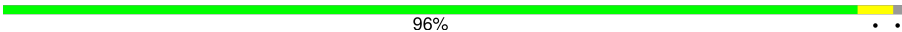
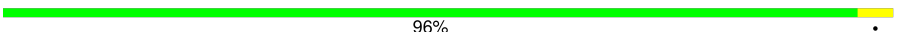










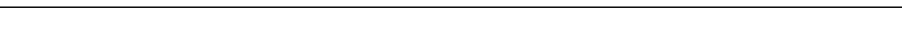

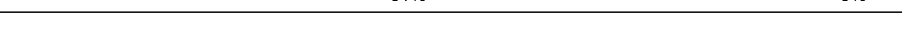

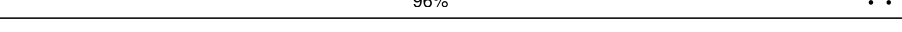







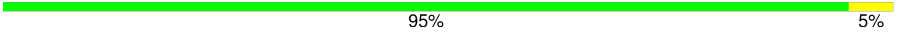
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	AA	120	
2	AB	2904	
3	AC	234	
4	AD	273	
5	AE	209	
6	AF	201	
7	AG	179	
8	AH	177	
9	AI	149	

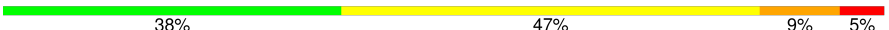

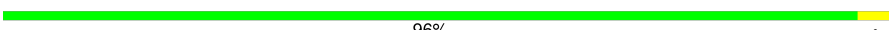
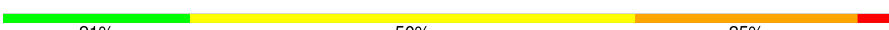








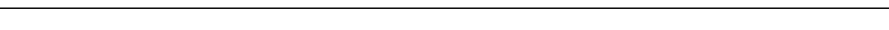
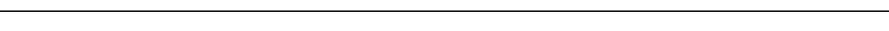
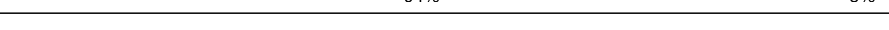
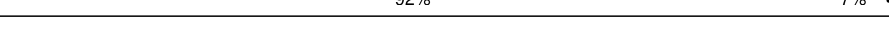
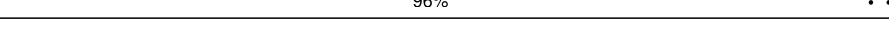

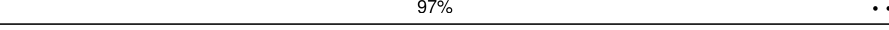
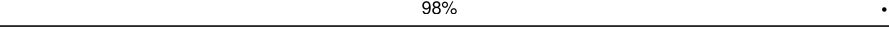
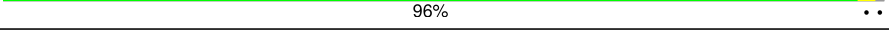


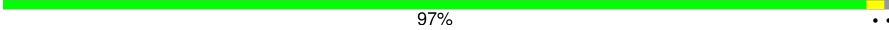
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Mol	Chain	Length	Quality of chain
10	AJ	142	 96% . .
11	AK	142	 96% .
12	AL	123	 90% 10%
13	AM	144	 96% .
14	AN	136	 93% 6% .
15	AO	127	 97% .
16	AP	117	 93% 7%
17	AQ	115	 90% 8% . .
18	AR	118	 91% 8% .
19	AS	103	 90% 10%
20	AT	110	 95% 5%
21	AU	100	 93% 7%
22	AV	104	 95% . .
23	AW	94	 91% 9%
24	AX	85	 93% 6% .
25	AY	78	 96% . .
26	AZ	63	 86% 13% .
27	Aa	59	 92% 7% .
28	Ab	70	 89% 11%
29	Ac	57	 88% 11% .
30	Ad	55	 93% 5% .
31	Ae	46	 87% 13%
32	Af	65	 95% . .
33	Ag	38	 95% 5%
34	BA	1542	 25% 50% 21% .

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Mol	Chain	Length	Quality of chain
35	BB	76	 38% 47% 9% 5%
35	BE	76	 34% 41% 21% .
36	BC	393	 96% .
37	BD	24	 21% 50% 25% .
38	BF	241	 94% 6%
39	BG	233	 92% 7%
40	BH	206	 94% 6%
41	BI	167	 92% 8% .
42	BJ	135	 94% 6%
43	BK	179	 93% 7% .
44	BL	130	 93% 6% .
45	BM	130	 90% 9% .
46	BN	103	 86% 14%
47	BO	129	 94% 5% .
48	BP	124	 92% 7% .
49	BQ	118	 96% . .
50	BR	101	 84% 14% . .
51	BS	89	 97% . .
52	BT	82	 98% .
53	BU	84	 96% . .
54	BV	75	 87% 9% . .
55	BW	92	 92% 5% . .
56	BX	87	 97% . .
57	BY	71	 85% 14% .

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 153634 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 ribosomal RNA 5S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	120	Total	C	N	O	P	0	0
			2566	1144	468	835	119		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	2904	Total	C	N	O	P	0	0
			62351	27824	11469	20155	2903		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	234	Total	C	N	O	S	0	0
			1733	1081	315	330	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	272	Total	C	N	O	S	0	0
			2092	1294	425	366	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 12 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 13 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 14 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	127	Total	C	N	O	S	0	0
			1008	621	204	178	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 18 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 19 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 20 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	100	Total	C	N	O	S	0	0
			787	496	146	143	2		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	103	Total	C	N	O	S	0	0
			789	498	148	143			

- Molecule 23 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	AZ	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Aa	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Ab	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Ac	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Ad	54	Total	C	N	O	S	0	0
			441	284	81	76			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ae	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Af	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Ag	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BA	1542	Total	C	N	O	P	0	0
			33089	14767	6064	10717	1541		

- Molecule 35 is a RNA chain called A/T-site tRNA Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	BB	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		
35	BE	76	Total	C	N	O	P	S	0	0
			1635	735	291	532	75	2		

- Molecule 36 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	BC	393	Total	C	N	O	S		0	0
			3036	1918	523	582	13			

- Molecule 37 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	BD	24	Total	C	N	O	P		0	0
			495	222	68	181	24			

- Molecule 38 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	BF	240	Total	C	N	O	S		0	0
			1872	1180	332	352	8			

- Molecule 39 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
39	BG	232	Total	C	N	O	S		0	0
			1822	1149	346	323	4			

- Molecule 40 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	BH	205	Total	C	N	O	S		0	0
			1643	1026	315	298	4			

- Molecule 41 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	BI	166	Total	C	N	O	S		0	0
			1225	761	232	226	6			

- Molecule 42 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BJ	135	Total	C	N	O	S	0	0
			1101	677	198	219	7		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BK	178	Total	C	N	O	S	0	0
			1400	874	269	253	4		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BL	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BM	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BN	103	Total	C	N	O	S	0	0
			825	514	158	151	2		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BO	128	Total	C	N	O	S	0	0
			965	595	196	171	3		

- Molecule 48 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BP	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 49 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	BQ	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 50 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BR	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 51 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	BS	88	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 52 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BT	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 53 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	BU	83	Total	C	N	O	S	0	0
			672	425	124	120	3		

- Molecule 54 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	BV	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 55 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	BW	91	Total	C	N	O	S	0	0
			727	464	139	122	2		

- Molecule 56 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	BX	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

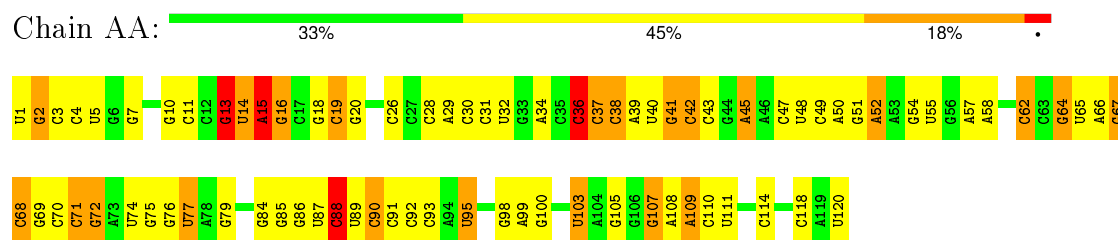
- Molecule 57 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	BY	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

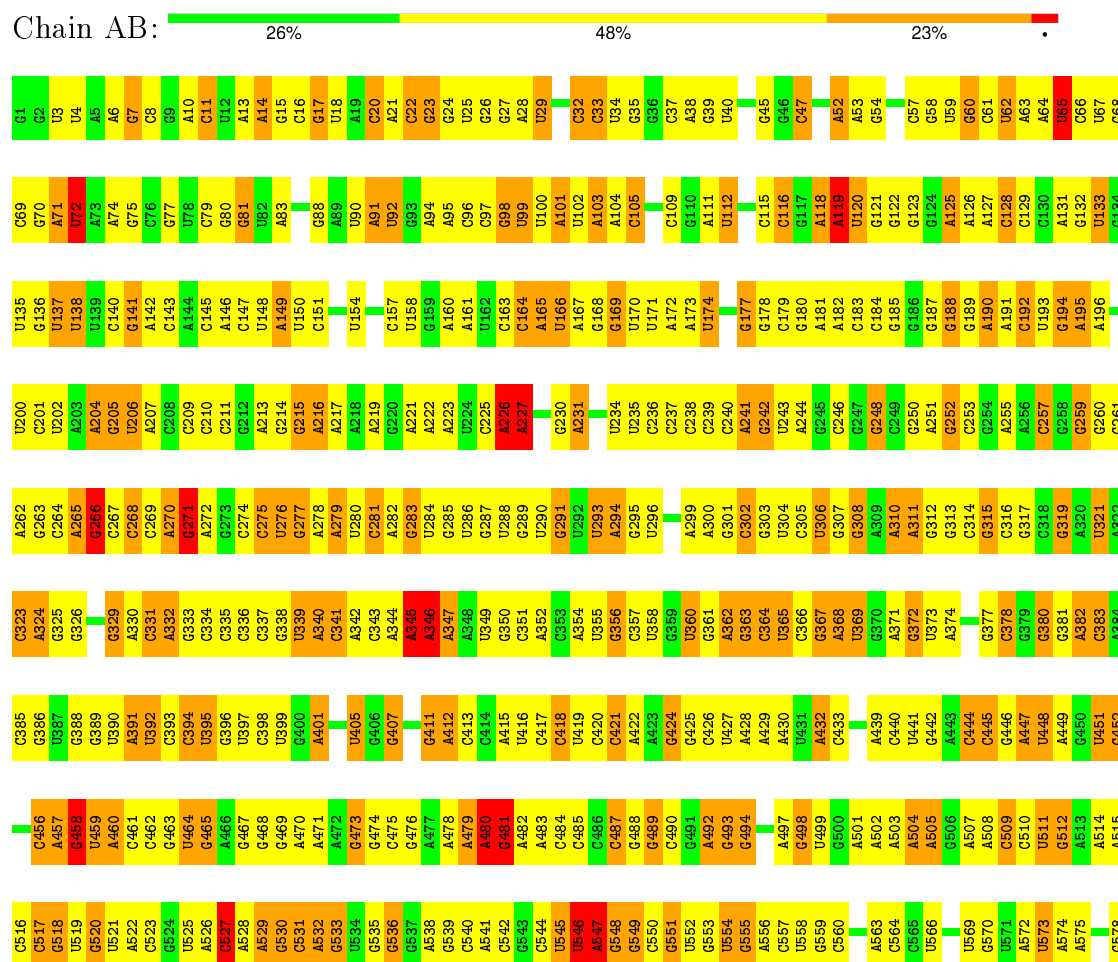
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

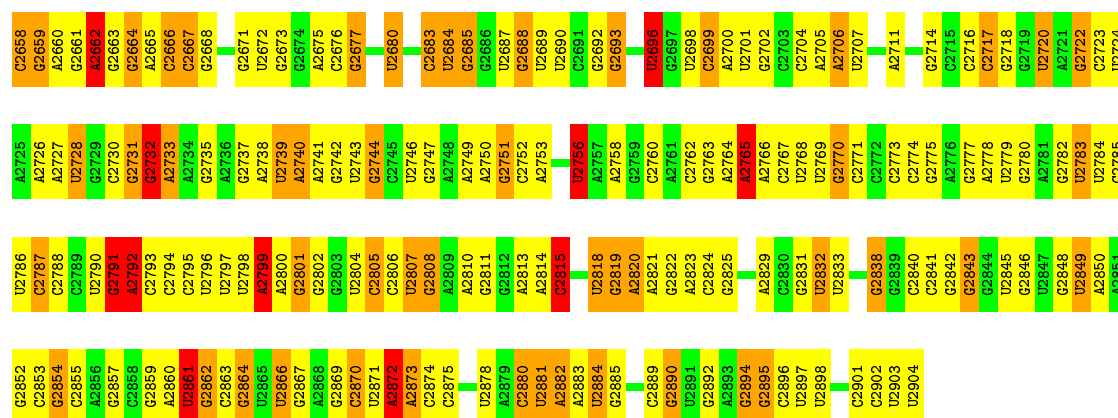
• Molecule 1: ribosomal RNA 5S



• Molecule 2: ribosomal RNA 23S



A1549	C1550	A1551	A1552	A1553	U1554	A1555		A1558	U1559	G1560	C1561	U1562	U1563	G1564	A1565	A1566	C1567	A1568	A1569	A1570	A1571	A1572	C1573	C1574	C1575	U1576	C1577	A1578	A1579	A1580	C1582	A1583	U1584	U1585	A1586	C1587	C1588	A1589	A1590	A1591	C1592	A1593	U1594	U1595	A1596	A1597	A1598	A1599	C1600	G1601	U1602	A1603	C1604	C1605	A1606	C1607	A1608	A1609		
U1486	U1487	C1488	C1489	A1490	A1491	A1492	C1493	A1494	A1495		C1498	U1499	U1500	G1501	A1502	A1503	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	C1512	U1513	U1514	U1515	U1516		U1520	C1521	A1522	U1523	A1524	A1525	C1526	U1527	C1528	A1529	U1530	C1531	A1532	C1533	U1534	U1535	C1536	C1537	U1538	U1539	C1600	G1601	A1602	A1603	C1604	C1605	A1606	C1607	A1608	A1609
G1416	C1417	G1418	A1419	A1420	G1421	C1422	G1423	G1424	G1425	G1426	A1427	A1433	A1434	G1435	G1436	G1437	U1440	U1441	U1442	U1443	U1444	U1445	C1446	C1447	U1448		C1451	G1452	A1453	C1454	G1455	U1456	U1457	U1458	U1459	C1460	C1461	C1462	C1463	U1467	G1471	C1472	G1473	U1474	G1475	U1476	A1477	G1478	G1479	C1480	U1481	G1482	A1483	U1484	U1485					
A1353	A1354	G1355	G1356	C1357	G1358	A1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	A1372	A1373	G1374	U1375	C1376	G1377	A1378	C1379	G1380	G1381	G1382	A1383	A1384	A1385	G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	C1398	C1399	U1400	G1401	U1402	A1403	C1404	U1405	G1406	G1407	G1408	U1409	U1410	U1411	U1412	C1413	C1414	U1415	
A1286	A1287	G1288	C1289	C1290	G1291	C1292	C1293	U1294	C1295	C1296	C1297	C1298	A1299	G1300	A1301	A1302	G1303	A1304	C1305	C1306	A1307	U1308	G1309	G1310	U1313	U1316	G1317	U1318	A1321	G1324	U1325	U1326	A1327	C1330	G1331	G1332	G1333	G1334	C1335	G1338	G1339	G1340	U1343	U1344	C1345	G1346	A1347	C1348	C1349	C1350	C1351	C1414	U1415							
U1219	G1220	C1221	U1222	G1223	U1224	G1225	A1226	G1227	C1228	C1229	A1230	U1231	G1232	U1233	A1234	G1235	G1236	A1237	G1238	U1241	U1242	C1243	A1244	G1245	A1246	U1247	G1248	U1249	G1250	A1254	U1255	G1256	C1257	U1258	C1261	A1262	U1263	G1266	U1267	A1268	A1276	G1271	A1272		A1275	A1276	G1277	C1278	G1279	G1280	G1281	U1282	G1283	A1285						
G1093	U1094	A1095	U1096	U1097	A1098	G1099	C1100	U1101	C1102	A1103	G1104	U1105	G1106	U1107	U1108	A1109	G1110	U1111	G1112	U1113	C1114	G1115	G1116	C1117	U1118	G1119	U1120	C1121	G1122	C1123	G1124	G1128	U1129	G1130	U1131	U1132	A1133	A1134	C1135	G1136	G1137	G1138	C1139	C1140	U1141	A1142	A1143	U1144	C1145	U1146	C1147	U1148	G1149	C1150	A1151	C1152	G1154			
U1159	G1160	C1161	G1162	G1163	C1164	A1165	A1166	C1167	C1170	U1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	U1179	U1180	U1181	G1182	U1183	U1184	G1185	U1186	G1187	U1188	A1189	U1190	G1191	G1192	G1193	A1194	U1195	C1196	G1197	U1198	U1199	C1200	U1201	G1202	U1203	A1204	G1206	C1207	C1208	U1209	G1210	C1211	G1212	A1213	A1214	G1215	G1216	U1217	G1218				
A1286	A1287	G1288	C1289	C1290	G1291	C1292	C1293	U1294	C1295	C1296	C1297	C1298	A1299	G1300	A1301	A1302	G1303	A1304	C1305	C1306	A1307	U1308	G1309	G1310	U1313	U1316	G1317	U1318	A1321	G1324	U1325	U1326	A1327	C1330	G1331	G1332	G1333	G1334	C1335	G1338	G1339	G1340	U1343	U1344	C1345	G1346	A1347	C1348	C1349	C1350	C1351	C1414	U1415							
A1353	A1354	G1355	G1356	C1357	G1358	A1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	G1371	A1372	A1373	G1374	U1375	C1376	G1377	A1378	C1379	G1380	G1381	G1382	A1383	A1384	A1385	G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	C1398	C1399	U1400	G1401	U1402	A1403	C1404	U1405	U1406	G1407	G1408	U1409	U1410	U1411	U1412	C1413	C1414	U1415	
G1416	C1417	G1418	A1419	A1420	G1421	C1422	G1423	G1424	G1425	G1426	A1427	A1433	A1434	G1435	G1436	C1437	U1440	U1441	U1442	U1443	U1444	U1445	C1446	C1447	U1448		C1451	G1452	A1453	C1454	G1455	U1456	U1457	U1458	U1459	C1460	C1461	C1462	C1463	U1467	G1471	C1472	G1473	U1474	G1475	U1476	A1477	G1478	G1479	C1480	U1481	G1482	A1483	U1484	U1485					
U1486	U1487	C1488	C1489	A1490	A1491	A1492	C1493	A1494	A1495		C1498	U1499	U1500	G1501	A1502	A1503	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	C1512	U1513	U1514	U1515	U1516		U1520	C1521	A1522	U1523	A1524	A1525	C1526	U1527	C1528	A1529	U1530	C1531	A1532	C1533	U1534	U1535	C1536	C1537	U1538	U1539	C1600	G1601	A1602	A1603	C1604	C1605	A1606	C1607	A1608	A1609



- Molecule 3: 50S ribosomal protein L1



- Molecule 4: 50S ribosomal protein L2



- Molecule 5: 50S ribosomal protein L3



- Molecule 6: 50S ribosomal protein L4

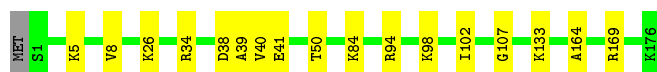


- Molecule 7: 50S ribosomal protein L5



- Molecule 8: 50S ribosomal protein L6





- Molecule 9: 50S ribosomal protein L9

Chain AI: 90% 9%



- Molecule 10: 50S ribosomal protein L11

Chain AJ: 96%



- Molecule 11: 50S ribosomal protein L13

Chain AK: 96%



- Molecule 12: 50S ribosomal protein L14

Chain AL: 90% 10%



- Molecule 13: 50S ribosomal protein L15

Chain AM: 96%



- Molecule 14: 50S ribosomal protein L16

Chain AN: 93% 6%



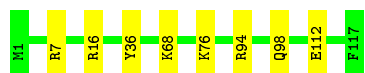
- Molecule 15: 50S ribosomal protein L17

Chain AO: 97%



- Molecule 16: 50S ribosomal protein L18

Chain AP:  93% 7%



- Molecule 17: 50S ribosomal protein L19

Chain AQ:  90% 8% ..



- Molecule 18: 50S ribosomal protein L20

Chain AR:  91% 8% .



- Molecule 19: 50S ribosomal protein L21

Chain AS:  90% 10%



- Molecule 20: 50S ribosomal protein L22

Chain AT:  95% 5%



- Molecule 21: 50S ribosomal protein L23

Chain AU:  93% 7%



- Molecule 22: 50S ribosomal protein L24

Chain AV:  95% . .



- Molecule 23: 50S ribosomal protein L25

Chain AW:  91% 9%



- Molecule 24: 50S ribosomal protein L27

Chain AX:  93% 6%




- Molecule 25: 50S ribosomal protein L28

Chain AY:  96% 4%



- Molecule 26: 50S ribosomal protein L29

Chain AZ:  86% 13%



- Molecule 27: 50S ribosomal protein L30

Chain Aa:  92% 7%



- Molecule 28: 50S ribosomal protein L31

Chain Ab:  89% 11%



- Molecule 29: 50S ribosomal protein L32

Chain Ac:  88% 11%



- Molecule 30: 50S ribosomal protein L33

Chain Ad:  93% 5%



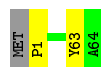
- Molecule 31: 50S ribosomal protein L34

Chain Ae: 87% 13%



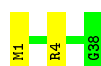
- Molecule 32: 50S ribosomal protein L35

Chain Af: 95% 5%



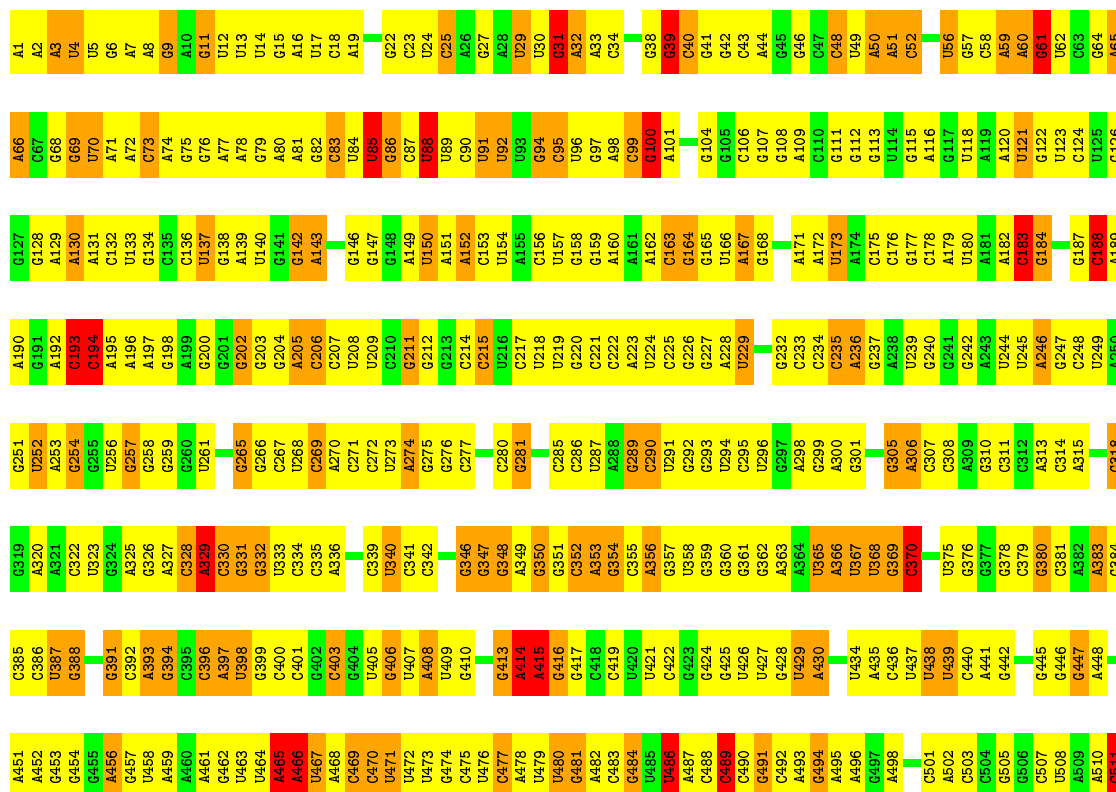
- Molecule 33: 50S ribosomal protein L36

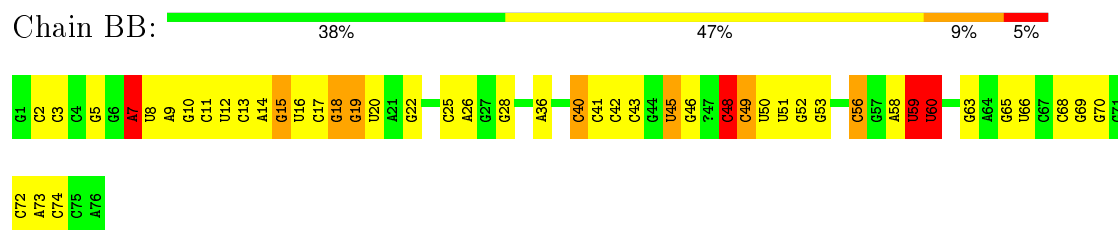
Chain Ag: 95% 5%



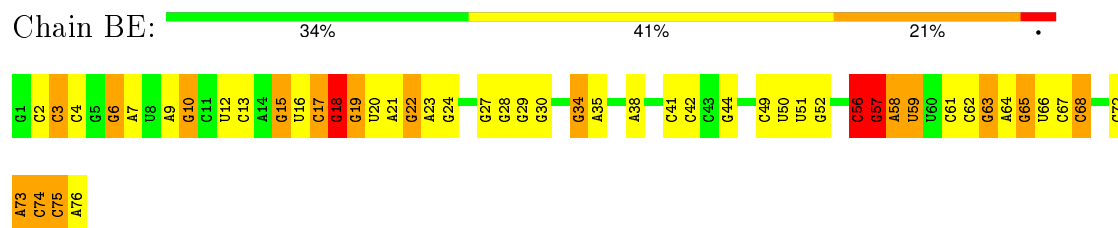
- Molecule 34: 16S ribosomal RNA

Chain BA: 25% 50% 21%

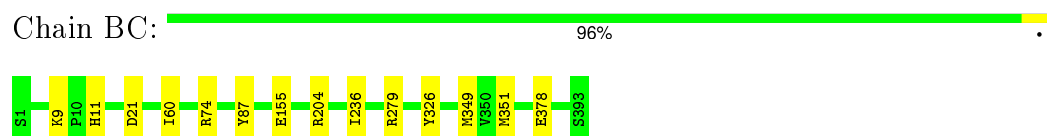




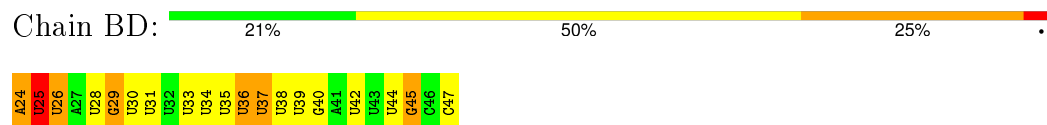
- Molecule 35: A/T-site tRNA Phe



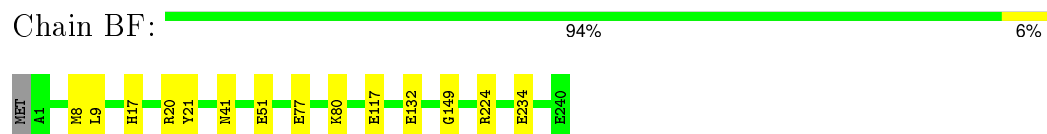
- Molecule 36: Elongation factor Tu 2



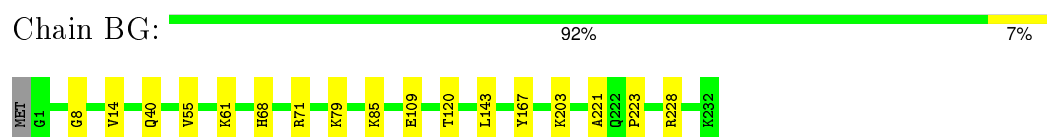
- Molecule 37: mRNA



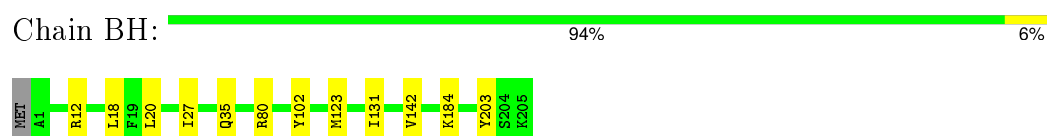
- Molecule 38: 30S ribosomal protein S2



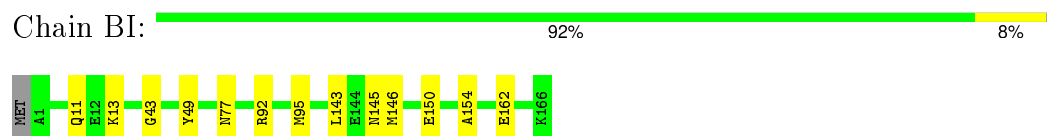
- Molecule 39: 30S ribosomal protein S3



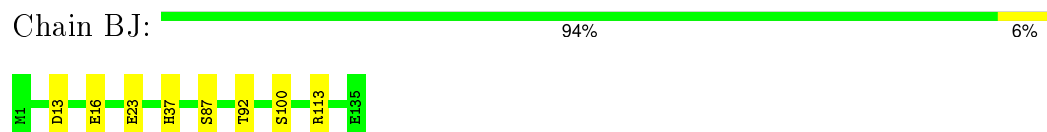
- Molecule 40: 30S ribosomal protein S4



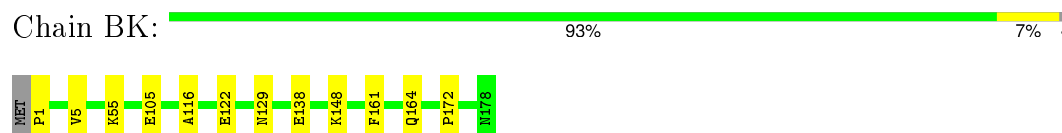
- Molecule 41: 30S ribosomal protein S5



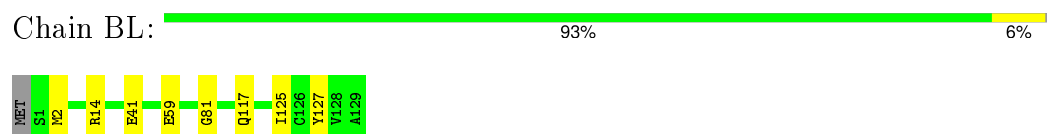
- Molecule 42: 30S ribosomal protein S6



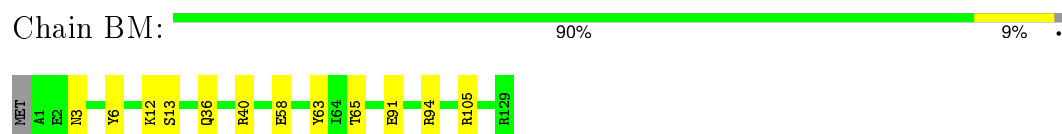
- Molecule 43: 30S ribosomal protein S7



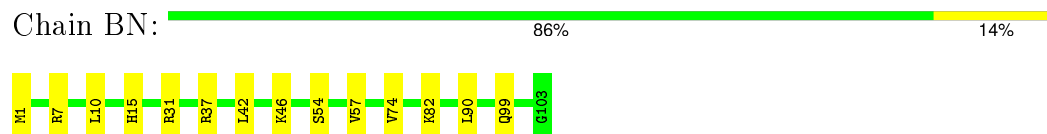
- Molecule 44: 30S ribosomal protein S8



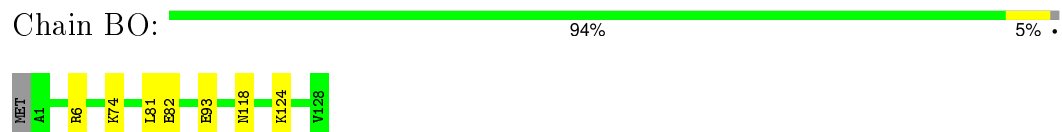
- Molecule 45: 30S ribosomal protein S9



- Molecule 46: 30S ribosomal protein S10

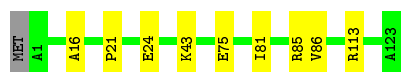


- Molecule 47: 30S ribosomal protein S11



- Molecule 48: 30S ribosomal protein S12

Chain BP:  92% 7% .




- Molecule 49: 30S ribosomal protein S13

Chain BQ:  96% ..



- Molecule 50: 30S ribosomal protein S14

Chain BR:  84% 14% ..



- Molecule 51: 30S ribosomal protein S15

Chain BS:  97% ..



- Molecule 52: 30S ribosomal protein S16

Chain BT:  98% .




- Molecule 53: 30S ribosomal protein S17

Chain BU:  96% ..



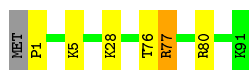
- Molecule 54: 30S ribosomal protein S18

Chain BV:  87% 9% . .



- Molecule 55: 30S ribosomal protein S19

Chain BW:  92% 5% ..



- Molecule 56: 30S ribosomal protein S20

Chain BX: 97% ..



- Molecule 57: 30S ribosomal protein S21

Chain BY: 85% 14% .



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	Not provided	Depositor
Microscope	Not provided	Depositor
Voltage (kV)	Not provided	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 5MU, CH, OMG, OMU, MA6, MIA, OMC, 1MG, H2U, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, 4SU, 7MG, 3AU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	AA	1.18	0/2869	2.04	104/4474 (2.3%)
10	AJ	0.57	0/1046	0.92	0/1410
11	AK	0.63	0/1152	0.99	0/1551
12	AL	0.57	0/956	1.00	0/1279
13	AM	0.60	0/1062	1.01	0/1413
14	AN	0.63	0/1093	1.05	1/1460 (0.1%)
15	AO	0.61	0/1021	1.03	0/1364
16	AP	0.60	0/910	1.00	0/1219
17	AQ	0.61	0/929	1.06	0/1242
18	AR	0.67	0/960	1.02	1/1278 (0.1%)
19	AS	0.62	0/829	1.01	0/1107
2	AB	1.17	0/69257	1.96	2261/108040 (2.1%)
20	AT	0.52	0/864	0.96	0/1156
21	AU	0.55	0/794	0.99	0/1060
22	AV	0.56	0/797	1.03	0/1062
23	AW	0.60	0/766	0.97	0/1025
24	AX	0.64	0/642	1.09	0/848
25	AY	0.64	0/635	1.06	0/848
26	AZ	0.56	0/510	1.10	1/677 (0.1%)
27	Aa	0.54	0/453	0.98	0/605
28	Ab	0.63	0/559	1.17	2/745 (0.3%)
29	Ac	0.59	0/450	1.05	0/599
3	AC	0.56	0/1748	0.96	1/2355 (0.0%)
30	Ad	0.61	0/448	1.00	0/594
31	Ae	0.63	0/380	1.11	1/498 (0.2%)
32	Af	0.58	0/513	1.01	1/676 (0.1%)
33	Ag	0.53	0/303	1.00	0/397
34	BA	1.17	1/36769 (0.0%)	1.96	1171/57354 (2.0%)
35	BB	1.23	0/1580	1.96	45/2459 (1.8%)
35	BE	1.20	0/1580	2.05	59/2459 (2.4%)
36	BC	0.61	0/3092	0.96	1/4183 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
37	BD	1.30	0/548	1.88	16/848 (1.9%)
38	BF	0.60	0/1904	1.00	0/2565
39	BG	0.60	0/1852	1.04	0/2490
4	AD	0.60	0/2131	1.07	1/2863 (0.0%)
40	BH	0.63	0/1665	1.02	0/2227
41	BI	0.56	0/1239	1.00	1/1664 (0.1%)
42	BJ	0.61	0/1121	1.05	0/1509
43	BK	0.62	0/1422	1.04	1/1908 (0.1%)
44	BL	0.58	0/989	0.97	0/1326
45	BM	0.65	0/1048	1.03	0/1394
46	BN	0.59	0/835	1.08	0/1127
47	BO	0.61	0/982	1.00	0/1323
48	BP	0.61	0/969	1.09	0/1300
49	BQ	0.57	0/919	1.01	0/1226
5	AE	0.58	0/1586	1.02	0/2134
50	BR	0.63	0/817	1.14	1/1088 (0.1%)
51	BS	0.58	0/724	1.00	1/966 (0.1%)
52	BT	0.63	0/659	1.04	0/884
53	BU	0.58	0/681	0.99	0/913
54	BV	0.71	0/637	1.06	0/851
55	BW	0.60	0/744	1.02	3/995 (0.3%)
56	BX	0.55	0/676	0.91	0/895
57	BY	0.69	0/598	1.17	1/792 (0.1%)
6	AF	0.57	0/1571	0.99	0/2113
7	AG	0.65	0/1444	1.10	4/1937 (0.2%)
8	AH	0.59	0/1343	1.02	0/1816
9	AI	0.57	0/1122	1.01	1/1515 (0.1%)
All	All	1.03	1/165193 (0.0%)	1.75	3679/246106 (1.5%)

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	AA	0	27
11	AK	0	2
15	AO	0	1
17	AQ	0	1
18	AR	0	1
2	AB	0	821
28	Ab	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AC	0	2
30	Ad	0	1
31	Ae	0	2
34	BA	0	473
35	BB	0	12
35	BE	0	15
37	BD	0	4
38	BF	0	1
39	BG	0	2
40	BH	0	2
41	BI	0	3
42	BJ	0	1
43	BK	0	2
45	BM	0	2
47	BO	0	1
48	BP	0	1
5	AE	0	3
50	BR	0	1
54	BV	0	1
55	BW	0	1
57	BY	0	3
6	AF	0	1
8	AH	0	2
9	AI	0	2
All	All	0	1392

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	BA	1535	C	P-O5'	5.14	1.64	1.59

The worst 5 of 3679 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	13	G	O4'-C1'-N9	15.20	120.36	108.20
2	AB	736	C	O4'-C1'-N1	14.43	119.74	108.20
34	BA	465	A	O4'-C1'-N9	13.60	119.08	108.20
2	AB	2832	U	O4'-C1'-N1	12.97	118.58	108.20
34	BA	1152	A	O4'-C1'-N9	12.96	118.57	108.20

There are no chirality outliers.

5 of 1392 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	13	G	Sidechain
1	AA	14	U	Sidechain
1	AA	15	A	Sidechain
1	AA	2	G	Sidechain
1	AA	7	G	Sidechain

5.2 Too-close contacts ⓘ

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	AA	2566	0	1302	0	0
2	AB	62351	0	31387	0	0
3	AC	1733	0	1824	0	0
4	AD	2092	0	2170	0	0
5	AE	1565	0	1616	0	0
6	AF	1552	0	1619	0	0
7	AG	1420	0	1460	0	0
8	AH	1323	0	1374	0	0
9	AI	1111	0	1148	0	0
10	AJ	1032	0	1088	0	0
11	AK	1129	0	1162	0	0
12	AL	947	0	1023	0	0
13	AM	1053	0	1129	0	0
14	AN	1074	0	1157	0	0
15	AO	1008	0	1045	0	0
16	AP	900	0	935	0	0
17	AQ	917	0	965	0	0
18	AR	947	0	1022	0	0
19	AS	816	0	839	0	0
20	AT	857	0	922	0	0
21	AU	787	0	846	0	0
22	AV	789	0	847	0	0
23	AW	753	0	780	0	0
24	AX	634	0	656	0	0
25	AY	625	0	655	0	0
26	AZ	509	0	543	0	0
27	Aa	449	0	491	0	0
28	Ab	549	0	552	0	0
29	Ac	444	0	461	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	Ad	441	0	485	0	0
31	Ae	377	0	418	0	0
32	Af	504	0	574	0	0
33	Ag	302	0	343	0	0
34	BA	33089	0	16678	0	0
35	BB	1635	0	849	0	0
35	BE	1635	0	849	0	0
36	BC	3036	0	3052	0	0
37	BD	495	0	249	0	0
38	BF	1872	0	1885	0	0
39	BG	1822	0	1913	0	0
40	BH	1643	0	1710	0	0
41	BI	1225	0	1273	0	0
42	BJ	1101	0	1050	0	0
43	BK	1400	0	1449	0	0
44	BL	979	0	1034	0	0
45	BM	1036	0	1084	0	0
46	BN	825	0	865	0	0
47	BO	965	0	997	0	0
48	BP	955	0	1019	0	0
49	BQ	910	0	981	0	0
50	BR	805	0	847	0	0
51	BS	716	0	742	0	0
52	BT	649	0	666	0	0
53	BU	672	0	716	0	0
54	BV	626	0	651	0	0
55	BW	727	0	769	0	0
56	BX	670	0	722	0	0
57	BY	590	0	631	0	0
All	All	153634	0	105519	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	232/234 (99%)	204 (88%)	25 (11%)	3 (1%)	15	60
4	AD	270/273 (99%)	239 (88%)	23 (8%)	8 (3%)	5	42
5	AE	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	6	43
6	AF	199/201 (99%)	182 (92%)	14 (7%)	3 (2%)	13	57
7	AG	176/179 (98%)	147 (84%)	27 (15%)	2 (1%)	17	63
8	AH	174/177 (98%)	163 (94%)	8 (5%)	3 (2%)	11	55
9	AI	147/149 (99%)	126 (86%)	16 (11%)	5 (3%)	5	40
10	AJ	139/142 (98%)	123 (88%)	15 (11%)	1 (1%)	26	71
11	AK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
12	AL	121/123 (98%)	106 (88%)	13 (11%)	2 (2%)	11	55
13	AM	142/144 (99%)	125 (88%)	15 (11%)	2 (1%)	14	58
14	AN	134/136 (98%)	122 (91%)	9 (7%)	3 (2%)	8	49
15	AO	125/127 (98%)	117 (94%)	7 (6%)	1 (1%)	24	69
16	AP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	21	67
17	AQ	112/115 (97%)	100 (89%)	10 (9%)	2 (2%)	11	53
18	AR	115/118 (98%)	110 (96%)	4 (4%)	1 (1%)	21	67
19	AS	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	4	35
20	AT	108/110 (98%)	98 (91%)	9 (8%)	1 (1%)	21	67
21	AU	98/100 (98%)	85 (87%)	11 (11%)	2 (2%)	9	51
22	AV	101/104 (97%)	89 (88%)	11 (11%)	1 (1%)	19	65
23	AW	92/94 (98%)	85 (92%)	5 (5%)	2 (2%)	8	49
24	AX	82/85 (96%)	67 (82%)	12 (15%)	3 (4%)	4	38
25	AY	75/78 (96%)	64 (85%)	9 (12%)	2 (3%)	6	45
26	AZ	61/63 (97%)	49 (80%)	9 (15%)	3 (5%)	3	31
27	Aa	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	11	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	Ab	68/70 (97%)	57 (84%)	10 (15%)	1 (2%)	13	57
29	Ac	54/57 (95%)	47 (87%)	5 (9%)	2 (4%)	4	38
30	Ad	52/55 (94%)	45 (86%)	7 (14%)	0	100	100
31	Ae	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
32	Af	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
33	Ag	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	6	44
36	BC	391/393 (100%)	368 (94%)	20 (5%)	3 (1%)	24	69
38	BF	238/241 (99%)	215 (90%)	20 (8%)	3 (1%)	15	60
39	BG	230/233 (99%)	211 (92%)	17 (7%)	2 (1%)	21	67
40	BH	203/206 (98%)	191 (94%)	10 (5%)	2 (1%)	19	65
41	BI	164/167 (98%)	144 (88%)	17 (10%)	3 (2%)	11	53
42	BJ	133/135 (98%)	128 (96%)	3 (2%)	2 (2%)	13	57
43	BK	176/179 (98%)	160 (91%)	14 (8%)	2 (1%)	17	63
44	BL	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	12	56
45	BM	127/130 (98%)	111 (87%)	14 (11%)	2 (2%)	12	56
46	BN	101/103 (98%)	86 (85%)	11 (11%)	4 (4%)	4	35
47	BO	126/129 (98%)	113 (90%)	11 (9%)	2 (2%)	12	56
48	BP	121/124 (98%)	104 (86%)	12 (10%)	5 (4%)	3	35
49	BQ	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
50	BR	98/101 (97%)	83 (85%)	8 (8%)	7 (7%)	1	22
51	BS	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
52	BT	80/82 (98%)	79 (99%)	1 (1%)	0	100	100
53	BU	81/84 (96%)	73 (90%)	8 (10%)	0	100	100
54	BV	72/75 (96%)	65 (90%)	5 (7%)	2 (3%)	6	44
55	BW	89/92 (97%)	80 (90%)	9 (10%)	0	100	100
56	BX	84/87 (97%)	78 (93%)	6 (7%)	0	100	100
57	BY	68/71 (96%)	60 (88%)	7 (10%)	1 (2%)	13	57
All	All	6548/6682 (98%)	5904 (90%)	536 (8%)	108 (2%)	17	56

5 of 108 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AD	260	LYS

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Mol	Chain	Res	Type
5	AE	122	VAL
5	AE	150	GLN
5	AE	170	VAL
9	AI	23	ALA

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	181/181 (100%)	171 (94%)	10 (6%)	27	63
4	AD	217/218 (100%)	204 (94%)	13 (6%)	24	60
5	AE	164/164 (100%)	154 (94%)	10 (6%)	23	60
6	AF	165/165 (100%)	158 (96%)	7 (4%)	36	70
7	AG	149/150 (99%)	138 (93%)	11 (7%)	17	54
8	AH	137/138 (99%)	125 (91%)	12 (9%)	12	45
9	AI	114/114 (100%)	106 (93%)	8 (7%)	19	56
10	AJ	109/110 (99%)	105 (96%)	4 (4%)	41	73
11	AK	116/116 (100%)	113 (97%)	3 (3%)	54	80
12	AL	104/104 (100%)	94 (90%)	10 (10%)	10	40
13	AM	103/103 (100%)	99 (96%)	4 (4%)	39	72
14	AN	109/109 (100%)	103 (94%)	6 (6%)	27	63
15	AO	103/103 (100%)	101 (98%)	2 (2%)	65	86
16	AP	87/87 (100%)	80 (92%)	7 (8%)	15	50
17	AQ	99/100 (99%)	91 (92%)	8 (8%)	15	50
18	AR	89/90 (99%)	82 (92%)	7 (8%)	15	51
19	AS	84/84 (100%)	78 (93%)	6 (7%)	18	55
20	AT	93/93 (100%)	89 (96%)	4 (4%)	35	70
21	AU	84/84 (100%)	79 (94%)	5 (6%)	24	60
22	AV	84/85 (99%)	81 (96%)	3 (4%)	42	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	AW	78/78 (100%)	72 (92%)	6 (8%)	16	52
24	AX	62/63 (98%)	60 (97%)	2 (3%)	46	76
25	AY	67/68 (98%)	67 (100%)	0	100	100
26	AZ	55/55 (100%)	49 (89%)	6 (11%)	8	35
27	Aa	48/49 (98%)	45 (94%)	3 (6%)	22	59
28	Ab	62/62 (100%)	58 (94%)	4 (6%)	21	58
29	Ac	47/48 (98%)	43 (92%)	4 (8%)	13	48
30	Ad	48/49 (98%)	46 (96%)	2 (4%)	36	70
31	Ae	38/38 (100%)	35 (92%)	3 (8%)	15	51
32	Af	51/52 (98%)	50 (98%)	1 (2%)	63	85
33	Ag	34/34 (100%)	33 (97%)	1 (3%)	50	78
36	BC	326/326 (100%)	316 (97%)	10 (3%)	47	77
38	BF	198/199 (100%)	188 (95%)	10 (5%)	29	66
39	BG	189/190 (100%)	176 (93%)	13 (7%)	19	56
40	BH	172/173 (99%)	164 (95%)	8 (5%)	32	68
41	BI	125/126 (99%)	118 (94%)	7 (6%)	26	62
42	BJ	116/116 (100%)	111 (96%)	5 (4%)	35	70
43	BK	146/147 (99%)	139 (95%)	7 (5%)	31	67
44	BL	104/105 (99%)	98 (94%)	6 (6%)	25	61
45	BM	106/107 (99%)	98 (92%)	8 (8%)	17	53
46	BN	90/90 (100%)	80 (89%)	10 (11%)	8	34
47	BO	98/99 (99%)	94 (96%)	4 (4%)	37	71
48	BP	103/104 (99%)	100 (97%)	3 (3%)	50	78
49	BQ	95/96 (99%)	91 (96%)	4 (4%)	36	70
50	BR	83/84 (99%)	76 (92%)	7 (8%)	14	48
51	BS	76/77 (99%)	75 (99%)	1 (1%)	76	89
52	BT	65/65 (100%)	63 (97%)	2 (3%)	47	77
53	BU	77/78 (99%)	75 (97%)	2 (3%)	54	80
54	BV	64/65 (98%)	56 (88%)	8 (12%)	6	30
55	BW	78/79 (99%)	74 (95%)	4 (5%)	29	66
56	BX	65/66 (98%)	63 (97%)	2 (3%)	47	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	BY	60/61 (98%)	55 (92%)	5 (8%)	14 49
All	All	5417/5447 (99%)	5119 (94%)	298 (6%)	31 63

5 of 298 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	AU	24	MET
30	Ad	34	GLU
52	BT	5	ARG
22	AV	85	ARG
26	AZ	30	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	119/120 (99%)	15 (12%)	3 (2%)
2	AB	2898/2904 (99%)	396 (13%)	130 (4%)
34	BA	1538/1542 (99%)	192 (12%)	77 (5%)
35	BB	73/76 (96%)	12 (16%)	2 (2%)
35	BE	73/76 (96%)	12 (16%)	6 (8%)
37	BD	24/24 (100%)	4 (16%)	5 (20%)
All	All	4725/4742 (99%)	631 (13%)	223 (4%)

5 of 631 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	13	G
1	AA	15	A
1	AA	16	G
1	AA	36	C

5 of 223 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AB	2130	U
2	AB	2732	G

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Mol	Chain	Res	Type
34	BA	1441	A
2	AB	2339	C
2	AB	2581	G

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

55 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	6MZ	AB	1618	2	17,25,26	0.92	1 (5%)	15,36,39	1.44	2 (13%)
2	2MG	AB	1835	2	18,26,27	1.32	1 (5%)	21,38,41	2.47	5 (23%)
2	PSU	AB	1911	2	15,21,22	1.32	1 (6%)	16,30,33	3.53	2 (12%)
2	3TD	AB	1915	2	15,22,23	0.97	0	17,32,35	1.42	3 (17%)
2	PSU	AB	1917	2	15,21,22	1.35	1 (6%)	16,30,33	3.57	3 (18%)
2	5MU	AB	1939	2	13,22,23	1.22	1 (7%)	16,32,35	4.86	4 (25%)
2	5MC	AB	1962	2	14,22,23	0.97	1 (7%)	17,32,35	1.17	3 (17%)
2	6MZ	AB	2030	2	17,25,26	0.91	1 (5%)	15,36,39	1.65	5 (33%)
2	7MG	AB	2069	2	20,26,27	2.22	3 (15%)	23,39,42	2.23	2 (8%)
2	OMG	AB	2251	2	18,26,27	1.25	2 (11%)	21,38,41	2.69	4 (19%)
2	2MG	AB	2445	2	18,26,27	1.29	2 (11%)	21,38,41	2.48	6 (28%)
2	H2U	AB	2449	2	17,21,22	0.84	1 (5%)	23,30,33	0.93	1 (4%)
2	PSU	AB	2457	2	15,21,22	1.32	1 (6%)	16,30,33	3.69	6 (37%)
2	OMC	AB	2498	2	15,22,23	0.83	0	20,31,34	1.06	2 (10%)
2	2MA	AB	2503	2	17,25,26	1.02	2 (11%)	18,37,40	1.80	1 (5%)
2	PSU	AB	2504	2	15,21,22	1.44	3 (20%)	16,30,33	3.57	5 (31%)
2	OMU	AB	2552	2	14,22,23	1.23	1 (7%)	19,31,34	2.84	4 (21%)
2	CH	AB	2575	2	14,21,22	0.97	1 (7%)	18,30,33	1.12	2 (11%)
2	PSU	AB	2580	2	15,21,22	1.34	1 (6%)	16,30,33	3.50	3 (18%)
2	PSU	AB	2605	2	15,21,22	1.29	1 (6%)	16,30,33	3.66	4 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1MG	AB	745	2	17,26,27	0.97	1 (5%)	19,39,42	1.85	4 (21%)
2	PSU	AB	746	2	15,21,22	1.36	2 (13%)	16,30,33	3.63	5 (31%)
2	5MU	AB	747	2	13,22,23	1.20	1 (7%)	16,32,35	4.79	5 (31%)
2	PSU	AB	955	2	15,21,22	1.25	1 (6%)	16,30,33	3.63	4 (25%)
34	2MG	BA	1207	34	18,26,27	1.29	2 (11%)	21,38,41	2.59	3 (14%)
34	4OC	BA	1402	34	15,23,24	1.01	1 (6%)	21,32,35	1.60	3 (14%)
34	5MC	BA	1407	34	14,22,23	0.96	1 (7%)	17,32,35	1.00	1 (5%)
34	UR3	BA	1498	34	13,22,23	0.93	0	18,32,35	1.21	2 (11%)
34	2MG	BA	1516	34	18,26,27	1.22	2 (11%)	21,38,41	2.77	5 (23%)
34	MA6	BA	1518	34	18,26,27	0.94	1 (5%)	15,38,41	1.32	1 (6%)
34	MA6	BA	1519	34	18,26,27	0.87	1 (5%)	15,38,41	1.92	5 (33%)
34	PSU	BA	516	34	15,21,22	1.28	1 (6%)	16,30,33	3.49	5 (31%)
34	7MG	BA	527	34	20,26,27	2.22	3 (15%)	23,39,42	2.42	3 (13%)
34	2MG	BA	966	34	18,26,27	1.26	2 (11%)	21,38,41	3.00	9 (42%)
34	5MC	BA	967	34	14,22,23	0.94	1 (7%)	17,32,35	0.79	0
35	H2U	BB	16	35	17,21,22	0.78	0	23,30,33	1.21	2 (8%)
35	H2U	BB	20	35	17,21,22	0.79	0	23,30,33	1.12	1 (4%)
35	PSU	BB	32	35	15,21,22	1.30	1 (6%)	16,30,33	3.53	4 (25%)
35	MIA	BB	37	35	22,31,32	1.08	4 (18%)	26,44,47	1.80	5 (19%)
35	PSU	BB	39	35	15,21,22	1.23	1 (6%)	16,30,33	3.64	5 (31%)
35	7MG	BB	46	35	20,26,27	2.23	3 (15%)	23,39,42	2.51	3 (13%)
35	3AU	BB	47	-	16,28,29	0.87	0	16,40,43	1.00	1 (6%)
35	5MU	BB	54	35	13,22,23	1.20	1 (7%)	16,32,35	4.68	3 (18%)
35	PSU	BB	55	35	15,21,22	1.28	2 (13%)	16,30,33	3.51	4 (25%)
35	4SU	BB	8	35	12,21,22	1.01	1 (8%)	15,30,33	1.71	1 (6%)
35	H2U	BE	16	35	17,21,22	0.79	0	23,30,33	1.03	2 (8%)
35	H2U	BE	20	35	17,21,22	0.77	0	23,30,33	1.36	4 (17%)
35	PSU	BE	32	35	15,21,22	1.29	1 (6%)	16,30,33	3.49	3 (18%)
35	MIA	BE	37	35	22,31,32	1.08	4 (18%)	26,44,47	1.68	6 (23%)
35	PSU	BE	39	35	15,21,22	1.30	1 (6%)	16,30,33	3.54	3 (18%)
35	7MG	BE	46	35	20,26,27	2.24	3 (15%)	23,39,42	2.30	2 (8%)
35	3AU	BE	47	-	16,28,29	0.90	0	16,40,43	2.06	4 (25%)
35	5MU	BE	54	35	13,22,23	1.24	1 (7%)	16,32,35	4.82	3 (18%)
35	PSU	BE	55	35	15,21,22	1.35	1 (6%)	16,30,33	3.44	3 (18%)
35	4SU	BE	8	35	12,21,22	0.94	0	15,30,33	2.20	5 (33%)

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
2	6MZ	AB	1618	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	1835	2	-	0/5/27/28	0/3/3/3
2	PSU	AB	1911	2	-	0/7/25/26	0/2/2/2
2	3TD	AB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	1917	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	1939	2	-	0/3/25/26	0/2/2/2
2	5MC	AB	1962	2	-	0/3/25/26	0/2/2/2
2	6MZ	AB	2030	2	-	0/5/27/28	0/3/3/3
2	7MG	AB	2069	2	-	0/7/37/38	0/3/3/3
2	OMG	AB	2251	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	2445	2	-	0/5/27/28	0/3/3/3
2	H2U	AB	2449	2	-	0/7/38/39	0/2/2/2
2	PSU	AB	2457	2	-	0/7/25/26	0/2/2/2
2	OMC	AB	2498	2	-	0/5/27/28	0/2/2/2
2	2MA	AB	2503	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2504	2	-	0/7/25/26	0/2/2/2
2	OMU	AB	2552	2	-	0/5/27/28	0/2/2/2
2	CH	AB	2575	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	2580	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	2605	2	-	0/7/25/26	0/2/2/2
2	1MG	AB	745	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	746	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	747	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	955	2	-	0/7/25/26	0/2/2/2
34	2MG	BA	1207	34	-	0/5/27/28	0/3/3/3
34	4OC	BA	1402	34	-	0/7/29/30	0/2/2/2
34	5MC	BA	1407	34	-	0/3/25/26	0/2/2/2
34	UR3	BA	1498	34	-	0/3/25/26	0/2/2/2
34	2MG	BA	1516	34	-	0/5/27/28	0/3/3/3
34	MA6	BA	1518	34	-	0/7/29/30	0/3/3/3
34	MA6	BA	1519	34	-	0/7/29/30	0/3/3/3
34	PSU	BA	516	34	-	0/7/25/26	0/2/2/2
34	7MG	BA	527	34	-	0/7/37/38	0/3/3/3
34	2MG	BA	966	34	-	0/5/27/28	0/3/3/3
34	5MC	BA	967	34	-	0/3/25/26	0/2/2/2
35	H2U	BB	16	35	-	0/7/38/39	0/2/2/2
35	H2U	BB	20	35	-	0/7/38/39	0/2/2/2
35	PSU	BB	32	35	-	0/7/25/26	0/2/2/2
35	MIA	BB	37	35	-	0/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	PSU	BB	39	35	-	0/7/25/26	0/2/2/2
35	7MG	BB	46	35	-	0/7/37/38	0/3/3/3
35	3AU	BB	47	-	-	0/8/34/35	0/2/2/2
35	5MU	BB	54	35	-	0/3/25/26	0/2/2/2
35	PSU	BB	55	35	-	0/7/25/26	0/2/2/2
35	4SU	BB	8	35	-	0/3/25/26	0/2/2/2
35	H2U	BE	16	35	-	0/7/38/39	0/2/2/2
35	H2U	BE	20	35	-	0/7/38/39	0/2/2/2
35	PSU	BE	32	35	-	0/7/25/26	0/2/2/2
35	MIA	BE	37	35	-	0/11/33/34	0/3/3/3
35	PSU	BE	39	35	-	0/7/25/26	0/2/2/2
35	7MG	BE	46	35	-	0/7/37/38	0/3/3/3
35	3AU	BE	47	-	-	0/8/34/35	0/2/2/2
35	5MU	BE	54	35	-	0/3/25/26	0/2/2/2
35	PSU	BE	55	35	-	0/7/25/26	0/2/2/2
35	4SU	BE	8	35	-	0/3/25/26	0/2/2/2

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	BB	46	7MG	C8-N9	-7.95	1.33	1.45
2	AB	2069	7MG	C8-N9	-7.91	1.34	1.45
35	BE	46	7MG	C8-N9	-7.89	1.34	1.45
34	BA	527	7MG	C8-N9	-7.84	1.34	1.45
2	AB	2069	7MG	C8-N7	-2.79	1.30	1.43

The worst 5 of 186 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	BE	54	5MU	C5-C4-N3	-13.38	114.12	125.35
2	AB	1939	5MU	C5-C4-N3	-13.30	114.19	125.35
2	AB	747	5MU	C5-C4-N3	-13.28	114.20	125.35
35	BB	54	5MU	C5-C4-N3	-13.25	114.23	125.35
34	BA	1516	2MG	C5-C6-N1	-8.68	112.17	123.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.