



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:00 PM BST

PDB ID : 4V6O
EMDB ID: : EMD-5359
Title : Structural characterization of mRNA-tRNA translocation intermediates (class 4a of the six classes)
Authors : Agirrezabala, X.; Liao, H.; Schreiner, E.; Fu, J.; Ortiz-Meoz, R.F.; Schulten, K.; Green, R.; Frank, J.
Deposited on : 2011-12-07
Resolution : 14.70 Å(reported)
Based on PDB ID : 2I2U

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>

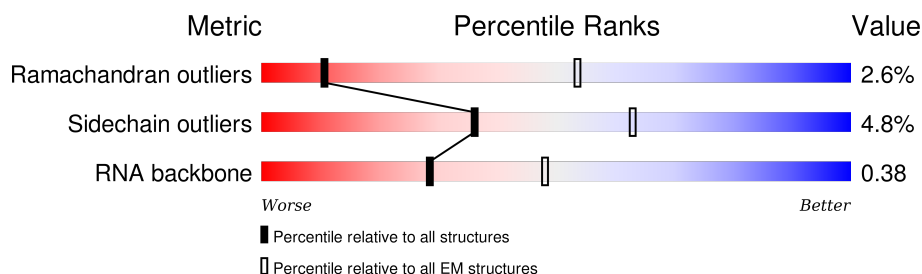
MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

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 14.70 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	1542	
2	AB	76	
3	AC	47	
4	AD	77	
5	AE	240	
6	AF	232	
7	AG	205	
8	AH	166	
9	AI	135	














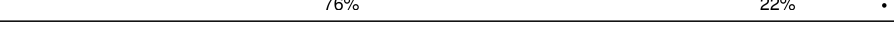







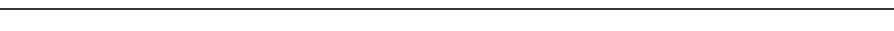


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Mol	Chain	Length	Quality of chain
10	AJ	178	
11	AK	129	
12	AL	129	
13	AM	103	
14	AN	128	
15	AO	123	
16	AP	117	
17	AQ	100	
18	AR	88	
19	AS	82	
20	AT	83	
21	AU	74	
22	AV	91	
23	AW	86	
24	AX	70	
25	BA	120	
26	BB	2904	
27	BC	234	
28	BD	272	
29	BE	209	
30	BF	201	
31	BG	178	
32	BH	176	
33	BI	149	
34	BJ	164	

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Mol	Chain	Length	Quality of chain
35	BK	141	 89% 11%
36	BL	142	 76% 21% .
37	BM	123	 74% 24% .
38	BN	144	 77% 18% 5%
39	BO	136	 78% 19% .
40	BP	127	 76% 20% .
41	BQ	117	 82% 14% .
42	BR	114	 66% 32% .
43	BS	117	 74% 23% .
44	BT	103	 80% 17% .
45	BU	110	 79% 17% .
46	BV	100	 79% 21%
47	BW	103	 79% 19% .
48	BX	94	 76% 22% .
49	BY	84	 77% 19% ..
50	BZ	77	 70% 23% 5% .
51	B0	63	 79% 19% .
52	B1	58	 78% 17% 5%
53	B2	70	 74% 21% .
54	B3	56	 73% 25% .
55	B4	54	 81% 17% .
56	B5	46	 57% 41% .
57	B6	64	 81% 17% .
58	B7	38	 68% 32%

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 152351 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 16S ribosomal RNA.

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

- Molecule 2 is a RNA chain called A site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	AB	76	Total	C	N	O	P	S	0	0
			1627	731	287	532	75	2		

- Molecule 3 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	47	Total	C	N	O	P	0	0
			993	445	167	335	46		

- Molecule 4 is a RNA chain called P site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	AD	77	Total	C	N	O	P	S	0	0
			1641	734	297	533	76	1		

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

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

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.

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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein S21.

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

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

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

- Molecule 27 is a protein called 50S ribosomal protein L1.

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

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BJ	164	Total	C	N	O	S	0	0
			1233	776	220	231	6		

- Molecule 35 is a protein called 50S ribosomal protein L11.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

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

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	117	Total	C	N	O	S	0	0
			947	604	192	151			

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

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

- Molecule 48 is a protein called 50S ribosomal protein L25.

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

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B0	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B2	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
55	B4	54	Total	C	N	O	0	0
			441	284	81	76		

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B5	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

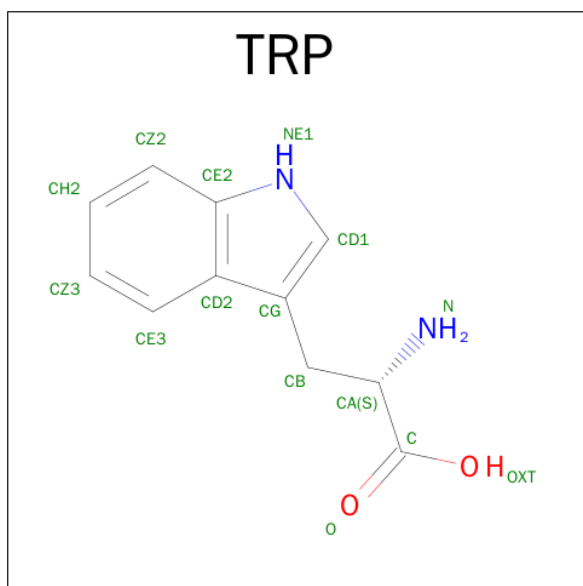
- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 58 is a protein called 50S ribosomal protein L36.

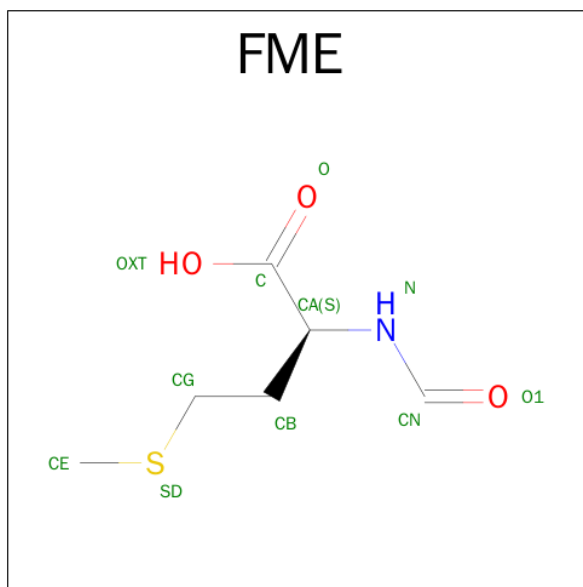
Mol	Chain	Residues	Atoms					AltConf	Trace
58	B7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 59 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
59	AB	1	Total	C	N	O	0
			14	11	2	1	

- Molecule 60 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).

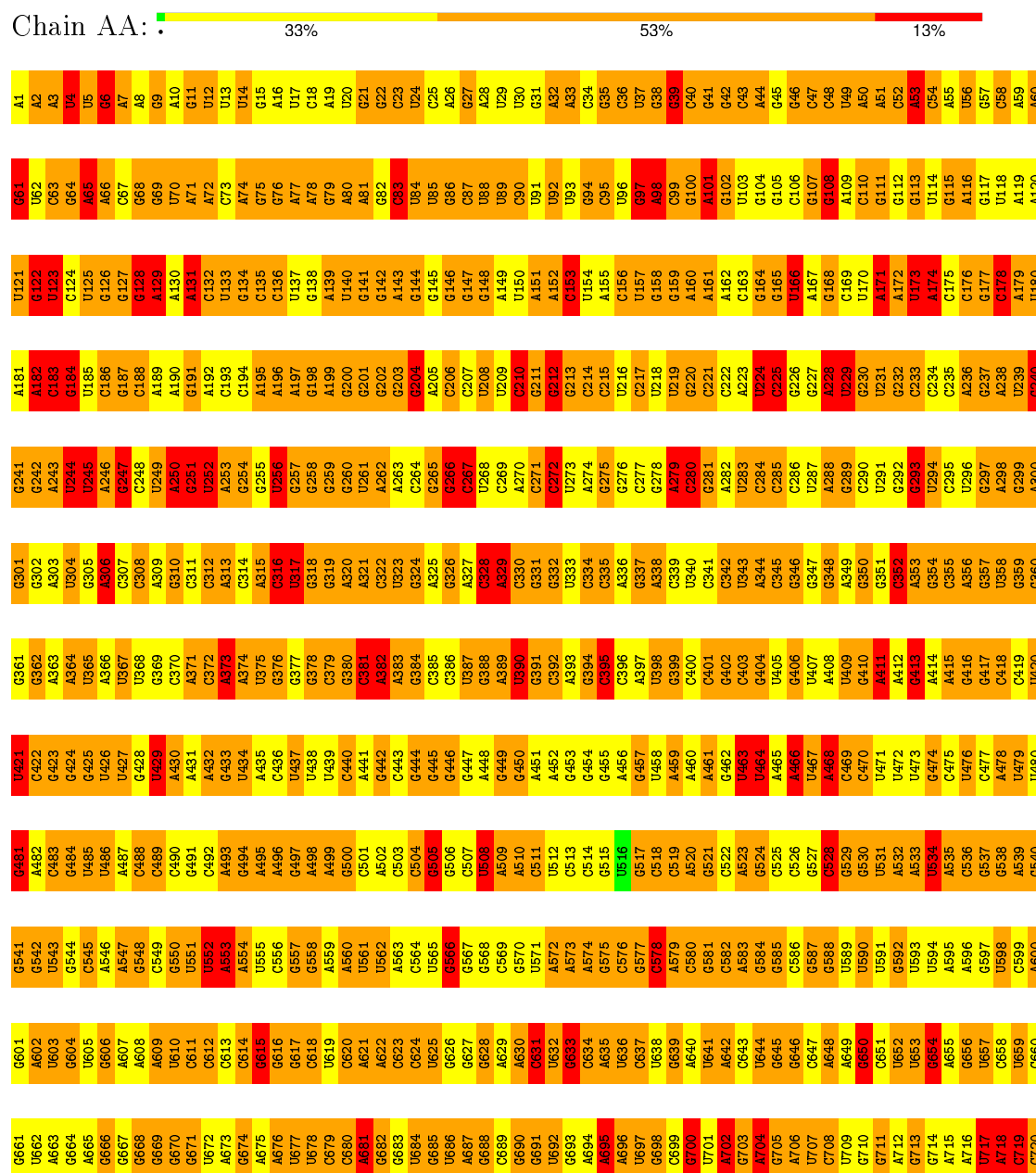


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
60	BB	1	10	6	1	2	1	0

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: 16S ribosomal RNA

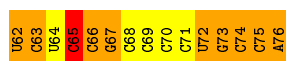


A1502	A1503	A1504	A1505	A1506	A1507	A1508	A1509	A1510	A1511	A1512	A1513	A1514	A1515	A1516	A1517	A1518	A1519	A1520	A1521	A1522	A1523	A1524	A1525	A1526	A1527	A1528	A1529	A1530	A1531	A1532	A1533	A1534	A1535	A1536	A1537	A1538	A1539	A1540	A1541	A1542																				
G1442	G1443	G1444	G1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	U1490	G1491	A1492	A1493	A1494	U1495	G1496	G1497	A1498	A1499	A1500	A1501	
C1382	C1383	C1384	G1385	G1386	G1387	C1388	C1389	U1390	U1391	G1392	U1393	G1394	C1395	A1396	G1397	A1398	C1399	A1340	G1401	C1402	G1403	G1404	A1405	G1406	G1407	A1408	A1409	A1410	C1411	C1412	G1413	G1414	G1415	G1416	G1417	A1418	G1419	U1420	G1421	G1422	A1423	A1424	U1425	G1426	G1427	A1428	A1429	A1430	A1431	A1432	A1433	A1434	U1435	G1436	A1437	G1438	A1439	A1500	A1501	
C1322	C1323	A1324	C1325	U1326	C1327	C1328	A1329	U1330	G1331	A1332	A1333	G1334	C1335	A1336	G1337	G1338	A1339	A1340	U1341	C1342	G1343	U1344	A1345	A1346	C1347	U1348	A1349	A1350	U1351	C1352	G1353	U1354	G1355	G1356	A1357	U1358	C1359	A1360	U1361	A1362	A1363	U1364	U1365	C1366	G1367	U1368	A1369	C1370	G1371	U1372	A1373	A1374	A1375	U1376	A1377	G1378	A1379	U1380	U1381	
C1262	C1263	U1264	C1265	G1266	G1267	C1268	C1269	C1270	A1271	C1272	C1273	A1274	C1275	A1276	C1277	G1278	G1279	C1280	C1281	C1282	U1283	U1284	A1285	C1286	C1287	A1288	A1289	G1290	U1291	C1292	C1293	G1294	U1295	C1296	C1297	U1298	A1299	G1300	U1301	A1302	C1303	G1304	G1305	A1306	U1307	U1308	G1309	G1310	G1311	C1312	U1313	A1314	U1315	U1316	C1317	A1318	A1319	C1320	U1321	
U1202	C1203	G1143	U1205	G1206	G1207	C1208	C1209	C1210	U1211	U1212	A1213	A1214	G1215	A1216	C1217	C1218	A1219	G1220	G1221	C1222	C1223	U1224	A1225	C1226	A1227	C1228	A1229	C1230	G1231	U1232	C1233	G1234	U1235	A1236	C1237	A1238	A1239	U1240	U1241	G1242	C1243	U1244	C1245	A1246	U1247	A1248	C1249	A1250	U1251	A1252	G1253	U1254	G1255	A1256	U1257	C1258	C1259	U1260	A1261	
G1142	U1083	G1143	U1085	U1086	G1087	C1088	U1089	U1090	U1091	A1092	A1093	G1094	U1095	G1096	C1097	C1098	U1099	C1100	A1101	C1102	A1103	G1104	U1105	G1106	C1107	U1108	C1109	A1110	A1111	C1112	G1113	U1114	U1115	U1116	A1117	U1118	C1119	A1120	C1121	U1122	U1123	G1124	U1125	G1126	U1127	C1128	C1129	A1130	C1131	C1132	G1133	U1134	U1135	C1136	C1137	U1138	U1139	C1140	A1141	
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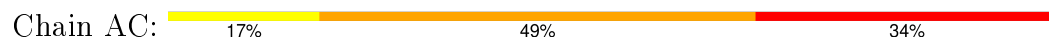
• Molecule 2: A site tRNA

Chain AB:  7% 33% 42% 18%

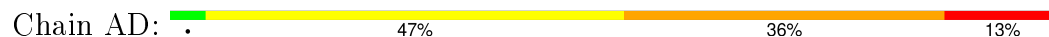
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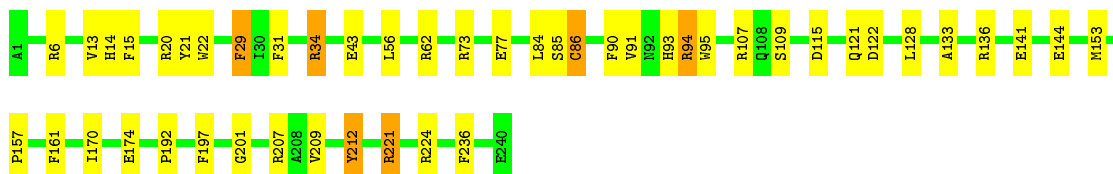
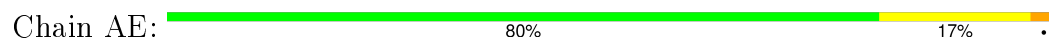
- Molecule 3: mRNA



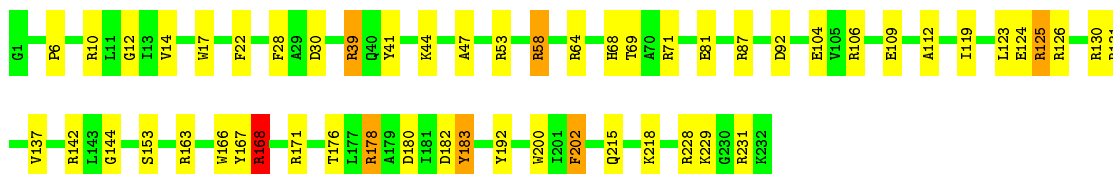
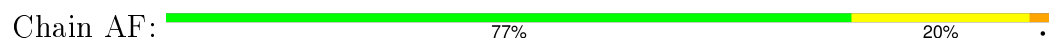
- Molecule 4: P site tRNA



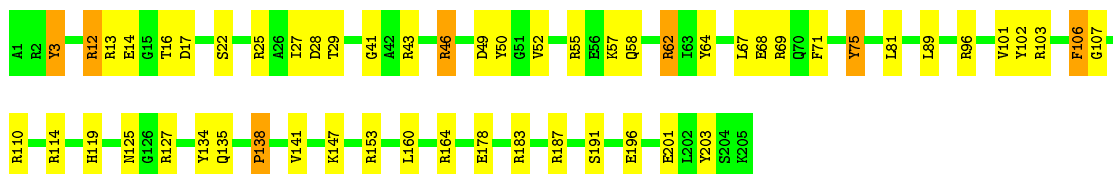
- Molecule 5: 30S ribosomal protein S2




- Molecule 6: 30S ribosomal protein S3

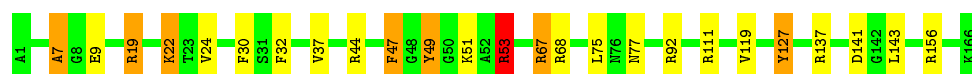


- Molecule 7: 30S ribosomal protein S4



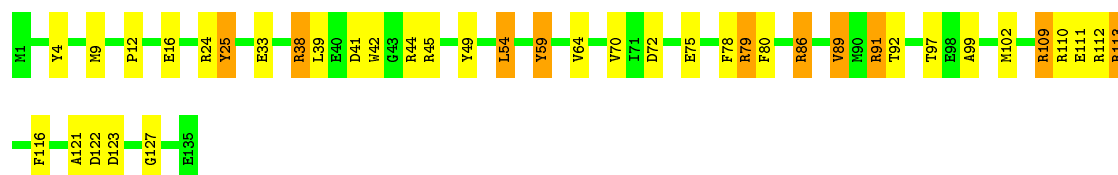
- Molecule 8: 30S ribosomal protein S5

Chain AH:  85% 10%



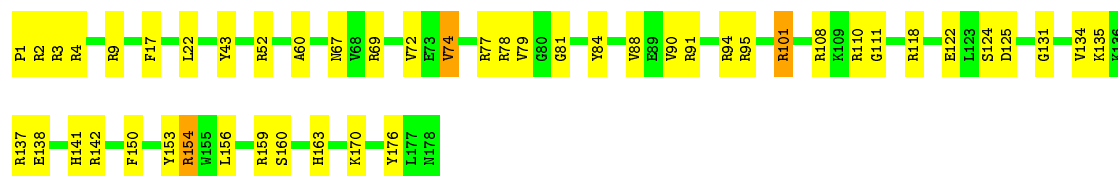
- Molecule 9: 30S ribosomal protein S6

Chain AI:  70% 22% 7%




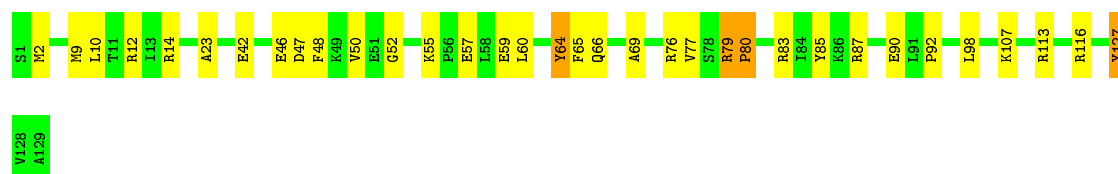
- Molecule 10: 30S ribosomal protein S7

Chain AJ:  73% 25%




- Molecule 11: 30S ribosomal protein S8

Chain AK:  74% 23%



- Molecule 12: 30S ribosomal protein S9

Chain AL:  75% 22%

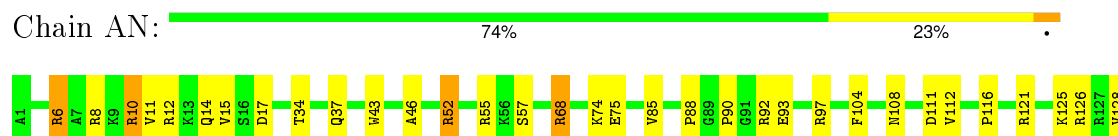


- Molecule 13: 30S ribosomal protein S10

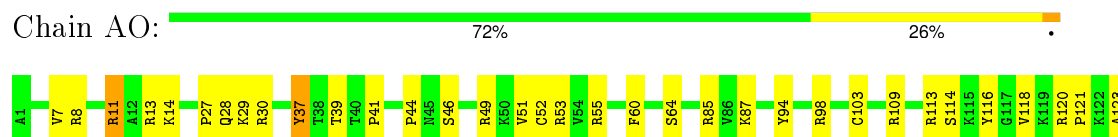
Chain AM:  70% 24% 6%



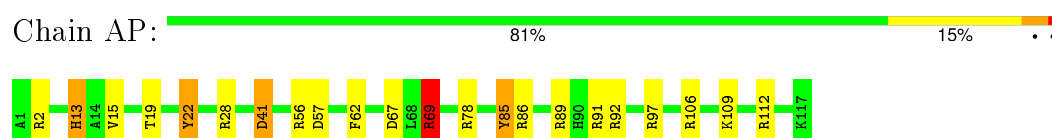
- Molecule 14: 30S ribosomal protein S11



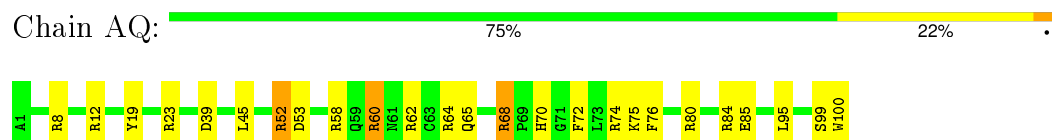
- Molecule 15: 30S ribosomal protein S12



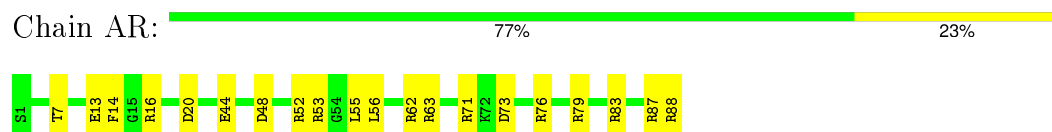
- Molecule 16: 30S ribosomal protein S13



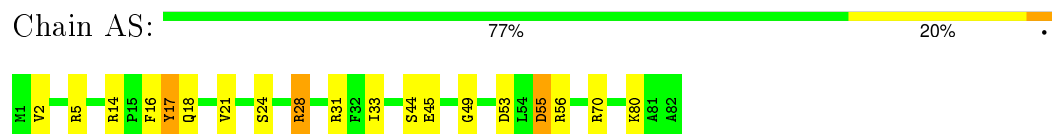
- Molecule 17: 30S ribosomal protein S14



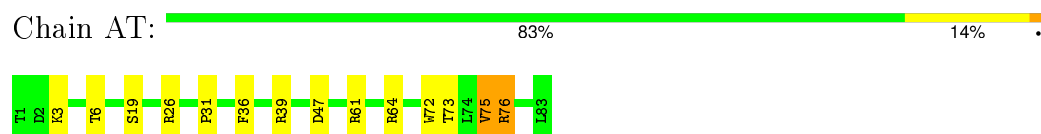
- Molecule 18: 30S ribosomal protein S15



- Molecule 19: 30S ribosomal protein S16



- Molecule 20: 30S ribosomal protein S17

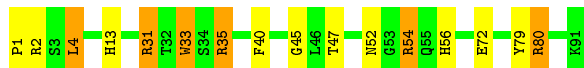
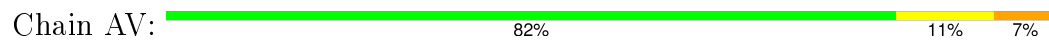


- Molecule 21: 30S ribosomal protein S18





- Molecule 22: 30S ribosomal protein S19



- Molecule 23: 30S ribosomal protein S20



- Molecule 24: 30S ribosomal protein S21



- Molecule 25: 5S ribosomal RNA



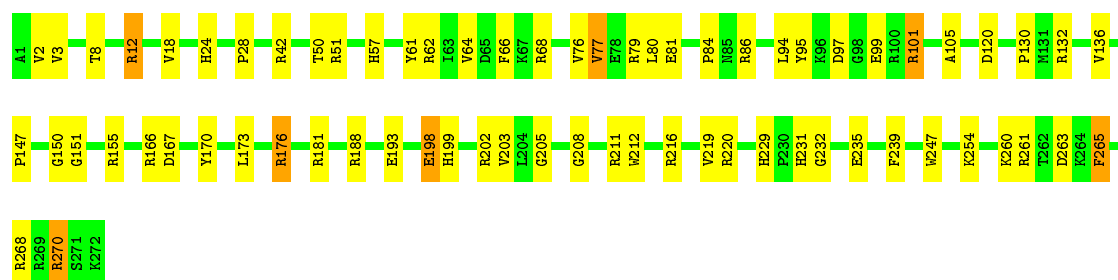
- Molecule 26: 23S ribosomal RNA



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A1264	A1204	A1144	A1084	G1024	C904	A844	G784	G723	G663	A603	G544	A483	A423	A363	G303
A1265	A1205	C1145	A1085	G1025	A905	A845	G785	U724	G664	G604	C545	A484	G424	C364	U304
U1266	G1206	C1146	A1086	G1026	U906	U846	G786	G725	U665	G605	U546	C485	G425	U365	C305
U1267	G1207	A1147	G1087	A1027	G907	U847	G787	G726	A666	U606	U547	C486	G426	C366	U306
A1268	U1208	U1148	A1088	A1028	C908	C848	A788	A727	U667	U607	A547	C487	U427	G367	G307
A1269	U1209	G1149	A1089	A1029	A909	A849	A789	G728	A668	A608	G548	A488	A428	A368	G308
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A1272	G1212	C1152	C1092	A1032	A912	U852	A792	G731	G671	C611	G551	A491	U431	A371	A311
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C1278	G1218	C1158	A1098	G1038	A918	G858	G798	G737	A677	G617	U558	A497	U437	G377	G317
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C1221	C1221	C1161	U1101	G1041	C921	A861	G801	C740	C680	G620	C560	G500	C440	G380	A320
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C1229	C1229	A1169	C1109	C1049	U929	G869	G809	A749	U688	G628	U568	A508	U448	G388	U328
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G1232	G1232	C1172	G1112	C1052	U932	U872	C812	A752	C691	A631	U571	U511	U451	A391	C331
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A1237	A1237	G1177	C1117	A1057	G937	A877	C817	G757	G696	G636	U576	C516	C456	G396	C336
G1238	G1238	C1178	U1118	U1058	G938	A878	G818	G758	G697	A637	A577	C517	A457	U397	C337
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G1300	G1240	U1180	G1120	U1060	G940	G880	A820	G760	A699	U639	G579	U519	U459	U399	U339
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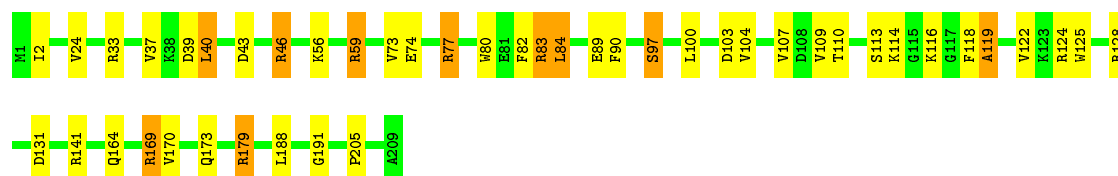
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U2229	A2169	U2109	G2049	G1989	G1929	C1869	A1809	A1749	U1689	U1629	A1569	A1509	G1449	G1389	U1329
G2230	A2170	G2110	C2050	C1990	G1930	C1870	A1810	G1750	A1690	A1630	A1570	G1510	G1450	U1390	C1330
U2231	A2171	U2111	A2051	U1991	U1931	A1871	G1811	U1751	G1691	A1631	A1571	G1511	C1451	U1391	G1331
C2232	U2172	G2112	A2052	G1992	A1932	A1872	U1812	C1752	U1692	A1632	A1572	C1512	G1452	A1392	G1332
A2233	C2173	G2113	G2053	U1993	G1933	C1873	G1813	G1753	U1693	G1633	G1573	A1513	A1453	A1393	G1333
C2234	C2174	A2114	A2054	C1994	C1934	C1874	G1814	A1754	G1694	A1634	G1574	G1514	C1454	U1394	G1334
G2235	C2175	G2115	C2055	U1995	G1935	G1875	A1815	A1755	G1695	A1635	C1575	A1515	G1455	A1395	C1335
U2236	A2176	G2116	G2056	C1996	A1936	A1876	C1816	G1756	G1696	U1636	U1576	G1516	G1456	A1396	C1336
G2237	C2177	A2117	C2057	C1997	A1937	A1877	G1817	A1757	G1697	A1637	C1577	U1517	U1457	U1397	G1337
G2238	C2178	U2118	A2058	A1998	A1938	C1878	U1818	U1758	A1698	C1638	A1578	G1518	U1458	C1398	G1338
G2239	C2179	G2119	A2059	C1999	U1939	C1879	A1819	A1759	G1699	C1639	A1579	G1519	G1459	C1399	G1339
U2240	U2180	G2120	A2060	C2000	U1940	U1880	U1820	C1760	A1700	A1640	U1580	U1520	U1460	U1400	U1340
A2241	U2181	G2121	G2061	C2001	C1941	C1881	A1821	C1761	A1701	A1641	G1581	G1521	C1461	G1401	G1341
G2242	U2182	U2122	A2062	G2002	C1942	U1882	G1822	A1762	G1702	G1642	G1582	A1522	C1462	U1402	A1342
U2243	A2183	G2123	C2063	A2003	U1943	U1883	G1823	C1763	G1703	A1643	U1583	U1523	C1463	A1403	G1343
U2244	A2184	G2124	C2064	G2004	U1944	C1884	G1824	C1764	C1704	A1644	U1584	G1524	G1464	A1404	U1344
U2245	U2185	G2125	A2065	A2005	G1945	A1885	U1825	U1765	A1705	G1645	C1585	A1525	G1465	U1405	G1345
G2246	G2186	A2126	C2066	C2006	U1946	U1886	G1826	G1766	C1706	C1646	A1586	C1526	U1466	U1406	G1346
A2247	U2187	G2127	G2067	U2007	C1947	C1887	U1827	G1767	G1707	U1647	G1587	G1527	U1467	G1407	A1347
G2248	U2188	G2128	U2068	C2008	G1948	G1888	G1828	C1768	C1708	U1648	G1588	A1528	U1468	G1408	C1348
U2249	C2189	C2129	C2069	A2009	G1949	A1889	A1829	U1769	U1709	G1649	U1589	G1529	A1469	U1409	C1349
G2250	G2190	U2130	A2070	G2010	G1950	A1890	C1830	G1770	G1710	A1650	A1590	G1530	A1470	G1410	C1350
G2251	A2191	U2131	A2071	U2011	U1951	G1891	G1831	C1771	A1711	G1651	A1591	C1531	G1471	U1411	C1351
G2252	U2192	U2132	C2072	G2012	A1952	C1892	C1832	U1772	U1712	A1652	C1592	A1532	C1472	U1412	U1352
G2253	G2193	G2133	C2073	A2013	A1953	C1893	C1833	A1773	A1713	G1653	A1593	C1533	G1473	A1413	A1353
C2254	U2194	A2134	C2074	A2014	G1954	C1894	U1834	C1774	U1714	A1654	U1594	U1534	U1474	C1414	A1354
G2255	C2195	A2135	U2075	U2015	U1955	G1895	G1835	G1775	G1715	A1655	C1595	A1535	G1475	U1415	G1355
G2256	G2196	G2136	U2076	A2016	G1956	G1896	C1836	G1776	U1716	C1656	A1596	C1536	U1476	G1416	G1356
U2257	U2197	U2137	A2077	U2017	C1957	G1897	C1837	U1777	A1717	U1657	A1597	G1537	A1477	C1417	C1357
C2258	A2198	G2138	C2078	G2018	C1958	U1898	C1838	U1778	G1718	C1658	A1598	G1538	G1478	G1418	G1358
U2259	A2199	U2139	U2079	A2019	G1959	A1899	G1839	U1779	G1719	C1659	U1599	U1539	G1479	A1419	A1359
C2260	C2200	G2140	A2080	A2020	A1960	A1900	G1840	U1780	U1720	G1660	C1600	G1540	U1480	A1420	G1360
G2261	G2201	G2141	U2081	C2021	C1961	A1901	U1841	U1781	G1721	G1661	G1601	C1541	U1481	G1421	G1361
U2262	U2202	A2142	A2082	U2022	C1962	G1902	G1842	U1782	A1722	U1662	U1602	U1542	G1482	G1422	C1362
C2263	U2203	C2143	G2083	C2023	U1963	G1903	C1843	A1783	G1723	C1663	A1603	G1543	G1483	G1423	C1363
G2264	G2204	G2144	C2084	G2024	G1964	G1904	A1844	A1784	U1724	A1664	C1604	A1544	U1484	G1424	G1364
U2265	A2205	C2145	U2085	C2025	C1965	G1905	G1845	A1785	U1725	A1665	C1605	A1545	U1485	G1425	A1365
A2266	C2206	G2146	U2086	U2026	A1966	G1906	G1846	A1786	C1726	G1666	C1606	G1546	U1486	G1426	A1366
A2267	C2207	A2147	G2087	G2027	C1967	C1907	A1847	A1787	C1727	G1667	C1607	C1547	U1487	A1427	A1367
A2268	C2208	G2148	A2088	U2028	G1968	C1908	A1848	C1788	C1728	A1668	A1608	A1548	U1488	C1428	G1368
G2269	G2209	U2149	C2089	G2029	A1969	G1909	G1849	U1789	U1729	A1669	A1609	A1549	C1489	G1429	G1369
A2270	U2210	C2150	A2090	U2030	A1970	G1910	G1850	C1790	U1730	C1670	A1610	C1550	A1490	G1430	C1370
G2271	A2211	U2151	C2091	U2031	U1971	U1911	U1851	A1791	G1731	U1671	C1611	A1551	G1491	A1431	G1371
U2272	A2212	G2152	U2092	G2032	G1972	A1912	U1852	G1792	C1732	A1672	C1612	A1552	G1492	G1432	U1372
A2273	C2213	C2153	G2093	A2033	G1973	C1913	A1853	C1793	G1733	G1673	G1613	C1493	A1433	A1373	A1373
A2274	C2214	A2154	A2094	U2034	C1974	C1914	A1854	U1794	G1734	G1674	A1614	U1554	A1494	A1434	G1374
C2275	C2215	U2155	A2095	G2035	G1975	G1915	U1855	C1795	A1735	C1675	C1615	G1555	A1495	G1435	U1375
G2276	G2216	G2156	C2096	C2036	U1976	A1916	U1856	U1796	U1736	A1676	A1616	C1556	A1496	G1436	C1376
G2277	G2217	G2157	A2097	U2037	A1977	U1917	G1857	G1797	G1737	A1677	C1617	C1557	U1497	C1437	G1377
A2278	G2218	A2158	U2098	G2038	A1978	A1918	A1858	U1798	G1738	A1678	C1618	C1558	C1498	U1438	A1378
G2279	U2219	G2159	U2099	U2039	A1979	A1919	U1859	G1799	A1739	A1679	G1619	U1559	C1499	A1439	U1379
G2280	G2220	C2160	G2040	G1980	C1980	C1920	G1860	C1740	G1740	A1680	G1620	U1560	G1500	U1440	G1380
A2281	G2221	C2161	A2101	U2041	A1981	G1921	G1861	A1801	C1741	G1681	U1621	C1561	G1501	G1441	G1381



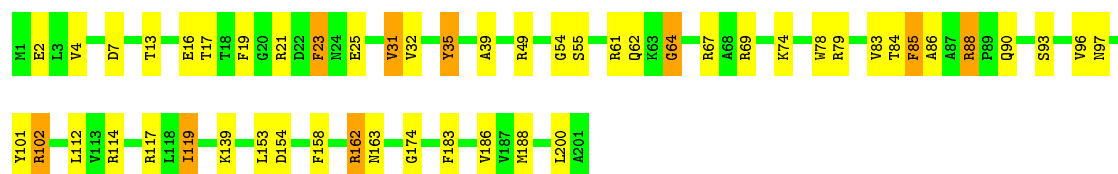
- Molecule 29: 50S ribosomal protein L3

Chain BE: 78% 17% 5%



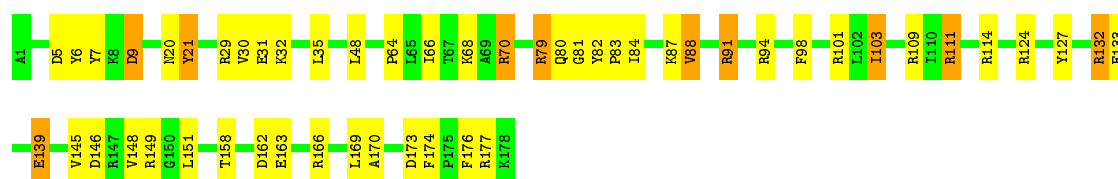
- Molecule 30: 50S ribosomal protein L4

Chain BF: 75% 21% 4%



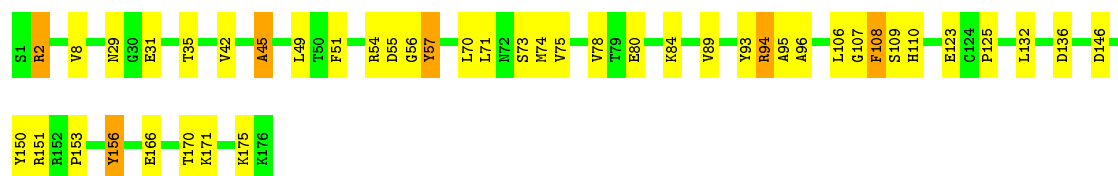
- Molecule 31: 50S ribosomal protein L5

Chain BG: 71% 24% 5%

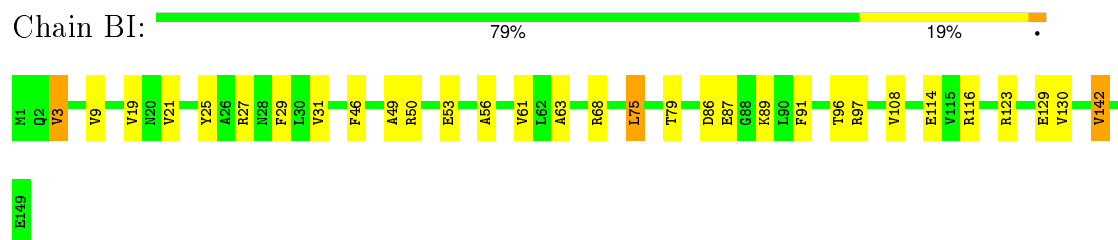


- Molecule 32: 50S ribosomal protein L6

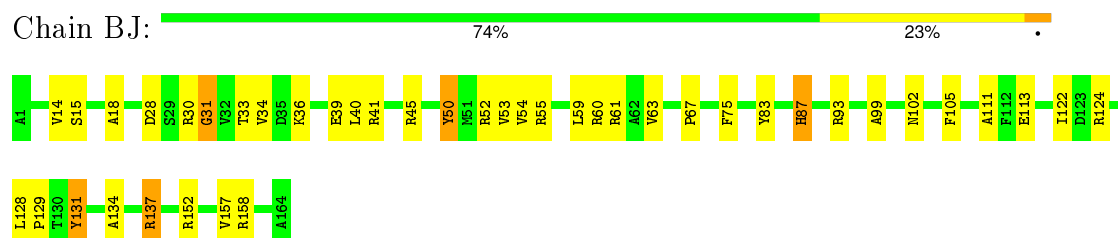
Chain BH: 75% 22% 3%



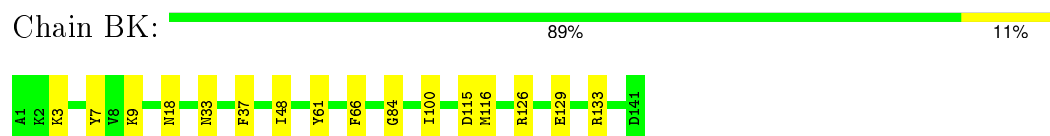
- Molecule 33: 50S ribosomal protein L9



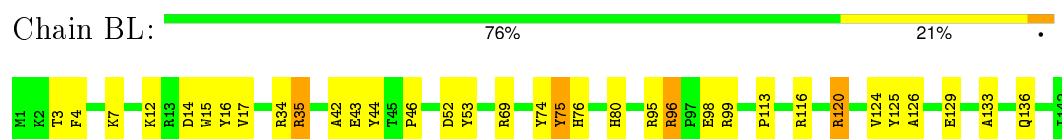
- Molecule 34: 50S ribosomal protein L10



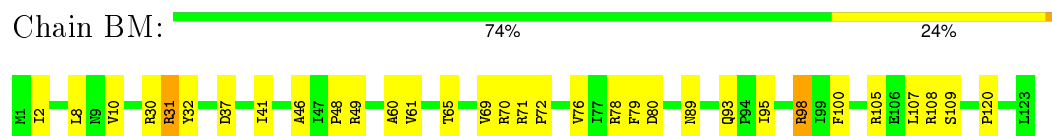
- Molecule 35: 50S ribosomal protein L11



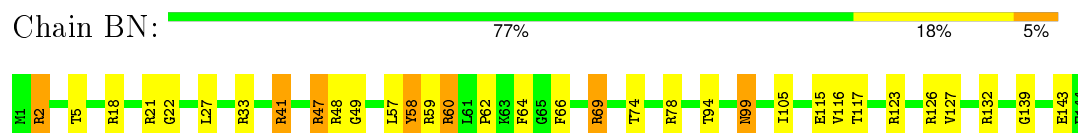
- Molecule 36: 50S ribosomal protein L13



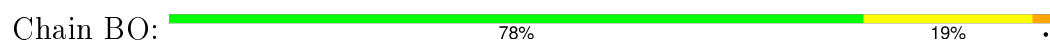
- Molecule 37: 50S ribosomal protein L14

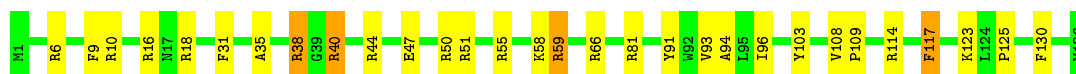


- Molecule 38: 50S ribosomal protein L15



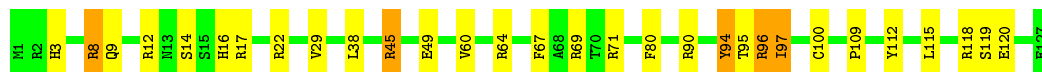
- Molecule 39: 50S ribosomal protein L16





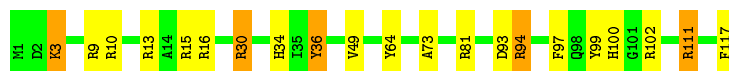
- Molecule 40: 50S ribosomal protein L17

Chain BP: 76% 20% •



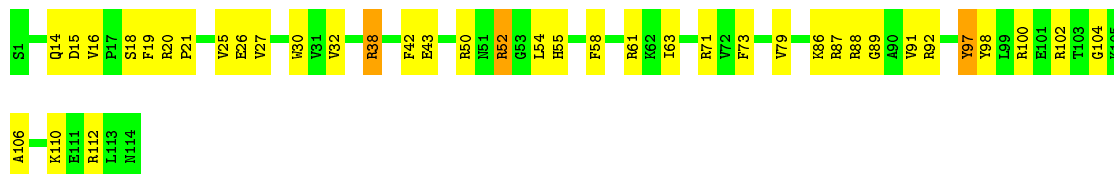
- Molecule 41: 50S ribosomal protein L18

Chain BQ: 82% 14% •



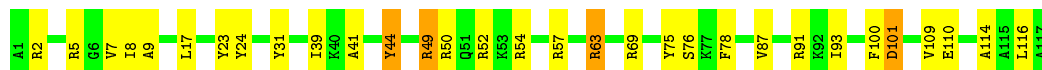
- Molecule 42: 50S ribosomal protein L19

Chain BR: 66% 32% •



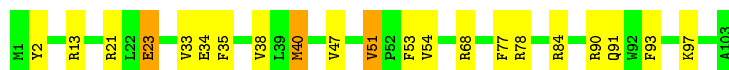
- Molecule 43: 50S ribosomal protein L20

Chain BS: 74% 23% •



- Molecule 44: 50S ribosomal protein L21

Chain BT: 80% 17% •



- Molecule 45: 50S ribosomal protein L22

Chain BU: 79% 17% •



- Molecule 46: 50S ribosomal protein L23

Chain BV: 79% 21% •



- Molecule 47: 50S ribosomal protein L24

Chain BW: 79% 19%



- Molecule 48: 50S ribosomal protein L25

Chain BX: 76% 22%



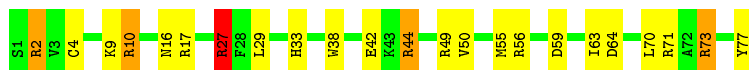
- Molecule 49: 50S ribosomal protein L27

Chain BY: 77% 19%



- Molecule 50: 50S ribosomal protein L28

Chain BZ: 70% 23% 5%



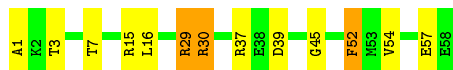
- Molecule 51: 50S ribosomal protein L29

Chain B0: 79% 19%



- Molecule 52: 50S ribosomal protein L30

Chain B1: 78% 17% 5%



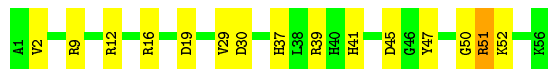
- Molecule 53: 50S ribosomal protein L31

Chain B2: 74% 21%




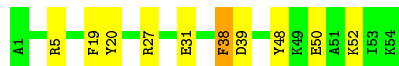
- Molecule 54: 50S ribosomal protein L32

Chain B3:  73% 25% •



- Molecule 55: 50S ribosomal protein L33

Chain B4:  81% 17% •




- Molecule 56: 50S ribosomal protein L34

Chain B5:  57% 41% •



- Molecule 57: 50S ribosomal protein L35

Chain B6:  81% 17% •



- Molecule 58: 50S ribosomal protein L36

Chain B7:  68% 32%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	21000	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	Volumes were CTF-corrected in defocus groups	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	25	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	59000	Depositor
Image detector	TVIPS TemCam-F415 (CCD)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: OMC, 3TD, CH, OMG, 5MC, MA6, MIA, H2U, 2MA, 6MZ, 2MG, OMU, UR3, 4OC, FME, 4SU, 7MG, 5MU, 1MG, 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	3.08	3882/36769 (10.6%)	3.52	8356/57354 (14.6%)
10	AJ	1.54	9/1422 (0.6%)	2.04	43/1908 (2.3%)
11	AK	1.56	5/989 (0.5%)	1.94	28/1326 (2.1%)
12	AL	1.54	2/1048 (0.2%)	2.06	39/1394 (2.8%)
13	AM	1.43	1/835 (0.1%)	2.03	27/1127 (2.4%)
14	AN	1.53	5/982 (0.5%)	1.98	26/1323 (2.0%)
15	AO	1.52	2/969 (0.2%)	2.34	41/1300 (3.2%)
16	AP	1.47	2/919 (0.2%)	2.23	25/1226 (2.0%)
17	AQ	1.48	1/817 (0.1%)	2.06	30/1088 (2.8%)
18	AR	1.52	0/724	2.00	27/966 (2.8%)
19	AS	1.54	4/659 (0.6%)	2.11	21/884 (2.4%)
2	AB	3.05	161/1600 (10.1%)	3.56	386/2492 (15.5%)
20	AT	1.56	2/681 (0.3%)	1.87	11/913 (1.2%)
21	AU	1.61	2/637 (0.3%)	2.24	27/851 (3.2%)
22	AV	1.45	4/744 (0.5%)	1.88	16/995 (1.6%)
23	AW	1.41	2/676 (0.3%)	1.66	7/895 (0.8%)
24	AX	1.56	2/598 (0.3%)	2.09	22/792 (2.8%)
25	BA	3.06	310/2869 (10.8%)	3.49	627/4474 (14.0%)
26	BB	3.07	7266/69257 (10.5%)	3.53	15668/108040 (14.5%)
27	BC	1.46	6/1748 (0.3%)	1.80	32/2355 (1.4%)
28	BD	1.54	14/2131 (0.7%)	1.94	53/2863 (1.9%)
29	BE	1.53	3/1586 (0.2%)	1.90	32/2134 (1.5%)
3	AC	3.23	133/1108 (12.0%)	3.55	250/1724 (14.5%)
30	BF	1.46	7/1571 (0.4%)	2.00	43/2113 (2.0%)
31	BG	1.53	5/1444 (0.3%)	1.95	36/1937 (1.9%)
32	BH	1.45	3/1343 (0.2%)	1.88	31/1816 (1.7%)
33	BI	1.49	0/1122	1.97	30/1515 (2.0%)
34	BJ	1.53	6/1247 (0.5%)	1.94	35/1679 (2.1%)
35	BK	1.44	1/1046 (0.1%)	1.79	14/1410 (1.0%)
36	BL	1.54	6/1152 (0.5%)	1.93	29/1551 (1.9%)
37	BM	1.48	4/956 (0.4%)	1.93	27/1279 (2.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	BN	1.58	5/1062 (0.5%)	2.01	28/1413 (2.0%)
39	BO	1.54	4/1093 (0.4%)	2.04	35/1460 (2.4%)
4	AD	3.02	174/1721 (10.1%)	3.61	441/2683 (16.4%)
40	BP	1.51	4/1021 (0.4%)	1.90	23/1364 (1.7%)
41	BQ	1.55	4/910 (0.4%)	2.05	22/1219 (1.8%)
42	BR	1.55	3/929 (0.3%)	2.15	32/1242 (2.6%)
43	BS	1.53	5/960 (0.5%)	2.10	34/1278 (2.7%)
44	BT	1.56	3/829 (0.4%)	1.93	17/1107 (1.5%)
45	BU	1.40	1/864 (0.1%)	1.89	21/1156 (1.8%)
46	BV	1.55	3/794 (0.4%)	2.06	19/1060 (1.8%)
47	BW	1.51	4/797 (0.5%)	1.86	18/1062 (1.7%)
48	BX	1.49	4/766 (0.5%)	1.82	17/1025 (1.7%)
49	BY	1.54	3/642 (0.5%)	1.90	17/848 (2.0%)
5	AE	1.50	9/1904 (0.5%)	1.89	37/2565 (1.4%)
50	BZ	1.49	0/635	2.10	24/848 (2.8%)
51	B0	1.49	1/510 (0.2%)	1.95	10/677 (1.5%)
52	B1	1.46	3/453 (0.7%)	1.77	12/605 (2.0%)
53	B2	1.56	4/559 (0.7%)	1.96	10/745 (1.3%)
54	B3	1.53	2/450 (0.4%)	2.12	19/599 (3.2%)
55	B4	1.49	1/448 (0.2%)	1.90	7/594 (1.2%)
56	B5	1.52	1/380 (0.3%)	2.36	24/498 (4.8%)
57	B6	1.52	3/513 (0.6%)	1.68	6/676 (0.9%)
58	B7	1.41	2/303 (0.7%)	2.14	10/397 (2.5%)
6	AF	1.54	11/1852 (0.6%)	2.09	63/2490 (2.5%)
7	AG	1.51	9/1665 (0.5%)	1.95	48/2227 (2.2%)
8	AH	1.48	1/1239 (0.1%)	1.94	30/1664 (1.8%)
9	AI	1.57	5/1121 (0.4%)	2.07	36/1509 (2.4%)
All	All	2.69	12119/164069 (7.4%)	3.18	27099/244735 (11.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	888
10	AJ	0	6
11	AK	0	3
12	AL	0	5
13	AM	0	4
14	AN	0	5
15	AO	0	2

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	AP	0	3
17	AQ	0	1
19	AS	0	3
2	AB	0	39
20	AT	0	1
21	AU	0	6
23	AW	0	2
24	AX	0	1
25	BA	0	71
26	BB	0	1680
27	BC	0	4
28	BD	0	11
29	BE	0	7
3	AC	0	23
30	BF	0	6
31	BG	0	8
32	BH	0	3
34	BJ	0	6
36	BL	0	6
37	BM	0	3
38	BN	0	3
39	BO	0	2
4	AD	0	34
40	BP	0	6
41	BQ	0	4
42	BR	0	4
43	BS	0	5
44	BT	0	1
45	BU	0	3
47	BW	0	2
48	BX	0	3
49	BY	0	5
5	AE	0	6
50	BZ	0	4
51	B0	0	2
52	B1	0	2
53	B2	0	1
55	B4	0	3
56	B5	0	1
57	B6	0	3
58	B7	0	1
6	AF	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	AG	0	11
8	AH	0	5
9	AI	0	11
All	All	0	2927

The worst 5 of 12119 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	1076	U	C2-N3	18.65	1.50	1.37
26	BB	757	G	P-O5'	16.91	1.76	1.59
25	BA	50	A	N7-C5	16.16	1.49	1.39
26	BB	2569	G	P-O5'	16.09	1.75	1.59
26	BB	1039	A	N7-C5	-15.99	1.29	1.39

The worst 5 of 27099 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	AO	55	ARG	NE-CZ-NH2	-27.98	106.31	120.30
26	BB	2063	C	N3-C4-C5	-21.69	113.22	121.90
26	BB	2163	A	O4'-C1'-N9	21.36	125.29	108.20
26	BB	337	C	O4'-C1'-N1	21.12	125.10	108.20
1	AA	190	A	C8-N9-C4	-20.93	97.43	105.80

There are no chirality outliers.

5 of 2927 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	3	A	Sidechain
1	AA	4	U	Sidechain
1	AA	6	G	Sidechain
1	AA	7	A	Sidechain
1	AA	9	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	33089	0	16610	0	0
2	AB	1627	0	843	0	0
3	AC	993	0	497	0	0
4	AD	1641	0	841	0	0
5	AE	1872	0	1885	0	0
6	AF	1822	0	1913	0	0
7	AG	1643	0	1710	0	0
8	AH	1225	0	1273	0	0
9	AI	1101	0	1050	0	0
10	AJ	1400	0	1449	0	0
11	AK	979	0	1034	0	0
12	AL	1036	0	1084	0	0
13	AM	825	0	865	0	0
14	AN	965	0	997	0	0
15	AO	955	0	1019	0	0
16	AP	910	0	981	0	0
17	AQ	805	0	847	0	0
18	AR	716	0	742	0	0
19	AS	649	0	666	0	0
20	AT	672	0	716	0	0
21	AU	626	0	651	0	0
22	AV	727	0	769	0	0
23	AW	670	0	722	0	0
24	AX	590	0	631	0	0
25	BA	2566	0	1302	0	0
26	BB	62351	0	31246	0	0
27	BC	1733	0	1824	0	0
28	BD	2092	0	2170	0	0
29	BE	1565	0	1616	0	0
30	BF	1552	0	1619	0	0
31	BG	1420	0	1460	0	0
32	BH	1323	0	1374	0	0
33	BI	1111	0	1148	0	0
34	BJ	1233	0	1283	0	0
35	BK	1032	0	1088	0	0
36	BL	1129	0	1162	0	0
37	BM	947	0	1023	0	0
38	BN	1053	0	1129	0	0
39	BO	1074	0	1157	0	0
40	BP	1008	0	1045	0	0
41	BQ	900	0	935	0	0
42	BR	917	0	965	0	0
43	BS	947	0	1022	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BT	816	0	839	0	0
45	BU	857	0	922	0	0
46	BV	787	0	846	0	0
47	BW	789	0	847	0	0
48	BX	753	0	780	0	0
49	BY	634	0	656	0	0
50	BZ	625	0	655	0	0
51	B0	509	0	543	0	0
52	B1	449	0	491	0	0
53	B2	549	0	552	0	0
54	B3	444	0	461	0	0
55	B4	441	0	485	0	0
56	B5	377	0	418	0	0
57	B6	504	0	574	0	0
58	B7	302	0	343	0	0
59	AB	14	0	9	0	0
60	BB	10	0	10	0	0
All	All	152351	0	103794	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 [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	238/240 (99%)	221 (93%)	13 (6%)	4 (2%)	11	55
6	AF	230/232 (99%)	200 (87%)	25 (11%)	5 (2%)	8	49
7	AG	203/205 (99%)	180 (89%)	18 (9%)	5 (2%)	7	46
8	AH	164/166 (99%)	141 (86%)	19 (12%)	4 (2%)	7	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	133/135 (98%)	118 (89%)	11 (8%)	4 (3%)	5	42
10	AJ	176/178 (99%)	164 (93%)	11 (6%)	1 (1%)	30	74
11	AK	127/129 (98%)	114 (90%)	11 (9%)	2 (2%)	12	56
12	AL	127/129 (98%)	109 (86%)	17 (13%)	1 (1%)	24	69
13	AM	101/103 (98%)	90 (89%)	7 (7%)	4 (4%)	4	35
14	AN	126/128 (98%)	105 (83%)	18 (14%)	3 (2%)	7	47
15	AO	121/123 (98%)	102 (84%)	16 (13%)	3 (2%)	7	46
16	AP	115/117 (98%)	104 (90%)	10 (9%)	1 (1%)	21	67
17	AQ	98/100 (98%)	84 (86%)	10 (10%)	4 (4%)	3	35
18	AR	86/88 (98%)	80 (93%)	6 (7%)	0	100	100
19	AS	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	7	46
20	AT	81/83 (98%)	71 (88%)	10 (12%)	0	100	100
21	AU	72/74 (97%)	63 (88%)	6 (8%)	3 (4%)	3	34
22	AV	89/91 (98%)	78 (88%)	10 (11%)	1 (1%)	17	63
23	AW	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	16	61
24	AX	68/70 (97%)	55 (81%)	9 (13%)	4 (6%)	2	27
27	BC	232/234 (99%)	208 (90%)	20 (9%)	4 (2%)	11	55
28	BD	270/272 (99%)	227 (84%)	37 (14%)	6 (2%)	8	49
29	BE	207/209 (99%)	171 (83%)	25 (12%)	11 (5%)	2	29
30	BF	199/201 (99%)	167 (84%)	26 (13%)	6 (3%)	5	42
31	BG	176/178 (99%)	144 (82%)	19 (11%)	13 (7%)	1	21
32	BH	174/176 (99%)	149 (86%)	16 (9%)	9 (5%)	2	30
33	BI	147/149 (99%)	132 (90%)	12 (8%)	3 (2%)	9	51
34	BJ	162/164 (99%)	140 (86%)	16 (10%)	6 (4%)	4	38
35	BK	139/141 (99%)	128 (92%)	9 (6%)	2 (1%)	14	58
36	BL	140/142 (99%)	118 (84%)	18 (13%)	4 (3%)	6	43
37	BM	121/123 (98%)	102 (84%)	14 (12%)	5 (4%)	3	35
38	BN	142/144 (99%)	113 (80%)	25 (18%)	4 (3%)	6	44
39	BO	134/136 (98%)	120 (90%)	13 (10%)	1 (1%)	26	71
40	BP	125/127 (98%)	116 (93%)	9 (7%)	0	100	100
41	BQ	115/117 (98%)	103 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BR	112/114 (98%)	90 (80%)	16 (14%)	6 (5%)	2	29
43	BS	115/117 (98%)	105 (91%)	7 (6%)	3 (3%)	7	45
44	BT	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	19	65
45	BU	108/110 (98%)	100 (93%)	4 (4%)	4 (4%)	4	38
46	BV	98/100 (98%)	85 (87%)	12 (12%)	1 (1%)	19	65
47	BW	101/103 (98%)	84 (83%)	15 (15%)	2 (2%)	9	51
48	BX	92/94 (98%)	79 (86%)	11 (12%)	2 (2%)	8	49
49	BY	82/84 (98%)	64 (78%)	15 (18%)	3 (4%)	4	38
50	BZ	75/77 (97%)	63 (84%)	9 (12%)	3 (4%)	4	35
51	B0	61/63 (97%)	53 (87%)	6 (10%)	2 (3%)	5	40
52	B1	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
53	B2	68/70 (97%)	51 (75%)	12 (18%)	5 (7%)	1	21
54	B3	54/56 (96%)	38 (70%)	14 (26%)	2 (4%)	4	38
55	B4	52/54 (96%)	47 (90%)	4 (8%)	1 (2%)	10	52
56	B5	44/46 (96%)	39 (89%)	4 (9%)	1 (2%)	8	48
57	B6	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
58	B7	36/38 (95%)	28 (78%)	6 (17%)	2 (6%)	2	28
All	All	6319/6423 (98%)	5497 (87%)	658 (10%)	164 (3%)	11	45

5 of 164 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	84	LEU
5	AE	93	HIS
7	AG	3	TYR
8	AH	77	ASN
9	AI	99	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	
5	AE	198/198 (100%)	193 (98%)	5 (2%)	55	81
6	AF	189/189 (100%)	181 (96%)	8 (4%)	36	70
7	AG	172/172 (100%)	164 (95%)	8 (5%)	32	68
8	AH	125/125 (100%)	121 (97%)	4 (3%)	46	76
9	AI	116/116 (100%)	110 (95%)	6 (5%)	29	65
10	AJ	146/146 (100%)	140 (96%)	6 (4%)	37	71
11	AK	104/104 (100%)	98 (94%)	6 (6%)	25	61
12	AL	106/106 (100%)	103 (97%)	3 (3%)	51	78
13	AM	90/90 (100%)	84 (93%)	6 (7%)	20	57
14	AN	98/98 (100%)	94 (96%)	4 (4%)	37	71
15	AO	103/103 (100%)	100 (97%)	3 (3%)	50	78
16	AP	95/95 (100%)	90 (95%)	5 (5%)	28	64
17	AQ	83/83 (100%)	80 (96%)	3 (4%)	42	74
18	AR	76/76 (100%)	75 (99%)	1 (1%)	76	89
19	AS	65/65 (100%)	63 (97%)	2 (3%)	47	77
20	AT	77/77 (100%)	73 (95%)	4 (5%)	29	65
21	AU	64/64 (100%)	59 (92%)	5 (8%)	16	51
22	AV	78/78 (100%)	71 (91%)	7 (9%)	12	44
23	AW	65/65 (100%)	64 (98%)	1 (2%)	72	88
24	AX	60/60 (100%)	58 (97%)	2 (3%)	45	76
27	BC	181/181 (100%)	172 (95%)	9 (5%)	30	66
28	BD	217/217 (100%)	204 (94%)	13 (6%)	24	60
29	BE	164/164 (100%)	150 (92%)	14 (8%)	13	48
30	BF	165/165 (100%)	154 (93%)	11 (7%)	20	57
31	BG	149/149 (100%)	138 (93%)	11 (7%)	17	54
32	BH	137/137 (100%)	129 (94%)	8 (6%)	25	61
33	BI	114/114 (100%)	108 (95%)	6 (5%)	28	64
34	BJ	122/122 (100%)	116 (95%)	6 (5%)	31	67
35	BK	109/109 (100%)	105 (96%)	4 (4%)	41	73
36	BL	116/116 (100%)	113 (97%)	3 (3%)	54	80
37	BM	104/104 (100%)	101 (97%)	3 (3%)	50	78
38	BN	103/103 (100%)	96 (93%)	7 (7%)	20	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	BO	109/109 (100%)	106 (97%)	3 (3%)	51	78
40	BP	103/103 (100%)	98 (95%)	5 (5%)	31	67
41	BQ	87/87 (100%)	84 (97%)	3 (3%)	44	75
42	BR	99/99 (100%)	93 (94%)	6 (6%)	23	60
43	BS	89/89 (100%)	87 (98%)	2 (2%)	60	83
44	BT	84/84 (100%)	79 (94%)	5 (6%)	24	60
45	BU	93/93 (100%)	90 (97%)	3 (3%)	46	76
46	BV	84/84 (100%)	77 (92%)	7 (8%)	14	49
47	BW	84/84 (100%)	80 (95%)	4 (5%)	31	67
48	BX	78/78 (100%)	73 (94%)	5 (6%)	22	58
49	BY	62/62 (100%)	60 (97%)	2 (3%)	46	76
50	BZ	67/67 (100%)	63 (94%)	4 (6%)	24	60
51	B0	55/55 (100%)	52 (94%)	3 (6%)	27	63
52	B1	48/48 (100%)	46 (96%)	2 (4%)	36	70
53	B2	62/62 (100%)	57 (92%)	5 (8%)	15	50
54	B3	47/47 (100%)	46 (98%)	1 (2%)	61	84
55	B4	48/48 (100%)	48 (100%)	0	100	100
56	B5	38/38 (100%)	37 (97%)	1 (3%)	54	80
57	B6	51/51 (100%)	48 (94%)	3 (6%)	24	61
58	B7	34/34 (100%)	33 (97%)	1 (3%)	50	78
All	All	5213/5213 (100%)	4964 (95%)	249 (5%)	36	67

5 of 249 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BE	24	VAL
31	BG	68	LYS
50	BZ	33	HIS
29	BE	46	ARG
30	BF	13	THR

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	1538/1542 (99%)	287 (18%)	93 (6%)
2	AB	74/76 (97%)	23 (31%)	7 (9%)
25	BA	119/120 (99%)	20 (16%)	13 (10%)
26	BB	2898/2904 (99%)	536 (18%)	180 (6%)
3	AC	47/47 (100%)	26 (55%)	14 (29%)
4	AD	76/77 (98%)	13 (17%)	4 (5%)
All	All	4752/4766 (99%)	905 (19%)	311 (6%)

5 of 905 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	6	G
1	AA	32	A
1	AA	36	C
1	AA	48	C

5 of 311 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BB	196	A
26	BB	611	C
26	BB	2515	C
26	BB	228	C
26	BB	404	A

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

49 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
1	2MG	AA	1207	1	18,26,27	1.82	4 (22%)	21,38,41	2.46	8 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	AA	1402	-	15,23,24	1.49	2 (13%)	21,32,35	2.60	3 (14%)
1	5MC	AA	1407	1	14,22,23	1.87	5 (35%)	17,32,35	1.80	4 (23%)
1	UR3	AA	1498	1	13,22,23	1.43	1 (7%)	18,32,35	1.34	1 (5%)
1	2MG	AA	1516	1	18,26,27	2.20	6 (33%)	21,38,41	3.33	12 (57%)
1	MA6	AA	1518	1	18,26,27	1.69	4 (22%)	15,38,41	2.16	3 (20%)
1	MA6	AA	1519	1	18,26,27	1.42	3 (16%)	15,38,41	2.42	7 (46%)
1	PSU	AA	516	1	15,21,22	1.28	3 (20%)	16,30,33	3.90	6 (37%)
1	7MG	AA	527	1	20,26,27	2.23	6 (30%)	23,39,42	2.12	9 (39%)
1	2MG	AA	966	1	18,26,27	1.56	3 (16%)	21,38,41	2.96	9 (42%)
1	5MC	AA	967	1	14,22,23	1.56	3 (21%)	17,32,35	1.45	1 (5%)
2	H2U	AB	16	2	17,21,22	1.52	2 (11%)	23,30,33	2.22	8 (34%)
2	H2U	AB	17	2	17,21,22	1.42	3 (17%)	23,30,33	1.19	3 (13%)
2	H2U	AB	20	2	17,21,22	1.41	2 (11%)	23,30,33	1.64	5 (21%)
2	OMC	AB	32	2	15,22,23	1.54	3 (20%)	20,31,34	2.05	7 (35%)
2	MIA	AB	37	2	22,31,32	1.72	4 (18%)	26,44,47	3.06	9 (34%)
2	7MG	AB	46	2	20,26,27	2.98	7 (35%)	23,39,42	2.66	9 (39%)
2	5MU	AB	54	2	13,22,23	1.94	4 (30%)	16,32,35	3.56	3 (18%)
2	PSU	AB	55	2	15,21,22	2.01	4 (26%)	16,30,33	3.93	5 (31%)
2	4SU	AB	8	2	12,21,22	1.28	1 (8%)	15,30,33	1.82	3 (20%)
4	H2U	AD	21	4	17,21,22	1.31	3 (17%)	23,30,33	2.08	6 (26%)
4	OMC	AD	33	4	15,22,23	1.57	3 (20%)	20,31,34	1.16	2 (10%)
4	5MU	AD	55	4	13,22,23	1.41	1 (7%)	16,32,35	5.11	5 (31%)
4	PSU	AD	56	4	15,21,22	2.17	5 (33%)	16,30,33	3.30	5 (31%)
4	4SU	AD	8	4	12,21,22	2.13	2 (16%)	15,30,33	2.66	4 (26%)
26	6MZ	BB	1618	26	17,25,26	1.78	4 (23%)	15,36,39	1.67	3 (20%)
26	2MG	BB	1835	26	18,26,27	1.78	5 (27%)	21,38,41	3.29	9 (42%)
26	PSU	BB	1911	26	15,21,22	1.99	2 (13%)	16,30,33	3.38	5 (31%)
26	3TD	BB	1915	26	15,22,23	2.08	5 (33%)	17,32,35	1.69	4 (23%)
26	PSU	BB	1917	26	15,21,22	1.98	3 (20%)	16,30,33	3.41	3 (18%)
26	5MU	BB	1939	26	13,22,23	2.53	5 (38%)	16,32,35	4.00	5 (31%)
26	5MC	BB	1962	26	14,22,23	1.47	3 (21%)	17,32,35	1.36	2 (11%)
26	6MZ	BB	2030	26	17,25,26	0.98	1 (5%)	15,36,39	2.40	5 (33%)
26	7MG	BB	2069	26	20,26,27	2.33	5 (25%)	23,39,42	2.56	7 (30%)
26	OMG	BB	2251	26	18,26,27	1.70	6 (33%)	21,38,41	3.46	9 (42%)
26	2MG	BB	2445	26	18,26,27	1.82	3 (16%)	21,38,41	2.57	10 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	H2U	BB	2449	26	17,21,22	1.73	3 (17%)	23,30,33	1.75	6 (26%)
26	PSU	BB	2457	26	15,21,22	1.46	3 (20%)	16,30,33	3.07	7 (43%)
26	OMC	BB	2498	26	15,22,23	1.51	3 (20%)	20,31,34	1.50	5 (25%)
26	2MA	BB	2503	26	17,25,26	2.00	5 (29%)	18,37,40	2.14	4 (22%)
26	PSU	BB	2504	26	15,21,22	2.09	5 (33%)	16,30,33	3.77	6 (37%)
26	OMU	BB	2552	26	14,22,23	1.97	5 (35%)	19,31,34	3.08	7 (36%)
26	CH	BB	2575	26	14,21,22	2.21	2 (14%)	18,30,33	1.93	4 (22%)
26	PSU	BB	2580	26	15,21,22	1.93	4 (26%)	16,30,33	3.09	6 (37%)
26	PSU	BB	2605	26	15,21,22	2.36	5 (33%)	16,30,33	4.21	2 (12%)
26	1MG	BB	745	26	17,26,27	1.94	3 (17%)	19,39,42	2.42	5 (26%)
26	PSU	BB	746	26	15,21,22	2.30	8 (53%)	16,30,33	4.52	9 (56%)
26	5MU	BB	747	26	13,22,23	1.83	3 (23%)	16,32,35	5.23	8 (50%)
26	PSU	BB	955	26	15,21,22	1.79	4 (26%)	16,30,33	4.53	2 (12%)

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
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
1	4OC	AA	1402	-	-	0/7/29/30	0/2/2/2
1	5MC	AA	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	AA	1519	1	-	0/7/29/30	0/3/3/3
1	PSU	AA	516	1	-	0/7/25/26	0/2/2/2
1	7MG	AA	527	1	-	0/7/37/38	0/3/3/3
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
1	5MC	AA	967	1	-	0/3/25/26	0/2/2/2
2	H2U	AB	16	2	-	0/7/38/39	0/2/2/2
2	H2U	AB	17	2	-	0/7/38/39	0/2/2/2
2	H2U	AB	20	2	-	0/7/38/39	0/2/2/2
2	OMC	AB	32	2	-	0/5/27/28	0/2/2/2
2	MIA	AB	37	2	-	0/11/33/34	0/3/3/3
2	7MG	AB	46	2	-	0/7/37/38	0/3/3/3
2	5MU	AB	54	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	55	2	-	0/7/25/26	0/2/2/2
2	4SU	AB	8	2	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	H2U	AD	21	4	-	0/7/38/39	0/2/2/2
4	OMC	AD	33	4	-	0/5/27/28	0/2/2/2
4	5MU	AD	55	4	-	0/3/25/26	0/2/2/2
4	PSU	AD	56	4	-	0/7/25/26	0/2/2/2
4	4SU	AD	8	4	-	0/3/25/26	0/2/2/2
26	6MZ	BB	1618	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	1835	26	-	0/5/27/28	0/3/3/3
26	PSU	BB	1911	26	-	0/7/25/26	0/2/2/2
26	3TD	BB	1915	26	-	0/7/25/26	0/2/2/2
26	PSU	BB	1917	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	1939	26	-	0/3/25/26	0/2/2/2
26	5MC	BB	1962	26	-	0/3/25/26	0/2/2/2
26	6MZ	BB	2030	26	-	0/5/27/28	0/3/3/3
26	7MG	BB	2069	26	-	0/7/37/38	0/3/3/3
26	OMG	BB	2251	26	-	0/5/27/28	0/3/3/3
26	2MG	BB	2445	26	-	0/5/27/28	0/3/3/3
26	H2U	BB	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	BB	2457	26	-	0/7/25/26	0/2/2/2
26	OMC	BB	2498	26	-	0/5/27/28	0/2/2/2
26	2MA	BB	2503	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	2504	26	-	0/7/25/26	0/2/2/2
26	OMU	BB	2552	26	-	0/5/27/28	0/2/2/2
26	CH	BB	2575	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	2580	26	-	1/7/25/26	0/2/2/2
26	PSU	BB	2605	26	-	0/7/25/26	0/2/2/2
26	1MG	BB	745	26	-	0/3/25/26	0/3/3/3
26	PSU	BB	746	26	-	0/7/25/26	0/2/2/2
26	5MU	BB	747	26	-	0/3/25/26	0/2/2/2
26	PSU	BB	955	26	-	0/7/25/26	0/2/2/2

The worst 5 of 179 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	46	7MG	C8-N9	-7.68	1.34	1.45
26	BB	2069	7MG	C8-N9	-6.90	1.35	1.45
1	AA	527	7MG	C8-N9	-6.57	1.35	1.45
26	BB	745	1MG	C8-N7	-5.15	1.24	1.34
26	BB	2605	PSU	C5-C1'	-4.92	1.48	1.52

The worst 5 of 270 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	747	5MU	C5-C4-N3	-14.25	113.39	125.35
4	AD	55	5MU	C5-C4-N3	-12.51	114.85	125.35
26	BB	1939	5MU	C5-C4-N3	-11.13	116.01	125.35
1	AA	966	2MG	C5-C6-N1	-10.06	110.37	123.52
2	AB	54	5MU	C5-C4-N3	-9.47	117.40	125.35

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	BB	2580	PSU	O4'-C1'-C5-C4

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](#)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	TRP	AB	101	60,2	14,15,16	1.55	2 (14%)	8,20,22	2.76	7 (87%)
60	FME	BB	3001	59	8,9,10	1.54	1 (12%)	5,9,11	2.05	2 (40%)

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
59	TRP	AB	101	60,2	-	0/5/6/8	0/2/2/2
60	FME	BB	3001	59	-	1/6/9/11	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AB	101	TRP	OXT-C	-3.85	1.25	1.42
60	BB	3001	FME	CA-N	-3.52	1.41	1.46
59	AB	101	TRP	C-CA	2.86	1.56	1.52

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AB	101	TRP	CB-CG-CD1	-3.98	123.06	127.97
60	BB	3001	FME	O-C-CA	-2.53	118.77	125.69
59	AB	101	TRP	CH2-CZ3-CE3	-2.51	116.83	120.45
59	AB	101	TRP	CZ2-CE2-CD2	-2.41	116.81	121.12
59	AB	101	TRP	CH2-CZ2-CE2	2.49	123.97	120.07

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	BB	3001	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

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.