



## wwPDB EM Map/Model Validation Report ⓘ

Sep 20, 2016 – 02:14 PM EDT

PDB ID : 5JTE  
EMDB ID: : EMD-8175  
Title : Cryo-EM structure of an ErmBL-stalled ribosome in complex with A-, P-, and E-tRNA  
Authors : Arenz, S.; Bock, L.V.; Graf, M.; Innis, C.A.; Beckmann, R.; Grubmueller, H.; Vaiana, A.C.; Wilson, D.N.  
Deposited on : 2016-05-09  
Resolution : 3.60 Å(reported)  
Based on PDB ID : 5AFI

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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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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) : rb-20027939

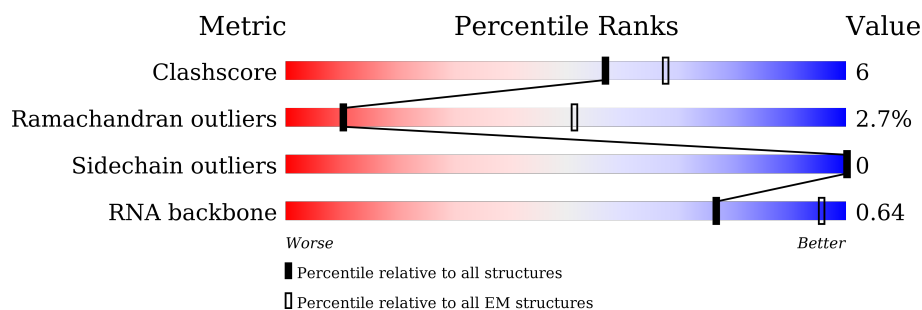
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)
Clashscore	114402	924
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  $\geq 3$ , 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	1539	53% 35% 11% .
2	AB	240	65% 25% . 9%
3	AC	233	64% 24% 12%
4	AD	206	55% 43% .
5	AE	167	66% 22% . 10%
6	AF	135	56% 18% . 26%
7	AG	179	66% 18% 16%
8	AH	130	75% 24% .

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Mol	Chain	Length	Quality of chain
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	10	
23	AW	74	
24	AX	77	
25	AY	71	
26	BA	2897	
27	BB	120	
28	BC	273	
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	
33	BH	149	

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Mol	Chain	Length	Quality of chain
34	BI	142	71%27%..
35	BJ	142	75%25%..
36	BK	123	66%33%..
37	BL	144	70%28%..
38	BM	136	75%25%..
39	BN	127	64%29%. 6%
40	BO	117	72%26%..
41	BP	115	70%30%.
42	BQ	118	87%12%.
43	BR	103	75%25%..
44	BS	110	83%16%.
45	BT	100	71%21%. 7%
46	BU	104	66%30%..
47	BV	94	83%17%..
48	BW	85	68%20%12%..
49	BX	78	77%22%.
50	BY	63	86%14%..
51	BZ	59	71%27%.
52	B0	57	77%21%.
53	B1	55	62%27%. 9%
54	B2	46	80%20%..
55	B3	65	71%28%.
56	B4	38	82%18%..
57	B5	9	33%67%..

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 146760 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	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0
			710	437	143	129	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	AR	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0
			218	98	44	66	10		

- Molecule 23 is a RNA chain called A-site Lysine tRNA Lysine.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AW	74	Total	C	N	O	P	S	0	0
			1593	716	280	522	73	2		

- Molecule 24 is a RNA chain called P-site tRNA Aspartate.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	AX	77	Total	C	N	O	P	S	0	0
			1656	741	290	547	77	1		

- Molecule 25 is a RNA chain called E-site tRNA Valine.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	AY	71	Total	C	N	O	P	S	0	0
			1525	682	276	496	70	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
28	BC	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BD	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	BE	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	BF	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BG	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	BH	47	Total	C	N	O	S	0	0
			359	233	62	63	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

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

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BO	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BT	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	BU	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

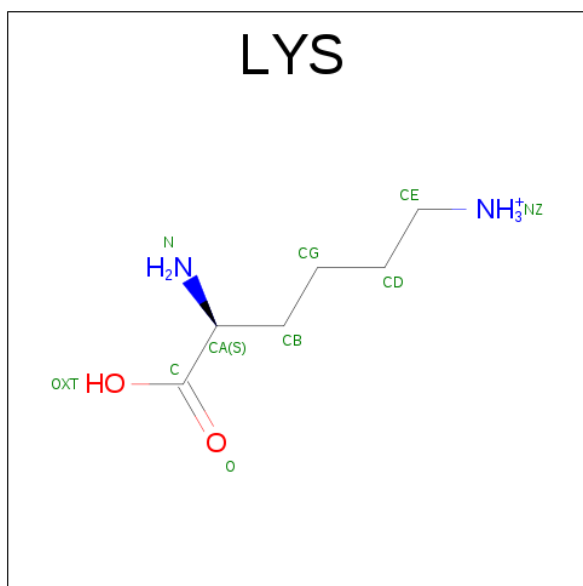
- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 57 is a protein called ErmBL.

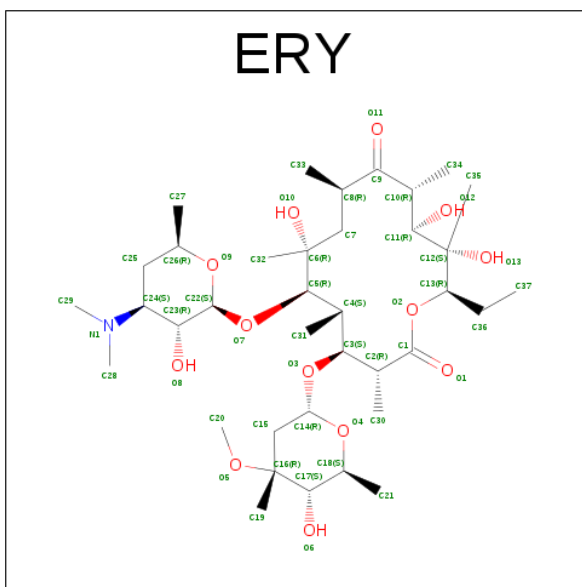
Mol	Chain	Residues	Atoms					AltConf	Trace
57	B5	9	Total	C	N	O	S	0	0
			74	46	14	13	1		

- Molecule 58 is LYSINE (three-letter code: LYS) (formula:  $C_6H_{15}N_2O_2$ ).



Mol	Chain	Residues	Atoms				AltConf
58	AW	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 59 is ERYTHROMYCIN A (three-letter code: ERY) (formula:  $C_{37}H_{67}NO_{13}$ ).

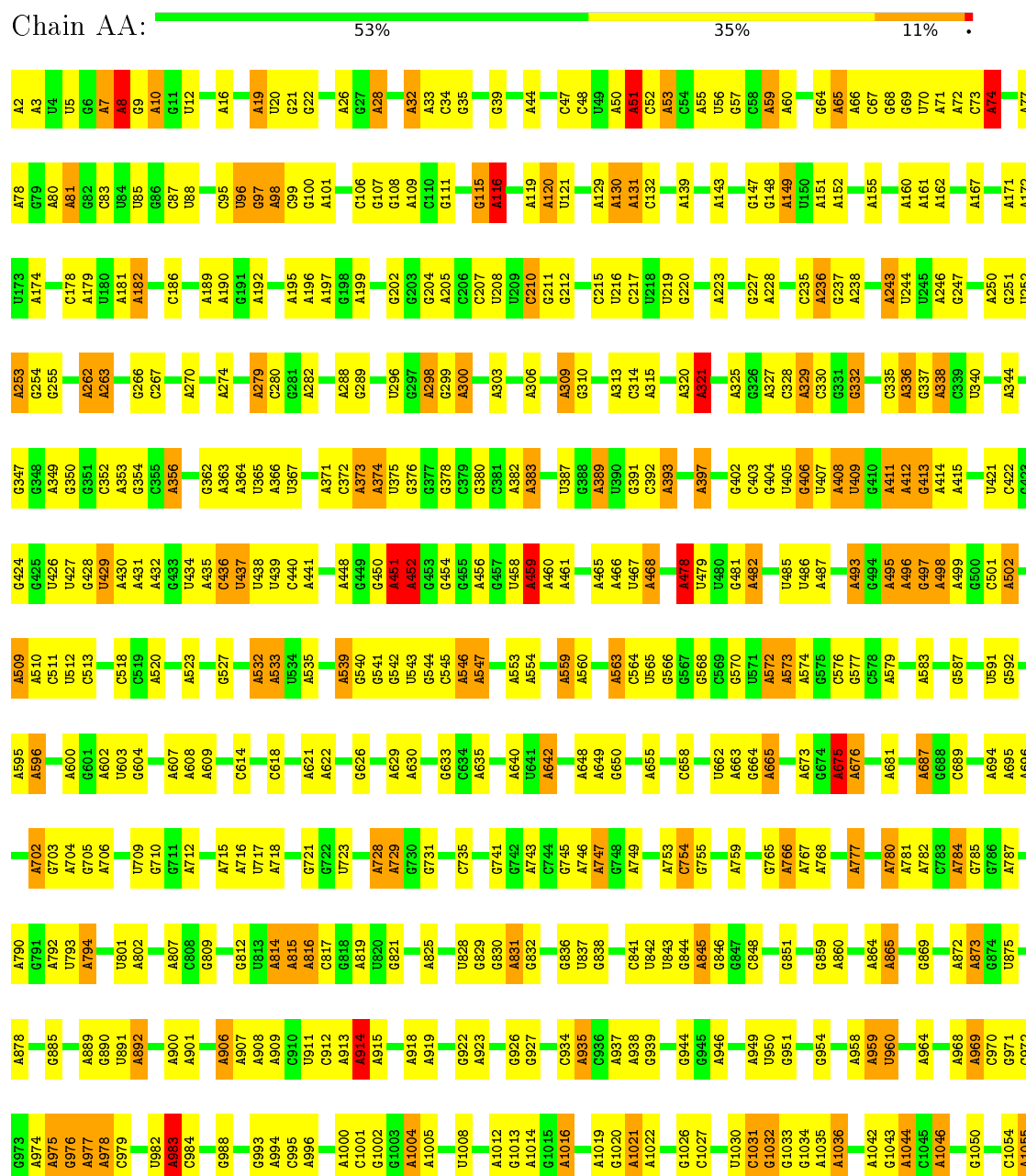


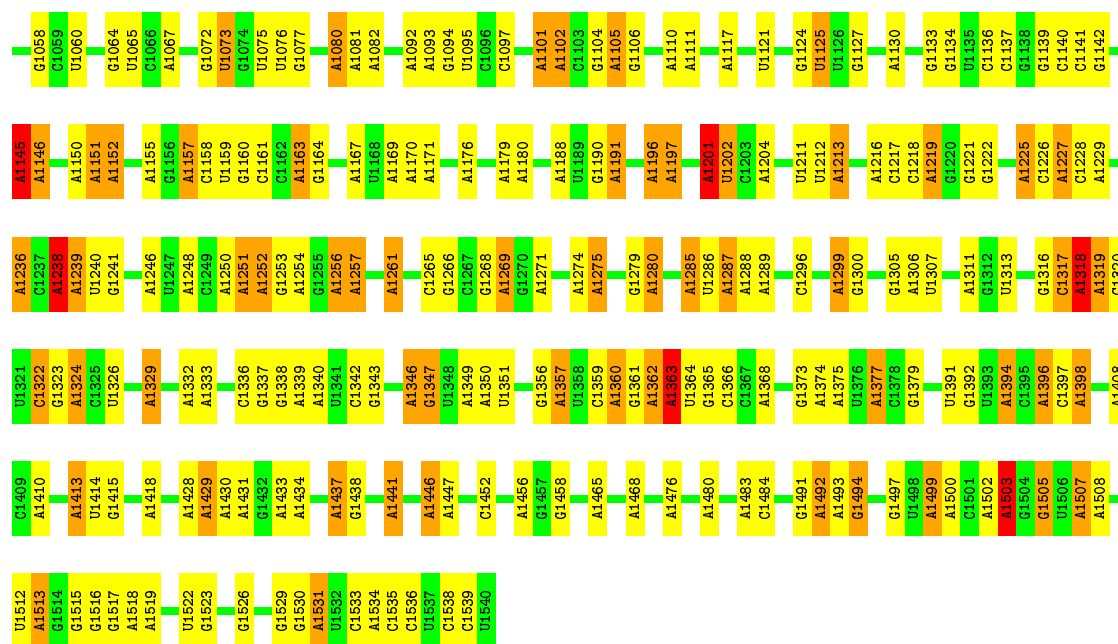
Mol	Chain	Residues	Atoms				AltConf
59	BA	1	Total	C	N	O	0
			51	37	1	13	

### 3 Residue-property plots

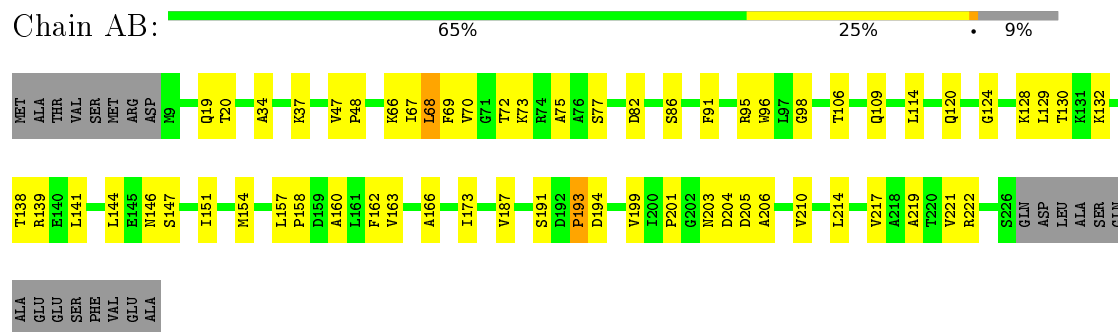
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric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

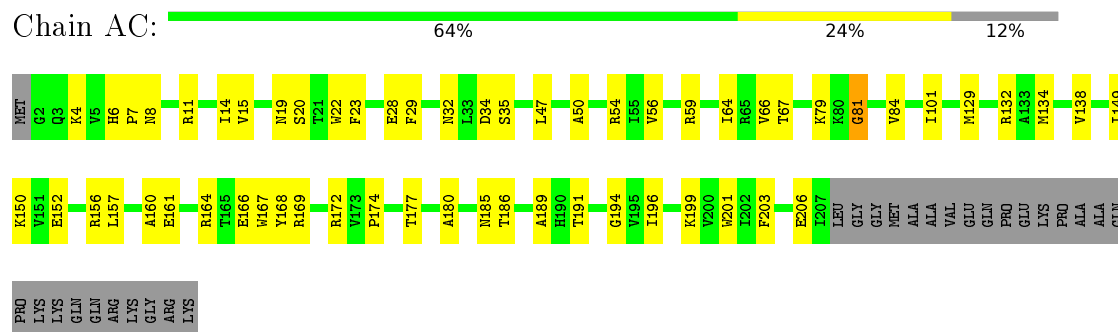




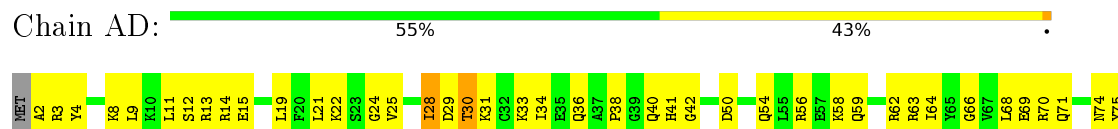
• Molecule 2: 30S ribosomal protein S2



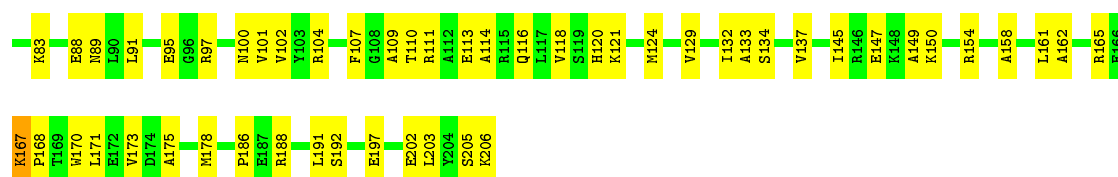
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4







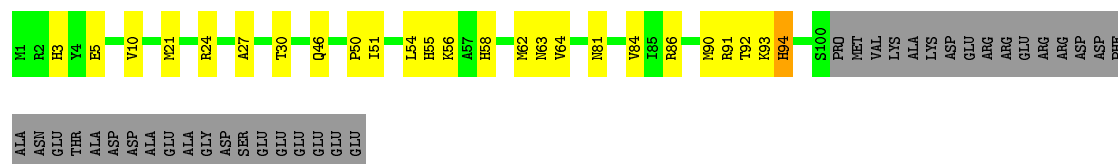
- Molecule 5: 30S ribosomal protein S5

Chain AE: 66% 22% 10%



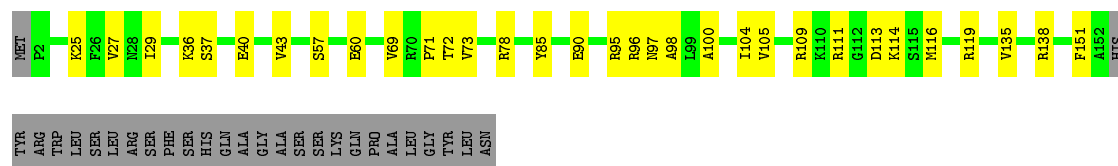
- Molecule 6: 30S ribosomal protein S6

Chain AF: 56% 18% 26%



- Molecule 7: 30S ribosomal protein S7

Chain AG: 66% 18% 16%



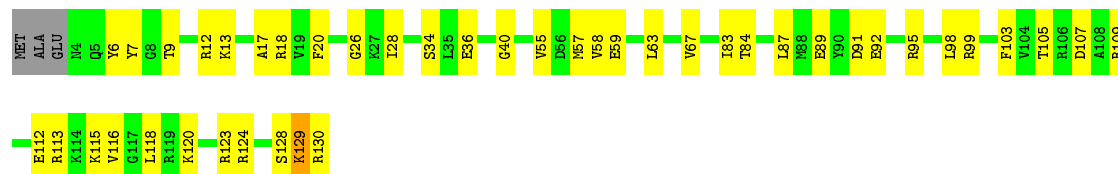
- Molecule 8: 30S ribosomal protein S8

Chain AH: 75% 24% 1%

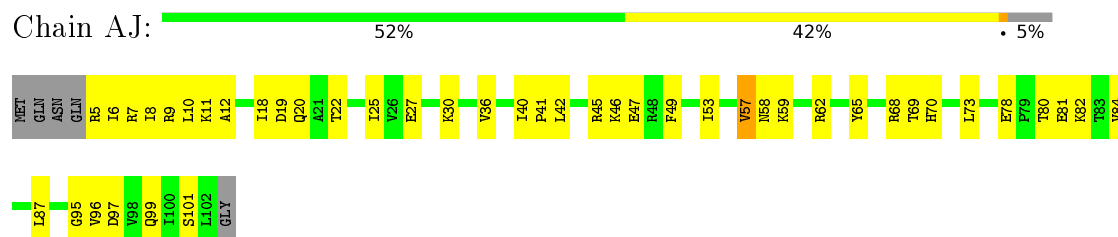


- Molecule 9: 30S ribosomal protein S9

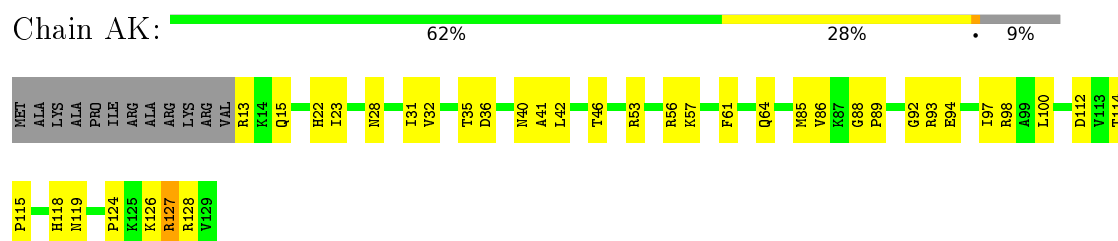
Chain AI: 65% 32% 3%



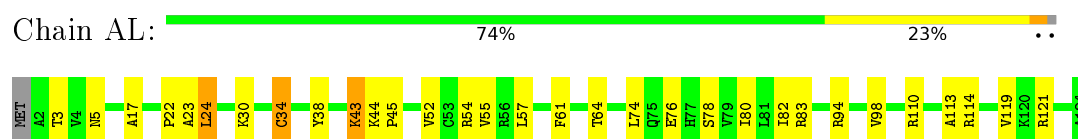
- Molecule 10: 30S ribosomal protein S10



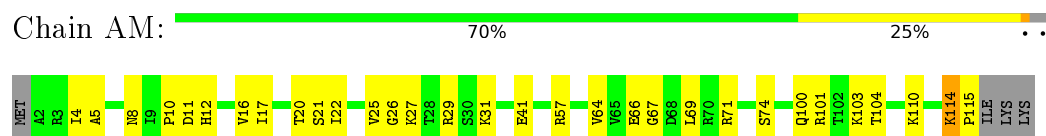
- Molecule 11: 30S ribosomal protein S11



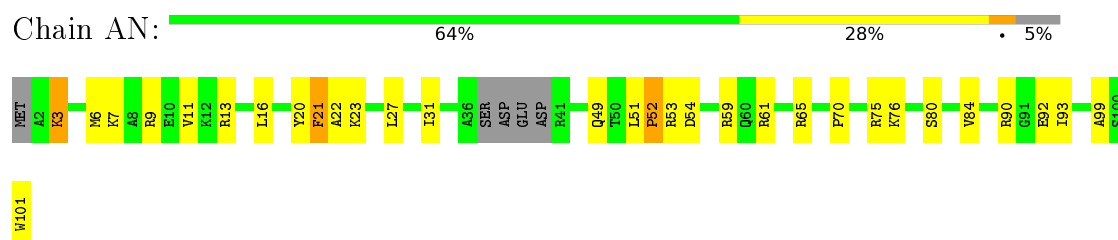
- Molecule 12: 30S ribosomal protein S12



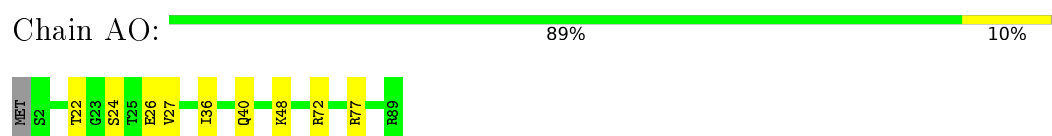
- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14



- Molecule 15: 30S ribosomal protein S15



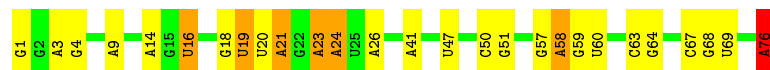
- Molecule 16: 30S ribosomal protein S16






• Molecule 24: P-site tRNA Aspartate

Chain AX: 65% 26% 8%



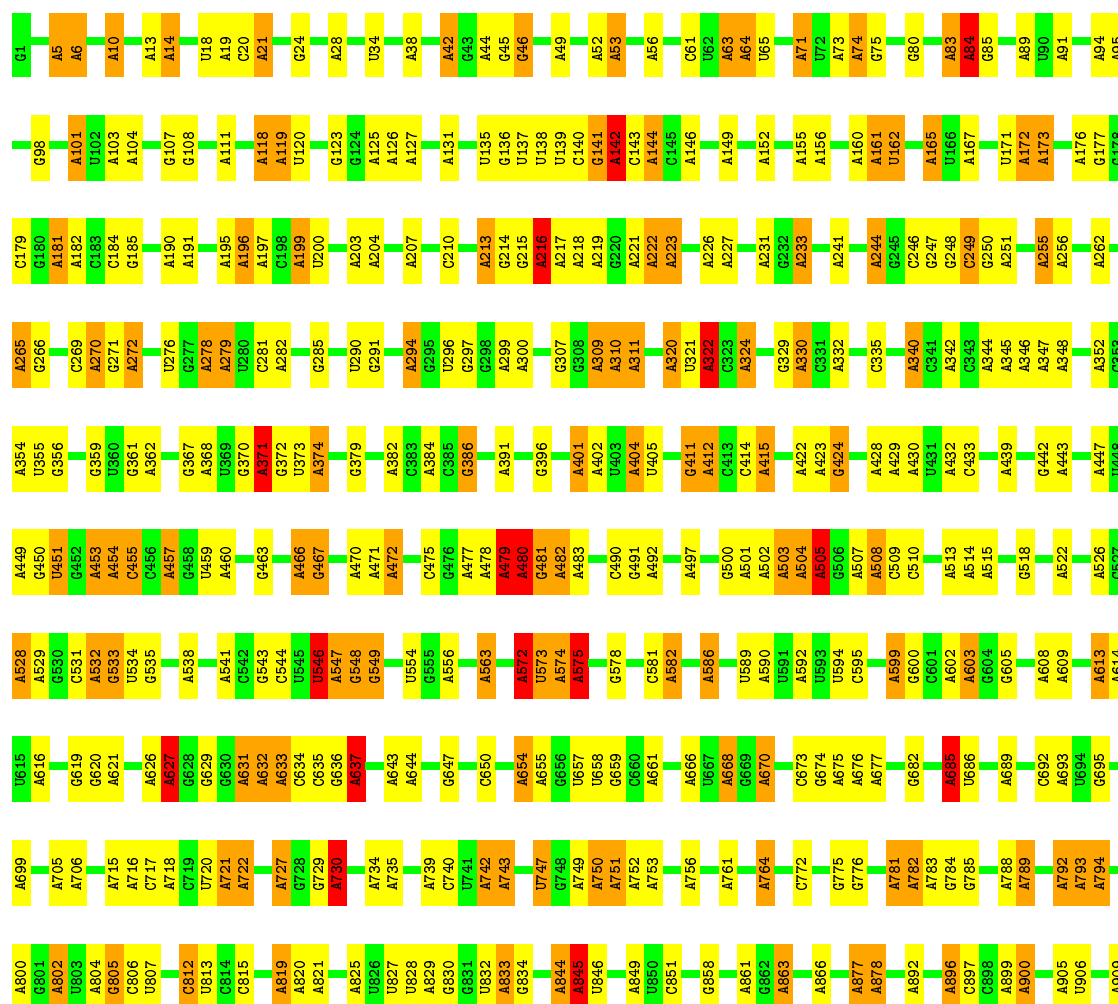
• Molecule 25: E-site tRNA Valine

Chain AY: 51% 37% 11%

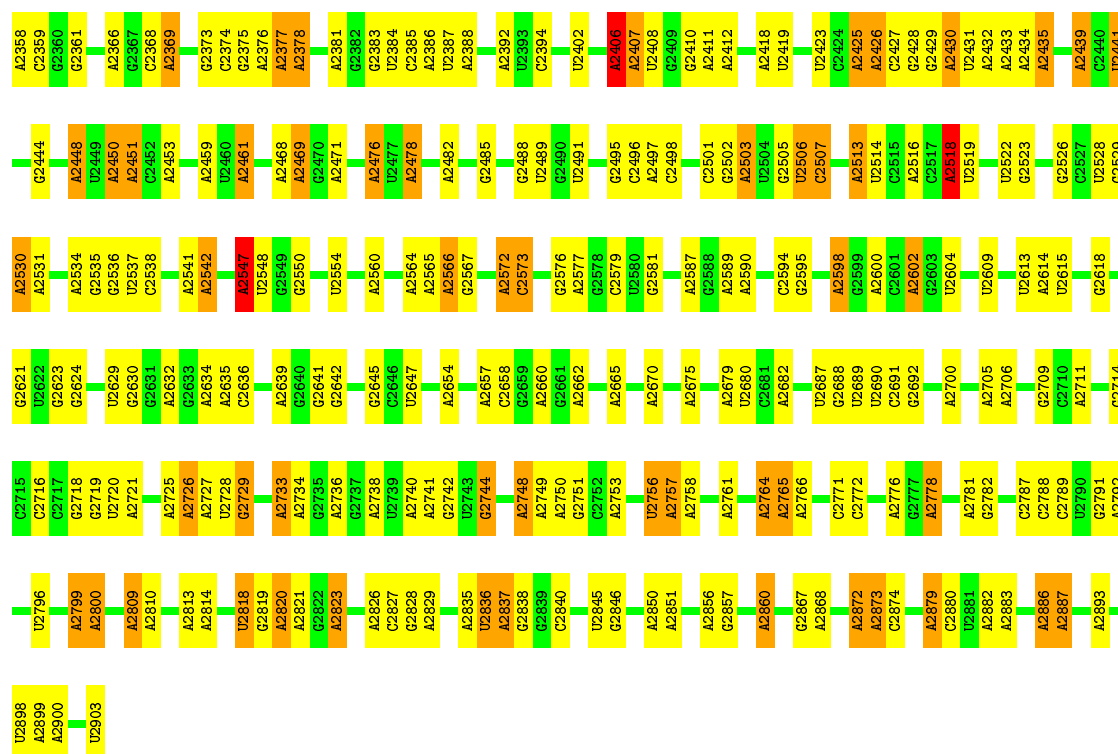


• Molecule 26: 23S ribosomal RNA

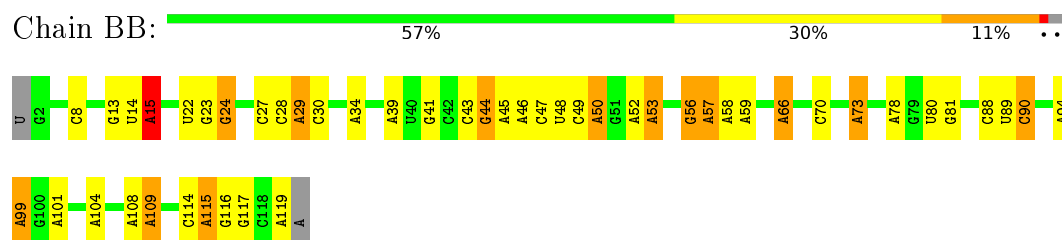
Chain BA: 55% 32% 11%



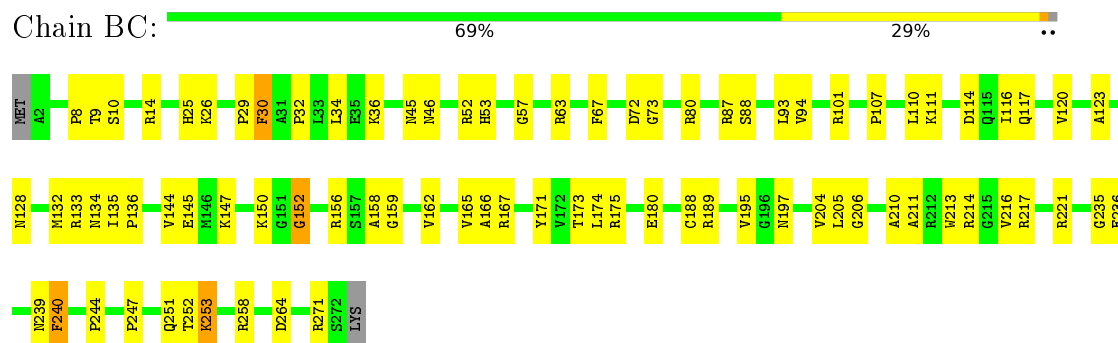
C2275	U2189	G2097	C1816	C1564	A1453	A1347	U1258	A1156	G1074	A990	A930
A2278	G2190	A2101	G1817	C1565	U1458	A1347	G1259	A1165	C1075	A995	A911
G2279	U2191	A2102	U1818	G1566	U1459	A1353	A1260	A1166	A1076	C995	G914
G2280	G2193	U2106	A1819	G1567	A1460	A1354	A1261	A1167	A1077	A996	C915
A2281	U2194	U2107	A1820	G1568	A1461	A1355	A1262	A1168	A1078	A1000	G916
G2282	G2195	U2108	A1821	A1570	A1477	A1359	A1263	A1169	A1079	A1001	A917
C2283	A2198	U2109	G1826	A1571	A1478	A1363	A1264	A1170	A1080	C1007	A918
A2284	U2199	U2110	U1827	A1572	G1478	A1364	A1265	G1177	U1081	C1008	U919
C2285	G2200	U2111	G1828	A1573	G1479	A1365	A1266	G1178	A1082	A1008	A920
G2286	G2201	U2112	A1829	A1574	A1482	A1366	A1267	G1179	A1083	A1009	G921
A2287	U2204	U2113	C1833	U1578	A1483	A1367	A1268	U1180	A1084	A1010	G922
A2288	A2205	U2114	U1834	A1579	A1490	A1368	A1269	U1181	A1085	G1011	G923
U2291	A2211	U2115	A1835	A1580	A1491	A1377	A1270	G1182	A1086	U1012	G924
U2292	U2212	U2116	G1836	A1581	C1493	A1378	A1271	G1183	A1087	C1013	A925
G2293	A2213	U2117	U1837	A1582	A1494	A1379	A1272	G1184	A1088	A1014	A926
G2294	U2214	U2118	A1838	A1583	A1495	A1380	A1273	G1185	A1089	A1015	A927
A2297	G2215	U2119	A1839	A1584	A1496	A1381	A1274	U1186	A1090	A1016	A928
A2298	G2216	A2126	A1840	A1585	A1502	A1382	A1275	G1187	A1091	A1020	U932
G2303	G2217	U2127	A1841	A1586	A1503	A1383	A1276	G1188	A1092	A1021	A933
G2304	U2223	U2131	U1842	A1587	A1504	A1384	A1277	G1189	A1093	G1022	A936
U2305	G2224	U2132	U1843	A1588	A1505	A1385	A1278	G1190	A1094	A1026	A937
A2309	A2225	G2133	G1844	A1589	A1506	A1386	A1279	G1191	A1095	A1027	A938
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A2312	A2227	A2135	U1846	A1591	A1508	A1388	A1281	G1195	A1097	A1029	G938
U2313	U2232	A2142	A1847	A1592	A1509	A1389	A1282	A1199	A1098	C1030	A941
G2314	G2233	U2143	U1848	A1593	A1510	A1390	A1283	G1200	A1099	G1031	G942
A2315	U2234	U2144	A1849	A1594	A1511	A1391	A1284	U1201	A1100	U1032	A943
G2316	G2235	A2145	U1850	A1595	A1512	A1392	A1285	G1202	A1101	U1033	G944
A2317	A2236	G2146	A1851	A1596	A1513	A1393	A1286	U1203	A1102	G1034	A945
U2322	U2237	A2147	A1852	A1597	A1514	A1394	A1287	G1204	A1103	A1035	A946
A2327	G2238	U2148	U1853	A1598	A1515	A1395	A1288	G1205	A1104	A1036	A947
A2328	U2239	A2149	A1854	A1599	A1516	A1396	A1289	G1206	A1105	A1037	A948
U2333	G2240	G2150	U1855	A1600	A1517	A1397	A1290	G1207	A1106	A1038	G949
A2334	A2241	U2151	A1856	A1601	A1518	A1403	A1291	G1208	A1107	A1039	A953
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U2337	G2243	A2153	A1858	A1603	A1520	A1405	A1293	G1212	A1109	A1041	A959
A2338	U2244	G2154	U1859	A1604	A1521	A1406	A1294	A1213	A1110	A1042	A960
U2339	A2245	U2154	A1860	A1605	A1522	A1407	A1295	A1214	A1111	A1043	C961
G2340	G2246	U2155	U1861	A1606	A1523	A1408	A1296	G1215	A1112	A1044	G968
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G2345	A2249	U2158	A1864	A1609	A1526	A1411	A1299	A1218	A1115	A1047	A973
A2346	U2250	A2159	U1865	A1610	A1527	A1412	A1300	A1219	A1116	A1048	A974
G2347	G2251	G2160	A1866	A1611	A1528	A1413	A1301	A1220	A1117	A1049	A975
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U2354	A2258	U2167	U1873	A1618	A1535	A1420	A1308	A1227	A1124	A1056	A989
G2355	G2259	A2168	A1874	A1619	A1536	A1421	A1309	A1228	A1125	A1057	A990
U2356	U2260	G2169	U1875	A1620	A1537	A1422	A1310	A1229	A1126	A1058	A991
A2357	C2261	U2169	U1876	A1621	A1538	A1423	A1311	A1230	A1127	A1059	A992
U2358	A2262	A2170	A1877	A1622	A1539	A1424	A1312	A1231	A1128	A1060	A993
G2359	U2263	U2171	U1878	A1623	A1540	A1425	A1313	A1232	A1129	U1061	A994
A2360	A2264	G2172	U1879	A1624	A1541	A1426	A1314	A1233	A1130	A1062	A995
U2361	G2265	A2173	U1880	A1625	A1542	A1427	A1315	A1234	A1131	A1063	A996
G2362	U2266	U2174	A1881	A1626	A1543	A1428	A1316	A1235	A1132	A1064	A997
A2363	A2267	G2175	U1882	A1627	A1544	A1429	A1317	A1236	A1133	A1065	A998
U2364	G2268	U2176	U1883	A1628	A1545	A1430	A1318	A1237	A1134	A1066	A999
G2365	U2269	A2177	A1884	A1629	A1546	A1431	A1319	A1238	A1135	A1067	A999
A2366	A2270	U2178	U1885	A1630	A1547	A1432	A1320	A1239	A1136	A1068	A999
U2367	G2271	U2179	U1886	A1631	A1548	A1433	A1321	A1240	A1137	A1069	A999
A2368	U2272	A2180	U1887	A1632	A1549	A1434	A1322	A1241	A1138	A1070	A999
G2369	A2273	U2181	U1888	A1633	A1550	A1435	A1323	A1242	A1139	A1071	A999
U2370	U2274	U2182	U1889	A1634	A1551	A1436	A1324	A1243	A1140	A1072	A999
A2371	G2275	A2183	U1890	A1635	A1552	A1437	A1325	A1244	A1141	A1073	A999
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G2380	A2284	U2192	U1899	A1644	A1561	A1446	A1334	A1253	A1150	A1082	A999
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A2385	U2289	U2197	U1904	A1649	A1566	A1451	A1339	A1258	A1155	A1087	A999
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G2389	A2293	U2201	U1908	A1653	A1570	A1455	A1343	A1262	A1159	A1091	A999
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G2397	U2301	U2209	U1916	A1661	A1578	A1463	A1351	A1270	A1167	A1099	A999
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G2400	A2304	U2212	U1919	A1664	A1581	A1466	A1354	A1273	A1170	A1102	A999
U2401	G2305	U2213	U1920	A1665	A1582	A1467	A1355	A1274	A1171	A1103	A999
A2402	U2306	U2214	U1921	A1666	A1583	A1468	A1356	A1275	A1172	A1104	A999
G2403	A2307	U2215	U1922	A1667	A1584	A1469	A1357	A1276	A1173	A1105	A999
U2404	U2308	U2216	U1923	A1668	A1585	A1470	A1358	A1277	A1174	A1106	A999
A2405	G2309	U2217	U1924	A1669	A1586	A1471	A1359	A1278	A1175	A1107	A999
G2406	U2310	U2218	U1925	A1670	A1587	A1472	A1360	A1279	A1176	A1108	A999
U2407	A2311	U2219	U1926	A1671	A1588	A1473	A1361	A1280	A1177	A1109	A999
G2408	U2312	U2220	U1927	A1672	A1589	A1474	A1362	A1281	A1178	A1110	A999
A2409	G2313	U2221	U1928	A1673	A1590	A1475	A1363	A1282	A1179	A1111	A999
U2410	U2314	U2222	U1929	A1674	A1591	A1476	A1364	A1283	A1180	A1112	A999
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U2412	G2316	U2224	U								



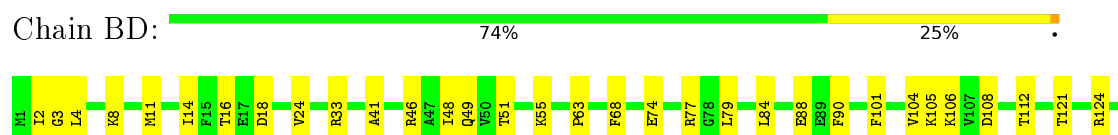
• Molecule 27: 5S ribosomal RNA



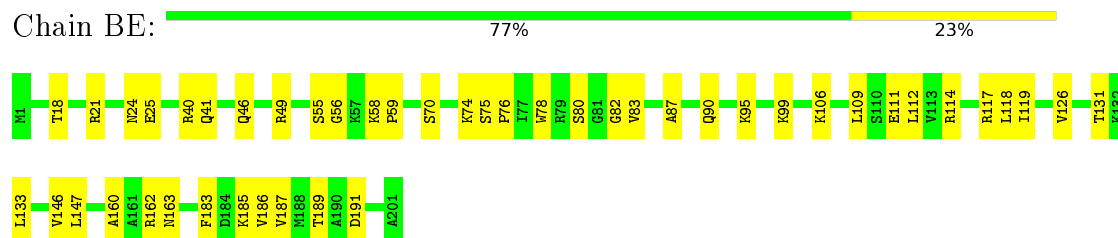
• Molecule 28: 50S ribosomal protein L2



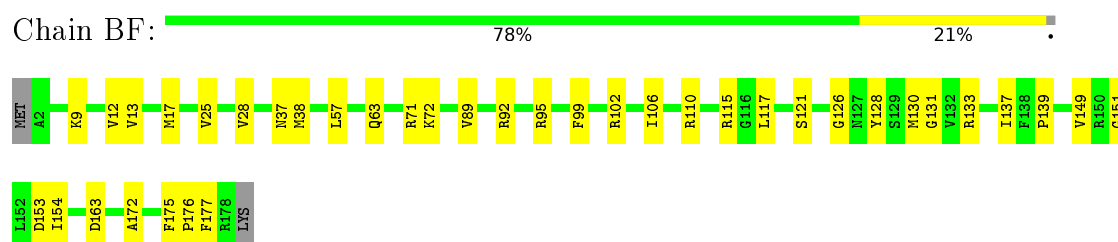
• Molecule 29: 50S ribosomal protein L3



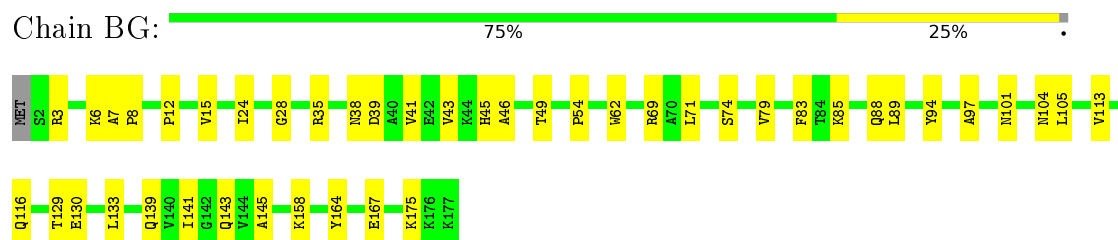
- Molecule 30: 50S ribosomal protein L4



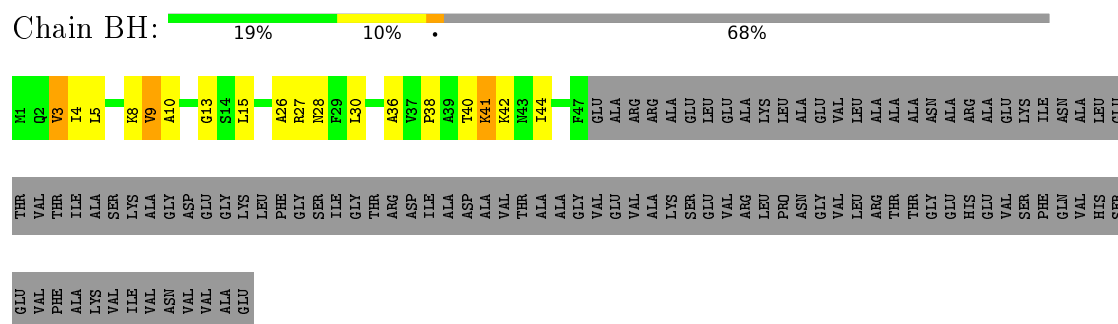
- Molecule 31: 50S ribosomal protein L5



- Molecule 32: 50S ribosomal protein L6

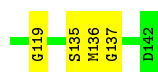


- Molecule 33: 50S ribosomal protein L9



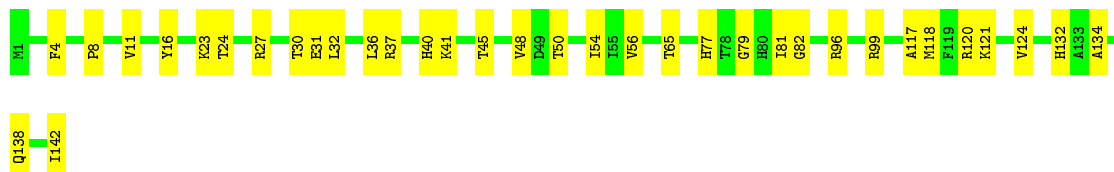
- Molecule 34: 50S ribosomal protein L11





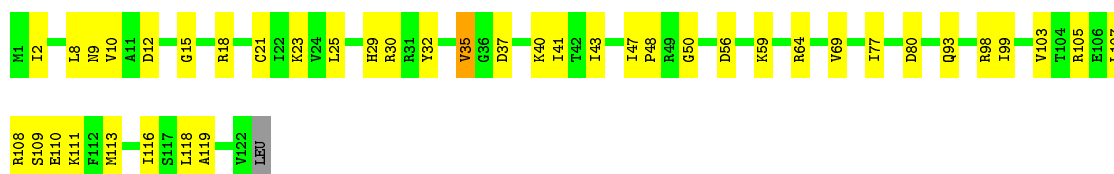
- Molecule 35: 50S ribosomal protein L13

Chain BJ: 75% 25%



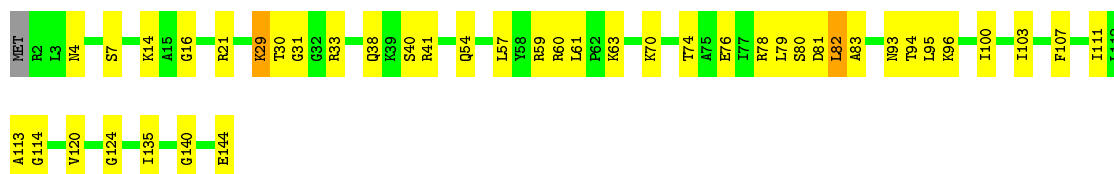
- Molecule 36: 50S ribosomal protein L14

Chain BK: 66% 33% ..



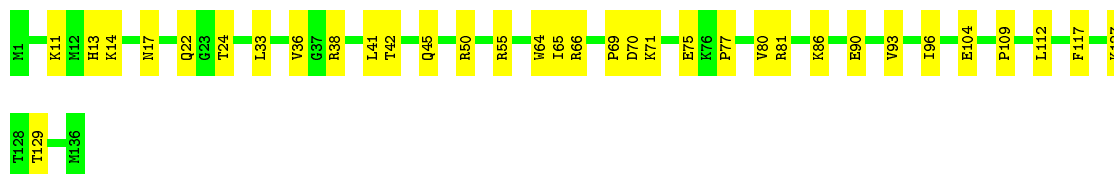
- Molecule 37: 50S ribosomal protein L15

Chain BL: 70% 28% ..



- Molecule 38: 50S ribosomal protein L16

Chain BM: 75% 25%



- Molecule 39: 50S ribosomal protein L17

Chain BN: 64% 29% 6%







- Molecule 40: 50S ribosomal protein L18

Chain BO: 72% 26% ..



- Molecule 41: 50S ribosomal protein L19

Chain BP: 70% 30% .



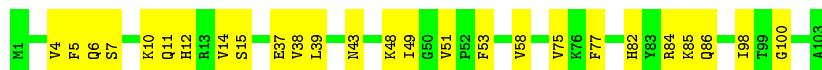
- Molecule 42: 50S ribosomal protein L20

Chain BQ: 87% 12% .



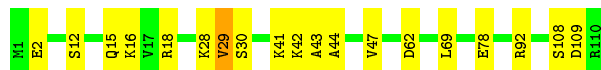
- Molecule 43: 50S ribosomal protein L21

Chain BR: 75% 25%



- Molecule 44: 50S ribosomal protein L22

Chain BS: 83% 16% .



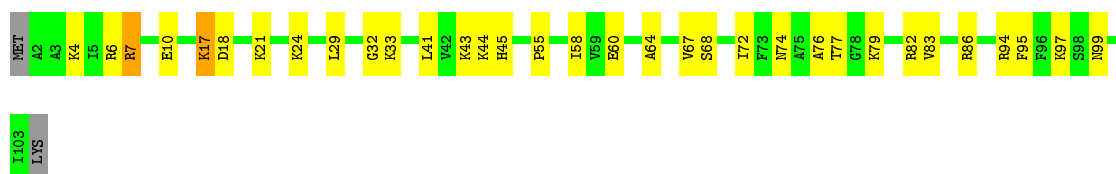
- Molecule 45: 50S ribosomal protein L23

Chain BT: 71% 21% 7%

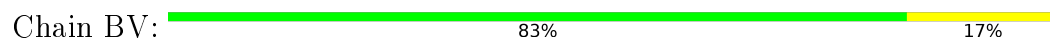


- Molecule 46: 50S ribosomal protein L24

Chain BU: 66% 30%



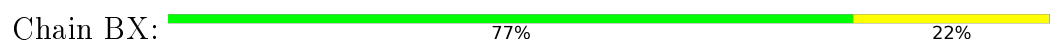
- Molecule 47: 50S ribosomal protein L25



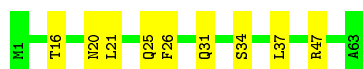
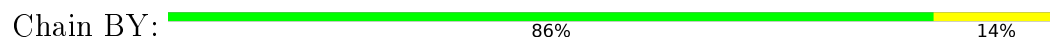
- Molecule 48: 50S ribosomal protein L27



- Molecule 49: 50S ribosomal protein L28



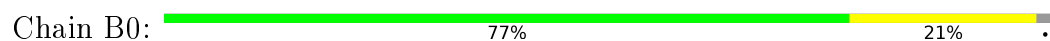
- Molecule 50: 50S ribosomal protein L29



- Molecule 51: 50S ribosomal protein L30

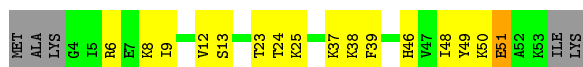


- Molecule 52: 50S ribosomal protein L32



- Molecule 53: 50S ribosomal protein L33





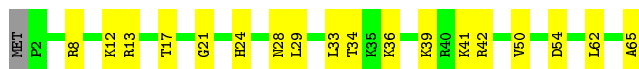
- Molecule 54: 50S ribosomal protein L34

Chain B2: 80% 20%



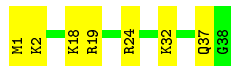
- Molecule 55: 50S ribosomal protein L35

Chain B3: 71% 28%



- Molecule 56: 50S ribosomal protein L36

Chain B4: 82% 18%



- Molecule 57: ErmBL

Chain B5: 33% 67%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	85393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	Not provided	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1200	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: 5MU, U8U, 7MG, ERY, PSU, 2MA, 6MZ, 3AU, 4SU, T6A, QUO, CM0

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	2.20	1353/36965 (3.7%)	3.39	4664/57662 (8.1%)
10	AJ	0.31	0/796	0.53	0/1077
11	AK	0.25	0/893	0.44	0/1205
12	AL	0.25	0/969	0.45	0/1300
13	AM	0.27	0/892	0.49	0/1193
14	AN	0.24	0/785	0.42	0/1043
15	AO	0.28	0/718	0.45	0/959
16	AP	0.26	0/659	0.44	0/884
17	AQ	0.26	0/657	0.49	0/881
18	AR	0.27	0/462	0.44	0/621
19	AS	0.26	0/652	0.43	0/877
2	AB	0.30	0/1735	0.49	0/2338
20	AT	0.25	0/671	0.43	0/888
21	AU	0.25	0/430	0.50	0/570
22	AV	3.36	21/245 (8.6%)	5.13	72/380 (18.9%)
23	AW	2.30	58/1569 (3.7%)	3.39	201/2437 (8.2%)
24	AX	2.07	48/1668 (2.9%)	2.69	139/2593 (5.4%)
25	AY	1.97	44/1554 (2.8%)	3.05	157/2416 (6.5%)
26	BA	2.25	2626/69659 (3.8%)	3.46	9154/108672 (8.4%)
27	BB	1.94	79/2828 (2.8%)	3.00	278/4410 (6.3%)
28	BC	0.25	0/2121	0.45	0/2852
29	BD	0.27	0/1586	0.45	0/2134
3	AC	0.25	0/1651	0.44	0/2225
30	BE	0.27	0/1571	0.45	0/2113
31	BF	0.30	0/1434	0.47	0/1926
32	BG	0.27	0/1343	0.44	0/1816
33	BH	0.29	0/364	0.52	0/490
34	BI	0.28	0/1046	0.49	0/1410
35	BJ	0.27	0/1152	0.44	0/1551
36	BK	0.26	0/947	0.46	0/1268
37	BL	0.24	0/1054	0.44	0/1403
38	BM	0.26	0/1093	0.43	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BN	0.25	0/973	0.43	0/1301
4	AD	0.27	0/1665	0.47	0/2227
40	BO	0.25	0/902	0.40	0/1209
41	BP	0.24	0/929	0.43	0/1242
42	BQ	0.24	0/960	0.38	0/1278
43	BR	0.25	0/829	0.43	0/1107
44	BS	0.29	0/864	0.48	0/1156
45	BT	0.23	0/744	0.43	0/994
46	BU	0.28	0/787	0.45	0/1051
47	BV	0.27	0/766	0.44	0/1025
48	BW	0.25	0/576	0.39	0/762
49	BX	0.23	0/635	0.39	0/848
5	AE	0.24	0/1118	0.46	0/1504
50	BY	0.22	0/510	0.38	0/677
51	BZ	0.23	0/453	0.44	0/605
52	B0	0.27	0/450	0.44	0/599
53	B1	0.24	0/416	0.43	0/554
54	B2	0.20	0/380	0.37	0/498
55	B3	0.22	0/513	0.41	0/676
56	B4	0.23	0/303	0.39	0/397
57	B5	0.36	0/74	0.59	0/98
6	AF	0.25	0/835	0.46	0/1128
7	AG	0.25	0/1195	0.42	0/1602
8	AH	0.27	0/989	0.45	0/1326
9	AI	0.28	0/1034	0.48	0/1375
All	All	1.89	4229/159069 (2.7%)	2.97	14665/238293 (6.2%)

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
29	BD	0	1

The worst 5 of 4229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	20	U	C5-C6	23.31	1.55	1.34
23	AW	20	U	C5-C6	23.29	1.55	1.34
24	AX	16	U	C5-C6	23.26	1.55	1.34
24	AX	19	U	C5-C6	23.18	1.55	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	BA	454	A	C6-N6	17.20	1.47	1.33

The worst 5 of 14665 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BA	278	A	C2-N3-C4	20.42	120.81	110.60
1	AA	983	A	C2-N3-C4	20.30	120.75	110.60
26	BA	2114	A	C2-N3-C4	20.19	120.70	110.60
26	BA	514	A	C2-N3-C4	19.99	120.60	110.60
26	BA	2451	A	N1-C6-N6	-19.89	106.67	118.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	BD	151	THR	Peptide

## 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	33015	0	16618	252	0
2	AB	1704	0	1732	31	0
3	AC	1624	0	1696	37	0
4	AD	1643	0	1707	74	0
5	AE	1105	0	1148	24	0
6	AF	817	0	808	12	0
7	AG	1181	0	1238	21	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	25	0
10	AJ	786	0	828	32	0
11	AK	877	0	887	25	0
12	AL	955	0	1016	20	0
13	AM	883	0	941	22	0
14	AN	774	0	824	26	0
15	AO	710	0	728	7	0
16	AP	649	0	666	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	AQ	648	0	691	17	0
18	AR	455	0	478	7	0
19	AS	637	0	665	15	0
20	AT	665	0	714	18	0
21	AU	425	0	449	7	0
22	AV	218	0	109	3	0
23	AW	1593	0	820	8	0
24	AX	1656	0	849	10	0
25	AY	1525	0	780	11	0
26	BA	62195	0	31280	431	0
27	BB	2529	0	1281	22	0
28	BC	2082	0	2154	53	0
29	BD	1565	0	1616	40	0
30	BE	1552	0	1619	32	0
31	BF	1410	0	1444	23	0
32	BG	1323	0	1371	27	0
33	BH	359	0	381	13	0
34	BI	1032	0	1085	26	0
35	BJ	1129	0	1162	22	0
36	BK	938	0	1012	26	0
37	BL	1045	0	1117	26	0
38	BM	1074	0	1157	25	0
39	BN	960	0	1000	29	0
40	BO	892	0	923	21	0
41	BP	917	0	962	22	0
42	BQ	947	0	1019	11	0
43	BR	816	0	839	15	0
44	BS	857	0	922	13	0
45	BT	738	0	807	14	0
46	BU	779	0	831	23	0
47	BV	753	0	780	9	0
48	BW	569	0	581	15	0
49	BX	625	0	652	13	0
50	BY	509	0	543	8	0
51	BZ	449	0	488	10	0
52	B0	444	0	458	8	0
53	B1	409	0	440	12	0
54	B2	377	0	418	7	0
55	B3	504	0	572	15	0
56	B4	302	0	343	8	0
57	B5	74	0	74	23	0
58	AW	9	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	BA	51	0	67	12	0
All	All	146760	0	97903	1470	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1470 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:BA:9000:ERY:C27	57:B5:-2:ASN:ND2	2.18	1.07
59:BA:9000:ERY:H271	57:B5:-2:ASN:HD21	1.13	1.06
59:BA:9000:ERY:H271	57:B5:-2:ASN:ND2	1.74	1.01
59:BA:9000:ERY:C27	57:B5:-2:ASN:HD21	1.72	0.98
58:AW:101:LYS:N	24:AX:76:A:HO2'	1.69	0.91

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	
2	AB	216/240 (90%)	190 (88%)	19 (9%)	7 (3%)	5	42
3	AC	204/233 (88%)	180 (88%)	20 (10%)	4 (2%)	9	53
4	AD	203/206 (98%)	188 (93%)	8 (4%)	7 (3%)	5	41
5	AE	148/167 (89%)	124 (84%)	17 (12%)	7 (5%)	3	30
6	AF	98/135 (73%)	85 (87%)	8 (8%)	5 (5%)	2	28
7	AG	149/179 (83%)	140 (94%)	8 (5%)	1 (1%)	26	72
8	AH	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	24	69
9	AI	125/130 (96%)	113 (90%)	6 (5%)	6 (5%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AJ	96/103 (93%)	82 (85%)	8 (8%)	6 (6%)	2	23
11	AK	115/129 (89%)	99 (86%)	13 (11%)	3 (3%)	7	46
12	AL	121/124 (98%)	108 (89%)	6 (5%)	7 (6%)	2	25
13	AM	112/118 (95%)	104 (93%)	7 (6%)	1 (1%)	21	67
14	AN	92/101 (91%)	79 (86%)	8 (9%)	5 (5%)	2	27
15	AO	86/89 (97%)	79 (92%)	7 (8%)	0	100	100
16	AP	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	7	48
17	AQ	78/84 (93%)	64 (82%)	11 (14%)	3 (4%)	4	37
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	77/92 (84%)	71 (92%)	5 (6%)	1 (1%)	15	60
20	AT	83/87 (95%)	76 (92%)	4 (5%)	3 (4%)	4	39
21	AU	49/71 (69%)	36 (74%)	8 (16%)	5 (10%)	1	11
28	BC	269/273 (98%)	247 (92%)	16 (6%)	6 (2%)	8	51
29	BD	207/209 (99%)	190 (92%)	15 (7%)	2 (1%)	19	66
30	BE	199/201 (99%)	188 (94%)	9 (4%)	2 (1%)	19	66
31	BF	175/179 (98%)	154 (88%)	16 (9%)	5 (3%)	6	44
32	BG	174/177 (98%)	161 (92%)	10 (6%)	3 (2%)	11	55
33	BH	45/149 (30%)	37 (82%)	4 (9%)	4 (9%)	1	13
34	BI	139/142 (98%)	116 (84%)	15 (11%)	8 (6%)	2	25
35	BJ	140/142 (99%)	131 (94%)	8 (6%)	1 (1%)	26	72
36	BK	120/123 (98%)	106 (88%)	9 (8%)	5 (4%)	3	33
37	BL	141/144 (98%)	117 (83%)	16 (11%)	8 (6%)	2	25
38	BM	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	8	51
39	BN	118/127 (93%)	104 (88%)	9 (8%)	5 (4%)	3	33
40	BO	114/117 (97%)	104 (91%)	7 (6%)	3 (3%)	7	46
41	BP	112/115 (97%)	105 (94%)	5 (4%)	2 (2%)	11	54
42	BQ	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
43	BR	101/103 (98%)	91 (90%)	6 (6%)	4 (4%)	4	35
44	BS	108/110 (98%)	97 (90%)	9 (8%)	2 (2%)	10	53
45	BT	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	8	51
46	BU	100/104 (96%)	82 (82%)	13 (13%)	5 (5%)	3	29

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	BV	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
48	BW	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
49	BX	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	BY	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
51	BZ	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	11	54
52	B0	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
53	B1	48/55 (87%)	45 (94%)	2 (4%)	1 (2%)	9	52
54	B2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	50
55	B3	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
56	B4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
57	B5	7/9 (78%)	3 (43%)	3 (43%)	1 (14%)	0	5
All	All	5522/5993 (92%)	4968 (90%)	406 (7%)	148 (3%)	10	46

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	105	ILE
9	AI	55	VAL
11	AK	127	ARG
12	AL	23	ALA
17	AQ	17	MET

### 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	
2	AB	180/198 (91%)	180 (100%)	0	100	100
3	AC	170/190 (90%)	170 (100%)	0	100	100
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	113/126 (90%)	113 (100%)	0	100	100
6	AF	87/116 (75%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	AG	124/147 (84%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	105 (100%)	0	100	100
10	AJ	86/90 (96%)	86 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	103/104 (99%)	103 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	79 (100%)	0	100	100
15	AO	75/77 (97%)	75 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	70/79 (89%)	70 (100%)	0	100	100
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	44/61 (72%)	44 (100%)	0	100	100
28	BC	216/218 (99%)	216 (100%)	0	100	100
29	BD	164/164 (100%)	164 (100%)	0	100	100
30	BE	165/165 (100%)	165 (100%)	0	100	100
31	BF	148/150 (99%)	148 (100%)	0	100	100
32	BG	137/138 (99%)	137 (100%)	0	100	100
33	BH	38/114 (33%)	38 (100%)	0	100	100
34	BI	109/110 (99%)	109 (100%)	0	100	100
35	BJ	116/116 (100%)	116 (100%)	0	100	100
36	BK	103/104 (99%)	103 (100%)	0	100	100
37	BL	102/103 (99%)	102 (100%)	0	100	100
38	BM	109/109 (100%)	109 (100%)	0	100	100
39	BN	100/103 (97%)	100 (100%)	0	100	100
40	BO	86/87 (99%)	86 (100%)	0	100	100
41	BP	99/100 (99%)	99 (100%)	0	100	100
42	BQ	89/90 (99%)	89 (100%)	0	100	100
43	BR	84/84 (100%)	84 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	BS	93/93 (100%)	93 (100%)	0	100	100
45	BT	80/84 (95%)	80 (100%)	0	100	100
46	BU	83/85 (98%)	83 (100%)	0	100	100
47	BV	78/78 (100%)	78 (100%)	0	100	100
48	BW	56/63 (89%)	56 (100%)	0	100	100
49	BX	67/68 (98%)	67 (100%)	0	100	100
50	BY	55/55 (100%)	55 (100%)	0	100	100
51	BZ	48/49 (98%)	48 (100%)	0	100	100
52	B0	47/48 (98%)	47 (100%)	0	100	100
53	B1	45/49 (92%)	45 (100%)	0	100	100
54	B2	38/38 (100%)	38 (100%)	0	100	100
55	B3	51/52 (98%)	51 (100%)	0	100	100
56	B4	34/34 (100%)	34 (100%)	0	100	100
57	B5	8/8 (100%)	8 (100%)	0	100	100
All	All	4594/4885 (94%)	4594 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
29	BD	164	GLN
32	BG	116	GLN
50	BY	25	GLN
30	BE	41	GLN
30	BE	97	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	218 (14%)	4 (0%)
22	AV	9/10 (90%)	0	0
23	AW	70/74 (94%)	13 (18%)	1 (1%)
24	AX	74/77 (96%)	6 (8%)	0
25	AY	67/71 (94%)	13 (19%)	1 (1%)
26	BA	2895/2897 (99%)	425 (14%)	10 (0%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	BB	117/120 (97%)	13 (11%)	0
All	All	4769/4788 (99%)	688 (14%)	16 (0%)

5 of 688 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	7	A
1	AA	8	A
1	AA	9	G
1	AA	32	A

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	404	A
26	BA	479	A
26	BA	2146	C
26	BA	271	G
26	BA	2225	A

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

21 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
23	U8U	AW	34	22,23	15,24,25	1.54	1 (6%)	17,34,37	3.48	2 (11%)
23	T6A	AW	37	23	23,34,35	1.19	2 (8%)	26,49,52	1.89	6 (23%)
23	PSU	AW	39	23	15,21,22	2.03	4 (26%)	16,30,33	2.85	5 (31%)
23	7MG	AW	46	23	20,26,27	1.85	5 (25%)	23,39,42	1.86	4 (17%)
23	3AU	AW	47	23	16,28,29	1.18	2 (12%)	16,40,43	0.78	1 (6%)
23	5MU	AW	54	23	13,22,23	1.42	1 (7%)	16,32,35	3.61	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	PSU	AW	55	23	15,21,22	2.05	4 (26%)	16,30,33	2.88	5 (31%)
23	4SU	AW	8	23	12,21,22	1.41	2 (16%)	15,30,33	2.03	1 (6%)
24	QUO	AX	34	24,22	27,35,36	1.66	4 (14%)	30,52,55	2.89	5 (16%)
24	2MA	AX	37	24	17,25,26	1.73	4 (23%)	18,37,40	1.63	1 (5%)
24	7MG	AX	46	24	20,26,27	1.89	5 (25%)	23,39,42	1.86	4 (17%)
24	5MU	AX	54	24	13,22,23	1.42	1 (7%)	16,32,35	3.59	2 (12%)
24	PSU	AX	55	24	15,21,22	2.03	4 (26%)	16,30,33	2.88	5 (31%)
24	PSU	AX	65	24	15,21,22	1.96	3 (20%)	16,30,33	2.88	3 (18%)
24	4SU	AX	8	24	12,21,22	1.41	2 (16%)	15,30,33	2.03	1 (6%)
25	CM0	AY	34	25	15,26,27	1.64	2 (13%)	18,37,40	2.72	3 (16%)
25	6MZ	AY	37	25	17,25,26	1.25	4 (23%)	15,36,39	0.93	1 (6%)
25	7MG	AY	46	25	20,26,27	1.87	5 (25%)	23,39,42	1.88	4 (17%)
25	5MU	AY	54	25	13,22,23	1.42	1 (7%)	16,32,35	3.61	2 (12%)
25	PSU	AY	55	25	15,21,22	2.00	4 (26%)	16,30,33	2.86	5 (31%)
25	4SU	AY	8	25	12,21,22	1.41	2 (16%)	15,30,33	2.03	1 (6%)

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
23	U8U	AW	34	22,23	-	0/5/28/29	0/2/2/2
23	T6A	AW	37	23	-	0/15/41/42	0/3/3/3
23	PSU	AW	39	23	-	0/7/25/26	0/2/2/2
23	7MG	AW	46	23	-	0/7/37/38	0/3/3/3
23	3AU	AW	47	23	-	0/8/34/35	0/2/2/2
23	5MU	AW	54	23	-	0/3/25/26	0/2/2/2
23	PSU	AW	55	23	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/3/25/26	0/2/2/2
24	QUO	AX	34	24,22	-	0/6/43/44	0/4/4/4
24	2MA	AX	37	24	-	0/3/25/26	0/3/3/3
24	7MG	AX	46	24	-	0/7/37/38	0/3/3/3
24	5MU	AX	54	24	-	0/3/25/26	0/2/2/2
24	PSU	AX	55	24	-	0/7/25/26	0/2/2/2
24	PSU	AX	65	24	-	0/7/25/26	0/2/2/2
24	4SU	AX	8	24	-	0/3/25/26	0/2/2/2
25	CM0	AY	34	25	-	0/6/30/31	0/2/2/2
25	6MZ	AY	37	25	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	7MG	AY	46	25	-	0/7/37/38	0/3/3/3
25	5MU	AY	54	25	-	0/3/25/26	0/2/2/2
25	PSU	AY	55	25	-	0/7/25/26	0/2/2/2
25	4SU	AY	8	25	-	0/3/25/26	0/2/2/2

The worst 5 of 62 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	55	PSU	C5-C1'	-2.77	1.49	1.52
23	AW	39	PSU	C5-C1'	-2.65	1.49	1.52
24	AX	55	PSU	C5-C1'	-2.63	1.49	1.52
24	AX	65	PSU	C6-C5	-2.48	1.35	1.38
23	AW	39	PSU	C6-C5	-2.48	1.35	1.38

The worst 5 of 63 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	34	QUO	C5-C6-N1	-14.01	113.38	124.15
23	AW	34	U8U	C5-C4-N3	-11.78	114.62	125.19
23	AW	54	5MU	C5-C4-N3	-10.41	116.61	125.35
25	AY	54	5MU	C5-C4-N3	-10.38	116.63	125.35
24	AX	54	5MU	C5-C4-N3	-10.35	116.66	125.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	AW	34	U8U	1	0
25	AY	34	CM0	1	0
25	AY	55	PSU	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.



## 5.6 Ligand geometry

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	$\# Z  > 2$
58	LYS	AW	101	23	6,8,9	0.79	0	6,8,10	1.55	1 (16%)
59	ERY	BA	9000	-	53,53,53	1.14	5 (9%)	82,82,82	1.66	22 (26%)

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
58	LYS	AW	101	23	-	0/5/7/9	0/0/0/0
59	ERY	BA	9000	-	-	0/72/107/107	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	BA	9000	ERY	O9-C26	-2.84	1.39	1.44
59	BA	9000	ERY	O13-C12	-2.84	1.39	1.44
59	BA	9000	ERY	O10-C6	-2.50	1.40	1.44
59	BA	9000	ERY	O2-C13	-2.45	1.42	1.46
59	BA	9000	ERY	C15-C14	2.01	1.56	1.51

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	BA	9000	ERY	C34-C10-C11	-3.58	109.62	114.44
59	BA	9000	ERY	C36-C13-C12	-3.48	107.79	115.13
58	AW	101	LYS	O-C-CA	-3.16	117.24	125.72
59	BA	9000	ERY	C12-C11-C10	-3.15	112.18	116.51
59	BA	9000	ERY	C16-C15-C14	-3.08	109.66	115.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	AW	101	LYS	3	0
59	BA	9000	ERY	12	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	AA	1
23	AW	1
25	AY	1
26	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.72
1	AW	15:G	O3'	18:G	P	9.77
1	AY	15:G	O3'	18:G	P	6.82
1	AA	99:C	O3'	100:G	P	4.17