



## wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:55 pm GMT

PDB ID : 4V6N  
EMDB ID: : EMD-5361  
Title : Structural characterization of mRNA-tRNA translocation intermediates (50S ribosome of class2 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 : 12.10 Å(reported)  
Based on PDB ID : 1ZAV, 1MZP, 2I2V

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report  
for a publicly released PDB/EMDB entry.

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>  
with specific help available everywhere you see the ⓘ symbol.

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MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc29047

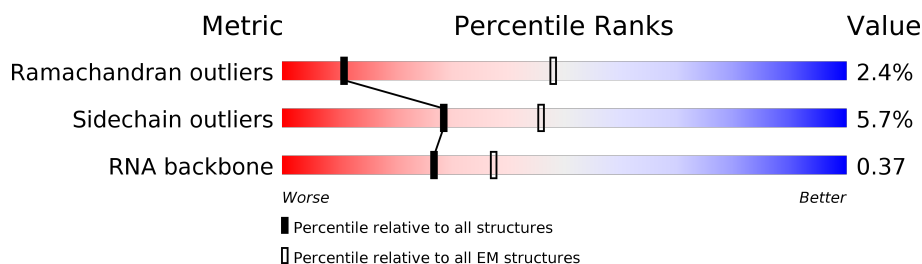
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 12.10 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.

















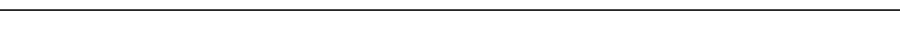




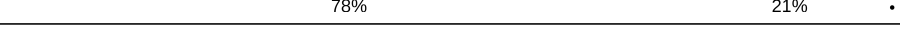





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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	120	
2	AB	2904	
3	AC	234	
4	AD	272	
5	AE	209	
6	AF	201	
7	AG	178	
8	AH	176	
9	AI	149	
















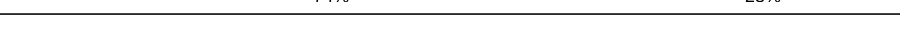

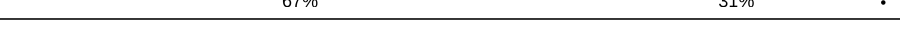
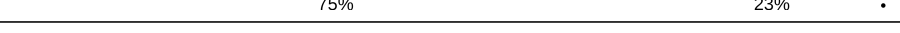
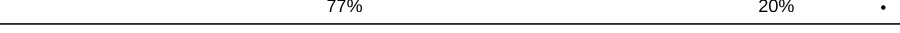




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Mol	Chain	Length	Quality of chain
10	AJ	164	 80% 18% .
11	AK	141	 84% 14% .
12	AL	142	 70% 25% 5%
13	AM	123	 74% 22% .
14	AN	144	 78% 20% .
15	AO	136	 79% 17% .
16	AP	127	 78% 20% .
17	AQ	117	 78% 20% .
18	AR	114	 74% 21% . .
19	AS	117	 78% 17% 5%
20	AT	103	 74% 23% .
21	AU	110	 72% 25% .
22	AV	100	 78% 21% .
23	AW	103	 77% 20% . .
24	AX	94	 84% 14% .
25	AY	84	 77% 18% 5%
26	AZ	77	 70% 25% 5%
27	A0	63	 79% 17% .
28	A1	58	 78% 21% .
29	A2	70	 77% 14% 9%
30	A3	56	 70% 21% 9%
31	A4	54	 72% 22% 6%
32	A5	46	 63% 33% .
33	A6	64	 80% 14% 6%
34	A7	38	 71% 29%

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Mol	Chain	Length	Quality of chain
35	BA	1542	
36	BB	76	
37	BC	47	
38	BD	77	
39	BE	240	
40	BF	232	
41	BG	205	
42	BH	166	
43	BI	135	
44	BJ	178	
45	BK	129	
46	BL	129	
47	BM	103	
48	BN	128	
49	BO	123	
50	BP	117	
51	BQ	100	
52	BR	88	
53	BS	82	
54	BT	83	
55	BU	74	
56	BV	91	
57	BW	86	
58	BX	70	

## 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 5S ribosomal RNA.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called 50S ribosomal protein L10.

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

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

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

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

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

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

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

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

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

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

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

- Molecule 16 is a protein called 50S ribosomal protein L17.

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

- Molecule 17 is a protein called 50S ribosomal protein L18.

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

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

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

- Molecule 20 is a protein called 50S ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

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

- Molecule 23 is a protein called 50S ribosomal protein L24.

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

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L27.

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

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	A0	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	A1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	A2	70	Total	C	N	O	S	0	0
			549	339	104	100	6		

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	A3	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	A4	54	Total	C	N	O	S	0	0
			441	284	81	76			

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A5	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	A6	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	A7	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a RNA chain called 16S ribosomal RNA.

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

- Molecule 36 is a RNA chain called A site tRNA.

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

- Molecule 37 is a RNA chain called mRNA.

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

- Molecule 38 is a RNA chain called P site tRNA.

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

- Molecule 39 is a protein called 30S ribosomal protein S2.

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

- Molecule 40 is a protein called 30S ribosomal protein S3.

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

- Molecule 41 is a protein called 30S ribosomal protein S4.

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

- Molecule 42 is a protein called 30S ribosomal protein S5.

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

- Molecule 43 is a protein called 30S ribosomal protein S6.

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

- Molecule 44 is a protein called 30S ribosomal protein S7.

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

- Molecule 45 is a protein called 30S ribosomal protein S8.

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

- Molecule 46 is a protein called 30S ribosomal protein S9.

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

- Molecule 47 is a protein called 30S ribosomal protein S10.

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

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

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

- Molecule 51 is a protein called 30S ribosomal protein S14.

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

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

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

- Molecule 55 is a protein called 30S ribosomal protein S18.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

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

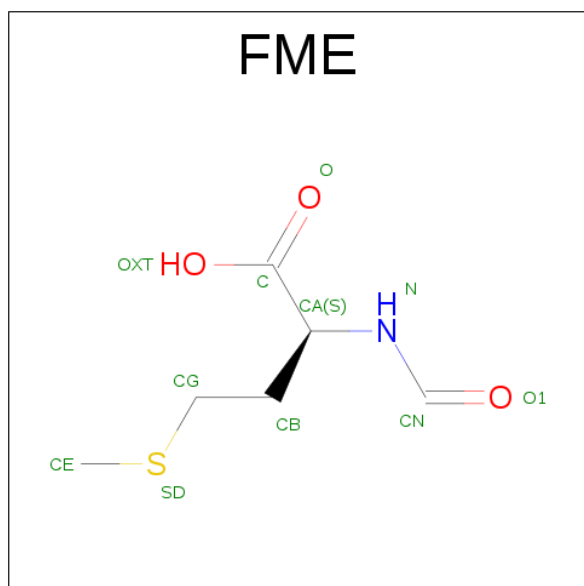
- Molecule 57 is a protein called 30S ribosomal protein S20.

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

- Molecule 58 is a protein called 30S ribosomal protein S21.

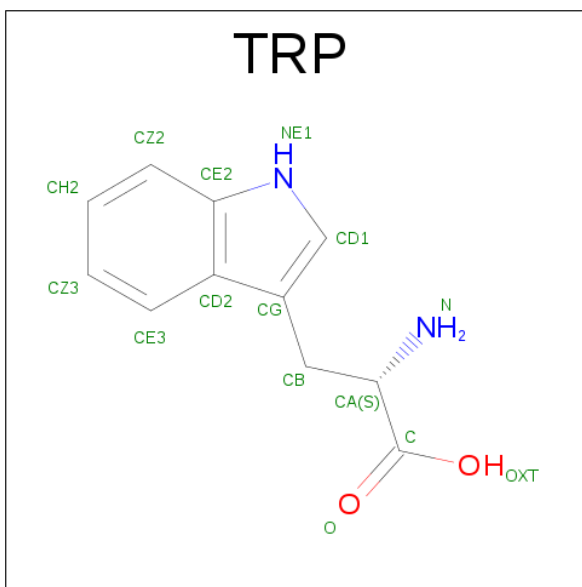
Mol	Chain	Residues	Atoms					AltConf	Trace
58	BX	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula:  $C_6H_{11}NO_3S$ ).



Mol	Chain	Residues	Atoms					AltConf
59	AB	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is TRYPTOPHAN (three-letter code: TRP) (formula:  $C_{11}H_{12}N_2O_2$ ).

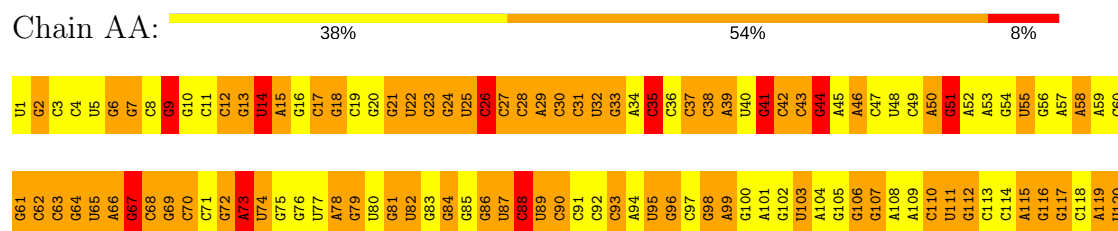


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	BB	1	14	11	2	1	0

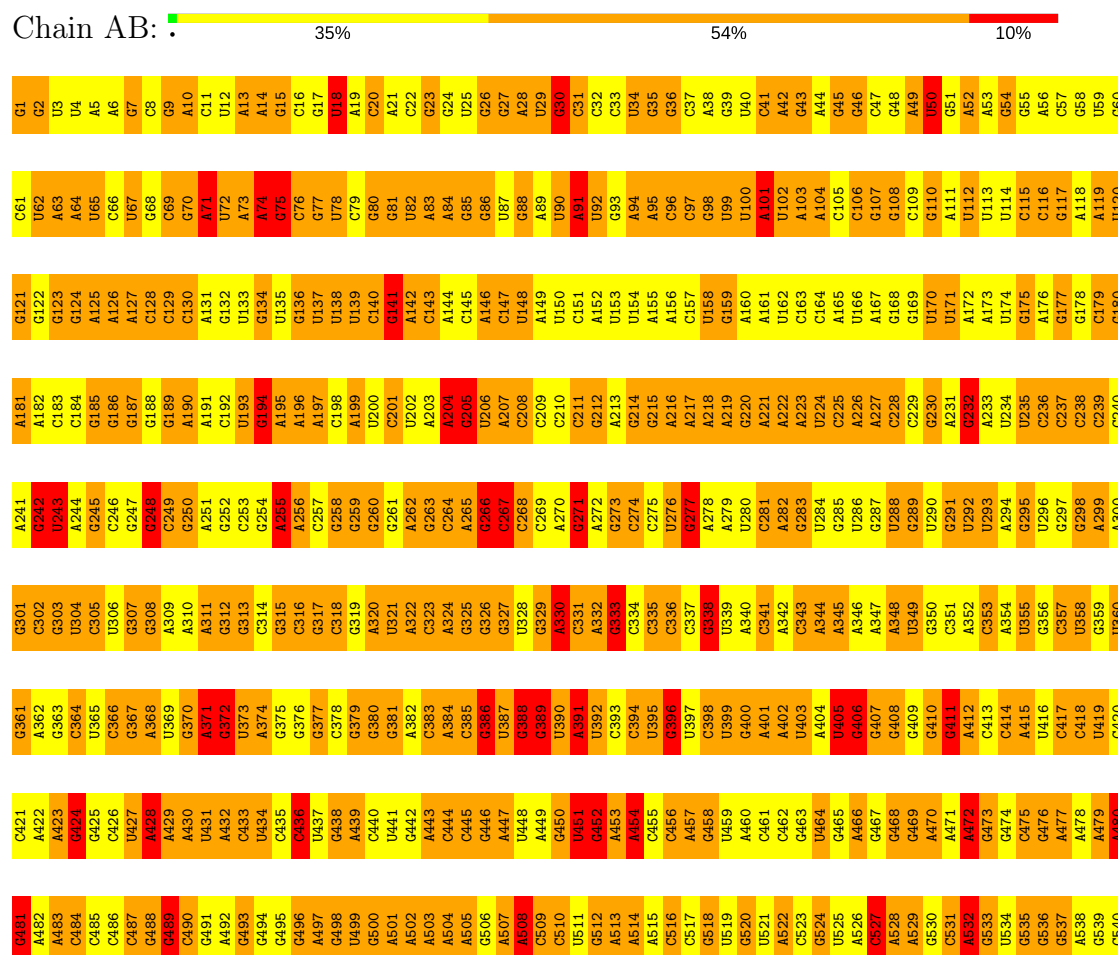
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: 5S ribosomal RNA



#### • Molecule 2: 23S ribosomal RNA



U1442	G1382	A1322	A1262	G1202	A1142	U1082	G1022	G962	C902	U842	A782	A721	G601	A541
U1443	A1383	C1323	U1263	U1203	A1143	U1083	U1023	U963	C903	G843	A783	A722	A602	C642
G1444	A1384	A1324	A1264	A1204	A1144	A1084	G1024	C964	G904	A844	G784	C723	A603	G543
G1445	U1385	A1325	A1265	A1205	A1145	A1085	G1025	C965	G905	A845	G785	U724	G604	G544
G1446	C1386	G1326	G1266	G1206	C1146	A1086	G1026	G966	U906	U846	C786	G725	G605	U545
G1447	A1387	U1327	U1267	G1207	U1147	A1087	A1027	U967	G907	U847	C787	G726	U606	U546
G1448	G1388	A1328	A1268	C1208	U1148	A1088	A1028	C968	C908	C848	A788	A727	U607	A547
G1449	G1389	A1329	A1269	U1209	G1149	A1089	A1029	G969	A909	A849	A789	G728	A608	G548
G1450	U1390	C1329	C1270	G1210	C1150	A1090	G1030	U970	A910	U850	U790	G729	A609	G549
G1451	U1391	G1271	G1271	C1211	A1151	G1091	A1031	G971	A911	C851	C791	A730	C611	C550
G1452	A1392	G1332	A1272	G1212	C1152	C1092	A1032	A972	C912	U852	A792	C731	G612	U552
A1453	G1393	G1333	U1273	A1213	G1153	G1093	U1033	A973	U913	C853	A793	G732	A613	G553
G1454	U1394	A1334	A1274	A1214	G1154	U1094	G1034	G974	G914	C854	A794	G733	C573	G554
G1455	A1395	C1335	A1275	G1215	A1155	A1095	U1035	A975	C915	G855	C795	A734	A614	U554
G1456	U1396	A1336	A1276	G1216	A1156	A1096	G1036	G976	A916	G856	A796	G735	U615	G555
G1457	G1397	G1337	U1277	U1217	G1157	U1097	G1037	G977	A917	G857	G797	C736	U616	A556
G1458	C1398	G1338	C1278	G1218	U1158	A1098	A1038	G978	A918	G858	A798	C737	G617	C557
G1459	G1399	G1339	G1279	U1219	U1159	G1099	U1039	A979	U919	G859	G799	G738	G618	U558
U1460	U1400	U1340	G1280	G1220	G1160	C1100	A1040	A980	A920	U860	A800	A739	G619	G559
C1461	G1401	G1341	G1281	C1221	C1161	U1101	G1041	A981	C921	A861	G801	C740	G620	C560
C1462	A1402	A1342	U1282	U1222	G1162	C1102	G1042	C982	C922	G862	A802	U741	A621	G561
C1463	G1343	G1343	G1283	G1223	C1163	A1103	C1043	A983	G923	A863	U803	A742	G622	U562
G1464	C1404	A1344	A1284	U1224	C1164	C1104	C1044	A984	G924	G864	A804	A743	C623	A563
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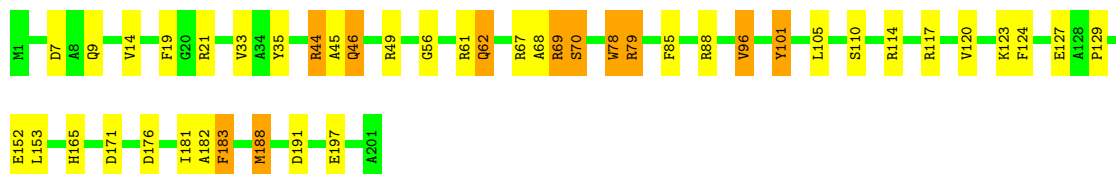
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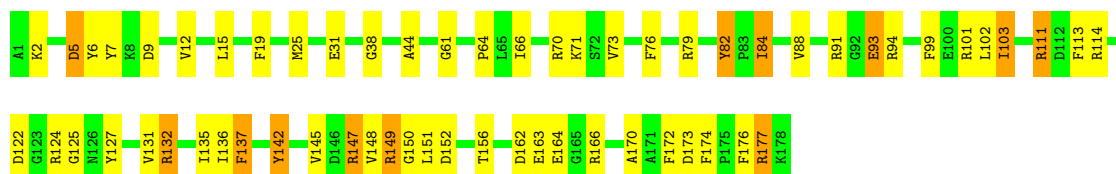
- Molecule 6: 50S ribosomal protein L4

Chain AF: 78% 16% 5%



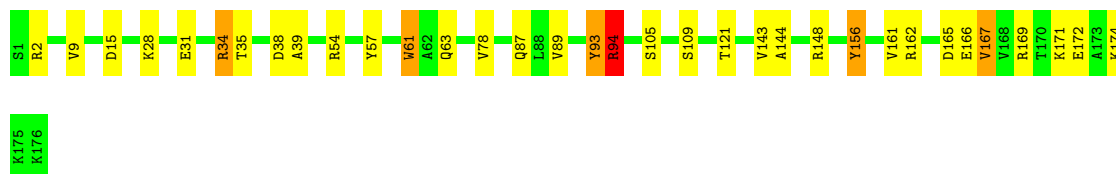
- Molecule 7: 50S ribosomal protein L5

Chain AG: 66% 28% 7%



- Molecule 8: 50S ribosomal protein L6

Chain AH: 81% 16% 3%



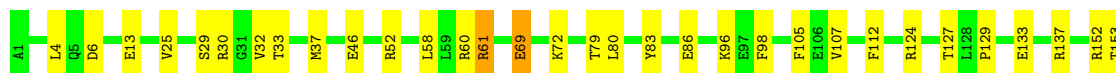
- Molecule 9: 50S ribosomal protein L9

Chain AI: 81% 15% 5%



- Molecule 10: 50S ribosomal protein L10

Chain AJ: 80% 18% 2%





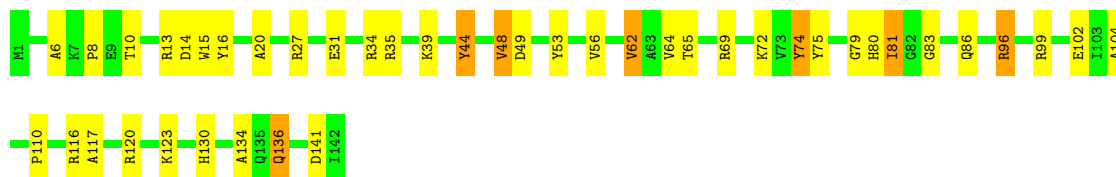
- Molecule 11: 50S ribosomal protein L11

Chain AK: 84% 14%



- Molecule 12: 50S ribosomal protein L13

Chain AL: 70% 25% 5%



- Molecule 13: 50S ribosomal protein L14

Chain AM: 74% 22%



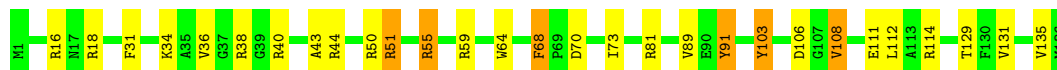
- Molecule 14: 50S ribosomal protein L15

Chain AN: 78% 20%



- Molecule 15: 50S ribosomal protein L16

Chain AO: 79% 17%



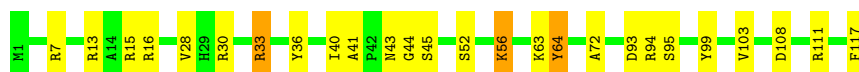
- Molecule 16: 50S ribosomal protein L17

Chain AP: 78% 20%



- Molecule 17: 50S ribosomal protein L18

Chain AQ: 78% 20%



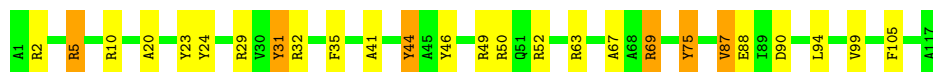
- Molecule 18: 50S ribosomal protein L19

Chain AR: 74% 21%



- Molecule 19: 50S ribosomal protein L20

Chain AS: 78% 17% 5%



- Molecule 20: 50S ribosomal protein L21

Chain AT: 74% 23%



- Molecule 21: 50S ribosomal protein L22

Chain AU: 72% 25%



- Molecule 22: 50S ribosomal protein L23

Chain AV: 78% 21%



- Molecule 23: 50S ribosomal protein L24

Chain AW: 77% 20%




- Molecule 24: 50S ribosomal protein L25

Chain AX: 84% 14%



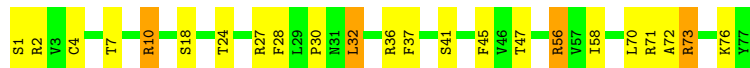
- Molecule 25: 50S ribosomal protein L27

Chain AY:  77% 18% 5%




- Molecule 26: 50S ribosomal protein L28

Chain AZ:  70% 25% 5%




- Molecule 27: 50S ribosomal protein L29

Chain A0:  79% 17% 4%




- Molecule 28: 50S ribosomal protein L30

Chain A1:  78% 21% 1%



- Molecule 29: 50S ribosomal protein L31

Chain A2:  77% 14% 9%



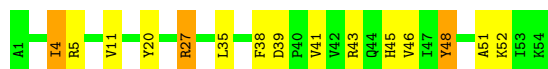
- Molecule 30: 50S ribosomal protein L32

Chain A3:  70% 21% 9%



- Molecule 31: 50S ribosomal protein L33

Chain A4:  72% 22% 6%

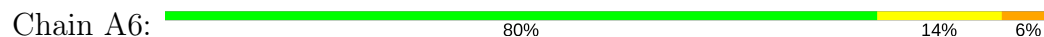


- Molecule 32: 50S ribosomal protein L34

Chain A5:  63% 33% 4%



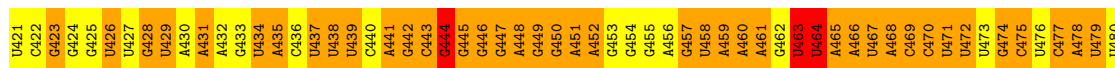
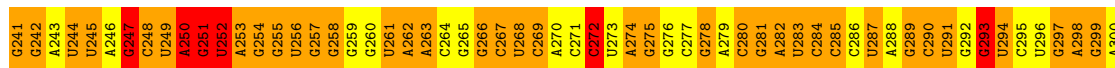
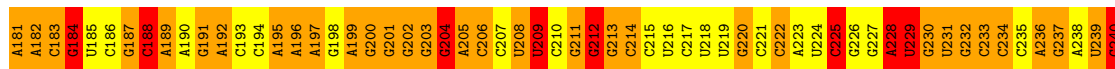
• Molecule 33: 50S ribosomal protein L35



• Molecule 34: 50S ribosomal protein L36



• Molecule 35: 16S ribosomal RNA



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A1503	U603	A663	U723	C783	U643	G903	G963	U1023	U1083	G1143	U1203	C1263	G1323	G1383	C1443	A1503
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A1508	A608	G668	A728	U788	C848	A908	A968	C1028	G1088	U1148	C1208	C1268	C1328	C1388	C1448	A1508
A1509	A609	G669	A729	U789	C849	A909	A969	U1029	G1089	C1149	C1209	A1269	A1329	C1389	C1449	A1509
C1510	U610	G670	G730	A790	U850	C910	C970	U1030	U1090	A1150	C1210	G1270	U1330	U1390	U1450	C1510
G1511	C611	G671	G731	G791	U851	U911	G971	C1031	U1091	A1151	U1211	A1271	G1331	G1391	U1451	G1511
U1512	C612	G672	C732	A792	G852	C912	G972	G1032	A1092	A1152	U1212	C1272	A1332	G1392	C1452	U1512
A1513	C613	U673	C733	U793	C853	A913	G973	G1033	A1093	G1153	U1213	C1273	A1333	U1393	G1453	A1513
G1514	G614	G674	G734	A794	U854	A914	A974	G1034	G1094	G1154	C1214	A1274	G1334	A1394	G1454	G1514
G1515	A615	A675	C735	C795	U855	A915	A975	A1035	U1095	A1155	G1215	A1275	U1335	C1395	G1455	G1515
G1516	A616	A676	C736	C796	C856	U916	G976	A1036	C1096	G1156	A1216	G1276	U1336	A1396	A1456	G1516
G1517	C617	U677	C737	C797	C857	G917	A977	C1037	U1097	A1157	C1217	C1277	G1337	C1397	G1457	G1517
C1520	C618	U678	C738	U798	G858	A918	A978	C1038	G1098	C1158	G1218	G1278	G1338	A1398	G1458	C1520
C1521	U619	C679	C739	G799	G859	A919	C979	G1039	G1099	U1159	A1219	G1279	G1339	C1399	G1459	C1521
U1522	C620	C680	U741	G800	A860	U920	C980	U1040	C1100	G1160	G1220	A1280	A1340	C1400	G1460	U1522
G1523	A621	A681	U742	U801	G861	U921	U981	G1041	A1101	C1161	G1221	C1281	U1341	U1401	G1461	G1523
C1524	A622	G682	G743	A802	C862	G922	U982	A1042	A1102	C1162	G1222	U1282	C1342	C1402	U1462	C1524
G1525	C624	G683	A744	G803	U863	A923	A983	G1043	C1103	A1163	C1223	U1283	G1343	C1403	U1463	G1525
U1526	U625	U684	C744	U804	A864	G924	C984	A1044	G1104	G1164	U1224	A1284	C1344	U1404	G1464	U1526
U1527	G626	G685	G745	C805	A865	G925	C985	A1045	A1105	U1165	A1225	U1285	C1345	G1405	A1465	U1527
U1528	G627	U686	A746	C806	C866	G926	U986	A1046	G1106	G1166	C1226	U1286	A1346	U1406	C1466	U1528
G1529	G628	A687	U747	A807	G867	G927	G987	G1047	C1107	A1167	C1227	A1287	U1347	U1407	G1467	G1529
U1530	A629	C689	G748	C808	C868	G928	U988	G1048	U1108	U1168	C1228	A1288	U1348	C1408	U1468	U1530
A1531	A630	U690	C750	A809	G869	G929	U989	G1049	C1109	A1169	A1229	A1289	A1349	U1409	G1469	A1531
U1532	C631	G691	U751	C810	U870	C930	C990	G1050	A1110	A1170	C1230	U1290	A1350	U1410	U1470	U1532
C1533	U632	G692	G752	C811	U871	C931	U991	C1051	C1111	A1171	G1231	U1291	U1351	C1411	U1471	C1533
A1534	G633	G693	G753	G812	A872	C932	U992	U1052	C1112	C1172	U1232	U1292	C1352	C1412	C1472	A1534
C1535	A634	A694	C754	U813	A873	G933	G993	G1053	C1113	U1173	U1233	C1293	C1353	G1413	G1473	C1535
U1537	U636	A695	G755	A815	G874	C934	A994	A1054	C1114	G1174	U1234	U1294	U1354	U1414	U1474	U1537
C1538	C637	A696	C756	U816	C875	C936	A996	U1056	U1116	A1176	A1236	C1296	G1356	G1416	A1476	C1538
U1539	U638	U697	U757	G817	G877	A937	U997	G1057	C1117	G1177	G1237	U1297	U1357	G1417	U1477	U1539
U1541	G639	G698	C758	C818	A878	A938	C998	G1058	U1118	G1178	A1238	U1298	U1358	A1418	U1478	U1541
A1542	A640	C699	A759	A819	C879	G939	C999	C1059	C1119	A1179	U1239	A1299	C1359	G1419	C1479	A1542
	U641	G700	G760	U820	C880	C940	A1000	U1060	C1120	A1180	U1240	A1300	U1360	U1420	C1480	
	A642	U701	G761	G821	C881	G941	C1001	G1061	U1121	G1181	G1241	U1301	U1361	G1421	U1481	
	C643	A702	U762	U822	C882	G942	G1002	U1062	U1122	G1182	C1242	C1302	U1362	G1422	G1482	
	U644	G703	G763	G823	C883	U943	C1003	C1063	U1123	U1183	C1243	C1303	U1363	G1423	U1483	
	A645	A704	C764	G824	U884	G944	A1004	G1064	G1124	G1184	C1244	C1304	U1364	U1424	C1484	
	G645	G705	G765	A825	C885	G945	A1005	U1065	U1125	G1185	C1245	G1305	U1365	U1425	U1485	
	A646	A706	A766	C826	G886	A946	C1006	C1066	U1126	G1186	A1246	A1306	C1366	G1426	U1486	
	U647	U707	A767	U827	C887	G947	U1007	A1067	U1127	G1187	U1247	U1307	C1367	G1427	G1487	
	A648	C708	A768	U828	G888	C948	U1008	G1068	C1128	A1188	A1248	U1308	U1368	A1428	G1488	
	U649	U709	G769	G829	A889	A949	U1009	C1069	C1129	U1189	C1249	G1309	C1369	A1429	G1489	
	G650	G710	C770	G830	C890	U950	U1010	U1070	A1130	G1190	A1250	G1310	U1370	A1430	U1490	
	C651	G711	U771	A831	U891	G951	C1011	C1071	C1131	A1191	A1251	A1311	U1371	A1431	G1491	
	U652	U772	G772	A832	A892	U952	C1012	G1072	C1132	C1192	A1252	G1312	U1372	A1432	A1492	
	G653	G713	G773	G833	C893	G953	G1013	U1073	G1133	G1193	G1253	U1313	U1373	A1433	A1493	
	A654	G714	G774	U834	G894	A1014	G1014	G1074	G1134	U1194	A1254	C1314	A1374	A1434	G1494	
	G655	A715	G775	U835	G895	U955	G1015	U1075	U1135	C1195	G1255	U1315	U1375	U1435	U1495	
	U657	G716	G776	G836	C896	U956	A1016	U1076	U1136	A1196	A1257	C1316	U1376	U1436	G1496	
	C658	U717	A777	U837	C897	U957	U1017	G1077	C1137	A1197	A1258	C1317	U1377	A1437	G1497	
	U659	G718	G778	G838	C898	A958	G1018	U1078	G1138	U1198	G1259	A1318	U1378	A1438	U1498	
	C660	C719	C779	C839	C899	A959	A1019	U1079	G1139	U1199	G1260	A1319	U1379	G1439	U1499	
		A780		C840	A900	U960	G1020	A1080	C1140	C1200						

• Molecule 36: A site tRNA

Chain BB:  5% 30% 50% 14%



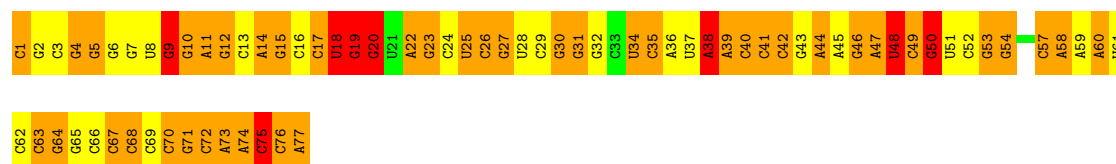
- Molecule 37: mRNA

Chain BC: 



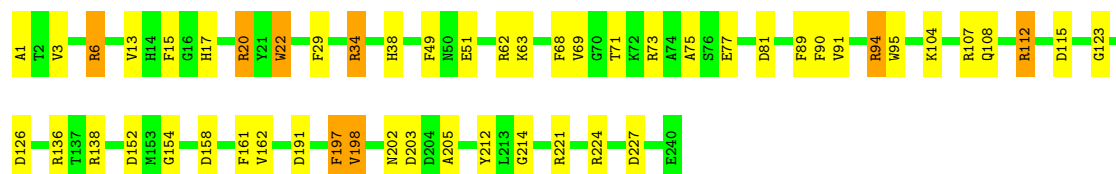
- Molecule 38: P site tRNA

Chain BD:  5% 30% 55% 10%




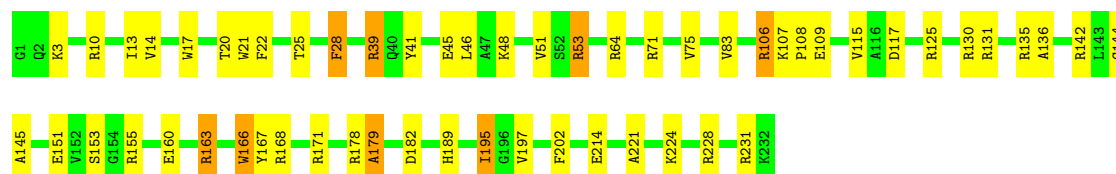
- Molecule 39: 30S ribosomal protein S2

Chain BE: 




- Molecule 40: 30S ribosomal protein S3

Chain BF:  76% 21%



- Molecule 41: 30S ribosomal protein S4

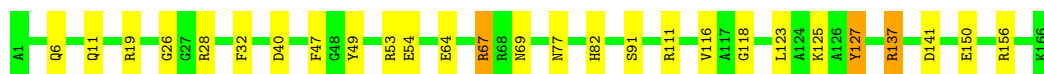
Chain BG:  76% 21%





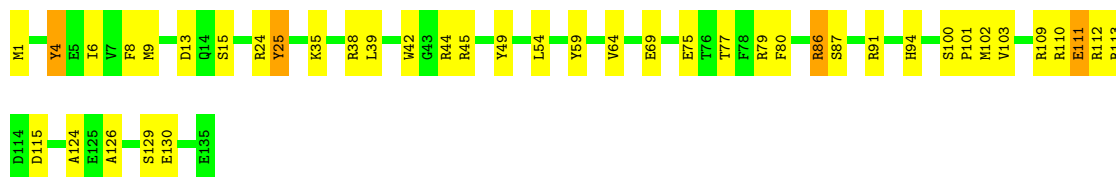
- Molecule 42: 30S ribosomal protein S5

Chain BH: 84% 14% •



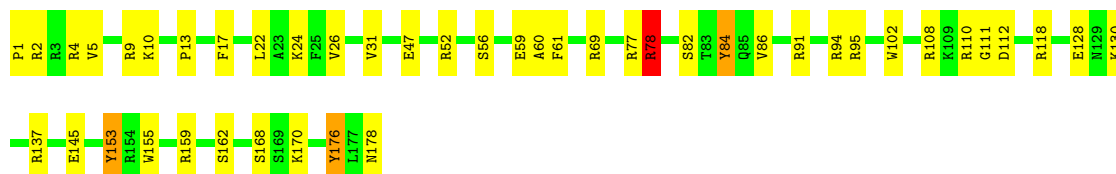
- Molecule 43: 30S ribosomal protein S6

Chain BI: 69% 28% •



- Molecule 44: 30S ribosomal protein S7

Chain BJ: 75% 23% ••



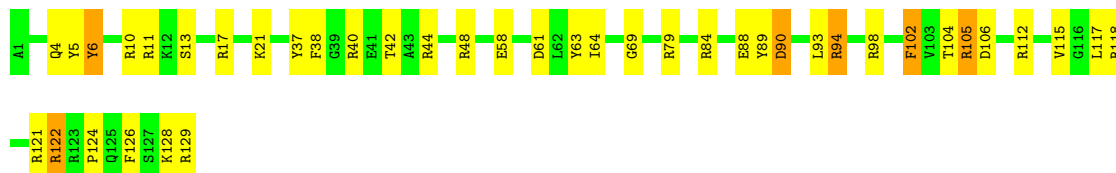
- Molecule 45: 30S ribosomal protein S8

Chain BK: 78% 16% 5%



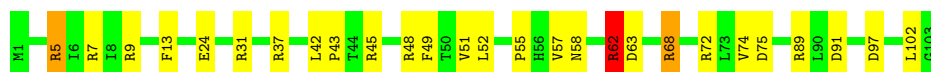
- Molecule 46: 30S ribosomal protein S9

Chain BL: 68% 27% 5%



- Molecule 47: 30S ribosomal protein S10

Chain BM: 74% 23% ••



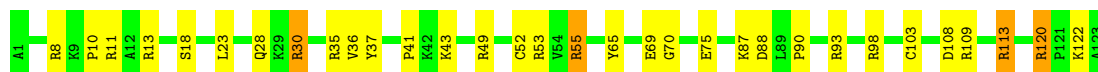
- Molecule 48: 30S ribosomal protein S11

Chain BN: 77% 18% 5%



- Molecule 49: 30S ribosomal protein S12

Chain BO: 74% 23% •



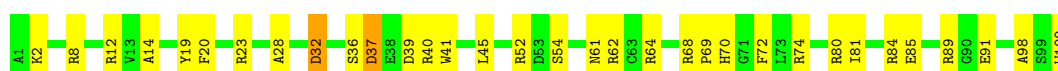
- Molecule 50: 30S ribosomal protein S13

Chain BP: 77% 19% •



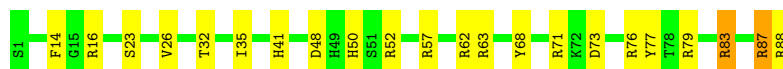
- Molecule 51: 30S ribosomal protein S14

Chain BQ: 67% 31% •



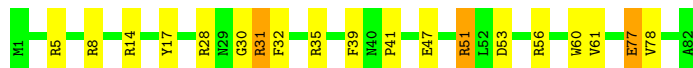
- Molecule 52: 30S ribosomal protein S15

Chain BR: 75% 23% •



- Molecule 53: 30S ribosomal protein S16

Chain BS: 77% 20% •

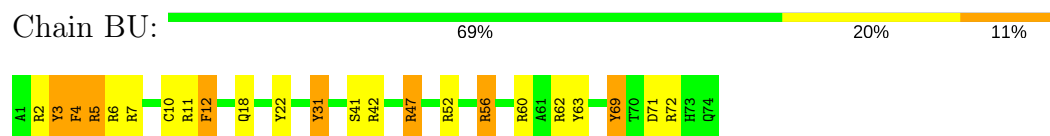


- Molecule 54: 30S ribosomal protein S17

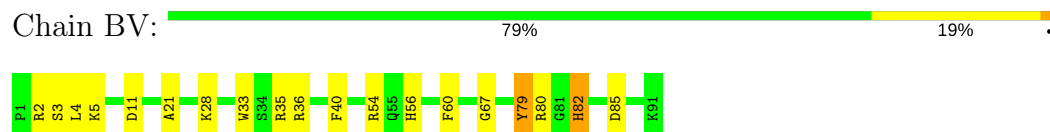
Chain BT: 75% 24% •



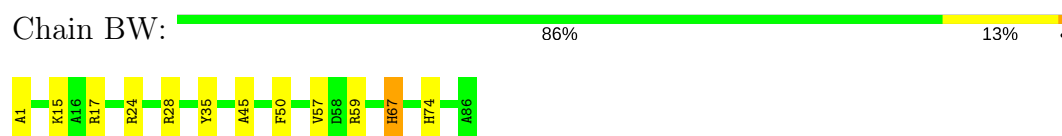
- Molecule 55: 30S ribosomal protein S18



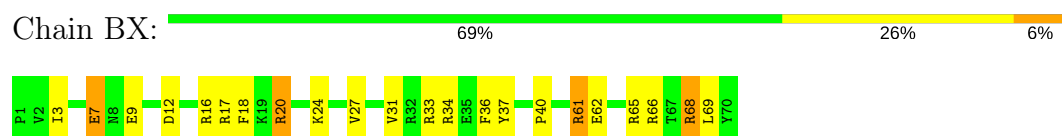
- Molecule 56: 30S ribosomal protein S19



- Molecule 57: 30S ribosomal protein S20



- Molecule 58: 30S ribosomal protein S21



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	36204	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	58269	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: 3TD, 5MU, CH, OMG, OMU, MA6, MIA, OMC, H2U, 2MA, 6MZ, 2MG, 5MC, UR3, 4OC, FME, 4SU, 7MG, 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	3.14	330/2869 (11.5%)	3.60	681/4474 (15.2%)
10	AJ	1.56	7/1247 (0.6%)	1.92	21/1679 (1.3%)
11	AK	1.50	3/1046 (0.3%)	1.84	19/1410 (1.3%)
12	AL	1.52	7/1152 (0.6%)	1.94	33/1551 (2.1%)
13	AM	1.41	1/956 (0.1%)	1.89	24/1279 (1.9%)
14	AN	1.52	2/1062 (0.2%)	1.98	27/1413 (1.9%)
15	AO	1.48	2/1093 (0.2%)	2.19	34/1460 (2.3%)
16	AP	1.48	4/1021 (0.4%)	2.00	21/1364 (1.5%)
17	AQ	1.49	3/910 (0.3%)	1.93	24/1219 (2.0%)
18	AR	1.56	6/929 (0.6%)	2.07	25/1242 (2.0%)
19	AS	1.57	5/960 (0.5%)	2.21	34/1278 (2.7%)
2	AB	3.07	7254/69257 (10.5%)	3.51	15515/108040 (14.4%)
20	AT	1.56	1/829 (0.1%)	1.93	19/1107 (1.7%)
21	AU	1.47	4/864 (0.5%)	2.01	27/1156 (2.3%)
22	AV	1.49	4/794 (0.5%)	1.86	17/1060 (1.6%)
23	AW	1.53	4/797 (0.5%)	1.94	20/1062 (1.9%)
24	AX	1.46	2/766 (0.3%)	1.80	14/1025 (1.4%)
25	AY	1.51	0/642	1.97	16/848 (1.9%)
26	AZ	1.57	3/635 (0.5%)	2.13	20/848 (2.4%)
27	A0	1.51	1/510 (0.2%)	1.90	10/677 (1.5%)
28	A1	1.41	1/453 (0.2%)	2.05	17/605 (2.8%)
29	A2	1.55	1/559 (0.2%)	2.18	16/745 (2.1%)
3	AC	1.50	7/1748 (0.4%)	1.83	37/2355 (1.6%)
30	A3	1.53	4/450 (0.9%)	2.15	17/599 (2.8%)
31	A4	1.50	0/448	1.96	12/594 (2.0%)
32	A5	1.49	4/380 (1.1%)	2.28	17/498 (3.4%)
33	A6	1.49	3/513 (0.6%)	1.89	11/676 (1.6%)
34	A7	1.42	1/303 (0.3%)	2.16	11/397 (2.8%)
35	BA	3.10	3971/36769 (10.8%)	3.53	8378/57354 (14.6%)
36	BB	3.03	178/1600 (11.1%)	3.53	372/2492 (14.9%)
37	BC	3.13	119/1108 (10.7%)	3.48	238/1724 (13.8%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
38	BD	3.05	179/1721 (10.4%)	3.56	400/2683 (14.9%)
39	BE	1.49	8/1904 (0.4%)	1.96	46/2565 (1.8%)
4	AD	1.51	4/2131 (0.2%)	1.99	62/2863 (2.2%)
40	BF	1.49	6/1852 (0.3%)	1.99	48/2490 (1.9%)
41	BG	1.57	9/1665 (0.5%)	2.08	56/2227 (2.5%)
42	BH	1.50	5/1239 (0.4%)	1.87	27/1664 (1.6%)
43	BI	1.55	5/1121 (0.4%)	2.04	41/1509 (2.7%)
44	BJ	1.54	8/1422 (0.6%)	1.94	39/1908 (2.0%)
45	BK	1.42	7/989 (0.7%)	1.98	21/1326 (1.6%)
46	BL	1.56	8/1048 (0.8%)	2.24	44/1394 (3.2%)
47	BM	1.49	3/835 (0.4%)	2.00	25/1127 (2.2%)
48	BN	1.48	2/982 (0.2%)	2.08	28/1323 (2.1%)
49	BO	1.52	4/969 (0.4%)	1.90	23/1300 (1.8%)
5	AE	1.50	6/1586 (0.4%)	1.92	28/2134 (1.3%)
50	BP	1.52	5/919 (0.5%)	2.05	25/1226 (2.0%)
51	BQ	1.62	9/817 (1.1%)	2.10	30/1088 (2.8%)
52	BR	1.47	1/724 (0.1%)	2.09	29/966 (3.0%)
53	BS	1.52	1/659 (0.2%)	2.18	22/884 (2.5%)
54	BT	1.55	4/681 (0.6%)	2.06	19/913 (2.1%)
55	BU	1.55	4/637 (0.6%)	2.18	28/851 (3.3%)
56	BV	1.52	2/744 (0.3%)	1.90	13/995 (1.3%)
57	BW	1.49	2/676 (0.3%)	1.78	7/895 (0.8%)
58	BX	1.58	2/598 (0.3%)	2.02	22/792 (2.8%)
6	AF	1.47	5/1571 (0.3%)	1.92	37/2113 (1.8%)
7	AG	1.60	10/1444 (0.7%)	2.03	49/1937 (2.5%)
8	AH	1.53	3/1343 (0.2%)	1.92	28/1816 (1.5%)
9	AI	1.45	3/1122 (0.3%)	1.96	24/1515 (1.6%)
All	All	2.70	12237/164069 (7.5%)	3.17	26948/244735 (11.0%)

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	68
10	AJ	0	3
11	AK	0	2
12	AL	0	4
13	AM	0	5
14	AN	0	4
15	AO	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
16	AP	0	8
17	AQ	0	2
18	AR	0	7
19	AS	0	5
2	AB	0	1652
20	AT	0	5
21	AU	0	2
22	AV	0	1
23	AW	0	1
24	AX	0	1
25	AY	0	7
26	AZ	0	2
27	A0	0	4
28	A1	0	1
29	A2	0	3
3	AC	0	2
30	A3	0	3
31	A4	0	2
33	A6	0	5
35	BA	0	910
36	BB	0	37
37	BC	0	28
38	BD	0	45
39	BE	0	4
4	AD	0	11
40	BF	0	7
41	BG	0	2
42	BH	0	3
43	BI	0	5
44	BJ	0	6
45	BK	0	4
46	BL	0	4
47	BM	0	2
48	BN	0	3
49	BO	0	8
5	AE	0	11
50	BP	0	2
51	BQ	0	3
52	BR	0	1
53	BS	0	4
54	BT	0	1
55	BU	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
56	BV	0	4
57	BW	0	2
58	BX	0	3
6	AF	0	3
7	AG	0	8
8	AH	0	5
9	AI	0	3
All	All	0	2936

The worst 5 of 12237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AB	2225	A	N3-C4	18.05	1.45	1.34
2	AB	2615	U	C2-N3	17.29	1.49	1.37
35	BA	729	A	P-O5'	15.61	1.75	1.59
2	AB	1970	A	N9-C4	15.52	1.47	1.37
2	AB	1008	A	N3-C4	15.09	1.44	1.34

The worst 5 of 26948 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	2855	C	N3-C4-C5	-23.45	112.52	121.90
2	AB	1264	A	N9-C4-C5	22.40	114.76	105.80
29	A2	25	ARG	NE-CZ-NH1	21.63	131.12	120.30
2	AB	248	G	C2-N3-C4	20.59	122.19	111.90
2	AB	6	A	C8-N9-C4	-20.57	97.57	105.80

There are no chirality outliers.

5 of 2936 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	C	Sidechain
1	AA	2	G	Sidechain
1	AA	6	G	Sidechain
1	AA	7	G	Sidechain
1	AA	9	G	Sidechain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	2566	0	1294	0	0
2	AB	62351	0	31238	0	0
3	AC	1733	0	1824	0	0
4	AD	2092	0	2170	0	0
5	AE	1565	0	1616	0	0
6	AF	1552	0	1619	0	0
7	AG	1420	0	1460	0	0
8	AH	1323	0	1374	0	0
9	AI	1111	0	1148	0	0
10	AJ	1233	0	1283	0	0
11	AK	1032	0	1088	0	0
12	AL	1129	0	1162	0	0
13	AM	947	0	1023	0	0
14	AN	1053	0	1129	0	0
15	AO	1074	0	1157	0	0
16	AP	1008	0	1045	0	0
17	AQ	900	0	935	0	0
18	AR	917	0	965	0	0
19	AS	947	0	1022	0	0
20	AT	816	0	839	0	0
21	AU	857	0	922	0	0
22	AV	787	0	846	0	0
23	AW	789	0	847	0	0
24	AX	753	0	780	0	0
25	AY	634	0	656	0	0
26	AZ	625	0	655	0	0
27	A0	509	0	543	0	0
28	A1	449	0	491	0	0
29	A2	549	0	552	0	0
30	A3	444	0	461	0	0
31	A4	441	0	485	0	0
32	A5	377	0	418	0	0
33	A6	504	0	574	0	0
34	A7	302	0	343	0	0
35	BA	33089	0	16604	0	0
36	BB	1627	0	845	0	0
37	BC	993	0	499	0	0
38	BD	1641	0	841	0	0
39	BE	1872	0	1885	0	0
40	BF	1822	0	1913	0	0
41	BG	1643	0	1710	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	BH	1225	0	1273	0	0
43	BI	1101	0	1050	0	0
44	BJ	1400	0	1449	0	0
45	BK	979	0	1034	0	0
46	BL	1036	0	1084	0	0
47	BM	825	0	865	0	0
48	BN	965	0	997	0	0
49	BO	955	0	1019	0	0
50	BP	910	0	981	0	0
51	BQ	805	0	847	0	0
52	BR	716	0	742	0	0
53	BS	649	0	666	0	0
54	BT	672	0	716	0	0
55	BU	626	0	651	0	0
56	BV	727	0	768	0	0
57	BW	670	0	722	0	0
58	BX	590	0	631	0	0
59	AB	10	0	10	0	0
60	BB	14	0	9	0	0
All	All	152351	0	103775	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	
3	AC	232/234 (99%)	214 (92%)	12 (5%)	6 (3%)	6	40
4	AD	270/272 (99%)	237 (88%)	24 (9%)	9 (3%)	4	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AE	207/209 (99%)	171 (83%)	28 (14%)	8 (4%)	3	31
6	AF	199/201 (99%)	172 (86%)	18 (9%)	9 (4%)	3	29
7	AG	176/178 (99%)	151 (86%)	16 (9%)	9 (5%)	2	26
8	AH	174/176 (99%)	158 (91%)	13 (8%)	3 (2%)	11	50
9	AI	147/149 (99%)	131 (89%)	10 (7%)	6 (4%)	3	30
10	AJ	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	28	71
11	AK	139/141 (99%)	135 (97%)	4 (3%)	0	100	100
12	AL	140/142 (99%)	119 (85%)	16 (11%)	5 (4%)	4	33
13	AM	121/123 (98%)	107 (88%)	9 (7%)	5 (4%)	3	30
14	AN	142/144 (99%)	127 (89%)	12 (8%)	3 (2%)	8	45
15	AO	134/136 (98%)	123 (92%)	8 (6%)	3 (2%)	8	44
16	AP	125/127 (98%)	114 (91%)	10 (8%)	1 (1%)	22	67
17	AQ	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
18	AR	112/114 (98%)	97 (87%)	13 (12%)	2 (2%)	10	49
19	AS	115/117 (98%)	107 (93%)	4 (4%)	4 (4%)	4	34
20	AT	101/103 (98%)	91 (90%)	8 (8%)	2 (2%)	9	46
21	AU	108/110 (98%)	100 (93%)	5 (5%)	3 (3%)	6	39
22	AV	98/100 (98%)	75 (76%)	20 (20%)	3 (3%)	5	37
23	AW	101/103 (98%)	89 (88%)	10 (10%)	2 (2%)	9	46
24	AX	92/94 (98%)	87 (95%)	4 (4%)	1 (1%)	17	60
25	AY	82/84 (98%)	63 (77%)	17 (21%)	2 (2%)	7	42
26	AZ	75/77 (97%)	66 (88%)	7 (9%)	2 (3%)	6	40
27	A0	61/63 (97%)	56 (92%)	4 (7%)	1 (2%)	11	51
28	A1	56/58 (97%)	54 (96%)	2 (4%)	0	100	100
29	A2	68/70 (97%)	64 (94%)	3 (4%)	1 (2%)	12	53
30	A3	54/56 (96%)	47 (87%)	4 (7%)	3 (6%)	2	25
31	A4	52/54 (96%)	49 (94%)	1 (2%)	2 (4%)	4	32
32	A5	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	3	29
33	A6	62/64 (97%)	59 (95%)	2 (3%)	1 (2%)	11	51
34	A7	36/38 (95%)	29 (81%)	5 (14%)	2 (6%)	2	25
39	BE	238/240 (99%)	220 (92%)	12 (5%)	6 (2%)	6	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	BF	230/232 (99%)	217 (94%)	8 (4%)	5 (2%)	8	44
41	BG	203/205 (99%)	189 (93%)	11 (5%)	3 (2%)	12	53
42	BH	164/166 (99%)	149 (91%)	13 (8%)	2 (1%)	15	57
43	BI	133/135 (98%)	123 (92%)	9 (7%)	1 (1%)	22	67
44	BJ	176/178 (99%)	164 (93%)	9 (5%)	3 (2%)	11	50
45	BK	127/129 (98%)	119 (94%)	7 (6%)	1 (1%)	22	67
46	BL	127/129 (98%)	115 (91%)	9 (7%)	3 (2%)	7	42
47	BM	101/103 (98%)	90 (89%)	6 (6%)	5 (5%)	2	27
48	BN	126/128 (98%)	112 (89%)	11 (9%)	3 (2%)	7	42
49	BO	121/123 (98%)	107 (88%)	12 (10%)	2 (2%)	11	50
50	BP	115/117 (98%)	110 (96%)	3 (3%)	2 (2%)	11	50
51	BQ	98/100 (98%)	84 (86%)	9 (9%)	5 (5%)	2	26
52	BR	86/88 (98%)	81 (94%)	4 (5%)	1 (1%)	15	57
53	BS	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
54	BT	81/83 (98%)	72 (89%)	8 (10%)	1 (1%)	15	57
55	BU	72/74 (97%)	62 (86%)	7 (10%)	3 (4%)	3	30
56	BV	89/91 (98%)	82 (92%)	6 (7%)	1 (1%)	17	60
57	BW	84/86 (98%)	79 (94%)	4 (5%)	1 (1%)	15	57
58	BX	68/70 (97%)	61 (90%)	4 (6%)	3 (4%)	3	29
All	All	6319/6423 (98%)	5710 (90%)	457 (7%)	152 (2%)	11	42

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	217	THR
4	AD	94	LEU
6	AF	62	GLN
6	AF	188	MET
7	AG	136	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	181/181 (100%)	177 (98%)	4 (2%)	57	79
4	AD	217/217 (100%)	212 (98%)	5 (2%)	56	79
5	AE	164/164 (100%)	148 (90%)	16 (10%)	9	34
6	AF	165/165 (100%)	156 (94%)	9 (6%)	25	58
7	AG	149/149 (100%)	140 (94%)	9 (6%)	22	55
8	AH	137/137 (100%)	125 (91%)	12 (9%)	12	39
9	AI	114/114 (100%)	107 (94%)	7 (6%)	22	55
10	AJ	122/122 (100%)	111 (91%)	11 (9%)	11	38
11	AK	109/109 (100%)	104 (95%)	5 (5%)	31	62
12	AL	116/116 (100%)	104 (90%)	12 (10%)	8	32
13	AM	104/104 (100%)	96 (92%)	8 (8%)	15	47
14	AN	103/103 (100%)	98 (95%)	5 (5%)	29	61
15	AO	109/109 (100%)	106 (97%)	3 (3%)	49	74
16	AP	103/103 (100%)	100 (97%)	3 (3%)	48	73
17	AQ	87/87 (100%)	81 (93%)	6 (7%)	18	51
18	AR	99/99 (100%)	91 (92%)	8 (8%)	14	44
19	AS	89/89 (100%)	87 (98%)	2 (2%)	57	79
20	AT	84/84 (100%)	77 (92%)	7 (8%)	13	43
21	AU	93/93 (100%)	87 (94%)	6 (6%)	20	52
22	AV	84/84 (100%)	80 (95%)	4 (5%)	30	61
23	AW	84/84 (100%)	79 (94%)	5 (6%)	22	55
24	AX	78/78 (100%)	74 (95%)	4 (5%)	28	60
25	AY	62/62 (100%)	60 (97%)	2 (3%)	44	71
26	AZ	67/67 (100%)	61 (91%)	6 (9%)	11	38
27	A0	55/55 (100%)	52 (94%)	3 (6%)	25	58
28	A1	48/48 (100%)	46 (96%)	2 (4%)	34	64
29	A2	62/62 (100%)	56 (90%)	6 (10%)	9	35
30	A3	47/47 (100%)	45 (96%)	2 (4%)	33	64
31	A4	48/48 (100%)	44 (92%)	4 (8%)	13	43
32	A5	38/38 (100%)	34 (90%)	4 (10%)	8	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	A6	51/51 (100%)	50 (98%)	1 (2%)	60	82
34	A7	34/34 (100%)	33 (97%)	1 (3%)	48	73
39	BE	198/198 (100%)	187 (94%)	11 (6%)	25	57
40	BF	189/189 (100%)	176 (93%)	13 (7%)	18	51
41	BG	172/172 (100%)	165 (96%)	7 (4%)	35	65
42	BH	125/125 (100%)	120 (96%)	5 (4%)	36	65
43	BI	116/116 (100%)	109 (94%)	7 (6%)	22	55
44	BJ	146/146 (100%)	138 (94%)	8 (6%)	25	58
45	BK	104/104 (100%)	93 (89%)	11 (11%)	8	31
46	BL	106/106 (100%)	99 (93%)	7 (7%)	19	52
47	BM	90/90 (100%)	87 (97%)	3 (3%)	43	70
48	BN	98/98 (100%)	93 (95%)	5 (5%)	28	60
49	BO	103/103 (100%)	96 (93%)	7 (7%)	18	51
50	BP	95/95 (100%)	90 (95%)	5 (5%)	26	59
51	BQ	83/83 (100%)	81 (98%)	2 (2%)	54	78
52	BR	76/76 (100%)	74 (97%)	2 (3%)	51	75
53	BS	65/65 (100%)	64 (98%)	1 (2%)	70	85
54	BT	77/77 (100%)	72 (94%)	5 (6%)	20	52
55	BU	64/64 (100%)	61 (95%)	3 (5%)	30	62
56	BV	78/78 (100%)	73 (94%)	5 (6%)	20	53
57	BW	65/65 (100%)	63 (97%)	2 (3%)	45	71
58	BX	60/60 (100%)	56 (93%)	4 (7%)	19	51
All	All	5213/5213 (100%)	4918 (94%)	295 (6%)	28	56

5 of 295 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	AU	4	ILE
29	A2	24	ILE
51	BQ	45	LEU
21	AU	102	HIS
24	AX	53	LYS

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

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	119/120 (99%)	17 (14%)	0
2	AB	2898/2904 (99%)	529 (18%)	0
35	BA	1538/1542 (99%)	299 (19%)	0
36	BB	74/76 (97%)	25 (33%)	0
37	BC	46/47 (97%)	16 (34%)	0
38	BD	76/77 (98%)	14 (18%)	0
All	All	4751/4766 (99%)	900 (18%)	0

5 of 900 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	13	G
1	AA	14	U
1	AA	25	U
1	AA	26	C

There are no RNA pucker outliers to report.

## 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	$\# Z  > 2$
2	6MZ	AB	1618	2	18,25,26	1.39	2 (11%)	16,36,39	1.75	3 (18%)
2	2MG	AB	1835	2	19,26,27	2.17	5 (26%)	20,38,41	3.20	5 (25%)
2	PSU	AB	1911	2	16,21,22	1.84	6 (37%)	20,30,33	7.29	9 (45%)
2	3TD	AB	1915	2	16,22,23	1.89	7 (43%)	19,32,35	2.44	7 (36%)
2	PSU	AB	1917	2	16,21,22	2.05	4 (25%)	20,30,33	6.31	9 (45%)
2	5MU	AB	1939	2	14,22,23	2.03	5 (35%)	16,32,35	3.48	4 (25%)
2	5MC	AB	1962	2	15,22,23	2.57	4 (26%)	17,32,35	2.45	6 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	6MZ	AB	2030	2	18,25,26	1.36	4 (22%)	16,36,39	2.52	4 (25%)
2	7MG	AB	2069	2	20,26,27	2.89	9 (45%)	22,39,42	2.71	6 (27%)
2	OMG	AB	2251	2	18,26,27	1.72	4 (22%)	22,38,41	2.54	6 (27%)
2	2MG	AB	2445	2	19,26,27	2.21	9 (47%)	20,38,41	2.94	8 (40%)
2	H2U	AB	2449	2	17,21,22	1.54	4 (23%)	21,30,33	1.54	4 (19%)
2	PSU	AB	2457	2	16,21,22	2.32	6 (37%)	20,30,33	7.62	8 (40%)
2	OMC	AB	2498	2	15,22,23	1.33	1 (6%)	19,31,34	1.50	6 (31%)
2	2MA	AB	2503	2	18,25,26	1.25	1 (5%)	17,37,40	1.72	3 (17%)
2	PSU	AB	2504	2	16,21,22	2.25	6 (37%)	20,30,33	6.38	9 (45%)
2	OMU	AB	2552	2	14,22,23	2.17	5 (35%)	18,31,34	3.01	7 (38%)
2	CH	AB	2575	2	15,21,22	1.25	0	16,30,33	1.40	2 (12%)
2	PSU	AB	2580	2	16,21,22	2.01	5 (31%)	20,30,33	6.86	11 (55%)
2	PSU	AB	2605	2	16,21,22	1.77	4 (25%)	20,30,33	6.49	6 (30%)
2	1MG	AB	745	2	18,26,27	1.83	6 (33%)	18,39,42	1.58	4 (22%)
2	PSU	AB	746	2	16,21,22	1.91	3 (18%)	20,30,33	6.94	6 (30%)
2	5MU	AB	747	2	14,22,23	2.10	4 (28%)	16,32,35	3.61	5 (31%)
2	PSU	AB	955	2	16,21,22	2.02	4 (25%)	20,30,33	6.50	8 (40%)
35	2MG	BA	1207	35	19,26,27	2.23	9 (47%)	20,38,41	2.66	8 (40%)
35	4OC	BA	1402	35	16,23,24	2.37	5 (31%)	19,32,35	1.95	3 (15%)
35	5MC	BA	1407	35	15,22,23	1.71	4 (26%)	17,32,35	1.79	5 (29%)
35	UR3	BA	1498	35	14,22,23	2.08	3 (21%)	16,32,35	1.63	3 (18%)
35	2MG	BA	1516	35	19,26,27	1.82	6 (31%)	20,38,41	2.78	8 (40%)
35	MA6	BA	1518	35	16,26,27	1.47	2 (12%)	18,38,41	1.58	3 (16%)
35	MA6	BA	1519	35	16,26,27	1.46	4 (25%)	18,38,41	1.57	3 (16%)
35	PSU	BA	516	35	16,21,22	2.69	6 (37%)	20,30,33	5.83	11 (55%)
35	7MG	BA	527	35	20,26,27	3.07	5 (25%)	22,39,42	2.16	3 (13%)
35	2MG	BA	966	35	19,26,27	2.16	6 (31%)	20,38,41	2.95	7 (35%)
35	5MC	BA	967	35	15,22,23	1.64	2 (13%)	17,32,35	1.52	3 (17%)
36	H2U	BB	16	36	17,21,22	1.81	4 (23%)	21,30,33	1.48	5 (23%)
36	H2U	BB	17	36	17,21,22	1.35	4 (23%)	21,30,33	2.19	8 (38%)
36	H2U	BB	20	36	17,21,22	2.00	7 (41%)	21,30,33	2.06	7 (33%)
36	OMC	BB	32	36	15,22,23	1.64	3 (20%)	19,31,34	1.97	6 (31%)
36	MIA	BB	37	36	23,31,32	1.87	5 (21%)	25,44,47	1.90	5 (20%)
36	7MG	BB	46	36	20,26,27	3.19	6 (30%)	22,39,42	2.63	6 (27%)
36	5MU	BB	54	36	14,22,23	1.93	3 (21%)	16,32,35	3.99	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
36	PSU	BB	55	36	16,21,22	2.16	7 (43%)	20,30,33	7.08	13 (65%)
36	4SU	BB	8	36	14,21,22	2.56	3 (21%)	15,30,33	1.85	4 (26%)
38	H2U	BD	21	38	17,21,22	1.05	1 (5%)	21,30,33	1.75	3 (14%)
38	OMC	BD	33	38	15,22,23	1.56	3 (20%)	19,31,34	1.45	5 (26%)
38	5MU	BD	55	38	14,22,23	1.86	4 (28%)	16,32,35	4.01	4 (25%)
38	PSU	BD	56	38	16,21,22	2.32	6 (37%)	20,30,33	6.36	7 (35%)
38	4SU	BD	8	38	14,21,22	1.75	3 (21%)	15,30,33	2.49	3 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	6MZ	AB	1618	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	1835	2	-	0/5/27/28	0/3/3/3
2	PSU	AB	1911	2	-	0/7/25/26	0/2/2/2
2	3TD	AB	1915	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	1917	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	1939	2	-	0/3/25/26	0/2/2/2
2	5MC	AB	1962	2	-	0/3/25/26	0/2/2/2
2	6MZ	AB	2030	2	-	0/5/27/28	0/3/3/3
2	7MG	AB	2069	2	-	0/7/37/38	0/3/3/3
2	OMG	AB	2251	2	-	0/5/27/28	0/3/3/3
2	2MG	AB	2445	2	-	0/5/27/28	0/3/3/3
2	H2U	AB	2449	2	-	0/7/38/39	0/2/2/2
2	PSU	AB	2457	2	-	0/7/25/26	0/2/2/2
2	OMC	AB	2498	2	-	0/5/27/28	0/2/2/2
2	2MA	AB	2503	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	2504	2	-	0/7/25/26	0/2/2/2
2	OMU	AB	2552	2	-	0/5/27/28	0/2/2/2
2	CH	AB	2575	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	2580	2	-	0/7/25/26	0/2/2/2
2	PSU	AB	2605	2	-	0/7/25/26	0/2/2/2
2	1MG	AB	745	2	-	0/3/25/26	0/3/3/3
2	PSU	AB	746	2	-	0/7/25/26	0/2/2/2
2	5MU	AB	747	2	-	0/3/25/26	0/2/2/2
2	PSU	AB	955	2	-	0/7/25/26	0/2/2/2
35	2MG	BA	1207	35	-	0/5/27/28	0/3/3/3
35	4OC	BA	1402	35	-	0/7/29/30	0/2/2/2
35	5MC	BA	1407	35	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	UR3	BA	1498	35	-	0/3/25/26	0/2/2/2
35	2MG	BA	1516	35	-	0/5/27/28	0/3/3/3
35	MA6	BA	1518	35	-	0/7/29/30	0/3/3/3
35	MA6	BA	1519	35	-	0/7/29/30	0/3/3/3
35	PSU	BA	516	35	-	0/7/25/26	0/2/2/2
35	7MG	BA	527	35	-	0/7/37/38	0/3/3/3
35	2MG	BA	966	35	-	0/5/27/28	0/3/3/3
35	5MC	BA	967	35	-	0/3/25/26	0/2/2/2
36	H2U	BB	16	36	-	0/7/38/39	0/2/2/2
36	H2U	BB	17	36	-	0/7/38/39	0/2/2/2
36	H2U	BB	20	36	-	0/7/38/39	0/2/2/2
36	OMC	BB	32	36	-	0/5/27/28	0/2/2/2
36	MIA	BB	37	36	-	0/11/33/34	0/3/3/3
36	7MG	BB	46	36	-	0/7/37/38	0/3/3/3
36	5MU	BB	54	36	-	0/3/25/26	0/2/2/2
36	PSU	BB	55	36	-	0/7/25/26	0/2/2/2
36	4SU	BB	8	36	-	0/3/25/26	0/2/2/2
38	H2U	BD	21	38	-	0/7/38/39	0/2/2/2
38	OMC	BD	33	38	-	0/5/27/28	0/2/2/2
38	5MU	BD	55	38	-	0/3/25/26	0/2/2/2
38	PSU	BD	56	38	-	0/7/25/26	0/2/2/2
38	4SU	BD	8	38	-	0/3/25/26	0/2/2/2

The worst 5 of 219 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BB	46	7MG	C8-N9	-11.38	1.29	1.45
35	BA	527	7MG	C8-N9	-9.08	1.32	1.45
2	AB	2069	7MG	C8-N9	-8.91	1.32	1.45
35	BA	516	PSU	C5-C1'	-7.28	1.45	1.52
35	BA	1402	4OC	O5'-C5'	-6.46	1.35	1.44

The worst 5 of 282 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AB	1911	PSU	N1-C2-N3	-25.19	110.28	128.40
2	AB	2457	PSU	N1-C2-N3	-23.59	111.44	128.40
38	BD	56	PSU	N1-C2-N3	-21.73	112.77	128.40
2	AB	2605	PSU	N1-C2-N3	-20.35	113.77	128.40
2	AB	2504	PSU	N1-C2-N3	-20.22	113.86	128.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	FME	AB	3001	60	9,9,10	2.02	4 (44%)	7,9,11	2.27	3 (42%)
60	TRP	BB	101	59,36	14,15,16	1.33	1 (7%)	13,20,22	2.08	3 (23%)

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	FME	AB	3001	60	-	1/6/9/11	0/0/0/0
60	TRP	BB	101	59,36	-	0/3/6/8	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AB	3001	FME	CA-N	-4.18	1.40	1.46
59	AB	3001	FME	CB-CA	2.14	1.57	1.53
59	AB	3001	FME	O-C	2.22	1.29	1.19
60	BB	101	TRP	CD1-NE1	2.41	1.41	1.36
59	AB	3001	FME	CA-C	2.89	1.54	1.50

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	AB	3001	FME	O-C-CA	-4.87	113.79	125.15
60	BB	101	TRP	CB-CG-CD1	-4.76	122.09	127.97
59	AB	3001	FME	CG-CB-CA	2.16	119.22	112.97
60	BB	101	TRP	CZ2-CE2-NE1	2.38	137.38	130.80
59	AB	3001	FME	CB-CA-C	2.42	115.64	111.65

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	AB	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.