



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 23, 2019 – 03:35 PM EST

PDB ID : 6TC3
EMDB ID: : EMD-10458
Title : Cryo-EM structure of an Escherichia coli ribosome-SpeFL complex stalled in response to L-ornithine (Replicate 1)
Authors : Innis, C.A.; Herrero del Valle, A.
Deposited on : 2019-11-05
Resolution : 2.70 Å(reported)
Based on PDB ID : 4YBB

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

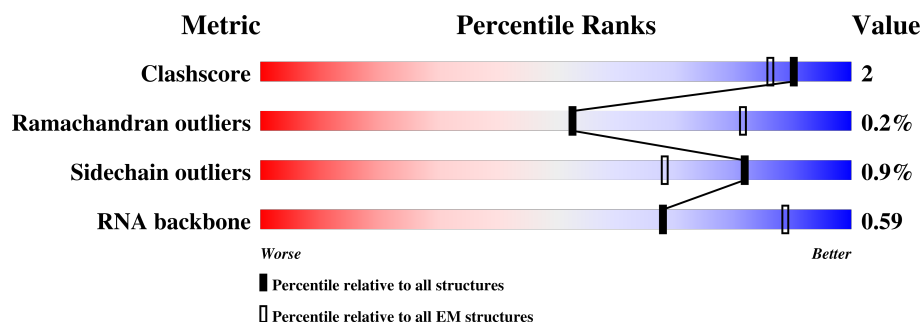
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 Å.

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






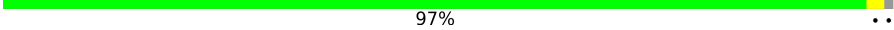

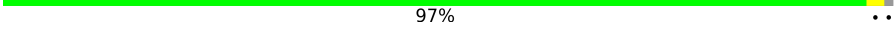
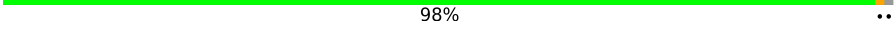
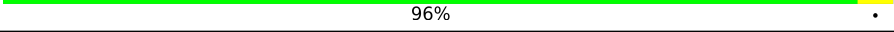
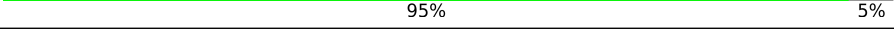


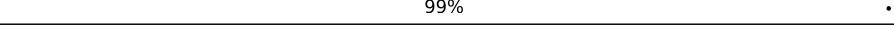



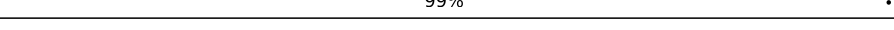
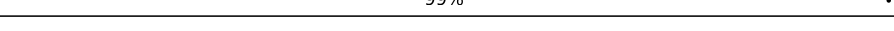
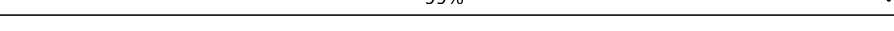
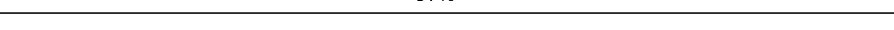
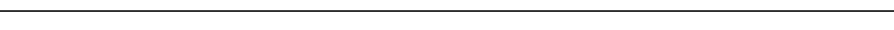

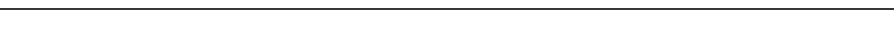
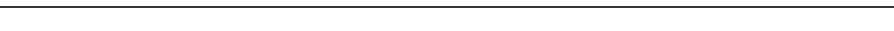


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531
RNA backbone	3747	458

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	16S1	1534	65% 30% 5%
2	S021	241	90% 7%
3	S031	233	88% 12%
4	S041	206	98% .
5	S051	167	92% 7%
6	S061	135	78% 21%
7	S071	179	83% 16%
8	S081	130	99% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	S091	130	 93% 5% .
10	S101	103	 88% 5% . .
11	S111	129	 91% 9%
12	S121	124	 97% . .
13	S131	118	 91% 6% .
14	S141	102	 97% . .
15	S151	89	 98% . .
16	S161	82	 96% .
17	S171	84	 95% 5%
18	S181	75	 71% . 27%
19	S191	92	 86% . . 11%
20	S201	87	 99% .
21	S211	71	 75% . 21%
22	23S1	2897	 64% 31% 5%
23	05S1	120	 69% 28% .
24	L021	273	 99% .
25	L031	209	 99% .
26	L041	201	 99% .
27	L051	179	 97% . .
28	L061	177	 99% . .
29	L091	149	 92% 7% .
30	L311	70	 93% . 6%
31	L131	142	 99% .
32	L141	123	 100%
33	L151	144	 98% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	L161	136	100%
35	L171	127	92% 7%
36	L181	117	100%
37	L191	115	99%
38	L201	118	98%
39	L211	103	100%
40	L221	110	99%
41	L231	100	93% 7%
42	L241	104	97%
43	L251	94	100%
44	L271	85	89% 11%
45	L281	78	96%
46	L291	63	98%
47	L301	59	98%
48	L321	57	96%
49	L331	55	93% 7%
50	L341	46	98%
51	L351	65	95%
52	L361	38	97%
53	SPE1	34	91% 9%
54	MRN1	7	29% 71%
55	PTR1	76	63% 32% 5%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 146672 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	16S1	1534	Total	C	N	O	P	0	0
			32930	14694	6041	10661	1534		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	S021	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S031	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	S041	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	S051	155	Total	C	N	O	S	0	0
			1144	711	216	211	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	S061	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	S071	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	S081	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	S091	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	S101	99	Total	C	N	O	S	0	0
			795	498	152	144	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S111	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	S121	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S131	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	S141	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S141	35	ALA	-	insertion	UNP P0AG59

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	S151	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	S161	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	S171	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	S181	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	S191	82	Total	C	N	O	S	0	0
			656	419	125	110	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S201	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S211	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	23S1	2897	Total	C	N	O	P	0	0
			62209	27759	11446	20107	2897		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	05S1	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L021	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 25 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L031	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 26 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L041	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L051	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 28 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L061	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L091	149	Total	C	N	O	S	0	0
			1110	699	197	213	1		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L311	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L131	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L141	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L151	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L161	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L171	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L181	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 37 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L191	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L201	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 39 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L211	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 40 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L221	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	L231	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	L241	102	Total	C	N	O		0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	L251	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L271	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	L281	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 46 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L291	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	L301	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	L321	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	L331	51	Total	C	N	O		0	0
			414	266	76	72			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	L341	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 51 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	L351	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 52 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	L361	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called SpeFL.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	SPE1	34	Total	C	N	O	S	0	0
			300	187	62	48	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
SPE1	5	SER	ASN	conflict	UNP A0A4S4NWS2
SPE1	7	THR	LEU	conflict	UNP A0A4S4NWS2

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	MRN1	7	Total	C	N	O	P	0	0
			146	65	23	51	7		

- Molecule 55 is a RNA chain called P-site Arg-tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	PTR1	76	Total	C	N	O	P	S	0	0
			1627	727	294	528	76	2		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	16S1	87	Total	Mg	0
			87	87	
56	23S1	249	Total	Mg	0
			249	249	
56	PTR1	1	Total	Mg	0
			1	1	
56	SPE1	1	Total	Mg	0
			1	1	
56	L231	1	Total	Mg	0
			1	1	

- Molecule 57 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	16S1	39	Total	K	0
			39	39	
57	23S1	106	Total	K	0
			106	106	
57	05S1	1	Total	K	0
			1	1	
57	L031	1	Total	K	0
			1	1	

- Molecule 58 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		AltConf
58	L231	1	Total	X	0
			1	1	
58	L151	5	Total	X	0
			5	5	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	PTR1	2	Total 2	X 2	0
58	16S1	145	Total 145	X 145	0
58	L281	2	Total 2	X 2	0
58	L161	5	Total 5	X 5	0
58	S171	1	Total 1	X 1	0
58	S031	1	Total 1	X 1	0
58	MRN1	1	Total 1	X 1	0
58	L321	3	Total 3	X 3	0
58	L221	8	Total 8	X 8	0
58	L271	3	Total 3	X 3	0
58	L331	1	Total 1	X 1	0
58	S111	2	Total 2	X 2	0
58	L031	17	Total 17	X 17	0
58	L171	5	Total 5	X 5	0
58	L131	6	Total 6	X 6	0
58	L341	8	Total 8	X 8	0
58	L021	26	Total 26	X 26	0
58	23S1	908	Total 908	X 908	0
58	L181	1	Total 1	X 1	0
58	SPE1	6	Total 6	X 6	0
58	L141	6	Total 6	X 6	0

Continued on next page...

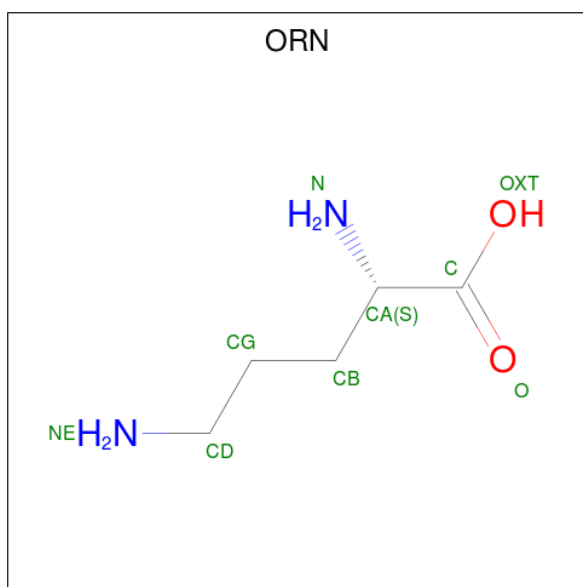
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	L191	4	Total 4	X 4	0
58	L211	1	Total 1	X 1	0
58	05S1	9	Total 9	X 9	0
58	L251	1	Total 1	X 1	0
58	L351	3	Total 3	X 3	0
58	L201	3	Total 3	X 3	0
58	L241	2	Total 2	X 2	0
58	S081	1	Total 1	X 1	0
58	S131	1	Total 1	X 1	0
58	S021	1	Total 1	X 1	0
58	S091	1	Total 1	X 1	0
58	L041	11	Total 11	X 11	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	L311	1	Total 1	Zn 1	0
59	S021	1	Total 1	Zn 1	0
59	L361	1	Total 1	Zn 1	0

- Molecule 60 is L-ornithine (three-letter code: ORN) (formula: C₅H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
60	23S1	1	Total	C	N	O	0
			9	5	2	2	

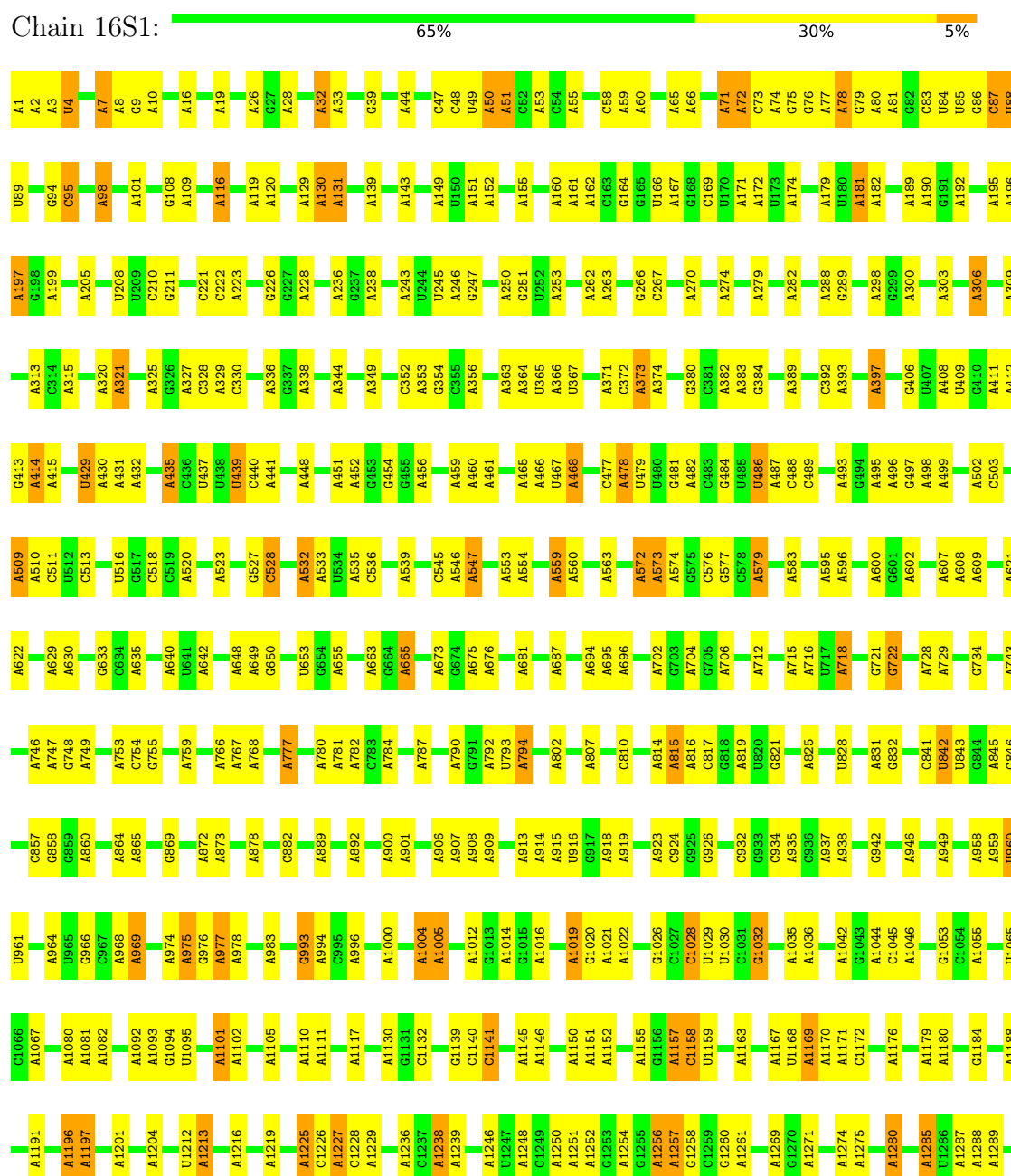
- Molecule 61 is water.

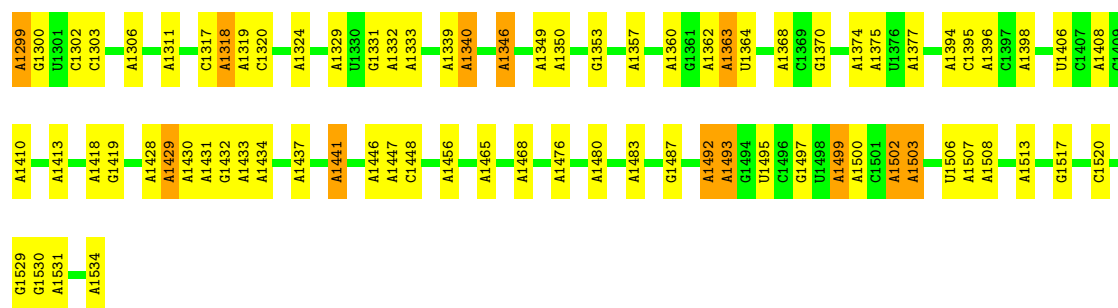
Mol	Chain	Residues	Atoms		AltConf
61	16S1	167	Total	O	0
			167	167	
61	S111	1	Total	O	0
			1	1	
61	S131	2	Total	O	0
			2	2	
61	S141	1	Total	O	0
			1	1	
61	S171	1	Total	O	0
			1	1	
61	23S1	619	Total	O	0
			619	619	
61	L021	3	Total	O	0
			3	3	
61	L031	2	Total	O	0
			2	2	
61	L151	2	Total	O	0
			2	2	
61	L171	2	Total	O	0
			2	2	

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.

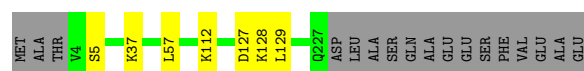
• Molecule 1: 16S rRNA





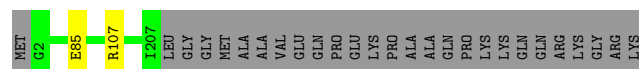
- Molecule 2: 30S ribosomal protein S2

Chain S021: 90% 7%



- Molecule 3: 30S ribosomal protein S3

Chain S031: 88% 12%



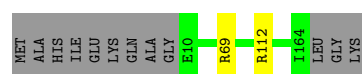
- Molecule 4: 30S ribosomal protein S4

Chain S041: 98% 0%



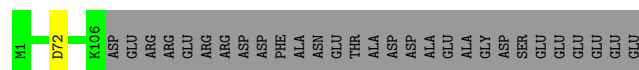
- Molecule 5: 30S ribosomal protein S5

Chain S051: 92% 7%



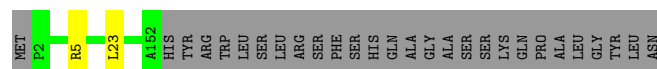
- Molecule 6: 30S ribosomal protein S6

Chain S061: 78% 21%



- Molecule 7: 30S ribosomal protein S7

Chain S071: 83% 16%



- Molecule 8: 30S ribosomal protein S8

Chain S081:  99% .



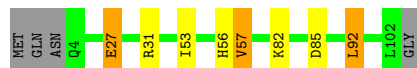
- Molecule 9: 30S ribosomal protein S9

Chain S091:  93% 5% .



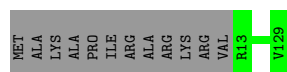
- Molecule 10: 30S ribosomal protein S10

Chain S101:  88% 5% . .



- Molecule 11: 30S ribosomal protein S11

Chain S111:  91% 9%



- Molecule 12: 30S ribosomal protein S12

Chain S121:  97% ..



- Molecule 13: 30S ribosomal protein S13

Chain S131:  91% 6% .



- Molecule 14: 30S ribosomal protein S14

Chain S141:  97% ..



- Molecule 15: 30S ribosomal protein S15

Chain S151:  98% ..



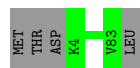
- Molecule 16: 30S ribosomal protein S16

Chain S161:  96% .




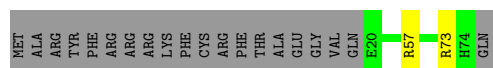
- Molecule 17: 30S ribosomal protein S17

Chain S171:  95% 5%



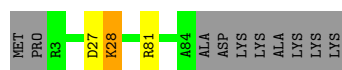
- Molecule 18: 30S ribosomal protein S18

Chain S181:  71% 27%



- Molecule 19: 30S ribosomal protein S19

Chain S191:  86% .. 11%




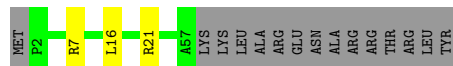
- Molecule 20: 30S ribosomal protein S20

Chain S201:  99% .



- Molecule 21: 30S ribosomal protein S21

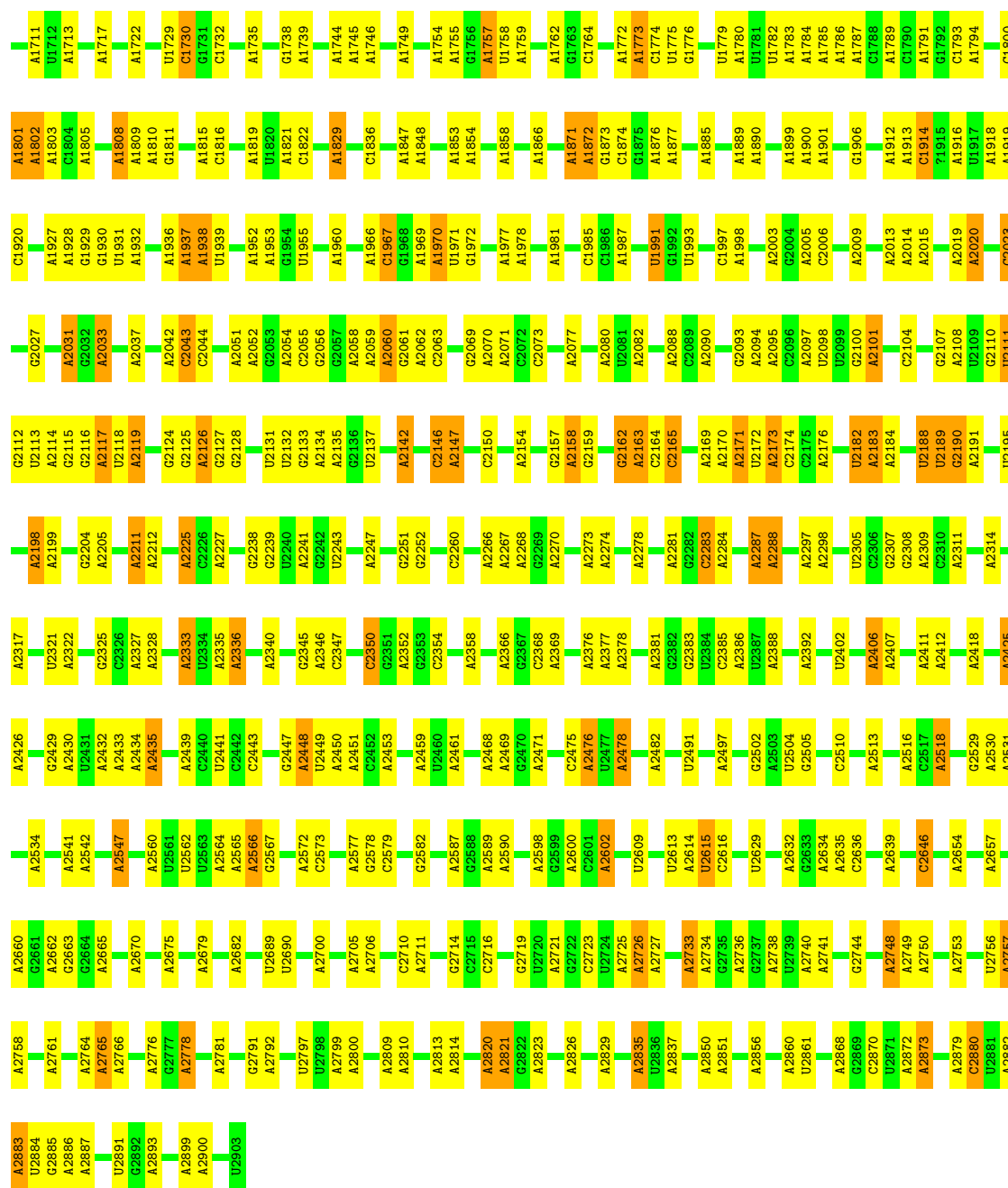
Chain S211:  75% 21%



- Molecule 22: 23S rRNA

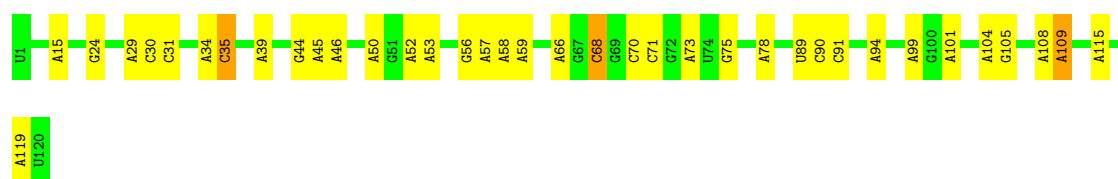
Chain 23S1:  64% 31% 5%

C1611	A1504	A1373	G1270	A1143	U1033	A936	A833	C740	C634	A526	A428	A310	A207	A111	G1
A1614	A1505	A1376	G1271	A1144	A1039	A941	C838	A741	C635	C527	A429	A311	A213	A116	A5
C1615	A1508	C1376	U1272	A1147	A1040	A941	U839	A742	A636	A528	A430	C116	G214	C116	A6
A1616	A1509	G1377	A1274	A1151	A1046	G942	C840	A743	A637	A529	U431	A117	G215	A118	A10
C1617	A1515	U1379	A1276	A1155	A1048	C944	A844	U747	A643	C531	A432	A119	A216	U120	C11
A1626	A1522	A1383	A1284	A1156	A1049	A945	U846	G748	A644	A532	A439	A125	A217	A125	U12
A1630	A1525	A1384	A1285	A1156	C1049	C946	U847	A749	C645	A538	A443	A126	A218	A13	A13
G1631	A1525	A1385	A1286	A1165	A1050	A947	U847	A751	A647	A541	A443	A127	A219	A14	A14
G1632	A1528	C1386	A1287	A1169	C1053	A959	C848	A752	U653	A544	A447	A128	A220	A128	A15
G1633	A1532	A1387	C1285	A1173	A1054	A960	A849	A753	A654	C544	U448	A129	A221	A129	A16
A1634	A1532	A1392	G1285	U1173	A1057	C961	G858	A756	A655	U546	U449	A131	A222	A131	A17
A1635	A1535	A1393	G1300	U1174	A1067	C965	G859	A757	A661	U547	A453	A132	A223	A132	A18
U1636	A1535	U1376	A1301	A1175	G1068	A972	U860	C758	A662	G548	A454	A133	A224	A133	A19
A1637	A1395	U1394	A1302	U1176	G1068	A973	A862	A761	A666	G549	A455	A134	A225	A134	A20
A1640	A1544	C1398	G1303	A1179	A1069	A974	A863	A762	U667	C550	A457	A135	A226	A135	A21
A1641	A1545	C1304	A1304	A1189	A1070	G974	A866	A763	A668	A556	A460	A136	A227	A136	A22
C1644	A1548	A1403	C1305	A1194	A1073	A975	A866	C765	G669	A566	A466	A137	A228	A137	A23
U1647	A1549	A1413	C1306	A1194	A1077	A979	A877	G775	C671	A563	A467	A138	A229	A138	A24
U1648	G1550	A1413	A1307	A1204	U1077	A980	A878	G776	C672	G564	G467	A139	A230	A139	A25
G1649	A1552	G1416	A1308	A1205	A1078	A981	A878	A781	C673	C565	A470	A140	A231	A140	A26
A1650	A1553	A1419	U1312	G1212	C1079	C982	U884	A782	A675	A572	A471	A141	A232	A141	A27
G1651	A1553	A1420	C1314	A1213	A1080	A983	C985	A783	A676	U573	A472	A142	A233	A142	A28
A1652	A1566	A1420	A1321	A1214	A1084	C985	C993	G784	A677	A574	A473	A143	A234	A143	A29
G1653	A1569	A1427	A1322	A1226	A1086	C987	U895	A788	A685	A575	A477	A144	A235	A144	A30
A1654	A1570	C1428	A1322	A1230	A1086	C987	U895	A789	U686	A582	A478	A145	A236	A145	A31
A1655	A1571	A1431	A1327	A1230	A1088	A988	C996	A792	A689	A586	A479	A146	A237	A146	A32
A1656	A1572	G1432	U1328	A1237	A1089	A990	C998	A793	A690	A586	A480	A147	A238	A147	A33
C1658	U1578	A1433	C1330	A1237	A1090	A996	A900	A794	A693	U591	A482	A148	A239	A148	A34
A1664	A1579	A1434	A1336	A1241	A1095	A996	A900	A794	A693	A592	A483	A149	A240	A149	A35
A1665	A1580	C1437	A1336	A1244	A1096	A1000	A905	A800	A699	A592	G491	A150	A241	A150	A36
A1668	A1583	U1438	U1340	G1244	U1097	A1001	U906	G801	U702	A599	A492	A151	A242	A151	A37
C1670	U1584	A1439	G1341	G1245	A1098	A1001	A909	A802	A705	A602	A497	A152	A243	A152	A38
U1671	C1585	A1439	A1342	A1246	C1005	C1005	A910	U803	A706	A603	A501	A153	A244	A153	A39
A1672	A1586	G1452	G1343	A1247	A1103	A1008	A911	A804	A706	A603	A502	A154	A245	A154	A40
G1673	A1590	A1453	A1343	G1250	A1111	A1009	C912	G806	A715	A608	A503	A155	A246	A155	A41
G1674	A1591	C1469	A1347	A1253	G1112	A1010	C915	U807	A716	A609	A504	A156	A247	A156	A42
C1675	A1591	A1470	C1348	A1254	C1117	G1011	G916	C812	C717	A505	A505	A157	A248	A157	A43
A1676	C1592	A1470	C1349	U1254	C1117	U1012	A917	A812	A718	A613	A506	A158	A249	A158	A44
A1677	A1593	A1477	C1350	G1255	A1126	C1013	A918	U806	A718	A614	A507	A159	A250	A159	A45
A1678	A1596	A1477	C1351	G1256	A1126	A1014	U919	C817	A721	U615	A508	A160	A251	A160	A46
A1679	A1597	G1482	U1352	C1257	A1127	A1014	U920	G818	A722	A616	A509	A161	A252	A161	A47
A1689	A1597	A1482	A1353	A1260	G1128	A1020	A925	A819	A722	A616	A510	A162	A253	A162	A48
A1690	A1598	A1490	A1354	C1261	A1129	A1021	A926	A820	A727	A621	A511	A163	A254	A163	A49
A1693	A1603	A1490	A1359	U1130	G1131	G1022	G926	A821	A727	A621	A512	A164	A255	A164	A50
G1698	A1606	A1494	A1363	U1132	G1131	G1026	A927	A825	A730	A626	A513	A165	A256	A165	A51
G1699	C1606	A1495	C1363	U1263	U1133	A1027	A928	U826	A730	A627	A514	A166	A257	A166	A52
A1700	C1607	A1496	G1364	A1264	A1134	A1028	A928	U827	A734	A631	A515	A167	A258	A167	A53
A1701	A1608	A1502	A1365	A1268	C1135	A1029	U931	U828	A735	A632	A522	A168	A259	A168	A54
A1705	A1610	A1503	A1367	A1269	A1142	A1032	U932	A829	A739	A633	A522	A169	A260	A169	A55



• Molecule 23: 5S rRNA

Chain 05S1: 69% 28%



• Molecule 24: 50S ribosomal protein L2

Chain L021:  99% .



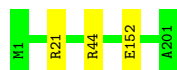
- Molecule 25: 50S ribosomal protein L3

Chain L031:  99% .



- Molecule 26: 50S ribosomal protein L4

Chain L041:  99% .



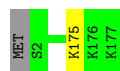
- Molecule 27: 50S ribosomal protein L5

Chain L051:  97% ..



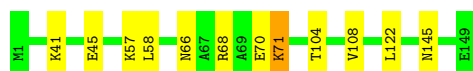
- Molecule 28: 50S ribosomal protein L6

Chain L061:  99% ..



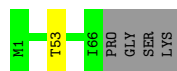
- Molecule 29: 50S ribosomal protein L9

Chain L091:  92% 7% .



- Molecule 30: 50S ribosomal protein L31

Chain L311:  93% 6% .



- Molecule 31: 50S ribosomal protein L13

Chain L131:  99% .



- Molecule 32: 50S ribosomal protein L14

Chain L141: 100%

There are no outlier residues recorded for this chain.

- Molecule 33: 50S ribosomal protein L15

Chain L151: 98%



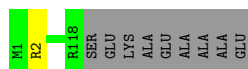
- Molecule 34: 50S ribosomal protein L16

Chain L161: 100%

There are no outlier residues recorded for this chain.

- Molecule 35: 50S ribosomal protein L17

Chain L171: 92%



- Molecule 36: 50S ribosomal protein L18

Chain L181: 100%

There are no outlier residues recorded for this chain.

- Molecule 37: 50S ribosomal protein L19

Chain L191: 99%



- Molecule 38: 50S ribosomal protein L20

Chain L201: 98%



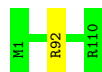
- Molecule 39: 50S ribosomal protein L21

Chain L211: 100%

There are no outlier residues recorded for this chain.

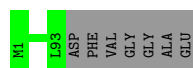
- Molecule 40: 50S ribosomal protein L22

Chain L221:  99%



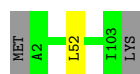
- Molecule 41: 50S ribosomal protein L23

Chain L231:  93% 7%



- Molecule 42: 50S ribosomal protein L24

Chain L241:  97%



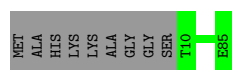
- Molecule 43: 50S ribosomal protein L25

Chain L251:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L27

Chain L271:  89% 11%



- Molecule 45: 50S ribosomal protein L28

Chain L281:  96%



- Molecule 46: 50S ribosomal protein L29

Chain L291:  98%



- Molecule 47: 50S ribosomal protein L30

Chain L301:  98% .



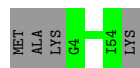
- Molecule 48: 50S ribosomal protein L32

Chain L321:  96% ..



- Molecule 49: 50S ribosomal protein L33

Chain L331:  93% 7%



- Molecule 50: 50S ribosomal protein L34

Chain L341:  98% .



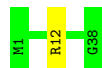
- Molecule 51: 50S ribosomal protein L35

Chain L351:  95% ..



- Molecule 52: 50S ribosomal protein L36

Chain L361:  97% .

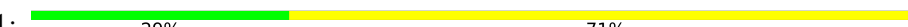


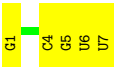
- Molecule 53: SpeFL

Chain SPE1:  91% 9%



- Molecule 54: mRNA

Chain MRN1:  29% 71%



● Molecule 55: P-site Arg-tRNA



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	68195	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	-500	Depositor
Maximum defocus (nm)	-1600	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MA6, 2MA, 2MG, 1MG, 3TD, G7M, D2T, UR3, 4D4, 5MU, ZN, OMU, UNX, K, 6MZ, FME, OMC, MG, OMG, ORN, MEQ, 5MC, 4OC, 4SU, RSP, 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	16S1	1.50	1056/36593 (2.9%)	3.49	4371/57081 (7.7%)
10	S101	0.95	1/805 (0.1%)	0.90	5/1089 (0.5%)
11	S111	0.81	0/893	0.58	0/1205
12	S121	0.89	0/960	0.65	1/1286 (0.1%)
13	S131	0.92	0/892	0.84	3/1193 (0.3%)
14	S141	0.91	0/811	0.67	0/1081
15	S151	0.87	0/722	0.53	1/964 (0.1%)
16	S161	0.87	0/659	0.67	1/884 (0.1%)
17	S171	0.76	0/657	0.57	0/881
18	S181	0.88	0/462	0.49	0/621
19	S191	0.83	0/672	0.75	1/904 (0.1%)
2	S021	0.67	0/1784	0.69	2/2403 (0.1%)
20	S201	0.74	0/676	0.56	0/895
21	S211	1.02	0/472	0.78	3/627 (0.5%)
22	23S1	1.58	1959/69120 (2.8%)	3.57	8521/107824 (7.9%)
23	05S1	1.36	69/2872 (2.4%)	3.12	276/4478 (6.2%)
24	L021	0.85	0/2121	0.60	0/2852
25	L031	0.70	0/1576	0.55	0/2119
26	L041	0.71	0/1571	0.57	0/2113
27	L051	0.78	0/1434	0.67	0/1926
28	L061	0.68	0/1343	0.64	0/1816
29	L091	0.71	0/1121	1.05	6/1515 (0.4%)
3	S031	0.80	0/1651	0.63	0/2225
30	L311	0.79	0/531	0.91	0/709
31	L131	0.76	1/1152 (0.1%)	0.52	0/1551
32	L141	0.84	0/955	0.61	0/1279
33	L151	0.82	0/1062	0.60	0/1413
34	L161	0.80	0/1081	0.55	0/1443
35	L171	0.95	0/958	0.61	0/1281
36	L181	0.84	0/910	0.54	0/1219
37	L191	0.85	0/929	0.58	0/1242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	L201	0.92	0/960	0.49	0/1278
39	L211	0.75	0/829	0.61	0/1107
4	S041	0.82	0/1665	0.54	0/2227
40	L221	0.80	0/864	0.54	0/1156
41	L231	0.75	0/744	0.63	0/994
42	L241	0.67	0/787	0.56	1/1051 (0.1%)
43	L251	0.66	0/766	0.51	0/1025
44	L271	0.84	0/587	0.50	0/776
45	L281	0.92	0/635	0.53	0/848
46	L291	0.76	0/502	0.51	0/667
47	L301	0.83	0/453	0.56	0/605
48	L321	0.90	0/450	0.69	1/599 (0.2%)
49	L331	0.65	0/421	0.62	0/561
5	S051	0.74	0/1157	0.67	1/1557 (0.1%)
50	L341	1.14	0/380	0.65	0/498
51	L351	0.78	0/513	0.64	0/676
52	L361	0.91	0/303	0.62	0/397
53	SPE1	0.93	0/299	0.69	0/399
54	MRN1	0.77	0/161	1.39	1/248 (0.4%)
55	PTR1	1.66	56/1672 (3.3%)	3.19	171/2598 (6.6%)
6	S061	0.71	0/881	0.61	1/1189 (0.1%)
7	S071	0.87	0/1195	0.70	1/1602 (0.1%)
8	S081	0.70	0/989	0.54	0/1326
9	S091	0.97	0/1034	0.82	3/1375 (0.2%)
All	All	1.37	3142/155692 (2.0%)	3.05	13371/232878 (5.7%)

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
10	S101	0	5
13	S131	0	3
19	S191	0	3
2	S021	0	2
26	L041	0	1
29	L091	0	5
3	S031	0	1
30	L311	0	1
33	L151	0	1
51	L351	0	1
All	All	0	23

The worst 5 of 3142 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	20	U	C5-C6	23.29	1.55	1.34
55	PTR1	17	U	C5-C6	22.31	1.54	1.34
22	23S1	2449	U	C5-C6	21.06	1.53	1.34
55	PTR1	17	U	N1-C6	10.30	1.47	1.38
55	PTR1	20	U	N1-C6	10.08	1.47	1.38

The worst 5 of 13371 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2872	A	N1-C6-N6	-26.65	102.61	118.60
22	23S1	504	A	N1-C2-N3	-25.85	116.38	129.30
22	23S1	1434	A	N1-C6-N6	-24.57	103.86	118.60
22	23S1	1937	A	N1-C6-N6	-23.75	104.35	118.60
1	16S1	1004	A	C2-N3-C4	23.60	122.40	110.60

There are no chirality outliers.

5 of 23 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S021	128	LYS	Peptide
2	S021	5	SER	Peptide
3	S031	85	GLU	Peptide
10	S101	27	GLU	Peptide
10	S101	56	HIS	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	16S1	32930	0	0	0	0
2	S021	1753	0	0	0	0
3	S031	1624	0	0	0	0
4	S041	1643	0	0	0	0
5	S051	1144	0	0	0	0
6	S061	862	0	0	0	0
7	S071	1181	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	S081	979	0	0	0	0
9	S091	1022	0	0	0	0
10	S101	795	0	0	0	0
11	S111	877	0	0	0	0
12	S121	957	0	0	0	0
13	S131	883	0	0	0	0
14	S141	799	0	0	0	0
15	S151	714	0	0	0	0
16	S161	649	0	0	0	0
17	S171	648	0	0	0	0
18	S181	455	0	0	0	0
19	S191	656	0	0	0	0
20	S201	670	0	0	0	0
21	S211	465	0	0	0	0
22	23S1	62209	0	0	0	0
23	05S1	2569	0	0	0	0
24	L021	2082	0	0	0	0
25	L031	1566	0	0	0	0
26	L041	1552	0	0	0	0
27	L051	1410	0	0	0	0
28	L061	1323	0	0	0	0
29	L091	1110	0	0	0	0
30	L311	522	0	0	0	0
31	L131	1129	0	0	0	0
32	L141	946	0	0	0	0
33	L151	1053	0	0	0	0
34	L161	1075	0	0	0	0
35	L171	945	0	0	0	0
36	L181	900	0	0	0	0
37	L191	917	0	0	0	0
38	L201	947	0	0	0	0
39	L211	816	0	0	0	0
40	L221	857	0	0	0	0
41	L231	738	0	0	0	0
42	L241	779	0	0	0	0
43	L251	753	0	0	0	0
44	L271	580	0	0	0	0
45	L281	625	0	0	0	0
46	L291	501	0	0	0	0
47	L301	449	0	0	0	0
48	L321	444	0	0	0	0
49	L331	414	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	L341	377	0	0	0	0
51	L351	504	0	0	0	0
52	L361	302	0	0	0	0
53	SPE1	300	0	0	0	0
54	MRN1	146	0	0	0	0
55	PTR1	1627	0	0	0	0
56	16S1	87	0	0	0	0
56	23S1	249	0	0	0	0
56	L231	1	0	0	0	0
56	PTR1	1	0	0	0	0
56	SPE1	1	0	0	0	0
57	05S1	1	0	0	0	0
57	16S1	39	0	0	0	0
57	23S1	106	0	0	0	0
57	L031	1	0	0	0	0
58	05S1	9	0	0	0	0
58	16S1	145	0	0	0	0
58	23S1	908	0	0	0	0
58	L021	26	0	0	0	0
58	L031	17	0	0	0	0
58	L041	11	0	0	0	0
58	L131	6	0	0	0	0
58	L141	6	0	0	0	0
58	L151	5	0	0	0	0
58	L161	5	0	0	0	0
58	L171	5	0	0	0	0
58	L181	1	0	0	0	0
58	L191	4	0	0	0	0
58	L201	3	0	0	0	0
58	L211	1	0	0	0	0
58	L221	8	0	0	0	0
58	L231	1	0	0	0	0
58	L241	2	0	0	0	0
58	L251	1	0	0	0	0
58	L271	3	0	0	0	0
58	L281	2	0	0	0	0
58	L321	3	0	0	0	0
58	L331	1	0	0	0	0
58	L341	8	0	0	0	0
58	L351	3	0	0	0	0
58	MRN1	1	0	0	0	0
58	PTR1	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	S021	1	0	0	0	0
58	S031	1	0	0	0	0
58	S081	1	0	0	0	0
58	S091	1	0	0	0	0
58	S111	2	0	0	0	0
58	S131	1	0	0	0	0
58	S171	1	0	0	0	0
58	SPE1	6	0	0	0	0
59	L311	1	0	0	0	0
59	L361	1	0	0	0	0
59	S021	1	0	0	0	0
60	23S1	9	0	0	0	0
61	16S1	167	0	0	0	0
61	23S1	619	0	0	0	0
61	L021	3	0	0	0	0
61	L031	2	0	0	0	0
61	L151	2	0	0	0	0
61	L171	2	0	0	0	0
61	S111	1	0	0	0	0
61	S131	2	0	0	0	0
61	S141	1	0	0	0	0
61	S171	1	0	0	0	0
All	All	146672	0	0	0	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 2.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S021	222/241 (92%)	208 (94%)	13 (6%)	1 (0%)	31	58
3	S031	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
4	S041	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	S051	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
6	S061	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	S071	149/179 (83%)	139 (93%)	10 (7%)	0	100	100
8	S081	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
9	S091	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	S101	97/103 (94%)	91 (94%)	5 (5%)	1 (1%)	17	41
11	S111	115/129 (89%)	106 (92%)	9 (8%)	0	100	100
12	S121	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	S131	112/118 (95%)	105 (94%)	6 (5%)	1 (1%)	19	44
14	S141	99/102 (97%)	85 (86%)	13 (13%)	1 (1%)	17	41
15	S151	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	S161	80/82 (98%)	75 (94%)	4 (5%)	1 (1%)	13	33
17	S171	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
18	S181	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	S191	80/92 (87%)	76 (95%)	4 (5%)	0	100	100
20	S201	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	S211	54/71 (76%)	54 (100%)	0	0	100	100
24	L021	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
25	L031	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	31	58
26	L041	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
27	L051	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
28	L061	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
29	L091	147/149 (99%)	129 (88%)	17 (12%)	1 (1%)	24	50
30	L311	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	L131	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
32	L141	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	L151	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	24	50
34	L161	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	L171	116/127 (91%)	111 (96%)	5 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	L181	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	L191	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
38	L201	115/118 (98%)	115 (100%)	0	0	100	100
39	L211	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
40	L221	108/110 (98%)	108 (100%)	0	0	100	100
41	L231	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
42	L241	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
43	L251	92/94 (98%)	92 (100%)	0	0	100	100
44	L271	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
45	L281	75/78 (96%)	75 (100%)	0	0	100	100
46	L291	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	L301	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	L321	54/57 (95%)	54 (100%)	0	0	100	100
49	L331	49/55 (89%)	49 (100%)	0	0	100	100
50	L341	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	L351	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	11	27
52	L361	36/38 (95%)	36 (100%)	0	0	100	100
53	SPE1	32/34 (94%)	32 (100%)	0	0	100	100
All	All	5607/5948 (94%)	5389 (96%)	209 (4%)	9 (0%)	53	77

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	S101	57	VAL
25	L031	149	ASN
51	L351	32	ILE
13	S131	66	GLU
14	S141	54	ASP

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	S021	186/199 (94%)	184 (99%)	2 (1%)	76	91
3	S031	170/190 (90%)	169 (99%)	1 (1%)	87	96
4	S041	172/173 (99%)	169 (98%)	3 (2%)	63	87
5	S051	118/126 (94%)	117 (99%)	1 (1%)	83	94
6	S061	92/116 (79%)	92 (100%)	0	100	100
7	S071	124/147 (84%)	123 (99%)	1 (1%)	83	94
8	S081	104/105 (99%)	104 (100%)	0	100	100
9	S091	105/107 (98%)	102 (97%)	3 (3%)	45	75
10	S101	87/90 (97%)	87 (100%)	0	100	100
11	S111	90/99 (91%)	90 (100%)	0	100	100
12	S121	102/103 (99%)	100 (98%)	2 (2%)	58	84
13	S131	92/96 (96%)	91 (99%)	1 (1%)	76	91
14	S141	79/84 (94%)	78 (99%)	1 (1%)	71	89
15	S151	76/77 (99%)	75 (99%)	1 (1%)	71	89
16	S161	65/65 (100%)	64 (98%)	1 (2%)	67	88
17	S171	74/78 (95%)	74 (100%)	0	100	100
18	S181	48/65 (74%)	46 (96%)	2 (4%)	32	62
19	S191	71/79 (90%)	71 (100%)	0	100	100
20	S201	65/66 (98%)	65 (100%)	0	100	100
21	S211	48/61 (79%)	47 (98%)	1 (2%)	56	83
24	L021	216/218 (99%)	215 (100%)	1 (0%)	90	97
25	L031	163/163 (100%)	161 (99%)	2 (1%)	74	90
26	L041	165/165 (100%)	163 (99%)	2 (1%)	74	90
27	L051	148/150 (99%)	145 (98%)	3 (2%)	58	84
28	L061	137/138 (99%)	136 (99%)	1 (1%)	85	95
29	L091	114/114 (100%)	112 (98%)	2 (2%)	62	86
30	L311	59/62 (95%)	59 (100%)	0	100	100
31	L131	116/116 (100%)	116 (100%)	0	100	100
32	L141	104/104 (100%)	104 (100%)	0	100	100
33	L151	103/103 (100%)	102 (99%)	1 (1%)	78	92
34	L161	108/108 (100%)	108 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	L171	98/103 (95%)	97 (99%)	1 (1%)	78	92
36	L181	87/87 (100%)	87 (100%)	0	100	100
37	L191	99/100 (99%)	99 (100%)	0	100	100
38	L201	89/90 (99%)	88 (99%)	1 (1%)	76	91
39	L211	84/84 (100%)	84 (100%)	0	100	100
40	L221	93/93 (100%)	92 (99%)	1 (1%)	76	91
41	L231	80/84 (95%)	80 (100%)	0	100	100
42	L241	83/85 (98%)	83 (100%)	0	100	100
43	L251	78/78 (100%)	78 (100%)	0	100	100
44	L271	57/63 (90%)	57 (100%)	0	100	100
45	L281	67/68 (98%)	65 (97%)	2 (3%)	44	74
46	L291	54/55 (98%)	54 (100%)	0	100	100
47	L301	48/49 (98%)	48 (100%)	0	100	100
48	L321	47/48 (98%)	46 (98%)	1 (2%)	56	83
49	L331	45/49 (92%)	45 (100%)	0	100	100
50	L341	38/38 (100%)	37 (97%)	1 (3%)	49	79
51	L351	51/52 (98%)	51 (100%)	0	100	100
52	L361	34/34 (100%)	33 (97%)	1 (3%)	45	75
53	SPE1	31/31 (100%)	28 (90%)	3 (10%)	9	21
All	All	4664/4858 (96%)	4621 (99%)	43 (1%)	82	93

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
21	S211	7	ARG
26	L041	44	ARG
52	L361	12	ARG
24	L021	80	ARG
25	L031	13	ARG

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	16S1	1530/1534 (99%)	175 (11%)	1 (0%)
22	23S1	2890/2897 (99%)	292 (10%)	18 (0%)
23	05S1	119/120 (99%)	8 (6%)	0
54	MRN1	6/7 (85%)	3 (50%)	1 (16%)
55	PTR1	73/76 (96%)	12 (16%)	1 (1%)
All	All	4618/4634 (99%)	490 (10%)	21 (0%)

5 of 490 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	16S1	4	U
1	16S1	7	A
1	16S1	9	G
1	16S1	32	A
1	16S1	39	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	23S1	1608	A
22	23S1	2146	C
22	23S1	2756	U
22	23S1	1508	A
22	23S1	2873	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	16S1	1207	1,57	18,26,27	4.25	8 (44%)	19,38,41	2.39	7 (36%)
1	4OC	16S1	1402	1,56	16,23,24	3.11	6 (37%)	20,32,35	1.27	1 (5%)
1	5MC	16S1	1407	1	14,22,23	2.74	5 (35%)	17,32,35	1.57	3 (17%)
1	UR3	16S1	1498	1	13,22,23	2.74	4 (30%)	15,32,35	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	16S1	1516	1	18,26,27	4.11	9 (50%)	19,38,41	2.42	7 (36%)
1	MA6	16S1	1518	1	16,26,27	1.38	2 (12%)	16,38,41	3.79	3 (18%)
1	MA6	16S1	1519	1	16,26,27	1.32	1 (6%)	16,38,41	3.85	4 (25%)
1	PSU	16S1	516	1,56	16,21,22	3.44	8 (50%)	20,30,33	3.25	6 (30%)
1	G7M	16S1	527	1,57	18,26,27	3.52	6 (33%)	18,39,42	2.99	7 (38%)
1	2MG	16S1	966	1	18,26,27	4.42	9 (50%)	19,38,41	2.40	8 (42%)
1	5MC	16S1	967	1	14,22,23	2.98	6 (42%)	17,32,35	1.25	2 (11%)
22	6MZ	23S1	1618	22	17,25,26	3.08	4 (23%)	15,36,39	2.32	3 (20%)
22	2MG	23S1	1835	22	18,26,27	3.96	8 (44%)	19,38,41	2.65	7 (36%)
22	PSU	23S1	1911	22	16,21,22	3.51	8 (50%)	20,30,33	2.96	6 (30%)
22	3TD	23S1	1915	22	16,22,23	4.67	7 (43%)	19,32,35	1.15	2 (10%)
22	PSU	23S1	1917	22	16,21,22	3.52	8 (50%)	20,30,33	3.33	6 (30%)
22	5MU	23S1	1939	57,22	13,22,23	1.22	2 (15%)	14,32,35	2.75	1 (7%)
22	5MC	23S1	1962	57,22	14,22,23	2.86	5 (35%)	17,32,35	1.27	2 (11%)
22	6MZ	23S1	2030	22	17,25,26	3.03	5 (29%)	15,36,39	3.02	5 (33%)
22	G7M	23S1	2069	57,22	18,26,27	3.39	7 (38%)	18,39,42	2.97	7 (38%)
22	OMG	23S1	2251	55,57,22	18,26,27	3.38	9 (50%)	22,38,41	2.14	7 (31%)
22	2MG	23S1	2445	22	18,26,27	4.10	9 (50%)	19,38,41	2.56	5 (26%)
22	PSU	23S1	2457	22	16,21,22	3.38	8 (50%)	20,30,33	2.90	7 (35%)
22	OMC	23S1	2498	56,22	15,22,23	3.04	7 (46%)	20,31,34	1.46	1 (5%)
22	2MA	23S1	2503	57,56,22	16,25,26	3.86	5 (31%)	17,37,40	1.95	4 (23%)
22	PSU	23S1	2504	57,22	16,21,22	3.48	7 (43%)	20,30,33	3.24	6 (30%)
22	OMU	23S1	2552	56,22	14,22,23	3.14	5 (35%)	17,31,34	0.57	0
22	PSU	23S1	2580	57,22	16,21,22	3.44	8 (50%)	20,30,33	2.90	7 (35%)
22	PSU	23S1	2604	22	16,21,22	3.40	8 (50%)	20,30,33	3.22	6 (30%)
22	PSU	23S1	2605	22	16,21,22	3.43	7 (43%)	20,30,33	3.35	7 (35%)
22	1MG	23S1	745	22	17,26,27	3.74	7 (41%)	17,39,42	1.68	3 (17%)
22	PSU	23S1	746	56,22	16,21,22	3.40	8 (50%)	20,30,33	3.13	7 (35%)
22	5MU	23S1	747	22	13,22,23	1.53	3 (23%)	14,32,35	2.70	1 (7%)
22	PSU	23S1	955	22	16,21,22	3.43	9 (56%)	20,30,33	2.96	6 (30%)
25	MEQ	L031	150	25	9,9,10	1.58	2 (22%)	6,10,12	1.75	1 (16%)
34	4D4	L161	81	34	9,11,12	1.67	2 (22%)	5,13,15	1.38	1 (20%)
55	RSP	PTR1	32	55	14,21,22	3.40	7 (50%)	15,30,33	2.00	3 (20%)
55	2MG	PTR1	37	55	18,26,27	4.26	9 (50%)	19,38,41	2.36	7 (36%)
55	G7M	PTR1	46	55	18,26,27	3.68	7 (38%)	18,39,42	3.19	7 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	5MU	PTR1	54	55	13,22,23	1.68	3 (23%)	14,32,35	2.64	1 (7%)
55	PSU	PTR1	55	55	16,21,22	3.62	7 (43%)	20,30,33	3.22	7 (35%)
55	4SU	PTR1	8	55	13,21,22	3.81	5 (38%)	14,30,33	1.72	2 (14%)
12	D2T	S121	89	12	5,9,10	1.42	1 (20%)	4,11,13	2.21	2 (50%)
53	FME	SPE1	1	53	9,9,10	1.15	1 (11%)	6,9,11	0.81	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MG	16S1	1207	1,57	-	0/5/27/28	0/3/3/3
1	4OC	16S1	1402	1,56	-	2/7/29/30	0/2/2/2
1	5MC	16S1	1407	1	-	0/3/25/26	0/2/2/2
1	UR3	16S1	1498	1	-	0/3/25/26	0/2/2/2
1	2MG	16S1	1516	1	-	0/5/27/28	0/3/3/3
1	MA6	16S1	1518	1	-	0/7/29/30	0/3/3/3
1	MA6	16S1	1519	1	-	3/7/29/30	0/3/3/3
1	PSU	16S1	516	1,56	-	0/7/25/26	0/2/2/2
1	G7M	16S1	527	1,57	-	2/3/25/26	0/3/3/3
1	2MG	16S1	966	1	-	2/5/27/28	0/3/3/3
1	5MC	16S1	967	1	-	0/3/25/26	0/2/2/2
22	6MZ	23S1	1618	22	-	0/5/27/28	0/3/3/3
22	2MG	23S1	1835	22	-	0/5/27/28	0/3/3/3
22	PSU	23S1	1911	22	-	0/7/25/26	0/2/2/2
22	3TD	23S1	1915	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	1917	22	-	0/7/25/26	0/2/2/2
22	5MU	23S1	1939	57,22	-	2/3/25/26	0/2/2/2
22	5MC	23S1	1962	57,22	-	0/3/25/26	0/2/2/2
22	6MZ	23S1	2030	22	-	2/5/27/28	0/3/3/3
22	G7M	23S1	2069	57,22	-	3/3/25/26	0/3/3/3
22	OMG	23S1	2251	55,57,22	-	1/5/27/28	0/3/3/3
22	2MG	23S1	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	23S1	2457	22	-	0/7/25/26	0/2/2/2
22	OMC	23S1	2498	56,22	-	0/5/27/28	0/2/2/2
22	2MA	23S1	2503	57,56,22	-	2/3/25/26	0/3/3/3
22	PSU	23S1	2504	57,22	-	2/7/25/26	0/2/2/2
22	OMU	23S1	2552	56,22	-	0/5/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	23S1	2580	57,22	-	1/7/25/26	0/2/2/2
22	PSU	23S1	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2605	22	-	0/7/25/26	0/2/2/2
22	1MG	23S1	745	22	-	0/3/25/26	0/3/3/3
22	PSU	23S1	746	56,22	-	2/7/25/26	0/2/2/2
22	5MU	23S1	747	22	-	0/3/25/26	0/2/2/2
22	PSU	23S1	955	22	-	0/7/25/26	0/2/2/2
25	MEQ	L031	150	25	-	2/7/9/11	-
34	4D4	L161	81	34	-	2/11/12/14	-
55	RSP	PTR1	32	55	-	2/3/25/26	0/2/2/2
55	2MG	PTR1	37	55	-	0/5/27/28	0/3/3/3
55	G7M	PTR1	46	55	-	1/3/25/26	0/3/3/3
55	5MU	PTR1	54	55	-	2/3/25/26	0/2/2/2
55	PSU	PTR1	55	55	-	0/7/25/26	0/2/2/2
55	4SU	PTR1	8	55	-	1/3/25/26	0/2/2/2
12	D2T	S121	89	12	-	1/2/12/14	-
53	FME	SPE1	1	53	-	3/6/9/11	-

The worst 5 of 262 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	23S1	1915	3TD	C5-C1'	-14.71	1.39	1.52
1	16S1	966	2MG	C2-N2	13.02	1.45	1.34
55	PTR1	37	2MG	C2-N2	12.41	1.44	1.34
1	16S1	1207	2MG	C2-N2	12.17	1.44	1.34
1	16S1	1516	2MG	C2-N2	11.73	1.44	1.34

The worst 5 of 185 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1519	MA6	N1-C6-N6	-12.35	104.06	117.06
1	16S1	1518	MA6	N1-C6-N6	-12.19	104.23	117.06
22	23S1	1917	PSU	N1-C2-N3	-11.54	119.25	128.43
1	16S1	516	PSU	N1-C2-N3	-11.28	119.46	128.43
22	23S1	2605	PSU	N1-C2-N3	-11.21	119.52	128.43

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16S1	966	2MG	O4'-C4'-C5'-O5'
1	16S1	966	2MG	C3'-C4'-C5'-O5'
1	16S1	527	G7M	O4'-C4'-C5'-O5'
1	16S1	527	G7M	C3'-C4'-C5'-O5'
1	16S1	1519	MA6	O4'-C4'-C5'-O5'

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](#)

Of 1691 ligands modelled in this entry, 1201 are unknown and 489 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
60	ORN	23S1	3001	-	4,8,8	0.34	0	3,9,9	0.38	0

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
60	ORN	23S1	3001	-	-	2/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	23S1	3001	ORN	N-CA-CB-CG
60	23S1	3001	ORN	C-CA-CB-CG

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	23S1	2
10	S101	1
55	PTR1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	23S1	885:C	O3'	892:A	P	13.12
1	PTR1	46:G7M	O3'	48:C	P	5.31
1	23S1	2099:U	O3'	2100:G	P	4.47
1	S101	53:ILE	C	54:SER	N	1.18