



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 02:24 pm GMT

PDB ID : 6TBV
EMDB ID : EMD-10453
Title : Cryo-EM structure of an Escherichia coli ribosome-SpeFL complex stalled in response to L-ornithine (Replicate 2)
Authors : Herrero del Valle, A.; Innis, C.A.
Deposited on : 2019-11-04
Resolution : 2.70 Å(reported)
Based on initial model : 4YBB

This is a wwPDB EM Validation Summary Report for a publicly released PDB 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

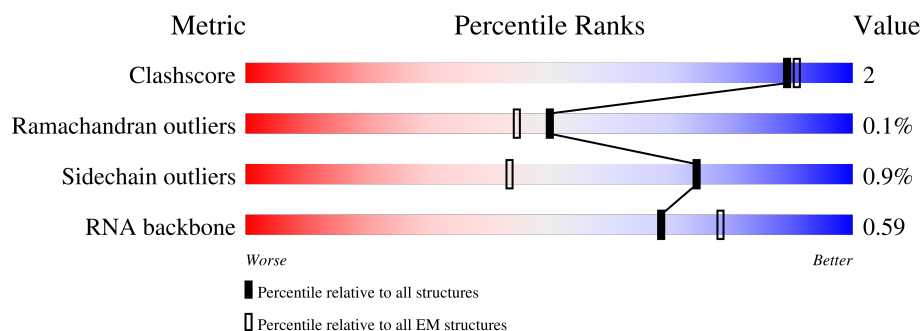
1 Overall quality at a glance

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.



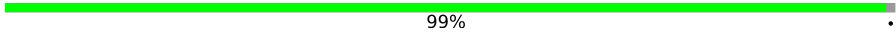
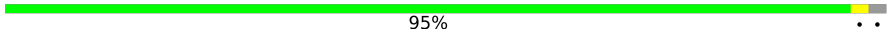
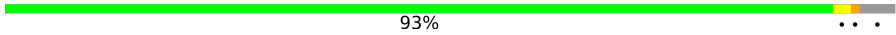

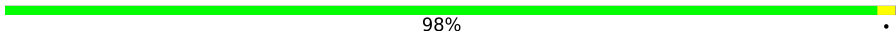
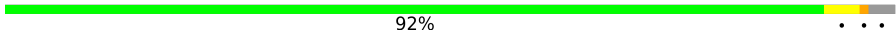
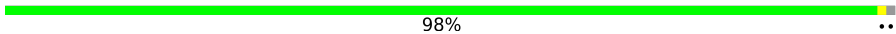
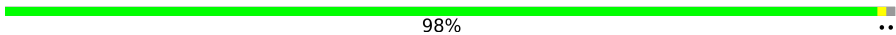
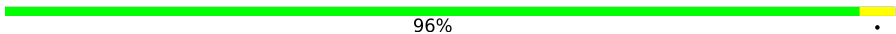
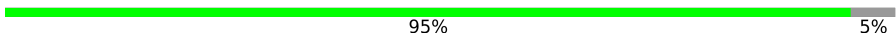


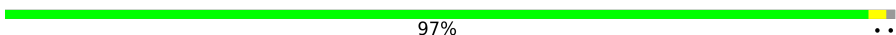



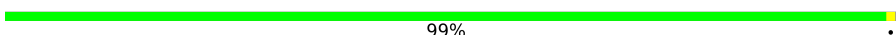
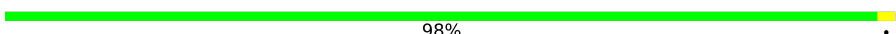
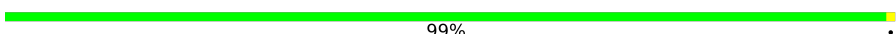
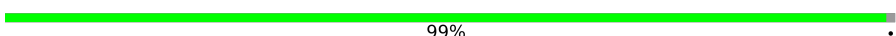
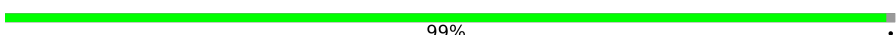
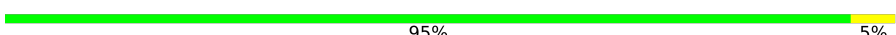

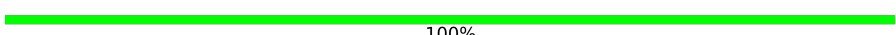
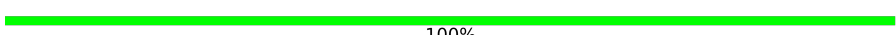
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	97% .
5	S051	167	92% 7%
6	S061	135	79% 21%
7	S071	179	82% 16%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	S081	130	 99%
9	S091	130	 95%
10	S101	103	 93%
11	S111	129	 91%
12	S121	124	 98%
13	S131	118	 92%
14	S141	102	 98%
15	S151	89	 98%
16	S161	82	 96%
17	S171	84	 95%
18	S181	75	 72%
19	S191	92	 88%
20	S201	87	 97%
21	S211	71	 76%
22	23S1	2897	 64%
23	05S1	120	 71%
24	L021	273	 99%
25	L031	209	 98%
26	L041	201	 99%
27	L051	179	 99%
28	L061	177	 99%
29	L091	149	 95%
30	L311	70	 89%
31	L131	142	 100%
32	L141	123	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	L151	144	99% .
34	L161	136	99% .
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	92% . 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	97% ..
48	L321	57	96% ..
49	L331	55	91% . 7%
50	L341	46	98% .
51	L351	65	95% ...
52	L361	38	97% .
53	SPE1	34	88% 12%
54	MRN1	7	43% 43% 14%
55	PTR1	76	59% 32% 9%

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	S	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	250	Total	Mg	0
			250	250	
56	L231	1	Total	Mg	0
			1	1	
56	PTR1	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	105	Total	K	0
			105	105	
57	05S1	1	Total	K	0
			1	1	
57	L031	1	Total	K	0
			1	1	
57	L161	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	16S1	148	Total	X	0
			148	148	
58	S021	1	Total	X	0
			1	1	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	S031	1	Total 1	X 1	0
58	S111	2	Total 2	X 2	0
58	S131	1	Total 1	X 1	0
58	S171	1	Total 1	X 1	0
58	23S1	919	Total 919	X 919	0
58	05S1	9	Total 9	X 9	0
58	L021	20	Total 20	X 20	0
58	L031	14	Total 14	X 14	0
58	L041	10	Total 10	X 10	0
58	L131	5	Total 5	X 5	0
58	L141	7	Total 7	X 7	0
58	L151	4	Total 4	X 4	0
58	L161	3	Total 3	X 3	0
58	L171	5	Total 5	X 5	0
58	L181	1	Total 1	X 1	0
58	L191	4	Total 4	X 4	0
58	L201	7	Total 7	X 7	0
58	L211	1	Total 1	X 1	0
58	L221	8	Total 8	X 8	0
58	L231	1	Total 1	X 1	0
58	L241	2	Total 2	X 2	0

Continued on next page...

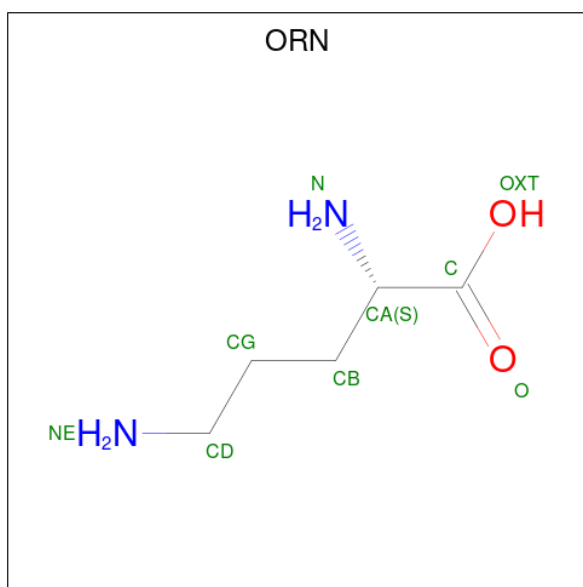
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
58	L251	1	Total 1	X 1	0
58	L271	1	Total 1	X 1	0
58	L281	1	Total 1	X 1	0
58	L321	2	Total 2	X 2	0
58	L331	1	Total 1	X 1	0
58	L341	7	Total 7	X 7	0
58	L351	4	Total 4	X 4	0
58	SPE1	6	Total 6	X 6	0
58	MRN1	1	Total 1	X 1	0
58	PTR1	3	Total 3	X 3	0

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

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

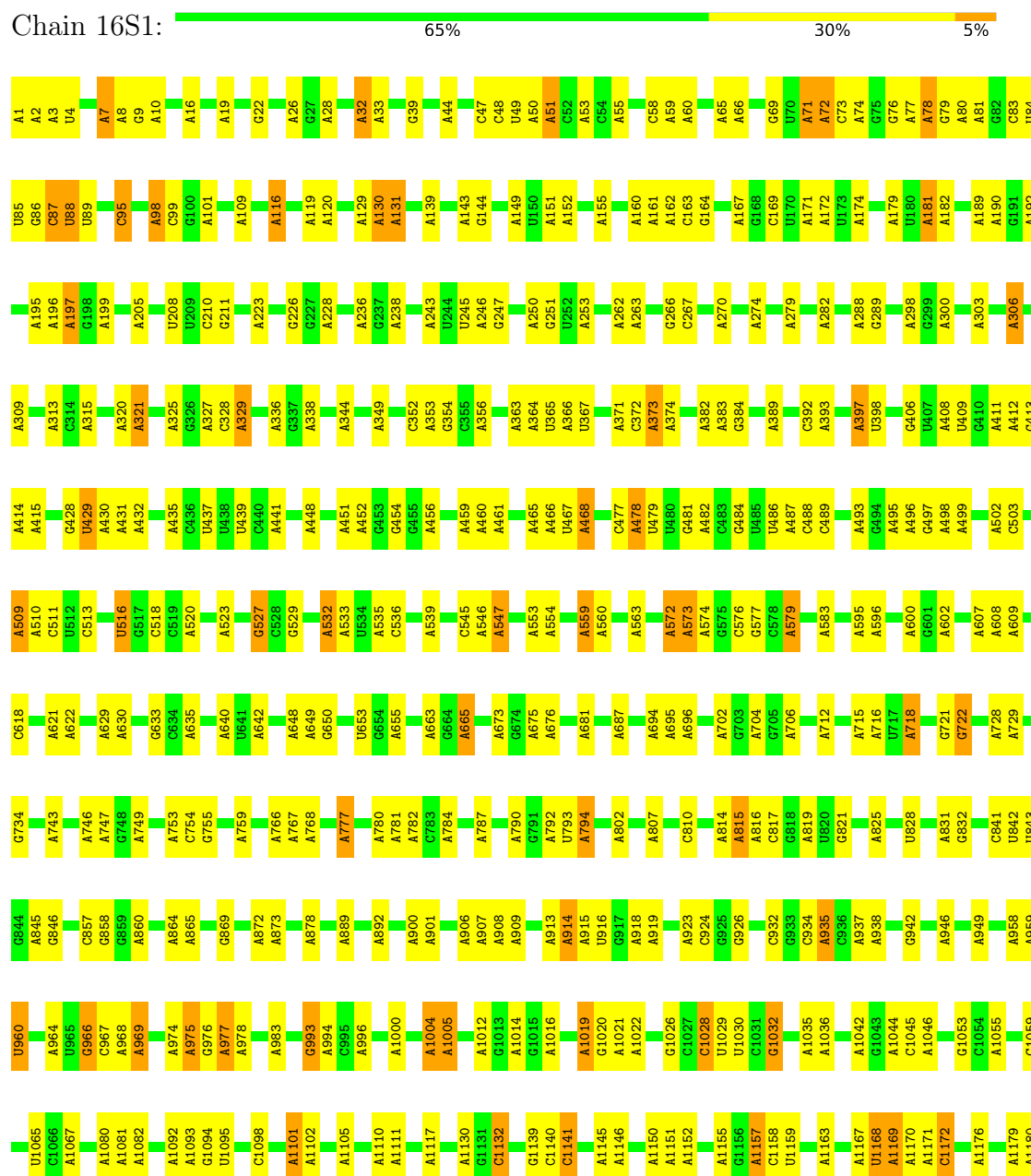
- Molecule 61 is water.

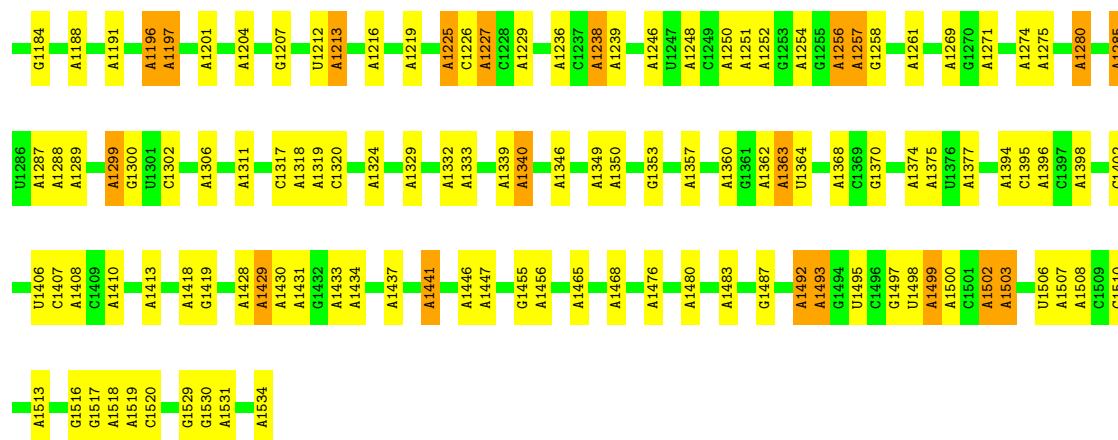
Mol	Chain	Residues	Atoms		AltConf
61	16S1	165	Total	O	0
			165	165	
61	S111	1	Total	O	0
			1	1	
61	S131	2	Total	O	0
			2	2	
61	S141	3	Total	O	0
			3	3	
61	S171	1	Total	O	0
			1	1	
61	23S1	616	Total	O	0
			616	616	
61	L021	6	Total	O	0
			6	6	
61	L031	2	Total	O	0
			2	2	
61	L151	2	Total	O	0
			2	2	
61	L171	2	Total	O	0
			2	2	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

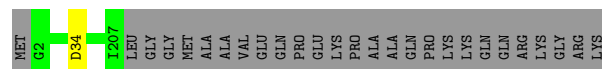




- Molecule 2: 30S ribosomal protein S2



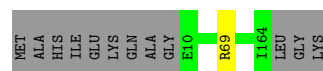
- Molecule 3: 30S ribosomal protein S3



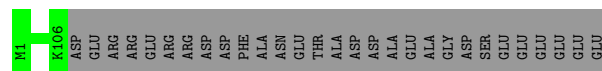
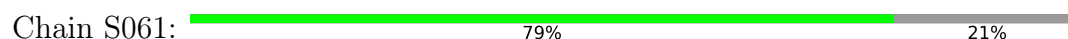
- Molecule 4: 30S ribosomal protein S4




- Molecule 5: 30S ribosomal protein S5

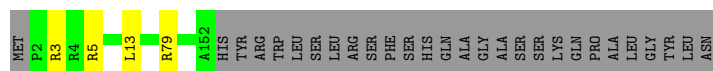


- Molecule 6: 30S ribosomal protein S6



- Molecule 7: 30S ribosomal protein S7

Chain S071:  82% 16%



- Molecule 8: 30S ribosomal protein S8

Chain S081:  99%



- Molecule 9: 30S ribosomal protein S9

Chain S091:  95%



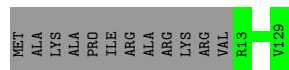
- Molecule 10: 30S ribosomal protein S10

Chain S101:  93%



- Molecule 11: 30S ribosomal protein S11

Chain S111:  91% 9%



- Molecule 12: 30S ribosomal protein S12

Chain S121:  98%



- Molecule 13: 30S ribosomal protein S13

Chain S131:  92%



- Molecule 14: 30S ribosomal protein S14

Chain S141:  98% ..



- Molecule 15: 30S ribosomal protein S15

Chain S151:  98% ..



- Molecule 16: 30S ribosomal protein S16

Chain S161:  96% .



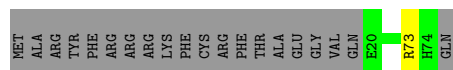
- Molecule 17: 30S ribosomal protein S17

Chain S171:  95% 5%



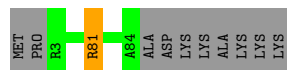
- Molecule 18: 30S ribosomal protein S18

Chain S181:  72% . 27%



- Molecule 19: 30S ribosomal protein S19

Chain S191:  88% . 11%




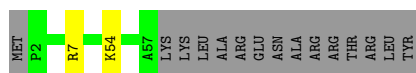
- Molecule 20: 30S ribosomal protein S20

Chain S201:  97% ..



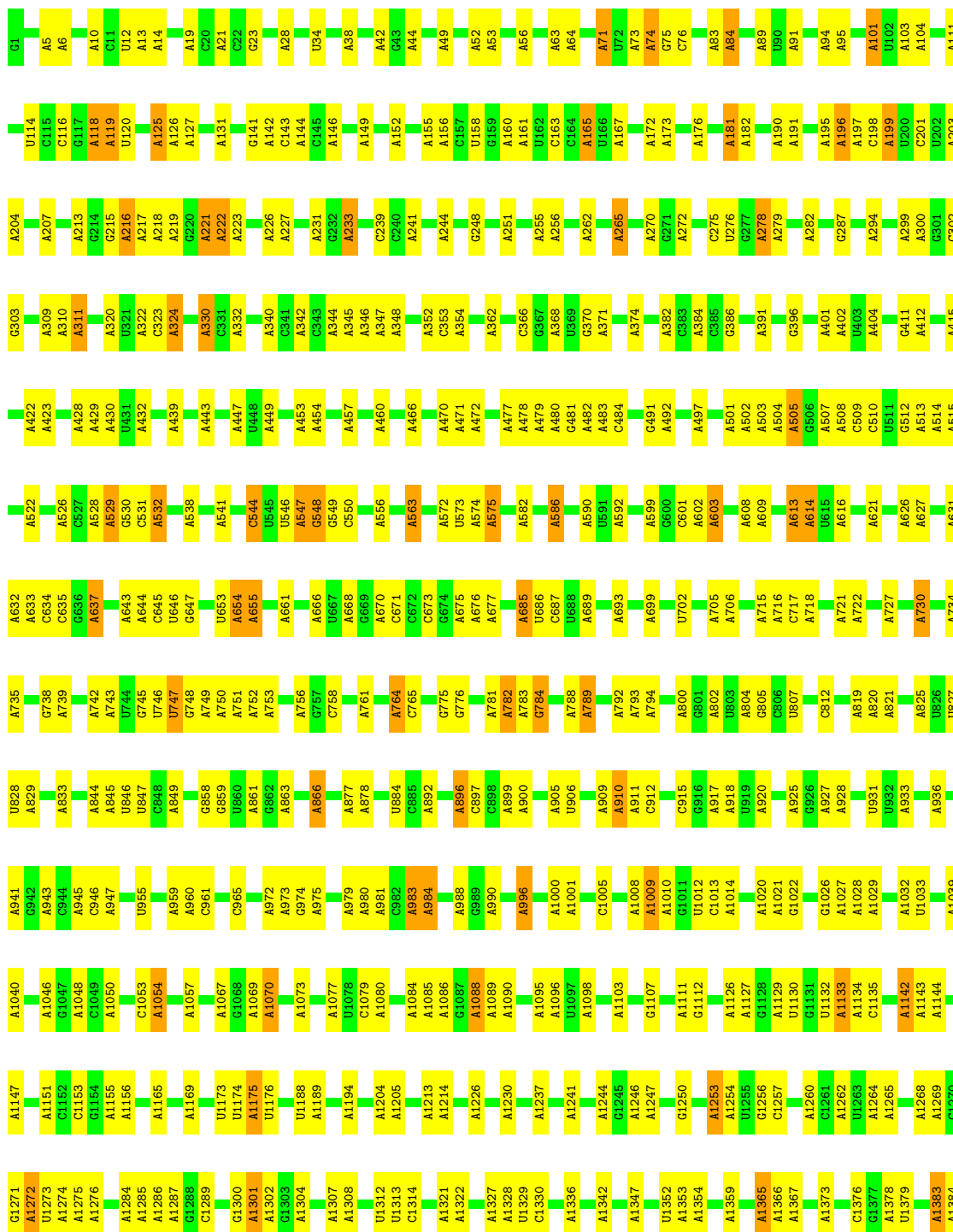
- Molecule 21: 30S ribosomal protein S21

Chain S211:  76% 21%



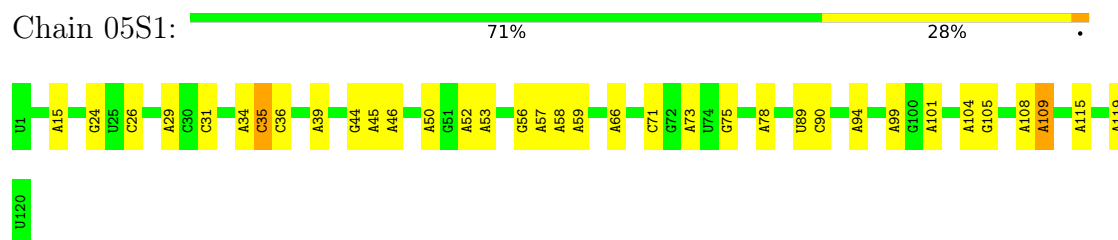
• Molecule 22: 23S rRNA

Chain 23S1:  64% 31% 5%



A2899	G2777	G2445	G2345	G2388	G2128	A2052	A1953	A1819	C1730	A1630	A1525	A1385
A2900	A2778	G2446	G2346	A2241	U2131	G2053	G1954	U1820	C1735	G1631	A1528	C1386
U2903	A2781	A2447	C2347	A2242	U2132	C2055	U1955	A1821	A1735	A1632	A1529	A1387
		A2448		U2243	G2133	G2056	A1960	A1829	G1738	A1634	A1532	A1392
		U2449	C2350	G2243	A2134	G2057	G1961	G1835	A1739	A1635	A1535	A1393
		A2450	G2351	A2247	A2135	A2058	C1962			U1636		U1394
		A2451	G2352		G2136	A2059			A1744	A1637	A1535	A1395
		C2452	A2353	G2251	U2137	A2060	A1966	A1847	A1745	A1644	A1544	
		A2453	G2354	G2252	A2142	A2062	C1967	A1848	A1746	A1641	G1546	C1398
		U2457	A2358			C2063	A1969	A1853	A1749		C1547	A1403
		G2458	A2366	A2266	C2146	G2069	A1970	A1854			A1548	
		A2459	G2367	A2267	A2147	A2070	C1968	A1858	A1754	C1644	A1549	A1413
		A2461	C2368	A2268	C2150	A2071	U1971	A1866	A1755	U1647	G1550	
			A2369	G2269	A2151	C2072	A1977	A1872	G1756	U1648	A1551	G1416
		A2468	A2376	A2270	A2154	C2073	A1978	A1871	U1758	G1649	A1552	
		A2469	A2377	A2273	A2157	A2077	A1981	A1872	A1759	A1650	A1553	A1419
		G2470	A2378	A2274	A2158			G1873		G1651		A1420
		A2471	A2379					A1877	A1762	A1652	A1566	
			A2381	A2278	A2162	A2080	A1987	A1885	A1763	G1653		A1427
		A2476	G2382	A2281	G2163	U2081	A1987	A1876	C1764	A1654	A1569	C1428
		U2477	C2383	G2282	A2164	A2082	U1991	A1877		A1655	A1570	
		A2478	U2384	A2284	C2165	A2088	G1992			A1656	A1571	A1431
		U2479	C2385	C2285		C2089	U1993	A1885	A1772		A1572	G1432
		C2480	G2386	A2287	A2169	A2090			A1773	A1664		A1433
		A2481	U2387	A2288	A2170	A2091	A1997	A1889	C1774	A1665		A1434
		G2482	U2388	A2289	A2171	G2093	A1998	A1890	U1775	A1668	U1578	
		U2491		A2290	U2172	A2094	A1998	A1891	A1779	A1669	A1580	U1437
		A2497	A2392	A2297	A2173	A2095	A2003	A1899	U1780	C1670	A1583	U1438
		C2498	U2402	A2298	A2176	C2096	G2004	A1901	A1781	U1671	U1584	A1439
		G2502	A2406	G2306	U2182	U2098	A2005	A1902	U1782	A1672	C1585	G1452
		U2503	A2407	G2307	A2183	U2098	C2006	A1903	A1783	G1673	A1586	A1453
		G2504	A2407	G2308	A2184			A1911	A1784	G1674	A1590	A1469
		G2505	A2411	A2309	A2188			A1912	A1785	C1675	A1591	A1470
		A2513	A2412	A2311	U2189	G2107	A2013	A1913	A1786	A1676	C1592	
			A2418	A2314	G2190	U2109	A2014	C1914	A1787	A1677	A1597	A1477
		A2516	A2425	A2317	A2191	U2110	A2015	3TD1915	C1788	A1678	A1596	G1482
		C2517	A2426	A2321	A2195	U2111	A2019	U1917	A1789	A1679	A1597	
		A2518	A2426	A2322	U2196	G2112	A2020	A1918	U1791	A1689	A1598	A1490
		G2529	G2429	A2325	C2196	U2113	C2023	A1919	A1794	A1690		A1494
		A2530	U2431	A2327	U2197	A2114	G2027	C1920		A1698	A1603	A1495
		A2531	A2432	A2328	A2198	G2115	A2030	A1927	C1800	G1699	A1496	
			A2433	A2329	A2199	G2116	A2031	A1928	A1801	A1700	C1606	
		A2534	A2434	A2330	A2204	U2117	G2032	G1929	A1802	A1701	C1607	A1502
		C2540	A2435	A2331	A2205	U2118	A2033	G1930	A1803	A1705	A1603	A1503
		A2541	A2439	A2332	A2211	G2120	A2033	U1931	C1804	A1705	A1610	A1504
		A2542	C2440	A2333	A2212	G2121	A2037	A1932	A1805	A1711	A1614	A1505
		A2547	U2441	A2334	A2212	G2122	A2042	A1936	A1808	U1712	A1615	A1508
		U2552	G2442	A2335	A2225	G2123	C2043	A1937	A1809	A1713	A1616	A1509
		A2560	C2443	A2336	A2226	G2124	C2044	A1938	G1811	A1717	C1617	A1515
			G2444	A2340	A2227	A2126	U1939	U1939	A1815	A1722	A1618	
						G2127	A2051	A1952	C1816		A1626	A1522

- Molecule 23: 5S rRNA



- Molecule 24: 50S ribosomal protein L2



- Molecule 25: 50S ribosomal protein L3



- Molecule 26: 50S ribosomal protein L4



- Molecule 27: 50S ribosomal protein L5



- Molecule 28: 50S ribosomal protein L6



- Molecule 29: 50S ribosomal protein L9





- Molecule 30: 50S ribosomal protein L31

Chain L311: 89% 6% 6%



- Molecule 31: 50S ribosomal protein L13

Chain L131: 100%

There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L14

Chain L141: 100%

There are no outlier residues recorded for this chain.

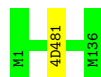
- Molecule 33: 50S ribosomal protein L15

Chain L151: 99% .



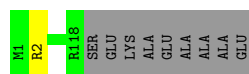
- Molecule 34: 50S ribosomal protein L16

Chain L161: 99% .



- Molecule 35: 50S ribosomal protein L17

Chain L171: 92% . 7%



- 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.

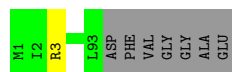
- Molecule 40: 50S ribosomal protein L22

Chain L221:  99%



- Molecule 41: 50S ribosomal protein L23

Chain L231:  92%



- Molecule 42: 50S ribosomal protein L24

Chain L241:  97%



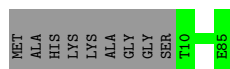
- Molecule 43: 50S ribosomal protein L25

Chain L251:  100%

There are no outlier residues recorded for this chain.

- Molecule 44: 50S ribosomal protein L27

Chain L271:  89%



- 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: 97%



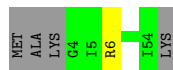
- Molecule 48: 50S ribosomal protein L32

Chain L321: 96%



- Molecule 49: 50S ribosomal protein L33

Chain L331: 91%



- Molecule 50: 50S ribosomal protein L34

Chain L341: 98%



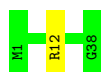
- Molecule 51: 50S ribosomal protein L35

Chain L351: 95%



- Molecule 52: 50S ribosomal protein L36

Chain L361: 97%



- Molecule 53: SpeFL

Chain SPE1: 88%



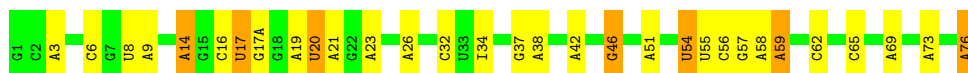
- Molecule 54: mRNA

Chain MRN1: 43%



- Molecule 55: P-site Arg-tRNA

Chain PTR1: 59%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	137494	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 ($e^-/\text{\AA}^2$)	29.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1500	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: 4SU, 1MG, ZN, 3TD, G7M, PSU, OMU, D2T, UNX, RSP, 5MC, UR3, 2MA, FME, OMG, 5MU, K, 2MG, MG, MEQ, MA6, 4OC, ORN, 6MZ, 4D4, OMC

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 >5	RMSZ	# Z >5
1	16S1	1.46	1103/36593 (3.0%)	3.48	4366/57081 (7.6%)
2	S021	0.68	0/1784	0.72	5/2403 (0.2%)
3	S031	0.78	0/1651	0.58	1/2225 (0.0%)
4	S041	0.83	0/1665	0.61	2/2227 (0.1%)
5	S051	0.72	0/1157	0.60	0/1557
6	S061	0.71	0/881	0.57	0/1189
7	S071	0.85	0/1195	0.65	1/1602 (0.1%)
8	S081	0.67	0/989	0.56	0/1326
9	S091	0.99	0/1034	0.83	0/1375
10	S101	0.88	0/805	0.70	1/1089 (0.1%)
11	S111	0.80	0/893	0.63	0/1205
12	S121	0.89	0/960	0.62	0/1286
13	S131	0.95	1/892 (0.1%)	0.78	1/1193 (0.1%)
14	S141	0.91	0/811	0.62	0/1081
15	S151	0.87	0/722	0.51	0/964
16	S161	0.87	0/659	0.68	0/884
17	S171	0.76	0/657	0.56	0/881
18	S181	0.87	0/462	0.56	0/621
19	S191	0.77	0/672	0.59	0/904
20	S201	0.72	0/676	0.53	1/895 (0.1%)
21	S211	1.01	0/472	0.53	0/627
22	23S1	1.53	2027/69120 (2.9%)	3.56	8534/107824 (7.9%)
23	05S1	1.32	71/2872 (2.5%)	3.09	276/4478 (6.2%)
24	L021	0.84	0/2121	0.60	1/2852 (0.0%)
25	L031	0.73	2/1576 (0.1%)	0.75	4/2119 (0.2%)
26	L041	0.70	0/1571	0.54	0/2113
27	L051	0.78	0/1434	0.63	0/1926
28	L061	0.65	0/1343	0.56	0/1816
29	L091	0.76	1/1121 (0.1%)	0.88	4/1515 (0.3%)
30	L311	0.77	0/531	0.87	3/709 (0.4%)
31	L131	0.72	0/1152	0.50	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L141	0.81	0/955	0.58	0/1279
33	L151	0.81	0/1062	0.55	0/1413
34	L161	0.79	0/1081	0.54	0/1443
35	L171	0.94	0/958	0.60	0/1281
36	L181	0.83	0/910	0.52	0/1219
37	L191	0.84	0/929	0.52	0/1242
38	L201	0.90	0/960	0.50	0/1278
39	L211	0.73	0/829	0.54	0/1107
40	L221	0.78	0/864	0.54	0/1156
41	L231	0.72	0/744	0.61	0/994
42	L241	0.68	0/787	0.60	1/1051 (0.1%)
43	L251	0.66	0/766	0.53	0/1025
44	L271	0.83	0/587	0.49	0/776
45	L281	0.96	0/635	0.55	0/848
46	L291	0.77	0/502	0.48	0/667
47	L301	0.82	0/453	0.56	0/605
48	L321	0.89	0/450	0.69	1/599 (0.2%)
49	L331	0.67	0/421	0.68	1/561 (0.2%)
50	L341	1.14	0/380	0.69	1/498 (0.2%)
51	L351	0.77	0/513	0.64	1/676 (0.1%)
52	L361	0.91	0/303	0.52	0/397
53	SPE1	0.91	0/299	0.71	0/399
54	MRN1	0.61	0/161	1.28	1/248 (0.4%)
55	PTR1	1.65	56/1672 (3.3%)	3.19	173/2598 (6.7%)
All	All	1.34	3261/155692 (2.1%)	3.04	13379/232878 (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
2	S021	0	3
9	S091	0	1
10	S101	0	2
13	S131	0	3
19	S191	0	1
21	S211	0	1
29	L091	0	2
33	L151	0	1
47	L301	0	1
51	L351	0	1
All	All	0	16

The worst 5 of 3261 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	20	U	C5-C6	23.07	1.54	1.34
55	PTR1	17	U	C5-C6	22.09	1.54	1.34
22	23S1	2449	U	C5-C6	20.84	1.52	1.34
55	PTR1	17	U	N1-C6	10.44	1.47	1.38
55	PTR1	20	U	N1-C6	10.04	1.47	1.38

The worst 5 of 13379 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	23S1	2189	U	O5'-P-OP1	-28.80	76.14	110.70
22	23S1	2872	A	N1-C6-N6	-26.88	102.47	118.60
22	23S1	2887	A	C2-N3-C4	26.20	123.70	110.60
22	23S1	504	A	N1-C2-N3	-25.31	116.65	129.30
22	23S1	1434	A	N1-C6-N6	-24.56	103.86	118.60

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S021	123	ASP	Peptide
2	S021	126	PHE	Sidechain
2	S021	5	SER	Peptide
9	S091	24	GLY	Peptide
10	S101	56	HIS	Peptide

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	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	250	0	0	0	0
56	L231	1	0	0	0	0
56	PTR1	1	0	0	0	0
57	05S1	1	0	0	0	0
57	16S1	39	0	0	0	0
57	23S1	105	0	0	0	0
57	L031	1	0	0	0	0
57	L161	1	0	0	0	0
58	05S1	9	0	0	0	0
58	16S1	148	0	0	0	0
58	23S1	919	0	0	0	0
58	L021	20	0	0	0	0
58	L031	14	0	0	0	0
58	L041	10	0	0	0	0
58	L131	5	0	0	0	0
58	L141	7	0	0	0	0
58	L151	4	0	0	0	0
58	L161	3	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	7	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	1	0	0	0	0
58	L281	1	0	0	0	0
58	L321	2	0	0	0	0
58	L331	1	0	0	0	0
58	L341	7	0	0	0	0
58	L351	4	0	0	0	0
58	MRN1	1	0	0	0	0
58	PTR1	3	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	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	165	0	0	0	0
61	23S1	616	0	0	0	0
61	L021	6	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	3	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	S021	222/241 (92%)	210 (95%)	12 (5%)	0	100	100
3	S031	204/233 (88%)	194 (95%)	10 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	S041	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	S051	153/167 (92%)	146 (95%)	7 (5%)	0	100	100
6	S061	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	S071	149/179 (83%)	140 (94%)	9 (6%)	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%)	92 (95%)	4 (4%)	1 (1%)	13	33
11	S111	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
12	S121	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
13	S131	112/118 (95%)	101 (90%)	10 (9%)	1 (1%)	14	35
14	S141	99/102 (97%)	87 (88%)	11 (11%)	1 (1%)	13	33
15	S151	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
16	S161	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
17	S171	78/84 (93%)	75 (96%)	3 (4%)	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%)	82 (98%)	2 (2%)	0	100	100
21	S211	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
24	L021	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
25	L031	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	25	49
26	L041	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
27	L051	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
28	L061	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
29	L091	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
30	L311	64/70 (91%)	59 (92%)	5 (8%)	0	100	100
31	L131	140/142 (99%)	140 (100%)	0	0	100	100
32	L141	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	L151	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
34	L161	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
35	L171	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	L181	115/117 (98%)	113 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	L191	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
38	L201	115/118 (98%)	115 (100%)	0	0	100	100
39	L211	101/103 (98%)	100 (99%)	1 (1%)	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%)	58 (97%)	2 (3%)	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%)	43 (98%)	1 (2%)	0	100	100
51	L351	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	8	21
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%)	5397 (96%)	205 (4%)	5 (0%)	50	73

All (5) 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%)	185 (100%)	1 (0%)	86	95
3	S031	170/190 (90%)	170 (100%)	0	100	100
4	S041	172/173 (99%)	168 (98%)	4 (2%)	45	74
5	S051	118/126 (94%)	117 (99%)	1 (1%)	79	91
6	S061	92/116 (79%)	92 (100%)	0	100	100
7	S071	124/147 (84%)	121 (98%)	3 (2%)	44	73
8	S081	104/105 (99%)	104 (100%)	0	100	100
9	S091	105/107 (98%)	103 (98%)	2 (2%)	52	79
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%)	101 (99%)	1 (1%)	73	89
13	S131	92/96 (96%)	91 (99%)	1 (1%)	70	87
14	S141	79/84 (94%)	79 (100%)	0	100	100
15	S151	76/77 (99%)	75 (99%)	1 (1%)	65	85
16	S161	65/65 (100%)	62 (95%)	3 (5%)	23	49
17	S171	74/78 (95%)	74 (100%)	0	100	100
18	S181	48/65 (74%)	47 (98%)	1 (2%)	48	76
19	S191	71/79 (90%)	70 (99%)	1 (1%)	62	84
20	S201	65/66 (98%)	64 (98%)	1 (2%)	60	83
21	S211	48/61 (79%)	47 (98%)	1 (2%)	48	76
24	L021	216/218 (99%)	215 (100%)	1 (0%)	86	95
25	L031	163/163 (100%)	162 (99%)	1 (1%)	84	94
26	L041	165/165 (100%)	163 (99%)	2 (1%)	67	86
27	L051	148/150 (99%)	148 (100%)	0	100	100
28	L061	137/138 (99%)	137 (100%)	0	100	100
29	L091	114/114 (100%)	113 (99%)	1 (1%)	75	90
30	L311	59/62 (95%)	57 (97%)	2 (3%)	32	61
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%)	73	89
34	L161	108/108 (100%)	108 (100%)	0	100	100
35	L171	98/103 (95%)	97 (99%)	1 (1%)	73	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	70	87
39	L211	84/84 (100%)	84 (100%)	0	100	100
40	L221	93/93 (100%)	92 (99%)	1 (1%)	70	87
41	L231	80/84 (95%)	79 (99%)	1 (1%)	65	85
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%)	36	65
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%)	48	76
49	L331	45/49 (92%)	45 (100%)	0	100	100
50	L341	38/38 (100%)	38 (100%)	0	100	100
51	L351	51/52 (98%)	51 (100%)	0	100	100
52	L361	34/34 (100%)	33 (97%)	1 (3%)	37	67
53	SPE1	31/31 (100%)	28 (90%)	3 (10%)	6	17
All	All	4664/4858 (96%)	4624 (99%)	40 (1%)	74	90

5 of 40 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	L151	78	ARG
48	L321	40	ARG
35	L171	2	ARG
41	L231	3	ARG
53	SPE1	4	ASN

Sometimes 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%)	173 (11%)	1 (0%)
22	23S1	2890/2897 (99%)	296 (10%)	18 (0%)
23	05S1	119/120 (99%)	7 (5%)	0
54	MRN1	6/7 (85%)	3 (50%)	1 (16%)
55	PTR1	73/76 (96%)	11 (15%)	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	7	A
1	16S1	9	G
1	16S1	22	G
1	16S1	32	A
1	16S1	39	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	23S1	2189	U
22	23S1	2756	U
55	PTR1	19	A
22	23S1	2873	A
22	23S1	2518	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$
22	PSU	23S1	955	22	18,21,22	4.02	7 (38%)	22,30,33	1.94	5 (22%)
22	G7M	23S1	2069	57,22	20,26,27	2.25	6 (30%)	17,39,42	1.27	3 (17%)
55	5MU	PTR1	54	55	19,22,23	1.01	2 (10%)	28,32,35	1.21	4 (14%)
1	MA6	16S1	1519	1	18,26,27	1.25	1 (5%)	19,38,41	3.34	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	4D4	L161	81	34	9,11,12	2.55	3 (33%)	8,13,15	1.21	1 (12%)
12	D2T	S121	89	12	7,9,10	1.02	0	6,11,13	2.29	2 (33%)
1	2MG	16S1	1516	1	18,26,27	2.33	7 (38%)	16,38,41	1.51	4 (25%)
55	PSU	PTR1	55	55	18,21,22	4.27	7 (38%)	22,30,33	1.76	5 (22%)
1	2MG	16S1	1207	57,1	18,26,27	2.40	7 (38%)	16,38,41	1.45	3 (18%)
1	G7M	16S1	527	57,1	20,26,27	2.40	6 (30%)	17,39,42	1.18	2 (11%)
22	5MU	23S1	1939	57,22	19,22,23	0.73	0	28,32,35	1.25	3 (10%)
22	PSU	23S1	2580	57,22	18,21,22	4.10	7 (38%)	22,30,33	2.04	6 (27%)
22	PSU	23S1	2605	22	18,21,22	4.04	7 (38%)	22,30,33	1.87	5 (22%)
55	4SU	PTR1	8	55	18,21,22	3.47	8 (44%)	26,30,33	1.65	4 (15%)
1	4OC	16S1	1402	56,1	20,23,24	2.93	8 (40%)	26,32,35	1.09	2 (7%)
1	2MG	16S1	966	1	18,26,27	2.41	7 (38%)	16,38,41	1.49	4 (25%)
1	PSU	16S1	516	56,1	18,21,22	4.07	8 (44%)	22,30,33	1.70	4 (18%)
22	PSU	23S1	2457	22	18,21,22	4.07	7 (38%)	22,30,33	2.05	5 (22%)
25	MEQ	L031	150	25	8,9,10	1.49	2 (25%)	5,10,12	1.81	2 (40%)
22	1MG	23S1	745	22	18,26,27	2.50	5 (27%)	19,39,42	1.52	4 (21%)
22	PSU	23S1	1917	22	18,21,22	4.13	7 (38%)	22,30,33	1.67	4 (18%)
22	PSU	23S1	1911	22	18,21,22	4.18	7 (38%)	22,30,33	1.89	5 (22%)
22	6MZ	23S1	2030	22	18,25,26	2.88	5 (27%)	16,36,39	2.80	4 (25%)
22	OMC	23S1	2498	56,22	19,22,23	2.73	7 (36%)	26,31,34	1.01	1 (3%)
22	5MU	23S1	747	22	19,22,23	0.78	0	28,32,35	1.21	2 (7%)
22	PSU	23S1	2604	22	18,21,22	4.00	7 (38%)	22,30,33	1.78	5 (22%)
22	2MG	23S1	1835	22	18,26,27	2.29	7 (38%)	16,38,41	1.47	4 (25%)
1	MA6	16S1	1518	1	18,26,27	1.22	1 (5%)	19,38,41	3.13	2 (10%)
55	G7M	PTR1	46	55	20,26,27	2.56	6 (30%)	17,39,42	1.23	3 (17%)
22	3TD	23S1	1915	22	18,22,23	4.10	8 (44%)	22,32,35	1.63	2 (9%)
22	2MG	23S1	2445	22	18,26,27	2.29	7 (38%)	16,38,41	1.49	3 (18%)
22	2MA	23S1	2503	56,22,57	19,25,26	3.25	6 (31%)	21,37,40	1.75	2 (9%)
1	UR3	16S1	1498	1	19,22,23	2.98	8 (42%)	26,32,35	1.39	2 (7%)
53	FME	SPE1	1	53	8,9,10	0.98	0	7,9,11	1.14	1 (14%)
22	6MZ	23S1	1618	22	18,25,26	2.96	4 (22%)	16,36,39	2.10	3 (18%)
22	PSU	23S1	746	56,22	18,21,22	4.04	7 (38%)	22,30,33	1.91	5 (22%)
55	RSP	PTR1	32	55	17,21,22	3.90	6 (35%)	22,30,33	1.15	2 (9%)
55	2MG	PTR1	37	55	18,26,27	2.40	7 (38%)	16,38,41	1.41	4 (25%)
22	OMG	23S1	2251	57,22,55	18,26,27	2.46	8 (44%)	19,38,41	1.99	7 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	5MC	23S1	1962	57,22	18,22,23	3.29	7 (38%)	26,32,35	1.03	2 (7%)
22	PSU	23S1	2504	57,22	18,21,22	4.16	7 (38%)	22,30,33	1.74	4 (18%)
22	OMU	23S1	2552	56,22	19,22,23	2.80	7 (36%)	26,31,34	1.83	5 (19%)
1	5MC	16S1	967	1	18,22,23	3.42	7 (38%)	26,32,35	1.04	2 (7%)
1	5MC	16S1	1407	1	18,22,23	3.38	7 (38%)	26,32,35	1.03	3 (11%)

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
22	PSU	23S1	955	22	-	0/7/25/26	0/2/2/2
22	G7M	23S1	2069	57,22	-	2/3/25/26	0/3/3/3
55	5MU	PTR1	54	55	-	2/7/25/26	0/2/2/2
1	MA6	16S1	1519	1	-	2/7/29/30	0/3/3/3
34	4D4	L161	81	34	-	3/11/12/14	-
12	D2T	S121	89	12	-	1/7/12/14	-
1	2MG	16S1	1516	1	-	0/5/27/28	0/3/3/3
55	PSU	PTR1	55	55	-	0/7/25/26	0/2/2/2
1	2MG	16S1	1207	57,1	-	0/5/27/28	0/3/3/3
1	G7M	16S1	527	57,1	-	2/3/25/26	0/3/3/3
22	5MU	23S1	1939	57,22	-	2/7/25/26	0/2/2/2
22	PSU	23S1	2580	57,22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2605	22	-	0/7/25/26	0/2/2/2
55	4SU	PTR1	8	55	-	0/7/25/26	0/2/2/2
1	4OC	16S1	1402	56,1	-	2/9/29/30	0/2/2/2
1	2MG	16S1	966	1	-	2/5/27/28	0/3/3/3
1	PSU	16S1	516	56,1	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2457	22	-	0/7/25/26	0/2/2/2
25	MEQ	L031	150	25	-	2/8/9/11	-
22	1MG	23S1	745	22	-	0/3/25/26	0/3/3/3
22	PSU	23S1	1917	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	1911	22	-	0/7/25/26	0/2/2/2
22	6MZ	23S1	2030	22	-	2/5/27/28	0/3/3/3
22	OMC	23S1	2498	56,22	-	0/9/27/28	0/2/2/2
22	5MU	23S1	747	22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2604	22	-	0/7/25/26	0/2/2/2
22	2MG	23S1	1835	22	-	0/5/27/28	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	16S1	1518	1	-	0/7/29/30	0/3/3/3
55	G7M	PTR1	46	55	-	1/3/25/26	0/3/3/3
22	3TD	23S1	1915	22	-	0/7/25/26	0/2/2/2
22	2MG	23S1	2445	22	-	2/5/27/28	0/3/3/3
22	2MA	23S1	2503	56,22,57	-	2/3/25/26	0/3/3/3
1	UR3	16S1	1498	1	-	0/7/25/26	0/2/2/2
53	FME	SPE1	1	53	-	6/7/9/11	-
22	6MZ	23S1	1618	22	-	0/5/27/28	0/3/3/3
22	PSU	23S1	746	56,22	-	1/7/25/26	0/2/2/2
55	RSP	PTR1	32	55	-	2/7/25/26	0/2/2/2
55	2MG	PTR1	37	55	-	1/5/27/28	0/3/3/3
22	OMG	23S1	2251	57,22,55	-	0/5/27/28	0/3/3/3
22	5MC	23S1	1962	57,22	-	0/7/25/26	0/2/2/2
22	PSU	23S1	2504	57,22	-	2/7/25/26	0/2/2/2
22	OMU	23S1	2552	56,22	-	1/9/27/28	0/2/2/2
1	5MC	16S1	967	1	-	0/7/25/26	0/2/2/2
1	5MC	16S1	1407	1	-	0/7/25/26	0/2/2/2

The worst 5 of 248 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	PTR1	32	RSP	C2-N3	11.95	1.49	1.36
22	23S1	1915	3TD	C6-C5	11.82	1.49	1.35
22	23S1	2504	PSU	C6-C5	11.47	1.48	1.35
22	23S1	1911	PSU	C6-C5	11.22	1.48	1.35
55	PTR1	55	PSU	C6-C5	11.21	1.48	1.35

The worst 5 of 147 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	16S1	1519	MA6	N1-C6-N6	-12.83	103.56	117.06
1	16S1	1518	MA6	N1-C6-N6	-11.96	104.47	117.06
22	23S1	2030	6MZ	C9-N6-C6	-7.25	116.63	122.87
22	23S1	2503	2MA	C2-N3-C4	6.28	120.62	115.52
1	16S1	1518	MA6	N3-C2-N1	-6.07	119.19	128.68

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	16S1	527	G7M	O4'-C4'-C5'-O5'
1	16S1	527	G7M	C3'-C4'-C5'-O5'
1	16S1	966	2MG	O4'-C4'-C5'-O5'
1	16S1	1519	MA6	O4'-C4'-C5'-O5'
25	L031	150	MEQ	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1691 ligands modelled in this entry, 489 are monoatomic and 1201 are unknown - 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	-	7,8,8	0.78	0	8,9,9	0.71	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	-	-	2/8/8/8	-

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
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	13.18
1	PTR1	46:G7M	O3'	48:C	P	5.16
1	23S1	2099:U	O3'	2100:G	P	4.33