



wwPDB EM Validation Summary Report ⓘ

Sep 18, 2021 – 08:42 am BST

PDB ID : 7O19
EMDB ID : EMD-12693
Title : Cryo-EM structure of an Escherichia coli TnaC-ribosome complex stalled in response to L-tryptophan
Authors : van der Stel, A.X.; Gordon, E.R.; Sengupta, A.; Martinez, A.K.; Klepacki, D.; Perry, T.N.; Herrero del Valle, A.; Vazquez-Laslop, N.; Sachs, M.S.; Cruz-Vera, L.R.; Innis, C.A.
Deposited on : 2021-03-29
Resolution : 2.90 Å(reported)
Based on initial model : 6TBV

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

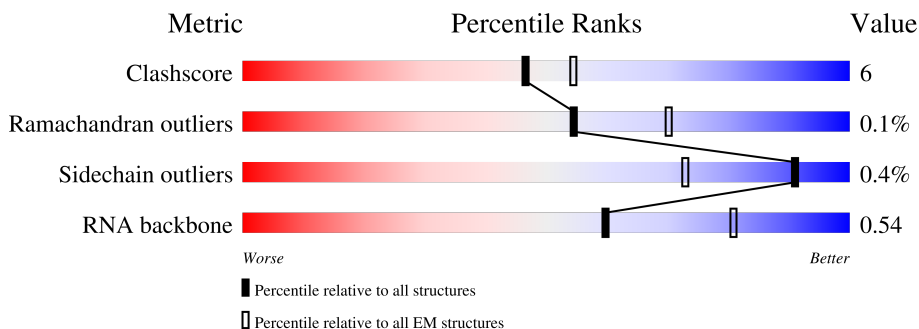
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

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 2.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	AA	1534	47% (green), 36% (yellow), 15% (orange), 2% (red), 0% (grey)
2	AB	241	66% (green), 24% (yellow), 7% (orange), 3% (red), 2% (grey)
3	AC	233	62% (green), 25% (yellow), 12% (orange), 1% (red), 0% (grey)
4	AD	206	71% (green), 28% (yellow), 1% (orange), 0% (red), 0% (grey)
5	AE	167	70% (green), 22% (yellow), 7% (orange), 1% (red), 0% (grey)
6	AF	135	50% (green), 27% (yellow), 21% (orange), 2% (red), 0% (grey)
7	AG	179	59% (green), 24% (yellow), 16% (orange), 1% (red), 0% (grey)











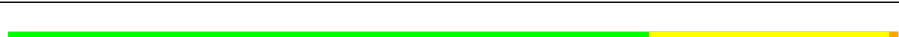


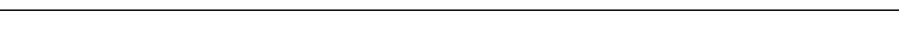
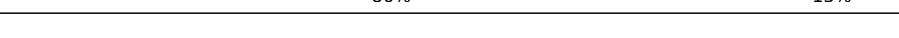
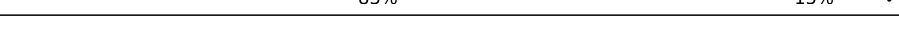

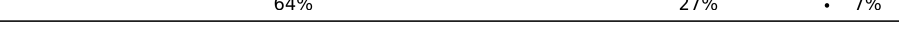

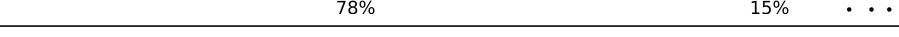


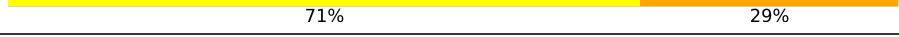
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Mol	Chain	Length	Quality of chain
8	AH	130	65% 34% ..
9	AI	130	62% 32% . .
10	AJ	103	51% 43% . .
11	AK	129	71% 20% 9%
12	AL	124	80% 19% ..
13	AM	118	57% 40% .
14	AN	102	69% 30% .
15	AO	89	78% 21% .
16	AP	82	73% 26% .
17	AQ	84	70% 24% . 5%
18	AR	75	61% 12% 27%
19	AS	92	49% 39% . 11%
20	AT	87	93% 6% .
21	AU	71	56% 21% . 21%
22	BA	2897	54% 33% 11% .
23	BB	120	66% 27% 6% .
24	BC	273	83% 15% ..
25	BD	209	88% 11% .
26	BE	201	86% 14%
27	BF	179	78% 20% ..
28	BG	177	79% 20% ..
29	BH	149	70% 30%
30	BI	70	64% 30% 6%
31	BJ	142	86% 13% .
32	BK	123	84% 15% .

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Mol	Chain	Length	Quality of chain
33	BL	144	 81% 18%
34	BM	136	 85% 14%
35	BN	127	 83% 10% 7%
36	BO	117	 84% 15%
37	BP	115	 86% 11%
38	BQ	118	 89% 10%
39	BR	103	 83% 17%
40	BS	110	 83% 16%
41	BT	100	 78% 15% 7%
42	BU	104	 76% 22%
43	BV	94	 72% 27%
44	BW	85	 78% 12% 11%
45	BX	78	 90% 9%
46	BY	63	 86% 13%
47	BZ	59	 83% 15%
48	B0	57	 84% 11%
49	B1	55	 64% 27% 7%
50	B2	46	 85% 15%
51	B3	65	 78% 15%
52	B4	38	 87% 13%
53	B5	17	 82% 12% 6%
54	B7	7	 71% 29%
55	B8	77	 55% 29% 14%

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 145019 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 Ribosomal RNA 16S.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	AE	155	1144	711	216	211	6	0	0

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	AJ	99	795	498	152	144	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	AL	123	957	591	196	165	5	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	AN	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	AS	82	656	419	125	110	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	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	AU	56	Total	C	N	O	S	0	0
			465	290	96	78	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BB	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	BC	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	BD	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	BE	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	BF	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	BG	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	BH	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	BI	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	BJ	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	BK	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	BL	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	BM	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	BN	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	BO	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	BP	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	BQ	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	BR	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	BS	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
			Total	C	N	O	S		
41	BT	93	738	466	139	131	2	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B0	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	B1	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	B2	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	B3	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	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 53 is a protein called Tryptophanase leader peptide.

Mol	Chain	Residues	Atoms			AltConf	Trace	
53	B5	17	Total	C	N	O	0	0
			146	94	27	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms				AltConf	Trace	
54	B7	7	Total	C	N	O	P	0	0
			146	65	24	50	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	B8	77	1646	733	295	541	77	0	0

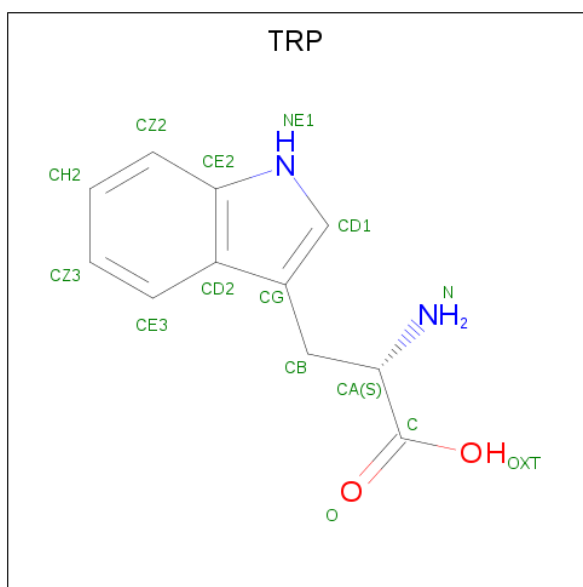
- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	AA	35	Total 35	Mg 35	0
56	BA	132	Total 132	Mg 132	0
56	BC	1	Total 1	Mg 1	0
56	BD	1	Total 1	Mg 1	0
56	B8	1	Total 1	Mg 1	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	AB	1	Total 1	Zn 1	0
57	BI	1	Total 1	Zn 1	0
57	B4	1	Total 1	Zn 1	0

- Molecule 58 is TRYPTOPHAN (three-letter code: TRP) (formula: C₁₁H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
58	BA	1	15	11	2	2	0

- Molecule 59 is water.

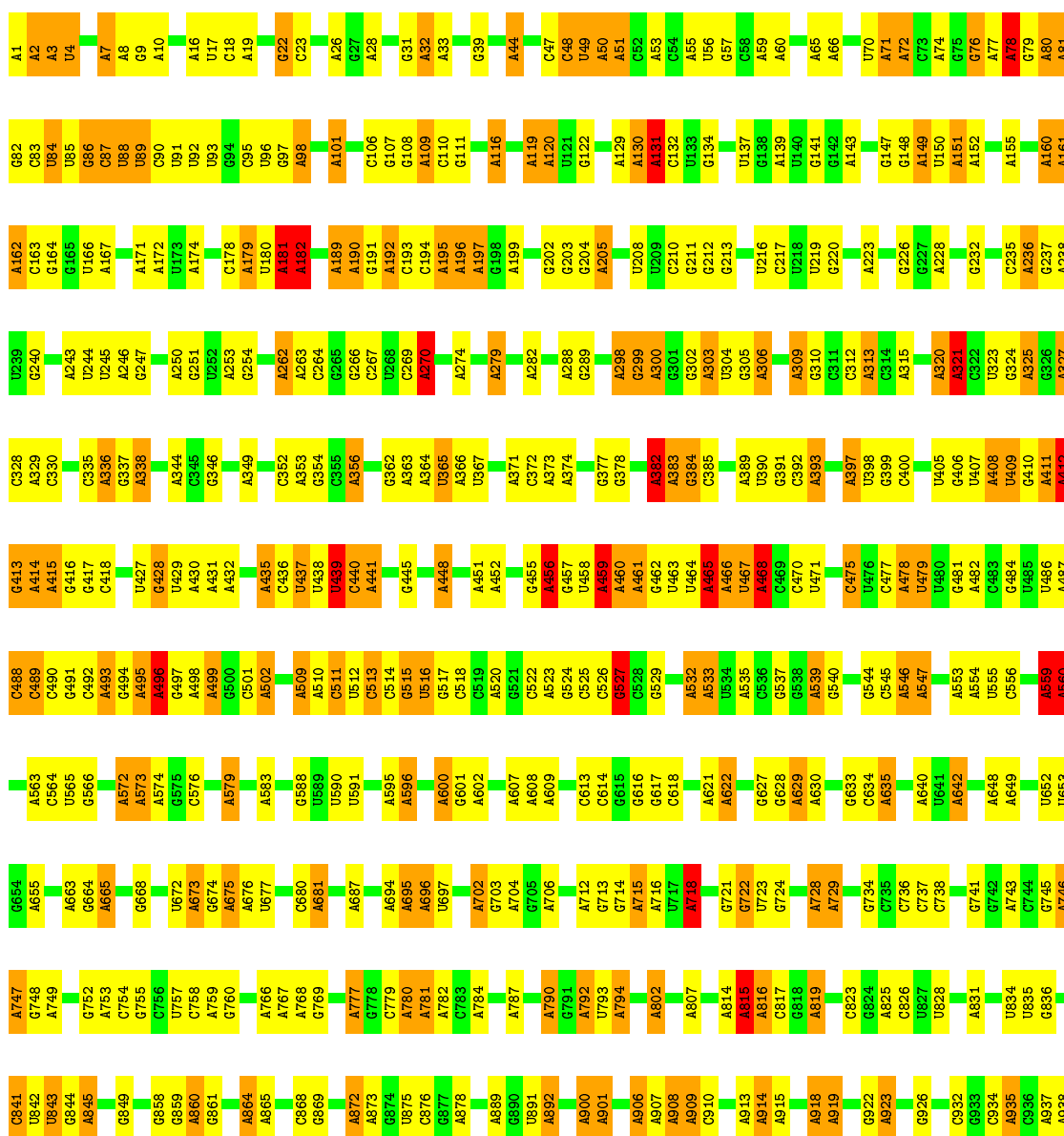
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
59	AA	168	168	168	0
59	AK	1	1	1	0
59	AM	1	1	1	0
59	AN	2	2	2	0
59	BA	608	608	608	0
59	BC	7	7	7	0
59	BD	1	1	1	0
59	BE	1	1	1	0
59	BL	2	2	2	0
59	BN	1	1	1	0
59	B8	1	1	1	0

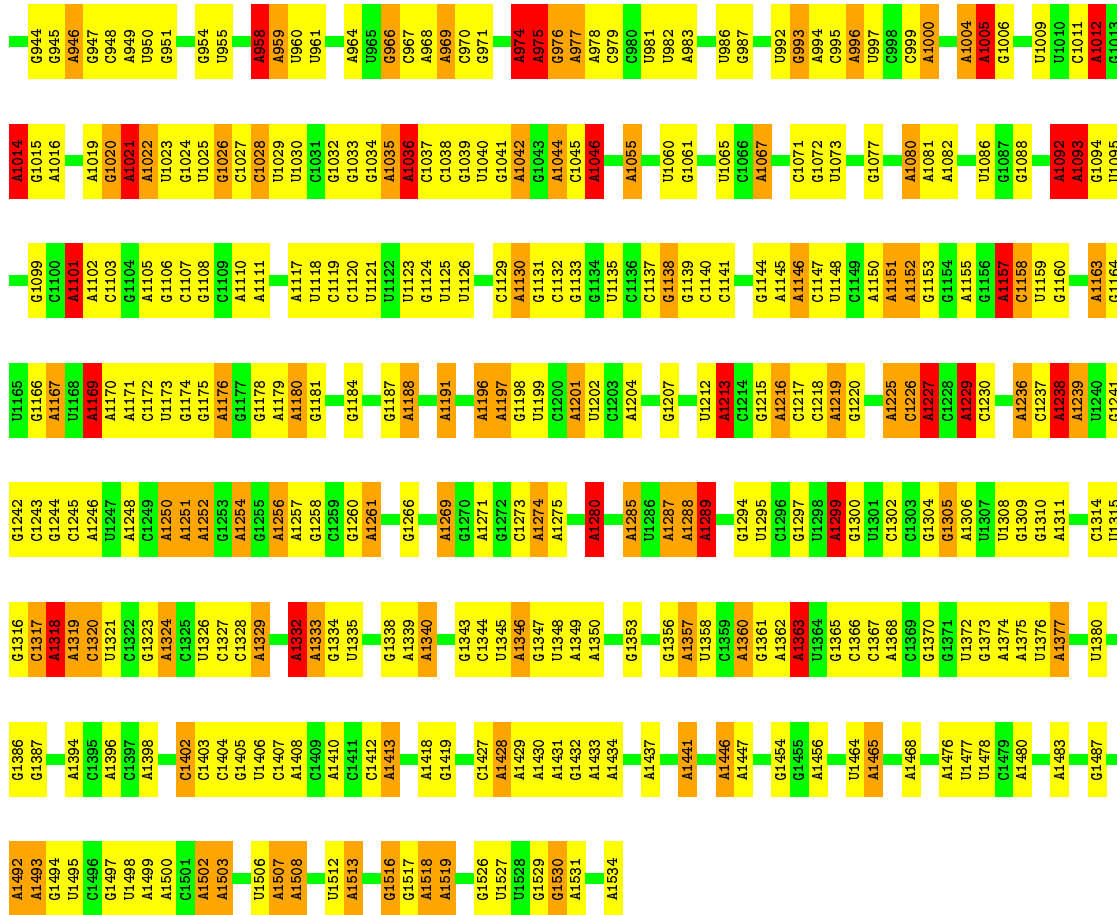
3 Residue-property plots

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.

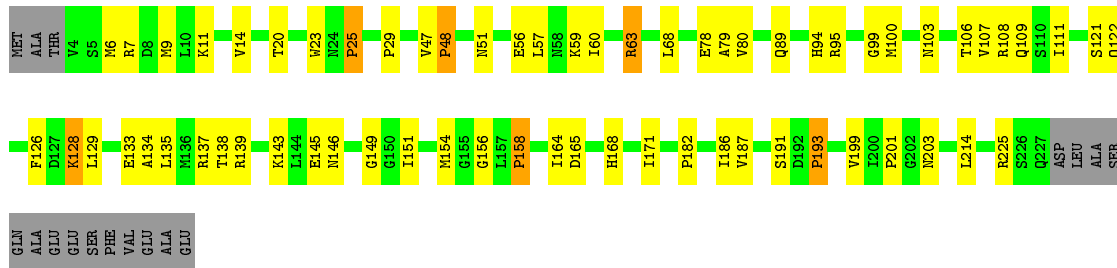
- Molecule 1: Ribosomal RNA 16S

Chain AA: 

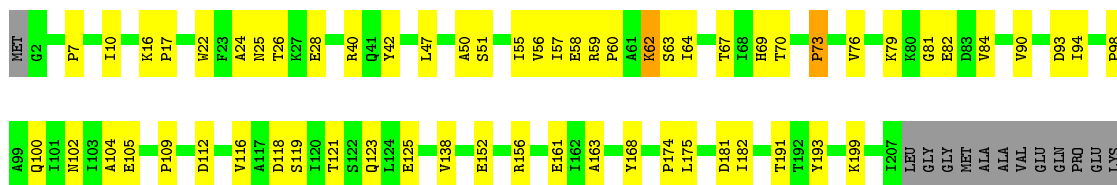




• Molecule 2: 30S ribosomal protein S2

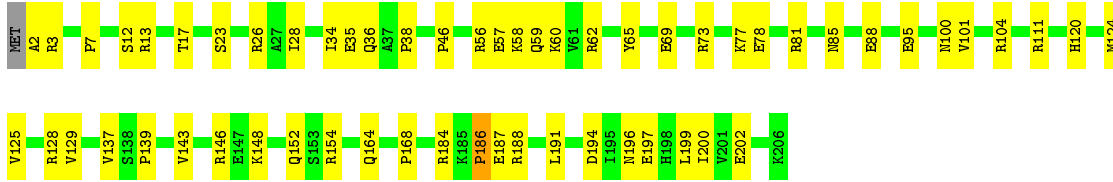


• Molecule 3: 30S ribosomal protein S3



PRO
ALA
ALA
ALA
GLN
PRO
PRO
LYS
LYS
GLN
GLN
ARG
LYS
GLY
ARG
LYS

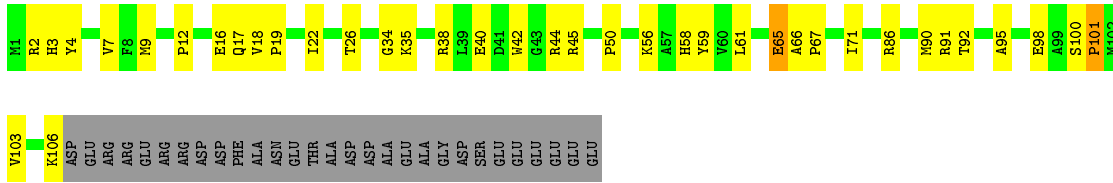
• Molecule 4: 30S ribosomal protein S4



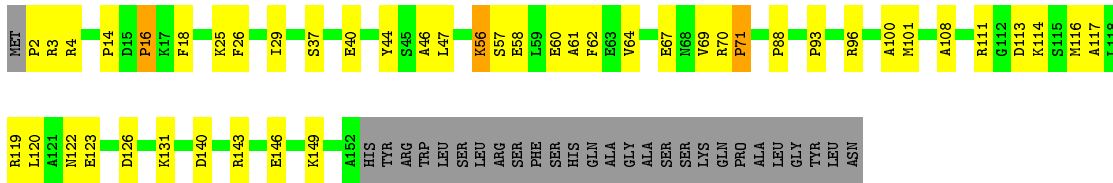
• Molecule 5: 30S ribosomal protein S5



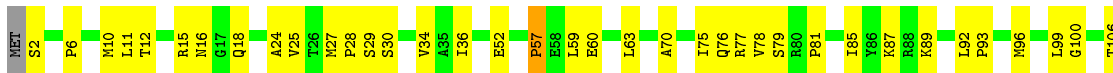
• Molecule 6: 30S ribosomal protein S6

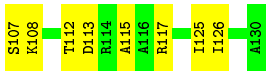


• Molecule 7: 30S ribosomal protein S7



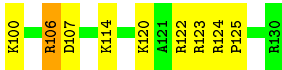
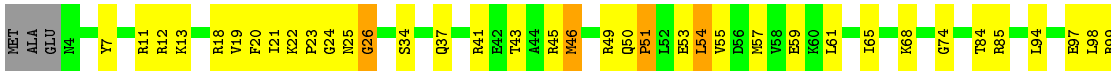
• Molecule 8: 30S ribosomal protein S8





- Molecule 9: 30S ribosomal protein S9

Chain AI: 62% 32%



- Molecule 10: 30S ribosomal protein S10

Chain AJ: 51% 43%



- Molecule 11: 30S ribosomal protein S11

Chain AK: 71% 20% 9%



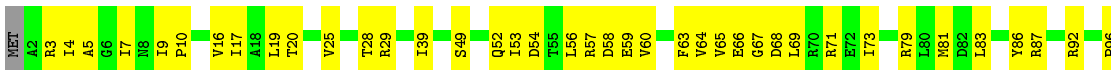
- Molecule 12: 30S ribosomal protein S12

Chain AL: 80% 19%



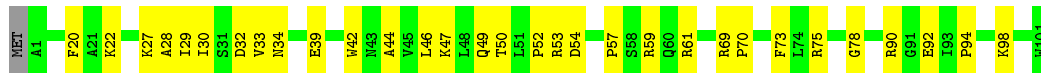
- Molecule 13: 30S ribosomal protein S13

Chain AM: 57% 40%




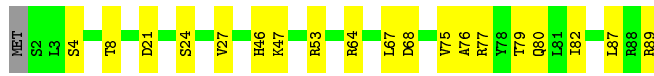
- Molecule 14: 30S ribosomal protein S14

Chain AN:  69% 30%



• Molecule 15: 30S ribosomal protein S15

Chain AO:  78% 21%



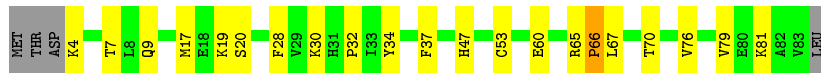
• Molecule 16: 30S ribosomal protein S16

Chain AP:  73% 26%



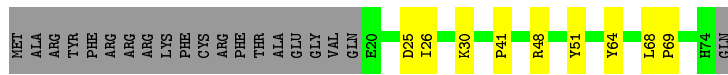
• Molecule 17: 30S ribosomal protein S17

Chain AQ:  70% 24% 5%



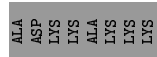
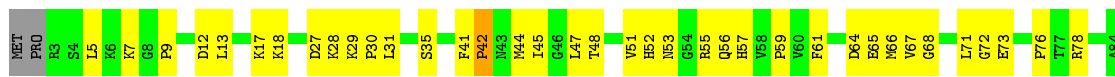
• Molecule 18: 30S ribosomal protein S18

Chain AR:  61% 12% 27%



• Molecule 19: 30S ribosomal protein S19

Chain AS:  49% 39% 11%

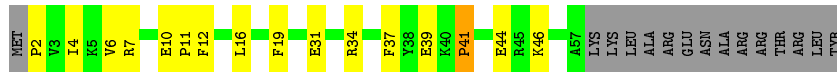


• Molecule 20: 30S ribosomal protein S20

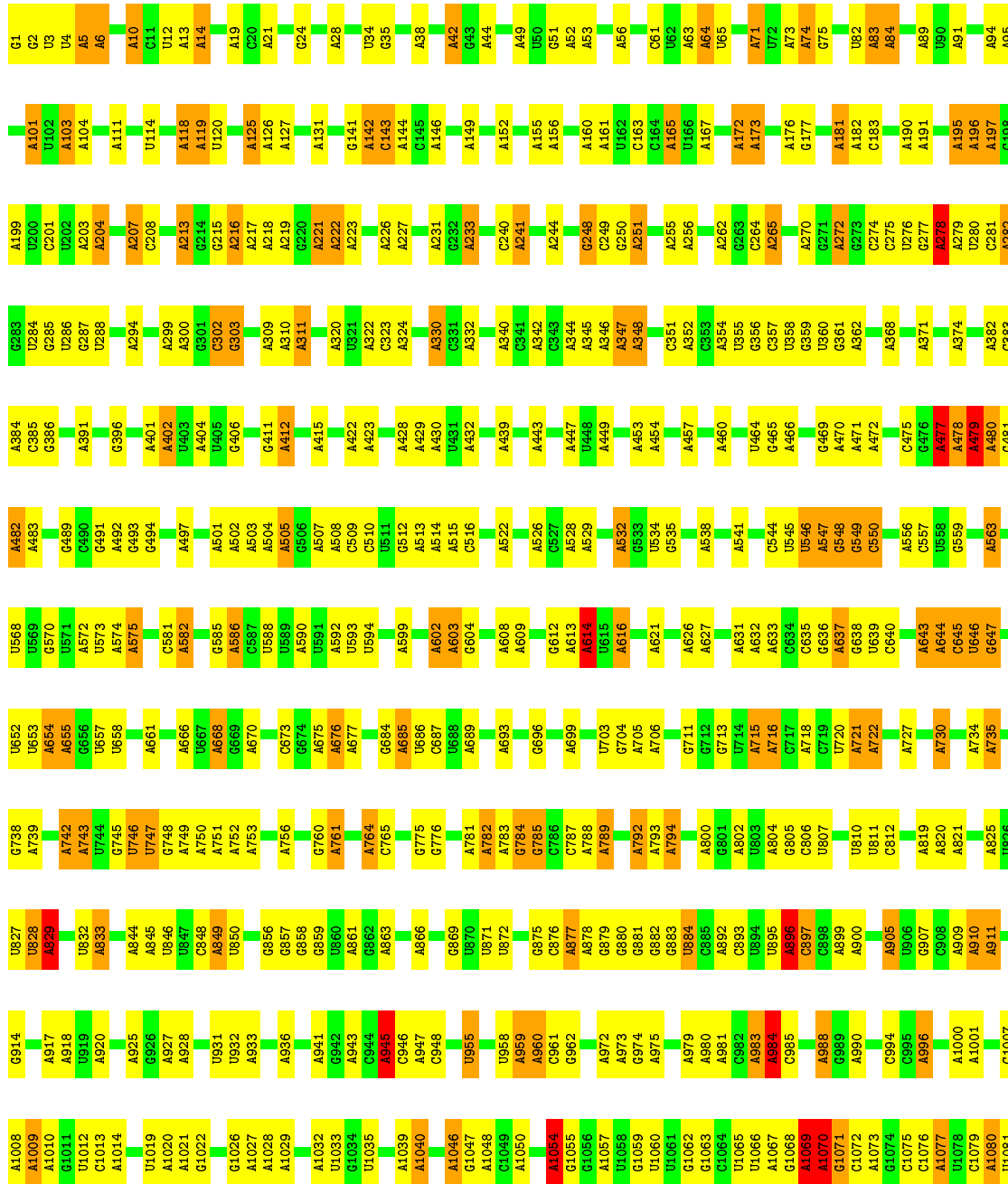
Chain AT:  93% 6%



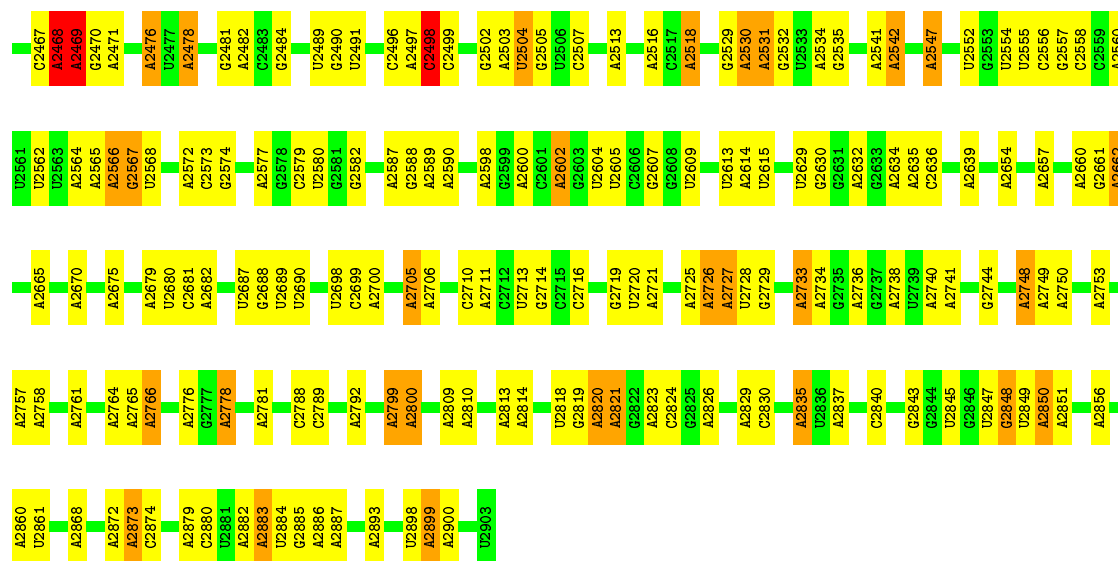
• Molecule 21: 30S ribosomal protein S21



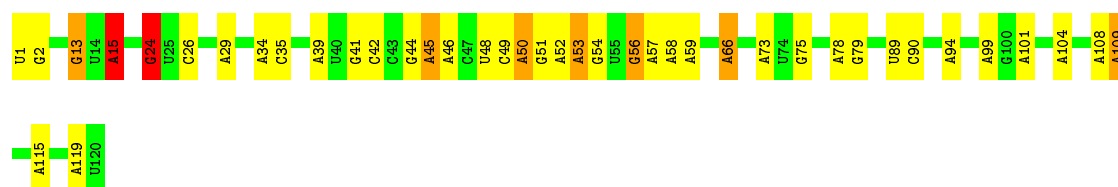
• Molecule 22: Ribosomal RNA 23S



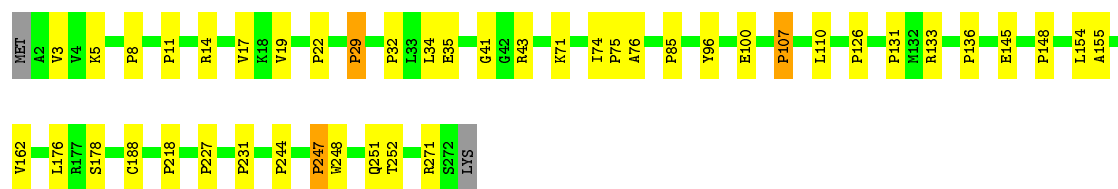
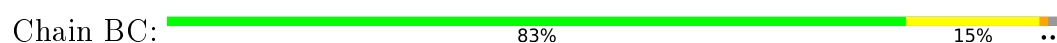
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G2037	G2038	G2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114																																																																																																																																								
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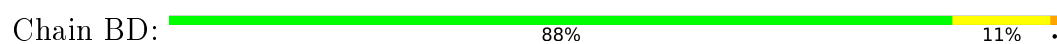
• Molecule 23: Ribosomal RNA 5S



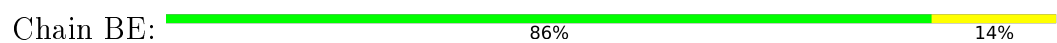
• Molecule 24: 50S ribosomal protein L2



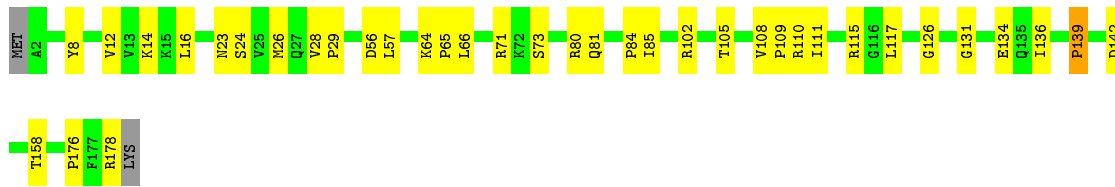
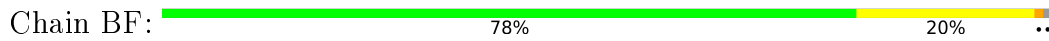
• Molecule 25: 50S ribosomal protein L3



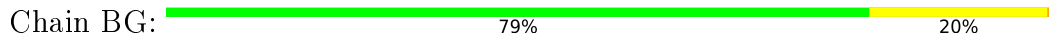
• Molecule 26: 50S ribosomal protein L4



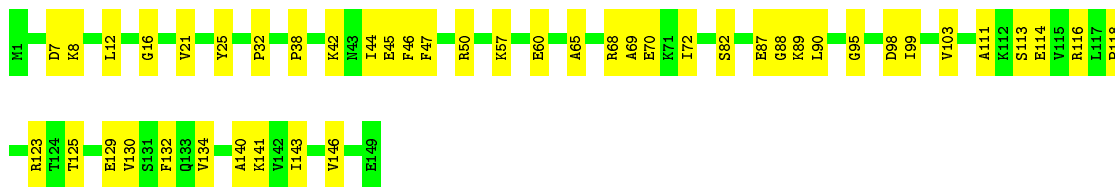
• Molecule 27: 50S ribosomal protein L5



• Molecule 28: 50S ribosomal protein L6



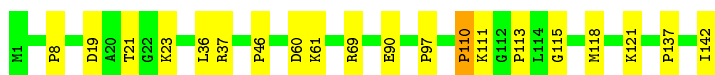
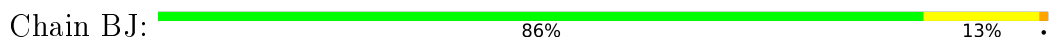
• Molecule 29: 50S ribosomal protein L9



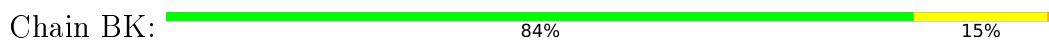
• Molecule 30: 50S ribosomal protein L31

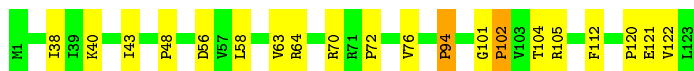


• Molecule 31: 50S ribosomal protein L13

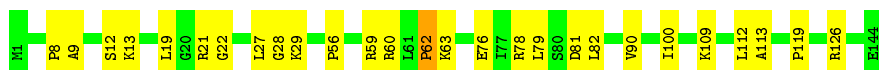
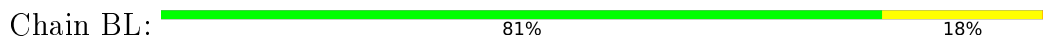


• Molecule 32: 50S ribosomal protein L14

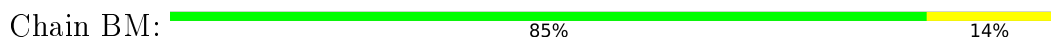




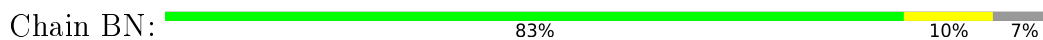
- Molecule 33: 50S ribosomal protein L15



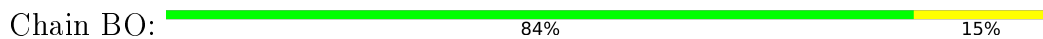
- Molecule 34: 50S ribosomal protein L16



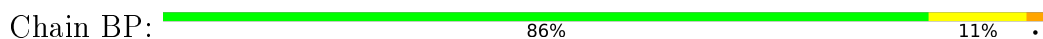
- Molecule 35: 50S ribosomal protein L17



- Molecule 36: 50S ribosomal protein L18



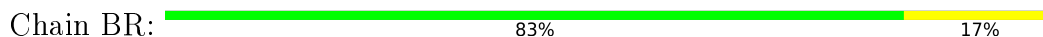
- Molecule 37: 50S ribosomal protein L19



- Molecule 38: 50S ribosomal protein L20

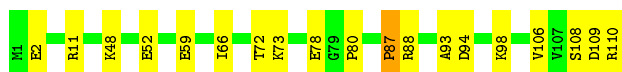
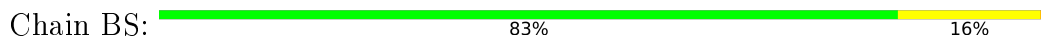


- Molecule 39: 50S ribosomal protein L21

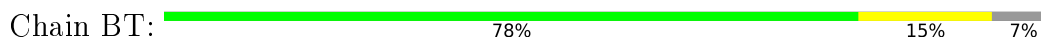




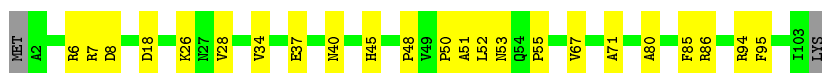
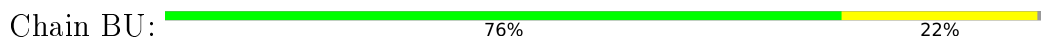
• Molecule 40: 50S ribosomal protein L22



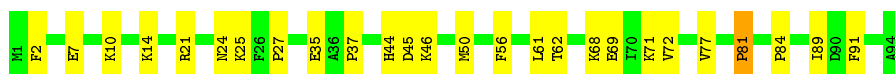
• Molecule 41: 50S ribosomal protein L23



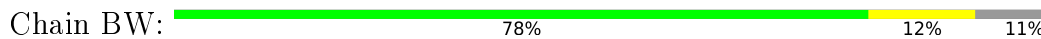
• Molecule 42: 50S ribosomal protein L24



• Molecule 43: 50S ribosomal protein L25



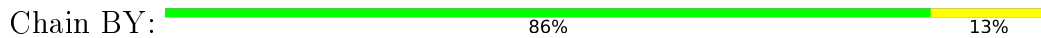
• Molecule 44: 50S ribosomal protein L27



• Molecule 45: 50S ribosomal protein L28

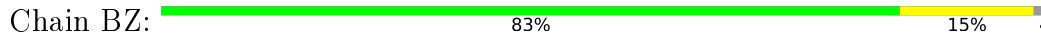


• Molecule 46: 50S ribosomal protein L29

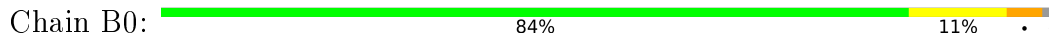




- Molecule 47: 50S ribosomal protein L30



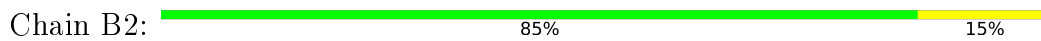
- Molecule 48: 50S ribosomal protein L32



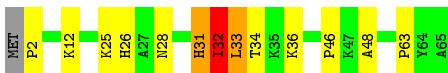
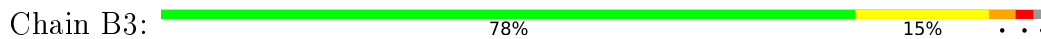
- Molecule 49: 50S ribosomal protein L33



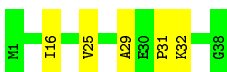
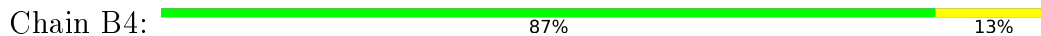
- Molecule 50: 50S ribosomal protein L34



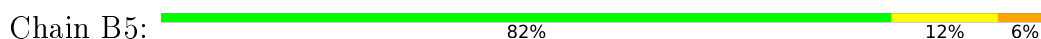
- Molecule 51: 50S ribosomal protein L35



- Molecule 52: 50S ribosomal protein L36



- Molecule 53: Tryptophanase leader peptide





- Molecule 54: mRNA



- Molecule 55: P-site tRNA-Pro



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93588	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2000	Depositor
Magnification	55127	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 3TD, 5MC, ZN, OMG, OMU, 2MA, MEQ, 2MG, 5MU, UR3, 6MZ, D2T, 4OC, OMC, MG, 1MG, PSU, MA6, 4D4, G7M

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	AA	1.49	1045/36593 (2.9%)	3.42	4438/57081 (7.8%)
2	AB	0.81	7/1784 (0.4%)	0.57	1/2403 (0.0%)
3	AC	0.83	7/1651 (0.4%)	0.51	0/2225
4	AD	0.78	6/1665 (0.4%)	0.47	0/2227
5	AE	0.87	5/1157 (0.4%)	0.57	0/1557
6	AF	1.05	7/881 (0.8%)	0.59	0/1189
7	AG	0.93	7/1195 (0.6%)	0.51	0/1602
8	AH	0.90	5/989 (0.5%)	0.55	0/1326
9	AI	0.73	3/1034 (0.3%)	0.66	3/1375 (0.2%)
10	AJ	1.03	6/805 (0.7%)	0.56	0/1089
11	AK	1.09	7/893 (0.8%)	0.57	0/1205
12	AL	1.12	8/960 (0.8%)	0.59	1/1286 (0.1%)
13	AM	0.93	5/892 (0.6%)	0.61	0/1193
14	AN	0.88	4/811 (0.5%)	0.53	0/1081
15	AO	0.36	0/722	0.47	0/964
16	AP	0.76	2/659 (0.3%)	0.54	0/884
17	AQ	0.76	2/657 (0.3%)	0.57	0/881
18	AR	0.87	2/462 (0.4%)	0.54	0/621
19	AS	1.08	5/672 (0.7%)	0.59	0/904
20	AT	0.54	1/676 (0.1%)	0.43	0/895
21	AU	1.08	4/472 (0.8%)	0.56	1/627 (0.2%)
22	BA	1.84	1753/69120 (2.5%)	3.52	8456/107824 (7.8%)
23	BB	1.53	58/2872 (2.0%)	3.02	271/4478 (6.1%)
24	BC	1.20	19/2121 (0.9%)	0.66	0/2852
25	BD	0.95	7/1576 (0.4%)	0.59	0/2119
26	BE	0.85	5/1571 (0.3%)	0.57	0/2113
27	BF	0.85	6/1434 (0.4%)	0.52	0/1926
28	BG	1.00	8/1343 (0.6%)	0.58	0/1816
29	BH	0.70	3/1121 (0.3%)	0.56	0/1515
30	BI	0.80	2/531 (0.4%)	0.60	0/709
31	BJ	1.03	6/1152 (0.5%)	0.56	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	BK	1.00	5/955 (0.5%)	0.67	1/1279 (0.1%)
33	BL	0.90	4/1062 (0.4%)	0.64	1/1413 (0.1%)
34	BM	1.09	7/1081 (0.6%)	0.59	0/1443
35	BN	0.98	4/958 (0.4%)	0.59	0/1281
36	BO	0.74	2/910 (0.2%)	0.54	0/1219
37	BP	0.90	3/929 (0.3%)	0.64	2/1242 (0.2%)
38	BQ	0.72	0/960	0.49	0/1278
39	BR	0.81	2/829 (0.2%)	0.56	0/1107
40	BS	0.76	2/864 (0.2%)	0.53	0/1156
41	BT	0.67	1/744 (0.1%)	0.56	0/994
42	BU	0.89	3/787 (0.4%)	0.58	0/1051
43	BV	1.01	4/766 (0.5%)	0.58	0/1025
44	BW	0.80	1/587 (0.2%)	0.57	0/776
45	BX	0.87	2/635 (0.3%)	0.59	0/848
46	BY	0.43	0/502	0.46	0/667
47	BZ	0.91	2/453 (0.4%)	0.57	0/605
48	B0	0.82	1/450 (0.2%)	0.64	1/599 (0.2%)
49	B1	1.19	5/421 (1.2%)	0.76	2/561 (0.4%)
50	B2	0.85	1/380 (0.3%)	0.60	0/498
51	B3	1.12	4/513 (0.8%)	0.74	1/676 (0.1%)
52	B4	0.88	1/303 (0.3%)	0.54	0/397
53	B5	1.51	2/150 (1.3%)	0.71	0/203
54	B7	0.31	0/161	1.06	0/248
55	B8	1.94	66/1839 (3.6%)	2.95	152/2866 (5.3%)
All	All	1.54	3127/155710 (2.0%)	3.00	13331/232950 (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	AJ	0	1
27	BF	0	1
51	B3	0	1
All	All	0	3

The worst 5 of 3127 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-21.93	1.29	1.53
22	BA	2449	U	C5-C6	20.02	1.52	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B8	14	A	C6-N6	17.45	1.48	1.33
55	B8	59	A	C6-N6	17.43	1.47	1.33
55	B8	76	A	C6-N6	17.33	1.47	1.33

The worst 5 of 13331 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	2451	A	N1-C6-N6	-24.52	103.89	118.60
22	BA	2872	A	N1-C6-N6	-23.89	104.27	118.60
22	BA	1668	A	N1-C6-N6	-23.68	104.39	118.60
22	BA	1668	A	C2-N3-C4	23.56	122.38	110.60
22	BA	1668	A	N1-C2-N3	-23.30	117.65	129.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
10	AJ	81	GLU	Peptide
51	B3	31	HIS	Peptide
27	BF	142	ASP	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	AA	32930	0	16591	430	0
2	AB	1753	0	1780	43	0
3	AC	1624	0	1696	36	0
4	AD	1643	0	1707	41	0
5	AE	1144	0	1185	26	0
6	AF	862	0	864	28	0
7	AG	1181	0	1238	35	0
8	AH	979	0	1031	32	0
9	AI	1022	0	1070	45	0
10	AJ	795	0	836	35	0
11	AK	877	0	887	24	0
12	AL	957	0	1017	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	AM	883	0	941	50	0
14	AN	799	0	841	26	0
15	AO	714	0	734	13	0
16	AP	649	0	666	16	0
17	AQ	648	0	691	13	0
18	AR	455	0	478	7	0
19	AS	656	0	680	34	0
20	AT	670	0	719	3	0
21	AU	465	0	491	17	0
22	BA	62209	0	31308	391	0
23	BB	2569	0	1301	15	0
24	BC	2082	0	2154	19	0
25	BD	1566	0	1618	15	0
26	BE	1552	0	1619	15	0
27	BF	1410	0	1444	30	0
28	BG	1323	0	1371	18	0
29	BH	1110	0	1148	32	0
30	BI	522	0	520	20	0
31	BJ	1129	0	1162	11	0
32	BK	946	0	1023	12	0
33	BL	1053	0	1129	18	0
34	BM	1075	0	1155	9	0
35	BN	945	0	989	8	0
36	BO	900	0	935	11	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	12	0
39	BR	816	0	839	11	0
40	BS	857	0	922	11	0
41	BT	738	0	807	12	0
42	BU	779	0	831	15	0
43	BV	753	0	780	15	0
44	BW	580	0	594	6	0
45	BX	625	0	652	4	0
46	BY	501	0	531	5	0
47	BZ	449	0	488	4	0
48	B0	444	0	458	5	0
49	B1	414	0	442	11	0
50	B2	377	0	418	7	0
51	B3	504	0	572	11	0
52	B4	302	0	340	3	0
53	B5	146	0	143	2	0
54	B7	146	0	77	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	B8	1646	0	831	19	0
56	AA	35	0	0	0	0
56	B8	1	0	0	0	0
56	BA	132	0	0	1	0
56	BC	1	0	0	0	0
56	BD	1	0	0	0	0
57	AB	1	0	0	0	0
57	B4	1	0	0	0	0
57	BI	1	0	0	0	0
58	BA	15	0	9	0	0
59	AA	168	0	0	3	0
59	AK	1	0	0	0	0
59	AM	1	0	0	0	0
59	AN	2	0	0	0	0
59	B8	1	0	0	1	0
59	BA	608	0	0	4	0
59	BC	7	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BL	2	0	0	0	0
59	BN	1	0	0	0	0
All	All	145019	0	96734	1531	0

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

The worst 5 of 1531 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:BA:962:G:OP1	59:BA:3201:HOH:O	1.58	1.19
22:BA:2107:G:H1	22:BA:2182:U:H3	1.03	1.01
22:BA:2133:G:N2	22:BA:2158:A:N6	2.12	0.98
13:AM:53:ILE:HG22	13:AM:57:ARG:HH21	1.26	0.97
22:BA:2133:G:N2	22:BA:2158:A:C6	2.35	0.94

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	AB	222/241 (92%)	209 (94%)	13 (6%)	0	100	100
3	AC	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
4	AD	203/206 (98%)	196 (97%)	7 (3%)	0	100	100
5	AE	153/167 (92%)	148 (97%)	5 (3%)	0	100	100
6	AF	104/135 (77%)	102 (98%)	2 (2%)	0	100	100
7	AG	149/179 (83%)	143 (96%)	6 (4%)	0	100	100
8	AH	127/130 (98%)	127 (100%)	0	0	100	100
9	AI	125/130 (96%)	115 (92%)	10 (8%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	7	26
11	AK	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
12	AL	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
13	AM	112/118 (95%)	104 (93%)	8 (7%)	0	100	100
14	AN	99/102 (97%)	88 (89%)	11 (11%)	0	100	100
15	AO	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
16	AP	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
17	AQ	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
18	AR	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
19	AS	80/92 (87%)	74 (92%)	6 (8%)	0	100	100
20	AT	84/87 (97%)	84 (100%)	0	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
25	BD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	29	61
26	BE	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
27	BF	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
28	BG	174/177 (98%)	173 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	BH	147/149 (99%)	133 (90%)	14 (10%)	0	100	100
30	BI	64/70 (91%)	58 (91%)	6 (9%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
33	BL	142/144 (99%)	134 (94%)	8 (6%)	0	100	100
34	BM	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
35	BN	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
36	BO	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
37	BP	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
38	BQ	115/118 (98%)	115 (100%)	0	0	100	100
39	BR	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
40	BS	108/110 (98%)	105 (97%)	3 (3%)	0	100	100
41	BT	91/100 (91%)	90 (99%)	1 (1%)	0	100	100
42	BU	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
43	BV	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	BW	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
45	BX	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
46	BY	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
47	BZ	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	B0	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
49	B1	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
50	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
51	B3	62/65 (95%)	57 (92%)	3 (5%)	2 (3%)	4	16
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	14 (93%)	1 (7%)	0	100	100
All	All	5590/5931 (94%)	5378 (96%)	207 (4%)	5 (0%)	54	82

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU

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Mol	Chain	Res	Type
10	AJ	57	VAL
10	AJ	58	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/199 (94%)	183 (98%)	3 (2%)	62	86
3	AC	170/190 (90%)	168 (99%)	2 (1%)	71	91
4	AD	172/173 (99%)	172 (100%)	0	100	100
5	AE	118/126 (94%)	118 (100%)	0	100	100
6	AF	92/116 (79%)	92 (100%)	0	100	100
7	AG	124/147 (84%)	123 (99%)	1 (1%)	81	94
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	104 (99%)	1 (1%)	76	92
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	90 (100%)	0	100	100
12	AL	102/103 (99%)	102 (100%)	0	100	100
13	AM	92/96 (96%)	92 (100%)	0	100	100
14	AN	79/84 (94%)	78 (99%)	1 (1%)	69	90
15	AO	76/77 (99%)	76 (100%)	0	100	100
16	AP	65/65 (100%)	65 (100%)	0	100	100
17	AQ	74/78 (95%)	74 (100%)	0	100	100
18	AR	48/65 (74%)	48 (100%)	0	100	100
19	AS	71/79 (90%)	70 (99%)	1 (1%)	67	89
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	162 (99%)	1 (1%)	86	96

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BE	165/165 (100%)	165 (100%)	0	100	100
27	BF	148/150 (99%)	147 (99%)	1 (1%)	84	95
28	BG	137/138 (99%)	136 (99%)	1 (1%)	84	95
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62 (95%)	58 (98%)	1 (2%)	60	86
31	BJ	116/116 (100%)	116 (100%)	0	100	100
32	BK	104/104 (100%)	103 (99%)	1 (1%)	76	92
33	BL	103/103 (100%)	103 (100%)	0	100	100
34	BM	108/108 (100%)	108 (100%)	0	100	100
35	BN	98/103 (95%)	98 (100%)	0	100	100
36	BO	87/87 (100%)	86 (99%)	1 (1%)	73	92
37	BP	99/100 (99%)	99 (100%)	0	100	100
38	BQ	89/90 (99%)	89 (100%)	0	100	100
39	BR	84/84 (100%)	84 (100%)	0	100	100
40	BS	93/93 (100%)	93 (100%)	0	100	100
41	BT	80/84 (95%)	80 (100%)	0	100	100
42	BU	83/85 (98%)	83 (100%)	0	100	100
43	BV	78/78 (100%)	78 (100%)	0	100	100
44	BW	57/63 (90%)	57 (100%)	0	100	100
45	BX	67/68 (98%)	67 (100%)	0	100	100
46	BY	54/55 (98%)	54 (100%)	0	100	100
47	BZ	48/49 (98%)	48 (100%)	0	100	100
48	B0	47/48 (98%)	46 (98%)	1 (2%)	53	81
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	38 (100%)	0	100	100
51	B3	51/52 (98%)	51 (100%)	0	100	100
52	B4	34/34 (100%)	34 (100%)	0	100	100
53	B5	17/17 (100%)	16 (94%)	1 (6%)	19	49
All	All	4650/4844 (96%)	4633 (100%)	17 (0%)	91	97

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	BO	63	LYS
53	B5	24	PRO
14	AN	27	LYS
19	AS	29	LYS
25	BD	33	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
53	B5	17	ASN
53	B5	14	ASN
28	BG	38	ASN
8	AH	18	GLN
36	BO	43	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	238 (15%)	7 (0%)
22	BA	2890/2897 (99%)	417 (14%)	23 (0%)
23	BB	119/120 (99%)	13 (10%)	1 (0%)
54	B7	6/7 (85%)	3 (50%)	1 (16%)
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4621/4635 (99%)	683 (14%)	34 (0%)

5 of 683 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	22	G
1	AA	32	A

5 of 34 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2518	A
22	BA	2873	A
55	B8	2	G
22	BA	984	A

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Mol	Chain	Res	Type
22	BA	784	G

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

37 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	5MC	BA	1962	22	15,22,23	2.54	5 (33%)	19,32,35	1.22	2 (10%)
1	4OC	AA	1402	1	16,23,24	3.13	6 (37%)	17,32,35	1.51	1 (5%)
22	PSU	BA	955	22	17,21,22	3.10	9 (52%)	20,30,33	2.78	5 (25%)
1	MA6	AA	1519	1	19,26,27	1.32	1 (5%)	18,38,41	3.66	2 (11%)
22	2MG	BA	1835	22	19,26,27	3.72	8 (42%)	21,38,41	2.64	5 (23%)
22	6MZ	BA	1618	22	18,25,26	2.93	5 (27%)	16,36,39	2.21	4 (25%)
22	G7M	BA	2069	22	20,26,27	3.15	6 (30%)	20,39,42	2.92	7 (35%)
1	PSU	AA	516	56,1	17,21,22	3.54	8 (47%)	20,30,33	3.13	6 (30%)
22	3TD	BA	1915	22	17,22,23	4.83	8 (47%)	19,32,35	1.25	3 (15%)
1	2MG	AA	966	1	19,26,27	4.34	7 (36%)	21,38,41	2.19	8 (38%)
1	2MG	AA	1516	1	19,26,27	4.07	8 (42%)	21,38,41	2.17	7 (33%)
34	4D4	BM	81	34	9,11,12	2.44	3 (33%)	8,13,15	1.06	0
22	PSU	BA	2580	22	17,21,22	3.17	9 (52%)	20,30,33	2.90	6 (30%)
1	MA6	AA	1518	1	19,26,27	1.34	2 (10%)	18,38,41	3.47	2 (11%)
22	2MG	BA	2445	22	19,26,27	3.73	8 (42%)	21,38,41	2.63	5 (23%)
22	PSU	BA	2604	22	17,21,22	3.18	7 (41%)	20,30,33	3.04	6 (30%)
22	PSU	BA	2605	22	17,21,22	3.10	9 (52%)	20,30,33	3.04	6 (30%)
22	PSU	BA	1911	22	17,21,22	3.45	9 (52%)	20,30,33	2.95	5 (25%)
22	1MG	BA	745	22	18,26,27	3.40	6 (33%)	19,39,42	1.59	2 (10%)
22	OMU	BA	2552	22	14,22,23	2.97	5 (35%)	14,31,34	0.78	0
22	2MA	BA	2503	56,22	17,25,26	3.56	5 (29%)	19,37,40	1.96	4 (21%)
22	PSU	BA	1917	22	17,21,22	3.44	9 (52%)	20,30,33	3.02	5 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	OMC	BA	2498	56,22	15,22,23	2.81	6 (40%)	17,31,34	1.29	2 (11%)
22	OMG	BA	2251	55,22	18,26,27	3.29	7 (38%)	20,38,41	2.23	7 (35%)
22	PSU	BA	746	56,22	17,21,22	2.09	4 (23%)	20,30,33	3.03	6 (30%)
22	5MU	BA	747	22	15,22,23	1.27	2 (13%)	16,32,35	2.44	1 (6%)
1	2MG	AA	1207	1	19,26,27	4.29	7 (36%)	21,38,41	2.32	7 (33%)
22	6MZ	BA	2030	22	18,25,26	2.95	5 (27%)	16,36,39	2.58	4 (25%)
22	PSU	BA	2457	22	17,21,22	3.01	9 (52%)	20,30,33	2.55	5 (25%)
1	G7M	AA	527	1	20,26,27	3.45	7 (35%)	20,39,42	3.16	5 (25%)
12	D2T	AL	89	12	4,9,10	1.19	0	3,11,13	2.66	1 (33%)
1	5MC	AA	967	1	15,22,23	2.90	5 (33%)	19,32,35	1.30	2 (10%)
22	5MU	BA	1939	22	15,22,23	1.13	2 (13%)	16,32,35	2.64	1 (6%)
22	PSU	BA	2504	22	17,21,22	3.26	9 (52%)	20,30,33	3.28	6 (30%)
1	UR3	AA	1498	1	14,22,23	2.68	5 (35%)	15,32,35	0.62	0
1	5MC	AA	1407	1	15,22,23	2.66	5 (33%)	19,32,35	1.31	2 (10%)
25	MEQ	BD	150	25	8,9,10	1.37	2 (25%)	5,10,12	1.46	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MC	BA	1962	22	-	2/5/25/26	0/2/2/2
1	4OC	AA	1402	1	-	1/9/29/30	0/2/2/2
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
22	6MZ	BA	1618	22	-	0/5/27/28	0/3/3/3
22	G7M	BA	2069	22	-	1/3/25/26	0/3/3/3
1	PSU	AA	516	56,1	-	0/7/25/26	0/2/2/2
22	3TD	BA	1915	22	-	3/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	2/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
34	4D4	BM	81	34	-	2/11/12/14	-
22	PSU	BA	2580	22	-	1/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	1911	22	-	2/7/25/26	0/2/2/2
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	OMU	BA	2552	22	-	0/7/27/28	0/2/2/2
22	2MA	BA	2503	56,22	-	1/3/25/26	0/3/3/3
22	PSU	BA	1917	22	-	0/7/25/26	0/2/2/2
22	OMC	BA	2498	56,22	-	2/7/27/28	0/2/2/2
22	OMG	BA	2251	55,22	-	3/5/27/28	0/3/3/3
22	PSU	BA	746	56,22	-	3/7/25/26	0/2/2/2
22	5MU	BA	747	22	-	0/5/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
22	PSU	BA	2457	22	-	0/7/25/26	0/2/2/2
1	G7M	AA	527	1	-	2/3/25/26	0/3/3/3
12	D2T	AL	89	12	-	1/3/12/14	-
1	5MC	AA	967	1	-	0/5/25/26	0/2/2/2
22	5MU	BA	1939	22	-	2/5/25/26	0/2/2/2
22	PSU	BA	2504	22	-	2/7/25/26	0/2/2/2
1	UR3	AA	1498	1	-	0/5/25/26	0/2/2/2
1	5MC	AA	1407	1	-	0/5/25/26	0/2/2/2
25	MEQ	BD	150	25	-	2/8/9/11	-

The worst 5 of 218 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C5-C1'	-15.87	1.38	1.52
1	AA	966	2MG	C2-N2	13.07	1.45	1.34
1	AA	1207	2MG	C2-N2	12.88	1.45	1.34
1	AA	1516	2MG	C2-N2	11.94	1.44	1.34
22	BA	1618	6MZ	C6-N6	10.93	1.52	1.35

The worst 5 of 141 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-13.95	102.37	117.06
1	AA	1518	MA6	N1-C6-N6	-13.36	103.00	117.06
1	AA	527	G7M	C1'-N9-C4	11.54	146.92	126.64
22	BA	2504	PSU	N1-C2-N3	-11.33	119.43	128.43
22	BA	1917	PSU	N1-C2-N3	-10.71	119.92	128.43

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	C3'-C4'-C5'-O5'
1	AA	966	2MG	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
34	BM	81	4D4	NE-CD-CG-CB
22	BA	746	PSU	O4'-C1'-C5-C4

There are no ring outliers.

12 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1402	4OC	1	0
22	BA	955	PSU	1	0
1	AA	1519	MA6	1	0
1	AA	1516	2MG	1	0
1	AA	1518	MA6	1	0
22	BA	2498	OMC	1	0
22	BA	2251	OMG	1	0
22	BA	746	PSU	1	0
22	BA	2030	6MZ	3	0
1	AA	527	G7M	1	0
12	AL	89	D2T	1	0
25	BD	150	MEQ	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 174 ligands modelled in this entry, 173 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
58	TRP	BA	3001	-	12,16,16	0.67	0	12,22,22	0.87	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
58	TRP	BA	3001	-	-	0/3/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.83
1	BA	2099:U	O3'	2100:G	P	3.52