



## wwPDB EM Validation Summary Report ⓘ

Mar 11, 2025 – 12:33 pm GMT

PDB ID : 7O1C  
EMDB ID : EMD-12695  
Title : Cryo-EM structure of an Escherichia coli TnaC(R23F)-ribosome-RF2 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 : 2.60 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](mailto: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>.

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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

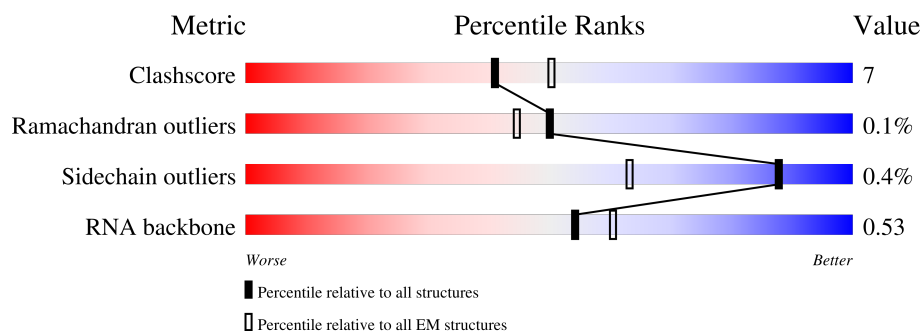
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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  $\geq 3$ , 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	50% 33% 15% .
2	AB	241	71% 20% . 7%
3	AC	233	62% 26% . 12%
4	AD	206	81% 18%
5	AE	167	74% 19% 7%
6	AF	135	56% 20% . 21%
7	AG	179	61% 23% . 16%









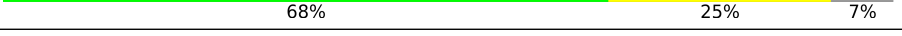
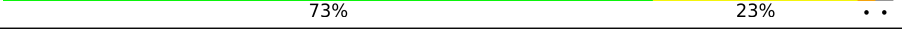
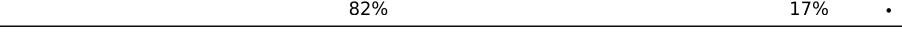

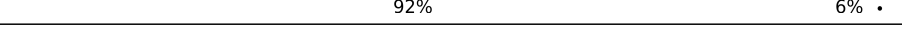
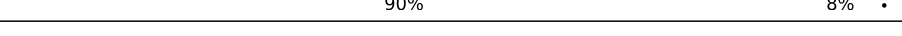
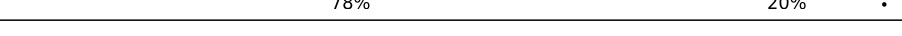


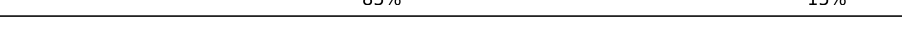
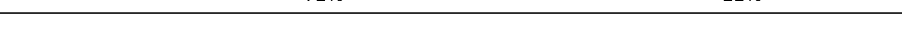

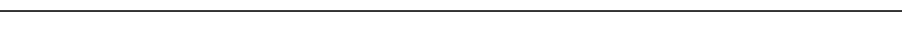

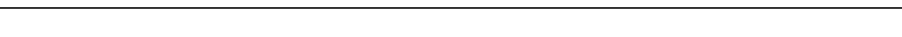
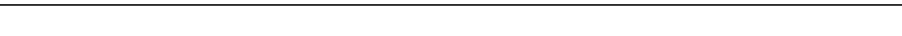
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Mol	Chain	Length	Quality of chain
8	AH	130	
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	102	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	BA	2897	
23	BB	120	
24	BC	273	
25	BD	209	
26	BE	201	
27	BF	179	
28	BG	177	
29	BH	149	
30	BI	70	
31	BJ	142	
32	BK	123	

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Mol	Chain	Length	Quality of chain
33	BL	144	 84% 15% .
34	BM	136	 82% 18% .
35	BN	127	 83% 9% 7%
36	BO	117	 89% 10% .
37	BP	115	 83% 17% .
38	BQ	118	 91% 8% .
39	BR	103	 87% 13%
40	BS	110	 81% 19%
41	BT	100	 68% 25% 7%
42	BU	104	 73% 23% . .
43	BV	94	 82% 17% .
44	BW	85	 73% 16% 11%
45	BX	78	 92% 6% .
46	BY	63	 90% 8% .
47	BZ	59	 78% 20% .
48	B0	57	 81% 18% .
49	B1	55	 71% 22% 7%
50	B2	46	 85% 15%
51	B3	65	 72% 22% . . .
52	B4	38	 87% 13%
53	B5	17	 59% 35% 6%
54	B7	10	 30% 60% 10%
55	B8	77	 42% 39% 18% .
56	B9	365	 61% 33% . 5%

## 2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 148175 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
1	AA	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	AB	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	AC	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	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
AN	35	ALA	-	insertion	UNP P0AG59

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	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	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
41	BT	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	BU	102	Total	C	N	O		0	0
			779	492	146	141			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BV	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	BW	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	BX	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	BY	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	BZ	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	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 TnaC-(R23F) - Tryptophanase leader peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B5	17	Total	C	N	O	0	0
			146	97	24	25		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B7	10	Total	C	N	O	P	0	0
			211	94	36	71	10		

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

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

- Molecule 56 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B9	348	Total	C	N	O	S	0	0
			2768	1705	482	571	10		

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	AA	87	Total	Mg	0
			87	87	
57	BA	243	Total	Mg	0
			243	243	
57	BB	1	Total	Mg	0
			1	1	
57	BC	1	Total	Mg	0
			1	1	
57	BD	2	Total	Mg	0
			2	2	
57	BL	3	Total	Mg	0
			3	3	
57	B8	2	Total	Mg	0
			2	2	

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	AA	38	Total	K	0
			38	38	
58	AM	1	Total	K	0
			1	1	
58	BA	104	Total	K	0
			104	104	
58	BB	1	Total	K	0
			1	1	
58	BC	1	Total	K	0
			1	1	
58	BD	1	Total	K	0
			1	1	

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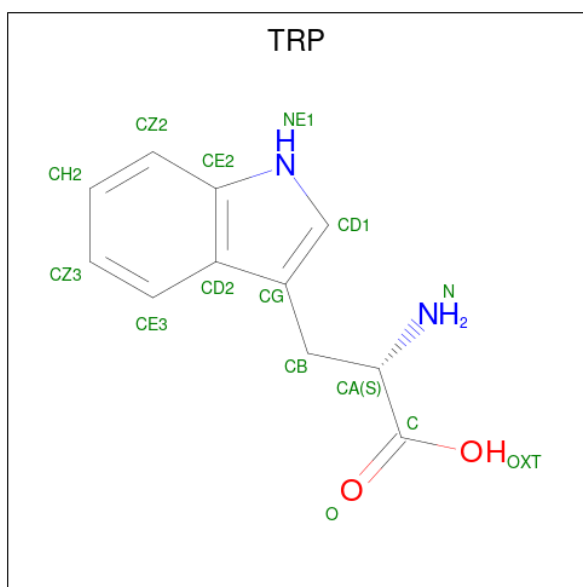
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Mol	Chain	Residues	Atoms		AltConf
58	BM	1	Total	K	0
			1	1	

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

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

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



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

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	AA	167	Total	O	0
			167	167	
61	AK	1	Total	O	0
			1	1	

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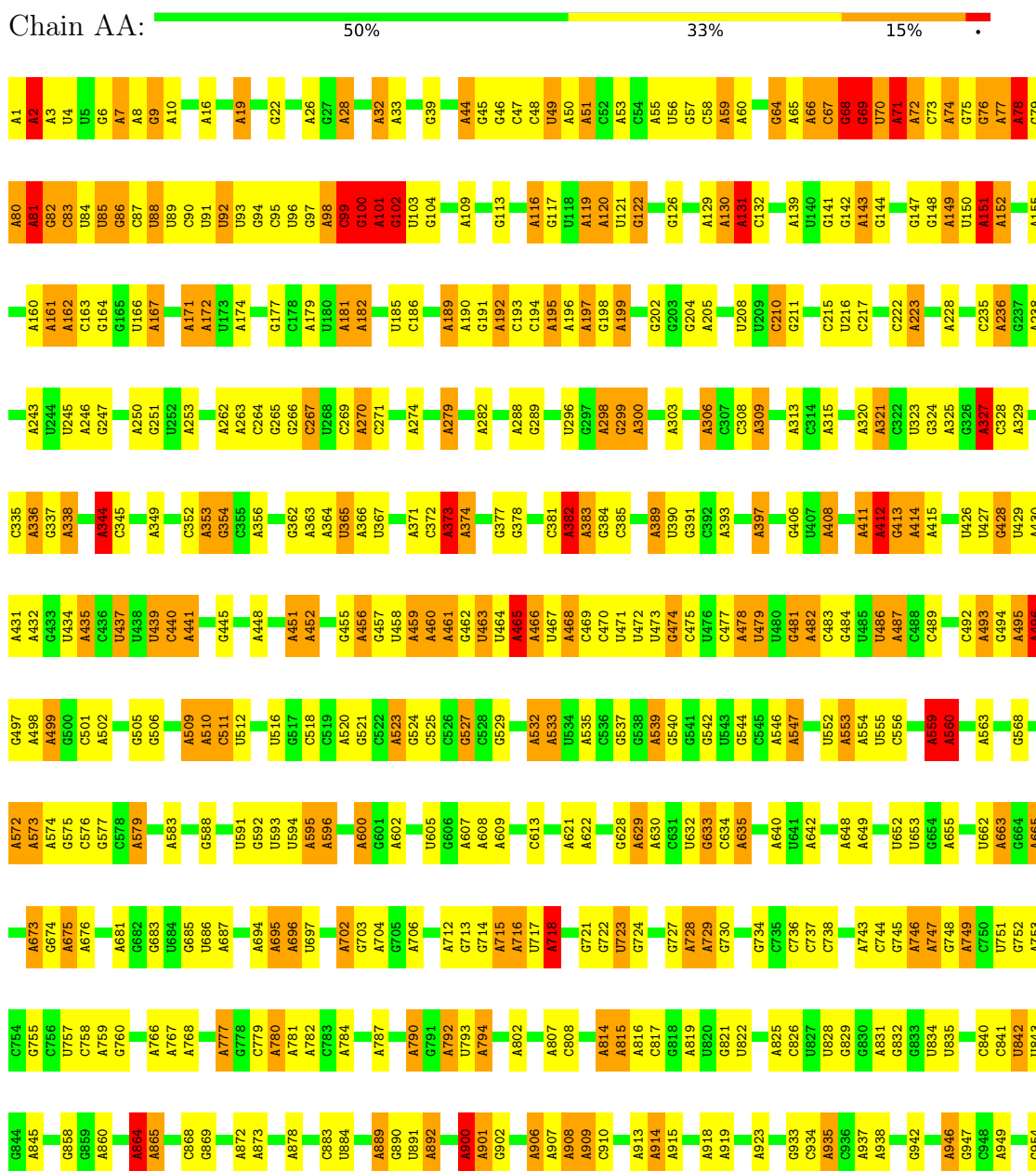
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Mol	Chain	Residues	Atoms		AltConf
61	AM	1	Total 1	O 1	0
61	AN	3	Total 3	O 3	0
61	BA	617	Total 617	O 617	0
61	BC	6	Total 6	O 6	0
61	BD	2	Total 2	O 2	0
61	BN	3	Total 3	O 3	0

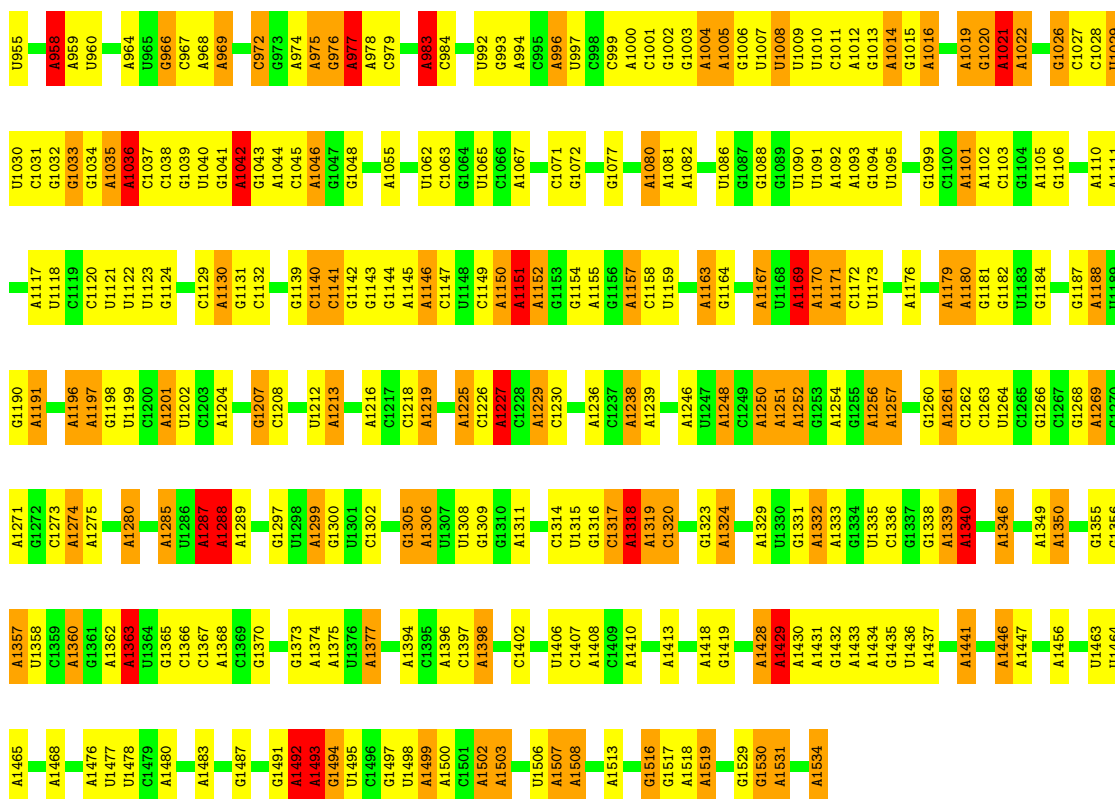
### 3 Residue-property plots

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.

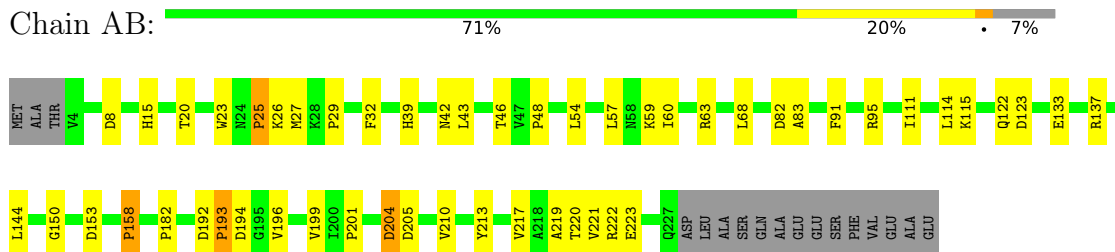
#### • Molecule 1: Ribosomal RNA 16S



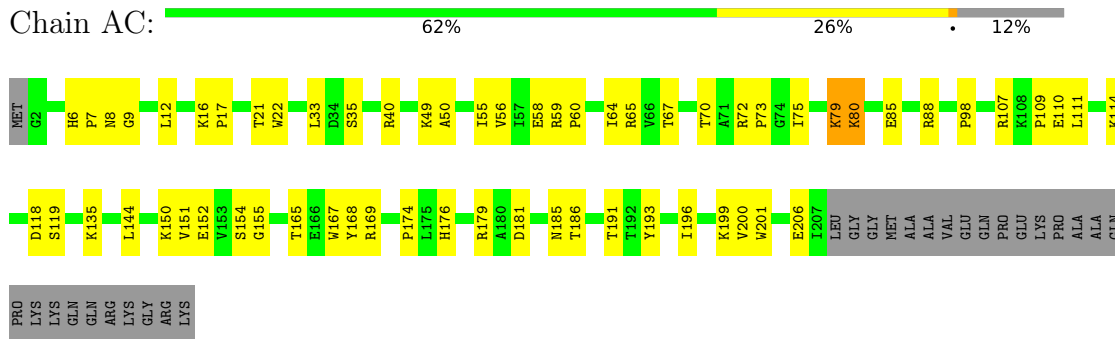




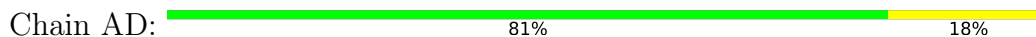
• Molecule 2: 30S ribosomal protein S2

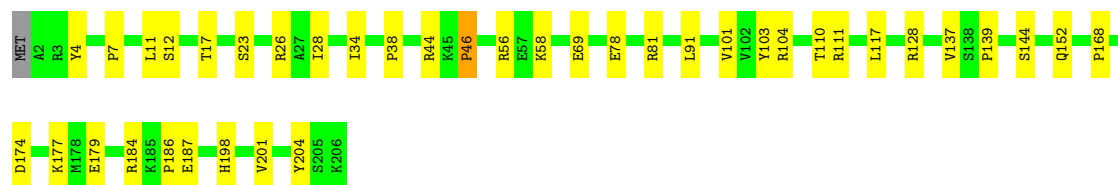


• Molecule 3: 30S ribosomal protein S3



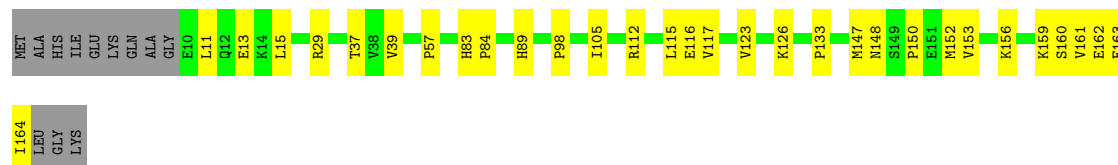
• Molecule 4: 30S ribosomal protein S4





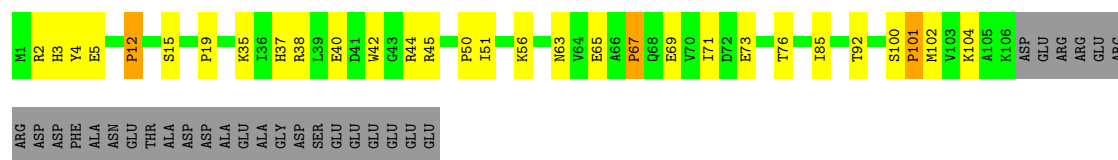
- Molecule 5: 30S ribosomal protein S5

Chain AE: 74% 19% 7%



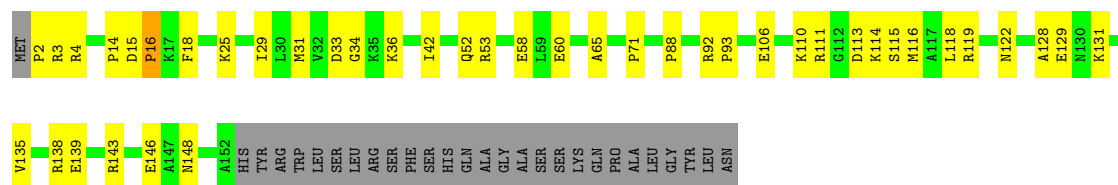
- Molecule 6: 30S ribosomal protein S6

Chain AF: 56% 20% 21%



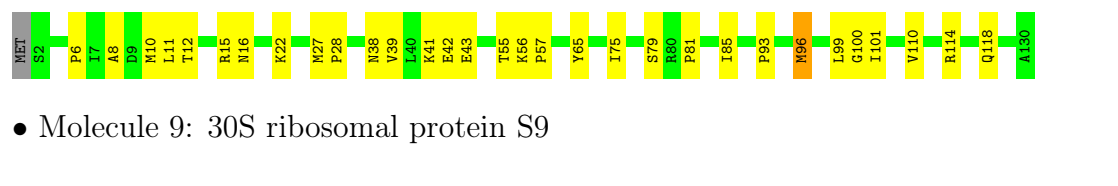
- Molecule 7: 30S ribosomal protein S7

Chain AG: 61% 23% 16%



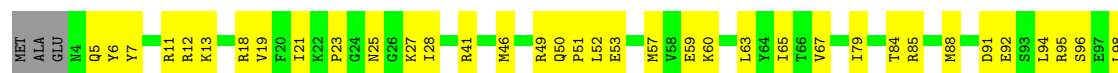
- Molecule 8: 30S ribosomal protein S8

Chain AH: 75% 23% 2%



- Molecule 9: 30S ribosomal protein S9

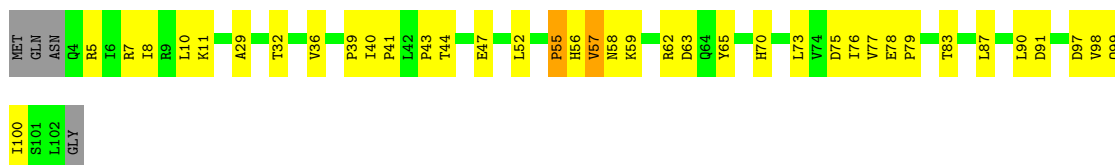
Chain AI: 62% 35% 3%





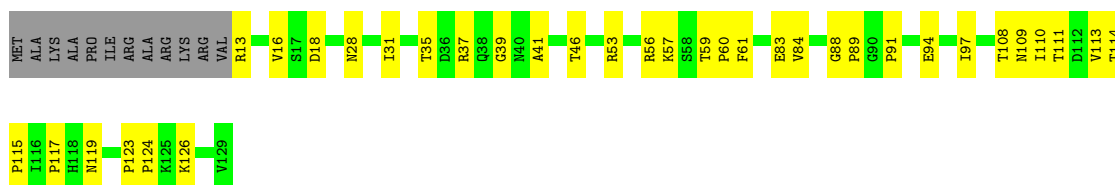
- Molecule 10: 30S ribosomal protein S10

Chain AJ: 59% 35%



- Molecule 11: 30S ribosomal protein S11

Chain AK: 64% 27% 9%



- Molecule 12: 30S ribosomal protein S12

Chain AL: 75% 23%



- Molecule 13: 30S ribosomal protein S13

Chain AM: 69% 28%



- Molecule 14: 30S ribosomal protein S14

Chain AN: 70% 28%

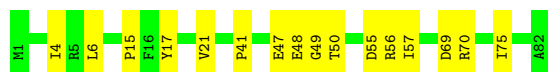
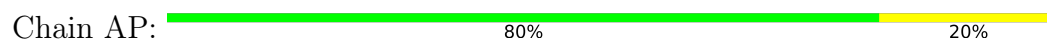


- Molecule 15: 30S ribosomal protein S15

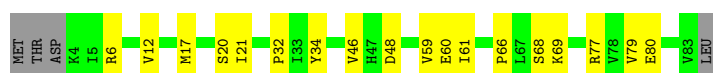
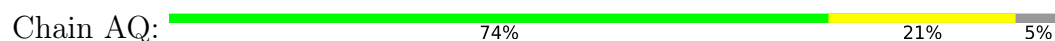
Chain AO: 96%



- Molecule 16: 30S ribosomal protein S16



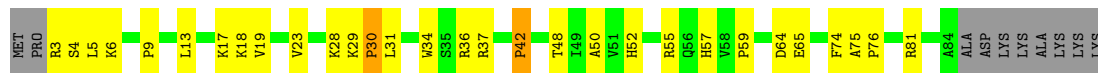
- Molecule 17: 30S ribosomal protein S17



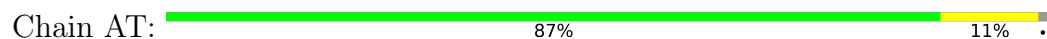
- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21

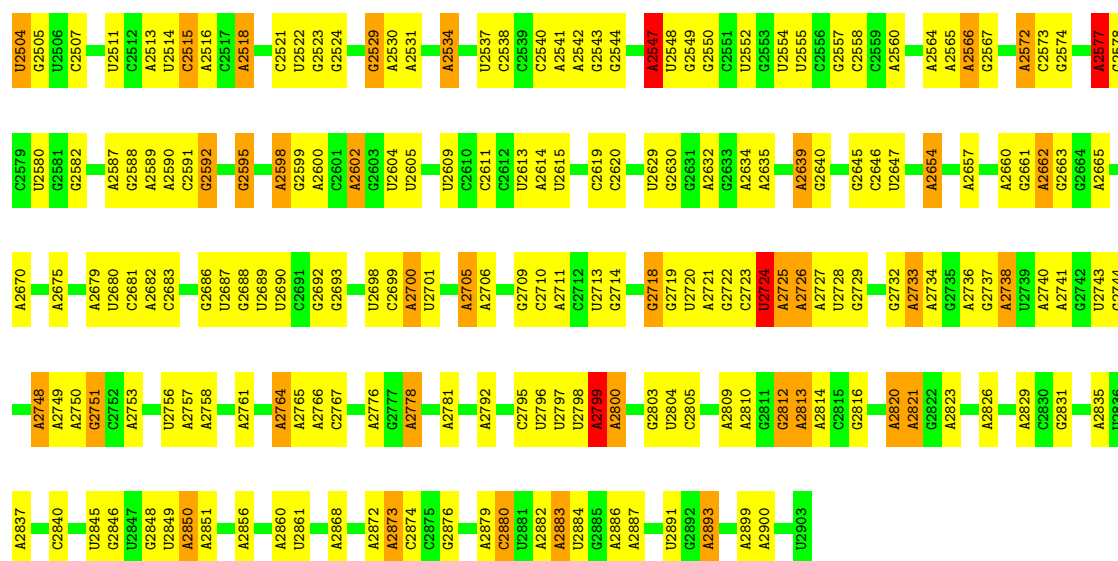


- Molecule 22: Ribosomal RNA 23S



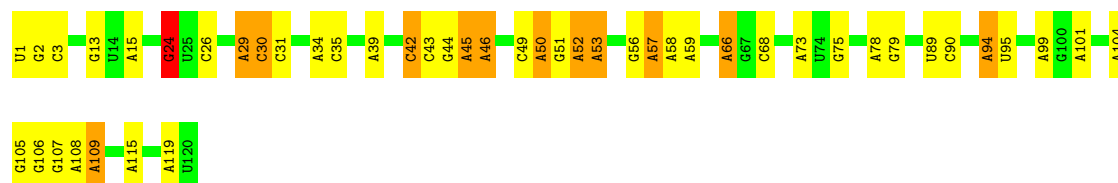
U1174	G1091	A1014	A941	C848	C785	U688	A532	A447	C364	A272	C192	A94	G1
A1175	C1092	A1020	A942	A849	C786	A689	G533	U448	U365	G273	U193	A95	G2
G1177	U1093	A1021	G942	U850	G771	G690	U534	A449	A368	C274	G194	A101	U3
C1178	U1094	A1022	A943	C851	G772	C691	C691	A454	A371	U276	A196	U102	U4
A1179	A1095	G1022	C944	G856	G775	C692	A538	A454	G372	G277	A197	A103	A5
U1180	U1097	G1025	C946	C857	G776	U615	A541	A457	U373	A278	C198	A104	A6
U1181	A1098	G1026	A947	G858	G696	A616	U545	G457	A374	A279	A199	A111	A10
G1182	C948	A1027	C948	G859	A699	A621	U546	G458	A374	U280	U200	A111	G11
U1183	U1098	A1028	A861	U860	A782	U627	U547	U459	C378	C281	U202	G117	U12
U1184	A1102	A1029	G952	A862	A783	A626	G548	A460	A382	A282	A203	A118	A13
G1185	A1103	G955	U955	A863	G784	A705	C550	A466	C383	G285	A204	A119	A14
U1186	G1110	U1033	A959	A866	A706	A631	G551	A466	A384	U286	G205	U120	G15
U1187	A1111	U1033	A960	U871	A706	A632	U552	A470	C385	G287	U206	A125	U18
A1188	G1112	G1038	A961	U872	G711	A633	G553	A471	G386	A294	C208	A126	C20
A1189	U1113	A1039	C961	U873	G712	C634	U554	A472	A391	A299	G213	A127	A21
A1194	C1114	A1040	G962	U874	G713	C635	G555	A477	G396	A300	A214	A131	C22
G1197	G1115	U1046	C964	C876	U714	A636	A556	A478	U397	G302	G215	U138	G23
U1201	G1124	G1047	C965	A877	A715	A637	C557	A479	G400	G303	G216	U139	G27
U1202	A1126	C1049	G966	A878	A716	U638	A563	A480	A401	A309	A217	C140	A28
A1204	G1127	A1050	U967	C877	C717	U639	G565	A481	A402	A310	A218	G141	A29
U1205	A1128	G1051	C968	C878	A718	C640	A566	A482	A403	A311	G220	A142	A38
G1206	G1130	C1052	G971	A879	C719	A643	U567	A483	U404	A320	A221	C143	A42
U1212	U1132	C1053	A972	U880	A720	A644	U568	A484	U405	A321	A222	A144	G43
A1213	A1133	A1054	C974	U881	A721	U646	U569	C490	G406	G322	A223	C145	A44
A1214	C1134	A1057	A975	C882	A722	C647	U570	A492	G407	C323	U224	A146	G45
G1225	G1135	U1061	G976	U883	G728	U652	U571	A497	G411	A324	A226	A149	G46
A1226	U1136	C1064	A979	A895	G729	U653	A572	A497	A412	A340	A227	A152	A49
U1230	G1137	U1065	A980	C897	A730	A654	A574	G500	C413	A341	C240	A160	A56
A1231	U1141	U1066	A981	C898	G733	A655	U575	A501	C414	A342	A241	U162	U50
G1237	A1142	G1067	C982	A899	A734	A656	G577	A502	A415	A343	G163	C61	G51
U1238	A1143	A1068	A984	A900	A735	U658	G578	A503	U416	A344	A244	U164	U62
G1239	A1144	U1070	C985	A905	G738	A661	A582	A504	C417	A345	A245	A165	A63
U1240	A1147	G1071	A988	A909	A739	A666	G583	A505	C421	A346	G247	U166	A64
A1241	U1148	C1072	G989	A910	A742	U667	C584	G506	A422	A347	G248	A167	A71
U1244	G1149	A1073	C991	A911	A743	U674	G585	A508	A423	A348	G249	A172	U72
G1245	C1150	G1074	C992	G914	A745	G669	A586	C509	A424	A349	G250	A173	A73
A1246	A1151	C1076	A996	C915	G746	A670	C587	C510	G425	A352	A251	A176	A74
U1247	C1152	U1077	A996	G916	U747	C671	U588	A514	A428	A353	A255	G177	G75
G1250	G1153	C1078	A1000	A917	G748	C672	A590	A515	A429	A354	A256	A181	A83
U1258	A1155	U1079	A1001	U919	A749	C673	U591	A522	A430	A355	A257	A182	G85
G1259	A1156	A1080	C1005	A920	A750	G674	A592	A522	U431	C353	A258	C183	A89
U1260	G1157	U1081	C1006	A925	A751	A675	U593	A522	A432	A356	A259	G189	U90
G1261	A1165	U1083	C1007	A926	A752	A676	U594	A522	C435	A357	A260	A190	A91
U1262	A1166	A1084	A1008	G926	A753	C678	C596	A522	A439	C357	A261	G189	U90
G1263	A1169	U1086	A1009	A927	A756	G682	U597	A522	A443	U358	A262	A191	A91
U1264	C1170	G1087	A1010	A928	A761	A685	U598	A522	C444	G359	A263	A191	A91
G1265	G1171	U1088	A1011	A933	U762	A686	A599	A522	G445	U360	A264	A191	A91
U1266	C1172	A1089	U1012	A934	U763	A687	A602	A522	G446	G361	A270	A191	A91
G1267	U1173	U1173	C1013	A936	A764	C687	A603	A522	G446	G362	G271	A191	A91





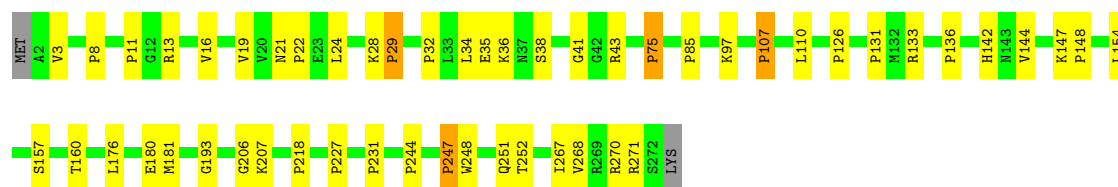
• Molecule 23: Ribosomal RNA 5S

Chain BB: 61% 28% 10% .



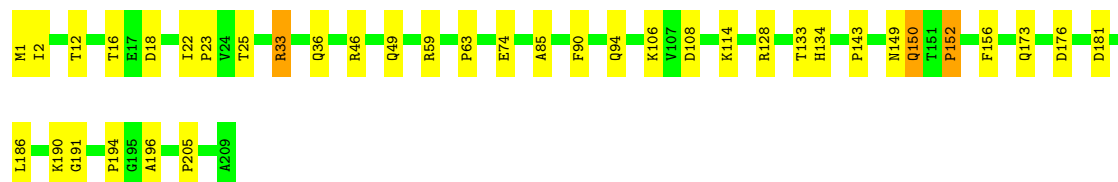
• Molecule 24: 50S ribosomal protein L2

Chain BC: 80% 18% ..



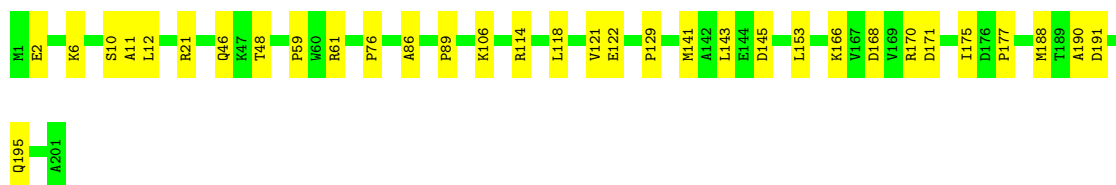
• Molecule 25: 50S ribosomal protein L3

Chain BD: 82% 17% .



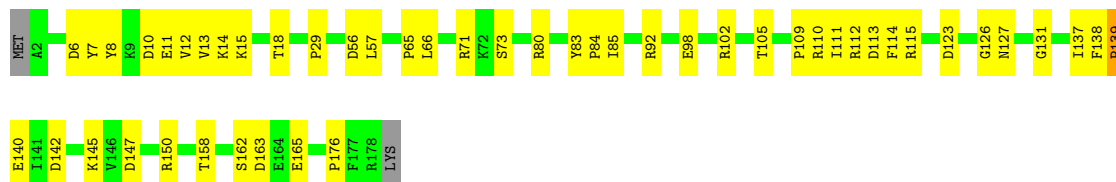
• Molecule 26: 50S ribosomal protein L4

Chain BE: 84% 16%



- Molecule 27: 50S ribosomal protein L5

Chain BF: 72% 27% ..



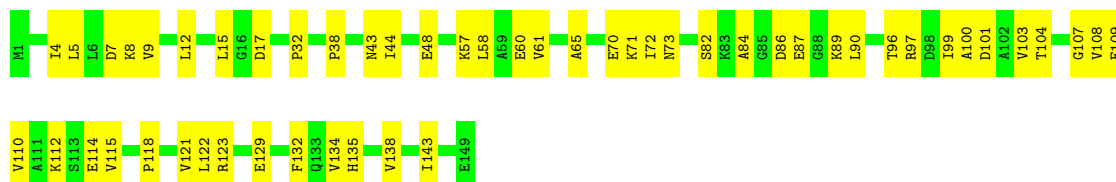
- Molecule 28: 50S ribosomal protein L6

Chain BG: 82% 16% ..



- Molecule 29: 50S ribosomal protein L9

Chain BH: 65% 35%



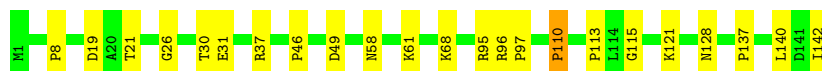
- Molecule 30: 50S ribosomal protein L31

Chain BI: 53% 40% 6%




- Molecule 31: 50S ribosomal protein L13

Chain BJ: 84% 15%




- Molecule 32: 50S ribosomal protein L14



Chain BK:  87% 13%




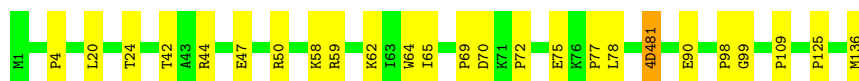
- Molecule 33: 50S ribosomal protein L15

Chain BL:  84% 15%



- Molecule 34: 50S ribosomal protein L16

Chain BM:  82% 18%



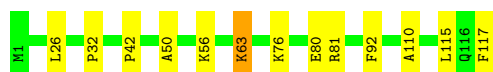
- Molecule 35: 50S ribosomal protein L17

Chain BN:  83% 9% 7%




- Molecule 36: 50S ribosomal protein L18

Chain BO:  89% 10%



- Molecule 37: 50S ribosomal protein L19

Chain BP:  83% 17%




- Molecule 38: 50S ribosomal protein L20

Chain BQ:  91% 8%




- Molecule 39: 50S ribosomal protein L21

Chain BR:  87% 13%



- Molecule 40: 50S ribosomal protein L22

Chain BS:  81% 19%



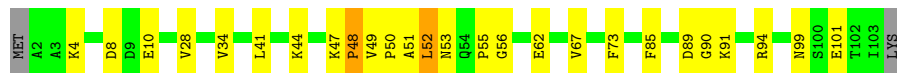
- Molecule 41: 50S ribosomal protein L23

Chain BT:  68% 25% 7%




- Molecule 42: 50S ribosomal protein L24

Chain BU:  73% 23% ..




- Molecule 43: 50S ribosomal protein L25

Chain BV:  82% 17% .



- Molecule 44: 50S ribosomal protein L27

Chain BW:  73% 16% 11%



- Molecule 45: 50S ribosomal protein L28

Chain BX:  92% 6% .




- Molecule 46: 50S ribosomal protein L29

Chain BY:  90% 8% .




- Molecule 47: 50S ribosomal protein L30

Chain BZ:  78% 20% .



- Molecule 48: 50S ribosomal protein L32

Chain B0:  81% 18% .




- Molecule 49: 50S ribosomal protein L33

Chain B1:  71% 22% 7%



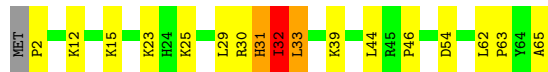
- Molecule 50: 50S ribosomal protein L34

Chain B2:  85% 15%




- Molecule 51: 50S ribosomal protein L35

Chain B3:  72% 22% . . .



- Molecule 52: 50S ribosomal protein L36

Chain B4:  87% 13%



- Molecule 53: TnaC-(R23F) - Tryptophanase leader peptide



C1	G2	C3	C4		G8	A9	U10
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C1	G2	G3	U4	G5	A6	A14	G17	U17A	G18	G19	U20	A21	G22	G23	G24	C25	A26	C30	G31	U32	C33	C34	A38	A41	A42	G46	U47	A51	G52	C56	G57	U58	A59	C62	U63	G64	U65	A66	U67	C68	A69	G70	G71	G72	A73	C74	G75	A76
----	----	----	----	----	----	-----	-----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

K303	E195	L70	MET
S315	R200	M73	PHE
	L201	K74	GLU
Q322	P206	L77	ILE
L323	P224	E78	ASN
R324	E225	V80	P6
D330			V7
S331	L230	L83	N8
R332	P236	E85	N9
I333	A237	L84	R10
G339	D238	L86	Q12
		A87	D13
T342	V243	V88	L14
R343	Y244	E89	E16
N344		A90	R17
T345	G248	P91	R18
L349	ALA	D92	D19
	GLY	E93	V20
L353	GLY	E94	L21
I357	GLN	T95	L22
E358	HLIS	F96	L25
	VAL	I97	D26
K362	ASN	E98	Y27
ALA	THR	A99	D28
GLY			A29
LEU	E258	L103	K30
		D104	K31
	V261	E107	E32
	R262	E108	R33
		K109	L34
	H265	I110	E40
	T266	A111	L41
	P267		E42
	T268	R116	E43
	G269	R117	Q43
	L270	M118	P44
	D277	G121	E49
		E122	P50
	Q280	Y123	E51
	H281	D124	R52
	K282		A53
	N283	Y129	Q54
	K284		A55
			L56
		E140	
	A287		E59
	N288	W144	R60
	K289	W155	S61
	Q290		S62
	H291	E170	L63
		I176	E64
	K294		A65
	E299		V66
		Y187	V67
			D68
			T69

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	113840	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA, FEI TITAN KRIOS	Depositor
Voltage (kV)	200, 300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40, 44	Depositor
Minimum defocus (nm)	-1000, -400	Depositor
Maximum defocus (nm)	-2000, -1600	Depositor
Magnification	55127, 59880	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k), 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: 6MZ, 4OC, K, ZN, D2T, MG, 5MU, PSU, 1MG, OMC, 5MC, 2MG, MA6, 4D4, 2MA, OMG, G7M, 3TD, UR3, OMU, MEQ

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	1.65	964/36593 (2.6%)	3.44	4347/57081 (7.6%)
2	AB	0.82	7/1784 (0.4%)	0.56	1/2403 (0.0%)
3	AC	0.86	7/1651 (0.4%)	0.62	2/2225 (0.1%)
4	AD	0.81	6/1665 (0.4%)	0.51	0/2227
5	AE	0.90	5/1157 (0.4%)	0.60	0/1557
6	AF	1.01	5/881 (0.6%)	0.56	0/1189
7	AG	0.96	7/1195 (0.6%)	0.54	0/1602
8	AH	0.94	5/989 (0.5%)	0.62	1/1326 (0.1%)
9	AI	0.76	3/1034 (0.3%)	0.56	0/1375
10	AJ	1.05	6/805 (0.7%)	0.59	0/1089
11	AK	1.11	7/893 (0.8%)	0.62	0/1205
12	AL	1.18	8/960 (0.8%)	0.65	0/1286
13	AM	0.93	5/892 (0.6%)	0.58	0/1193
14	AN	0.89	4/811 (0.5%)	0.55	0/1081
15	AO	0.44	0/722	0.48	0/964
16	AP	0.76	2/659 (0.3%)	0.60	0/884
17	AQ	0.83	2/657 (0.3%)	0.55	0/881
18	AR	0.97	2/462 (0.4%)	0.58	0/621
19	AS	1.09	5/672 (0.7%)	0.65	0/904
20	AT	0.60	1/676 (0.1%)	0.46	0/895
21	AU	1.09	4/472 (0.8%)	0.53	0/627
22	BA	2.12	2046/69120 (3.0%)	3.57	8225/107824 (7.6%)
23	BB	1.74	59/2872 (2.1%)	3.03	258/4478 (5.8%)
24	BC	1.29	23/2121 (1.1%)	0.68	0/2852
25	BD	1.05	11/1576 (0.7%)	0.64	0/2119
26	BE	0.91	6/1571 (0.4%)	0.60	0/2113
27	BF	0.89	6/1434 (0.4%)	0.56	0/1926
28	BG	1.03	8/1343 (0.6%)	0.60	0/1816
29	BH	0.73	3/1121 (0.3%)	0.54	0/1515
30	BI	0.82	2/531 (0.4%)	0.55	0/709
31	BJ	1.09	7/1152 (0.6%)	0.62	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	BK	1.08	5/955 (0.5%)	0.68	0/1279
33	BL	0.95	5/1062 (0.5%)	0.67	0/1413
34	BM	1.16	8/1081 (0.7%)	0.66	0/1443
35	BN	1.07	5/958 (0.5%)	0.68	0/1281
36	BO	0.81	2/910 (0.2%)	0.57	1/1219 (0.1%)
37	BP	0.99	3/929 (0.3%)	0.62	0/1242
38	BQ	0.93	0/960	0.58	0/1278
39	BR	0.91	2/829 (0.2%)	0.64	0/1107
40	BS	0.84	3/864 (0.3%)	0.60	0/1156
41	BT	0.79	1/744 (0.1%)	0.63	0/994
42	BU	0.96	3/787 (0.4%)	0.68	1/1051 (0.1%)
43	BV	1.06	4/766 (0.5%)	0.61	0/1025
44	BW	0.91	1/587 (0.2%)	0.63	0/776
45	BX	0.96	3/635 (0.5%)	0.66	1/848 (0.1%)
46	BY	0.55	0/502	0.56	0/667
47	BZ	0.97	2/453 (0.4%)	0.64	0/605
48	B0	0.89	2/450 (0.4%)	0.61	0/599
49	B1	1.09	2/421 (0.5%)	0.64	0/561
50	B2	0.97	1/380 (0.3%)	0.64	0/498
51	B3	1.21	4/513 (0.8%)	0.82	1/676 (0.1%)
52	B4	1.02	1/303 (0.3%)	0.67	0/397
53	B5	1.33	2/151 (1.3%)	0.81	0/205
54	B7	1.47	3/233 (1.3%)	2.72	14/358 (3.9%)
55	B8	1.87	57/1839 (3.1%)	2.96	169/2866 (5.9%)
56	B9	0.73	8/2806 (0.3%)	0.55	0/3778
All	All	1.72	3353/158589 (2.1%)	3.01	13021/236840 (5.5%)

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
5	AE	0	1
51	B3	0	1
All	All	0	2

The worst 5 of 3353 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	C2'-C1'	-22.33	1.28	1.53
22	BA	2449	U	C5-C6	18.12	1.50	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	892	A	O4'-C1'	16.77	1.63	1.41
55	B8	59	A	C6-N6	16.71	1.47	1.33
55	B8	58	A	C6-N6	16.69	1.47	1.33

The worst 5 of 13021 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	752	A	N1-C6-N6	-27.47	102.12	118.60
22	BA	2872	A	N1-C6-N6	-24.44	103.94	118.60
22	BA	1668	A	N1-C6-N6	-24.16	104.11	118.60
22	BA	2062	A	N1-C2-N3	-23.43	117.58	129.30
22	BA	1668	A	N1-C2-N3	-23.24	117.68	129.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	AE	89	HIS	Peptide
51	B3	31	HIS	Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32930	0	16583	454	0
2	AB	1753	0	1780	34	0
3	AC	1624	0	1696	33	0
4	AD	1643	0	1707	20	0
5	AE	1144	0	1185	18	0
6	AF	862	0	864	21	0
7	AG	1181	0	1238	28	0
8	AH	979	0	1031	18	0
9	AI	1022	0	1070	39	0
10	AJ	795	0	836	25	0
11	AK	877	0	887	19	0
12	AL	957	0	1017	19	0
13	AM	883	0	941	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	AN	799	0	841	23	0
15	AO	714	0	734	2	0
16	AP	649	0	666	9	0
17	AQ	648	0	691	10	0
18	AR	455	0	478	10	0
19	AS	656	0	680	24	0
20	AT	670	0	719	7	0
21	AU	465	0	491	11	0
22	BA	62209	0	31287	446	0
23	BB	2569	0	1301	19	0
24	BC	2082	0	2154	26	0
25	BD	1566	0	1618	18	0
26	BE	1552	0	1619	18	0
27	BF	1410	0	1444	38	0
28	BG	1323	0	1371	14	0
29	BH	1110	0	1148	31	0
30	BI	522	0	520	23	0
31	BJ	1129	0	1162	14	0
32	BK	946	0	1023	8	0
33	BL	1053	0	1128	15	0
34	BM	1075	0	1155	13	0
35	BN	945	0	989	7	0
36	BO	900	0	935	7	0
37	BP	917	0	962	12	0
38	BQ	947	0	1019	11	0
39	BR	816	0	839	7	0
40	BS	857	0	922	12	0
41	BT	738	0	807	17	0
42	BU	779	0	831	18	0
43	BV	753	0	780	10	0
44	BW	580	0	594	11	0
45	BX	625	0	652	2	0
46	BY	501	0	531	4	0
47	BZ	449	0	488	8	0
48	B0	444	0	458	7	0
49	B1	414	0	442	6	0
50	B2	377	0	418	3	0
51	B3	504	0	572	16	0
52	B4	302	0	340	3	0
53	B5	146	0	139	5	0
54	B7	211	0	110	5	0
55	B8	1646	0	831	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	B9	2768	0	2666	86	0
57	AA	87	0	0	0	0
57	B8	2	0	0	0	0
57	BA	243	0	0	0	0
57	BB	1	0	0	0	0
57	BC	1	0	0	0	0
57	BD	2	0	0	0	0
57	BL	3	0	0	0	0
58	AA	38	0	0	0	0
58	AM	1	0	0	0	0
58	BA	104	0	0	0	0
58	BB	1	0	0	0	0
58	BC	1	0	0	0	0
58	BD	1	0	0	0	0
58	BM	1	0	0	0	0
59	AB	1	0	0	0	0
59	B4	1	0	0	0	0
59	BI	1	0	0	0	0
60	BA	15	0	9	0	0
61	AA	167	0	0	0	0
61	AK	1	0	0	0	0
61	AM	1	0	0	0	0
61	AN	3	0	0	0	0
61	BA	617	0	0	3	0
61	BC	6	0	0	0	0
61	BD	2	0	0	0	0
61	BN	3	0	0	0	0
All	All	148175	0	99399	1626	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 7.

The worst 5 of 1626 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)
55:B8:1:C:H5'	56:B9:282:LYS:NZ	1.70	1.05
22:BA:2185:U:C4	22:BA:2186:G:O6	2.13	1.00
1:AA:1088:G:N2	1:AA:1167:A:H61	1.59	1.00
1:AA:1026:G:C6	1:AA:1035:A:N6	2.32	0.98
22:BA:884:U:O4	22:BA:892:A:C5	2.21	0.93

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%)	210 (95%)	12 (5%)	0	100	100
3	AC	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
4	AD	203/206 (98%)	195 (96%)	8 (4%)	0	100	100
5	AE	153/167 (92%)	144 (94%)	9 (6%)	0	100	100
6	AF	104/135 (77%)	101 (97%)	3 (3%)	0	100	100
7	AG	149/179 (83%)	135 (91%)	14 (9%)	0	100	100
8	AH	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
9	AI	125/130 (96%)	116 (93%)	9 (7%)	0	100	100
10	AJ	97/103 (94%)	89 (92%)	6 (6%)	2 (2%)	5	11
11	AK	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
12	AL	120/124 (97%)	109 (91%)	11 (9%)	0	100	100
13	AM	112/118 (95%)	98 (88%)	14 (12%)	0	100	100
14	AN	99/102 (97%)	84 (85%)	15 (15%)	0	100	100
15	AO	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	AP	80/82 (98%)	71 (89%)	9 (11%)	0	100	100
17	AQ	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
18	AR	53/75 (71%)	51 (96%)	2 (4%)	0	100	100
19	AS	80/92 (87%)	75 (94%)	5 (6%)	0	100	100
20	AT	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	AU	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
24	BC	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
25	BD	206/209 (99%)	196 (95%)	9 (4%)	1 (0%)	25	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
27	BF	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
28	BG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
29	BH	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
30	BI	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
31	BJ	140/142 (99%)	140 (100%)	0	0	100	100
32	BK	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
33	BL	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
34	BM	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
35	BN	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
36	BO	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
37	BP	112/115 (97%)	108 (96%)	4 (4%)	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%)	89 (89%)	10 (10%)	1 (1%)	13	29
43	BV	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
44	BW	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	BX	75/78 (96%)	69 (92%)	6 (8%)	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%)	52 (96%)	2 (4%)	0	100	100
49	B1	49/55 (89%)	45 (92%)	4 (8%)	0	100	100
50	B2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	B3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	3	5
52	B4	36/38 (95%)	36 (100%)	0	0	100	100
53	B5	15/17 (88%)	13 (87%)	2 (13%)	0	100	100
56	B9	344/365 (94%)	325 (94%)	19 (6%)	0	100	100
All	All	5934/6296 (94%)	5626 (95%)	302 (5%)	6 (0%)	50	71

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	BD	149	ASN
51	B3	32	ILE
51	B3	33	LEU
10	AJ	57	VAL
10	AJ	58	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	186/199 (94%)	186 (100%)	0	100	100
3	AC	170/190 (90%)	168 (99%)	2 (1%)	67	85
4	AD	172/173 (99%)	171 (99%)	1 (1%)	84	94
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%)	124 (100%)	0	100	100
8	AH	104/105 (99%)	104 (100%)	0	100	100
9	AI	105/107 (98%)	104 (99%)	1 (1%)	73	88
10	AJ	87/90 (97%)	87 (100%)	0	100	100
11	AK	90/99 (91%)	89 (99%)	1 (1%)	70	86
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%)	65	84
15	AO	76/77 (99%)	75 (99%)	1 (1%)	65	84
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%)	47 (98%)	1 (2%)	48	73
19	AS	71/79 (90%)	70 (99%)	1 (1%)	62	82
20	AT	65/66 (98%)	65 (100%)	0	100	100
21	AU	48/61 (79%)	48 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	BC	216/218 (99%)	216 (100%)	0	100	100
25	BD	163/163 (100%)	161 (99%)	2 (1%)	67	85
26	BE	165/165 (100%)	165 (100%)	0	100	100
27	BF	148/150 (99%)	148 (100%)	0	100	100
28	BG	137/138 (99%)	137 (100%)	0	100	100
29	BH	114/114 (100%)	114 (100%)	0	100	100
30	BI	59/62 (95%)	59 (100%)	0	100	100
31	BJ	116/116 (100%)	115 (99%)	1 (1%)	75	90
32	BK	104/104 (100%)	104 (100%)	0	100	100
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%)	70	86
37	BP	99/100 (99%)	98 (99%)	1 (1%)	73	88
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%)	47 (100%)	0	100	100
49	B1	45/49 (92%)	45 (100%)	0	100	100
50	B2	38/38 (100%)	37 (97%)	1 (3%)	41	67
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%)	16	35
56	B9	298/311 (96%)	296 (99%)	2 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	4948/5155 (96%)	4930 (100%)	18 (0%)	88 96

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	B2	41	ARG
56	B9	116	ARG
56	B9	33	ARG
19	AS	81	ARG
37	BP	37	LYS

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

Mol	Chain	Res	Type
56	B9	281	HIS
41	BT	48	GLN
11	AK	119	ASN
8	AH	118	GLN
26	BE	97	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1530/1534 (99%)	241 (15%)	8 (0%)
22	BA	2890/2897 (99%)	438 (15%)	24 (0%)
23	BB	119/120 (99%)	15 (12%)	1 (0%)
54	B7	8/10 (80%)	2 (25%)	0
55	B8	76/77 (98%)	12 (15%)	2 (2%)
All	All	4623/4638 (99%)	708 (15%)	35 (0%)

5 of 708 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	4	U
1	AA	7	A
1	AA	9	G
1	AA	19	A

5 of 35 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	2474	U
22	BA	2518	A
23	BB	66	A
22	BA	685	A
22	BA	276	U

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

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	OMU	BA	2552	57,22	19,22,23	2.56	7 (36%)	26,31,34	2.05	6 (23%)
1	5MC	AA	1407	1	18,22,23	3.14	7 (38%)	26,32,35	1.22	2 (7%)
22	2MG	BA	1835	22	18,26,27	2.05	5 (27%)	16,38,41	1.78	4 (25%)
1	UR3	AA	1498	1	19,22,23	2.91	8 (42%)	26,32,35	1.43	2 (7%)
22	3TD	BA	1915	22	18,22,23	4.04	7 (38%)	22,32,35	1.75	3 (13%)
1	G7M	AA	527	1,58	20,26,27	2.31	6 (30%)	17,39,42	1.26	1 (5%)
1	PSU	AA	516	1,57	18,21,22	4.01	7 (38%)	22,30,33	1.98	6 (27%)
22	PSU	BA	955	22	18,21,22	3.56	6 (33%)	22,30,33	2.31	5 (22%)
22	PSU	BA	2457	57,22	18,21,22	3.44	7 (38%)	22,30,33	2.45	5 (22%)
1	MA6	AA	1518	1	18,26,27	1.44	5 (27%)	19,38,41	3.33	2 (10%)
1	4OC	AA	1402	1,57	20,23,24	2.76	8 (40%)	26,32,35	0.96	2 (7%)
22	5MC	BA	1962	58,22	18,22,23	2.90	7 (38%)	26,32,35	1.10	2 (7%)
1	MA6	AA	1519	1	18,26,27	1.39	3 (16%)	19,38,41	3.70	2 (10%)
22	6MZ	BA	2030	22	18,25,26	2.87	6 (33%)	16,36,39	2.91	4 (25%)
1	2MG	AA	1516	1	18,26,27	2.21	6 (33%)	16,38,41	1.81	4 (25%)
22	5MU	BA	747	22	19,22,23	0.76	0	28,32,35	1.13	2 (7%)
22	PSU	BA	1917	22	18,21,22	3.88	6 (33%)	22,30,33	1.96	5 (22%)
22	PSU	BA	2580	22	18,21,22	3.58	7 (38%)	22,30,33	1.97	4 (18%)
1	5MC	AA	967	1	18,22,23	3.36	7 (38%)	26,32,35	1.12	1 (3%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	AA	966	1	18,26,27	2.37	7 (38%)	16,38,41	1.41	4 (25%)
22	PSU	BA	2504	58,22	18,21,22	3.52	6 (33%)	22,30,33	1.74	4 (18%)
22	5MU	BA	1939	58,22	19,22,23	1.05	3 (15%)	28,32,35	1.32	4 (14%)
22	2MA	BA	2503	57,58,22	19,25,26	2.95	7 (36%)	21,37,40	2.14	3 (14%)
22	G7M	BA	2069	58,22	20,26,27	1.98	5 (25%)	17,39,42	1.22	2 (11%)
25	MEQ	BD	150	25	8,9,10	1.43	2 (25%)	5,10,12	1.50	1 (20%)
34	4D4	BM	81	34	9,11,12	2.44	4 (44%)	8,13,15	1.26	1 (12%)
12	D2T	AL	89	12	7,9,10	1.02	0	6,11,13	2.65	3 (50%)
1	2MG	AA	1207	1,58	18,26,27	2.37	7 (38%)	16,38,41	1.43	3 (18%)
22	PSU	BA	746	57,22	18,21,22	3.95	8 (44%)	22,30,33	1.73	6 (27%)
22	PSU	BA	2604	22	18,21,22	3.40	6 (33%)	22,30,33	2.74	6 (27%)
22	PSU	BA	2605	22	18,21,22	3.54	8 (44%)	22,30,33	2.06	4 (18%)
22	2MG	BA	2445	22	18,26,27	2.12	5 (27%)	16,38,41	2.12	4 (25%)
22	6MZ	BA	1618	22	18,25,26	2.84	5 (27%)	16,36,39	2.95	4 (25%)
22	OMG	BA	2251	55,58,22	18,26,27	2.14	5 (27%)	19,38,41	1.50	5 (26%)
22	PSU	BA	1911	22	18,21,22	3.98	7 (38%)	22,30,33	2.22	5 (22%)
22	1MG	BA	745	22	18,26,27	2.41	5 (27%)	19,39,42	1.52	3 (15%)
22	OMC	BA	2498	57,22	19,22,23	2.45	7 (36%)	26,31,34	0.97	2 (7%)

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	OMU	BA	2552	57,22	-	0/9/27/28	0/2/2/2
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
22	2MG	BA	1835	22	-	0/5/27/28	0/3/3/3
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
22	3TD	BA	1915	22	-	2/7/25/26	0/2/2/2
1	G7M	AA	527	1,58	-	2/3/25/26	0/3/3/3
1	PSU	AA	516	1,57	-	1/7/25/26	0/2/2/2
22	PSU	BA	955	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2457	57,22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	0/7/29/30	0/3/3/3
1	4OC	AA	1402	1,57	-	2/9/29/30	0/2/2/2
22	5MC	BA	1962	58,22	-	0/7/25/26	0/2/2/2
1	MA6	AA	1519	1	-	2/7/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	6MZ	BA	2030	22	-	2/5/27/28	0/3/3/3
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
22	5MU	BA	747	22	-	3/7/25/26	0/2/2/2
22	PSU	BA	1917	22	-	1/7/25/26	0/2/2/2
22	PSU	BA	2580	22	-	2/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
1	2MG	AA	966	1	-	0/5/27/28	0/3/3/3
22	PSU	BA	2504	58,22	-	2/7/25/26	0/2/2/2
22	5MU	BA	1939	58,22	-	0/7/25/26	0/2/2/2
22	2MA	BA	2503	57,58,22	-	2/3/25/26	0/3/3/3
22	G7M	BA	2069	58,22	-	2/3/25/26	0/3/3/3
25	MEQ	BD	150	25	-	4/8/9/11	-
34	4D4	BM	81	34	-	2/11/12/14	-
12	D2T	AL	89	12	-	1/7/12/14	-
1	2MG	AA	1207	1,58	-	0/5/27/28	0/3/3/3
22	PSU	BA	746	57,22	-	3/7/25/26	0/2/2/2
22	PSU	BA	2604	22	-	0/7/25/26	0/2/2/2
22	PSU	BA	2605	22	-	0/7/25/26	0/2/2/2
22	2MG	BA	2445	22	-	2/5/27/28	0/3/3/3
22	6MZ	BA	1618	22	-	0/5/27/28	0/3/3/3
22	OMG	BA	2251	55,58,22	-	2/5/27/28	0/3/3/3
22	PSU	BA	1911	22	-	0/7/25/26	0/2/2/2
22	1MG	BA	745	22	-	0/3/25/26	0/3/3/3
22	OMC	BA	2498	57,22	-	0/9/27/28	0/2/2/2

The worst 5 of 212 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	1915	3TD	C6-C5	11.61	1.48	1.35
22	BA	1911	PSU	C6-C5	10.71	1.47	1.35
22	BA	1917	PSU	C6-C5	10.44	1.47	1.35
1	AA	516	PSU	C6-C5	10.41	1.47	1.35
22	BA	2030	6MZ	C6-N6	10.36	1.52	1.35

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1519	MA6	N1-C6-N6	-14.58	101.71	117.06
1	AA	1518	MA6	N1-C6-N6	-13.26	103.10	117.06
22	BA	2030	6MZ	C9-N6-C6	-8.27	115.75	122.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BA	1618	6MZ	C9-N6-C6	-7.09	116.76	122.87
22	BA	2503	2MA	C2-N3-C4	7.09	121.28	115.52

There are no chirality outliers.

5 of 37 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	527	G7M	O4'-C4'-C5'-O5'
1	AA	527	G7M	C3'-C4'-C5'-O5'
25	BD	150	MEQ	O-C-CA-CB
22	BA	746	PSU	C2'-C1'-C5-C4
22	BA	747	5MU	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1519	MA6	1	0
22	BA	2030	6MZ	2	0
1	AA	1516	2MG	1	0
25	BD	150	MEQ	1	0
34	BM	81	4D4	1	0
1	AA	1207	2MG	1	0
22	BA	2251	OMG	1	0
22	BA	2498	OMC	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 490 ligands modelled in this entry, 489 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
60	TRP	BA	3001	-	14,16,16	0.84	1 (7%)	16,22,22	1.04	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	TRP	BA	3001	-	-	0/7/8/8	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	BA	3001	TRP	OXT-C	-2.11	1.23	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	BA	3001	TRP	OXT-C-O	-2.32	118.81	124.09

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
54	B7	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	885:C	O3'	892:A	P	13.97
1	BA	2099:U	O3'	2100:G	P	3.25
1	B7	7:U	O3'	8:G	P	2.92