



## wwPDB EM Validation Summary Report ⓘ

Mar 11, 2025 – 03:51 pm GMT

PDB ID : 6ZTL  
EMDB ID : EMD-11419  
Title : E. coli 70S-RNAP expressome complex in collided state bound to NusG  
Authors : Webster, M.W.; Takacs, M.; Weixlbaumer, A.  
Deposited on : 2020-07-20  
Resolution : 3.50 Å (reported)  
Based on initial models : 4YBB, 6ALH

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

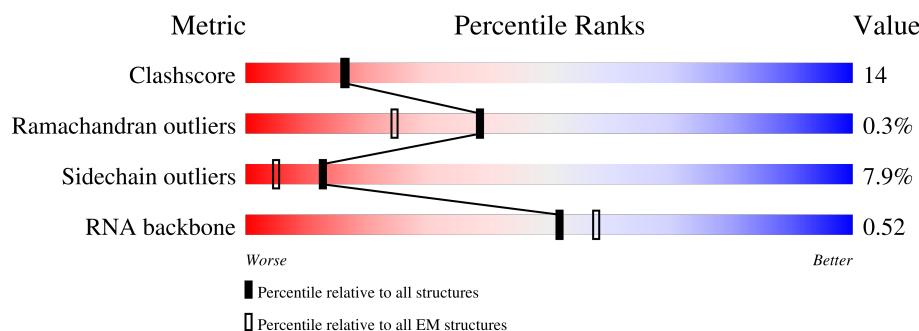
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.50 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.












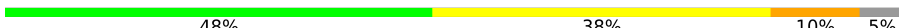






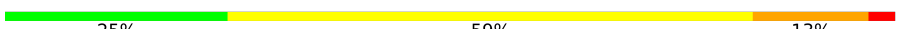
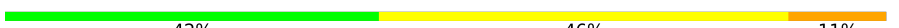







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	1542	
2	AB	241	
3	AC	233	
4	AD	206	
5	AE	167	
6	AF	131	
7	AG	156	


























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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	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	49	
23	AW	77	
24	AX	76	
25	BA	2904	
26	BB	120	
27	BC	273	
28	BD	209	
29	BE	201	
30	BF	179	
31	BG	177	
32	BH	149	




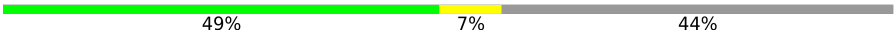
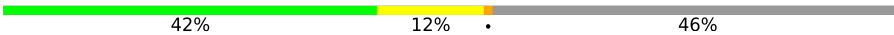
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Mol	Chain	Length	Quality of chain
33	BK	142	 61% 37% .
34	BL	123	 65% 33% .
35	BM	144	 74% 24% .
36	BN	136	 74% 24% .
37	BO	127	 62% 28% . 7%
38	BP	117	 62% 32% 6%
39	BQ	115	 59% 37% ..
40	BR	118	 69% 28% ..
41	BS	103	 67% 29% .
42	BT	110	 63% 32% 5%
43	BU	100	 67% 26% . 5%
44	BV	104	 64% 30% ..
45	BW	94	 62% 34% .
46	BX	85	 60% 26% . 11%
47	BY	78	 64% 33% ..
48	BZ	63	 60% 35% ..
49	B1	59	 59% 37% ..
50	B2	57	 67% 30% ..
51	B3	55	 44% 45% 5% 5%
52	B4	46	 74% 22% .
53	B5	65	 72% 18% 5% ..
54	B6	50	 54% 22% 24%
55	CN	39	 18% 49% 10% 23%
56	CT	39	 8% 44% 26% 23%
57	CA	329	 57% 12% . 30%

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Mol	Chain	Length	Quality of chain
57	CB	329	 56% 9% • 33%
58	CC	1342	 75% 19% • •
59	CD	1407	 76% 17% • 5%
60	CE	91	 49% 7% 44%
61	CF	181	 42% 12% • 46%

## 2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 173008 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1533	Total	C	N	O	P	0	0
			32908	14683	6037	10655	1533		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	226	Total	C	N	O	S	0	0
			1764	1116	316	324	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- 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	156	Total	C	N	O	S	0	0
			1148	715	217	210	6		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AE	9	CYS	GLY	conflict	UNP P0A7W1
AE	151	ALA	GLU	conflict	UNP P0A7W1

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	154	Total	C	N	O	S	0	0
			1214	756	235	219	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	128	Total	C	N	O	S	0	0
			1031	639	207	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	102	Total	C	N	O	S	0	0
			817	509	157	150	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	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	89	Total	C	N	O	S	0	0
			722	444	145	131	2		

- 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	57	Total	C	N	O	0	0
			474	298	90	86		

- 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	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	34	Total	C	N	O	P	0	0
			720	323	130	233	34		

- Molecule 23 is a RNA chain called tRNA(fmet) P-site.

Mol	Chain	Residues	Atoms					AltConf	Trace	
23	AW	77	Total	C	N	O	P	S	0	0
			1645	734	297	536	77	1		

- Molecule 24 is a RNA chain called Phe-NH-tRNA(Phe) A-site.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	AX	76	Total	C	N	O	P	S	0	0
			1629	729	290	533	76	1		

- Molecule 25 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BA	2899	Total	C	N	O	P	0	0
			62248	27776	11451	20122	2899		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	?	-	G	deletion	GB CP023165.1
BA	?	-	C	deletion	GB CP023165.1
BA	1211	U	C	conflict	GB CP023165.1
BA	1723	G	A	conflict	GB CP023165.1
BA	2211	G	A	conflict	GB CP023165.1

- Molecule 26 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

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

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

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

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BG	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BL	123	Total	C	N	O	S	0	0
			946	592	181	167	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BM	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BU	95	Total	C	N	O	S	0	0
			757	479	141	135	2		

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BX	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B1	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B2	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 51 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	B3	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 52 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B4	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 53 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	B5	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 54 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B6	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 55 is a DNA chain called Non-template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	CN	30	Total	C	N	O	P	0	0
			618	294	114	180	30		

- Molecule 56 is a DNA chain called Template DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CT	30	Total	C	N	O	P	0	0
			606	288	105	183	30		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	CA	229	Total	C	N	O	S	0	0
			1775	1106	313	350	6		
57	CB	219	Total	C	N	O	S	0	0
			1684	1051	295	332	6		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	CC	1320	Total	C	N	O	S	0	0
			10415	6535	1815	2021	44		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	CD	1333	Total	C	N	O	S	0	0
			10375	6518	1851	1956	50		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	CE	51	Total	C	N	O	S	0	0
			399	246	77	75	1		

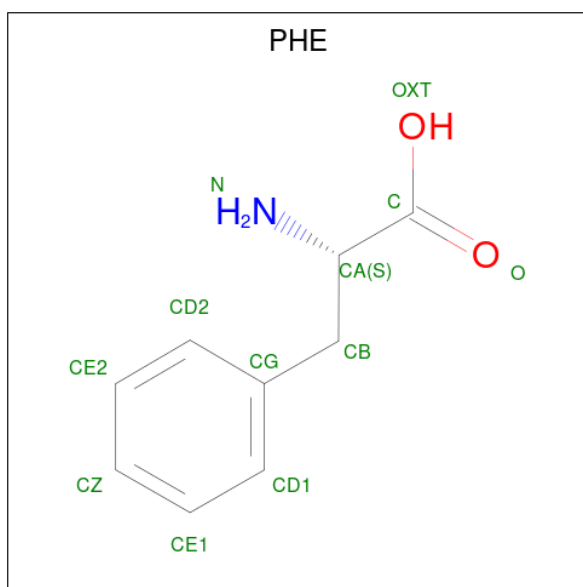
- Molecule 61 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	CF	98	Total	C	N	O	S	0	0
			790	505	139	140	6		

- Molecule 62 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	AA	115	Total	Mg	0
			115	115	
62	AL	1	Total	Mg	0
			1	1	
62	AM	1	Total	Mg	0
			1	1	
62	AN	1	Total	Mg	0
			1	1	
62	AP	1	Total	Mg	0
			1	1	
62	AX	1	Total	Mg	0
			1	1	
62	BA	304	Total	Mg	0
			304	304	
62	BB	8	Total	Mg	0
			8	8	
62	BC	4	Total	Mg	0
			4	4	
62	BD	2	Total	Mg	0
			2	2	
62	BQ	1	Total	Mg	0
			1	1	
62	BR	1	Total	Mg	0
			1	1	
62	CD	1	Total	Mg	0
			1	1	

- Molecule 63 is PHENYLALANINE (three-letter code: PHE) (formula: C<sub>9</sub>H<sub>11</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				AltConf
63	AX	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 64 is ZINC ION (three-letter code: ZN) (formula: Zn).

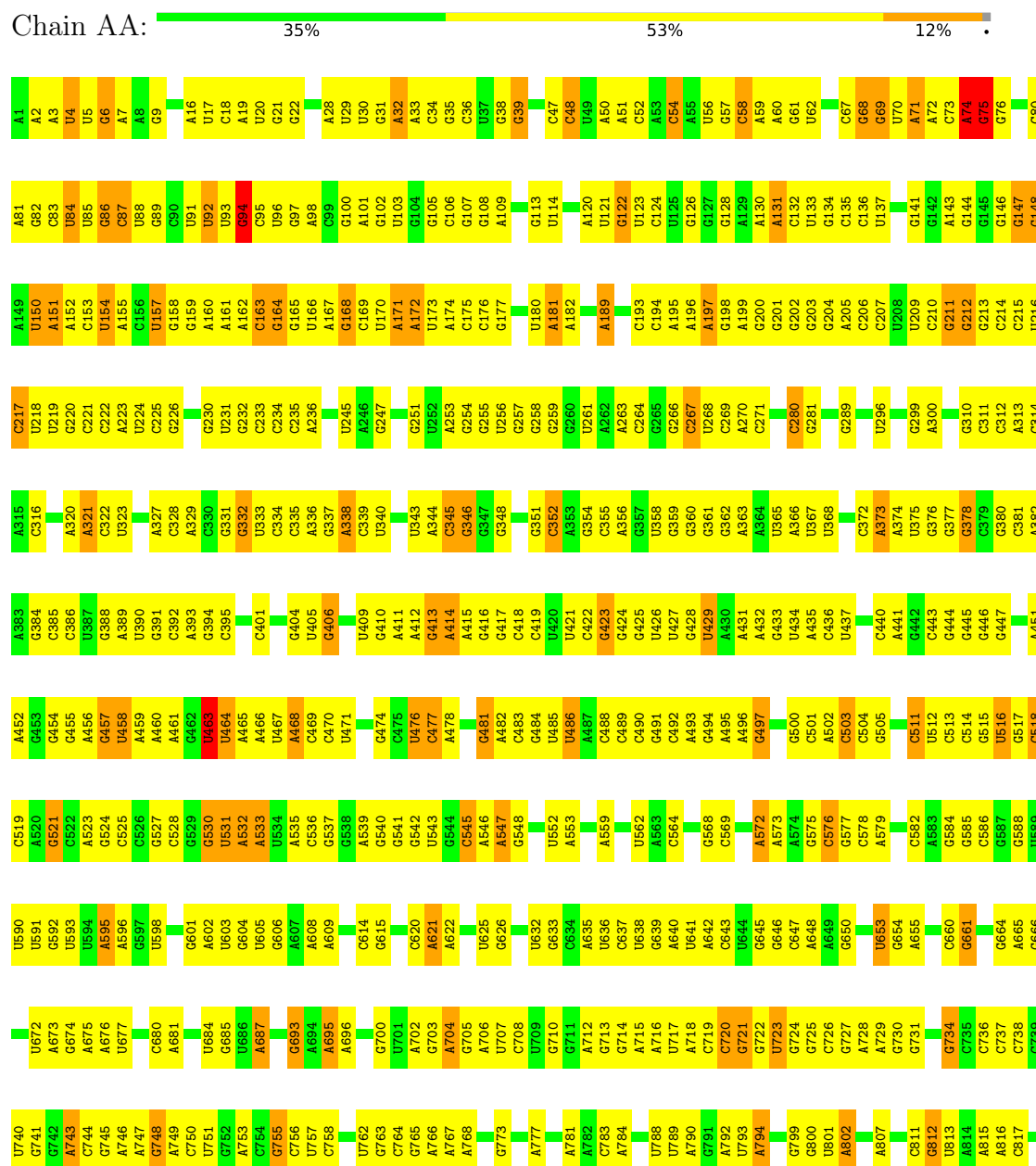
Mol	Chain	Residues	Atoms		AltConf
64	B6	1	Total	Zn	0
			1	1	
64	CD	2	Total	Zn	0
			2	2	



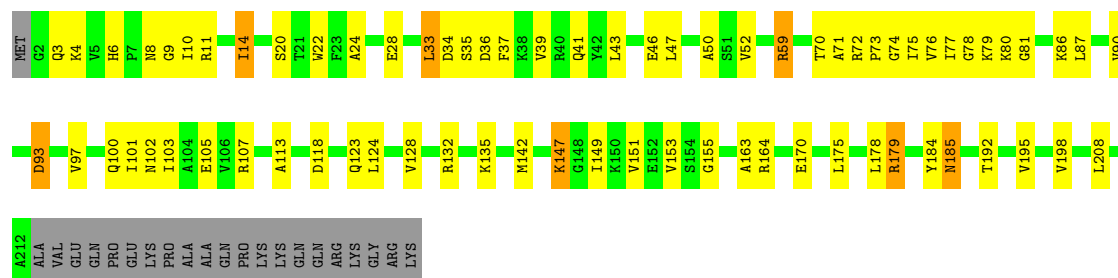
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 16S ribosomal RNA

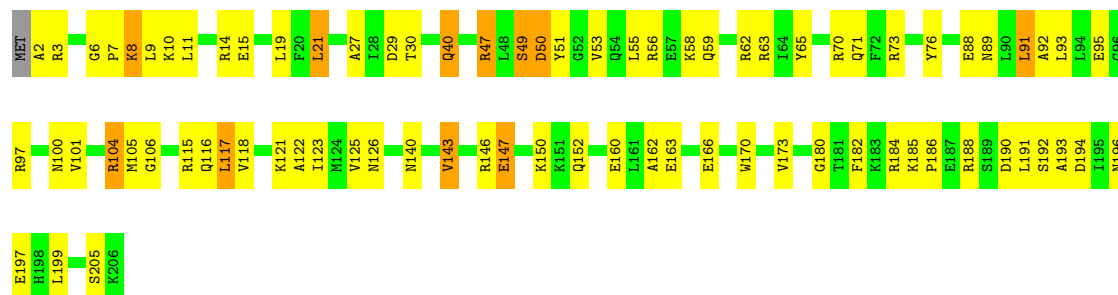






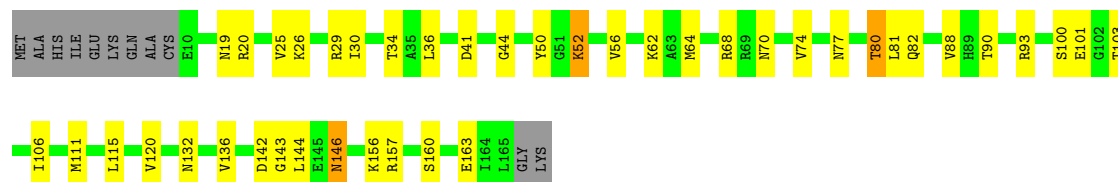
- Molecule 4: 30S ribosomal protein S4

Chain AD: 61% 33% 5%



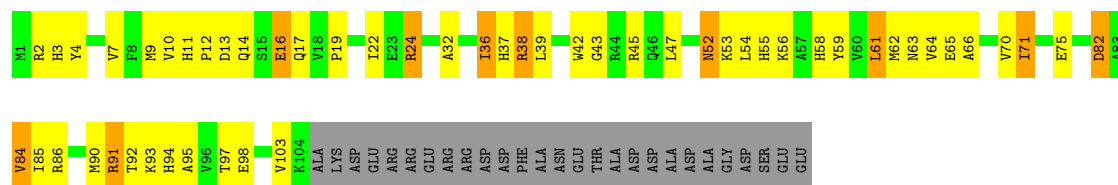
- Molecule 5: 30S ribosomal protein S5

Chain AE: 68% 23% 7%



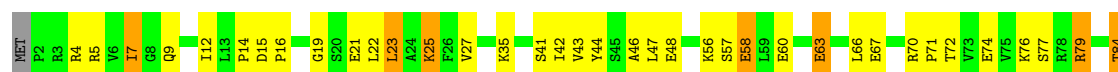
- Molecule 6: 30S ribosomal protein S6

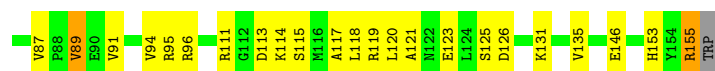
Chain AF: 39% 33% 8% 21%



- Molecule 7: 30S ribosomal protein S7

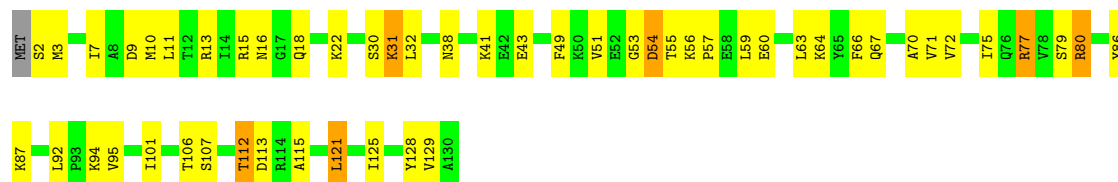
Chain AG: 60% 33% 6%





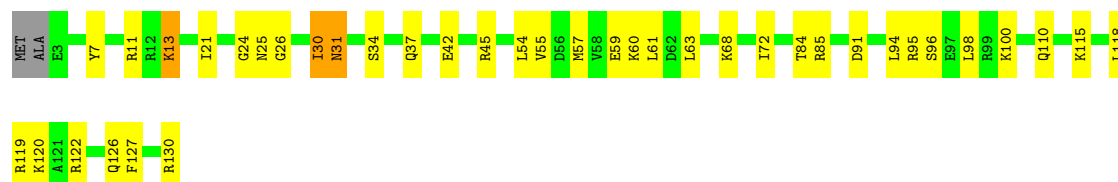
• Molecule 8: 30S ribosomal protein S8

Chain AH: 59% 35% 5% .



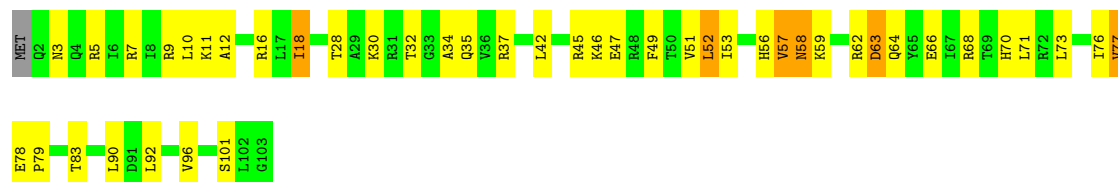
• Molecule 9: 30S ribosomal protein S9

Chain AI: 68% 28% . .



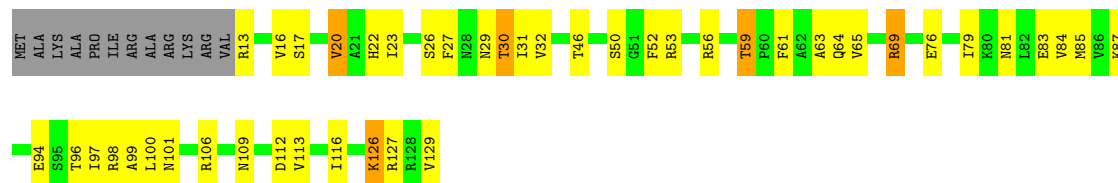
• Molecule 10: 30S ribosomal protein S10

Chain AJ: 56% 37% 6% .



• Molecule 11: 30S ribosomal protein S11

Chain AK: 56% 31% . 9%



• Molecule 12: 30S ribosomal protein S12

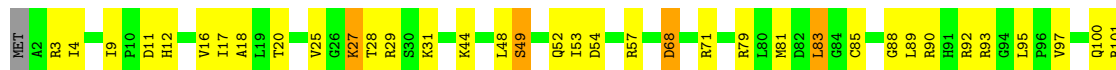
Chain AL: 59% 34% 6% . .





- Molecule 13: 30S ribosomal protein S13

Chain AM: 62% 31%



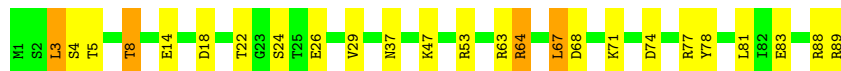
- Molecule 14: 30S ribosomal protein S14

Chain AN: 68% 29%



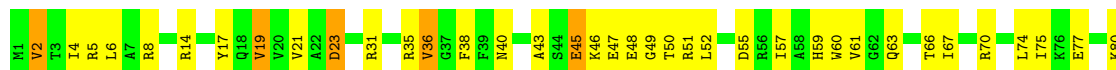
- Molecule 15: 30S ribosomal protein S15

Chain AO: 72% 24%



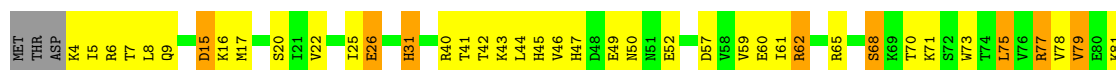
- Molecule 16: 30S ribosomal protein S16

Chain AP: 55% 39% 6%



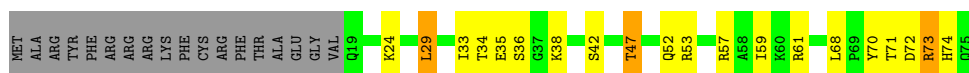
- Molecule 17: 30S ribosomal protein S17

Chain AQ: 48% 38% 10% 5%

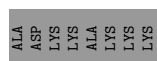
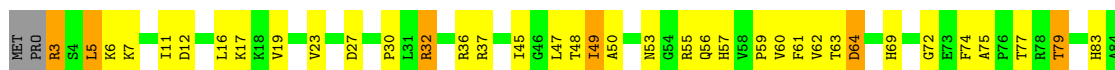


- Molecule 18: 30S ribosomal protein S18

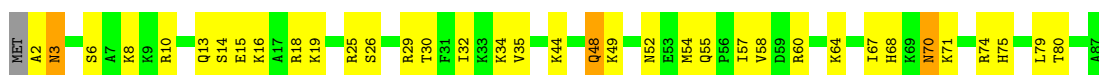
Chain AR: 49% 23% 24%



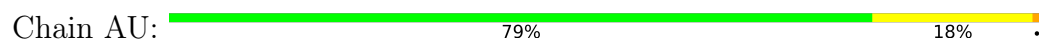
• Molecule 19: 30S ribosomal protein S19



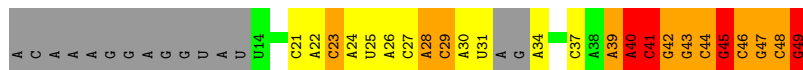
• Molecule 20: 30S ribosomal protein S20



• Molecule 21: 30S ribosomal protein S21



• Molecule 22: mRNA



• Molecule 23: tRNA(fmet) P-site



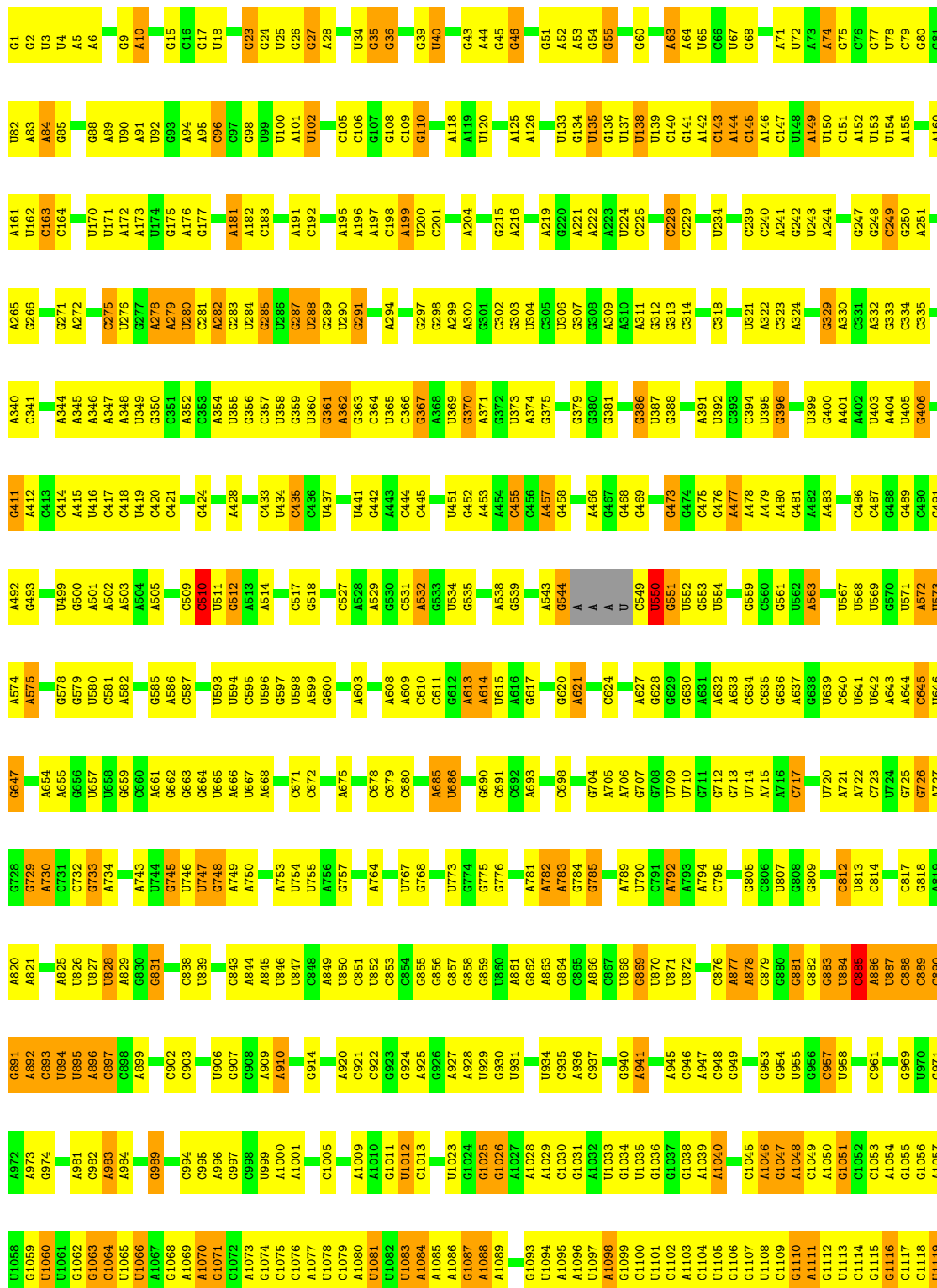
• Molecule 24: Phe-NH-tRNA(Phe) A-site





• Molecule 25: 23S ribosomal RNA

Chain BA: 42% 46% 11%



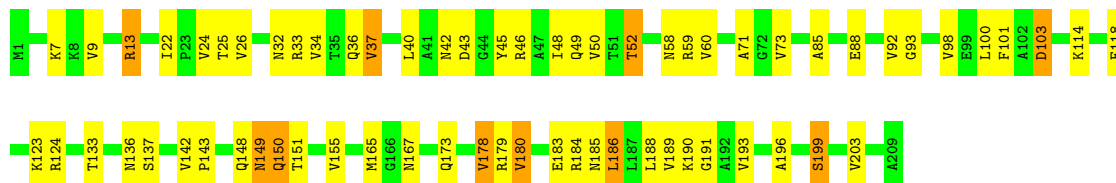
G2285	U2167	G2032	U1923	C1844	C1748	U1880	A1598	U1523	G1452	A1383	A1287	A1204	G1120
U2236	G2168	A2033	G1929	G1845	A1749	G1681	U1599	G1524	A1453	A1384	G1288	A1205	G1128
G2237	A2169	G1929	G1930	G1846	G1750	U1682	C1600	G1524	A1453	A1385	G1292	G1206	G1132
G2239	A2170	G1930	G1931	G1847	U1751	U1683	G1601	G1524	A1453	C1386	G1294	G1212	G1131
	A2171	G2038	U1931	A1848	C1753	G1685		G1528	U1457	A1387	U1294	G1218	U1132
U2243	A2173	G2040	C1934	A1853	G1756	C1856	C1604	A1529	G1458		C1295	G1218	A1133
U2244	C2174	U2041	G1935	A1854	G1756	C1887	C1605	G1530	G1459		C1295	G1218	A1133
U2245	C2175	A2042	A1936	G1854	G1756	U1688	C1606	C1531	U1460		C1297	G1223	A1134
G2246	A2176	C2043	A1937	G1857	C1760	A1689	C1607	A1532	U1461		C1297	G1227	A1134
A2247	C2177	G2044	A1938	A1858	C1760	A1690	A1608	U1534	C1462		C1297	G1227	G1139
C2248	C2178	C2045	U1939	U1859	C1764	C1691	A1610	A1535	G1464		G1300	G1230	U1140
U2249	A2117	G2046		U1864	A1773	U1692	A1614	C1536	G1465		A1301	A1230	U1141
G2250	A2119	C2047	U1985	U1864	A1773	U1693	C1615	C1537	U1466		C1306	U1231	A1142
G2251	G2120	G2048	A1986	U1865	C1774		C1616	G1538	U1467		C1306	U1232	C1145
	U2182	G2121	A1987	U1866	U1775	G1696	A1616	U1539	U1468		C1306	C1233	C1146
U2259	A2183	A2052	C1981	G1867	U1775	G1697	C1617	G1540	A1469		U1313	U1234	A1147
C2260	A2184	G2122	C1982	C1868	U1779	A1698	A1618	G1541	A1470		U1314	G1235	C1147
C2261	U2185	U1963	U1963	G1869	U1779	A1699		U1542	G1471		U1315	G1236	U1148
	G2125	C2055		C1870	A1784	G1702	G1622	G1543	C1472		U1316	A1237	G1149
C2264	G2126	G2056	A1966	A1871	A1784	G1703		A1544	G1473		U1317	G1238	C1150
U2285	G2127	A2058	C1967	G1872	A1789	C1704	C1625		U1474		U1318	A1151	C1152
A2286	G2128	A2059	G1968	A1873	C1790	G1705		A1548	G1475		C1319	C1152	C1152
A2287	C2129	A2060	A1969	C1874	A1791	G1706	U1629	A1549	U1476		C1320	C1153	G1153
A2287	U2130	G2061	A1970	G1875	A1791	G1707	A1630		U1477		A1321	G1154	C1154
	U2131	A2062	U1971	A1876	A1794	U1709	G1631	C1558			A1322	G1248	
U2272	G2132	C2063	G1972	U1880	C1795	U1710			G1482		U1325	U1249	C1161
A2273	U2133	C2064	A1987	G1887	U1796	A1711	A1634	U1563	G1483		U1325	G1250	C1162
A2274	G2134	C2065	G1988	U1882	U1797	U1712	A1635	C1564	U1484		U1325	G1251	
	A2135		A1988	U1883	U1798	U1713	A1636	C1565	U1485		G1333	A1252	A1165
U2279	A2136	U2068	U1991	U1884	G1799	U1714	A1637	C1566	U1486		G1334	A1254	A1166
G2280	U2137	C2069	G1992	G1884	C1800	G1715	C1638	C1567	U1487		A1336	U1255	G1167
A2281	G2138	A2070	G1992	C1887	A1801			G1568			G1341	G1257	G1168
C2282	C2200	A2071	U1993	U1888	A1802	U1720	C1646	U1569	A1490		G1341	G1261	G1171
C2283	G2140	C2072	C1996	A1889	A1803	G1721	U1647	A1570	C1493		C1345	A1262	C1172
A2284	G2141	C2073	C1997	A1890	A1803	G1722	U1648	A1571	A1494		C1345	U1263	U1173
C2285	A2142	U2074	C1997	A1890	A1808	G1723	G1649	A1572	A1495		C1345	A1264	U1174
G2286	C2143	U2075	G2004	G1896	U1812	G1724	A1650	G1573	A1495		C1349	A1265	U1175
A2287	G2144	U2076	A2005	G1897	G1813	C1727	G1651	C1574	U1496		C1350	A1266	U1176
A2288	A2147	U2079	C2006	U1897	G1814	C1728	G1652	C1575	U1497		C1350	G1266	G1177
G2289	G2148	A2080	A2009	U1898	A1815	U1729	G1653	U1576	C1498		C1350	G1266	G1177
U2291	U2149	U2081	A2009	G1903	G1816	G1730	A1654	C1577	C1499		A1353	U1267	C1178
U2292	C2150	A2082	G2010	C1904	G1817	G1731	G1659	U1578	G1500		A1354	A1268	G1179
G2293	U2151		U2011	C1905	U1818	C1732		A1579	G1501		A1355	A1269	U1180
C2294	G2152	C2091	G2012	G1906	G1826	G1733	A1664	C1582	A1502		A1359	C1270	U1181
C2295	C2153	U2092	A2013	G1907	G1827	G1734	G1665	A1583	A1503		A1359	G1271	G1182
U2296	A2154	G2093	A2014	G1907	U1827	U1735	G1666	U1584	A1504		A1360	A1272	U1183
A2297	U2155	A2094	A2015	G1910	G1828	U1736	G1667	C1585	A1506		A1361	U1273	U1184
U2298	G2156	A2095	A2015	U1911	A1829	G1737	A1668	A1586	C1507		G1361	A1274	G1185
U2299	G2157	C2096	C2021	U1912	C1830	G1738	A1669	A1587	A1508		G1364	A1275	G1186
	A2158	A2097	U2022	A1913	G1831	G1739	C1670	G1588	A1509		G1364	C1278	G1187
G2303	G2159	U2098	C2023	C1914	C1832	A1739	U1671	U1589	A1510		A1365	C1278	U1188
C2304	C2160	U2099	G2024	3TD1915	C1833	C1741	A1672	A1590	G1511		A1367	G1279	G1197
U2305	G2161	G2100	C2025	U1834	U1834	U1742	G1673	A1591	G1512		A1368	G1280	G1198
C2306	U1917	A2101	U2026	G1835	G1835	G1743	G1674	C1592	U1513		A1369	G1281	U1199
G2307	A2163	G2102	U2026	A1918	C1838	A1744	C1675	A1593	G1514		C1370	G1283	G1200
	C2164	C2103	G2029	G1921	C1838	A1745		U1594	G1515		G1371	A1284	U1201
A2309	U2166	U2105	A2031	G1922	C1843	U1747	A1678	G1516	G1517		G1371	A1285	U1202
													U1203






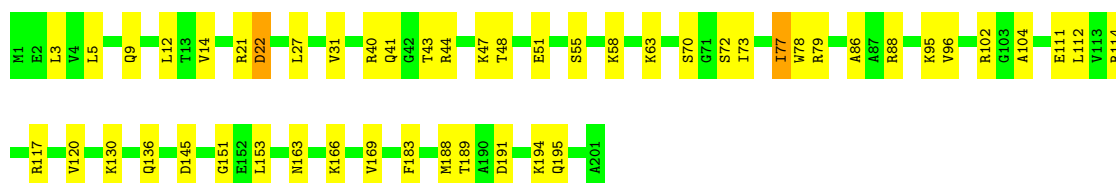
- Molecule 28: 50S ribosomal protein L3

Chain BD:  68% 27% 5%



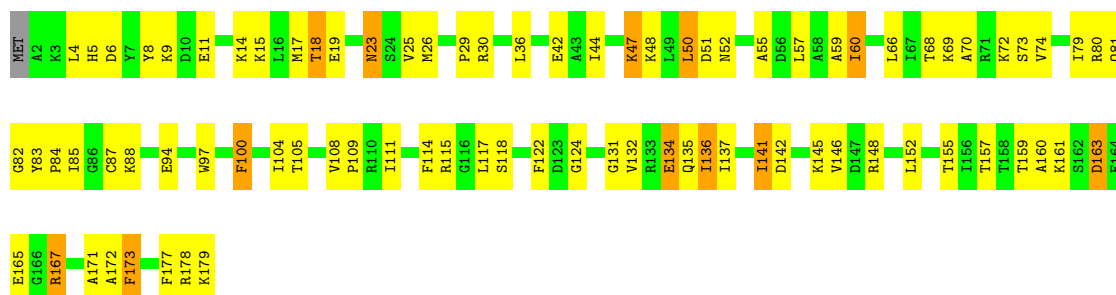
- Molecule 29: 50S ribosomal protein L4

Chain BE:  75% 24% .



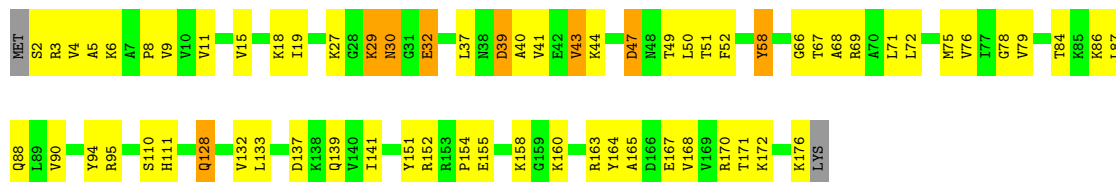
- Molecule 30: 50S ribosomal protein L5

Chain BF:  53% 40% 7% .




- Molecule 31: 50S ribosomal protein L6

Chain BG:  61% 33% 5% .

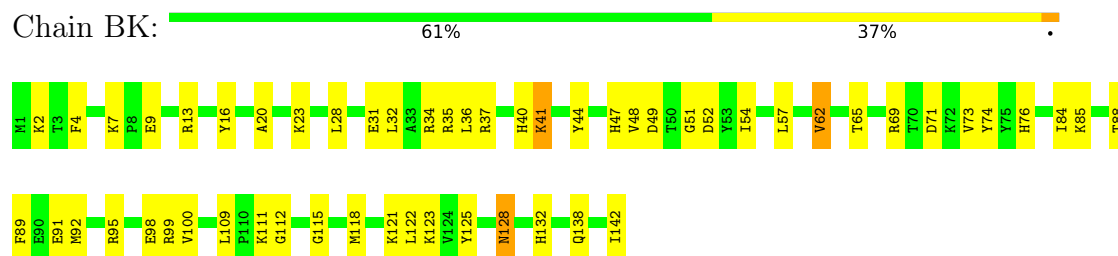


- Molecule 32: 50S ribosomal protein L9

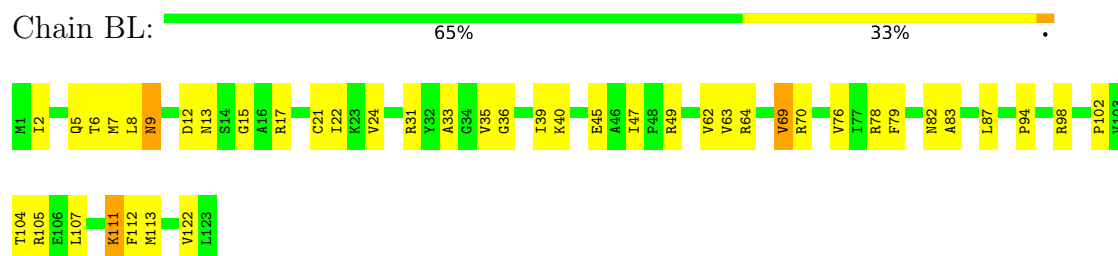
Chain BH:  85% 14% .



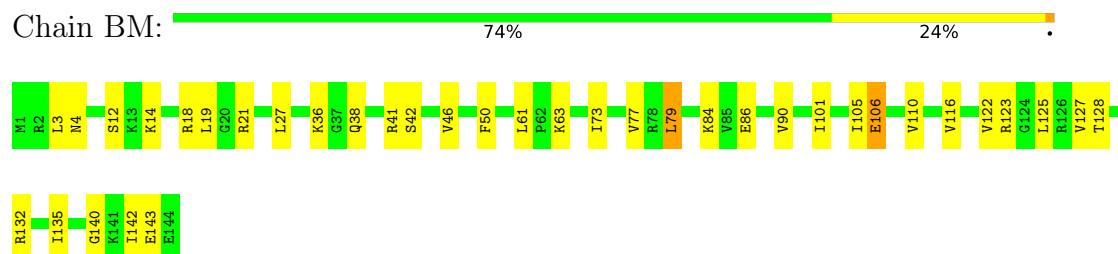
- Molecule 33: 50S ribosomal protein L13



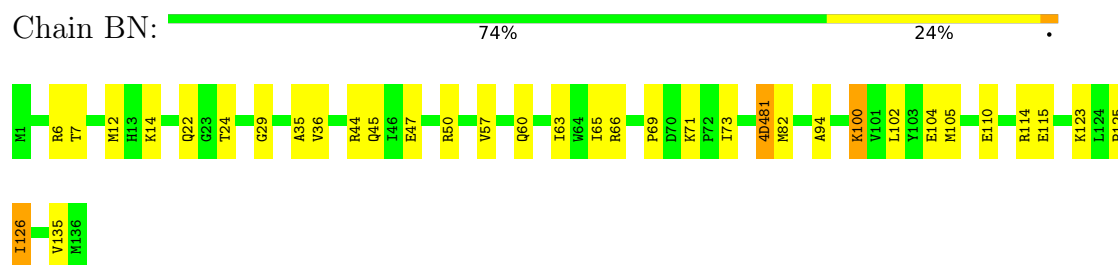
- Molecule 34: 50S ribosomal protein L14



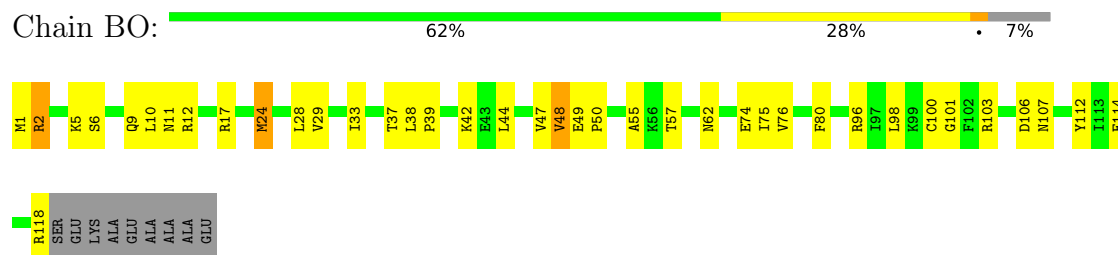
- Molecule 35: 50S ribosomal protein L15



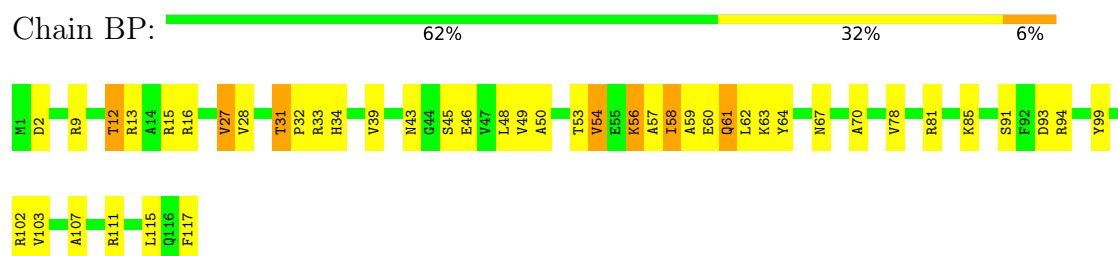
- Molecule 36: 50S ribosomal protein L16



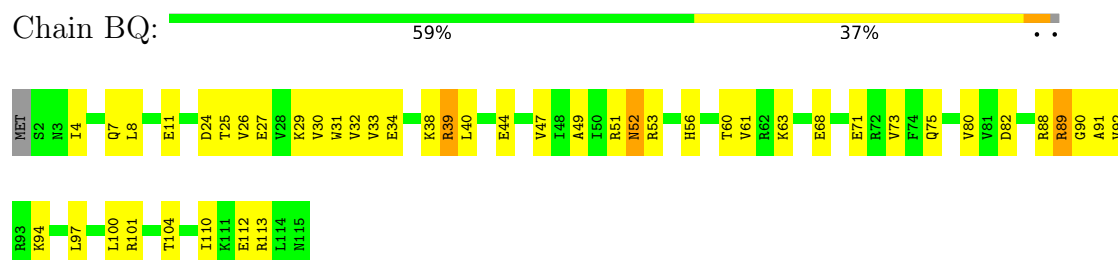
- Molecule 37: 50S ribosomal protein L17



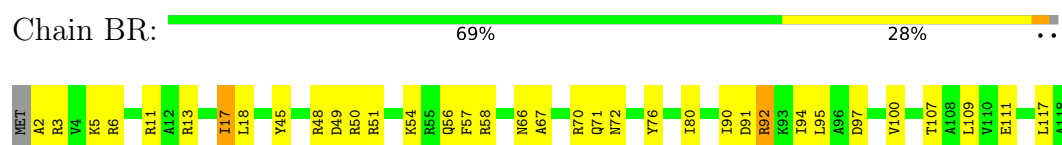
- Molecule 38: 50S ribosomal protein L18



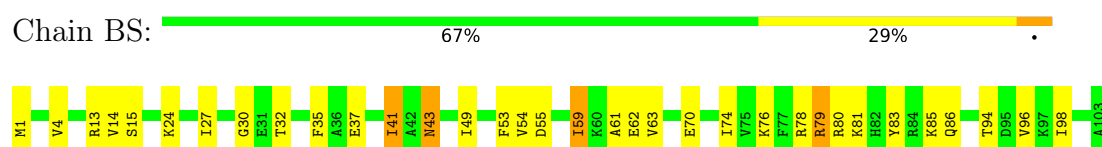
- Molecule 39: 50S ribosomal protein L19



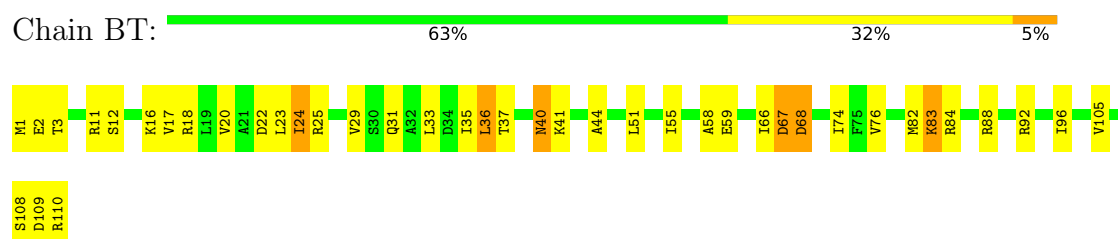
- Molecule 40: 50S ribosomal protein L20



- Molecule 41: 50S ribosomal protein L21



- Molecule 42: 50S ribosomal protein L22



- Molecule 43: 50S ribosomal protein L23





- Molecule 44: 50S ribosomal protein L24

Chain BV: 64% 30%



- Molecule 45: 50S ribosomal protein L25

Chain BW: 62% 34%



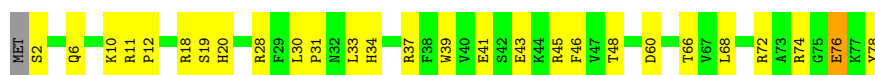
- Molecule 46: 50S ribosomal protein L27

Chain BX: 60% 26% 11%



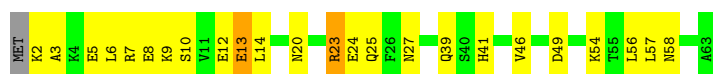
- Molecule 47: 50S ribosomal protein L28

Chain BY: 64% 33%



- Molecule 48: 50S ribosomal protein L29

Chain BZ: 60% 35%



- Molecule 49: 50S ribosomal protein L30

Chain B1: 59% 37%



- Molecule 50: 50S ribosomal protein L32

Chain B2:  67% 30% . .




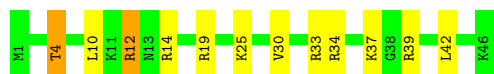
- Molecule 51: 50S ribosomal protein L33

Chain B3:  44% 45% 5% 5%



- Molecule 52: 50S ribosomal protein L34

Chain B4:  74% 22% .



- Molecule 53: 50S ribosomal protein L35

Chain B5:  72% 18% 5% . .




- Molecule 54: 50S ribosomal protein L36

Chain B6:  54% 22% 24%




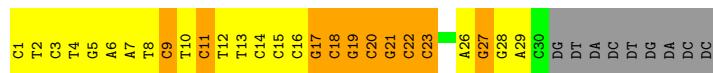
- Molecule 55: Non-template DNA strand

Chain CN:  18% 49% 10% 23%



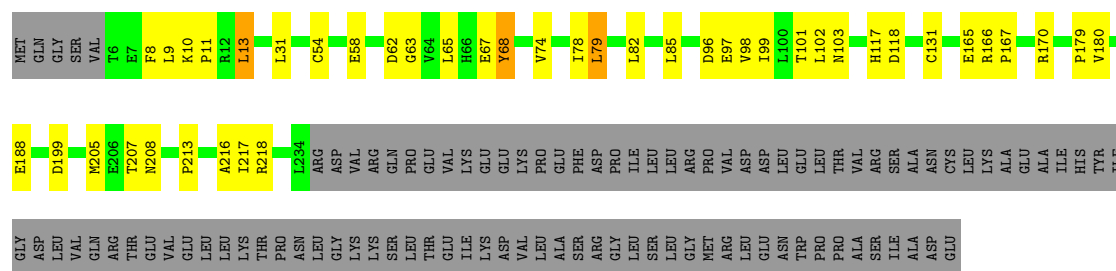
- Molecule 56: Template DNA strand

Chain CT:  8% 44% 26% 23%



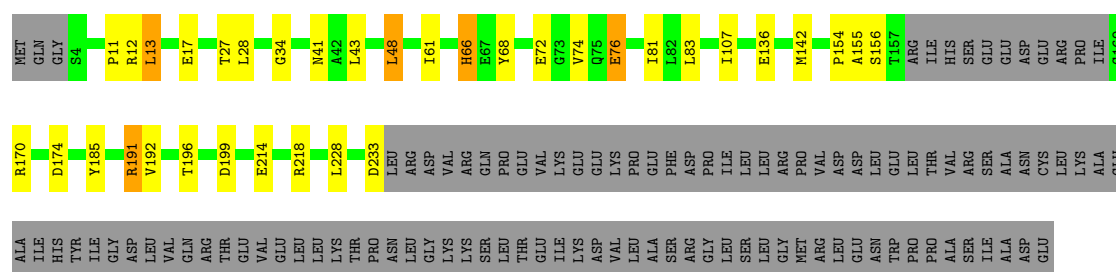
- Molecule 57: DNA-directed RNA polymerase subunit alpha

Chain CA:  57% 12% 30%




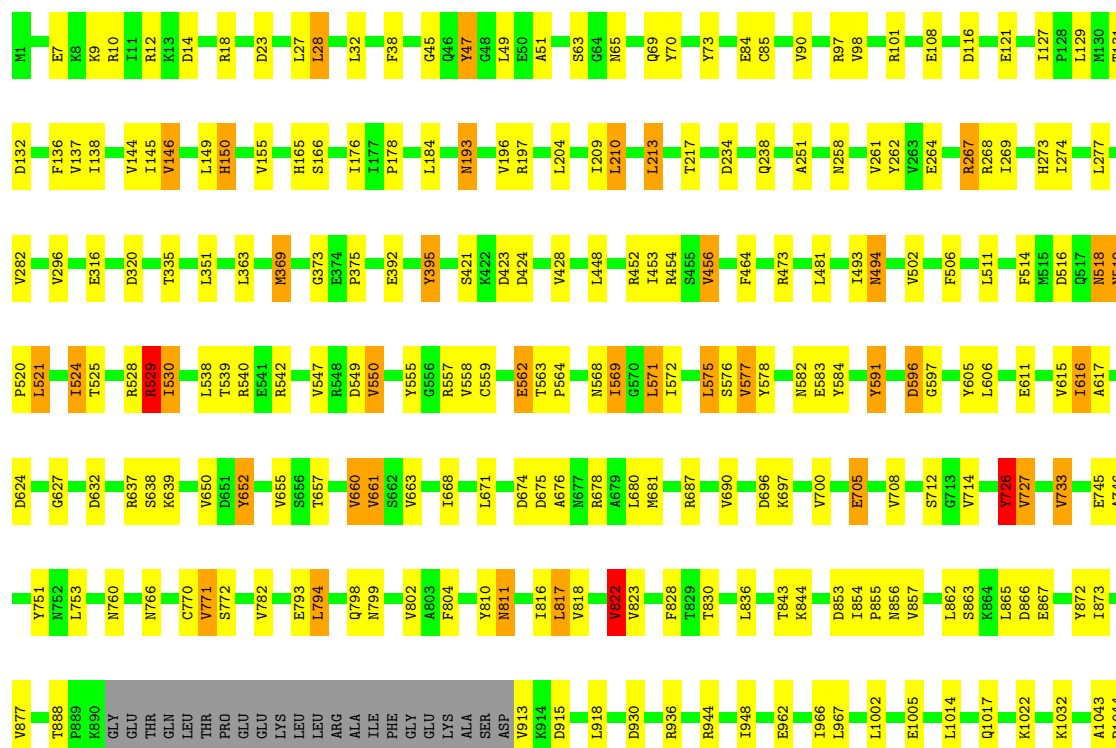
- Molecule 57: DNA-directed RNA polymerase subunit alpha

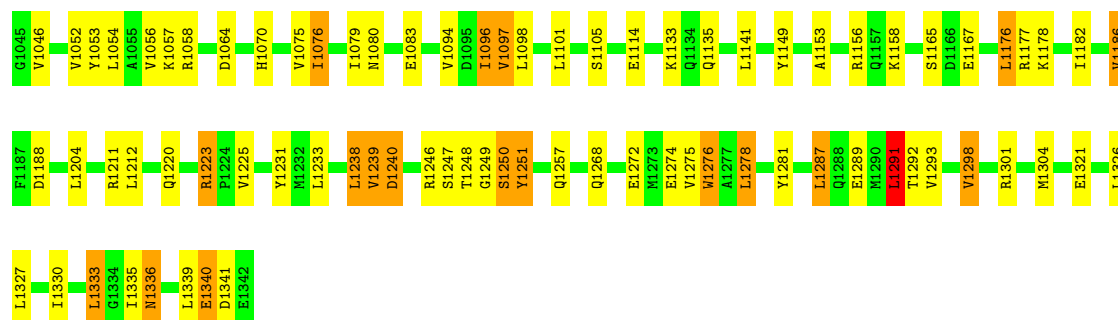
Chain CB:  56% 9% 33%



- Molecule 58: DNA-directed RNA polymerase subunit beta

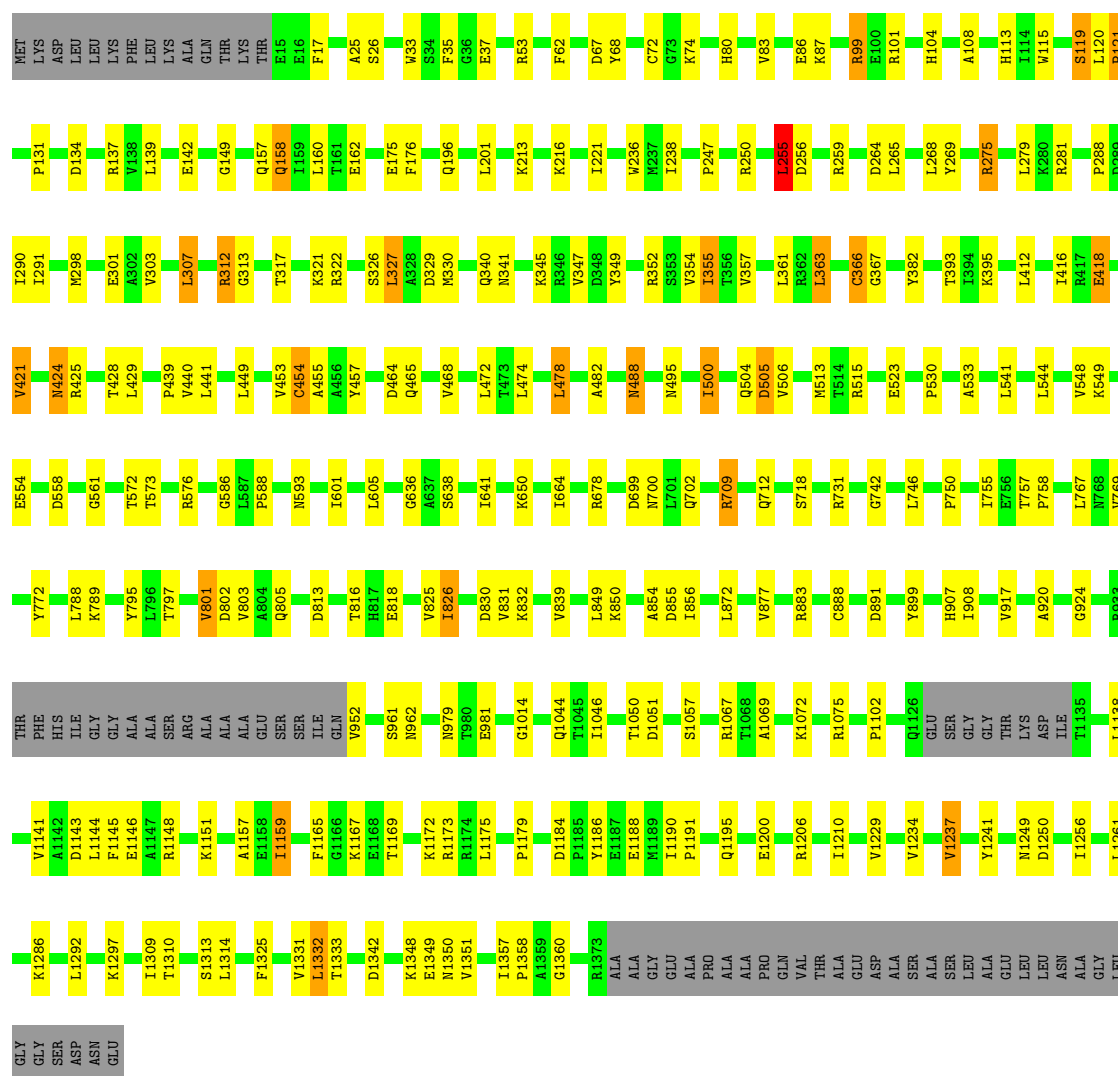
Chain CC:  75% 19% 6%





- Molecule 59: DNA-directed RNA polymerase subunit beta'

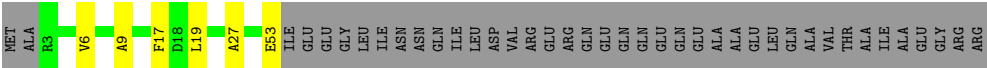
Chain CD: 76% 17% 5%



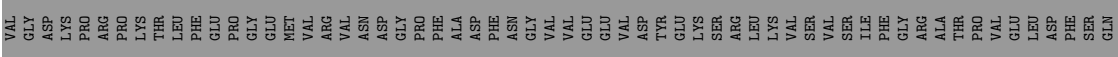
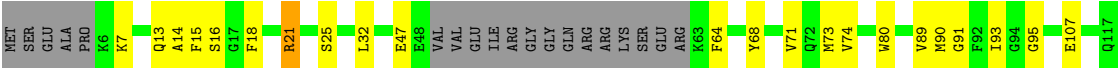
- Molecule 60: DNA-directed RNA polymerase subunit omega

Chain CE: 49% 7% 44%





● Molecule 61: Transcription termination/antitermination protein NusG



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MIA, 2MA, 3TD, H2U, G7M, 3AU, MA6, 4D4, 6MZ, PSU, 4OC, OMC, 7MG, MEQ, OMU, D2T, UR3, 4SU, OMG, MG, 1MG, 5MC, 5MU, ZN, 2MG

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	0.73	0/36569	0.92	19/57044 (0.0%)
2	AB	0.31	0/1795	0.49	0/2418
3	AC	0.37	0/1680	0.48	0/2263
4	AD	0.34	0/1665	0.48	0/2227
5	AE	0.39	0/1161	0.50	0/1563
6	AF	0.37	0/867	0.52	0/1171
7	AG	0.30	0/1230	0.45	0/1649
8	AH	0.37	0/989	0.50	0/1326
9	AI	0.35	0/1043	0.63	0/1387
10	AJ	0.34	0/827	0.53	0/1117
11	AK	0.35	0/893	0.46	0/1205
12	AL	0.45	1/960 (0.1%)	0.51	0/1286
13	AM	0.33	0/900	0.50	0/1204
14	AN	0.32	0/817	0.43	0/1088
15	AO	0.32	0/730	0.43	0/974
16	AP	0.34	0/659	0.50	0/884
17	AQ	0.37	0/657	0.50	0/881
18	AR	0.37	0/481	0.49	0/645
19	AS	0.31	0/672	0.46	0/904
20	AT	0.30	0/676	0.42	0/895
21	AU	0.30	0/598	0.51	0/792
22	AV	1.76	27/803 (3.4%)	1.63	32/1245 (2.6%)
23	AW	0.70	1/1725 (0.1%)	0.94	2/2687 (0.1%)
24	AX	0.58	1/1584 (0.1%)	0.86	0/2463
25	BA	0.89	1/69143 (0.0%)	0.93	43/107862 (0.0%)
26	BB	0.67	0/2872	0.86	1/4478 (0.0%)
27	BC	0.48	1/2131 (0.0%)	0.52	0/2863
28	BD	0.44	0/1576	0.53	0/2119
29	BE	0.40	0/1571	0.48	0/2113
30	BF	0.34	0/1444	0.47	0/1937
31	BG	0.35	0/1333	0.47	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	BH	0.31	0/1122	0.62	0/1515
33	BK	0.45	0/1152	0.48	0/1551
34	BL	0.43	0/955	0.53	0/1277
35	BM	0.42	0/1061	0.51	0/1412
36	BN	0.44	0/1081	0.50	0/1443
37	BO	0.41	0/958	0.49	0/1281
38	BP	0.33	0/910	0.49	0/1219
39	BQ	0.40	0/929	0.51	0/1242
40	BR	0.52	0/960	0.48	0/1278
41	BS	0.45	0/829	0.52	0/1107
42	BT	0.40	0/864	0.51	0/1156
43	BU	0.37	0/764	0.49	0/1021
44	BV	0.37	0/787	0.50	0/1051
45	BW	0.38	0/766	0.47	0/1025
46	BX	0.44	0/589	0.49	0/779
47	BY	0.42	0/635	0.48	0/848
48	BZ	0.32	0/502	0.44	0/667
49	B1	0.39	0/453	0.51	0/605
50	B2	0.40	0/450	0.56	0/599
51	B3	0.36	0/433	0.55	0/576
52	B4	0.42	0/380	0.48	0/498
53	B5	0.39	0/513	0.49	0/676
54	B6	0.41	0/302	0.47	0/397
55	CN	1.78	12/693 (1.7%)	1.24	2/1068 (0.2%)
56	CT	2.53	41/676 (6.1%)	1.33	9/1039 (0.9%)
57	CA	1.13	6/1797 (0.3%)	0.91	2/2436 (0.1%)
57	CB	0.81	1/1703 (0.1%)	0.86	3/2308 (0.1%)
58	CC	1.41	122/10581 (1.2%)	0.97	31/14275 (0.2%)
59	CD	1.12	57/10532 (0.5%)	0.91	16/14219 (0.1%)
60	CE	0.48	0/401	0.75	0/540
61	CF	0.41	0/808	0.58	0/1088
All	All	0.84	271/184637 (0.1%)	0.86	160/272691 (0.1%)

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
9	AI	0	1
13	AM	0	2
22	AV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
53	B5	0	1
All	All	0	5

The worst 5 of 271 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	AW	1	C	OP3-P	-10.66	1.48	1.61
24	AX	1	G	OP3-P	-10.41	1.48	1.61
56	CT	18	DC	C3'-O3'	-10.24	1.30	1.44
59	CD	1357	ILE	C-N	-9.76	1.15	1.34
56	CT	14	DC	C3'-O3'	-9.59	1.31	1.44

The worst 5 of 160 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	2902	C	N3-C2-O2	-11.33	113.97	121.90
56	CT	19	DG	O4'-C1'-N9	10.14	115.10	108.00
25	BA	2902	C	N1-C2-O2	9.98	124.89	118.90
22	AV	48	C	C6-N1-C2	-9.65	116.44	120.30
25	BA	2164	C	C2-N1-C1'	9.05	128.76	118.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	AI	30	ILE	Peptide
13	AM	48	LEU	Peptide
13	AM	49	SER	Peptide
22	AV	41	C	Sidechain
53	B5	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	32908	0	16576	926	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1764	0	1788	63	0
3	AC	1653	0	1725	140	0
4	AD	1643	0	1706	100	0
5	AE	1148	0	1195	26	0
6	AF	848	0	846	41	0
7	AG	1214	0	1267	42	0
8	AH	979	0	1031	41	0
9	AI	1031	0	1076	31	0
10	AJ	817	0	853	36	0
11	AK	877	0	887	29	0
12	AL	957	0	1017	32	0
13	AM	891	0	952	29	0
14	AN	805	0	844	21	0
15	AO	722	0	746	14	0
16	AP	649	0	666	34	0
17	AQ	648	0	691	29	0
18	AR	474	0	494	13	0
19	AS	656	0	680	36	0
20	AT	670	0	719	26	0
21	AU	590	0	629	10	0
22	AV	720	0	369	45	0
23	AW	1645	0	842	39	0
24	AX	1629	0	835	37	0
25	BA	62248	0	31320	1337	0
26	BB	2569	0	1301	55	0
27	BC	2092	0	2167	51	0
28	BD	1566	0	1618	46	0
29	BE	1552	0	1618	27	0
30	BF	1420	0	1457	49	0
31	BG	1313	0	1358	39	0
32	BH	1111	0	1148	13	0
33	BK	1129	0	1162	37	0
34	BL	946	0	1019	34	0
35	BM	1052	0	1127	27	0
36	BN	1075	0	1154	22	0
37	BO	945	0	989	25	0
38	BP	900	0	935	32	0
39	BQ	917	0	962	34	0
40	BR	947	0	1019	32	0
41	BS	816	0	839	23	0
42	BT	857	0	922	26	0
43	BU	757	0	820	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BV	779	0	830	22	0
45	BW	753	0	780	24	0
46	BX	582	0	599	19	0
47	BY	625	0	652	19	0
48	BZ	501	0	531	14	0
49	B1	449	0	488	16	0
50	B2	444	0	458	15	0
51	B3	426	0	464	23	0
52	B4	377	0	418	9	0
53	B5	504	0	572	18	0
54	B6	301	0	340	8	0
55	CN	618	0	336	67	0
56	CT	606	0	338	39	0
57	CA	1775	0	1799	41	0
57	CB	1684	0	1713	19	0
58	CC	10415	0	10431	277	0
59	CD	10375	0	10596	191	0
60	CE	399	0	417	4	0
61	CF	790	0	781	61	0
62	AA	115	0	0	0	0
62	AL	1	0	0	0	0
62	AM	1	0	0	0	0
62	AN	1	0	0	0	0
62	AP	1	0	0	0	0
62	AX	1	0	0	0	0
62	BA	304	0	0	0	0
62	BB	8	0	0	0	0
62	BC	4	0	0	0	0
62	BD	2	0	0	0	0
62	BQ	1	0	0	0	0
62	BR	1	0	0	0	0
62	CD	1	0	0	0	0
63	AX	11	0	8	1	0
64	B6	1	0	0	0	0
64	CD	2	0	0	0	0
All	All	173008	0	123920	4047	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 14.

The worst 5 of 4047 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)
4:AD:192:SER:CA	59:CD:74:LYS:HE2	1.36	1.52
3:AC:80:LYS:CE	58:CC:873:ILE:HG21	1.42	1.49
3:AC:107:ARG:CD	57:CA:165:GLU:HG2	1.05	1.48
4:AD:192:SER:HB3	59:CD:74:LYS:CE	1.43	1.46
3:AC:80:LYS:HE3	58:CC:873:ILE:CG2	1.40	1.46

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	224/241 (93%)	200 (89%)	24 (11%)	0	100	100
3	AC	209/233 (90%)	197 (94%)	12 (6%)	0	100	100
4	AD	203/206 (98%)	191 (94%)	12 (6%)	0	100	100
5	AE	154/167 (92%)	140 (91%)	14 (9%)	0	100	100
6	AF	102/131 (78%)	94 (92%)	8 (8%)	0	100	100
7	AG	152/156 (97%)	140 (92%)	12 (8%)	0	100	100
8	AH	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
9	AI	126/130 (97%)	115 (91%)	10 (8%)	1 (1%)	16	51
10	AJ	100/103 (97%)	88 (88%)	10 (10%)	2 (2%)	6	33
11	AK	115/129 (89%)	105 (91%)	10 (9%)	0	100	100
12	AL	120/124 (97%)	107 (89%)	12 (10%)	1 (1%)	16	51
13	AM	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
14	AN	98/101 (97%)	93 (95%)	5 (5%)	0	100	100
15	AO	87/89 (98%)	84 (97%)	3 (3%)	0	100	100
16	AP	80/82 (98%)	68 (85%)	12 (15%)	0	100	100
17	AQ	78/84 (93%)	72 (92%)	6 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AR	55/75 (73%)	51 (93%)	4 (7%)	0	100	100
19	AS	80/92 (87%)	73 (91%)	7 (9%)	0	100	100
20	AT	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	AU	68/71 (96%)	66 (97%)	2 (3%)	0	100	100
27	BC	270/273 (99%)	244 (90%)	25 (9%)	1 (0%)	30	64
28	BD	206/209 (99%)	198 (96%)	7 (3%)	1 (0%)	25	59
29	BE	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
30	BF	176/179 (98%)	159 (90%)	17 (10%)	0	100	100
31	BG	173/177 (98%)	158 (91%)	15 (9%)	0	100	100
32	BH	147/149 (99%)	134 (91%)	11 (8%)	2 (1%)	9	40
33	BK	140/142 (99%)	132 (94%)	8 (6%)	0	100	100
34	BL	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
35	BM	142/144 (99%)	131 (92%)	11 (8%)	0	100	100
36	BN	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
37	BO	116/127 (91%)	108 (93%)	8 (7%)	0	100	100
38	BP	115/117 (98%)	102 (89%)	13 (11%)	0	100	100
39	BQ	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
40	BR	115/118 (98%)	112 (97%)	3 (3%)	0	100	100
41	BS	101/103 (98%)	94 (93%)	7 (7%)	0	100	100
42	BT	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
43	BU	93/100 (93%)	83 (89%)	10 (11%)	0	100	100
44	BV	100/104 (96%)	87 (87%)	13 (13%)	0	100	100
45	BW	92/94 (98%)	85 (92%)	7 (8%)	0	100	100
46	BX	74/85 (87%)	66 (89%)	8 (11%)	0	100	100
47	BY	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
48	BZ	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
49	B1	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
50	B2	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
51	B3	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
52	B4	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
53	B5	62/65 (95%)	52 (84%)	9 (14%)	1 (2%)	8	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B6	36/50 (72%)	35 (97%)	1 (3%)	0	100	100
57	CA	227/329 (69%)	217 (96%)	10 (4%)	0	100	100
57	CB	215/329 (65%)	203 (94%)	11 (5%)	1 (0%)	25	59
58	CC	1316/1342 (98%)	1197 (91%)	110 (8%)	9 (1%)	19	53
59	CD	1327/1407 (94%)	1223 (92%)	94 (7%)	10 (1%)	16	51
60	CE	49/91 (54%)	40 (82%)	8 (16%)	1 (2%)	6	33
61	CF	94/181 (52%)	88 (94%)	6 (6%)	0	100	100
All	All	8773/9507 (92%)	8089 (92%)	654 (8%)	30 (0%)	38	68

5 of 30 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	AI	13	LYS
32	BH	89	LYS
58	CC	165	HIS
59	CD	1159	ILE
32	BH	15	LEU

### 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	187/199 (94%)	163 (87%)	24 (13%)	3	18
3	AC	172/190 (90%)	151 (88%)	21 (12%)	4	20
4	AD	172/173 (99%)	154 (90%)	18 (10%)	5	25
5	AE	118/126 (94%)	108 (92%)	10 (8%)	8	32
6	AF	91/112 (81%)	76 (84%)	15 (16%)	2	11
7	AG	127/129 (98%)	104 (82%)	23 (18%)	1	7
8	AH	104/105 (99%)	91 (88%)	13 (12%)	3	19
9	AI	106/107 (99%)	102 (96%)	4 (4%)	28	57
10	AJ	89/90 (99%)	79 (89%)	10 (11%)	5	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	AK	90/99 (91%)	80 (89%)	10 (11%)	5	23
12	AL	102/103 (99%)	84 (82%)	18 (18%)	1	8
13	AM	93/96 (97%)	82 (88%)	11 (12%)	4	21
14	AN	83/84 (99%)	74 (89%)	9 (11%)	5	24
15	AO	77/77 (100%)	66 (86%)	11 (14%)	2	16
16	AP	65/65 (100%)	57 (88%)	8 (12%)	4	20
17	AQ	74/78 (95%)	56 (76%)	18 (24%)	0	3
18	AR	50/65 (77%)	43 (86%)	7 (14%)	3	16
19	AS	71/79 (90%)	62 (87%)	9 (13%)	3	18
20	AT	65/66 (98%)	60 (92%)	5 (8%)	10	34
21	AU	60/61 (98%)	56 (93%)	4 (7%)	13	40
27	BC	217/218 (100%)	201 (93%)	16 (7%)	11	36
28	BD	163/163 (100%)	144 (88%)	19 (12%)	4	21
29	BE	165/165 (100%)	148 (90%)	17 (10%)	6	26
30	BF	149/150 (99%)	122 (82%)	27 (18%)	1	7
31	BG	136/138 (99%)	114 (84%)	22 (16%)	2	11
32	BH	114/114 (100%)	111 (97%)	3 (3%)	41	66
33	BK	116/116 (100%)	107 (92%)	9 (8%)	10	34
34	BL	104/104 (100%)	99 (95%)	5 (5%)	21	50
35	BM	103/103 (100%)	96 (93%)	7 (7%)	13	39
36	BN	108/108 (100%)	100 (93%)	8 (7%)	11	36
37	BO	98/103 (95%)	89 (91%)	9 (9%)	7	29
38	BP	87/87 (100%)	76 (87%)	11 (13%)	3	19
39	BQ	99/100 (99%)	90 (91%)	9 (9%)	7	30
40	BR	89/90 (99%)	81 (91%)	8 (9%)	8	30
41	BS	84/84 (100%)	76 (90%)	8 (10%)	7	28
42	BT	93/93 (100%)	84 (90%)	9 (10%)	6	27
43	BU	82/84 (98%)	75 (92%)	7 (8%)	8	32
44	BV	83/85 (98%)	71 (86%)	12 (14%)	2	15
45	BW	78/78 (100%)	72 (92%)	6 (8%)	10	34
46	BX	58/63 (92%)	54 (93%)	4 (7%)	13	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
47	BY	67/68 (98%)	63 (94%)	4 (6%)	16	43
48	BZ	54/55 (98%)	47 (87%)	7 (13%)	3	18
49	B1	48/49 (98%)	43 (90%)	5 (10%)	5	25
50	B2	47/48 (98%)	43 (92%)	4 (8%)	8	32
51	B3	47/49 (96%)	41 (87%)	6 (13%)	3	18
52	B4	38/38 (100%)	35 (92%)	3 (8%)	10	34
53	B5	51/52 (98%)	45 (88%)	6 (12%)	4	21
54	B6	34/44 (77%)	33 (97%)	1 (3%)	37	64
57	CA	197/286 (69%)	193 (98%)	4 (2%)	50	72
57	CB	187/286 (65%)	177 (95%)	10 (5%)	19	46
58	CC	1139/1157 (98%)	1097 (96%)	42 (4%)	29	58
59	CD	1118/1168 (96%)	1096 (98%)	22 (2%)	50	72
60	CE	43/75 (57%)	42 (98%)	1 (2%)	45	69
61	CF	86/158 (54%)	85 (99%)	1 (1%)	67	82
All	All	7378/7883 (94%)	6798 (92%)	580 (8%)	13	34

5 of 580 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
46	BX	77	ARG
59	CD	1165	PHE
49	B1	11	ARG
46	BX	70	GLU
58	CC	262	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
40	BR	72	ASN
48	BZ	58	ASN
48	BZ	41	HIS
19	AS	57	HIS
39	BQ	7	GLN

### 5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	299 (19%)	8 (0%)
22	AV	32/49 (65%)	13 (40%)	1 (3%)
23	AW	76/77 (98%)	19 (25%)	2 (2%)
24	AX	73/76 (96%)	22 (30%)	1 (1%)
25	BA	2893/2904 (99%)	561 (19%)	7 (0%)
26	BB	119/120 (99%)	17 (14%)	1 (0%)
All	All	4722/4768 (99%)	931 (19%)	20 (0%)

5 of 931 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	2	A
1	AA	4	U
1	AA	6	G
1	AA	9	G
1	AA	16	A

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	784	G
25	BA	2225	A
26	BB	41	G
25	BA	2609	U
1	AA	1166	G

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

53 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	$\# Z  > 2$
25	OMC	BA	2498	62,25	18,21,23	2.81	7 (38%)	26,30,34	0.60	0
25	5MC	BA	1962	25	18,22,23	3.80	7 (38%)	26,32,35	1.03	1 (3%)
24	PSU	AX	39	24	18,21,22	1.01	1 (5%)	22,30,33	1.78	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	4SU	AW	8	23	18,21,22	4.05	8 (44%)	26,30,33	2.41	5 (19%)
25	6MZ	BA	2030	25	18,25,26	1.90	4 (22%)	16,36,39	2.73	4 (25%)
24	PSU	AX	55	24	18,21,22	1.06	2 (11%)	22,30,33	1.79	4 (18%)
25	OMU	BA	2552	25	19,22,23	2.78	7 (36%)	26,31,34	1.77	5 (19%)
1	G7M	AA	527	1	20,26,27	2.30	8 (40%)	17,39,42	1.24	3 (17%)
23	PSU	AW	55	23	18,21,22	1.11	1 (5%)	22,30,33	1.77	4 (18%)
25	H2U	BA	2449	25	18,21,22	2.76	5 (27%)	21,30,33	2.44	5 (23%)
25	G7M	BA	2069	25	20,26,27	2.21	8 (40%)	17,39,42	1.12	1 (5%)
28	MEQ	BD	150	28	8,9,10	0.94	0	5,10,12	1.08	1 (20%)
25	6MZ	BA	1618	25	18,25,26	1.95	3 (16%)	16,36,39	2.21	4 (25%)
1	2MG	AA	966	1	18,25,27	2.50	8 (44%)	19,37,41	1.51	4 (21%)
25	PSU	BA	1917	25	18,21,22	1.06	2 (11%)	22,30,33	1.73	4 (18%)
25	PSU	BA	2604	62,25	18,21,22	0.98	2 (11%)	22,30,33	1.69	4 (18%)
1	5MC	AA	1407	1	18,22,23	3.82	7 (38%)	26,32,35	1.12	2 (7%)
24	H2U	AX	20	24	18,21,22	3.12	5 (27%)	21,30,33	1.97	4 (19%)
25	3TD	BA	1915	25	18,22,23	4.39	9 (50%)	22,32,35	1.67	2 (9%)
25	OMG	BA	2251	62,23,25	18,26,27	2.56	8 (44%)	19,38,41	1.52	4 (21%)
25	PSU	BA	2605	25	18,21,22	1.04	2 (11%)	22,30,33	1.79	5 (22%)
36	4D4	BN	81	36	9,11,12	2.31	2 (22%)	8,13,15	1.10	1 (12%)
25	PSU	BA	746	62,25	18,21,22	1.08	3 (16%)	22,30,33	1.80	4 (18%)
1	5MC	AA	967	1	18,22,23	3.95	7 (38%)	26,32,35	1.15	2 (7%)
25	2MA	BA	2503	62,25	19,25,26	3.42	9 (47%)	21,37,40	2.32	4 (19%)
24	PSU	AX	32	24	18,21,22	0.97	1 (5%)	22,30,33	1.83	5 (22%)
1	4OC	AA	1402	62,1	20,23,24	3.42	9 (45%)	26,32,35	0.88	1 (3%)
25	PSU	BA	2504	25	18,21,22	1.04	1 (5%)	22,30,33	1.84	4 (18%)
25	5MU	BA	747	25	19,22,23	1.40	4 (21%)	28,32,35	2.11	6 (21%)
25	PSU	BA	1911	25	18,21,22	1.03	2 (11%)	22,30,33	1.93	4 (18%)
1	PSU	AA	516	62,1	18,21,22	0.97	1 (5%)	22,30,33	1.80	5 (22%)
1	MA6	AA	1518	1	18,26,27	1.37	3 (16%)	19,38,41	4.23	2 (10%)
25	PSU	BA	955	25	18,21,22	1.08	3 (16%)	22,30,33	1.73	4 (18%)
23	OMC	AW	32	23	19,22,23	2.91	8 (42%)	26,31,34	0.83	0
25	1MG	BA	745	25	18,26,27	2.58	6 (33%)	19,39,42	1.48	4 (21%)
1	MA6	AA	1519	1	18,26,27	1.35	3 (16%)	19,38,41	4.08	2 (10%)
25	2MG	BA	1835	25	18,26,27	2.21	7 (38%)	16,38,41	1.70	4 (25%)
24	4SU	AX	8	24	18,21,22	4.14	8 (44%)	26,30,33	2.27	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	2MG	AA	1516	1	18,26,27	2.24	7 (38%)	16,38,41	1.57	4 (25%)
24	7MG	AX	46	24	20,25,27	3.22	10 (50%)	27,37,42	2.23	8 (29%)
25	PSU	BA	2580	25	18,21,22	1.08	2 (11%)	22,30,33	1.98	5 (22%)
24	H2U	AX	16	24	18,21,22	3.05	5 (27%)	21,30,33	2.05	5 (23%)
25	5MU	BA	1939	25	19,22,23	1.43	4 (21%)	28,32,35	2.34	6 (21%)
12	D2T	AL	89	12	7,9,10	1.00	0	6,11,13	2.26	3 (50%)
24	3AU	AX	47	24	18,21,29	3.49	8 (44%)	26,30,43	1.62	4 (15%)
24	5MU	AX	54	24	19,22,23	1.38	4 (21%)	28,32,35	2.24	6 (21%)
23	H2U	AW	20	23	18,21,22	3.15	5 (27%)	21,30,33	2.02	5 (23%)
1	UR3	AA	1498	1	19,22,23	2.55	6 (31%)	26,32,35	1.40	3 (11%)
23	5MU	AW	54	23	19,22,23	1.40	6 (31%)	28,32,35	2.20	9 (32%)
24	MIA	AX	37	24	22,29,32	2.88	4 (18%)	22,41,47	2.85	7 (31%)
25	2MG	BA	2445	25	18,26,27	2.20	7 (38%)	16,38,41	1.58	4 (25%)
25	PSU	BA	2457	25	18,21,22	1.04	3 (16%)	22,30,33	1.97	5 (22%)
1	2MG	AA	1207	1	18,26,27	2.34	7 (38%)	16,38,41	1.52	4 (25%)

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
25	OMC	BA	2498	62,25	-	2/7/25/28	0/2/2/2
25	5MC	BA	1962	25	-	4/7/25/26	0/2/2/2
24	PSU	AX	39	24	-	0/7/25/26	0/2/2/2
23	4SU	AW	8	23	-	0/7/25/26	0/2/2/2
25	6MZ	BA	2030	25	-	2/5/27/28	0/3/3/3
24	PSU	AX	55	24	-	1/7/25/26	0/2/2/2
25	OMU	BA	2552	25	-	0/9/27/28	0/2/2/2
1	G7M	AA	527	1	-	1/3/25/26	0/3/3/3
23	PSU	AW	55	23	-	1/7/25/26	0/2/2/2
25	H2U	BA	2449	25	-	0/7/38/39	0/2/2/2
25	G7M	BA	2069	25	-	2/3/25/26	0/3/3/3
28	MEQ	BD	150	28	-	1/8/9/11	-
25	6MZ	BA	1618	25	-	5/5/27/28	0/3/3/3
1	2MG	AA	966	1	-	2/3/25/28	0/3/3/3
25	PSU	BA	1917	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	2604	62,25	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	AA	1407	1	-	0/7/25/26	0/2/2/2
24	H2U	AX	20	24	-	3/7/38/39	0/2/2/2
25	3TD	BA	1915	25	-	0/7/25/26	0/2/2/2
25	OMG	BA	2251	62,23,25	-	1/5/27/28	0/3/3/3
25	PSU	BA	2605	25	-	0/7/25/26	0/2/2/2
36	4D4	BN	81	36	-	4/11/12/14	-
25	PSU	BA	746	62,25	-	1/7/25/26	0/2/2/2
1	5MC	AA	967	1	-	0/7/25/26	0/2/2/2
25	2MA	BA	2503	62,25	-	3/3/25/26	0/3/3/3
24	PSU	AX	32	24	-	0/7/25/26	0/2/2/2
1	4OC	AA	1402	62,1	-	2/9/29/30	0/2/2/2
25	PSU	BA	2504	25	-	2/7/25/26	0/2/2/2
25	5MU	BA	747	25	-	0/7/25/26	0/2/2/2
25	PSU	BA	1911	25	-	1/7/25/26	0/2/2/2
1	PSU	AA	516	62,1	-	0/7/25/26	0/2/2/2
1	MA6	AA	1518	1	-	4/7/29/30	0/3/3/3
25	PSU	BA	955	25	-	0/7/25/26	0/2/2/2
23	OMC	AW	32	23	-	0/9/27/28	0/2/2/2
25	1MG	BA	745	25	-	0/3/25/26	0/3/3/3
1	MA6	AA	1519	1	-	4/7/29/30	0/3/3/3
25	2MG	BA	1835	25	-	2/5/27/28	0/3/3/3
24	4SU	AX	8	24	-	3/7/25/26	0/2/2/2
1	2MG	AA	1516	1	-	0/5/27/28	0/3/3/3
24	7MG	AX	46	24	-	6/7/34/38	0/3/3/3
25	PSU	BA	2580	25	-	0/7/25/26	0/2/2/2
24	H2U	AX	16	24	-	4/7/38/39	0/2/2/2
25	5MU	BA	1939	25	-	0/7/25/26	0/2/2/2
12	D2T	AL	89	12	-	1/7/12/14	-
24	3AU	AX	47	24	-	2/7/25/35	0/2/2/2
24	5MU	AX	54	24	-	0/7/25/26	0/2/2/2
23	H2U	AW	20	23	-	1/7/38/39	0/2/2/2
1	UR3	AA	1498	1	-	0/7/25/26	0/2/2/2
23	5MU	AW	54	23	-	0/7/25/26	0/2/2/2
24	MIA	AX	37	24	-	4/9/31/34	0/3/3/3
25	2MG	BA	2445	25	-	2/5/27/28	0/3/3/3
25	PSU	BA	2457	25	-	0/7/25/26	0/2/2/2
1	2MG	AA	1207	1	-	0/5/27/28	0/3/3/3

The worst 5 of 259 bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1915	3TD	C6-C5	11.77	1.49	1.35
23	AW	20	H2U	C2-N1	9.77	1.49	1.35
24	AX	20	H2U	C2-N1	9.66	1.49	1.35
25	BA	1915	3TD	C2-N1	9.63	1.49	1.37
24	AX	37	MIA	C13-C14	9.61	1.60	1.32

The worst 5 of 204 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1518	MA6	N1-C6-N6	-17.41	98.73	117.06
1	AA	1519	MA6	N1-C6-N6	-16.80	99.38	117.06
24	AX	37	MIA	C12-C13-C14	-8.98	109.67	127.14
25	BA	2449	H2U	C4-N3-C2	-8.53	118.71	125.79
23	AW	8	4SU	C4-N3-C2	-8.33	119.25	127.34

There are no chirality outliers.

5 of 71 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AA	1518	MA6	O4'-C4'-C5'-O5'
1	AA	1519	MA6	O4'-C4'-C5'-O5'
12	AL	89	D2T	CG-CB-SB-CB1
24	AX	8	4SU	C3'-C4'-C5'-O5'
24	AX	8	4SU	O4'-C4'-C5'-O5'

There are no ring outliers.

26 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	BA	2030	6MZ	2	0
25	BA	2552	OMU	2	0
25	BA	2069	G7M	1	0
28	BD	150	MEQ	3	0
25	BA	1618	6MZ	1	0
25	BA	1917	PSU	1	0
1	AA	1407	5MC	1	0
24	AX	20	H2U	2	0
25	BA	2251	OMG	1	0
25	BA	2605	PSU	1	0
36	BN	81	4D4	1	0
25	BA	2503	2MA	2	0
1	AA	1402	4OC	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	AA	1518	MA6	1	0
23	AW	32	OMC	1	0
25	BA	745	1MG	1	0
1	AA	1519	MA6	1	0
1	AA	1516	2MG	1	0
24	AX	46	7MG	2	0
24	AX	16	H2U	1	0
12	AL	89	D2T	2	0
24	AX	47	3AU	1	0
23	AW	20	H2U	2	0
1	AA	1498	UR3	1	0
23	AW	54	5MU	2	0
1	AA	1207	2MG	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 445 ligands modelled in this entry, 444 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	$\# Z  > 2$
63	PHE	AX	102	24	10,11,12	0.53	0	10,13,15	0.28	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
63	PHE	AX	102	24	-	4/5/6/8	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	AX	102	PHE	N-CA-CB-CG
63	AX	102	PHE	CA-CB-CG-CD1
63	AX	102	PHE	CA-CB-CG-CD2
63	AX	102	PHE	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	AX	102	PHE	1	0

## 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
59	CD	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CD	1357:ILE	C	1358:PRO	N	1.15