



## wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 03:13 PM BST

PDB ID : 4V7B  
EMDB ID: : EMD-5775  
Title : Visualization of two tRNAs trapped in transit during EF-G-mediated translocation  
Authors : Ramrath, D.J.F.; Lancaster, L.; Sprink, T.; Mielke, T.; Loerke, J.; Noller, H.F.; Spahn, C.M.T.  
Deposited on : 2013-10-27  
Resolution : 6.80 Å(reported)  
Based on PDB ID : 4KIY

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.  
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>

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MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk27241

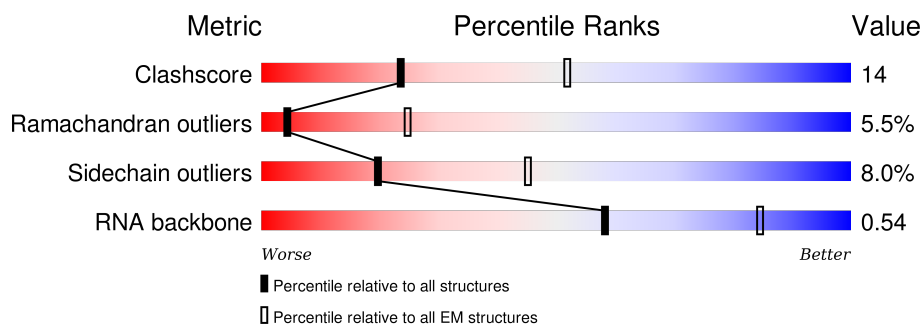
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 6.80 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	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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

Mol	Chain	Length	Quality of chain
1	AA	1542	58% 31% 8% ..
2	AB	241	54% 32% 5% 10%
3	AC	233	63% 22% .. 12%
4	AD	206	63% 31% 6%
5	AE	167	50% 36% .. 10%
6	AF	135	53% 16% .. 24%
7	AG	179	61% 21% . 16%
8	AH	130	71% 23% 5% .
















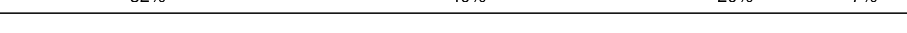









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Mol	Chain	Length	Quality of chain
9	AI	130	
10	AJ	103	
11	AK	129	
12	AL	124	
13	AM	118	
14	AN	101	
15	AO	89	
16	AP	82	
17	AQ	84	
18	AR	75	
19	AS	92	
20	AT	87	
21	AU	71	
22	AV	77	
23	AW	77	
24	AX	19	
25	AY	704	
26	BB	120	
27	BC	273	
28	BA	2904	
29	BD	209	
30	BE	201	
31	BF	179	
32	BG	177	
33	BH	50	

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Mol	Chain	Length	Quality of chain
34	BI	142	
35	BJ	142	
36	BK	123	
37	BL	144	
38	BM	136	
39	BN	127	
40	BO	117	
41	BP	115	
42	BQ	118	
43	BR	103	
44	BS	110	
45	BT	100	
46	BU	104	
47	BV	94	
48	BW	85	
49	BX	78	
50	BY	63	
51	BZ	59	
52	B0	57	
53	B1	55	
54	B2	46	
55	B3	65	
56	B4	38	
57	B5	165	
58	B6	121	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
59	FUA	AY	801	-	-	X	-
60	GDP	AY	802	-	-	X	-

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 150958 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
			32895	14671	6036	10655	1533		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- 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	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	102	Total	C	N	O	S	0	0
			832	525	150	150	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	98	Total	C	N	O	S	0	0
			786	493	150	142	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
			955	590	196	165	4		

- 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	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- 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	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 22 is a RNA chain called modified formyl-methionine specific initiator transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 23 is a RNA chain called formyl-methionine specific initiator transfer RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0
			1635	732	291	536	76		

- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AX	19	Total	C	N	O	P	0	0
			416	187	86	124	19		

- Molecule 25 is a protein called Elongation Factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	AY	671	Total	C	N	O	S	0	0
			5194	3278	895	998	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BB	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

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

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

- Molecule 28 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BA	2854	Total	C	N	O	P	0	0
			61274	27334	11279	19807	2854		

- Molecule 29 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BD	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

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

- Molecule 33 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	50	Total	C	N	O	S	0	0
			384	247	68	68	1		

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BI	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BM	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	BO	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

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

- Molecule 43 is a protein called 50S ribosomal protein L21.

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

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L25.

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

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	BW	79	Total	C	N	O	S	0	0
			596	367	120	108	1		

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	BY	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	B1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	B2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	B3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	B4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

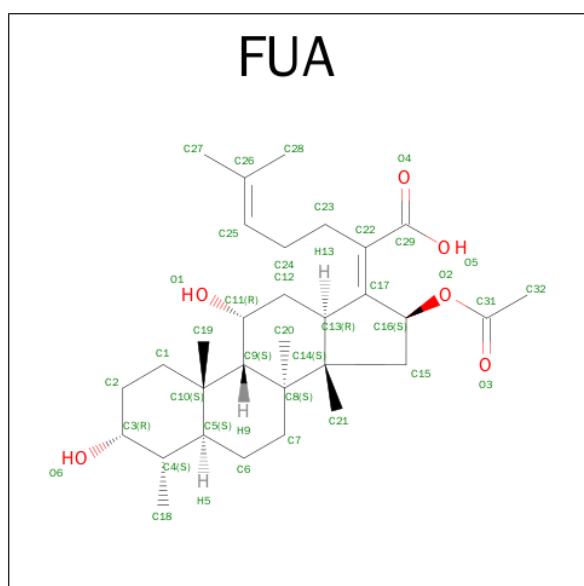
- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	B5	148	Total	C	N	O	S	0	0
			1117	705	196	209	7		

- Molecule 58 is a protein called 50S ribosomal protein L7/L12.

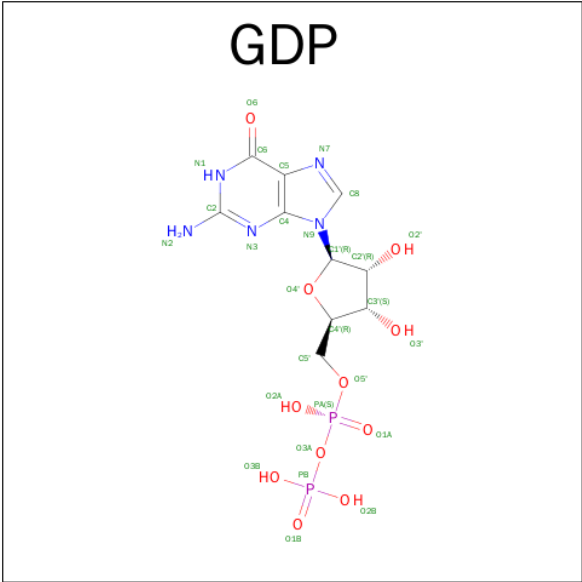
Mol	Chain	Residues	Atoms					AltConf	Trace
58	B6	30	Total	C	N	O	S	0	0
			227	144	33	47	3		

- Molecule 59 is FUSIDIC ACID (three-letter code: FUA) (formula:  $C_{31}H_{48}O_6$ ).



Mol	Chain	Residues	Atoms			AltConf
59	AY	1	Total	C	O	0
			37	31	6	

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).

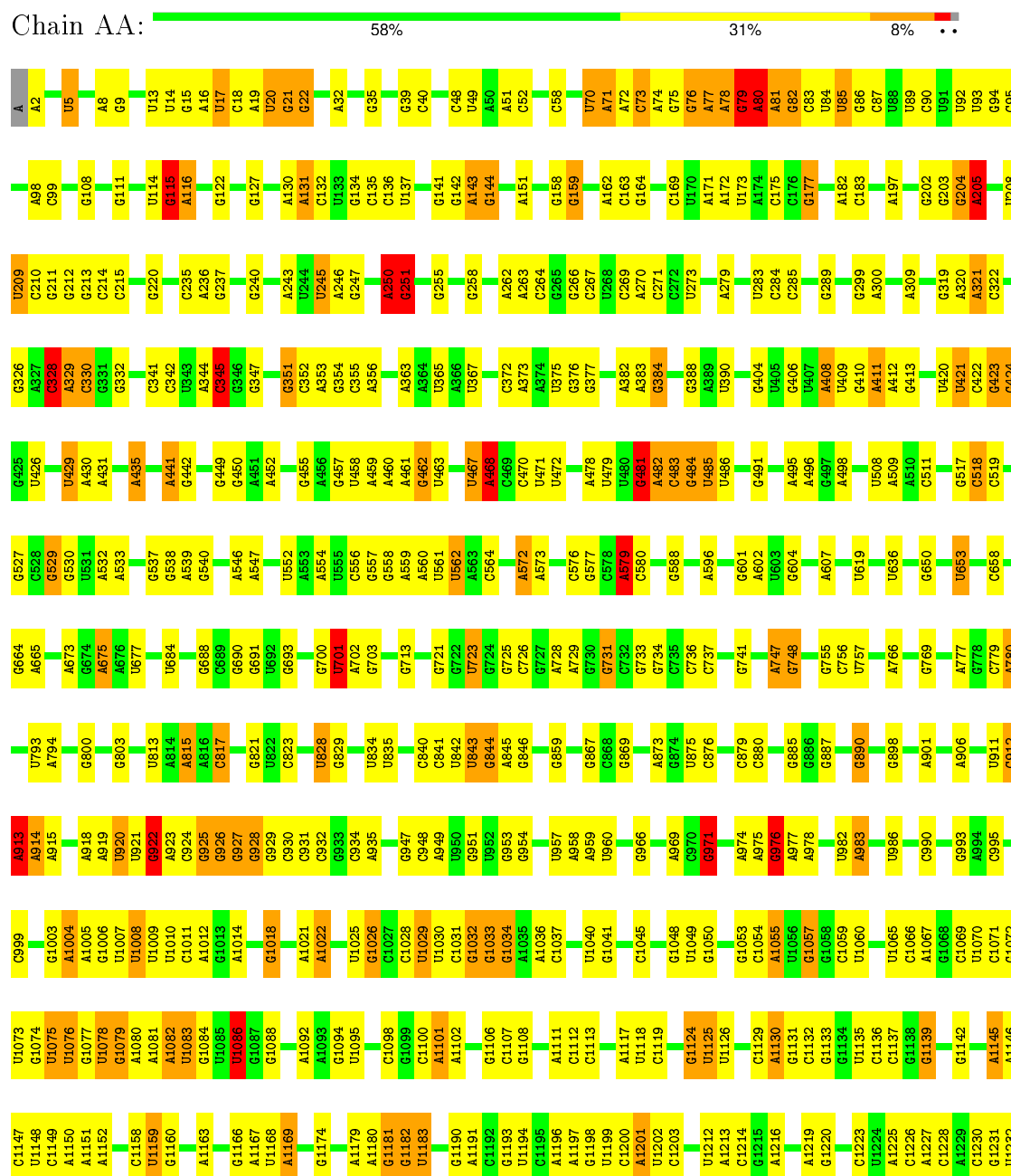


Mol	Chain	Residues	Atoms					AltConf
60	AY	1	Total	C	N	O	P	0
			28	10	5	11	2	

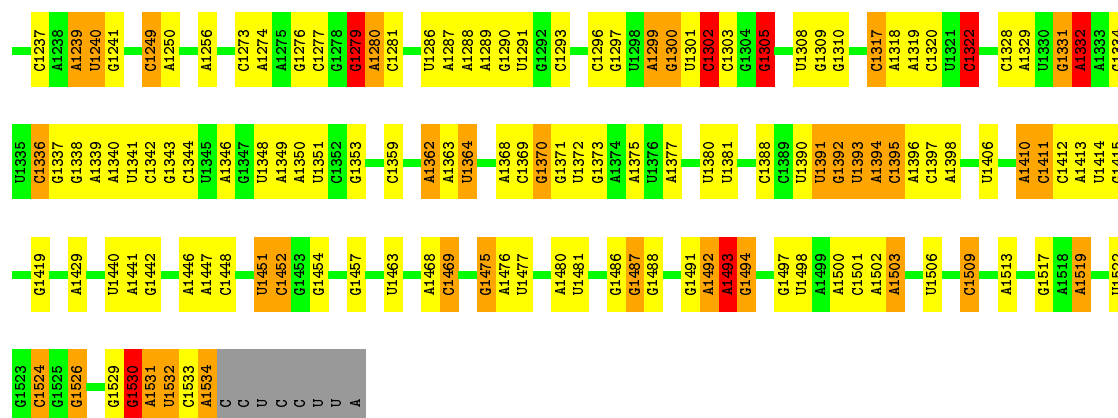
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

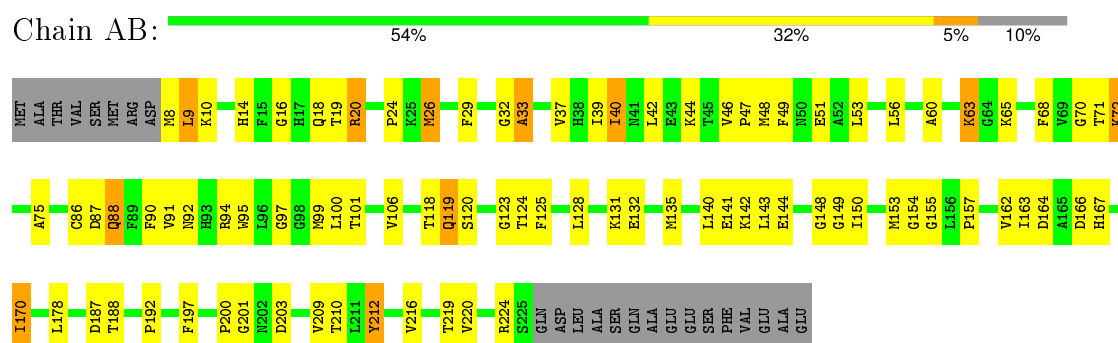
#### • Molecule 1: 16S ribosomal RNA



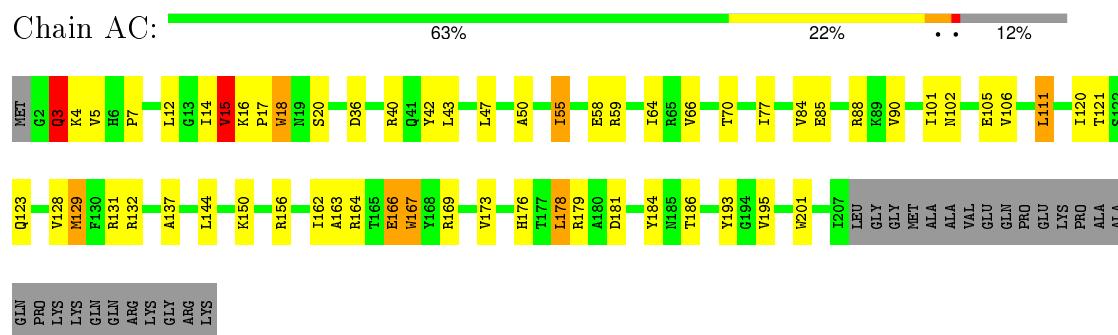




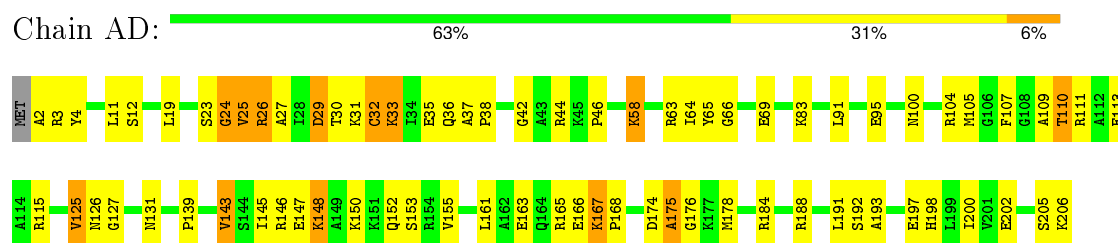
• Molecule 2: 30S ribosomal protein S2



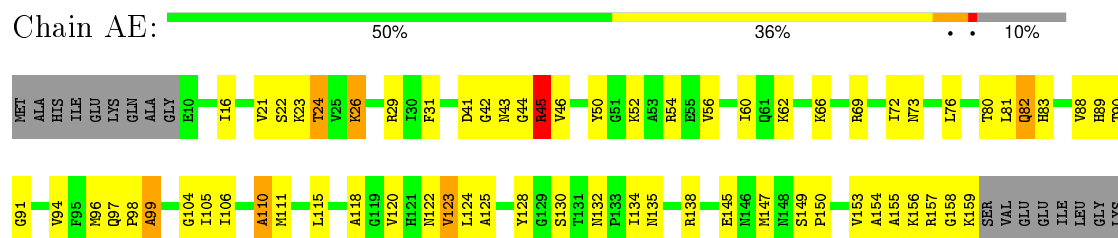
• Molecule 3: 30S ribosomal protein S3



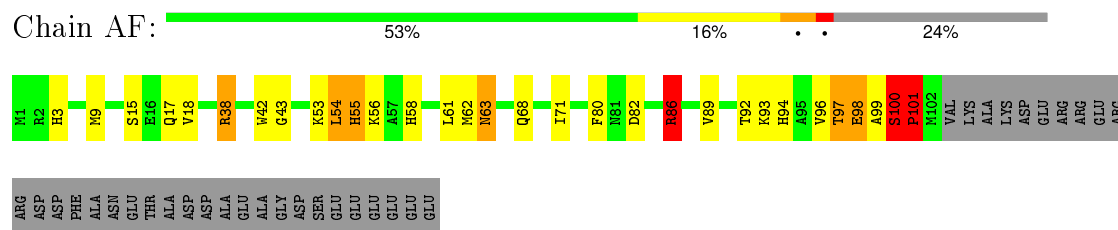
• Molecule 4: 30S ribosomal protein S4



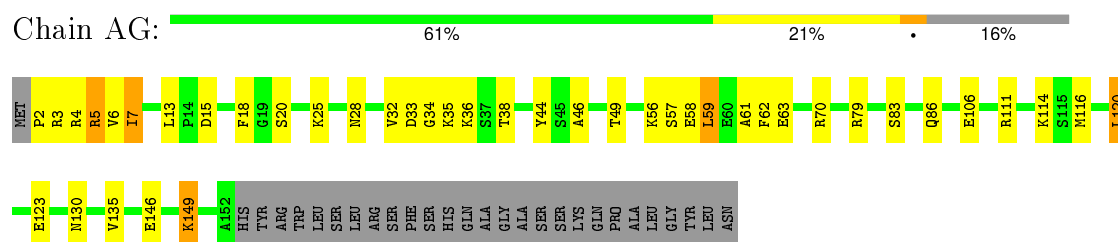
• Molecule 5: 30S ribosomal protein S5



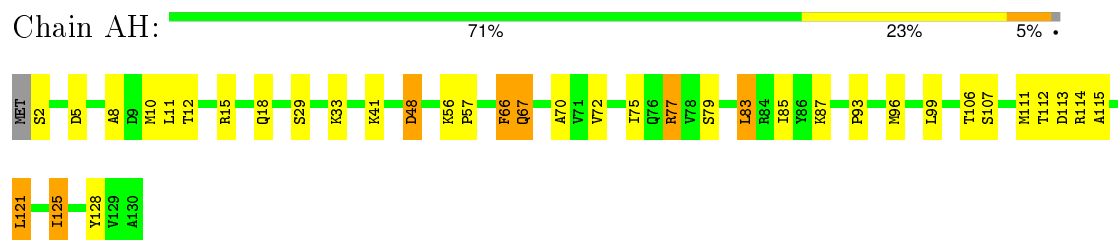
- Molecule 6: 30S ribosomal protein S6



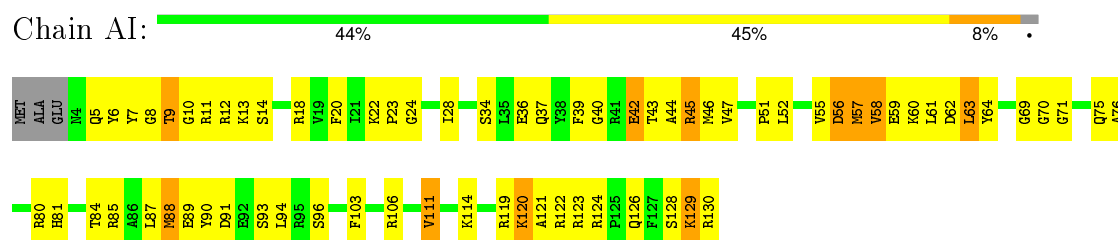
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8

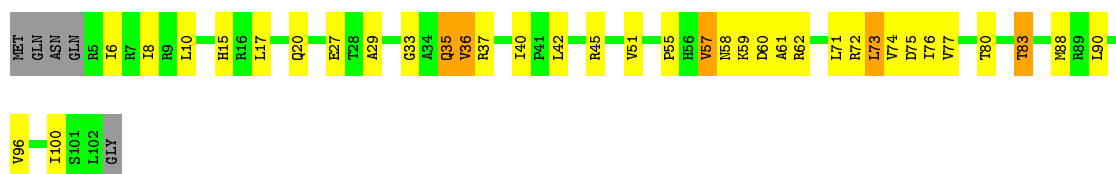


- Molecule 9: 30S ribosomal protein S9



- Molecule 10: 30S ribosomal protein S10





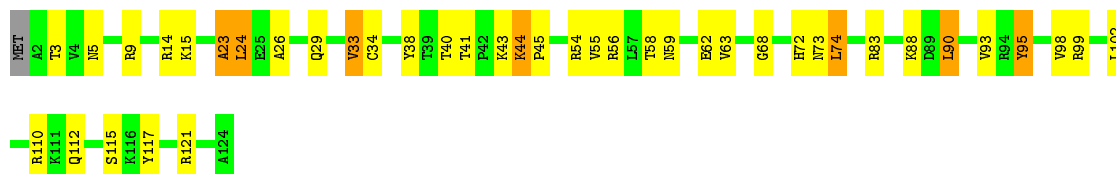
- Molecule 11: 30S ribosomal protein S11

Chain AK: 66% 21% 9%



- Molecule 12: 30S ribosomal protein S12

Chain AL: 66% 27% 6%



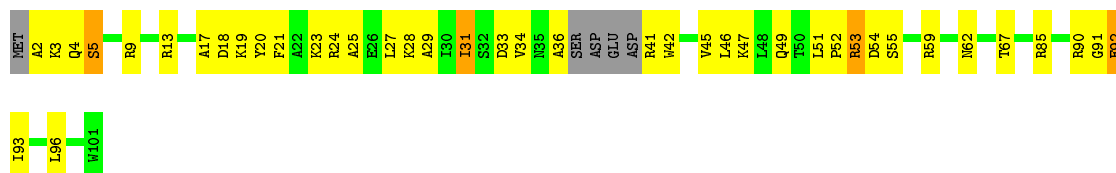
- Molecule 13: 30S ribosomal protein S13

Chain AM: 69% 21% 7%



- Molecule 14: 30S ribosomal protein S14

Chain AN: 54% 37% 5%

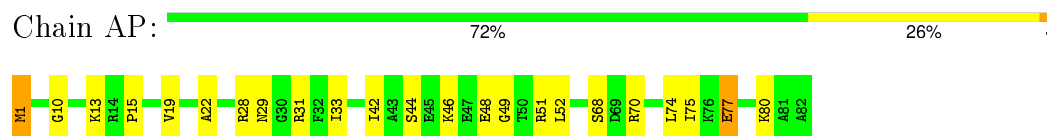


- Molecule 15: 30S ribosomal protein S15

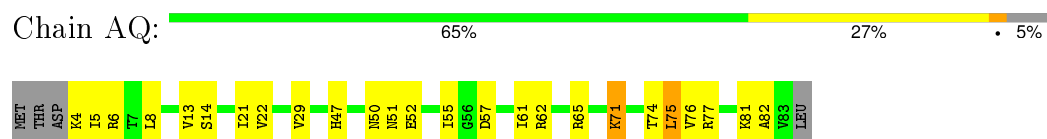
Chain AO: 78% 20% 2%



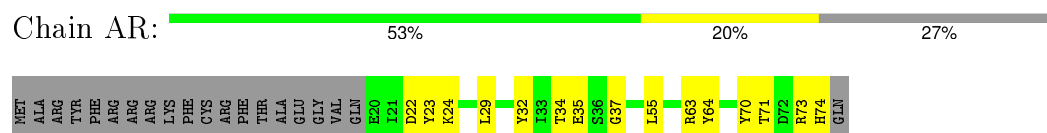
- Molecule 16: 30S ribosomal protein S16



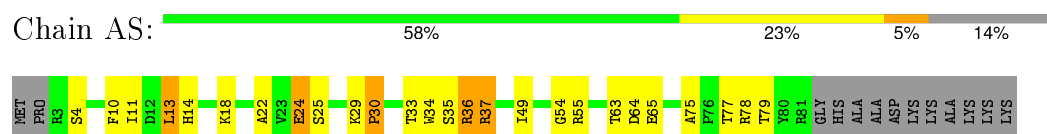
- Molecule 17: 30S ribosomal protein S17



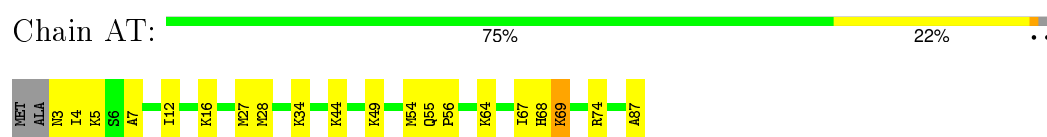
- Molecule 18: 30S ribosomal protein S18



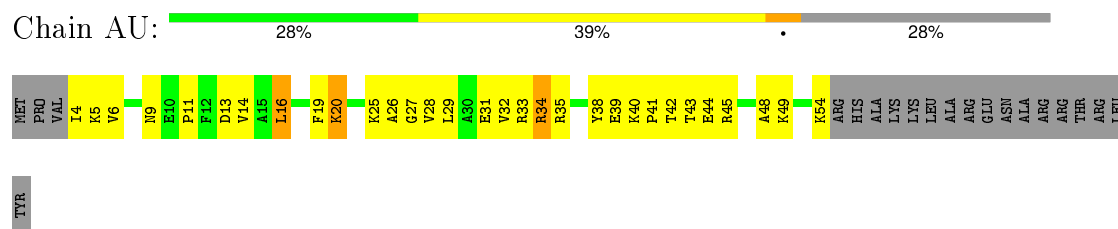
- Molecule 19: 30S ribosomal protein S19



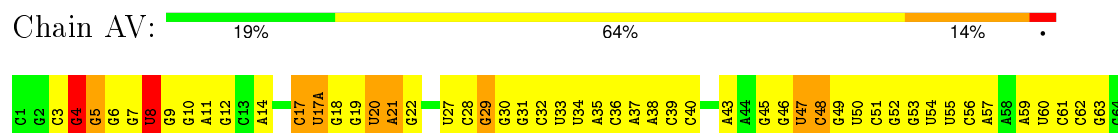
- Molecule 20: 30S ribosomal protein S20



- Molecule 21: 30S ribosomal protein S21



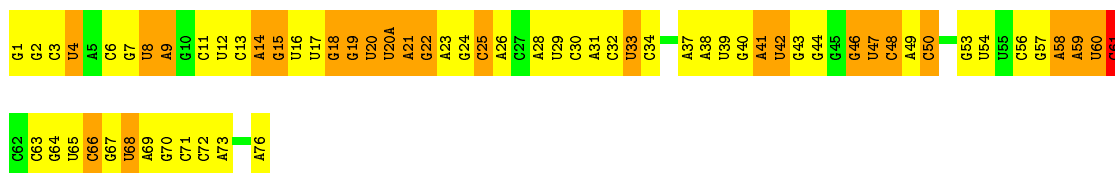
- Molecule 22: modified formyl-methionine specific initiator transfer RNA





- Molecule 23: formyl-methionine specific initiator transfer RNA

Chain AW: 16% 52% 31%



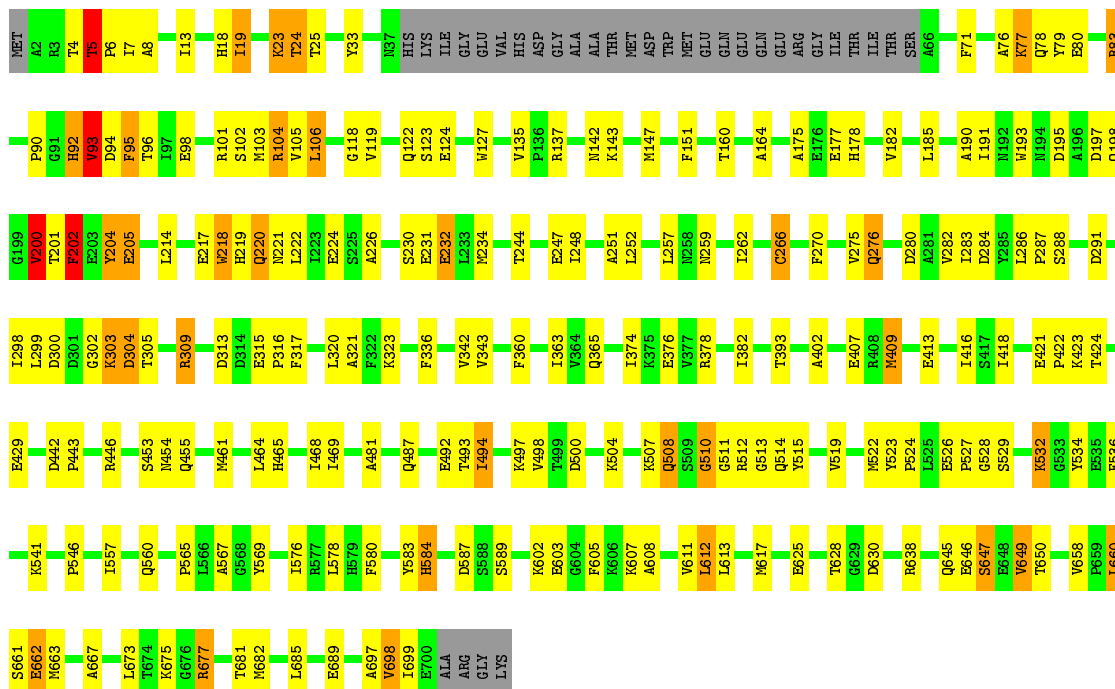
- Molecule 24: messenger RNA

Chain AX: 26% 74%



- Molecule 25: Elongation Factor G

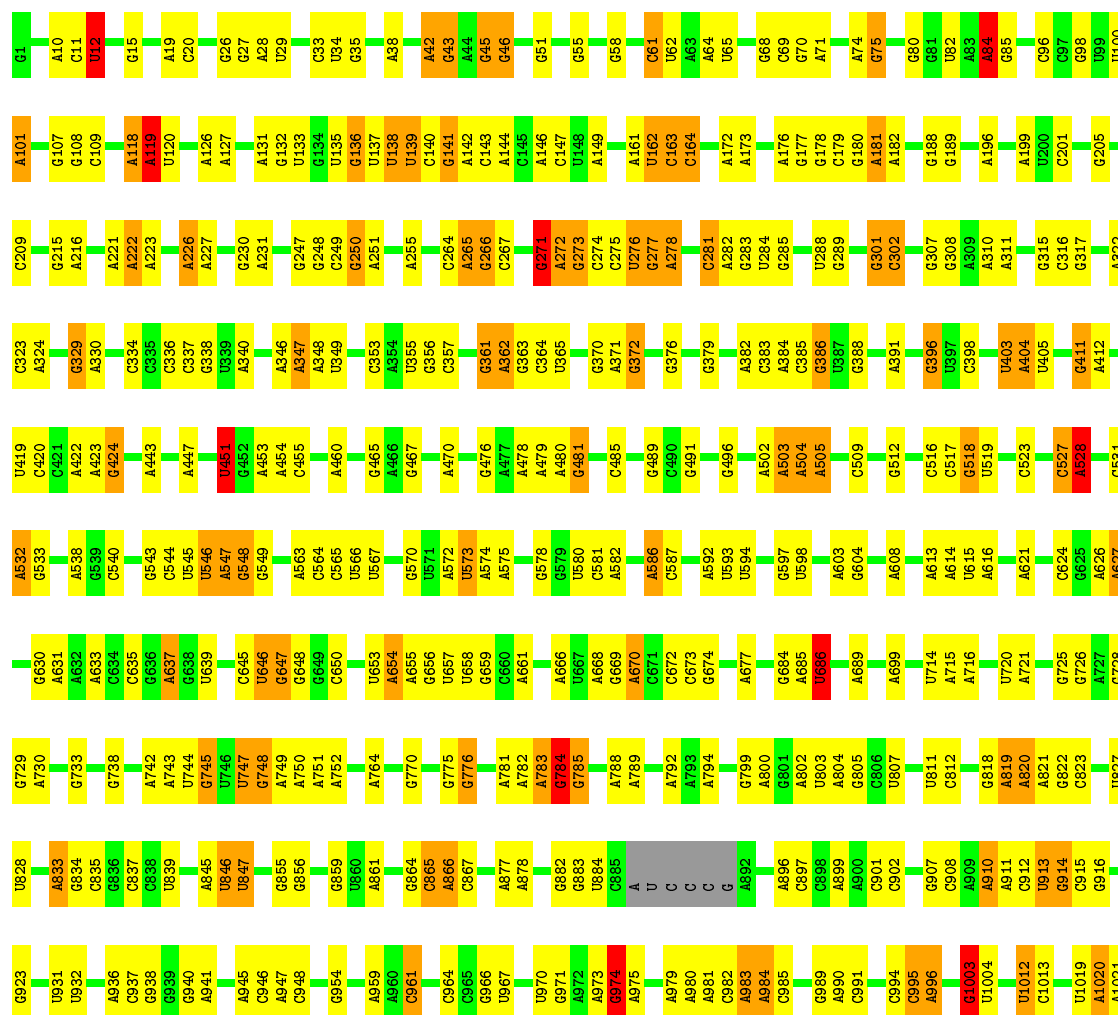
Chain AY: 64% 26% 5%



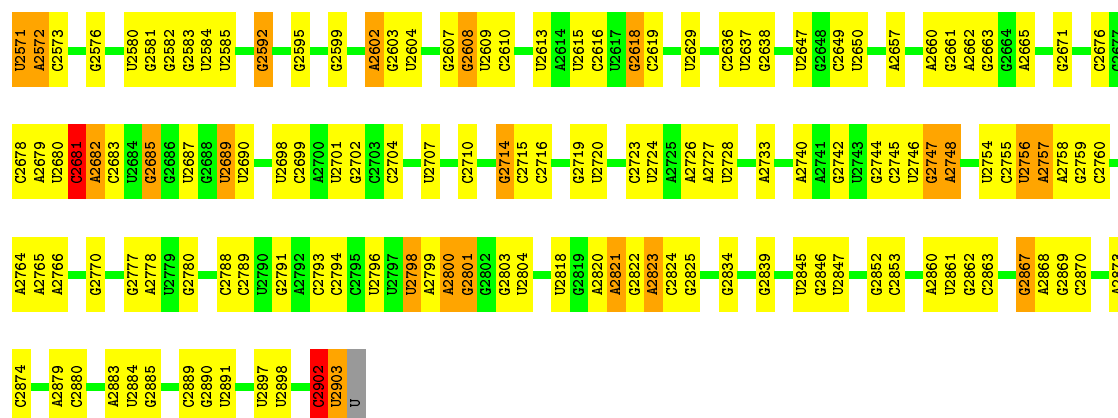
- Molecule 26: 5S ribosomal RNA

Chain BB: 66% 25% 8%



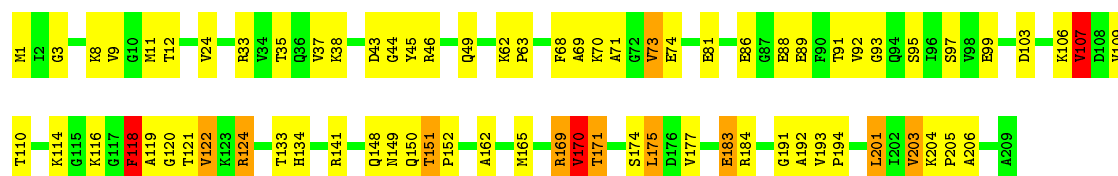


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A2469	G2373	C2283	U2182	U	A1928	A1802	U1714	A1603	G1479	G1382	G1288	A1189	G1102	U1023
G2470	G2373	A2284	A2183	G	G1929	A1803	G1715	G1603	G1482	A1383	G1289	G1190	G1106	G1024
A2476	G2383	C2285	A2184	G	G1930	A1804	G1715	G1606	G1482	A1384	C1290	G1191	G1107	G1025
U2477	U2384	A2287	U2185	G	G1935	A1805	A1722	C1607	U1485	C1385	G1298	G1193	G1110	A1027
A2478	C2385	A2288	G2289	G	A1936	G1807	G1723	A1608	U1486	A1386	G1299	A1194	A1111	G1031
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A2482	U2387	A2297	U2195	C	A1938	G1811	U1729	C1612	C1493	A1392	G1300	C1196	G1112	U1033
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	G2490	G2204												



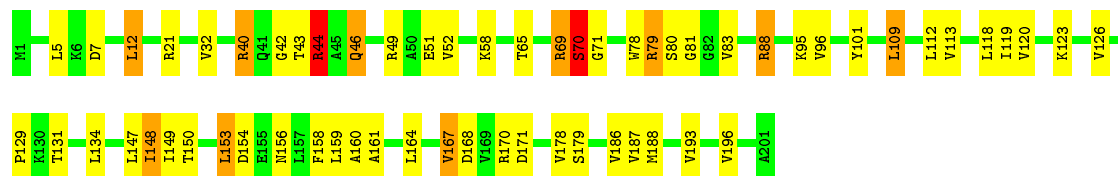
- Molecule 29: 50S ribosomal protein L3

Chain BD: 65% 29% 5% •



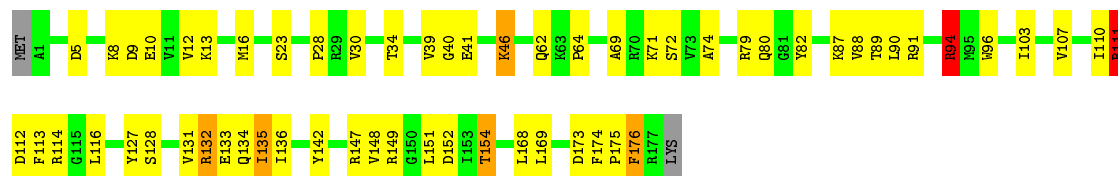
- Molecule 30: 50S ribosomal protein L4

Chain BE: 70% 24% 5% •



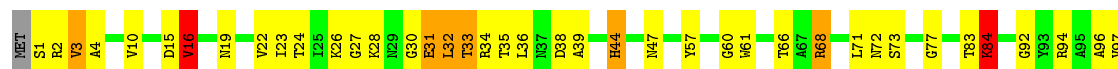
- Molecule 31: 50S ribosomal protein L5

Chain BF: 65% 30% 5% •



- Molecule 32: 50S ribosomal protein L6

Chain BG: 62% 29% 8% •

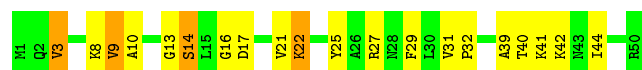






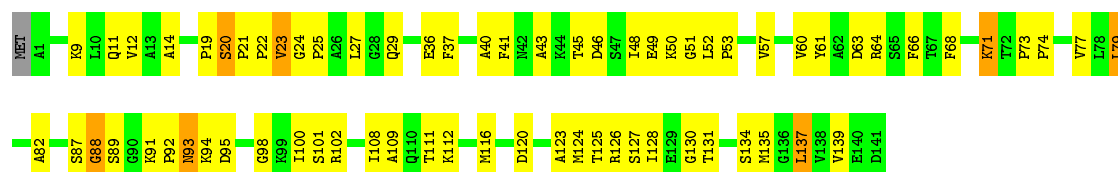
- Molecule 33: 50S ribosomal protein L9

Chain BH: 60% 32% 8%



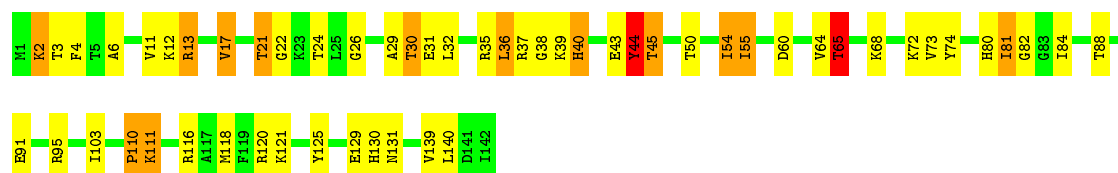
- Molecule 34: 50S ribosomal protein L11

Chain BI: 51% 44% 5%



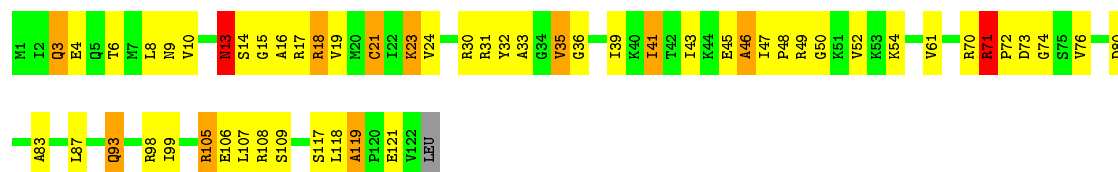
- Molecule 35: 50S ribosomal protein L13

Chain BJ: 61% 28% 9%



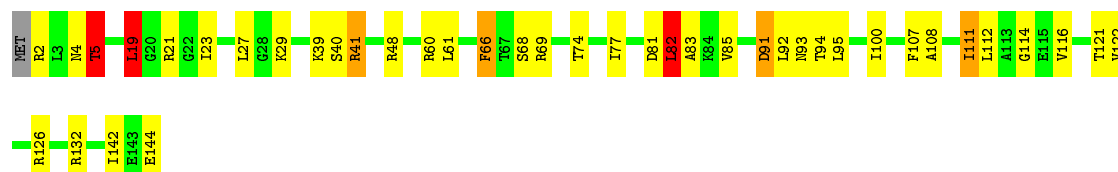
- Molecule 36: 50S ribosomal protein L14

Chain BK: 54% 35% 8%

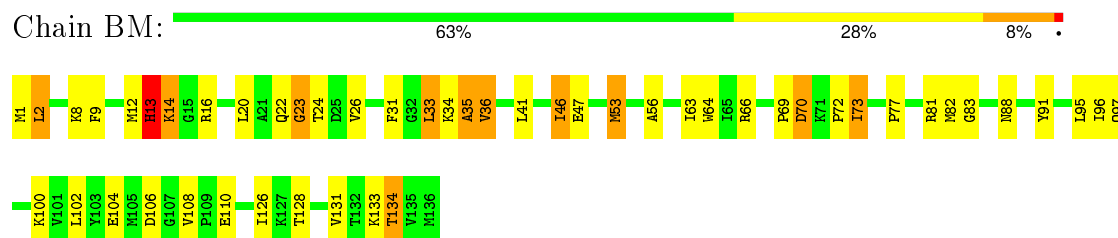


- Molecule 37: 50S ribosomal protein L15

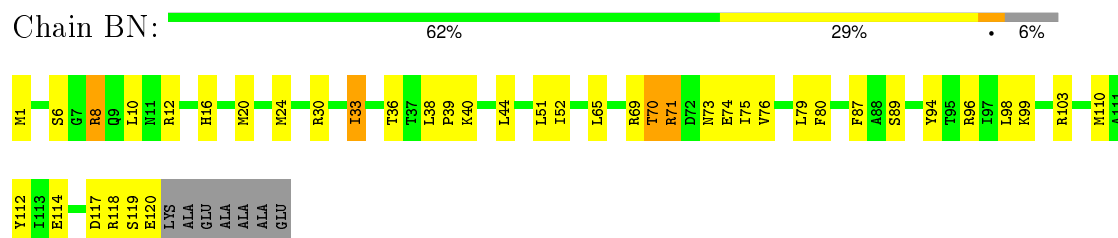
Chain BL: 71% 24% 5%



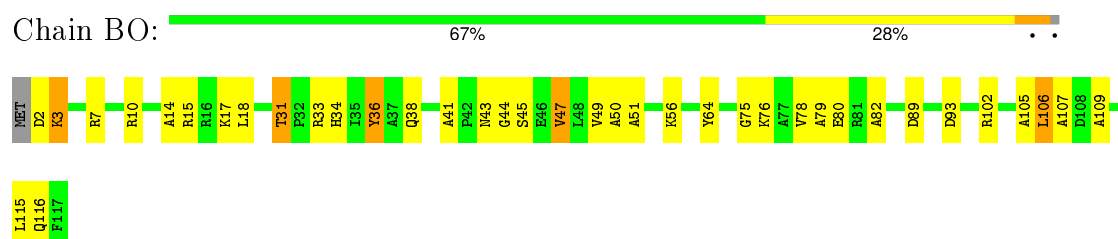
- Molecule 38: 50S ribosomal protein L16



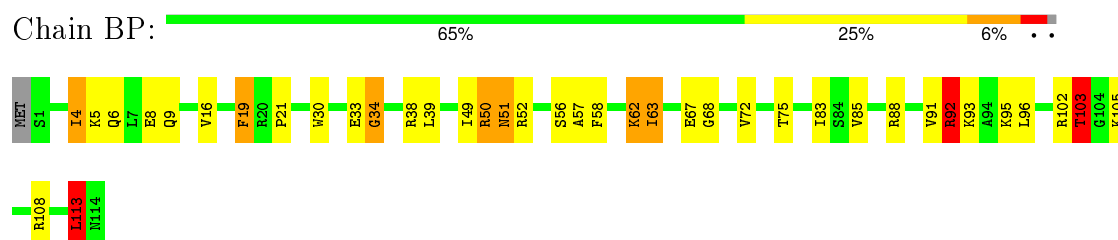
- Molecule 39: 50S ribosomal protein L17



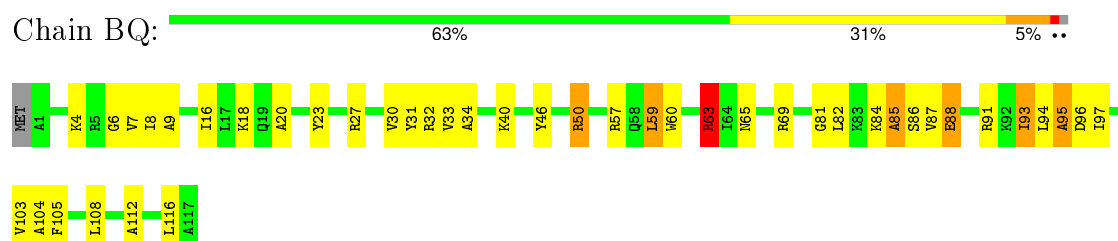
- Molecule 40: 50S ribosomal protein L18



- Molecule 41: 50S ribosomal protein L19

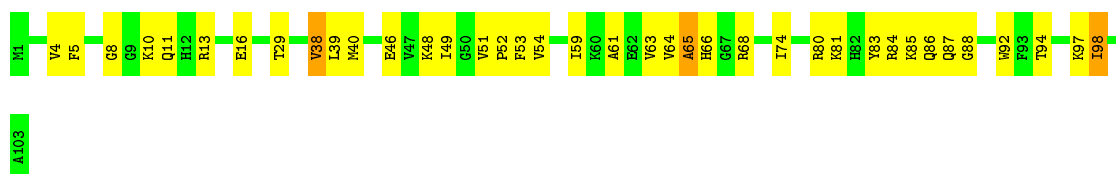


- Molecule 42: 50S ribosomal protein L20



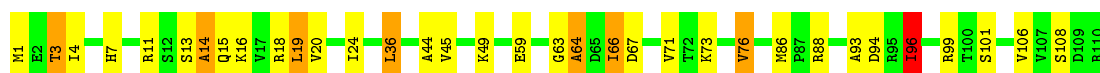
- Molecule 43: 50S ribosomal protein L21





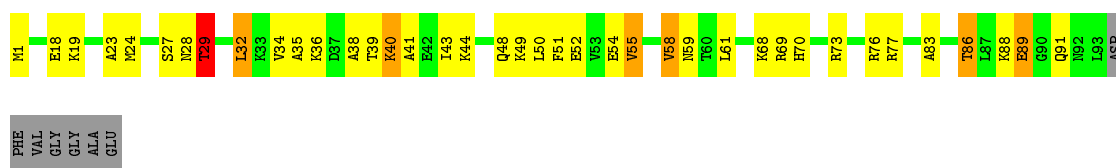
- Molecule 44: 50S ribosomal protein L22

Chain BS: 69% 24% 6% •



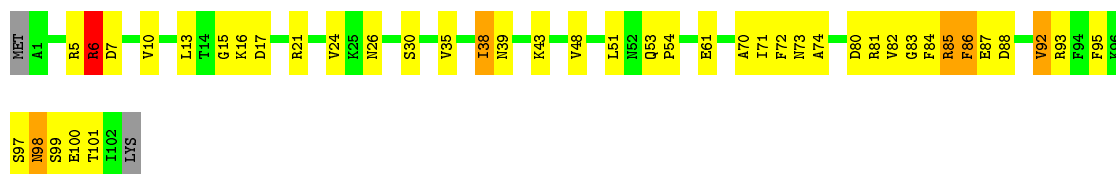
- Molecule 45: 50S ribosomal protein L23

Chain BT: 54% 32% 6% • 7%



- Molecule 46: 50S ribosomal protein L24

Chain BU: 57% 36% 5% ••



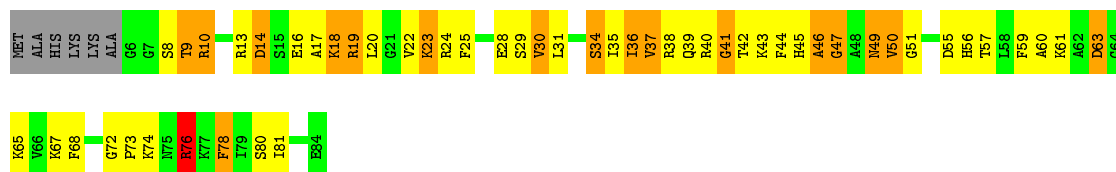
- Molecule 47: 50S ribosomal protein L25

Chain BV: 76% 22% •



- Molecule 48: 50S ribosomal protein L27

Chain BW: 32% 40% 20% • 7%



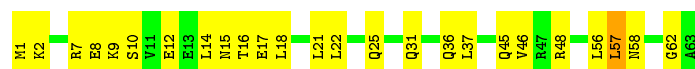
- Molecule 49: 50S ribosomal protein L28

Chain BX: 



- Molecule 50: 50S ribosomal protein L29

Chain BY: 



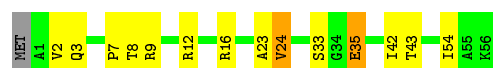
- Molecule 51: 50S ribosomal protein L30

Chain BZ: 



- Molecule 52: 50S ribosomal protein L32

Chain B0: 




- Molecule 53: 50S ribosomal protein L33

Chain B1: 




- Molecule 54: 50S ribosomal protein L34

Chain B2: 



- Molecule 55: 50S ribosomal protein L35

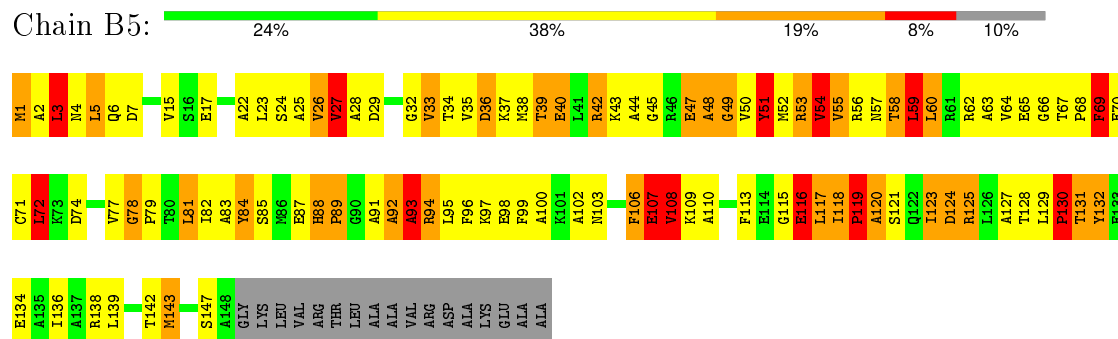
Chain B3: 



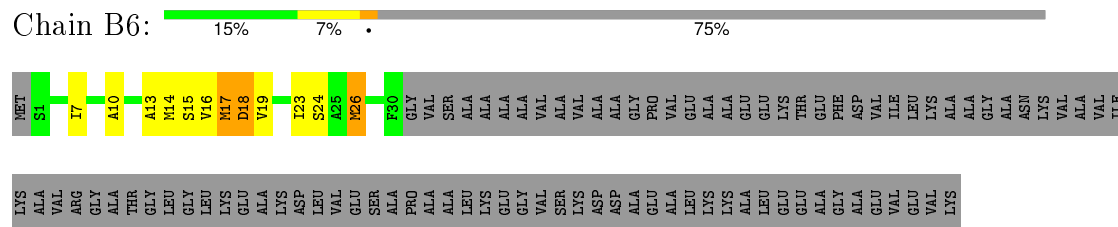
- Molecule 56: 50S ribosomal protein L36

Chain B4: 

- Molecule 57: 50S ribosomal protein L10



- Molecule 58: 50S ribosomal protein L7/L12



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	279309	Depositor
Resolution determination method	FSC at 0.5 cut-off	Depositor
CTF correction method	The volumes were CTF-corrected in defocus groups with an average of approximately 906 individual images per group.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	20.00	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163 FILM	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, 5MU, FUA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	AA	0.65	4/36834 (0.0%)	1.13	100/57462 (0.2%)
10	AJ	0.54	0/796	0.80	0/1077
11	AK	0.50	0/893	0.74	0/1205
12	AL	0.54	0/969	0.82	0/1300
13	AM	0.48	0/892	0.70	0/1193
14	AN	0.48	0/785	0.78	0/1043
15	AO	0.44	0/722	0.66	0/964
16	AP	0.48	0/659	0.74	0/884
17	AQ	0.46	0/657	0.73	0/881
18	AR	0.45	0/462	0.62	0/621
19	AS	0.47	0/652	0.81	0/877
2	AB	0.49	0/1735	0.72	0/2338
20	AT	0.47	0/671	0.61	0/888
21	AU	0.66	0/430	0.84	0/570
22	AV	0.57	0/1810	0.74	0/2821
23	AW	0.43	0/1827	1.14	6/2845 (0.2%)
24	AX	0.30	0/469	0.70	0/730
25	AY	0.46	0/5291	0.67	2/7160 (0.0%)
26	BB	0.66	0/2828	1.10	2/4410 (0.0%)
27	BC	0.54	0/2121	0.79	2/2852 (0.1%)
28	BA	0.81	17/68626 (0.0%)	1.22	303/107056 (0.3%)
29	BD	0.57	0/1586	0.77	1/2134 (0.0%)
3	AC	0.45	0/1651	0.69	0/2225
30	BE	0.53	0/1571	0.76	2/2113 (0.1%)
31	BF	0.49	0/1434	0.71	1/1926 (0.1%)
32	BG	0.55	0/1343	0.73	0/1816
33	BH	0.53	0/389	0.73	0/523
34	BI	0.62	0/1046	0.84	1/1410 (0.1%)
35	BJ	0.63	1/1152 (0.1%)	0.78	0/1551
36	BK	0.65	1/947 (0.1%)	0.77	0/1268
37	BL	0.56	0/1054	0.79	2/1403 (0.1%)
38	BM	0.61	0/1093	0.77	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
39	BN	0.51	0/973	0.68	0/1301
4	AD	0.53	0/1665	0.79	0/2227
40	BO	0.46	0/902	0.70	0/1209
41	BP	0.52	0/929	0.78	1/1242 (0.1%)
42	BQ	0.62	0/960	0.71	1/1278 (0.1%)
43	BR	0.61	1/829 (0.1%)	0.76	0/1107
44	BS	0.54	0/864	0.73	0/1156
45	BT	0.55	0/744	0.85	1/994 (0.1%)
46	BU	0.56	0/787	0.78	0/1051
47	BV	0.48	0/766	0.67	1/1025 (0.1%)
48	BW	0.69	0/603	1.00	1/797 (0.1%)
49	BX	0.50	0/635	0.79	1/848 (0.1%)
5	AE	0.49	0/1118	0.76	0/1504
50	BY	0.46	0/510	0.75	0/677
51	BZ	0.54	0/453	0.84	1/605 (0.2%)
52	B0	0.54	0/450	0.69	0/599
53	B1	0.53	0/416	0.74	0/554
54	B2	0.53	0/380	0.70	0/498
55	B3	0.53	0/513	0.75	0/676
56	B4	0.58	0/303	0.84	0/397
57	B5	0.74	0/1131	1.32	26/1524 (1.7%)
58	B6	0.59	0/227	0.65	0/304
6	AF	0.50	0/851	0.70	0/1150
7	AG	0.49	0/1195	0.67	0/1602
8	AH	0.48	0/989	0.65	0/1326
9	AI	0.54	0/1034	0.81	0/1375
All	All	0.69	24/163622 (0.0%)	1.08	455/244032 (0.2%)

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
12	AL	0	1
22	AV	0	3
25	AY	0	1
27	BC	0	1
29	BD	0	1
35	BJ	0	1
36	BK	0	1
57	B5	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	AF	0	1
All	All	0	11

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AA	922	G	O3'-P	9.48	1.72	1.61
28	BA	984	A	N9-C4	-8.58	1.32	1.37
1	AA	1362	A	N7-C5	7.93	1.44	1.39
28	BA	528	A	N9-C4	-6.68	1.33	1.37
28	BA	1142	A	N9-C4	-6.58	1.33	1.37

The worst 5 of 455 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	BA	1073	A	N1-C6-N6	-20.01	106.59	118.60
28	BA	1073	A	C5-C6-N6	14.04	134.94	123.70
28	BA	2053	G	N1-C6-O6	13.92	128.25	119.90
1	AA	922	G	P-O3'-C3'	13.08	135.40	119.70
28	BA	2504	U	N3-C4-O4	13.06	128.54	119.40

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	AF	101	PRO	Peptide
12	AL	23	ALA	Peptide
22	AV	29	G	Sidechain
22	AV	4	G	Sidechain
22	AV	8	U	Sidechain

## 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	32895	0	16542	956	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	AB	1704	0	1732	90	0
3	AC	1624	0	1696	41	0
4	AD	1643	0	1707	68	0
5	AE	1105	0	1147	147	0
6	AF	832	0	824	26	0
7	AG	1181	0	1236	53	0
8	AH	979	0	1031	28	0
9	AI	1022	0	1067	121	0
10	AJ	786	0	828	23	0
11	AK	877	0	887	32	0
12	AL	955	0	1016	36	0
13	AM	883	0	941	31	0
14	AN	774	0	824	35	0
15	AO	714	0	733	11	0
16	AP	649	0	666	14	0
17	AQ	648	0	691	11	0
18	AR	455	0	478	10	0
19	AS	637	0	665	39	0
20	AT	665	0	714	11	0
21	AU	425	0	449	43	0
22	AV	1640	0	832	136	0
23	AW	1635	0	829	97	0
24	AX	416	0	207	169	0
25	AY	5194	0	5170	222	0
26	BB	2529	0	1281	21	0
27	BC	2082	0	2157	50	0
28	BA	61274	0	30812	852	0
29	BD	1565	0	1616	52	0
30	BE	1552	0	1619	37	0
31	BF	1410	0	1442	59	0
32	BG	1323	0	1374	45	0
33	BH	384	0	405	35	0
34	BI	1032	0	1088	57	0
35	BJ	1129	0	1162	52	0
36	BK	938	0	1012	40	0
37	BL	1045	0	1117	34	0
38	BM	1074	0	1156	48	0
39	BN	960	0	1000	30	0
40	BO	892	0	923	22	0
41	BP	917	0	965	51	0
42	BQ	947	0	1022	50	0
43	BR	816	0	839	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BS	857	0	922	28	0
45	BT	738	0	807	35	0
46	BU	779	0	834	29	0
47	BV	753	0	780	14	0
48	BW	596	0	610	82	0
49	BX	625	0	655	16	0
50	BY	509	0	543	12	0
51	BZ	449	0	491	17	0
52	B0	444	0	461	17	0
53	B1	409	0	440	16	0
54	B2	377	0	418	5	0
55	B3	504	0	574	10	0
56	B4	302	0	340	15	0
57	B5	1117	0	1155	120	0
58	B6	227	0	237	7	0
59	AY	37	0	44	59	0
60	AY	28	0	12	26	0
All	All	150958	0	103225	3593	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 3593 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)
25:AY:92:HIS:CE1	59:AY:801:FUA:H283	1.23	1.69
1:AA:1498:U:C5	24:AX:12:U:H5''	1.26	1.64
1:AA:1498:U:C4	24:AX:12:U:H5''	1.32	1.61
24:AX:14:A:H2'	24:AX:15:A:C5'	1.24	1.58
24:AX:14:A:C2'	24:AX:15:A:H5''	1.16	1.57

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	216/241 (90%)	151 (70%)	51 (24%)	14 (6%)	1	25
3	AC	204/233 (88%)	181 (89%)	18 (9%)	5 (2%)	7	46
4	AD	203/206 (98%)	162 (80%)	30 (15%)	11 (5%)	2	29
5	AE	148/167 (89%)	123 (83%)	18 (12%)	7 (5%)	3	32
6	AF	100/135 (74%)	79 (79%)	15 (15%)	6 (6%)	2	26
7	AG	149/179 (83%)	128 (86%)	20 (13%)	1 (1%)	26	71
8	AH	127/130 (98%)	114 (90%)	12 (9%)	1 (1%)	24	69
9	AI	125/130 (96%)	104 (83%)	15 (12%)	6 (5%)	3	32
10	AJ	96/103 (93%)	69 (72%)	20 (21%)	7 (7%)	1	21
11	AK	115/129 (89%)	97 (84%)	12 (10%)	6 (5%)	2	30
12	AL	121/124 (98%)	101 (84%)	16 (13%)	4 (3%)	5	40
13	AM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	2	29
14	AN	92/101 (91%)	73 (79%)	13 (14%)	6 (6%)	1	25
15	AO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	8	48
16	AP	80/82 (98%)	60 (75%)	17 (21%)	3 (4%)	4	37
17	AQ	78/84 (93%)	59 (76%)	15 (19%)	4 (5%)	2	30
18	AR	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
19	AS	77/92 (84%)	65 (84%)	11 (14%)	1 (1%)	15	60
20	AT	83/87 (95%)	74 (89%)	7 (8%)	2 (2%)	7	47
21	AU	49/71 (69%)	26 (53%)	20 (41%)	3 (6%)	2	26
25	AY	667/704 (95%)	541 (81%)	92 (14%)	34 (5%)	2	30
27	BC	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	28
29	BD	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	23
30	BE	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	3	31
31	BF	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	8	48
32	BG	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	1	14
33	BH	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	1	12
34	BI	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	25
35	BJ	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	2	25
36	BK	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	1	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	BL	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	4	39
38	BM	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	18
39	BN	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	24	69
40	BO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	21	67
41	BP	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	19
42	BQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	39
43	BR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	42
44	BS	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	3	32
45	BT	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	11
46	BU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	1	14
47	BV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
48	BW	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	3
49	BX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	4	35
50	BY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	24
51	BZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	38
52	B0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	21
53	B1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	2	25
54	B2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
55	B3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	41
56	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	18
57	B5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	3
58	B6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	4	38
All	All	6365/6876 (93%)	5040 (79%)	977 (15%)	348 (6%)	4	29

5 of 348 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	33	ALA
2	AB	40	ILE
2	AB	119	GLN
3	AC	101	ILE
4	AD	24	GLY

### 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	180/199 (90%)	170 (94%)	10 (6%)	26	62
3	AC	170/190 (90%)	156 (92%)	14 (8%)	14	49
4	AD	172/173 (99%)	165 (96%)	7 (4%)	37	71
5	AE	113/126 (90%)	108 (96%)	5 (4%)	35	69
6	AF	89/116 (77%)	82 (92%)	7 (8%)	15	51
7	AG	124/147 (84%)	115 (93%)	9 (7%)	17	54
8	AH	104/105 (99%)	96 (92%)	8 (8%)	16	52
9	AI	105/107 (98%)	96 (91%)	9 (9%)	13	47
10	AJ	86/90 (96%)	83 (96%)	3 (4%)	43	74
11	AK	90/99 (91%)	85 (94%)	5 (6%)	26	62
12	AL	103/104 (99%)	96 (93%)	7 (7%)	20	57
13	AM	92/96 (96%)	88 (96%)	4 (4%)	35	70
14	AN	79/84 (94%)	75 (95%)	4 (5%)	29	66
15	AO	76/77 (99%)	72 (95%)	4 (5%)	28	64
16	AP	65/65 (100%)	61 (94%)	4 (6%)	23	60
17	AQ	74/78 (95%)	66 (89%)	8 (11%)	8	35
18	AR	48/65 (74%)	47 (98%)	1 (2%)	61	84
19	AS	70/79 (89%)	64 (91%)	6 (9%)	13	47
20	AT	65/66 (98%)	60 (92%)	5 (8%)	16	52
21	AU	44/61 (72%)	36 (82%)	8 (18%)	2	15
25	AY	552/578 (96%)	505 (92%)	47 (8%)	13	48
27	BC	216/218 (99%)	202 (94%)	14 (6%)	21	58
29	BD	164/164 (100%)	151 (92%)	13 (8%)	15	51
30	BE	165/165 (100%)	146 (88%)	19 (12%)	7	32
31	BF	148/150 (99%)	138 (93%)	10 (7%)	20	57
32	BG	137/138 (99%)	122 (89%)	15 (11%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BH	40/40 (100%)	38 (95%)	2 (5%)	30	66
34	BI	109/110 (99%)	105 (96%)	4 (4%)	41	73
35	BJ	116/116 (100%)	100 (86%)	16 (14%)	4	27
36	BK	103/104 (99%)	92 (89%)	11 (11%)	8	36
37	BL	102/103 (99%)	95 (93%)	7 (7%)	19	56
38	BM	109/109 (100%)	93 (85%)	16 (15%)	4	24
39	BN	100/103 (97%)	93 (93%)	7 (7%)	19	56
40	BO	86/87 (99%)	78 (91%)	8 (9%)	11	42
41	BP	99/100 (99%)	91 (92%)	8 (8%)	15	49
42	BQ	89/90 (99%)	81 (91%)	8 (9%)	12	44
43	BR	84/84 (100%)	78 (93%)	6 (7%)	18	55
44	BS	93/93 (100%)	84 (90%)	9 (10%)	10	40
45	BT	80/84 (95%)	77 (96%)	3 (4%)	40	73
46	BU	83/85 (98%)	76 (92%)	7 (8%)	14	48
47	BV	78/78 (100%)	75 (96%)	3 (4%)	40	73
48	BW	59/63 (94%)	53 (90%)	6 (10%)	9	37
49	BX	67/68 (98%)	61 (91%)	6 (9%)	12	44
50	BY	55/55 (100%)	52 (94%)	3 (6%)	27	63
51	BZ	48/49 (98%)	40 (83%)	8 (17%)	3	19
52	B0	47/48 (98%)	46 (98%)	1 (2%)	61	84
53	B1	45/49 (92%)	42 (93%)	3 (7%)	20	57
54	B2	38/38 (100%)	35 (92%)	3 (8%)	15	51
55	B3	51/52 (98%)	46 (90%)	5 (10%)	10	39
56	B4	34/34 (100%)	31 (91%)	3 (9%)	12	45
57	B5	112/123 (91%)	93 (83%)	19 (17%)	2	18
58	B6	26/85 (31%)	22 (85%)	4 (15%)	3	22
All	All	5284/5590 (94%)	4862 (92%)	422 (8%)	20	50

5 of 422 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BD	37	VAL
32	BG	94	ARG

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Mol	Chain	Res	Type
54	B2	24	THR
29	BD	170	VAL
30	BE	118	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
25	AY	92	HIS
25	AY	276	GLN
50	BY	41	HIS
25	AY	122	GLN
25	AY	465	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1532/1542 (99%)	282 (18%)	18 (1%)
22	AV	76/77 (98%)	15 (19%)	0
23	AW	76/77 (98%)	27 (35%)	2 (2%)
24	AX	18/19 (94%)	14 (77%)	1 (5%)
26	BB	117/120 (97%)	17 (14%)	0
28	BA	2850/2904 (98%)	462 (16%)	41 (1%)
All	All	4669/4739 (98%)	817 (17%)	62 (1%)

5 of 817 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	9	G
1	AA	17	U
1	AA	20	U
1	AA	21	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
28	BA	527	C
28	BA	882	G
28	BA	2326	C
28	BA	784	G

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Mol	Chain	Res	Type
28	BA	1020	A

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

1 non-standard protein/DNA/RNA residue is 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	5MU	AV	54	22	13,21,23	1.27	2 (15%)	17,30,35	3.13	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	AV	54	22	-	0/3/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	AV	54	5MU	C6-N1	2.27	1.38	1.35
22	AV	54	5MU	C4-N3	3.24	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	AV	54	5MU	C5-C4-N3	-3.16	115.53	123.28
22	AV	54	5MU	C4-N3-C2	12.40	127.28	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	AV	54	5MU	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z  > 2$
59	FUA	AY	801	-	37,40,40	1.67	5 (13%)	51,64,64	1.64	9 (17%)
60	GDP	AY	802	-	24,30,30	1.32	2 (8%)	26,47,47	1.84	5 (19%)

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
59	FUA	AY	801	-	-	0/10/92/92	0/4/4/4
60	GDP	AY	802	-	-	0/12/32/32	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	AY	801	FUA	C23-C22	-6.24	1.39	1.51
59	AY	801	FUA	C23-C24	-4.08	1.39	1.53
59	AY	801	FUA	C24-C25	-2.96	1.39	1.50
59	AY	801	FUA	C14-C8	-2.85	1.53	1.58
59	AY	801	FUA	C25-C26	2.34	1.39	1.32

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
60	AY	802	GDP	N3-C2-N1	-5.45	120.14	127.56
59	AY	801	FUA	C13-C12-C11	-4.65	105.81	111.98
59	AY	801	FUA	C16-O2-C31	-3.82	111.11	117.14
60	AY	802	GDP	C5-C6-N1	-3.75	118.61	123.52
60	AY	802	GDP	C4'-O4'-C1'	-3.50	105.94	109.64

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 85 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	AY	801	FUA	59	0
60	AY	802	GDP	26	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.