



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Mar 2, 2017 – 12:28 pm GMT

PDB ID : 4V4W
EMDB ID: : EMD-1143
Title : Structure of a SecM-stalled E. coli ribosome complex obtained by fitting atomic models for RNA and protein components into cryo-EM map EMD-1143
Authors : Mitra, K.; Frank, J.
Deposited on : 2006-05-09
Resolution : 15.00 Å(reported)

This is a wwPDB/EMDatabank EM Map/Model Validation Summary Report for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

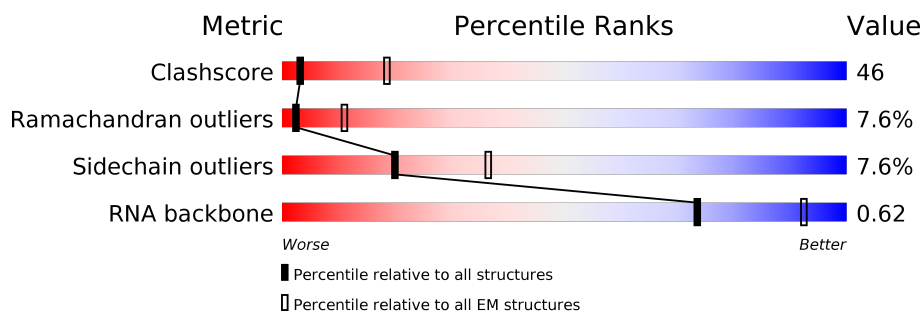
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 15.00 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.



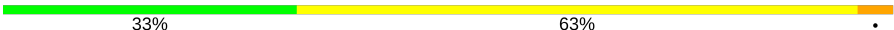

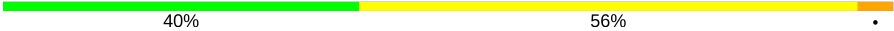













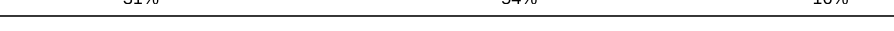

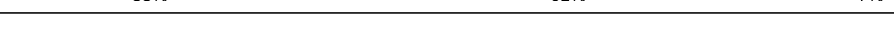
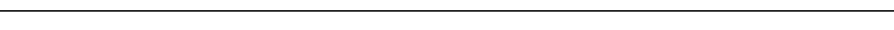
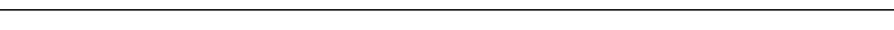
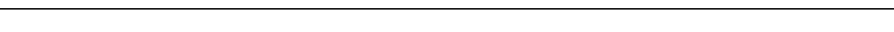
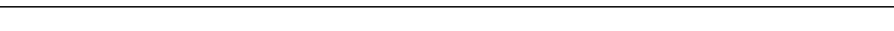
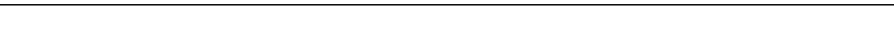

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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 ≥ 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	1488	28% 56% 15% .
2	AU	76	28% 59% 13%
2	AV	76	30% 59% 11%
2	AW	76	26% 61% 13%
3	AB	236	44% 51% .
4	AC	206	40% 54% 5%
5	AD	204	41% 57% .
6	AE	148	40% 57% .



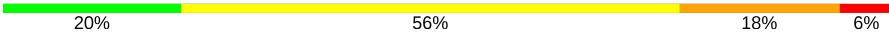
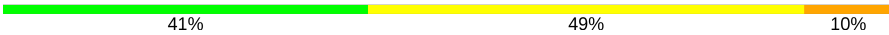
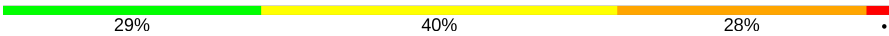
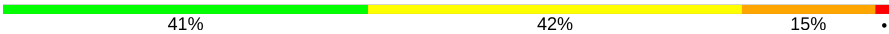
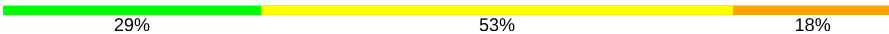

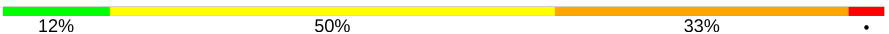
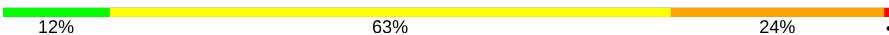
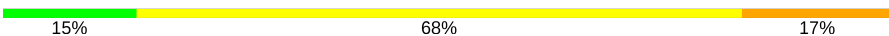
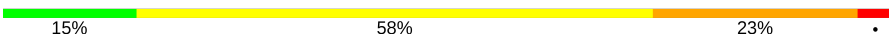
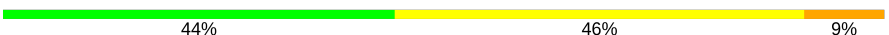

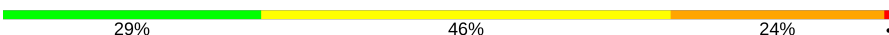




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Mol	Chain	Length	Quality of chain
7	AF	95	
8	AG	137	
9	AH	127	
10	AI	126	
11	AJ	96	
12	AK	116	
13	AL	101	
14	AM	115	
15	AN	61	
16	AO	86	
17	AP	78	
18	AQ	79	
19	AR	69	
20	AS	87	
21	AT	83	
22	B0	2740	
23	B9	108	
24	B2	222	
25	B3	119	
25	B5	119	
26	BA	227	
27	BB	209	
28	BC	198	
29	BD	177	
30	BE	167	

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Mol	Chain	Length	Quality of chain
31	BF	149	
32	BG	139	
33	BH	142	
34	BI	122	
35	BJ	140	
36	BK	131	
37	BL	114	
38	BM	113	
39	BN	114	
40	BO	115	
41	BQ	106	
42	BR	92	
43	BS	99	
44	BT	94	
45	BU	84	
46	BW	60	
47	BX	56	
48	BZ	29	
49	B1	52	

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 141668 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	1488	Total	C	N	O	P	0	0
			31924	14238	5854	10345	1487		

- Molecule 2 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AU	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		
2	AV	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		
2	AW	76	Total	C	N	O	P	0	0
			1622	725	293	529	75		

- Molecule 3 is a protein called 30S ribosomal subunit protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AB	236	Total	C	N	O	S	0	0
			1847	1165	328	346	8		

- Molecule 4 is a protein called 30S ribosomal subunit protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AC	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 5 is a protein called 30S ribosomal subunit protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AD	204	Total	C	N	O	S	0	0
			1638	1023	314	297	4		

- Molecule 6 is a protein called 30S ribosomal subunit protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AE	148	Total	C	N	O	S	0	0
			1093	679	208	200	6		

- Molecule 7 is a protein called 30S ribosomal subunit protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AF	95	Total	C	N	O	S	0	0
			784	495	143	140	6		

- Molecule 8 is a protein called 30S ribosomal subunit protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AG	137	Total	C	N	O	S	0	0
			1079	671	204	200	4		

- Molecule 9 is a protein called 30S ribosomal subunit protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AH	127	Total	C	N	O	S	0	0
			968	610	171	181	6		

- Molecule 10 is a protein called 30S ribosomal subunit protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AI	126	Total	C	N	O	S	0	0
			1014	630	204	177	3		

- Molecule 11 is a protein called 30S ribosomal subunit protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AJ	96	Total	C	N	O	S	0	0
			773	484	148	140	1		

- Molecule 12 is a protein called 30S ribosomal subunit protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AK	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 13 is a protein called 30S ribosomal subunit protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AL	101	Total	C	N	O	S	0	0
			787	486	159	138	4		

- Molecule 14 is a protein called 30S ribosomal subunit protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AM	115	Total	C	N	O	S	0	0
			892	552	179	158	3		

- Molecule 15 is a protein called 30S ribosomal subunit protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AN	61	Total	C	N	O	S	0	0
			500	310	108	80	2		

- Molecule 16 is a protein called 30S ribosomal subunit protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AO	86	Total	C	N	O	S	0	0
			697	430	139	127	1		

- Molecule 17 is a protein called 30S ribosomal subunit protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AP	78	Total	C	N	O	S	0	0
			622	390	122	109	1		

- Molecule 18 is a protein called 30S ribosomal subunit protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AQ	79	Total	C	N	O	S	0	0
			640	405	119	113	3		

- Molecule 19 is a protein called 30S ribosomal subunit protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AR	69	Total	C	N	O	S	0	0
			576	362	112	101	1		

- Molecule 20 is a protein called 30S ribosomal subunit protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AS	87	Total	C	N	O	S	0	0
			695	443	132	118	2		

- Molecule 21 is a protein called 30S ribosomal subunit protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AT	83	Total	C	N	O	S	0	0
			649	401	134	111	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	B0	2740	Total	C	N	O	P	0	0
			58824	26239	10826	19019	2740		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	B9	108	Total	C	N	O	P	0	0
			2310	1030	423	750	107		

- Molecule 24 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	B2	222	Total	C	N	O	S	0	0
			1652	1031	301	314	6		

- Molecule 25 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B3	119	Total	C	N	O	S	0	0
			845	531	137	174	3		
25	B5	119	Total	C	N	O	S	0	0
			845	531	137	174	3		

- Molecule 26 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BA	227	Total	C	N	O	S	0	0
			1733	1064	352	311	6		

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BC	198	Total	C	N	O	S	0	0
			1531	960	280	287	4		

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BD	177	Total	C	N	O	S	0	0
			1415	902	250	257	6		

- Molecule 30 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BE	167	Total	C	N	O	S	0	0
			1253	789	228	234	2		

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BG	139	Total	C	N	O	S	0	0
			1019	644	177	192	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BH	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	BI	122	Total	C	N	O	S	0	0
			939	588	180	166	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BJ	140	Total	C	N	O	S	0	0
			1017	632	200	184	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BK	131	Total	C	N	O	S	0	0
			1036	661	200	171	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BL	114	Total	C	N	O	S	0	0
			908	564	184	156	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	BM	113	Total	C	N	O	0	0
			864	534	174	156		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BN	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	BO	115	Total	C	N	O	0	0
			937	598	190	149		

- Molecule 41 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BQ	106	Total	C	N	O	S	0	0
			825	512	162	149	2		

- Molecule 42 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BR	92	Total	C	N	O	S	0	0
			717	455	132	129	1		

- Molecule 43 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BS	99	Total	C	N	O	S	0	0
			762	480	143	139			

- Molecule 44 is a protein called 50S ribosomal protein L25.

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

- Molecule 45 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BU	84	Total	C	N	O	S	0	0
			634	391	129	113	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BW	60	Total	C	N	O	S	0	0
			495	305	96	92	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BX	56	Total	C	N	O	S	0	0
			435	272	84	77	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
48	BZ	29	Total	C	N	O	0	0
			234	145	47	42		

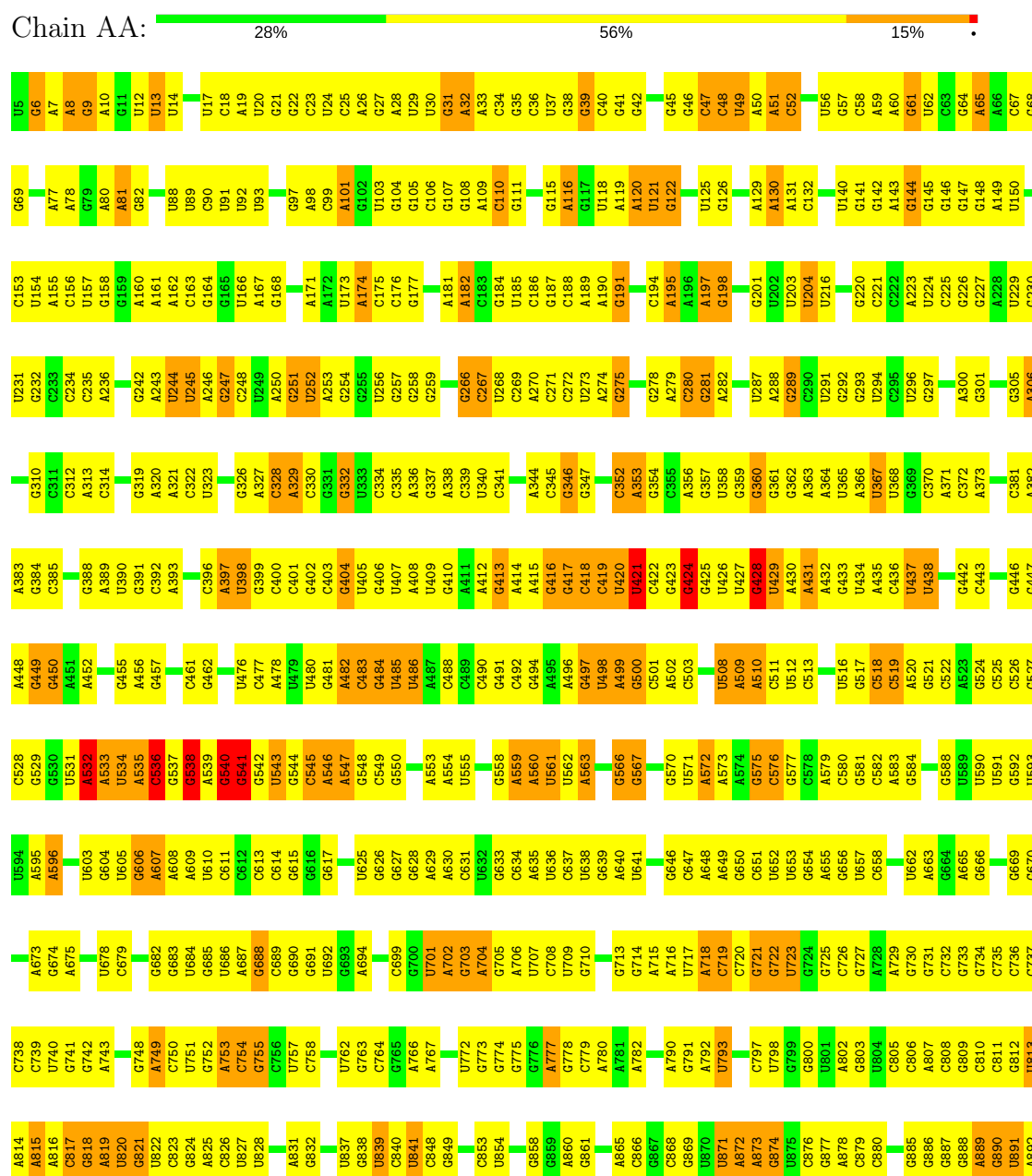
- Molecule 49 is a protein called 50S ribosomal protein L33.

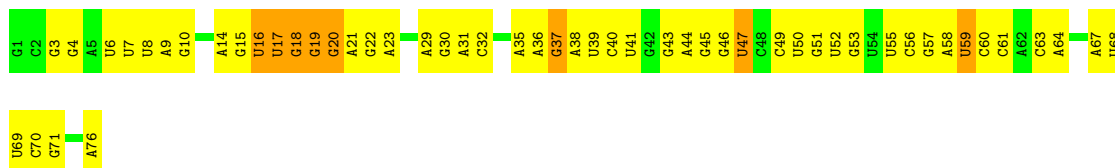
Mol	Chain	Residues	Atoms				AltConf	Trace
49	B1	52	Total	C	N	O	0	0
			424	272	78	74		

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 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.

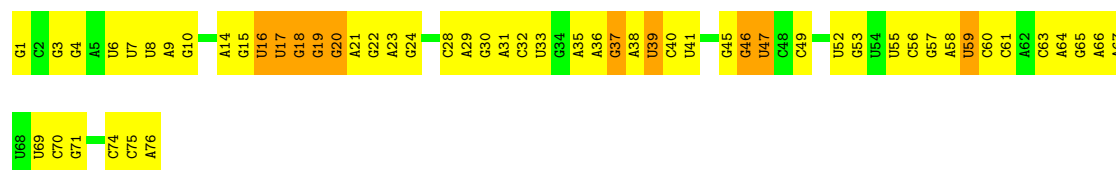
• Molecule 1: 16S ribosomal RNA





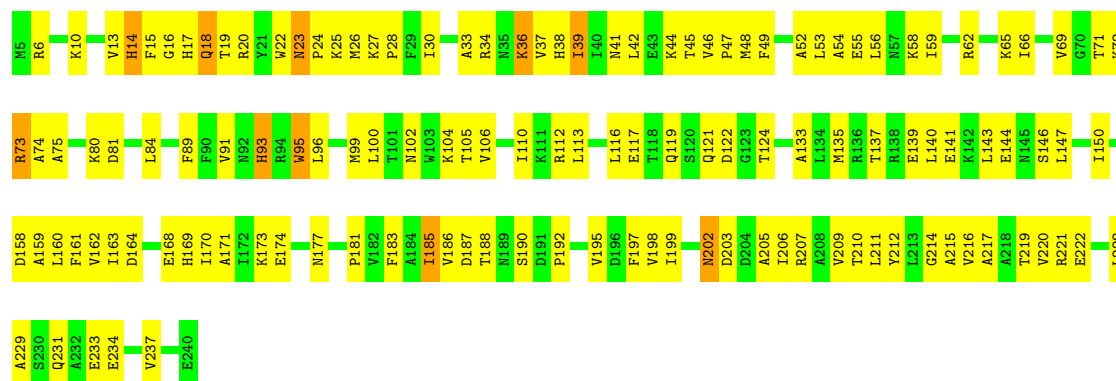
- Molecule 2: tRNA

Chain AW: 



- Molecule 3: 30S ribosomal subunit protein S2

Chain AB: 



- Molecule 4: 30S ribosomal subunit protein S3

Chain AC: 



- Molecule 5: 30S ribosomal subunit protein S4

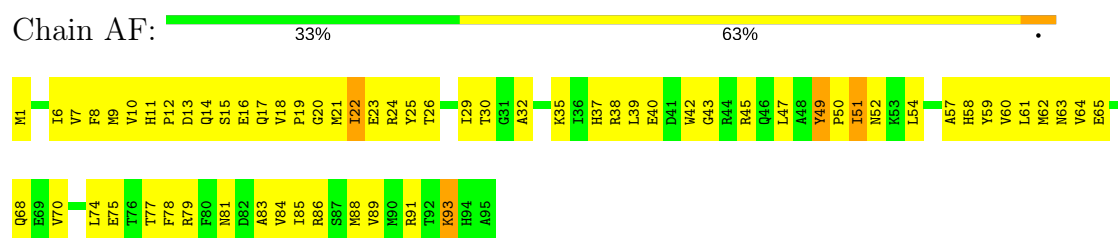
Chain AD: 



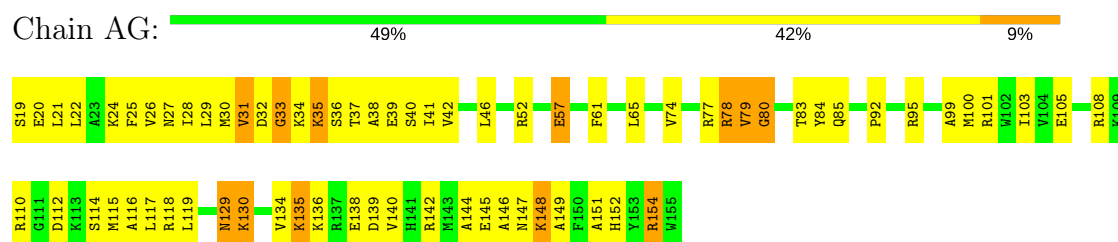
• Molecule 6: 30S ribosomal subunit protein S5



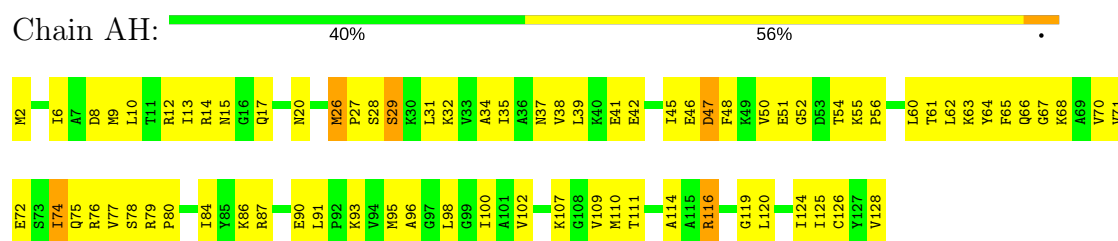
• Molecule 7: 30S ribosomal subunit protein S6



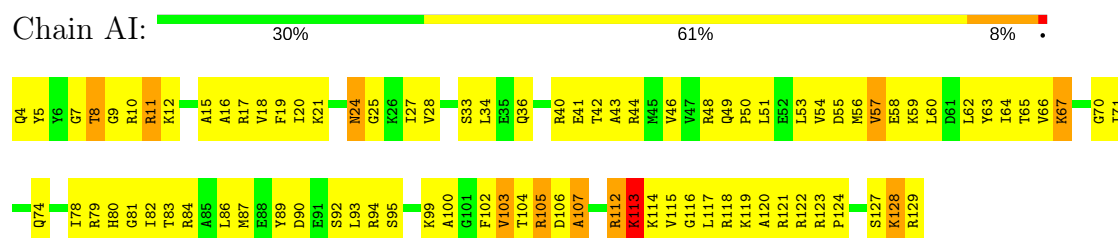
• Molecule 8: 30S ribosomal subunit protein S7



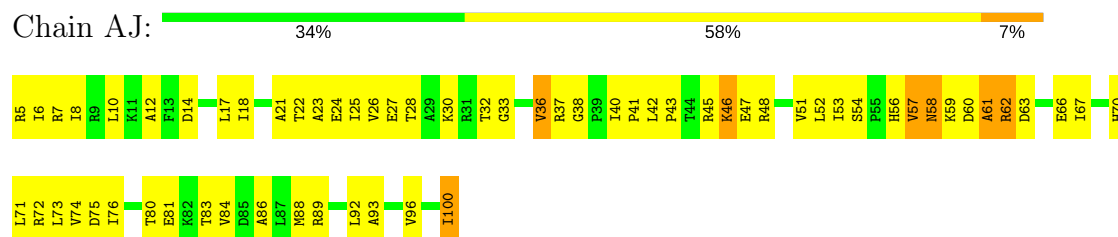
• Molecule 9: 30S ribosomal subunit protein S8



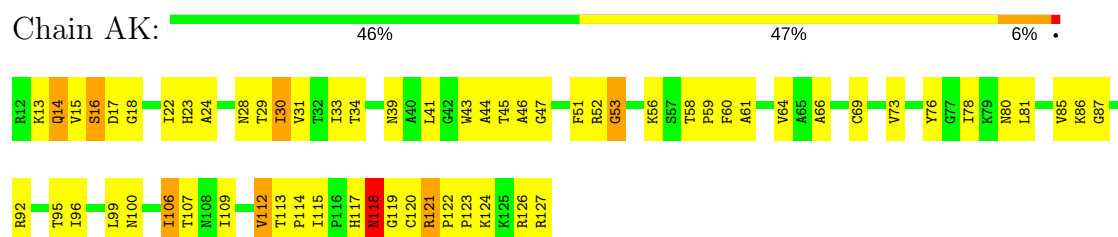
• Molecule 10: 30S ribosomal subunit protein S9



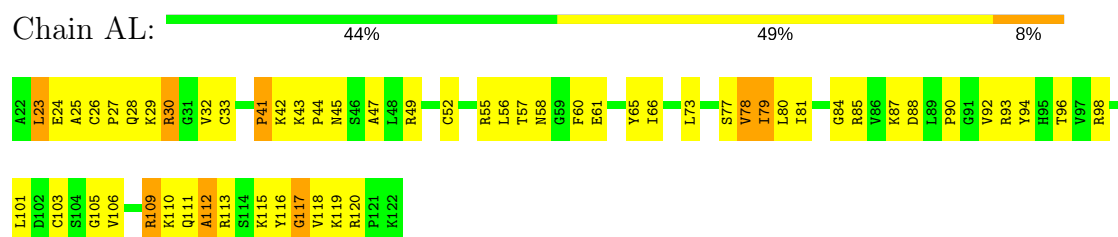
- Molecule 11: 30S ribosomal subunit protein S10



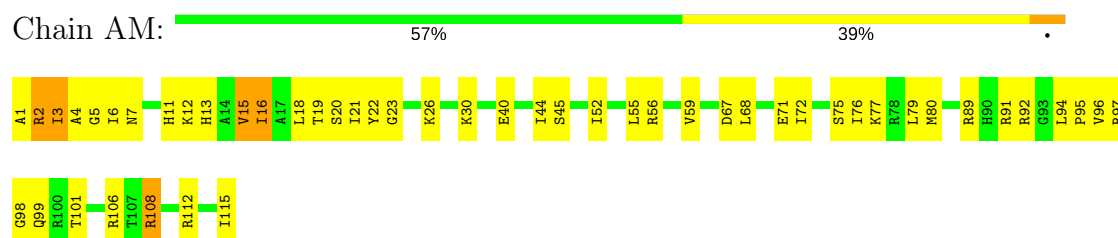
- Molecule 12: 30S ribosomal subunit protein S11



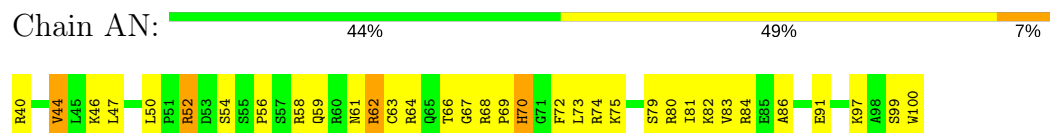
- Molecule 13: 30S ribosomal subunit protein S12



- Molecule 14: 30S ribosomal subunit protein S13



- Molecule 15: 30S ribosomal subunit protein S14



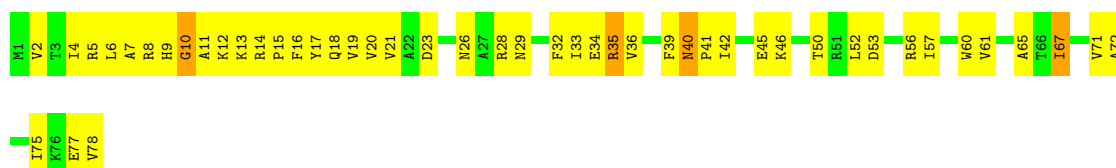
- Molecule 16: 30S ribosomal subunit protein S15





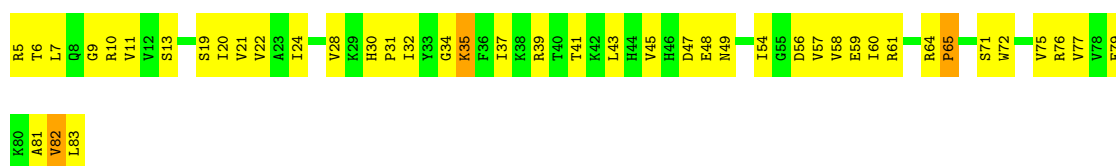
- Molecule 17: 30S ribosomal subunit protein S16

Chain AP: 38% 56% 5%



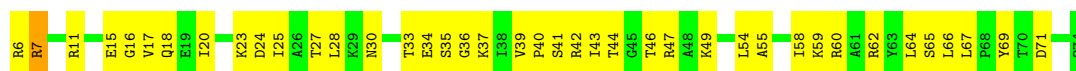
- Molecule 18: 30S ribosomal subunit protein S17

Chain AQ: 44% 52%



- Molecule 19: 30S ribosomal subunit protein S18

Chain AR: 42% 57%



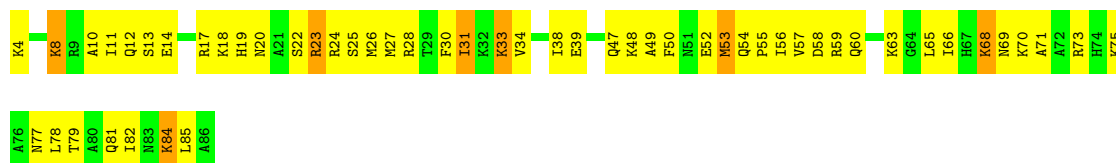
- Molecule 20: 30S ribosomal subunit protein S19

Chain AS: 37% 56% 7%



- Molecule 21: 30S ribosomal subunit protein S20

Chain AT: 36% 55% 8%



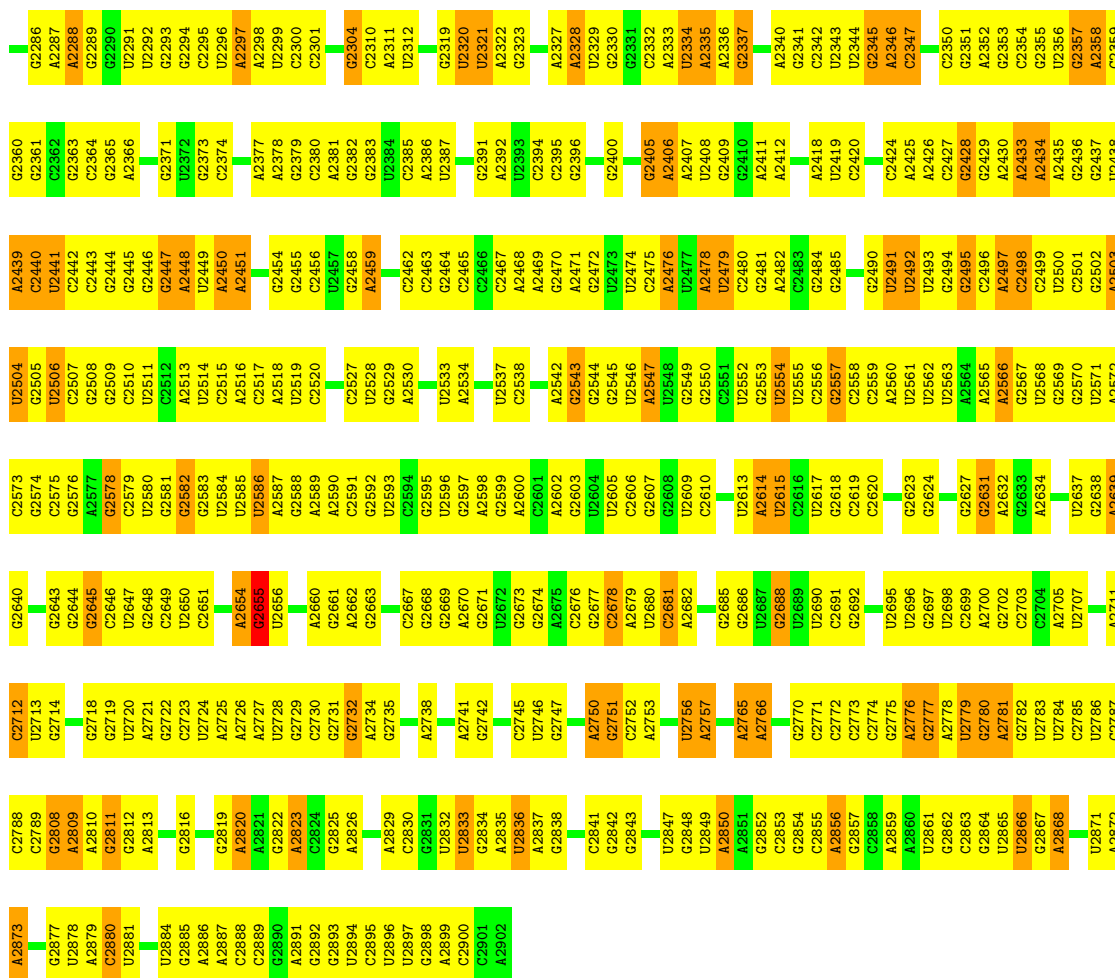
● Molecule 22: 23S ribosomal RNA

Chain B0:



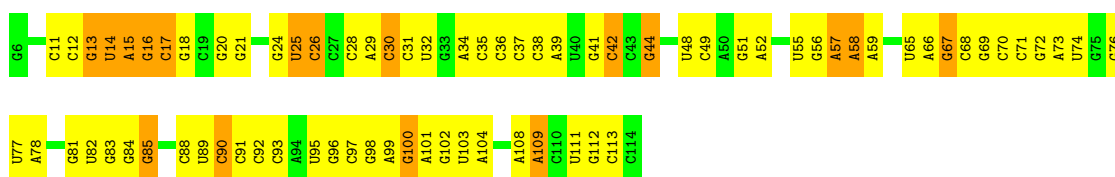
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A1014	A1088	A878	C817	U755	C692	G622	C550	C487	C414	C341	C274	U193	A94	G17
A1089	A1089	G882	C818	U756	A693	C523	C551	C488	A415	A342	C275	G194	A95	U18
A1090	A1090	G883	A819	G757	G694	G624	U554	C489	A416	C347	U276	A195	C96	U18
	U1094	U884	A820	G758	G695	G625	U555	C490	C417	A348	A278	A196	C97	C20
		G885	A821	G759	G696	A626	U556	C491	C418	U349	A279	A197	G98	A21
		G886	G822	G760	G697	G627	A556	C492	U419	U349	U280	C198	U99	
		G887	C823	U761	C698	G628	A557	A492	C420	G350	C281	A199	U100	G24
		G888	U824	U762	A699	G629	G558	C493	C421	C351	A282	U102	U102	
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		G890	U826	A764	G701	A631	C560	C495	A423	C353	U284	A204	C109	
		G891	U827	G765	U702	A632	G561	C496	A423	A354	G285	A205	G27	
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		G893	A829	U767	G704	C634	G563	C498	U427	U355	U286	U206	U111	U34
		G894	G830	U768	A705	C635	C564	U499	U428	U358	G287		U112	G35
		G895	G831	U769		G636	C565	U499	A428	U358			U113	
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		A933	C866	A804	U741	C678	G605	C535	A472	A401	U328		G177	G80
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A2227	C2150	A2020	G1955	A1794	U1636	A1569	A1493	A1427	G1360	C1292	G1229	U1159
G2228	U2151	C2021	U1956	G1795	A1637	A1570	A1494	C1428	G1361	C1293	A1230	G1160
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U2196	U2196	G2068	G2002	U1842	G1682	A1616	A1554	U1484	U1214	A1343	G1277	U1214
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U2199	U2199	C2071	C2005	G1845	U1685	A1619	A1557	U1487	U1217	A1346	G1283	G1220
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C2202	C2202	A2074	G2008	U1849	C1691	G1627	U1560	U1490	U1220	U1349	A1286	G1223
C2203	C2203	U2075	G2010	G1850	U1692	G1628	U1561	U1491	U1221	U1350	A1287	U1221
C2204	C2204	U2076	U2011	U1851	U1693	U1629	U1562	U1492	U1222	U1351	A1288	U1222
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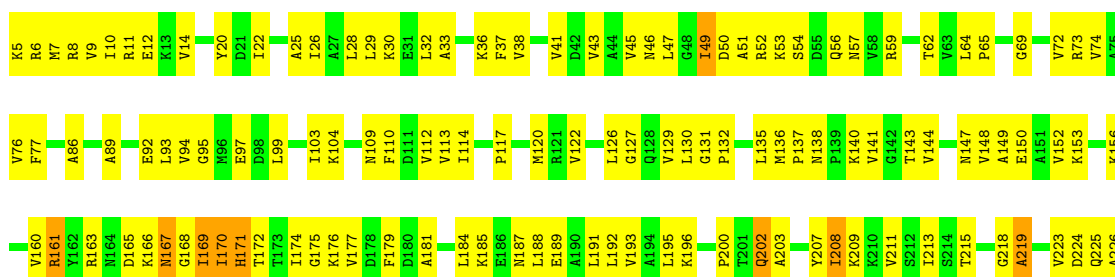
- Molecule 23: 5S ribosomal RNA

Chain B9:  31% 54% 16%

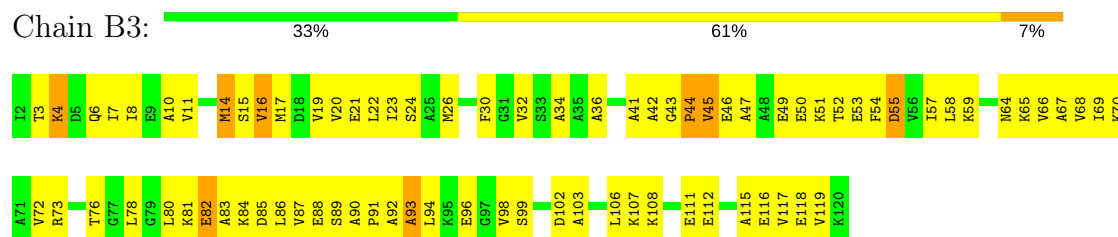


- Molecule 24: 50S ribosomal protein L1

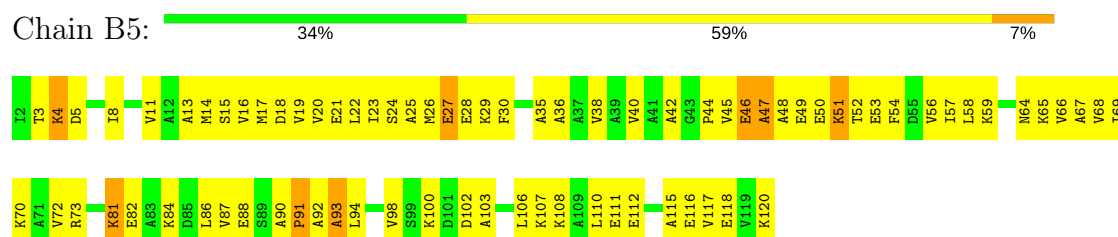
Chain B2: 44% 52%



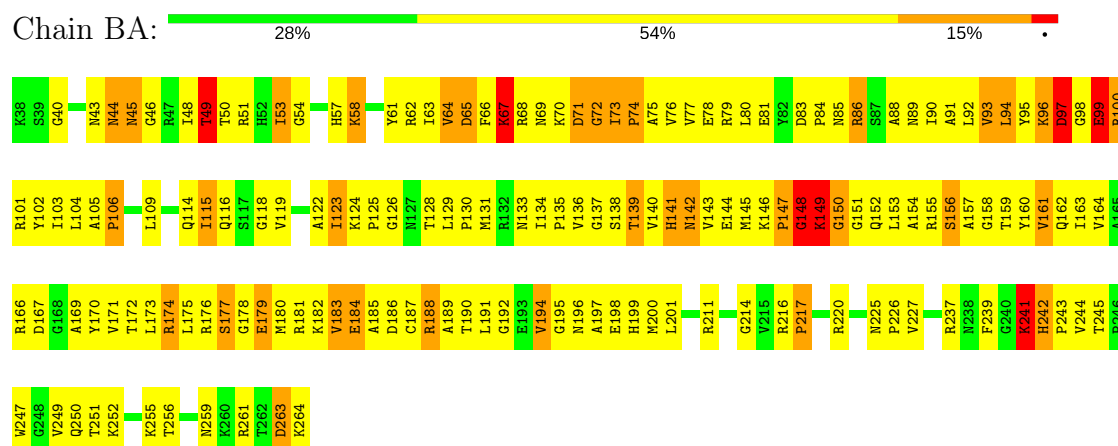
- Molecule 25: 50S ribosomal protein L7/L12



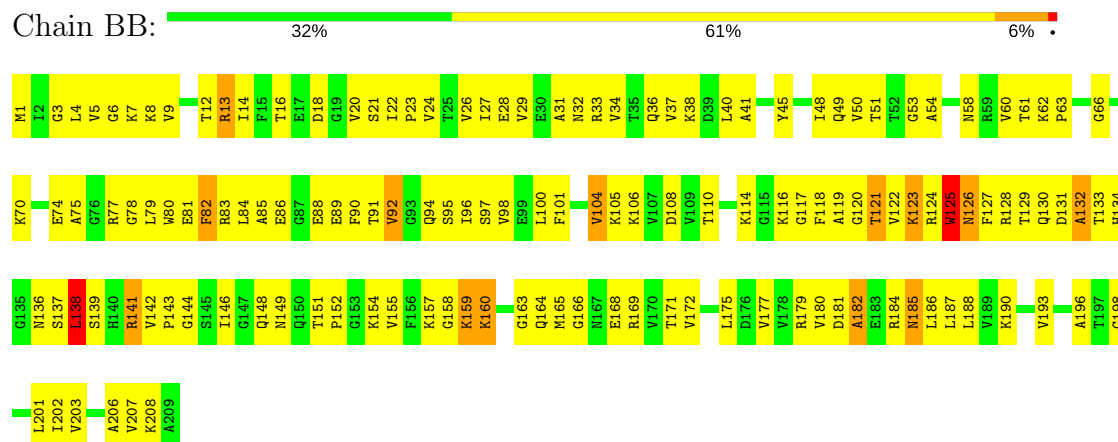
- Molecule 25: 50S ribosomal protein L7/L12



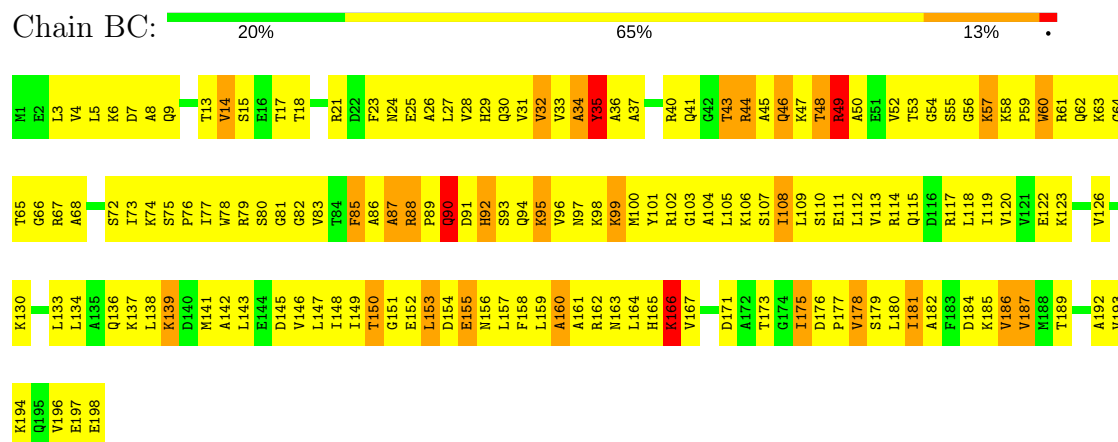
- Molecule 26: 50S ribosomal protein L2



- Molecule 27: 50S ribosomal protein L3



- Molecule 28: 50S ribosomal protein L4



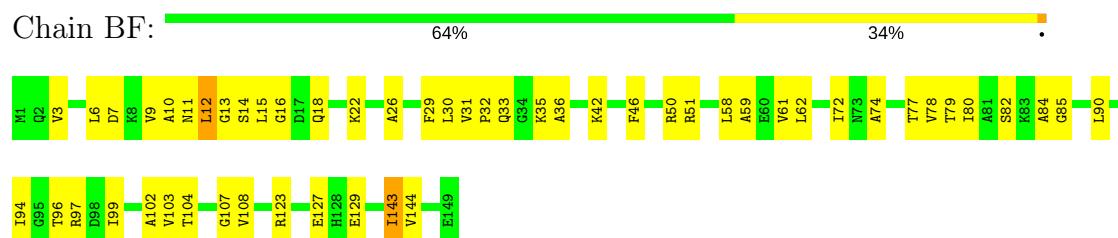
- Molecule 29: 50S ribosomal protein L5



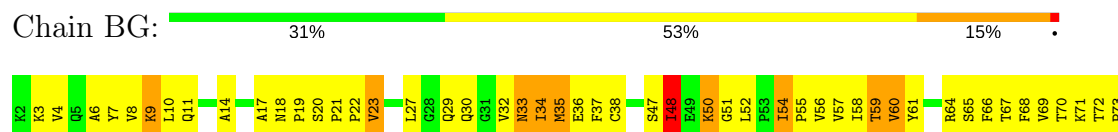
- Molecule 30: 50S ribosomal protein L6



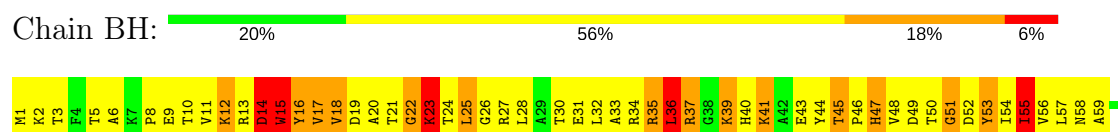
- Molecule 31: 50S ribosomal protein L9



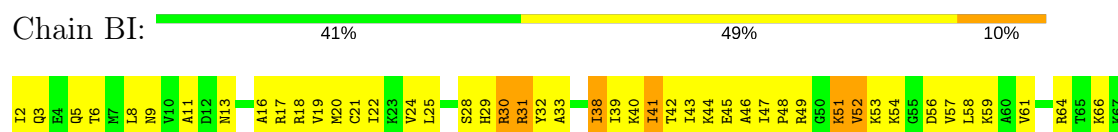
- Molecule 32: 50S ribosomal protein L11



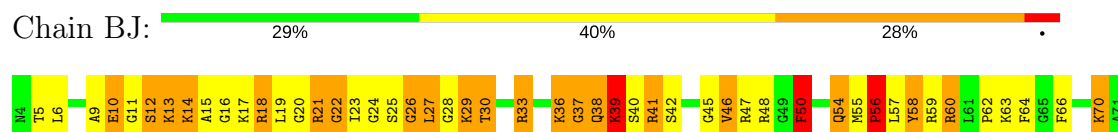
• Molecule 33: 50S ribosomal protein L13



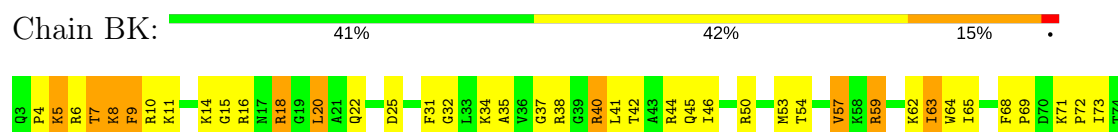
• Molecule 34: 50S ribosomal protein L14



• Molecule 35: 50S ribosomal protein L15



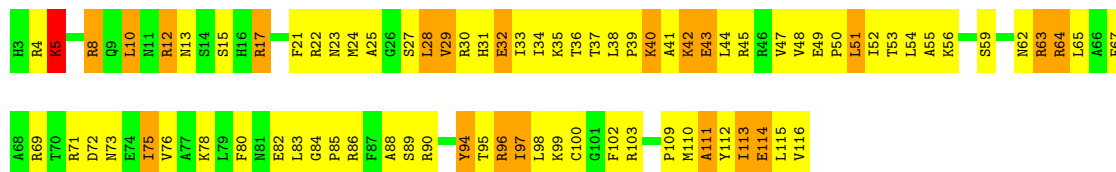
• Molecule 36: 50S ribosomal protein L16





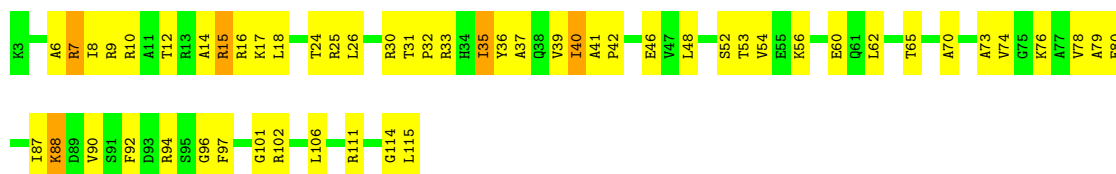
• Molecule 37: 50S ribosomal protein L17

Chain BL: 29% 53% 18%



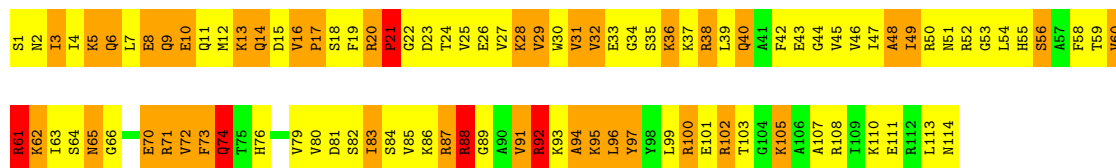
• Molecule 38: 50S ribosomal protein L18

Chain BM: 52% 43%



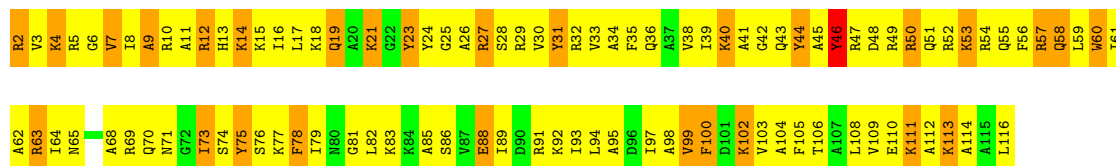
• Molecule 39: 50S ribosomal protein L19

Chain BN: 12% 50% 33%



• Molecule 40: 50S ribosomal protein L20

Chain BO: 12% 63% 24%

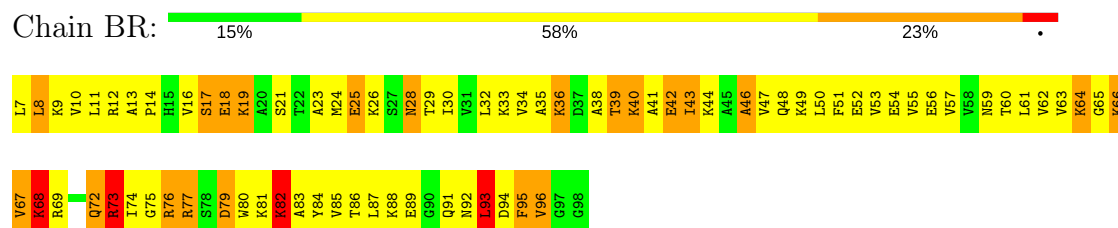


• Molecule 41: 50S ribosomal protein L22

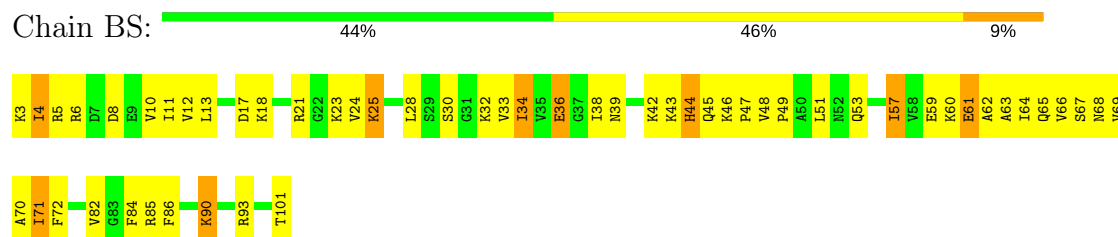
Chain BQ: 15% 68% 17%



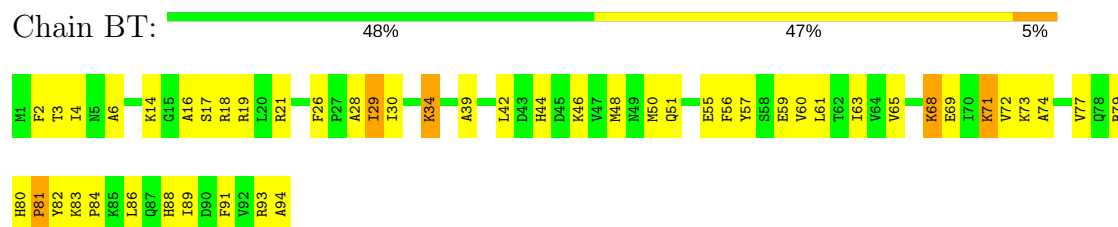
- Molecule 42: 50S ribosomal protein L23



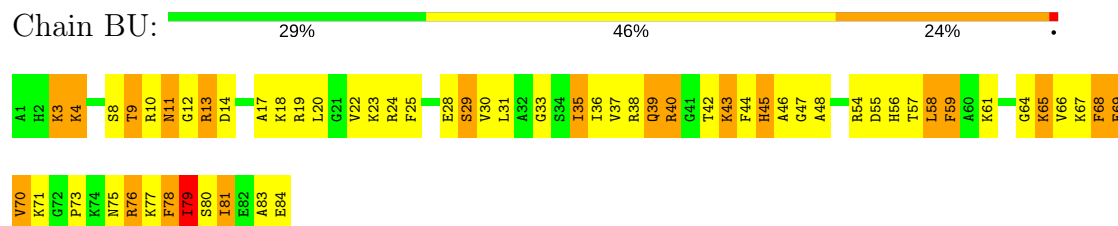
- Molecule 43: 50S ribosomal protein L24



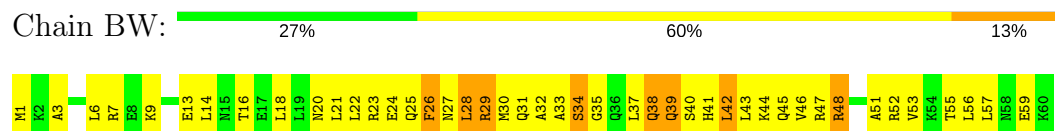
- Molecule 44: 50S ribosomal protein L25



- Molecule 45: 50S ribosomal protein L27

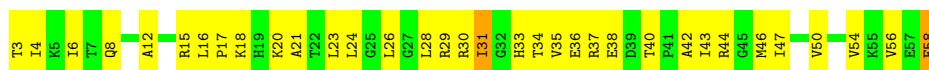


- Molecule 46: 50S ribosomal protein L29

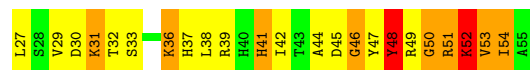
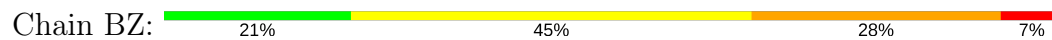


- Molecule 47: 50S ribosomal protein L30





- Molecule 48: 50S ribosomal protein L32



- Molecule 49: 50S ribosomal protein L33



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction of 3D-maps by Wiener filtration	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1100	Depositor
Minimum defocus (nm)	1.5	Depositor
Maximum defocus (nm)	4.3	Depositor
Magnification	39000	Depositor
Image detector	KODAK SO163 film	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.67	96/35745 (0.3%)	0.93	170/55764 (0.3%)
10	AI	0.24	0/1026	0.44	0/1364
11	AJ	0.23	0/783	0.46	0/1058
12	AK	0.24	0/886	0.44	0/1195
13	AL	0.22	0/799	0.44	0/1070
14	AM	0.21	0/900	0.43	0/1201
15	AN	0.25	0/510	0.39	0/679
16	AO	0.23	0/705	0.42	0/942
17	AP	0.26	0/632	0.44	0/848
18	AQ	0.24	0/649	0.45	0/870
19	AR	0.25	0/585	0.39	0/782
2	AU	0.17	0/1814	0.65	0/2827
2	AV	0.17	0/1814	0.64	0/2827
2	AW	0.18	0/1814	0.63	0/2827
20	AS	0.25	0/712	0.46	0/955
21	AT	0.24	0/655	0.38	0/866
22	B0	0.40	23/65882 (0.0%)	0.67	20/102783 (0.0%)
23	B9	0.20	0/2583	0.64	0/4028
24	B2	0.22	0/1665	0.44	0/2240
25	B3	0.22	0/842	0.43	0/1123
25	B5	0.22	0/844	0.46	0/1129
26	BA	0.72	4/1758 (0.2%)	0.65	2/2353 (0.1%)
27	BB	0.56	1/1582 (0.1%)	0.61	1/2122 (0.0%)
28	BC	0.25	0/1549	0.52	0/2082
29	BD	0.26	0/1438	0.46	0/1927
3	AB	0.25	0/1877	0.40	0/2523
30	BE	0.23	0/1273	0.43	0/1725
31	BF	0.24	0/1120	0.43	0/1509
32	BG	0.25	0/1032	0.54	0/1388
33	BH	0.27	0/1152	0.62	1/1551 (0.1%)
34	BI	0.23	0/948	0.45	0/1269
35	BJ	0.25	0/1025	0.56	0/1363
36	BK	0.27	0/1055	0.48	0/1409
37	BL	0.26	0/920	0.61	0/1229

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
38	BM	0.22	0/873	0.40	0/1170
39	BN	0.25	0/929	0.51	0/1242
4	AC	0.23	0/1652	0.42	0/2225
40	BO	1.30	6/949 (0.6%)	3.57	8/1261 (0.6%)
41	BQ	0.23	0/832	0.58	0/1113
42	BR	0.24	0/720	0.54	0/956
43	BS	0.25	0/769	0.42	0/1023
44	BT	0.25	0/766	0.41	0/1025
45	BU	0.27	0/642	0.50	0/848
46	BW	0.24	0/496	0.50	0/658
47	BX	0.23	0/439	0.45	0/587
48	BZ	0.24	0/238	0.45	0/316
49	B1	0.27	0/431	0.46	0/572
5	AD	0.22	0/1660	0.40	0/2220
6	AE	0.23	0/1106	0.42	0/1488
7	AF	0.24	0/802	0.45	0/1081
8	AG	0.23	0/1093	0.42	0/1467
9	AH	0.23	0/978	0.43	0/1311
All	All	0.46	130/153949 (0.1%)	0.75	202/230391 (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
1	AA	1	3
22	B0	5	4
All	All	6	7

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	B0	1996	C	N1-C2	33.93	1.74	1.40
22	B0	1579	A	N1-C2	27.63	1.59	1.34
22	B0	1421	G	N1-C2	25.25	1.57	1.37
1	AA	545	C	O3'-P	24.31	1.90	1.61
1	AA	536	C	N1-C6	24.27	1.51	1.37

The worst 5 of 202 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	BO	100	PHE	CZ-CE2-CD2	-69.61	36.57	120.10
40	BO	100	PHE	CD1-CE1-CZ	-69.56	36.62	120.10
40	BO	100	PHE	CE1-CZ-CE2	-53.35	23.98	120.00
40	BO	100	PHE	CG-CD1-CE1	-32.88	84.64	120.80
40	BO	100	PHE	CG-CD2-CE2	-32.87	84.64	120.80

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	428	G	C1'
22	B0	1593	G	C1'
22	B0	1653	G	C1'
22	B0	2143	C	C1'
22	B0	2250	G	C1'

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	538	G	Sidechain
1	AA	540	G	Sidechain
1	AA	541	G	Sidechain
22	B0	1418	G	Sidechain
22	B0	1579	A	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	31924	0	16066	1600	0
2	AU	1622	0	821	102	0
2	AV	1622	0	821	75	0
2	AW	1622	0	821	80	0
3	AB	1847	0	1855	120	0
4	AC	1625	0	1699	164	0
5	AD	1638	0	1702	185	0
6	AE	1093	0	1132	117	0
7	AF	784	0	776	100	0
8	AG	1079	0	1108	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	AH	968	0	1021	96	0
10	AI	1014	0	1064	153	0
11	AJ	773	0	812	71	0
12	AK	870	0	878	98	0
13	AL	787	0	825	81	0
14	AM	892	0	954	65	0
15	AN	500	0	526	51	0
16	AO	697	0	716	72	0
17	AP	622	0	637	77	0
18	AQ	640	0	678	49	0
19	AR	576	0	599	55	0
20	AS	695	0	725	118	0
21	AT	649	0	697	67	0
22	B0	58824	0	29589	3943	0
23	B9	2310	0	1173	79	0
24	B2	1652	0	1730	181	0
25	B3	845	0	876	139	0
25	B5	845	0	878	133	0
26	BA	1733	0	1764	643	0
27	BB	1565	0	1612	264	0
28	BC	1531	0	1593	499	0
29	BD	1415	0	1451	166	0
30	BE	1253	0	1289	87	0
31	BF	1111	0	1146	48	0
32	BG	1019	0	1076	134	0
33	BH	1129	0	1162	273	0
34	BI	939	0	1011	95	0
35	BJ	1017	0	1086	283	0
36	BK	1036	0	1109	154	0
37	BL	908	0	946	174	0
38	BM	864	0	902	60	0
39	BN	917	0	965	236	0
40	BO	937	0	1008	249	0
41	BQ	825	0	886	220	0
42	BR	717	0	770	187	0
43	BS	762	0	809	72	0
44	BT	753	0	780	45	0
45	BU	634	0	656	172	0
46	BW	495	0	530	76	0
47	BX	435	0	470	41	0
48	BZ	234	0	235	43	0
49	B1	424	0	461	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	141668	0	94896	10859	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 46.

The worst 5 of 10859 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B0:1579:A:C2	26:BA:67:LYS:CA	1.76	1.66
22:B0:1996:C:C2	27:BB:138:LEU:CA	1.77	1.62
22:B0:1579:A:C4	26:BA:67:LYS:CA	1.86	1.52
22:B0:1579:A:C4	26:BA:67:LYS:HA	1.38	1.52
22:B0:1421:G:N1	26:BA:149:LYS:CA	1.71	1.51

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	
3	AB	230/236 (98%)	193 (84%)	28 (12%)	9 (4%)	3	31
4	AC	204/206 (99%)	160 (78%)	34 (17%)	10 (5%)	2	27
5	AD	202/204 (99%)	177 (88%)	22 (11%)	3 (2%)	12	53
6	AE	146/148 (99%)	135 (92%)	10 (7%)	1 (1%)	25	68
7	AF	93/95 (98%)	81 (87%)	10 (11%)	2 (2%)	8	44
8	AG	135/137 (98%)	114 (84%)	13 (10%)	8 (6%)	2	23
9	AH	125/127 (98%)	113 (90%)	9 (7%)	3 (2%)	7	42
10	AI	124/126 (98%)	93 (75%)	20 (16%)	11 (9%)	1	15
11	AJ	94/96 (98%)	73 (78%)	15 (16%)	6 (6%)	1	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	AK	114/116 (98%)	91 (80%)	14 (12%)	9 (8%)	1	17
13	AL	99/101 (98%)	75 (76%)	19 (19%)	5 (5%)	2	26
14	AM	111/115 (96%)	90 (81%)	18 (16%)	3 (3%)	6	40
15	AN	59/61 (97%)	50 (85%)	5 (8%)	4 (7%)	1	20
16	AO	84/86 (98%)	76 (90%)	8 (10%)	0	100	100
17	AP	76/78 (97%)	62 (82%)	13 (17%)	1 (1%)	14	56
18	AQ	77/79 (98%)	65 (84%)	10 (13%)	2 (3%)	6	40
19	AR	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
20	AS	85/87 (98%)	69 (81%)	12 (14%)	4 (5%)	3	28
21	AT	81/83 (98%)	68 (84%)	11 (14%)	2 (2%)	6	41
24	B2	216/222 (97%)	183 (85%)	27 (12%)	6 (3%)	6	39
25	B3	108/119 (91%)	84 (78%)	18 (17%)	6 (6%)	2	25
25	B5	112/119 (94%)	89 (80%)	16 (14%)	7 (6%)	1	22
26	BA	215/227 (95%)	128 (60%)	56 (26%)	31 (14%)	0	5
27	BB	199/209 (95%)	148 (74%)	37 (19%)	14 (7%)	1	19
28	BC	194/198 (98%)	124 (64%)	45 (23%)	25 (13%)	0	6
29	BD	173/177 (98%)	96 (56%)	54 (31%)	23 (13%)	0	6
30	BE	165/167 (99%)	141 (86%)	22 (13%)	2 (1%)	15	57
31	BF	143/149 (96%)	121 (85%)	16 (11%)	6 (4%)	3	30
32	BG	135/139 (97%)	85 (63%)	33 (24%)	17 (13%)	0	7
33	BH	140/142 (99%)	77 (55%)	41 (29%)	22 (16%)	0	4
34	BI	120/122 (98%)	93 (78%)	20 (17%)	7 (6%)	2	24
35	BJ	136/140 (97%)	69 (51%)	37 (27%)	30 (22%)	0	2
36	BK	129/131 (98%)	93 (72%)	24 (19%)	12 (9%)	1	14
37	BL	110/114 (96%)	67 (61%)	32 (29%)	11 (10%)	1	12
38	BM	111/113 (98%)	90 (81%)	16 (14%)	5 (4%)	3	29
39	BN	112/114 (98%)	50 (45%)	35 (31%)	27 (24%)	0	2
40	BO	111/115 (96%)	59 (53%)	39 (35%)	13 (12%)	0	8
41	BQ	104/106 (98%)	68 (65%)	29 (28%)	7 (7%)	1	21
42	BR	83/92 (90%)	39 (47%)	25 (30%)	19 (23%)	0	2
43	BS	95/99 (96%)	69 (73%)	21 (22%)	5 (5%)	2	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BT	92/94 (98%)	76 (83%)	13 (14%)	3 (3%)	4	35
45	BU	82/84 (98%)	43 (52%)	23 (28%)	16 (20%)	0	3
46	BW	58/60 (97%)	49 (84%)	5 (9%)	4 (7%)	1	20
47	BX	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
48	BZ	27/29 (93%)	11 (41%)	6 (22%)	10 (37%)	0	0
49	B1	50/52 (96%)	27 (54%)	19 (38%)	4 (8%)	1	17
All	All	5480/5639 (97%)	4077 (74%)	988 (18%)	415 (8%)	2	18

5 of 415 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AB	14	HIS
3	AB	93	HIS
4	AC	126	ARG
4	AC	178	ARG
8	AG	31	VAL

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	
3	AB	195/195 (100%)	190 (97%)	5 (3%)	51	75
4	AC	170/170 (100%)	164 (96%)	6 (4%)	41	69
5	AD	172/172 (100%)	170 (99%)	2 (1%)	75	88
6	AE	112/112 (100%)	108 (96%)	4 (4%)	40	68
7	AF	83/83 (100%)	80 (96%)	3 (4%)	40	68
8	AG	112/112 (100%)	108 (96%)	4 (4%)	40	68
9	AH	103/103 (100%)	100 (97%)	3 (3%)	48	73
10	AI	104/104 (100%)	100 (96%)	4 (4%)	38	67
11	AJ	84/84 (100%)	80 (95%)	4 (5%)	30	61
12	AK	89/89 (100%)	86 (97%)	3 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	AL	85/85 (100%)	82 (96%)	3 (4%)	41	69
14	AM	93/93 (100%)	90 (97%)	3 (3%)	44	71
15	AN	52/52 (100%)	51 (98%)	1 (2%)	62	82
16	AO	74/74 (100%)	74 (100%)	0	100	100
17	AP	63/63 (100%)	60 (95%)	3 (5%)	30	61
18	AQ	73/73 (100%)	72 (99%)	1 (1%)	71	86
19	AR	60/60 (100%)	59 (98%)	1 (2%)	66	84
20	AS	75/75 (100%)	73 (97%)	2 (3%)	50	74
21	AT	63/63 (100%)	56 (89%)	7 (11%)	7	29
24	B2	172/172 (100%)	166 (96%)	6 (4%)	41	69
25	B3	83/83 (100%)	81 (98%)	2 (2%)	54	78
25	B5	83/83 (100%)	80 (96%)	3 (4%)	40	68
26	BA	176/176 (100%)	159 (90%)	17 (10%)	9	35
27	BB	164/164 (100%)	160 (98%)	4 (2%)	54	78
28	BC	163/163 (100%)	152 (93%)	11 (7%)	19	51
29	BD	149/149 (100%)	124 (83%)	25 (17%)	2	16
30	BE	130/130 (100%)	123 (95%)	7 (5%)	26	58
31	BF	114/114 (100%)	112 (98%)	2 (2%)	64	84
32	BG	108/108 (100%)	91 (84%)	17 (16%)	3	18
33	BH	116/116 (100%)	94 (81%)	22 (19%)	2	11
34	BI	103/103 (100%)	97 (94%)	6 (6%)	23	56
35	BJ	99/99 (100%)	74 (75%)	25 (25%)	0	5
36	BK	104/104 (100%)	90 (86%)	14 (14%)	4	24
37	BL	94/94 (100%)	80 (85%)	14 (15%)	3	20
38	BM	83/83 (100%)	78 (94%)	5 (6%)	22	55
39	BN	99/99 (100%)	74 (75%)	25 (25%)	0	5
40	BO	89/89 (100%)	70 (79%)	19 (21%)	1	8
41	BQ	89/89 (100%)	76 (85%)	13 (15%)	3	21
42	BR	77/77 (100%)	65 (84%)	12 (16%)	3	18
43	BS	82/82 (100%)	77 (94%)	5 (6%)	22	55
44	BT	78/78 (100%)	75 (96%)	3 (4%)	38	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	BU	62/62 (100%)	52 (84%)	10 (16%)	3	17
46	BW	55/55 (100%)	50 (91%)	5 (9%)	11	38
47	BX	47/47 (100%)	45 (96%)	2 (4%)	33	64
48	BZ	24/24 (100%)	18 (75%)	6 (25%)	1	5
49	B1	46/46 (100%)	37 (80%)	9 (20%)	1	10
All	All	4551/4551 (100%)	4203 (92%)	348 (8%)	20	47

5 of 348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	BH	23	LYS
35	BJ	79	LEU
45	BU	45	HIS
33	BH	41	LYS
34	BI	41	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 139 such sidechains are listed below:

Mol	Chain	Res	Type
21	AT	54	GLN
27	BB	36	GLN
44	BT	44	HIS
24	B2	56	GLN
26	BA	52	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1487/1488 (99%)	248 (16%)	0
2	AU	75/76 (98%)	13 (17%)	0
2	AV	75/76 (98%)	10 (13%)	0
2	AW	75/76 (98%)	13 (17%)	0
22	B0	2739/2740 (99%)	541 (19%)	0
23	B9	107/108 (99%)	20 (18%)	0
All	All	4558/4564 (99%)	845 (18%)	0

5 of 845 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	31	G

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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
25	B3	6
26	BA	5
25	B5	4
27	BB	4
42	BR	4
3	AB	2
31	BF	2
24	B2	2
40	BO	1
37	BL	1

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Mol	Chain	Number of breaks
29	BD	1
43	BS	1
35	BJ	1
32	BG	1
28	BC	1
14	AM	1

The worst 5 of 37 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B5	52:THR	C	53:GLU	N	10.02
1	BA	60:ALA	C	61:TYR	N	9.99
1	B5	50:GLU	C	51:LYS	N	9.70
1	BB	167:ASN	C	168:GLU	N	8.31
1	BC	96:VAL	C	97:ASN	N	7.51