



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:44 PM BST

PDB ID : 4V61
EMDB ID: : EMD-1417
Title : Homology model for the Spinach chloroplast 30S subunit fitted to 9.4Å cryo-EM map of the 70S chlororibosome.
Authors : Sharma, M.R.; Wilson, D.N.; Datta, P.P.; Barat, C.; Schlutzenzen, F.; Fucini, P.; Agrawal, R.K.
Deposited on : 2007-11-09
Resolution : 9.40 Å (reported)
Based on PDB ID : 2XYZ and 2ZXY for small and large subunit respectively

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

A user guide is available at

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

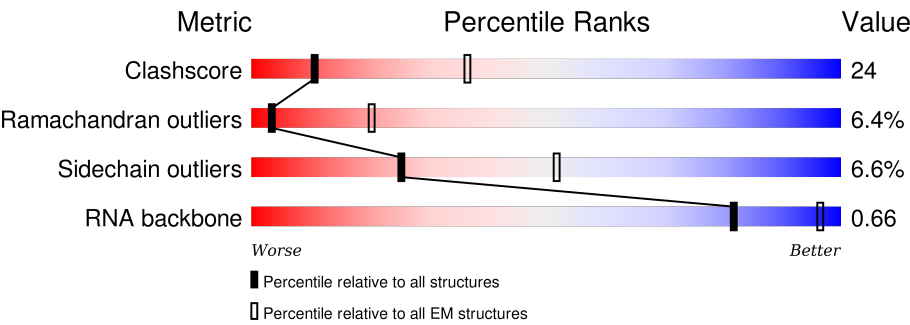
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 9.40 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.











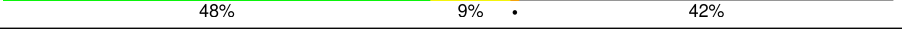
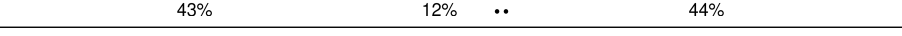
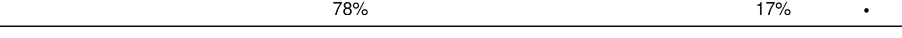
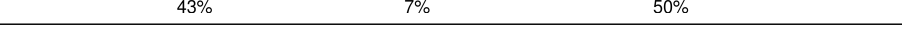

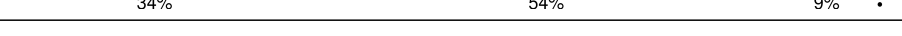


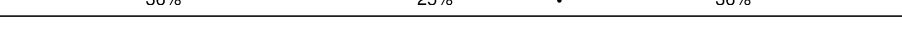

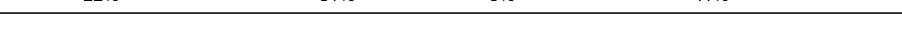






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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 ≥ 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	1491	<div><div>39%</div><div>46%</div><div>14%</div><div>.</div></div>
2	AB	231	<div><div>84%</div><div>13%</div><div>.</div></div>
3	AC	218	<div><div>85%</div><div>13%</div><div>.</div></div>
4	AD	201	<div><div>84%</div><div>15%</div><div>.</div></div>
5	AE	308	<div><div>43%</div><div>7%</div><div>.</div><div>49%</div></div>
6	AF	168	<div><div>48%</div><div>15%</div><div>.</div><div>36%</div></div>
7	AG	155	<div><div>87%</div><div>10%</div><div>..</div></div>
8	AH	134	<div><div>84%</div><div>13%</div><div>.</div></div>

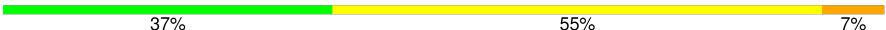


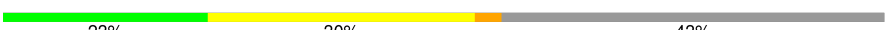
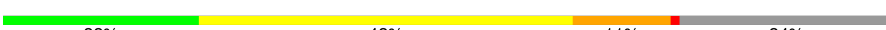





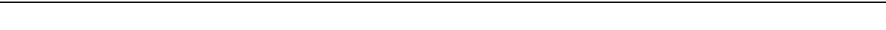

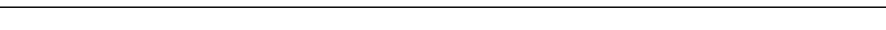
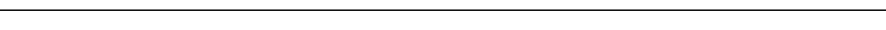
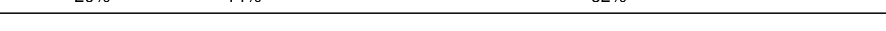
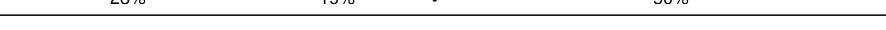
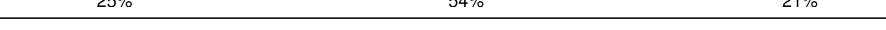



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Mol	Chain	Length	Quality of chain
9	AI	197	
10	AJ	197	
11	AK	140	
12	AL	123	
13	AM	145	
14	AN	100	
15	AO	90	
16	AP	88	
17	AQ	142	
18	AR	103	
19	AS	92	
20	AT	202	
21	AU	190	
22	BA	2810	
23	BB	117	
24	BC	103	
25	BD	352	
26	BE	269	
27	BF	259	
28	BG	293	
29	BH	220	
30	BI	223	
31	BJ	197	
32	BK	224	
33	BL	250	

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Mol	Chain	Length	Quality of chain
34	BM	121	
35	BN	257	
36	BO	135	
37	BP	205	
38	BQ	161	
39	BR	233	
40	BS	119	
41	BT	257	
42	BU	199	
43	BV	198	
44	BW	191	
45	BX	198	
46	BY	151	
47	BZ	173	
48	B1	144	
49	B2	57	
50	B3	66	
51	B4	152	
52	B5	159	
53	B6	104	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 142250 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 rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	1478	Total	C	N	O	P	0	0
			31745	14154	5865	10249	1477		

- Molecule 2 is a protein called Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	231	Total	C	N	O	S	0	0
			1827	1152	334	328	13		

- Molecule 3 is a protein called Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	217	Total	C	N	O	S	0	0
			1744	1113	314	310	7		

- Molecule 4 is a protein called Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	199	Total	C	N	O	S	0	0
			1632	1032	318	277	5		

- Molecule 5 is a protein called Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AE	158	Total	C	N	O	S	0	0
			1190	742	230	212	6		

- Molecule 6 is a protein called Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	107	Total	C	N	O	S	0	0
			872	558	145	166	3		

- Molecule 7 is a protein called Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AG	154	Total	C	N	O	S	0	0
			1211	753	244	211	3		

- Molecule 8 is a protein called Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AH	134	Total	C	N	O	S	0	0
			1088	684	211	187	6		

- Molecule 9 is a protein called Ribosomal Protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0
			988	627	188	172	1		

- Molecule 10 is a protein called Ribosomal Protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0
			803	515	144	139	5		

- Molecule 11 is a protein called Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	118	Total	C	N	O	S	0	0
			888	549	182	152	5		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AK	21	SER	-	INSERTION	UNP P06506
AK	22	ALA	-	INSERTION	UNP P06506

- Molecule 12 is a protein called Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0
			968	604	198	163	3		

- Molecule 13 is a protein called Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	AM	99	Total	C	N	O	S	0	0
			824	513	168	141	2		

- Molecule 14 is a protein called Ribosomal Protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	AN	99	Total	C	N	O	S	0	0
			820	507	174	136	3		

- Molecule 15 is a protein called Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	AO	85	Total	C	N	O	S	0	0
			713	454	134	124	1		

- Molecule 16 is a protein called Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AP	80	Total	C	N	O	S	0	0
			664	425	123	114	2		

- Molecule 17 is a protein called Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AQ	83	Total	C	N	O	S	0	0
			662	416	130	112	4		

- Molecule 18 is a protein called Ribosomal Protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	AR	58	Total	C	N	O	S	0	0
			478	300	94	83	1		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AR	81	GLU	-	INSERTION	UNP Q9M3K7
AR	82	LYS	-	INSERTION	UNP Q9M3K7

- Molecule 19 is a protein called Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	AS	92	Total	C	N	O	S	0	0
			747	472	146	126	3		

- Molecule 20 is a protein called Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	AT	102	Total	C	N	O	S	0	0
			799	493	163	142	1		

- Molecule 21 is a protein called Ribosomal Protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	AU	53	Total	C	N	O	S	0	0
			455	276	96	81	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BA	2732	Total	C	N	O	P	0	0
			58665	26173	10857	18904	2731		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	BB	117	Total	C	N	O	P	0	0
			2497	1116	452	813	116		

- Molecule 24 is a RNA chain called 4.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	BC	103	Total	C	N	O	P	0	0
			2207	987	408	710	102		

- Molecule 25 is a protein called Ribosomal Protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BD	227	Total	C	N	O	S	0	0
			1760	1117	307	329	7		

- Molecule 26 is a protein called Ribosomal Protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	BE	266	Total	C	N	O	S	0	0
			2049	1268	418	357	6		

- Molecule 27 is a protein called Ribosomal Protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	BF	154	Total	C	N	O	S	0	0
			1196	756	230	205	5		

- Molecule 28 is a protein called Ribosomal Protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BG	211	Total	C	N	O	S	0	0
			1664	1057	309	295	3		

- Molecule 29 is a protein called Ribosomal Protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	BH	175	Total	C	N	O	S	0	0
			1351	862	233	248	8		

- Molecule 30 is a protein called Ribosomal Protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	BI	182	Total	C	N	O	S	0	0
			1429	907	257	262	3		

- Molecule 31 is a protein called Ribosomal Protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	BJ	148	Total	C	N	O	S	0	0
			1177	753	206	215	3		

- Molecule 32 is a protein called Ribosomal Protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	BK	145	Total	C	N	O	S	0	0
			1060	679	177	198	6		

- Molecule 33 is a protein called Ribosomal Protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	BL	125	Total	C	N	O	S	0	0
			998	634	192	169	3		

- Molecule 34 is a protein called Ribosomal Protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	BM	121	Total	C	N	O	S	0	0
			943	588	179	171	5		

- Molecule 35 is a protein called Ribosomal Protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	BN	176	Total	C	N	O	S	0	0
			1333	835	257	235	6		

- Molecule 36 is a protein called Ribosomal Protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	BO	135	Total	C	N	O	S	0	0
			1076	677	218	175	6		

- Molecule 37 is a protein called Ribosomal Protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	BP	116	Total	C	N	O	S	0	0
			948	594	195	155	4		

- Molecule 38 is a protein called Ribosomal Protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	BQ	122	Total	C	N	O	S	0	0
			962	597	183	178	4		

- Molecule 39 is a protein called Ribosomal Protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	BR	113	Total	C	N	O	S	0	0
			915	586	177	151	1		

- Molecule 40 is a protein called Ribosomal Protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	BS	119	Total	C	N	O	S	0	0
			1030	653	213	161	3		

- Molecule 41 is a protein called Ribosomal Protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	BT	104	Total	C	N	O	S	0	0
			826	537	150	139			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	122	ILE	-	INSERTION	UNP P24613

- Molecule 42 is a protein called Ribosomal Protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	BU	122	Total	C	N	O	S	0	0
			986	627	178	175	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	126	LEU	LYS	CONFLICT	UNP P09594

- Molecule 43 is a protein called Ribosomal Protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	BV	85	Total	C	N	O	S	0	0
			677	436	115	124	2		

- Molecule 44 is a protein called Ribosomal Protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	BW	110	Total	C	N	O	S	0	0
			869	548	160	160	1		

- Molecule 45 is a protein called Ribosomal Protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	BX	86	Total	C	N	O	S	0	0
			660	419	127	114			

- Molecule 46 is a protein called Ribosomal Protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	BY	76	Total	C	N	O	S	0	0
			619	395	120	103	1		

- Molecule 47 is a protein called Ribosomal Protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	BZ	65	Total	C	N	O	S	0	0
			551	341	106	101	3		

- Molecule 48 is a protein called Ribosomal Protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	B1	72	Total	C	N	O	S	0	0
			581	369	99	109	4		

- Molecule 49 is a protein called Ribosomal Protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	B2	57	Total	C	N	O	S	0	0
			469	305	87	76	1		

- Molecule 50 is a protein called Ribosomal Protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	B3	65	Total	C	N	O	S	0	0
			524	326	105	88	5		

- Molecule 51 is a protein called Ribosomal Protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	B4	37	Total	C	N	O	S	0	0
			297	180	70	45	2		

- Molecule 52 is a protein called Ribosomal Protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	B5	62	Total	C	N	O	S	0	0
			504	315	107	81	1		

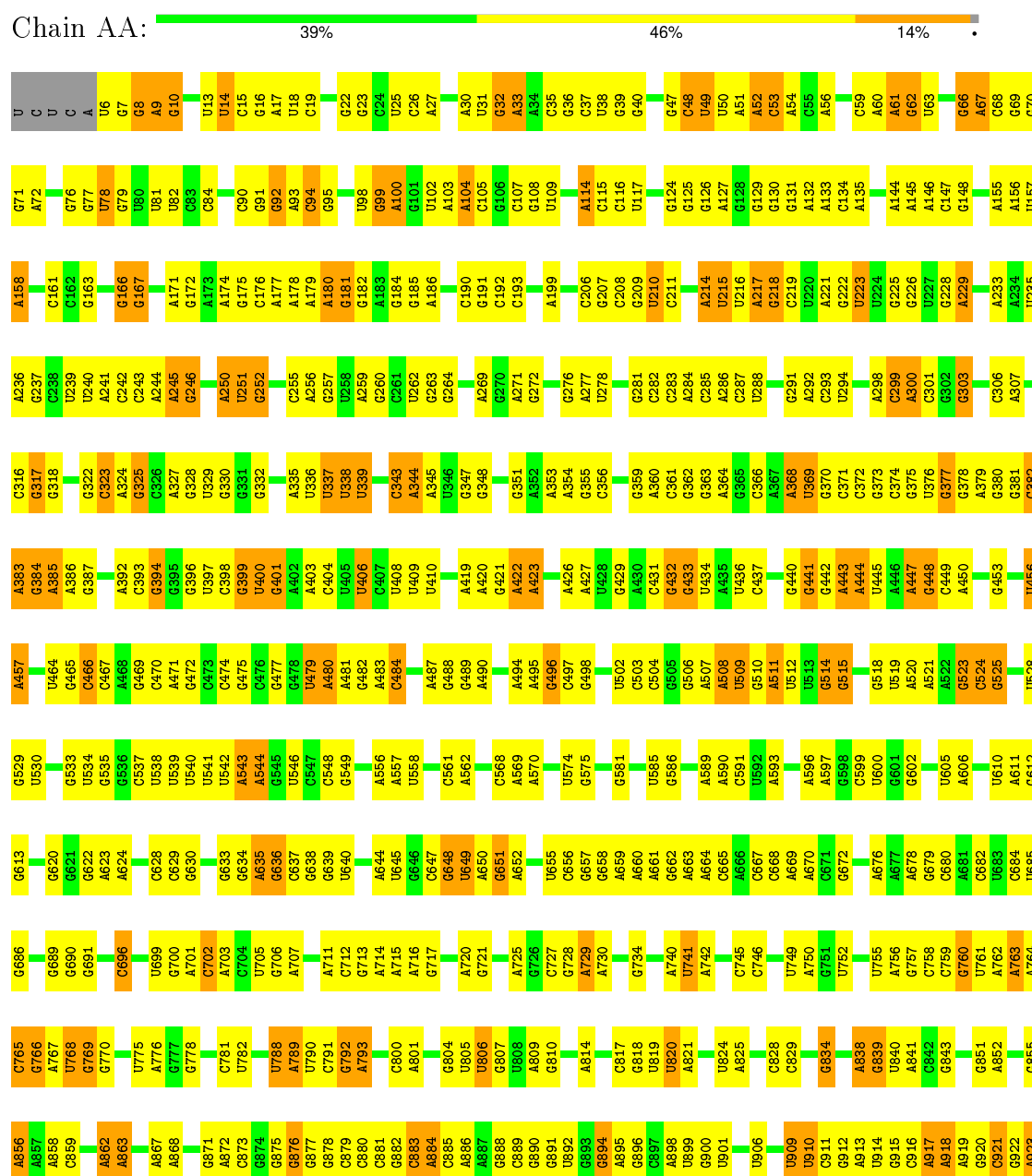
- Molecule 53 is a protein called Ribosomal Protein L36.

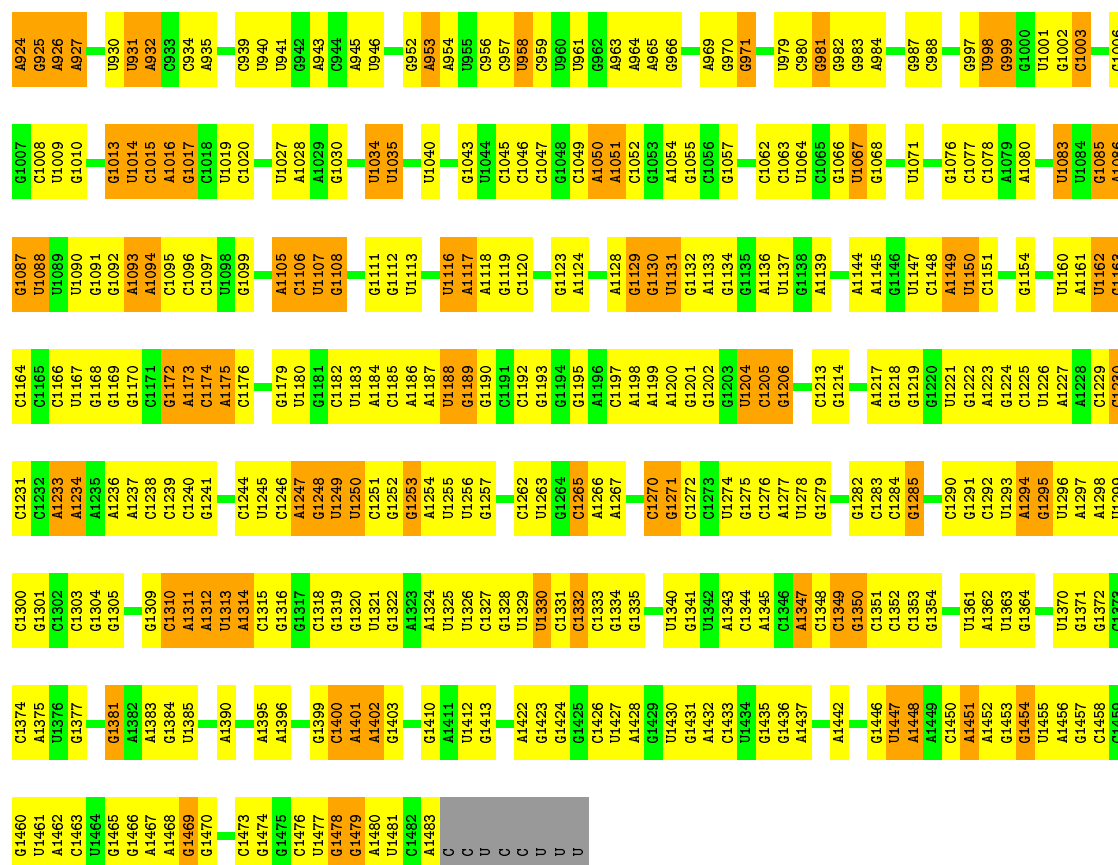
Mol	Chain	Residues	Atoms					AltConf	Trace
53	B6	38	Total	C	N	O	S	0	0
			309	190	65	49	5		

3 Residue-property plots [i](#)

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.

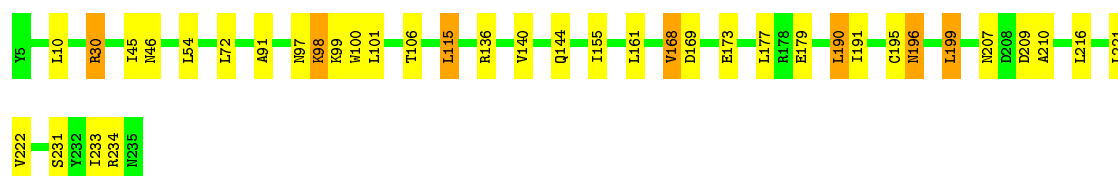
• Molecule 1: 16S rRNA





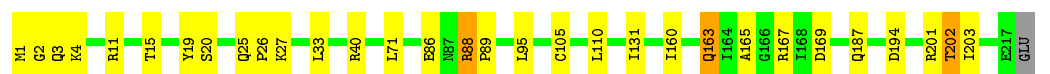
• Molecule 2: Ribosomal Protein S2

Chain AB: 84% 13%



• Molecule 3: Ribosomal Protein S3

Chain AC: 85% 13%



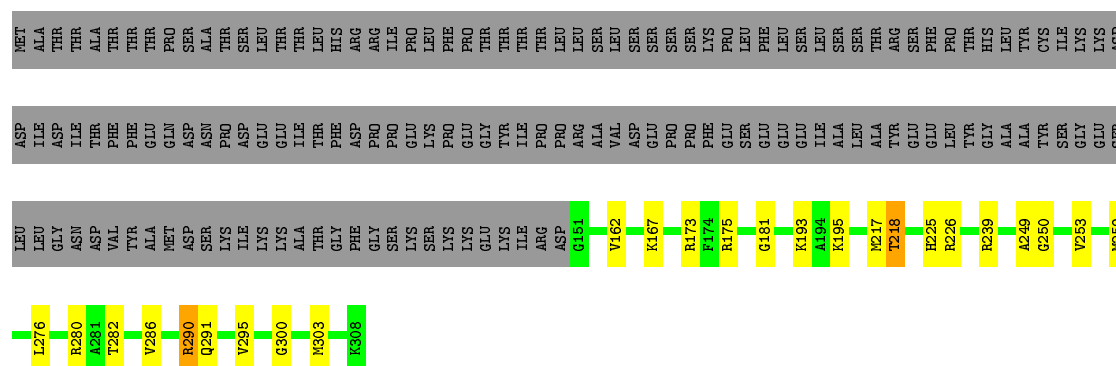
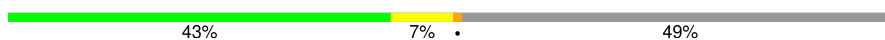
• Molecule 4: Ribosomal Protein S4

Chain AD: 84% 15%



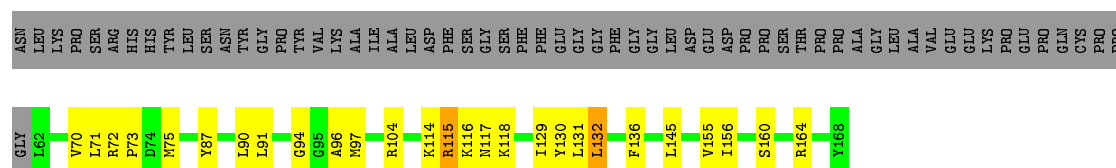
• Molecule 5: Ribosomal Protein S5

Chain AE:



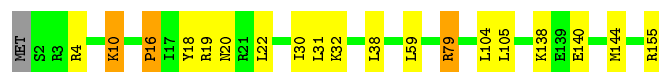
- Molecule 6: Ribosomal Protein S6

Chain AF:



- Molecule 7: Ribosomal Protein S7

Chain AG:



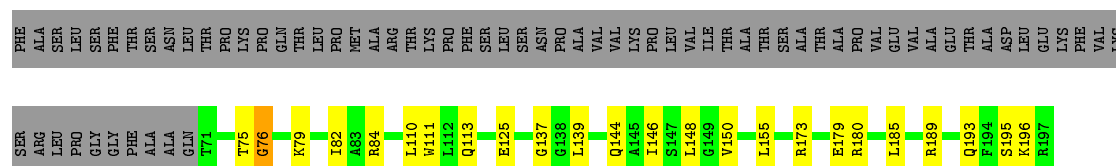
- Molecule 8: Ribosomal Protein S8

Chain AH:



- Molecule 9: Ribosomal Protein S9

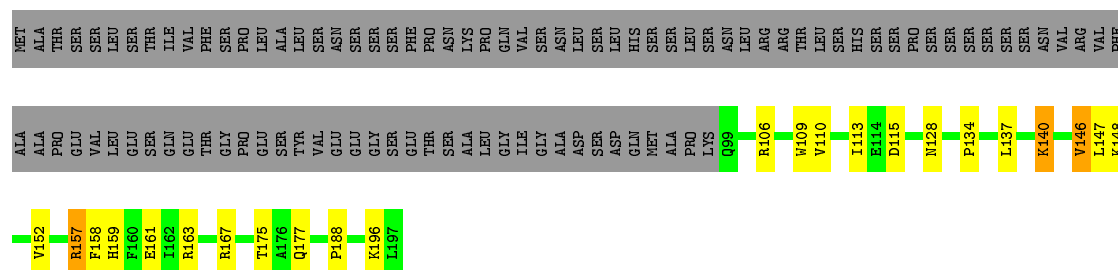
Chain AI:



- Molecule 10: Ribosomal Protein S10

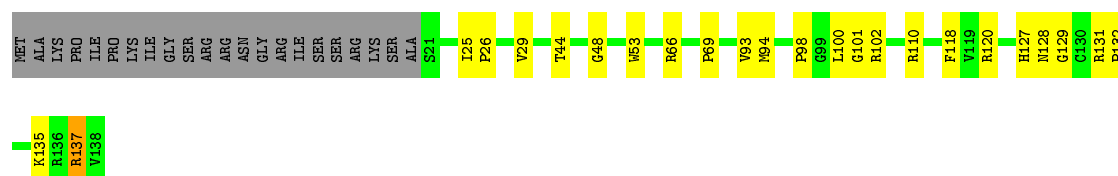
Chain AJ:





- Molecule 11: Ribosomal Protein S11

Chain AK: 67% 16% 16%



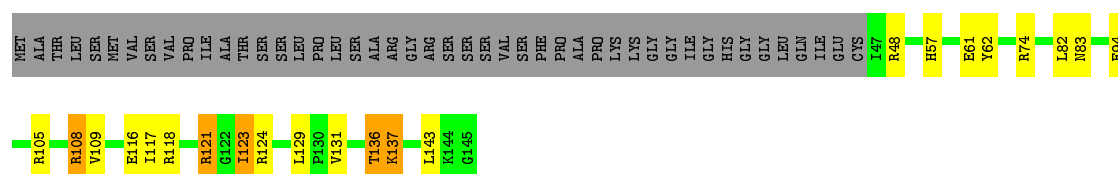
- Molecule 12: Ribosomal Protein S12

Chain AL: 82% 15%



- Molecule 13: Ribosomal Protein S13

Chain AM: 53% 12% 32%



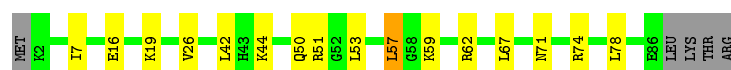
- Molecule 14: Ribosomal Protein S14

Chain AN: 76% 20%



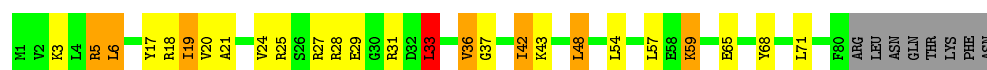
- Molecule 15: Ribosomal Protein S15

Chain AO: 77% 17% 6%



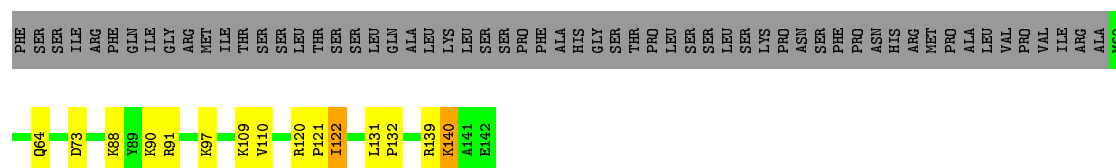
- Molecule 16: Ribosomal Protein S16

Chain AP: 



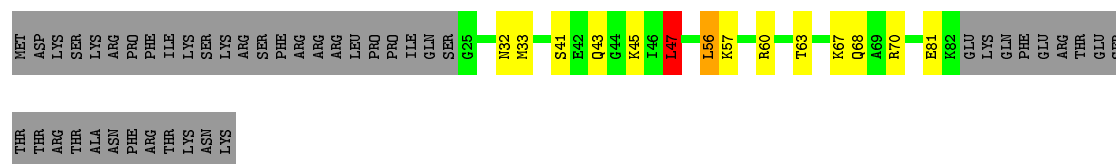
• Molecule 17: Ribosomal Protein S17

Chain AQ: 




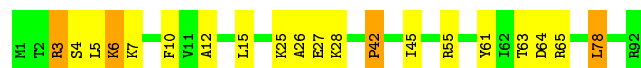
• Molecule 18: Ribosomal Protein S18

Chain AR: 



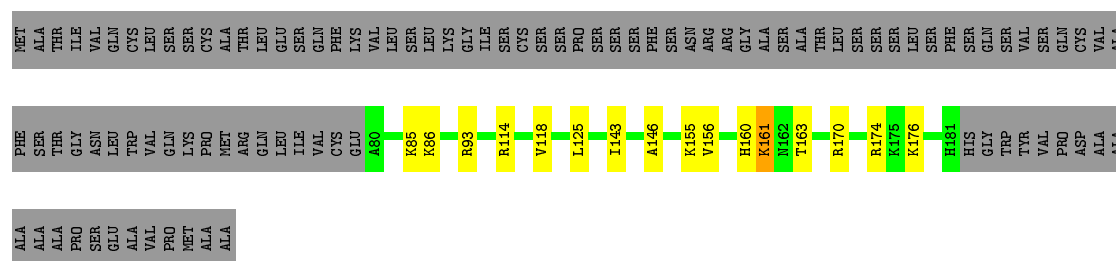
• Molecule 19: Ribosomal Protein S19

Chain AS: 



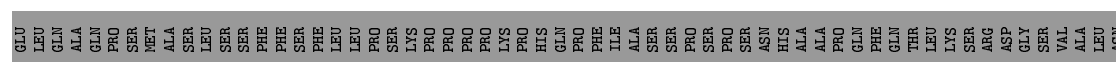
• Molecule 20: Ribosomal Protein S20

Chain AT: 

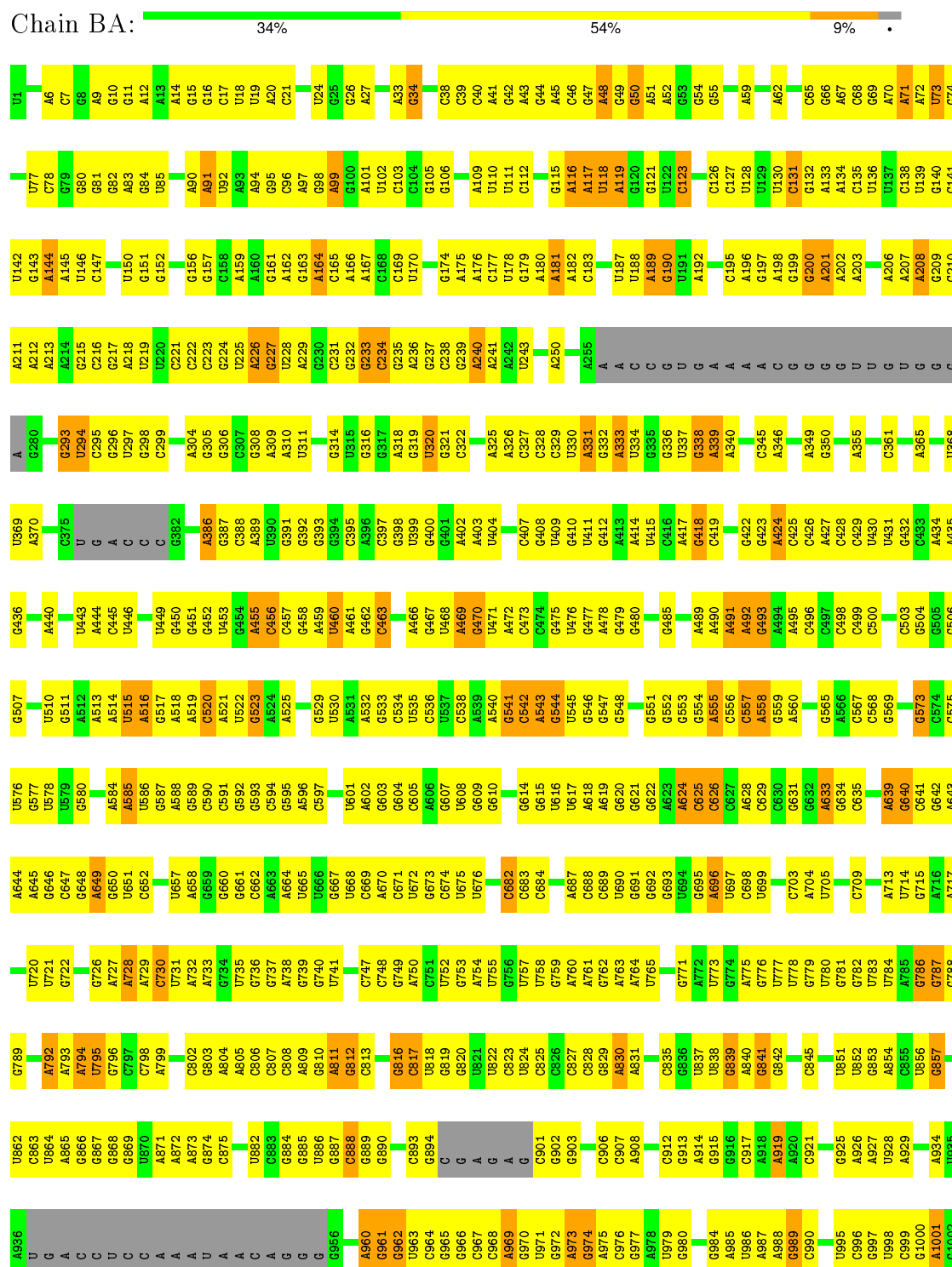


• Molecule 21: Ribosomal Protein S21

Chain AU: 

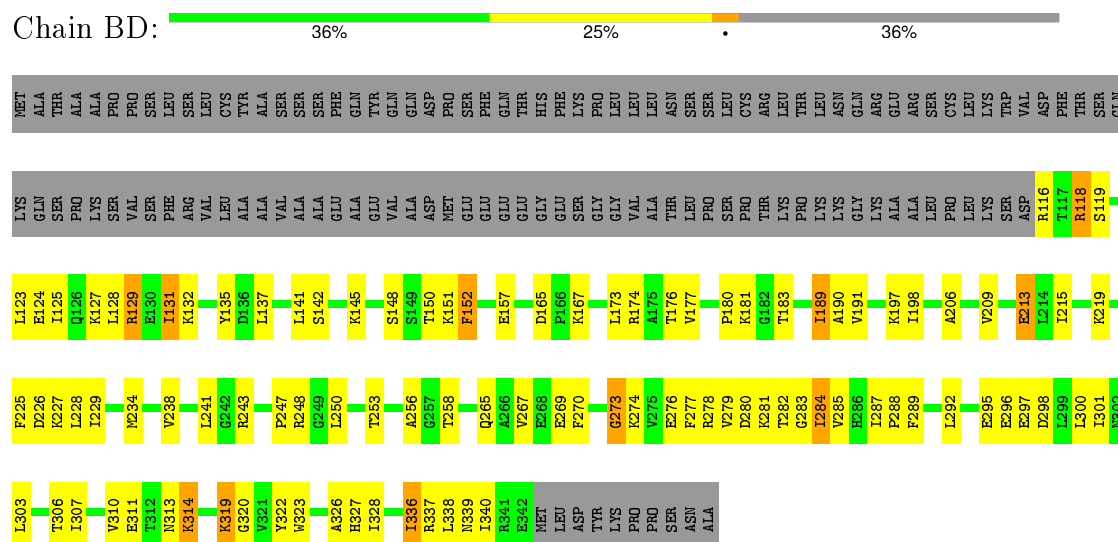


- Molecule 22: 23S rRNA

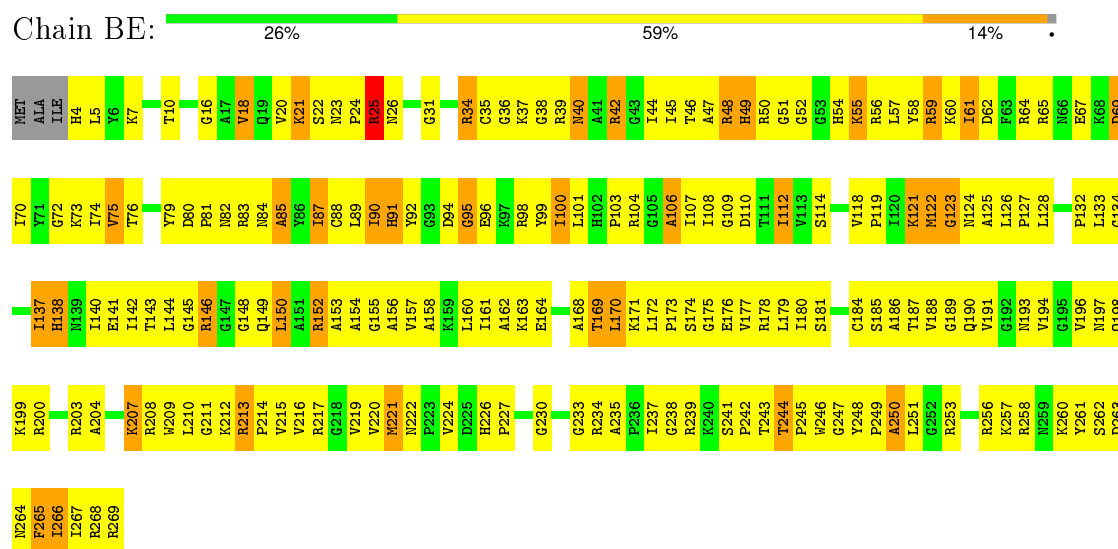




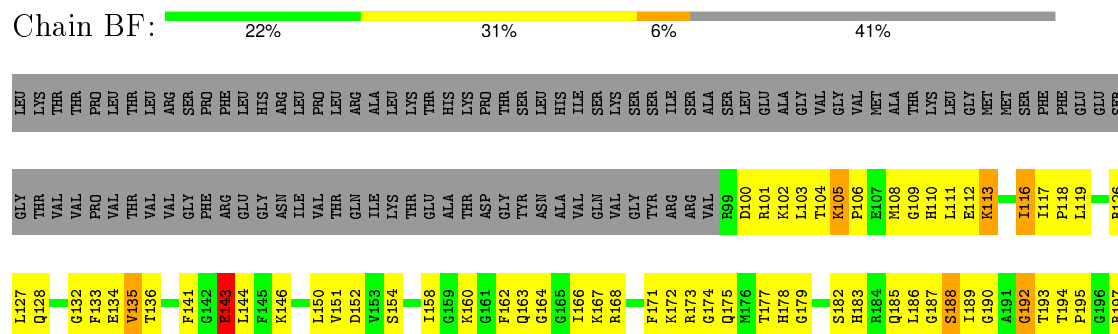

- Molecule 25: Ribosomal Protein L1



- Molecule 26: Ribosomal Protein L2



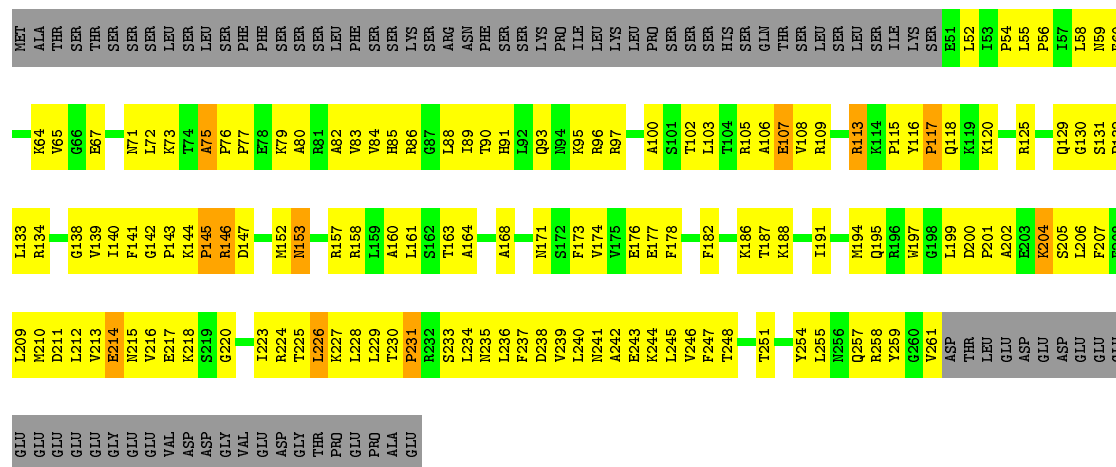
- Molecule 27: Ribosomal Protein L3





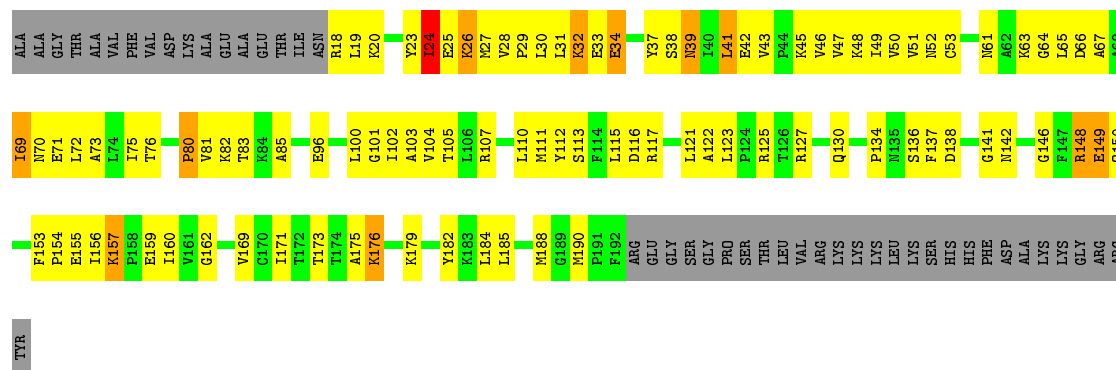
• Molecule 28: Ribosomal Protein L4

Chain BG: 26% 43% • 28%



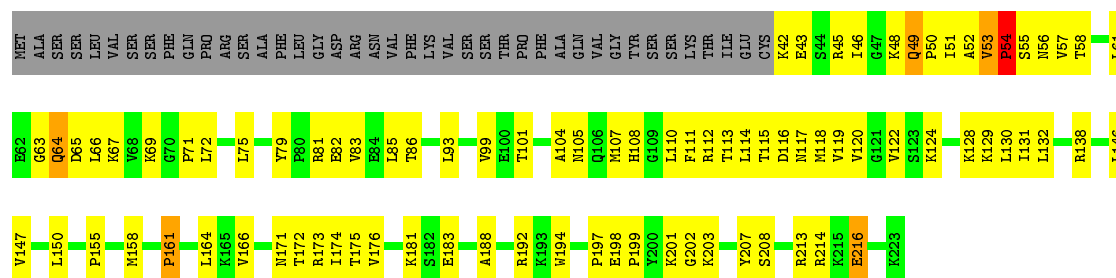
• Molecule 29: Ribosomal Protein L5

Chain BH: 35% 39% 5% 20%

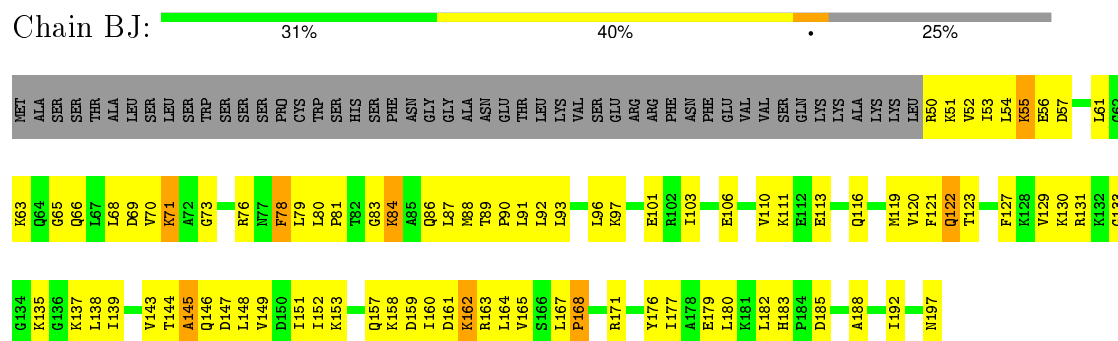


• Molecule 30: Ribosomal Protein L6

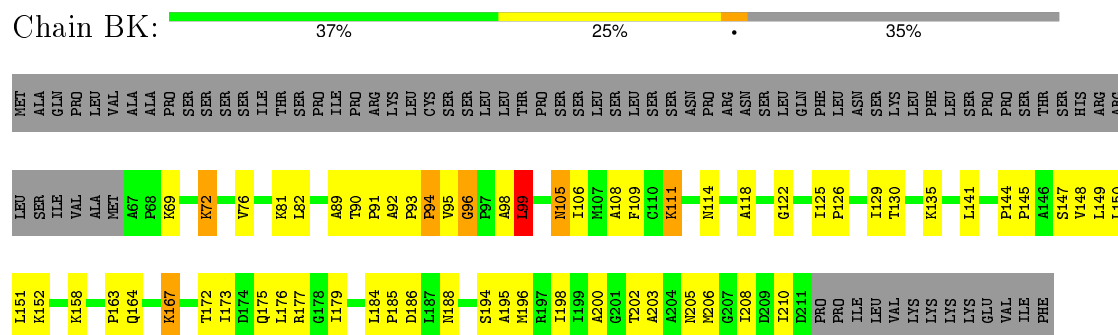
Chain BI: 43% 36% • 18%



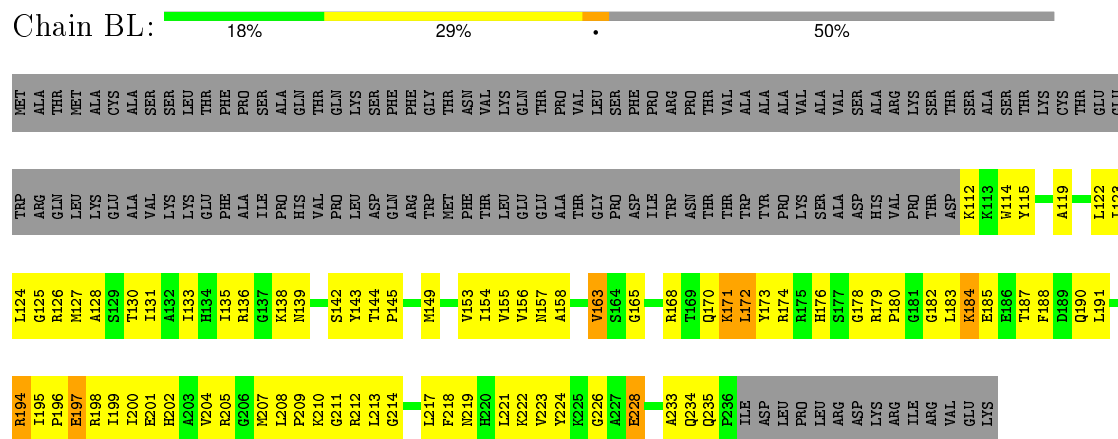
• Molecule 31: Ribosomal Protein L9



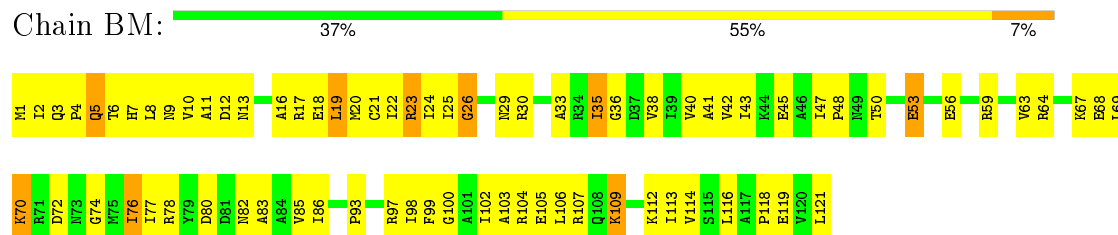
- Molecule 32: Ribosomal Protein L11



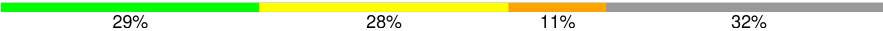
- Molecule 33: Ribosomal Protein L13

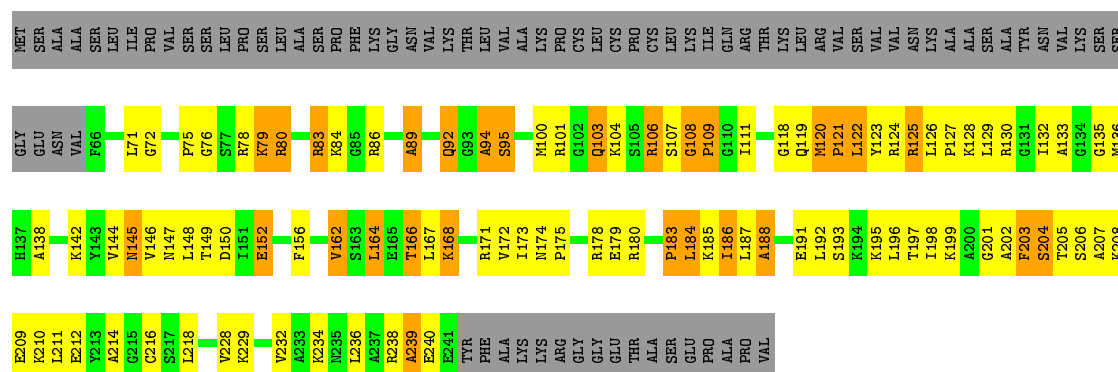


- Molecule 34: Ribosomal Protein L14



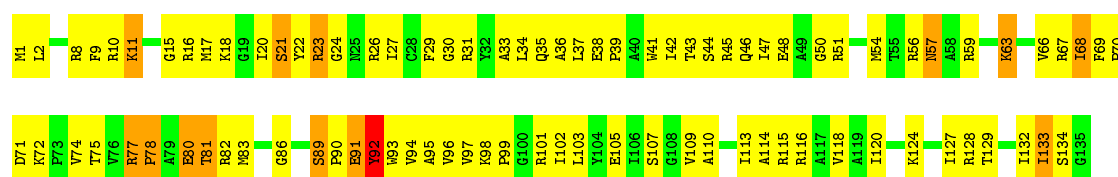
- Molecule 35: Ribosomal Protein L15

Chain BN: 




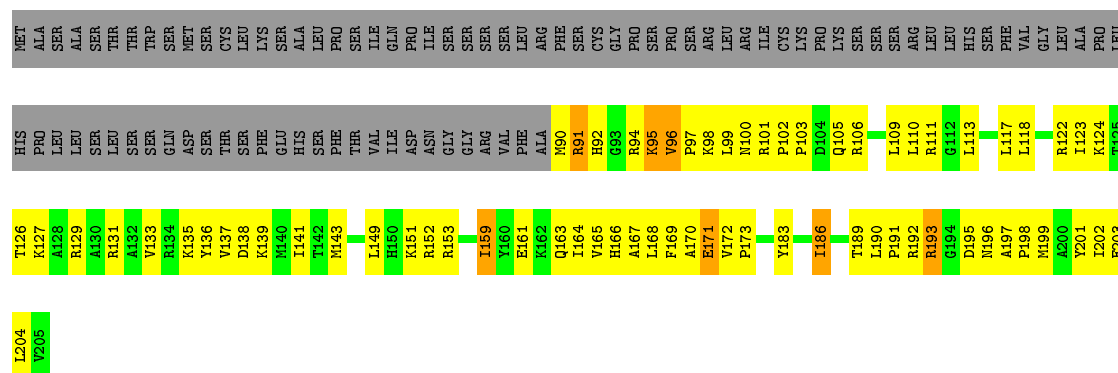
• Molecule 36: Ribosomal Protein L16

Chain BO: 




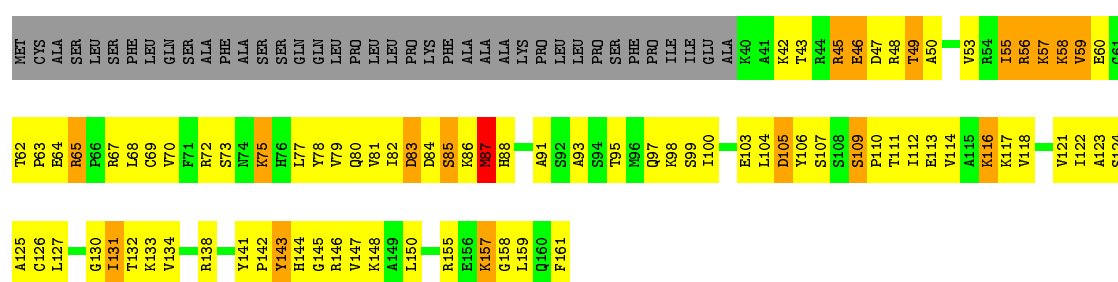
• Molecule 37: Ribosomal Protein L17

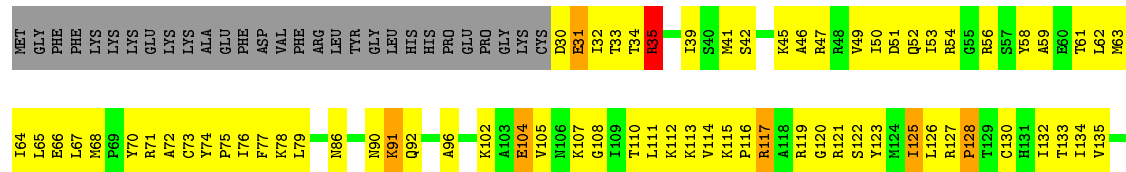
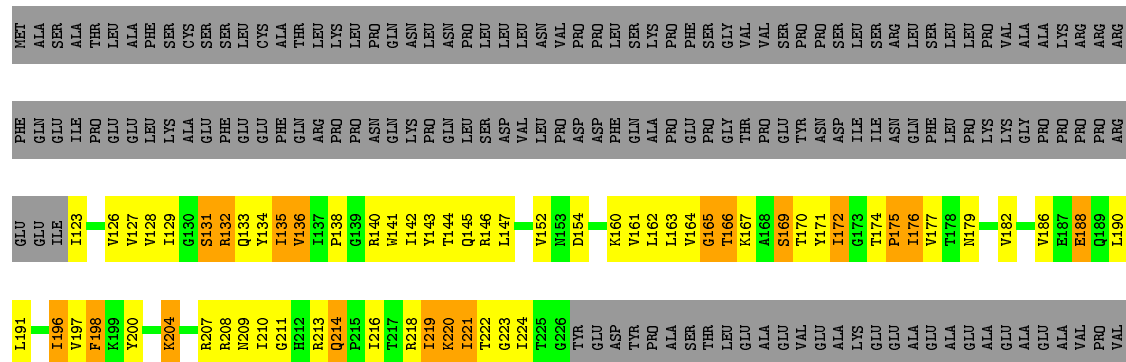
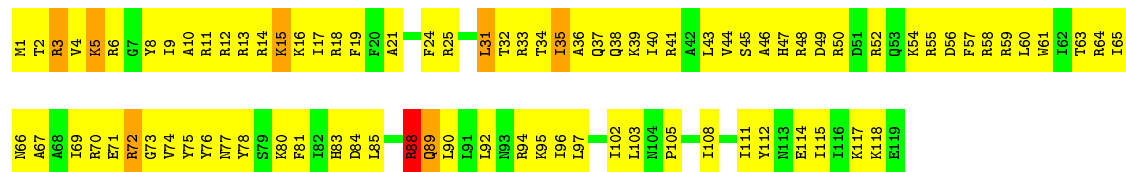
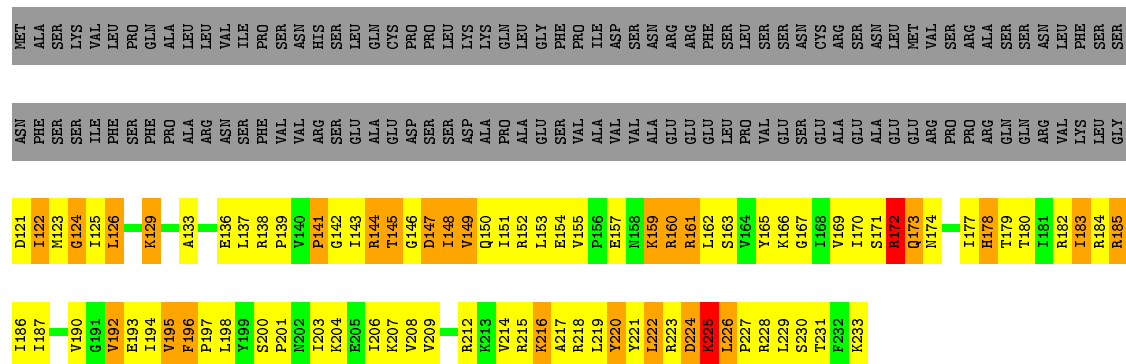
Chain BP: 

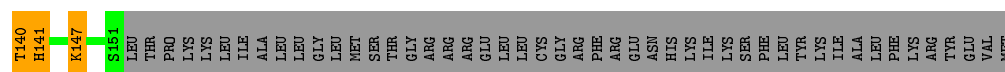


• Molecule 38: Ribosomal Protein L18

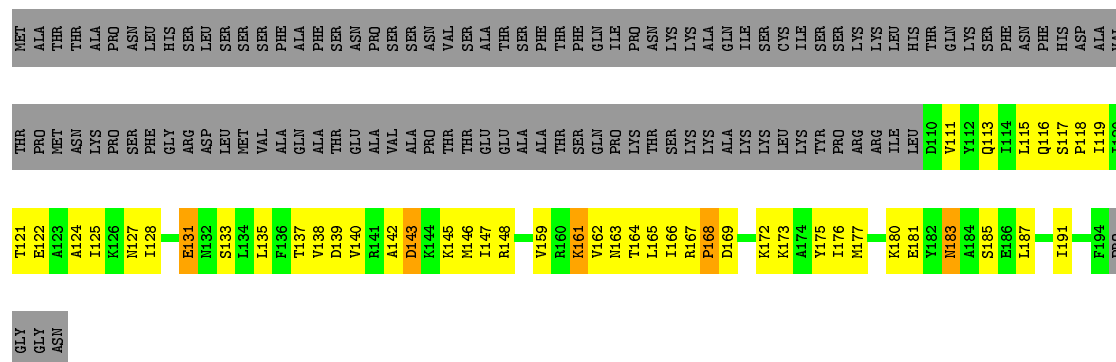
Chain BQ: 



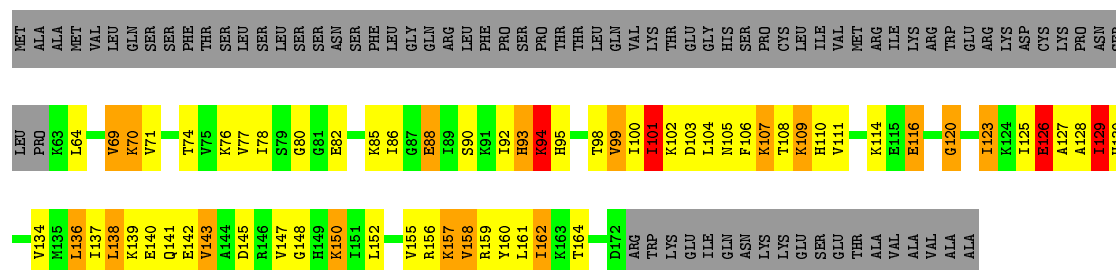




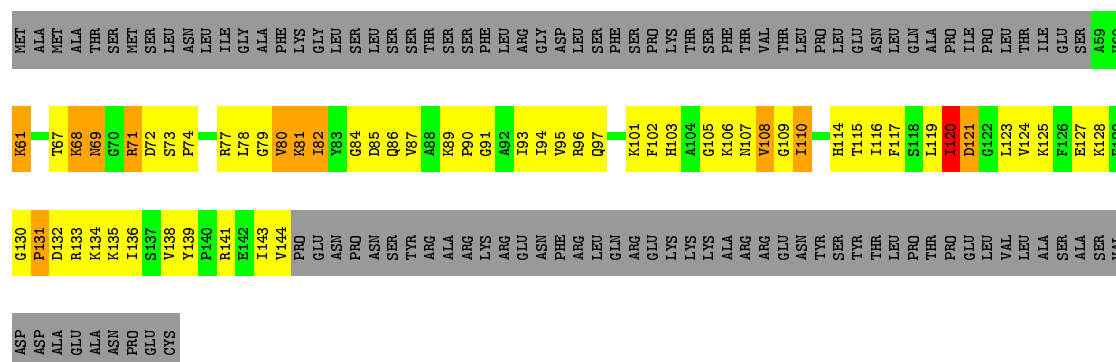
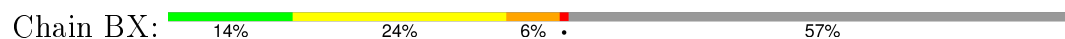
• Molecule 43: Ribosomal Protein L23



• Molecule 44: Ribosomal Protein L24



• Molecule 45: Ribosomal Protein L27



• Molecule 46: Ribosomal Protein L28



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	CTF correction for each Micrograph	Depositor
Microscope	Phillips Tecnai F20 FEG	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2000	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	50000	Depositor
Image detector	Kodak S0163 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	0.22	0/35552	0.66	1/55472 (0.0%)
10	AJ	0.59	0/820	0.69	0/1108
11	AK	0.57	0/902	0.68	0/1214
12	AL	0.56	0/984	0.71	1/1323 (0.1%)
13	AM	0.60	0/833	0.78	1/1108 (0.1%)
14	AN	0.53	0/836	0.77	0/1116
15	AO	0.63	0/721	0.69	0/956
16	AP	0.72	0/674	0.86	2/902 (0.2%)
17	AQ	0.57	0/672	0.69	1/898 (0.1%)
18	AR	0.57	0/481	0.79	1/641 (0.2%)
19	AS	0.59	0/762	0.67	0/1021
2	AB	0.62	0/1860	0.69	3/2512 (0.1%)
20	AT	0.47	0/803	0.64	0/1063
21	AU	0.59	0/458	0.76	0/608
22	BA	0.13	0/65708	0.63	0/102501
23	BB	0.13	0/2793	0.63	0/4353
24	BC	0.13	0/2472	0.63	0/3854
25	BD	0.24	0/1786	0.40	0/2397
26	BE	0.21	0/2085	0.42	0/2800
27	BF	0.24	0/1214	0.42	0/1613
28	BG	0.25	0/1696	0.43	0/2283
29	BH	0.24	0/1372	0.41	0/1848
3	AC	0.63	0/1771	0.75	3/2380 (0.1%)
30	BI	0.23	0/1451	0.42	0/1944
31	BJ	0.24	0/1189	0.40	0/1589
32	BK	0.23	0/1077	0.43	0/1456
33	BL	0.23	0/1019	0.40	0/1369
34	BM	0.22	0/952	0.42	0/1282
35	BN	0.23	0/1354	0.40	0/1806
36	BO	0.24	0/1098	0.41	0/1471
37	BP	0.23	0/964	0.41	0/1288
38	BQ	0.23	0/976	0.41	0/1305
39	BR	0.22	0/929	0.46	0/1248
4	AD	0.61	0/1660	0.74	1/2228 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	BS	0.24	0/1047	0.40	0/1394
41	BT	0.23	0/839	0.43	0/1135
42	BU	0.23	0/1003	0.40	0/1348
43	BV	0.24	0/685	0.40	0/920
44	BW	0.21	0/878	0.42	0/1171
45	BX	0.25	0/672	0.41	0/896
46	BY	0.25	0/629	0.44	0/835
47	BZ	0.25	0/553	0.40	0/728
48	B1	0.26	0/594	0.37	0/797
49	B2	0.28	0/478	0.39	0/633
5	AE	0.56	0/1204	0.64	0/1620
50	B3	0.23	0/532	0.40	0/708
51	B4	0.25	0/298	0.39	0/390
52	B5	0.23	0/509	0.38	0/672
53	B6	0.25	0/312	0.37	0/409
6	AF	0.71	0/887	0.76	2/1195 (0.2%)
7	AG	0.56	0/1227	0.70	2/1641 (0.1%)
8	AH	0.59	0/1103	0.70	0/1477
9	AI	0.63	0/1004	0.75	1/1347 (0.1%)
All	All	0.27	0/154378	0.62	19/230273 (0.0%)

There are no bond length outliers.

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	AF	132	LEU	CA-CB-CG	7.67	132.94	115.30
13	AM	82	LEU	CA-CB-CG	7.39	132.30	115.30
16	AP	6	LEU	CA-CB-CG	7.02	131.45	115.30
7	AG	31	LEU	CA-CB-CG	6.96	131.32	115.30
16	AP	33	LEU	CA-CB-CG	6.96	131.30	115.30

There are no chirality outliers.

There are no planarity outliers.

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	31745	0	15984	1134	0
2	AB	1827	0	1867	17	0
3	AC	1744	0	1831	18	0
4	AD	1632	0	1734	17	0
5	AE	1190	0	1245	18	0
6	AF	872	0	884	41	0
7	AG	1211	0	1284	11	0
8	AH	1088	0	1149	14	0
9	AI	988	0	1047	12	0
10	AJ	803	0	845	14	0
11	AK	888	0	933	10	0
12	AL	968	0	1046	12	0
13	AM	824	0	872	26	0
14	AN	820	0	858	13	0
15	AO	713	0	765	48	0
16	AP	664	0	703	13	0
17	AQ	662	0	715	11	0
18	AR	478	0	519	14	0
19	AS	747	0	787	22	0
20	AT	799	0	879	11	0
21	AU	455	0	466	10	0
22	BA	58665	0	29550	2028	0
23	BB	2497	0	1264	51	0
24	BC	2207	0	1114	89	0
25	BD	1760	0	1834	107	0
26	BE	2049	0	2128	412	0
27	BF	1196	0	1282	135	0
28	BG	1664	0	1731	187	0
29	BH	1351	0	1405	129	0
30	BI	1429	0	1510	94	0
31	BJ	1177	0	1259	86	0
32	BK	1060	0	1129	59	0
33	BL	998	0	1038	94	0
34	BM	943	0	996	101	0
35	BN	1333	0	1406	155	0
36	BO	1076	0	1134	127	0
37	BP	948	0	1009	96	0
38	BQ	962	0	992	120	0
39	BR	915	0	1001	153	0
40	BS	1030	0	1100	150	0
41	BT	826	0	900	83	0
42	BU	986	0	1025	106	0
43	BV	677	0	716	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	BW	869	0	929	107	0
45	BX	660	0	693	92	0
46	BY	619	0	672	97	0
47	BZ	551	0	587	38	0
48	B1	581	0	562	46	0
49	B2	469	0	516	77	0
50	B3	524	0	557	64	0
51	B4	297	0	336	40	0
52	B5	504	0	559	77	0
53	B6	309	0	340	25	0
All	All	142250	0	97687	5825	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 24.

The worst 5 of 5825 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)
1:AA:755:U:H3	26:BE:5:LEU:CD1	1.02	1.62
1:AA:1423:G:C4'	22:BA:1737:A:C2	1.80	1.61
15:AO:44:LYS:HE3	26:BE:7:LYS:CE	1.25	1.61
1:AA:660:A:C5'	26:BE:161:ILE:HA	1.32	1.54
1:AA:1423:G:H4'	22:BA:1737:A:C2	1.37	1.49

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	229/231 (99%)	201 (88%)	25 (11%)	3 (1%)	15 60
3	AC	215/218 (99%)	179 (83%)	29 (14%)	7 (3%)	5 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	197/201 (98%)	179 (91%)	17 (9%)	1 (0%)	34	77
5	AE	156/308 (51%)	138 (88%)	16 (10%)	2 (1%)	15	60
6	AF	105/168 (62%)	92 (88%)	10 (10%)	3 (3%)	6	43
7	AG	152/155 (98%)	136 (90%)	14 (9%)	2 (1%)	15	60
8	AH	132/134 (98%)	118 (89%)	13 (10%)	1 (1%)	24	69
9	AI	125/197 (64%)	110 (88%)	13 (10%)	2 (2%)	12	56
10	AJ	97/197 (49%)	85 (88%)	10 (10%)	2 (2%)	9	50
11	AK	116/140 (83%)	95 (82%)	16 (14%)	5 (4%)	3	34
12	AL	121/123 (98%)	99 (82%)	17 (14%)	5 (4%)	3	35
13	AM	97/145 (67%)	75 (77%)	15 (16%)	7 (7%)	1	22
14	AN	97/100 (97%)	83 (86%)	13 (13%)	1 (1%)	19	65
15	AO	83/90 (92%)	77 (93%)	6 (7%)	0	100	100
16	AP	78/88 (89%)	59 (76%)	12 (15%)	7 (9%)	1	17
17	AQ	81/142 (57%)	69 (85%)	11 (14%)	1 (1%)	16	61
18	AR	56/103 (54%)	51 (91%)	4 (7%)	1 (2%)	11	53
19	AS	90/92 (98%)	75 (83%)	12 (13%)	3 (3%)	5	40
20	AT	100/202 (50%)	93 (93%)	7 (7%)	0	100	100
21	AU	51/190 (27%)	37 (72%)	10 (20%)	4 (8%)	1	20
25	BD	225/352 (64%)	189 (84%)	33 (15%)	3 (1%)	15	60
26	BE	264/269 (98%)	126 (48%)	94 (36%)	44 (17%)	0	5
27	BF	152/259 (59%)	91 (60%)	32 (21%)	29 (19%)	0	3
28	BG	209/293 (71%)	159 (76%)	39 (19%)	11 (5%)	2	29
29	BH	173/220 (79%)	130 (75%)	32 (18%)	11 (6%)	2	25
30	BI	180/223 (81%)	143 (79%)	30 (17%)	7 (4%)	4	36
31	BJ	146/197 (74%)	105 (72%)	33 (23%)	8 (6%)	2	29
32	BK	143/224 (64%)	115 (80%)	22 (15%)	6 (4%)	3	34
33	BL	123/250 (49%)	92 (75%)	24 (20%)	7 (6%)	2	28
34	BM	119/121 (98%)	96 (81%)	20 (17%)	3 (2%)	7	46
35	BN	174/257 (68%)	98 (56%)	48 (28%)	28 (16%)	0	5
36	BO	133/135 (98%)	93 (70%)	30 (23%)	10 (8%)	1	21
37	BP	114/205 (56%)	94 (82%)	16 (14%)	4 (4%)	4	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	BQ	120/161 (74%)	81 (68%)	23 (19%)	16 (13%)	0	7
39	BR	111/233 (48%)	66 (60%)	25 (22%)	20 (18%)	0	4
40	BS	117/119 (98%)	96 (82%)	12 (10%)	9 (8%)	1	20
41	BT	102/257 (40%)	62 (61%)	23 (22%)	17 (17%)	0	5
42	BU	120/199 (60%)	92 (77%)	20 (17%)	8 (7%)	1	24
43	BV	83/198 (42%)	63 (76%)	15 (18%)	5 (6%)	2	26
44	BW	108/191 (56%)	59 (55%)	34 (32%)	15 (14%)	0	6
45	BX	84/198 (42%)	52 (62%)	21 (25%)	11 (13%)	0	7
46	BY	74/151 (49%)	43 (58%)	20 (27%)	11 (15%)	0	5
47	BZ	63/173 (36%)	58 (92%)	5 (8%)	0	100	100
48	B1	70/144 (49%)	52 (74%)	14 (20%)	4 (6%)	2	28
49	B2	55/57 (96%)	32 (58%)	11 (20%)	12 (22%)	0	2
50	B3	63/66 (96%)	33 (52%)	23 (36%)	7 (11%)	0	11
51	B4	35/152 (23%)	28 (80%)	7 (20%)	0	100	100
52	B5	60/159 (38%)	39 (65%)	15 (25%)	6 (10%)	1	14
53	B6	36/104 (35%)	26 (72%)	6 (17%)	4 (11%)	0	11
All	All	5834/8791 (66%)	4464 (76%)	997 (17%)	373 (6%)	3	25

5 of 373 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	88	ARG
3	AC	89	PRO
3	AC	202	THR
5	AE	218	THR
6	AF	155	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	
2	AB	196/196 (100%)	177 (90%)	19 (10%)	10	40
3	AC	187/188 (100%)	177 (95%)	10 (5%)	28	64
4	AD	178/180 (99%)	167 (94%)	11 (6%)	23	60
5	AE	121/255 (48%)	118 (98%)	3 (2%)	55	81
6	AF	95/144 (66%)	84 (88%)	11 (12%)	7	32
7	AG	125/126 (99%)	113 (90%)	12 (10%)	10	40
8	AH	117/117 (100%)	105 (90%)	12 (10%)	9	37
9	AI	101/159 (64%)	93 (92%)	8 (8%)	15	51
10	AJ	91/178 (51%)	79 (87%)	12 (13%)	5	28
11	AK	92/110 (84%)	86 (94%)	6 (6%)	21	58
12	AL	106/106 (100%)	98 (92%)	8 (8%)	17	53
13	AM	90/126 (71%)	80 (89%)	10 (11%)	8	34
14	AN	89/90 (99%)	77 (86%)	12 (14%)	5	27
15	AO	80/85 (94%)	75 (94%)	5 (6%)	22	59
16	AP	71/79 (90%)	58 (82%)	13 (18%)	2	14
17	AQ	72/125 (58%)	67 (93%)	5 (7%)	19	56
18	AR	54/98 (55%)	49 (91%)	5 (9%)	11	42
19	AS	81/81 (100%)	74 (91%)	7 (9%)	13	47
20	AT	80/163 (49%)	72 (90%)	8 (10%)	9	38
21	AU	49/170 (29%)	46 (94%)	3 (6%)	23	60
25	BD	190/297 (64%)	181 (95%)	9 (5%)	32	68
26	BE	212/214 (99%)	205 (97%)	7 (3%)	45	76
27	BF	127/217 (58%)	123 (97%)	4 (3%)	47	77
28	BG	177/254 (70%)	172 (97%)	5 (3%)	51	78
29	BH	148/183 (81%)	139 (94%)	9 (6%)	23	60
30	BI	156/192 (81%)	152 (97%)	4 (3%)	54	80
31	BJ	128/171 (75%)	125 (98%)	3 (2%)	58	83
32	BK	114/189 (60%)	109 (96%)	5 (4%)	35	69
33	BL	104/213 (49%)	101 (97%)	3 (3%)	50	78
34	BM	101/101 (100%)	94 (93%)	7 (7%)	19	56
35	BN	136/203 (67%)	126 (93%)	10 (7%)	17	54
36	BO	108/108 (100%)	100 (93%)	8 (7%)	17	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BP	97/177 (55%)	92 (95%)	5 (5%)	29	65
38	BQ	103/135 (76%)	94 (91%)	9 (9%)	13	45
39	BR	100/207 (48%)	89 (89%)	11 (11%)	8	34
40	BS	106/106 (100%)	101 (95%)	5 (5%)	32	68
41	BT	90/224 (40%)	86 (96%)	4 (4%)	35	69
42	BU	108/176 (61%)	104 (96%)	4 (4%)	41	73
43	BV	74/171 (43%)	72 (97%)	2 (3%)	52	79
44	BW	98/171 (57%)	88 (90%)	10 (10%)	9	37
45	BX	68/167 (41%)	62 (91%)	6 (9%)	12	45
46	BY	66/133 (50%)	63 (96%)	3 (4%)	34	69
47	BZ	61/149 (41%)	55 (90%)	6 (10%)	10	39
48	B1	62/126 (49%)	61 (98%)	1 (2%)	70	88
49	B2	50/50 (100%)	46 (92%)	4 (8%)	15	50
50	B3	59/60 (98%)	55 (93%)	4 (7%)	20	57
51	B4	31/125 (25%)	29 (94%)	2 (6%)	21	58
52	B5	53/140 (38%)	50 (94%)	3 (6%)	25	62
53	B6	36/87 (41%)	36 (100%)	0	100	100
All	All	5038/7522 (67%)	4705 (93%)	333 (7%)	25	57

5 of 333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
16	AP	59	LYS
25	BD	314	LYS
45	BX	81	LYS
17	AQ	122	ILE
20	AT	85	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
29	BH	130	GLN
32	BK	105	ASN
49	B2	53	ASN
29	BH	140	HIS

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Mol	Chain	Res	Type
30	BI	159	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1477/1491 (99%)	245 (16%)	51 (3%)
22	BA	2726/2810 (97%)	387 (14%)	12 (0%)
23	BB	116/117 (99%)	12 (10%)	0
24	BC	102/103 (99%)	14 (13%)	0
All	All	4421/4521 (97%)	658 (14%)	63 (1%)

5 of 658 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	A
1	AA	10	G
1	AA	14	U
1	AA	15	C
1	AA	32	G

5 of 63 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AA	862	A
1	AA	1014	U
22	BA	1878	C
1	AA	883	C
1	AA	924	A

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

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

5.5 Carbohydrates ⓘ

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](#)

There are no chain breaks in this entry.