



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 17, 2024 – 04:17 AM EST

PDB ID : 4V4Y
Title : Crystal structure of the 70S *Thermus thermophilus* ribosome with translocated and rotated Shine-Dalgarno Duplex.
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.
Deposited on : 2006-06-27
Resolution : 5.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

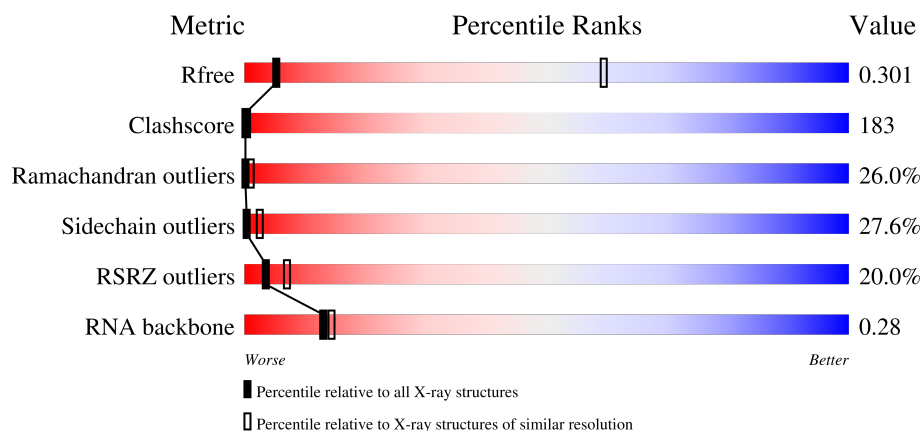
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1029 (7.00-4.00)
Clashscore	180529	1069 (7.00-4.00)
Ramachandran outliers	177936	1010 (7.04-3.96)
Sidechain outliers	177891	1004 (7.04-3.94)
RSRZ outliers	164620	1023 (7.00-4.00)
RNA backbone	3690	1172 (7.80-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1522	<div> <div>9%</div> <div>56%</div> <div>34%</div> <div>8%</div> </div>
2	A1	50	<div> <div>68%</div> <div>48%</div> <div>48%</div> </div>
3	AB	76	<div> <div>49%</div> <div>7%</div> <div>50%</div> <div>36%</div> <div>8%</div> </div>
3	AC	76	<div> <div>3%</div> <div>59%</div> <div>34%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
3	AD	76	
4	AE	256	
5	AF	239	
6	AG	209	
7	AH	162	
8	AI	101	
9	AJ	156	
10	AK	138	
11	AL	128	
12	AM	105	
13	AN	129	
14	AO	132	
15	AP	126	
16	AQ	61	
17	AR	89	
18	AS	88	
19	AT	105	
20	AU	88	
21	AV	93	
22	AW	106	
23	AX	27	
24	BA	2916	
25	BB	123	
26	BC	229	
27	BD	276	

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Mol	Chain	Length	Quality of chain
28	BE	206	
29	BF	210	
30	BG	182	
31	BH	180	
32	BK	148	
33	BL	147	
34	BM	140	
35	BN	122	
36	BO	150	
37	BP	141	
38	BQ	118	
39	BR	112	
40	BS	146	
41	BT	118	
42	BU	101	
43	BV	113	
44	BW	96	
45	BX	110	
46	BY	206	
47	BZ	85	
48	B1	67	
49	B2	60	
50	B3	71	
51	B4	60	
52	B5	54	

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Mol	Chain	Length	Quality of chain
53	B6	49	<p>12% 53% 37% 10%</p>
54	B7	65	<p>3% 52% 38% 8%</p>
55	B8	37	<p>14% 8% 57% 30% 5%</p>

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 151691 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	AA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 2 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A1	50	Total	C	N	O	P	0	0	0
			1025	459	128	388	50			

- Molecule 3 is a RNA chain called tRNA PHE (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
3	AD	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
3	AB	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	98	Total	C	N	O	S	0	0	0
			794	499	156	138	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
20	AU	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 23 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	AX	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 24 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2889	Total	C	N	O	P	0	0	0
			62218	27691	11629	20009	2889			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	493	G	-	insertion	GB 48268

- Molecule 25 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BB	123	Total	C	N	O	P	0	0	0
			2641	1175	488	855	123			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BB	-1	A	-	insertion	GB 48271

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Chain	Residue	Modelled	Actual	Comment	Reference
BB	120	U	-	insertion	GB 48271

- Molecule 26 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BC	228	Total	C	N	O	S	0	0	0
			1742	1102	318	319	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BD	272	Total	C	N	O	S	0	0	0
			2124	1339	424	358	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BE	206	Total	C	N	O	S	0	0	0
			1578	997	302	273	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	208	Total	C	N	O	S	0	0	0
			1625	1034	303	286	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BG	182	Total	C	N	O	S	0	0	0
			1482	947	269	261	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BH	174	Total	C	N	O	S	0	0	0
			1328	844	248	235	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	148	Total	C	N	O	S	0	0	0
			1155	737	205	212	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	138	Total	C	N	O	S	0	0	0
			1025	654	181	185	5			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BM	139	Total	C	N	O	S	0	0	0
			1113	717	207	186	3			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	122	Total	C	N	O	S	0	0	0
			932	587	171	170	4			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	145	Total	C	N	O	S	0	0	0
			1106	688	226	190	2			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BP	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	BR	110	Total	C	N	O			
			877	553	175	149	0	0	0

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BS	117	Total	C	N	O	S			
			976	614	197	164	1	0	0	0

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	117	Total	C	N	O	S			
			964	610	202	151	1	0	0	0

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	101	Total	C	N	O	S			
			779	501	142	135	1	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BV	110	Total	C	N	O	S			
			876	552	171	151	2	0	0	0

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	94	Total	C	N	O			
			742	483	133	126	0	0	0

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BX	110	Total	C	N	O	S			
			844	539	158	141	6	0	0	0

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BY	180	Total	C	N	O	S	0	0	0
			1435	916	256	260	3			

- Molecule 47 is a protein called Ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BZ	85	Total	C	N	O	S	0	0	0
			670	415	141	112	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	B1	67	Total	C	N	O	S	0	0	0
			567	350	116	99	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	59	Total	C	N	O	S	0	0	0
			469	298	90	81				

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	57	Total	C	N	O	S	0	0	0
			445	279	87	74	5			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B5	49	Total	C	N	O	S	0	0	0
			426	265	87	70	4			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B7	64	Total	C	N	O	S	0	0	0
			515	331	102	79	3			

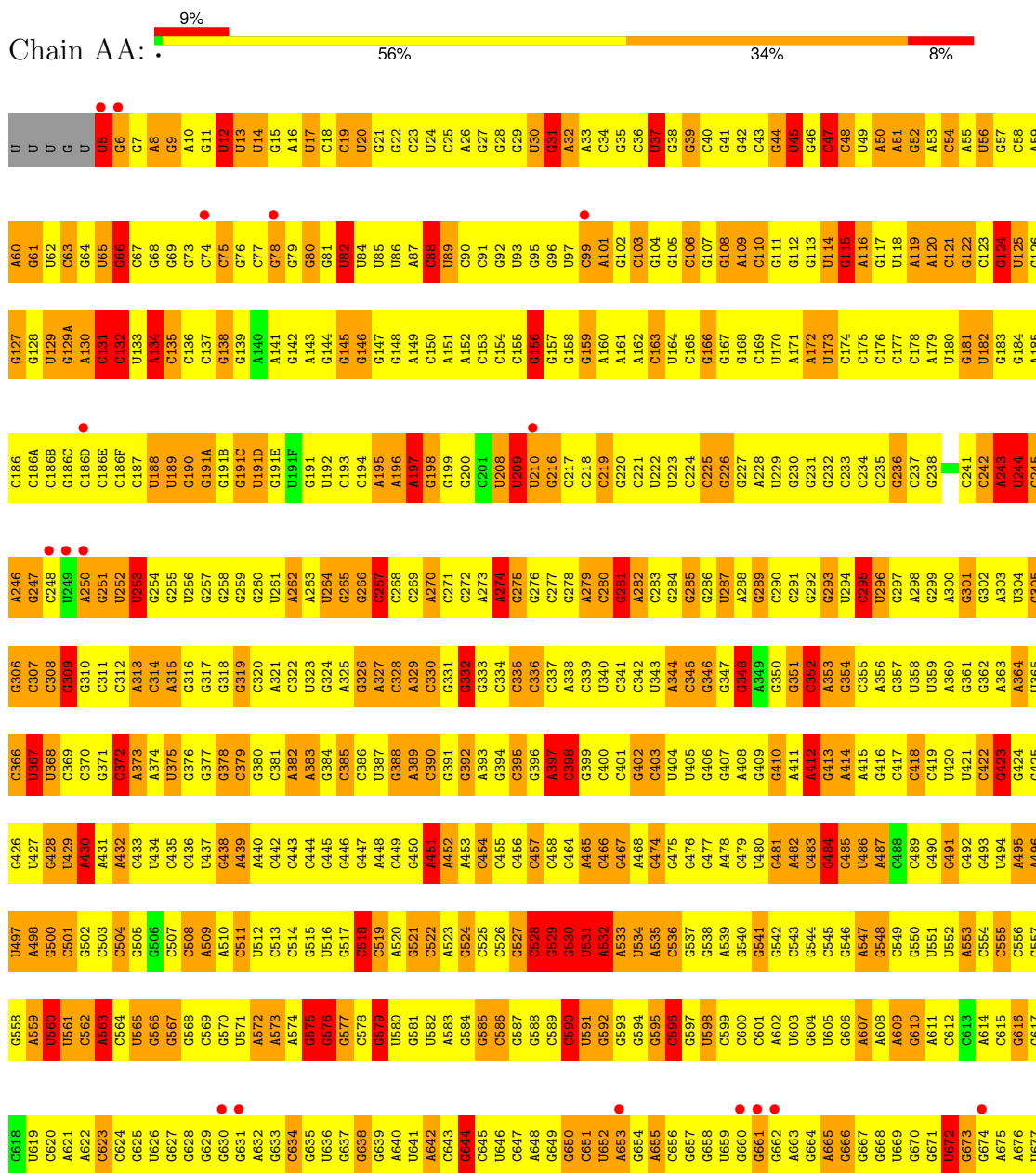
- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B8	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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

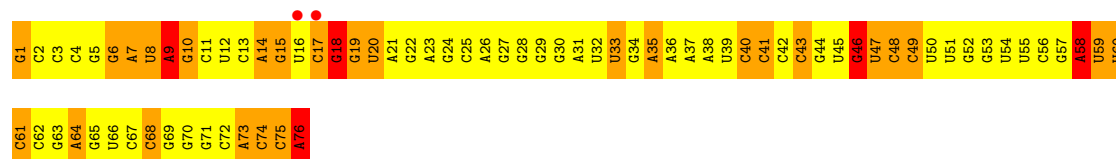




• Molecule 2: mRNA



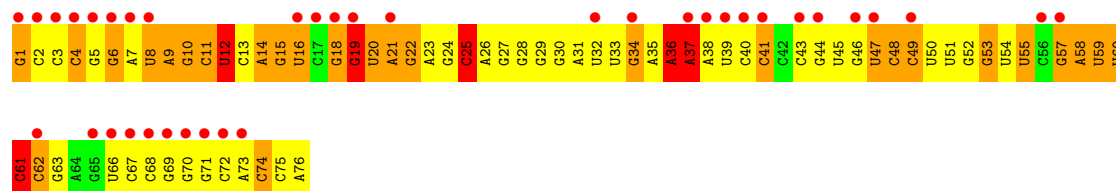
• Molecule 3: tRNA PHE (unmodified bases)



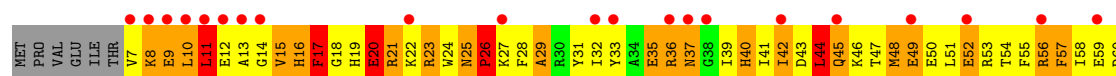
• Molecule 3: tRNA PHE (unmodified bases)

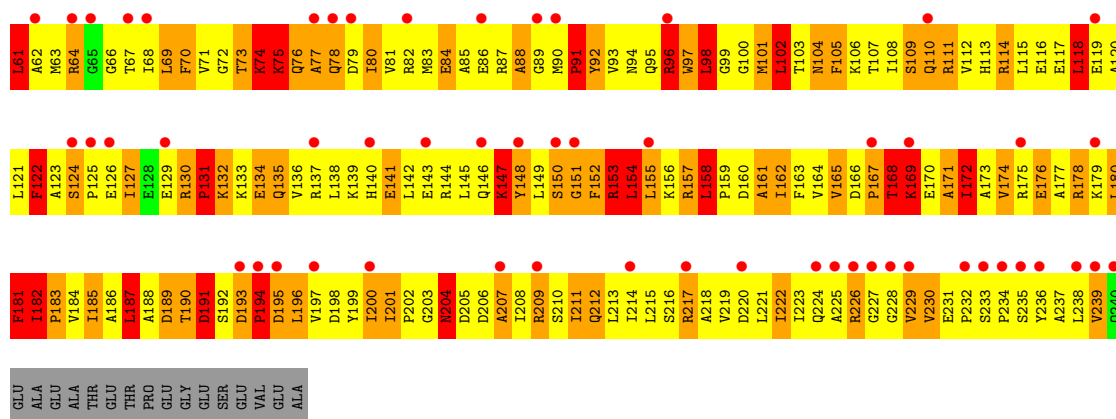


• Molecule 3: tRNA PHE (unmodified bases)

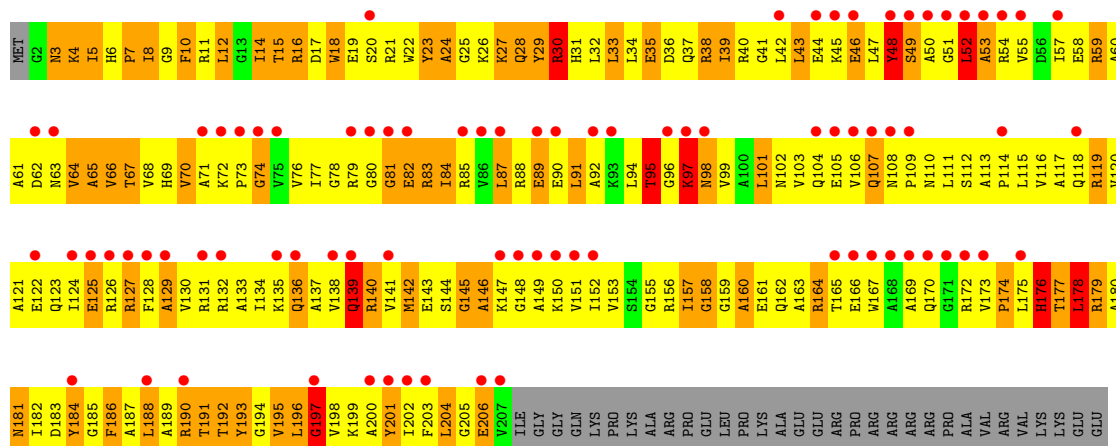


• Molecule 4: 30S ribosomal protein S2

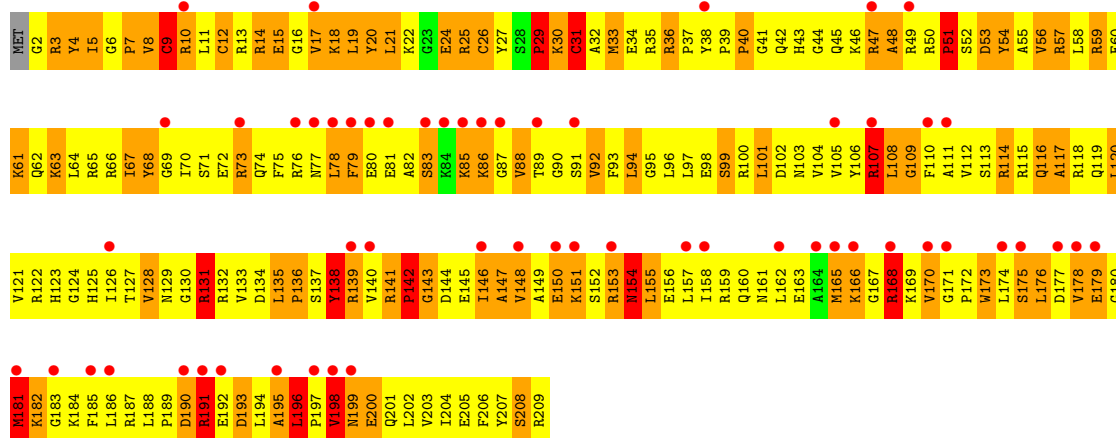




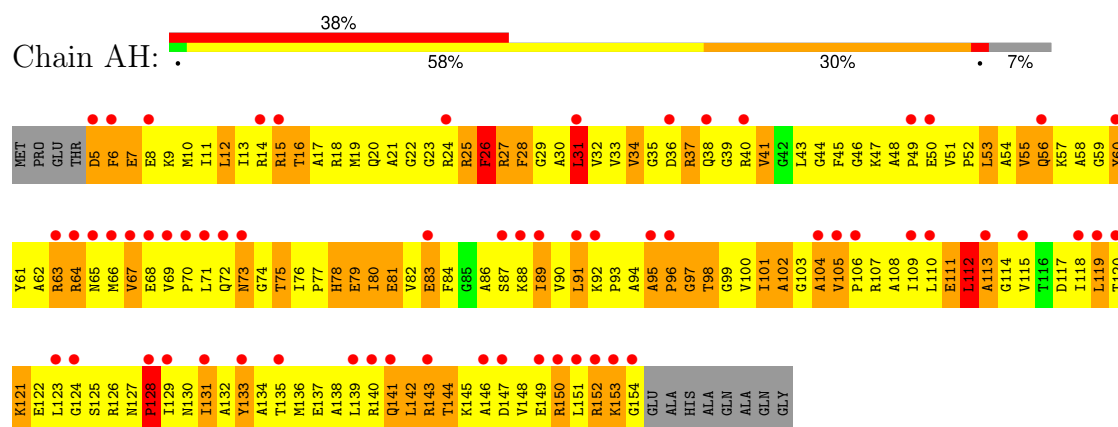
• Molecule 5: 30S ribosomal protein S3



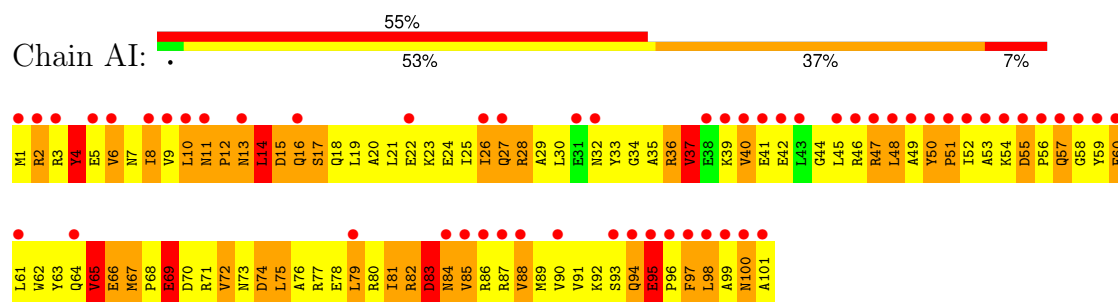
• Molecule 6: 30S ribosomal protein S4



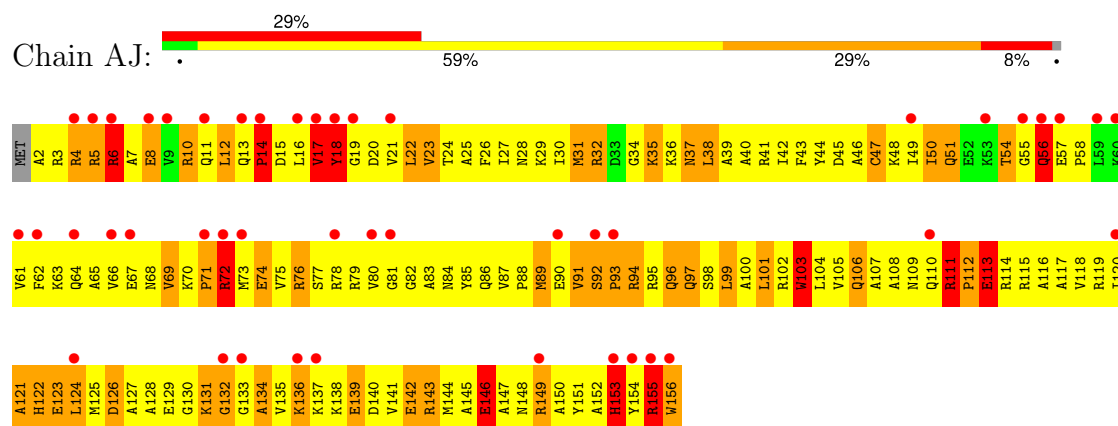
• Molecule 7: 30S ribosomal protein S5



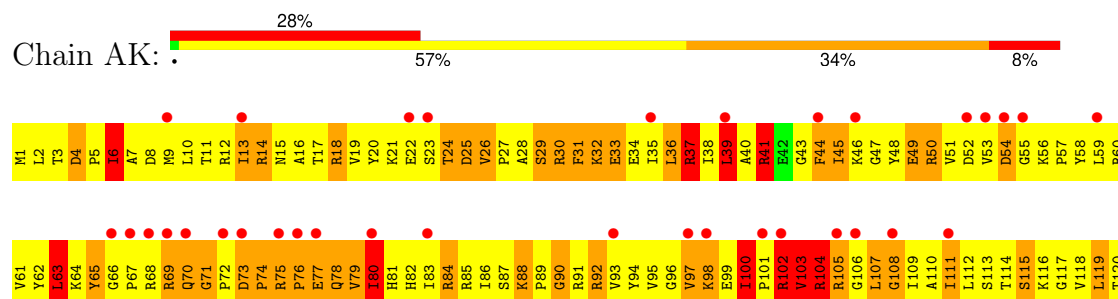
• Molecule 8: 30S ribosomal protein S6



• Molecule 9: 30S ribosomal protein S7

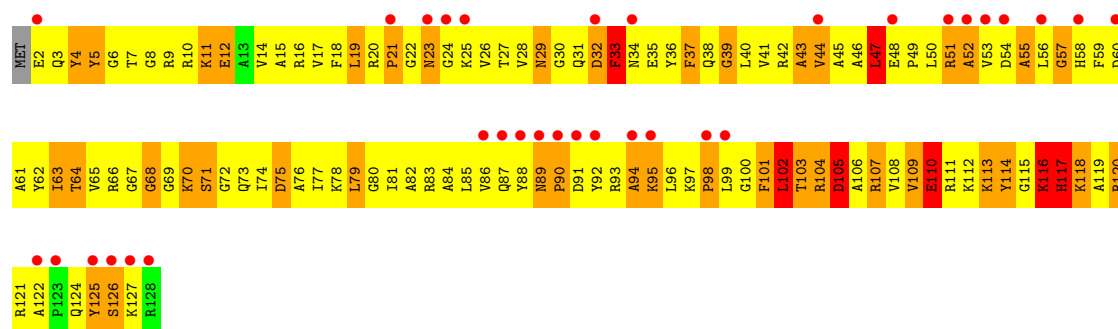


• Molecule 10: 30S ribosomal protein S8

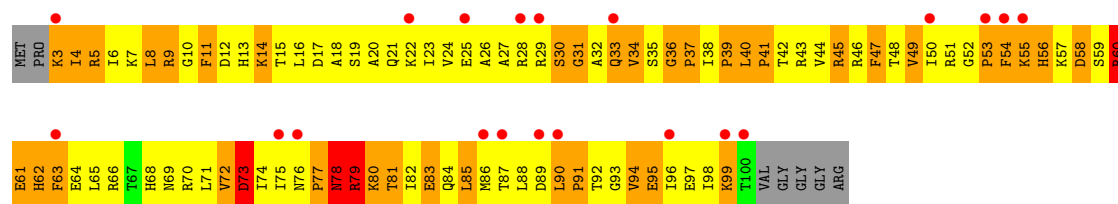




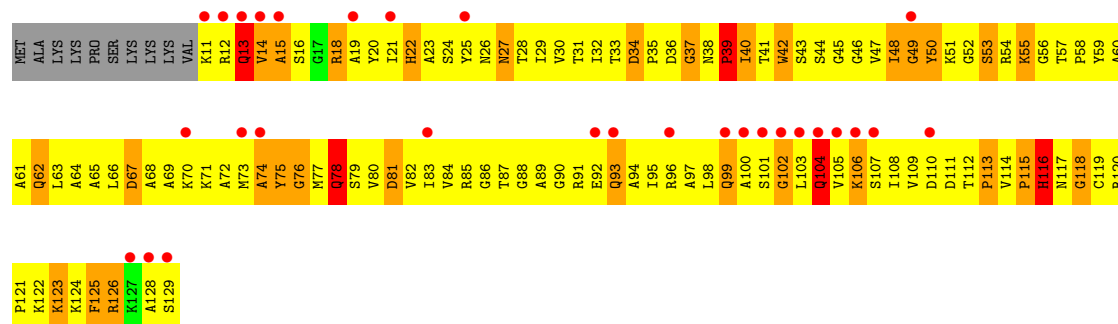
• Molecule 11: 30S ribosomal protein S9



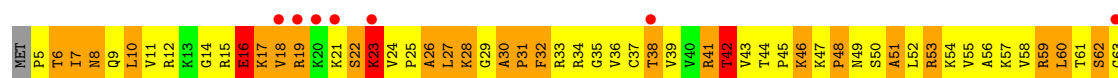
• Molecule 12: 30S ribosomal protein S10

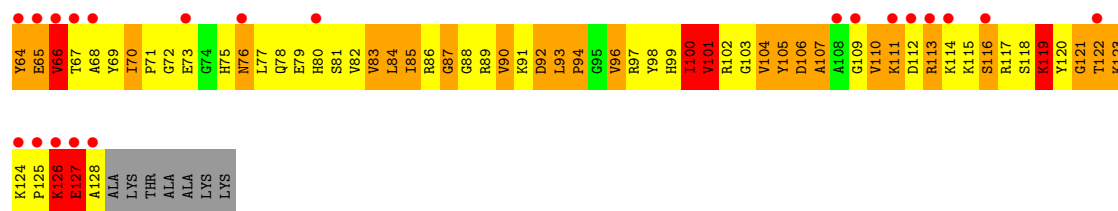


• Molecule 13: 30S ribosomal protein S11

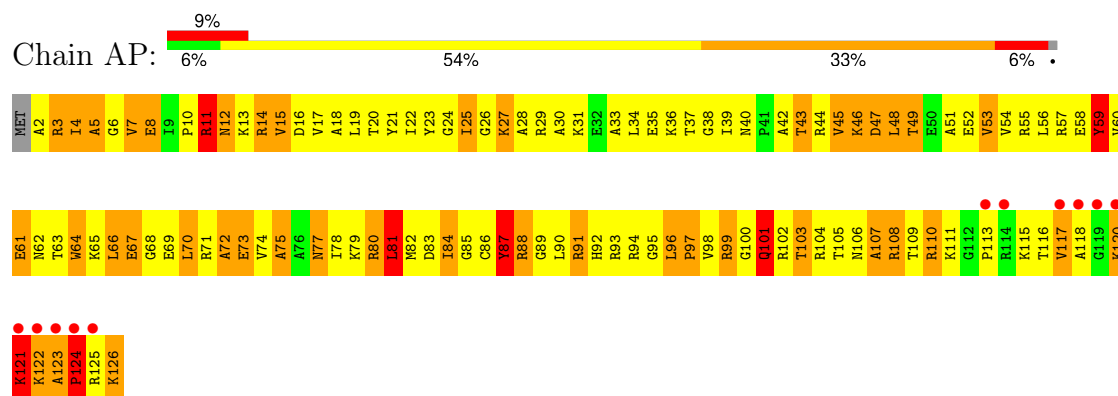


• Molecule 14: 30S ribosomal protein S12

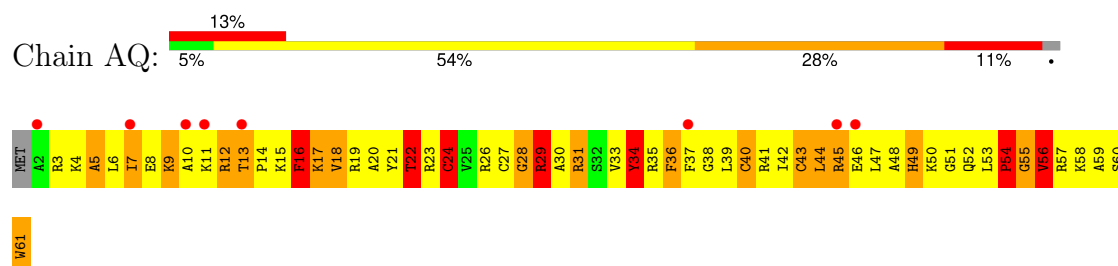




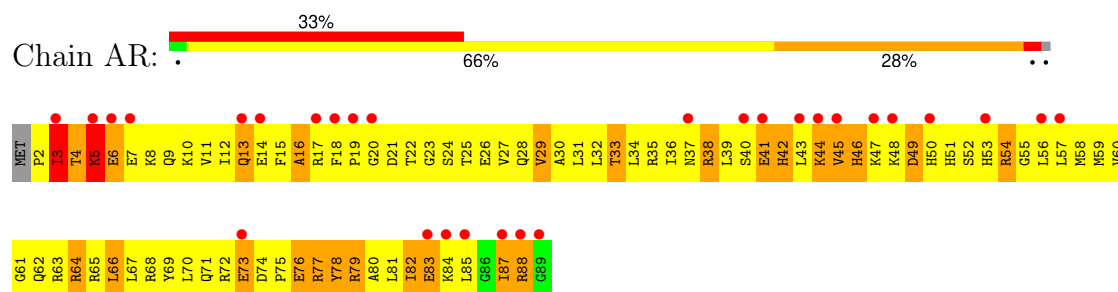
• Molecule 15: 30S ribosomal protein S13



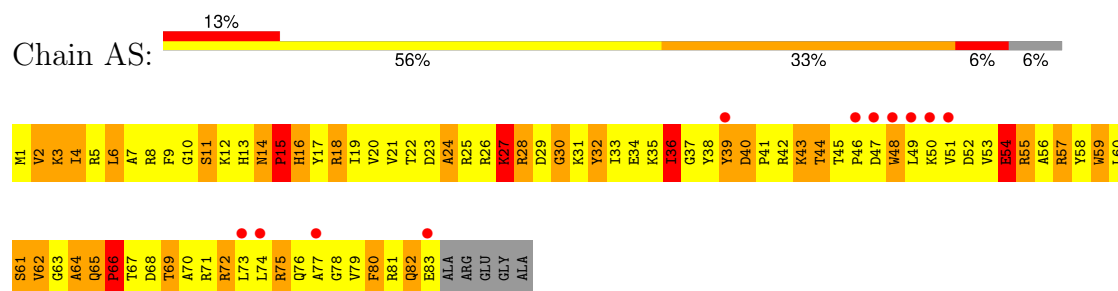
• Molecule 16: 30S ribosomal protein S14



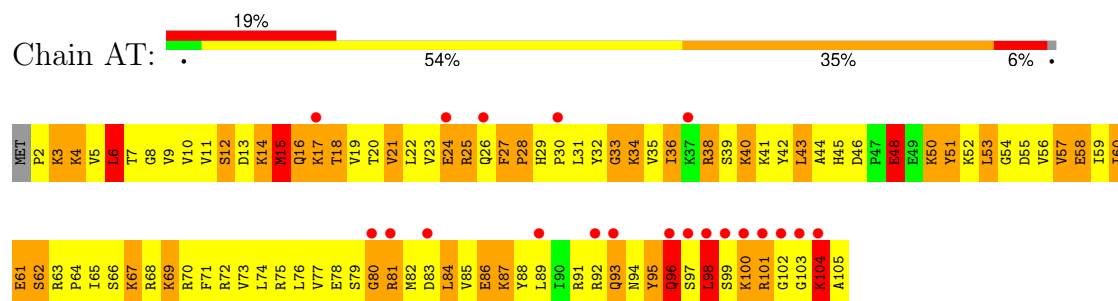
• Molecule 17: 30S ribosomal protein S15



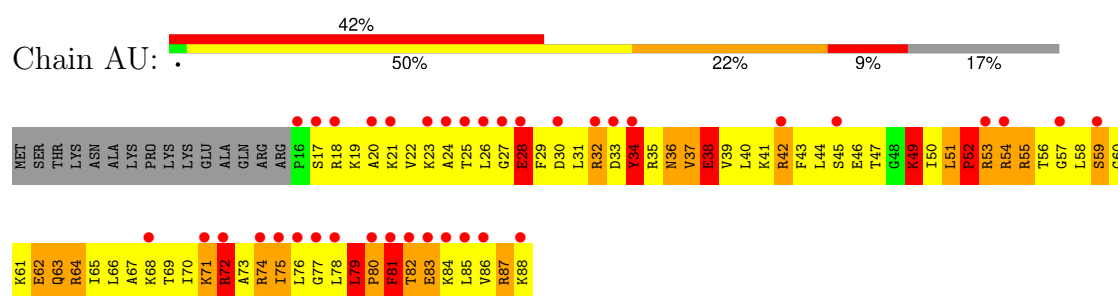
• Molecule 18: 30S ribosomal protein S16



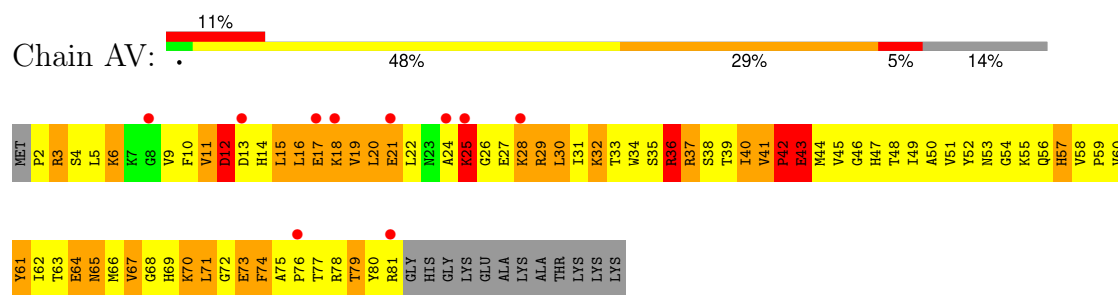
- Molecule 19: 30S ribosomal protein S17



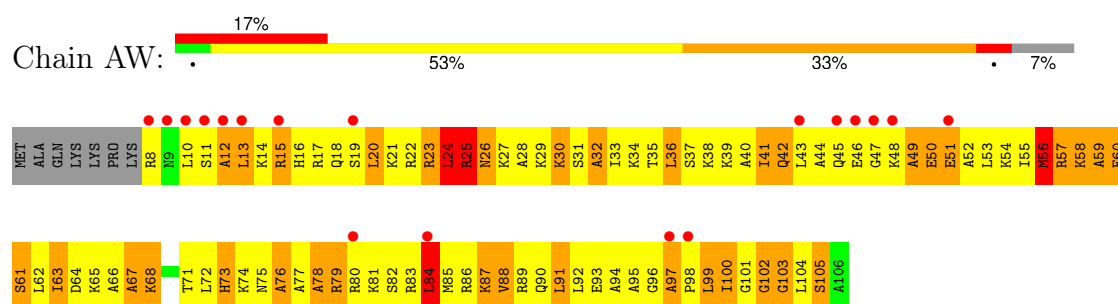
- Molecule 20: 30S ribosomal protein S18



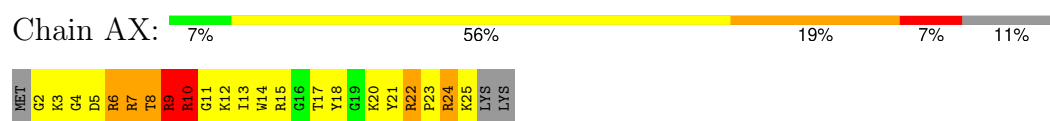
- Molecule 21: 30S ribosomal protein S19



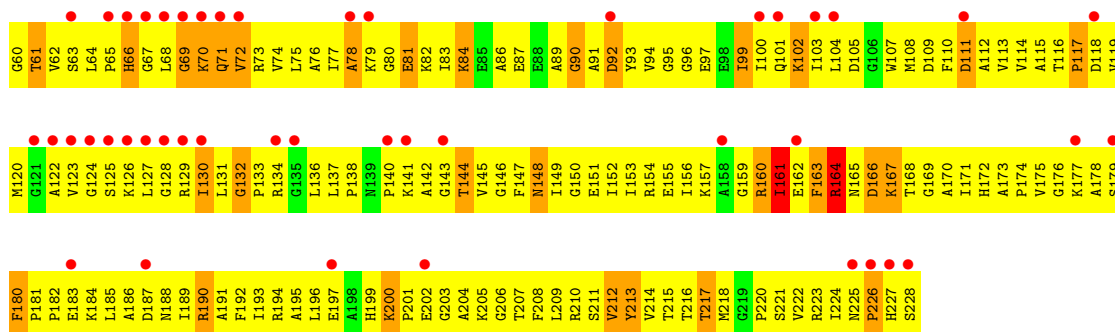
- Molecule 22: 30S ribosomal protein S20



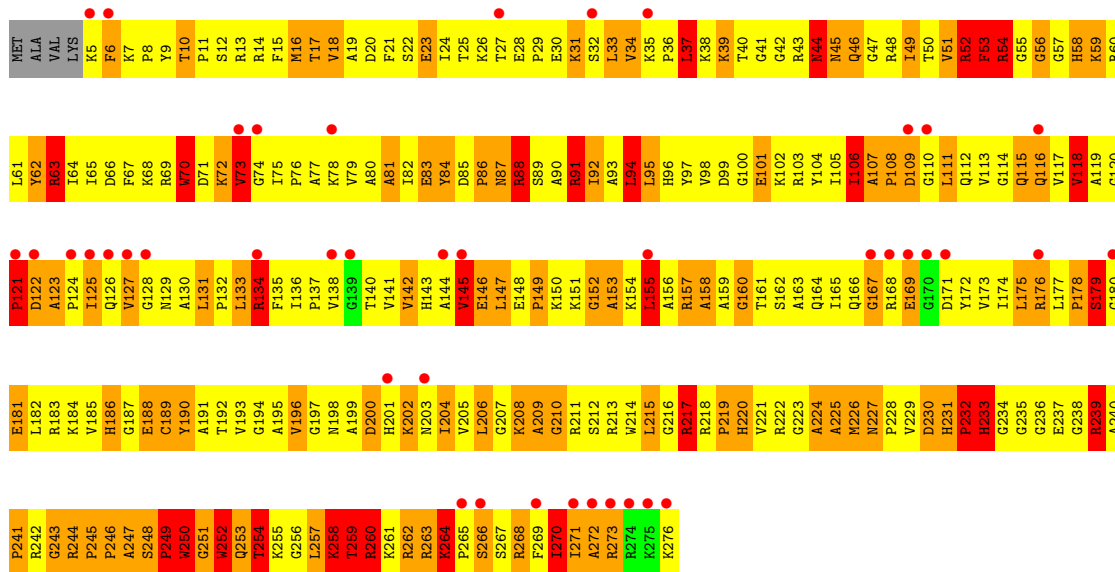
- Molecule 23: 30S ribosomal protein Thx



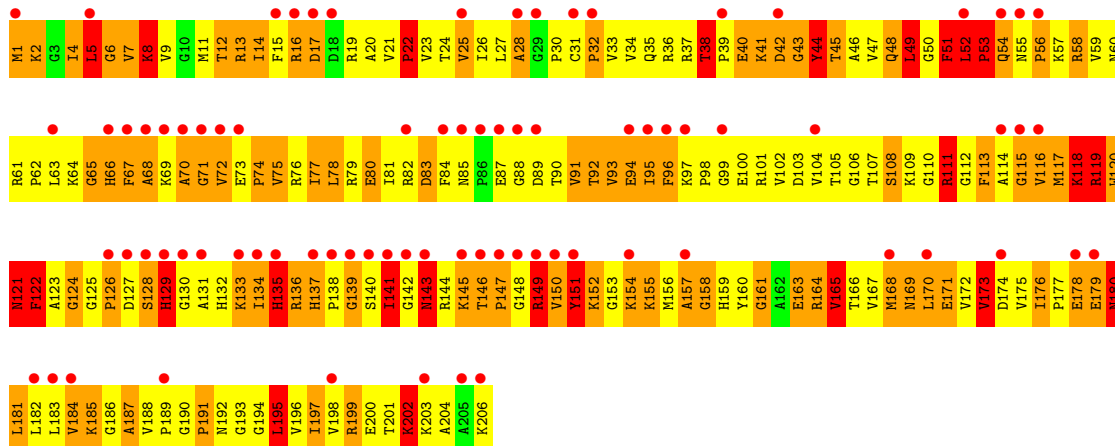
- Molecule 24: 23S ribosomal RNA



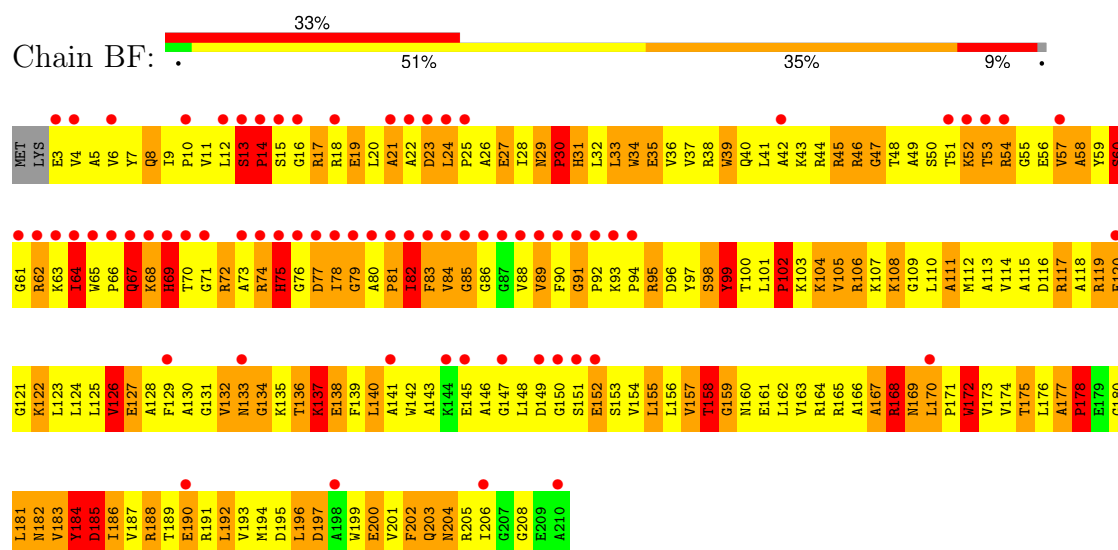
• Molecule 27: 50S ribosomal protein L2



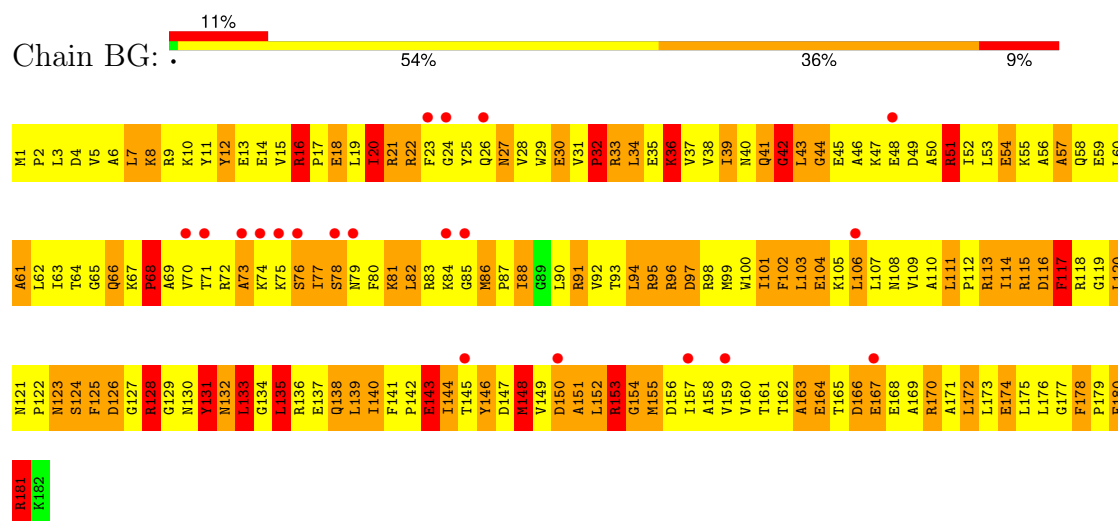
• Molecule 28: 50S ribosomal protein L3



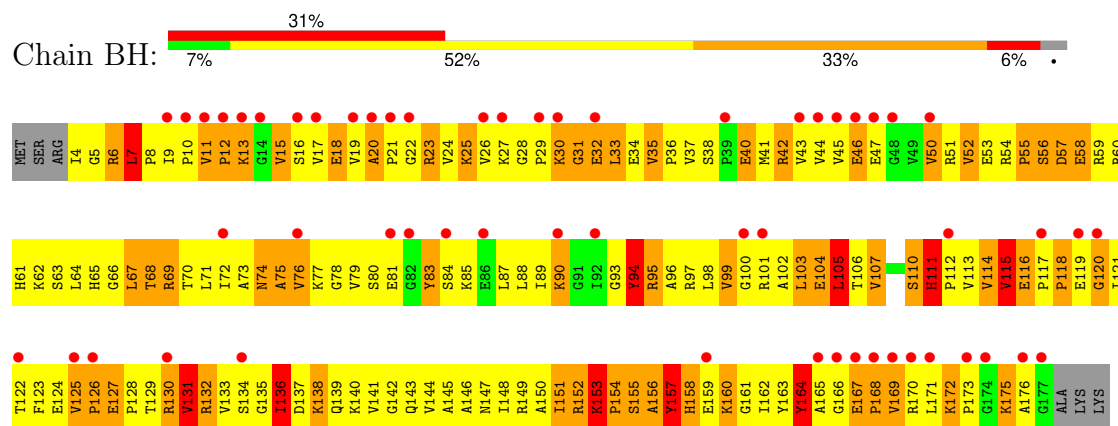
• Molecule 29: 50S ribosomal protein L4



• Molecule 30: 50S ribosomal protein L5

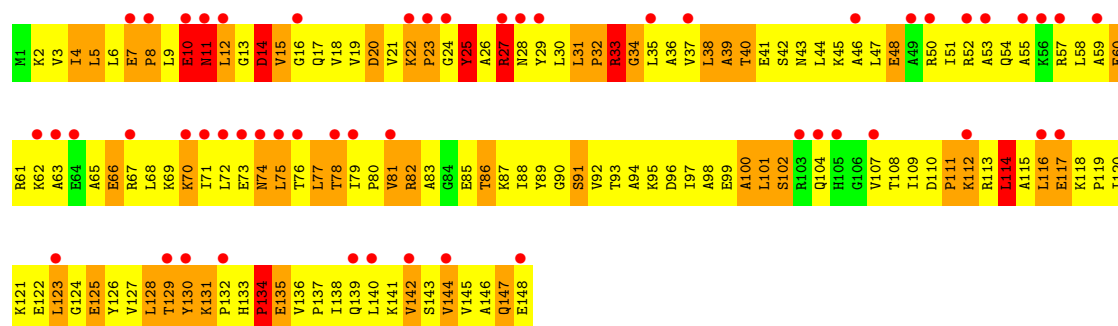


• Molecule 31: 50S ribosomal protein L6

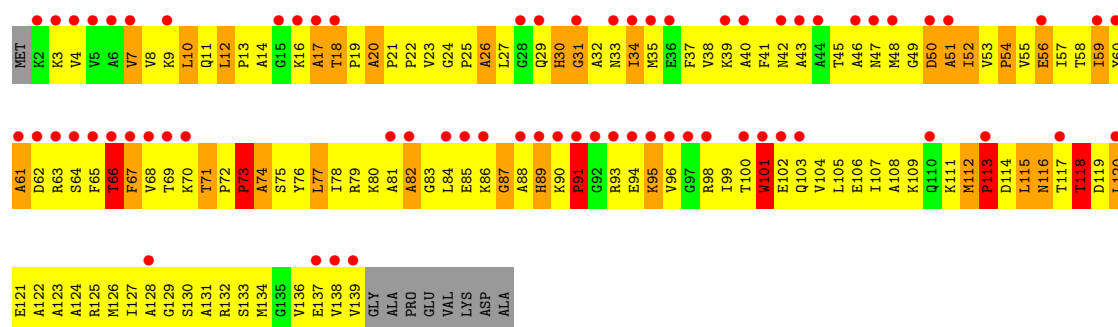
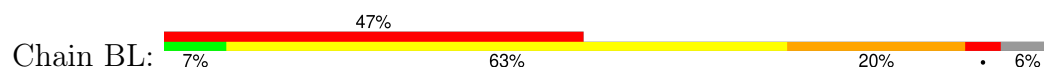


• Molecule 32: 50S ribosomal protein L9

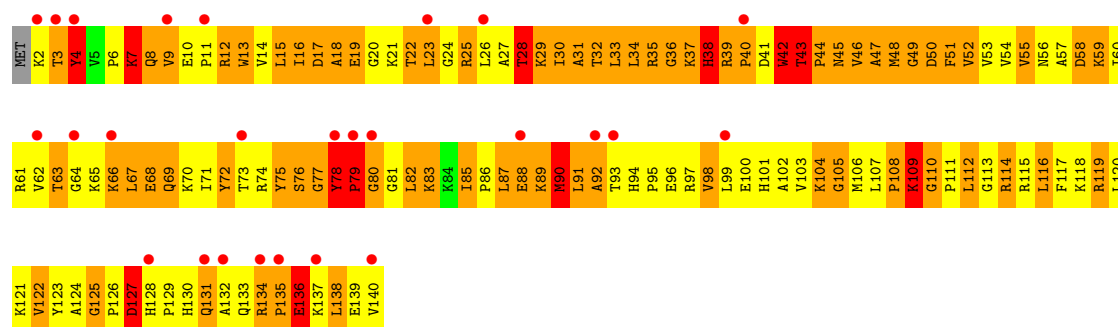




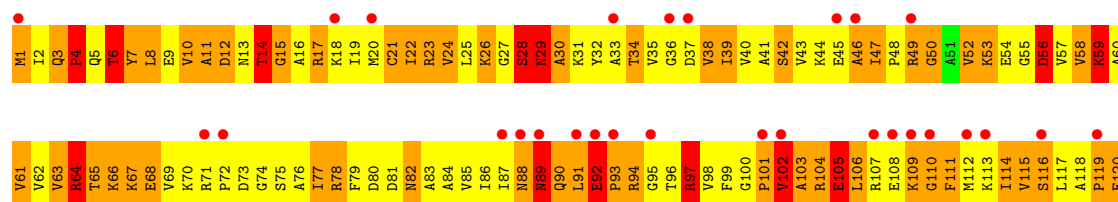
• Molecule 33: 50S ribosomal protein L11



• Molecule 34: 50S ribosomal protein L13



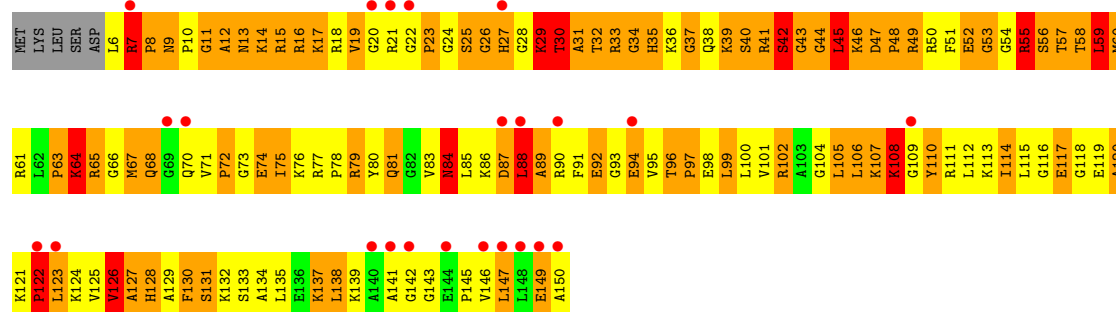
• Molecule 35: 50S ribosomal protein L14



V121
L122

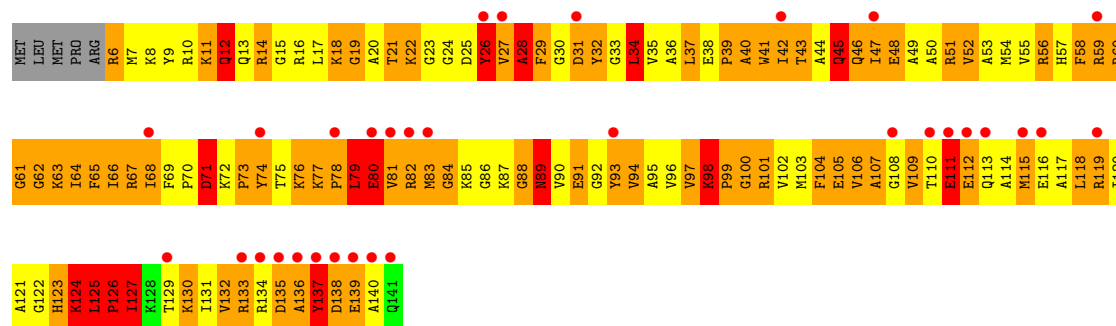
• Molecule 36: 50S ribosomal protein L15

Chain BO: 5% 15% 37% 45% 9% .



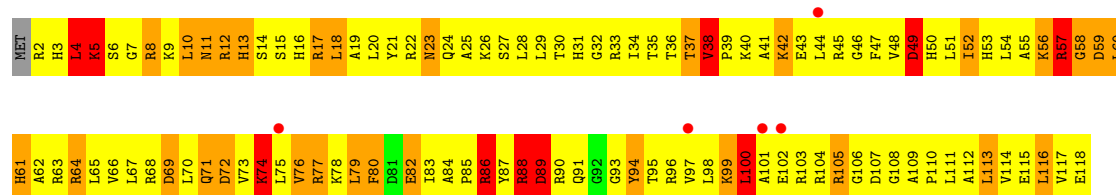
• Molecule 37: 50S ribosomal protein L16

Chain BP: 23% 35% 48% 11% .



• Molecule 38: 50S ribosomal protein L17

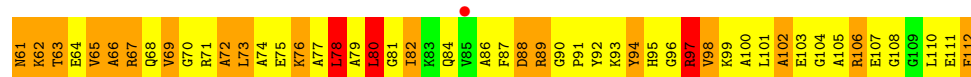
Chain BQ: 4% 64% 25% 8% .



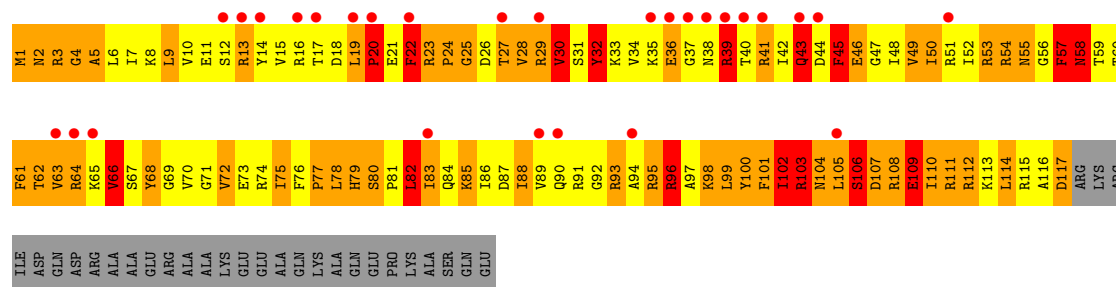
• Molecule 39: 50S ribosomal protein L18

Chain BR: 48% 39% 6% .

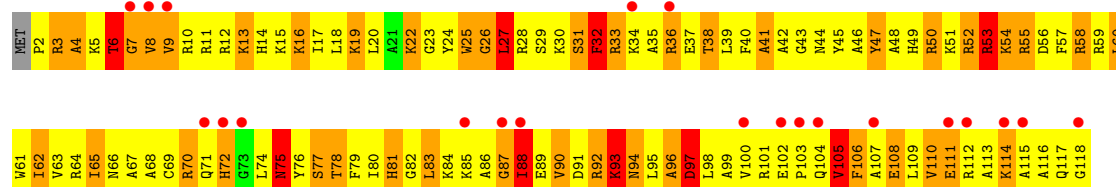




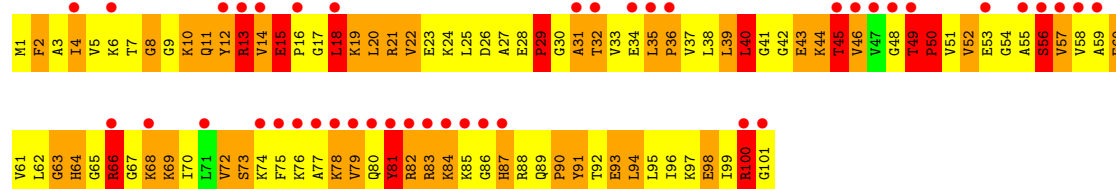
• Molecule 40: 50S ribosomal protein L19



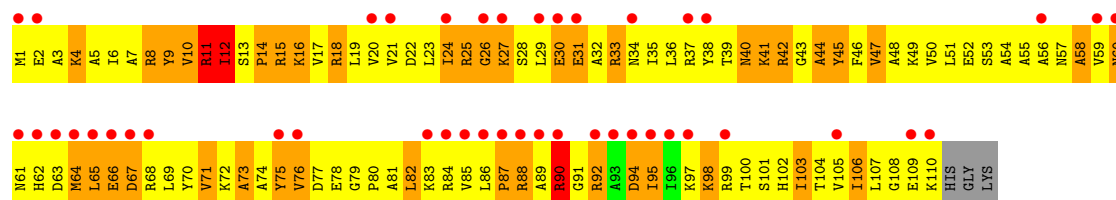
• Molecule 41: 50S ribosomal protein L20



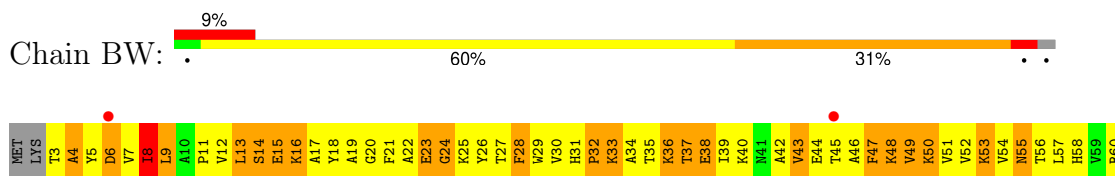
• Molecule 42: 50S ribosomal protein L21



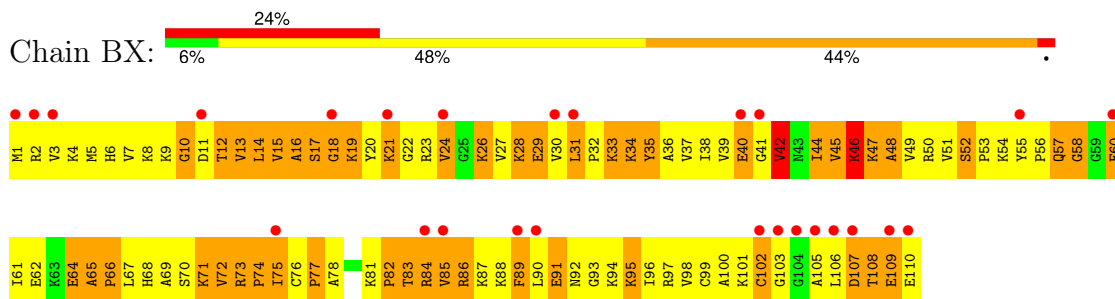
• Molecule 43: 50S ribosomal protein L22



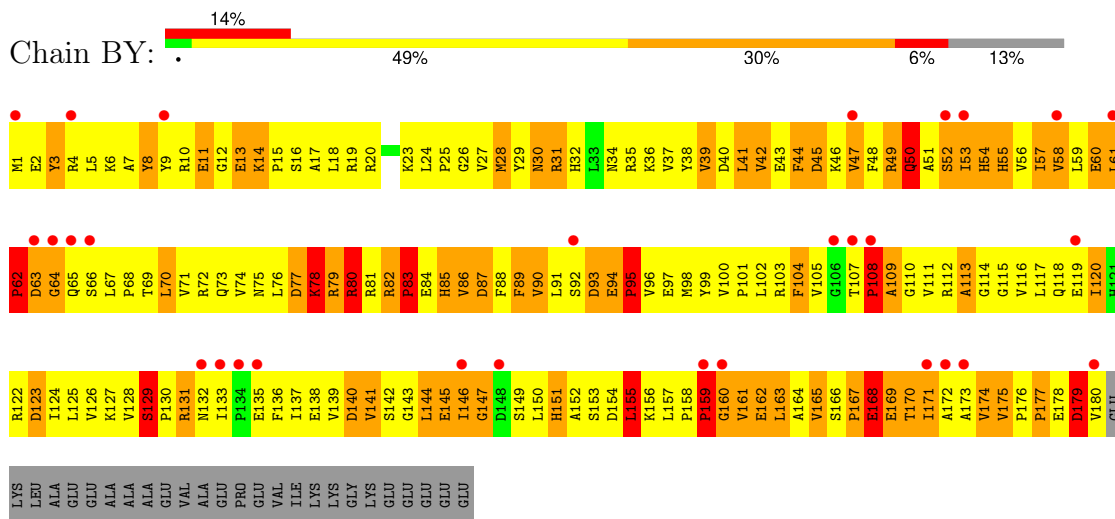
• Molecule 44: 50S ribosomal protein L23



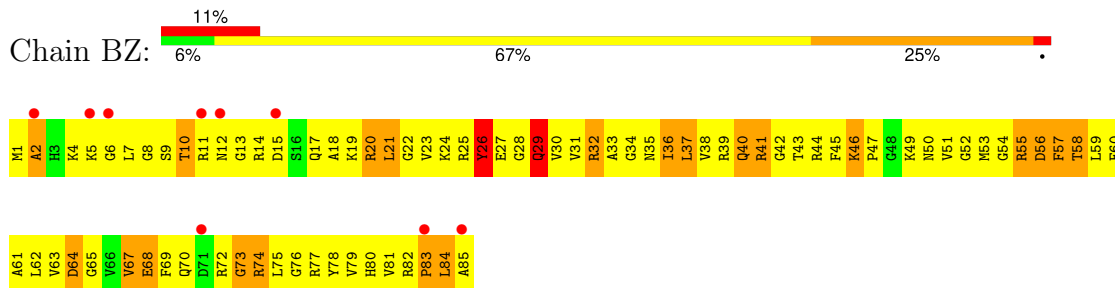
• Molecule 45: 50S ribosomal protein L24



• Molecule 46: 50S ribosomal protein L25



• Molecule 47: Ribosomal protein L27

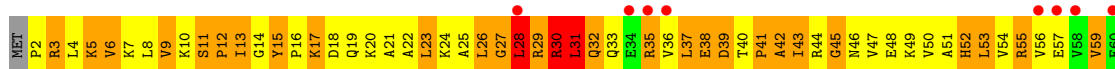


• Molecule 48: 50S ribosomal protein L29

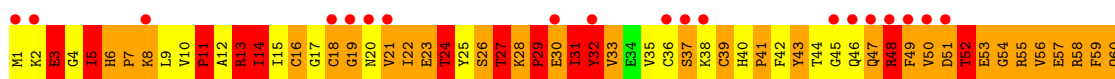




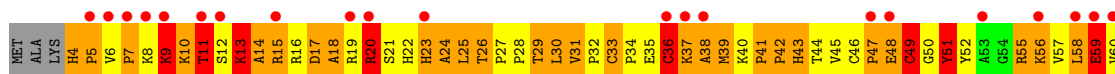
- Molecule 49: 50S ribosomal protein L30



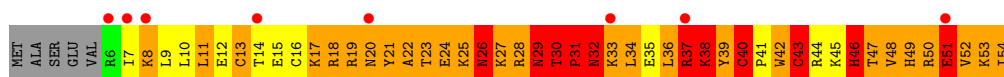
- Molecule 50: 50S ribosomal protein L31



- Molecule 51: 50S ribosomal protein L32



- Molecule 52: 50S ribosomal protein L33

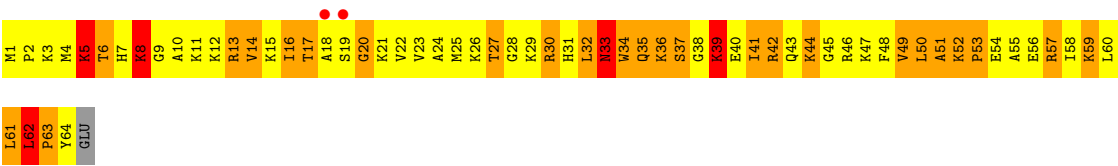


- Molecule 53: 50S ribosomal protein L34

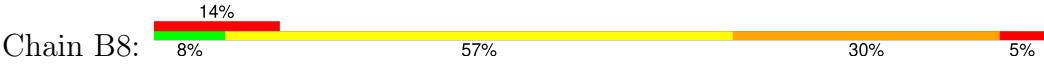


- Molecule 54: 50S ribosomal protein L35





● Molecule 55: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.54Å 508.54Å 806.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 300.00 – 5.50	Depositor EDS
% Data completeness (in resolution range)	96.7 (300.00-5.50) 99.0 (300.00-5.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.00 (at 4.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.243 , 0.326 0.245 , 0.301	Depositor DCC
R_{free} test set	8057 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	108.9	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.12 , 80.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	151691	wwPDB-VP
Average B, all atoms (Å ²)	226.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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 > 5$	RMSZ	# $ Z > 5$
1	AA	0.87	32/36438 (0.1%)	1.08	147/56869 (0.3%)
2	A1	0.67	1/1133 (0.1%)	0.93	2/1753 (0.1%)
3	AB	0.70	1/1813 (0.1%)	1.02	9/2823 (0.3%)
3	AC	0.98	2/1813 (0.1%)	0.93	2/2823 (0.1%)
3	AD	0.69	1/1813 (0.1%)	0.92	2/2823 (0.1%)
4	AE	0.64	0/1935	1.00	4/2609 (0.2%)
5	AF	0.55	0/1636	0.92	4/2205 (0.2%)
6	AG	0.64	1/1733 (0.1%)	0.98	3/2318 (0.1%)
7	AH	0.63	0/1162	1.01	3/1564 (0.2%)
8	AI	0.60	0/856	0.95	0/1154
9	AJ	0.57	0/1276	0.90	3/1709 (0.2%)
10	AK	0.62	0/1136	1.01	3/1527 (0.2%)
11	AL	0.54	0/1029	0.83	0/1379
12	AM	0.48	0/807	0.89	1/1085 (0.1%)
13	AN	0.62	0/900	0.98	0/1213
14	AO	0.60	0/986	1.00	3/1320 (0.2%)
15	AP	0.50	0/1008	0.91	2/1347 (0.1%)
16	AQ	0.55	0/501	0.96	1/664 (0.2%)
17	AR	0.62	0/745	0.95	0/992
18	AS	0.62	0/716	0.95	1/963 (0.1%)
19	AT	0.68	1/870 (0.1%)	0.99	2/1159 (0.2%)
20	AU	0.59	0/603	1.01	1/799 (0.1%)
21	AV	0.51	0/661	0.92	0/890
22	AW	0.65	0/765	1.00	2/1007 (0.2%)
23	AX	0.45	0/212	0.80	0/277
24	BA	0.98	108/69685 (0.2%)	1.10	361/108786 (0.3%)
25	BB	0.83	4/2954 (0.1%)	0.99	7/4606 (0.2%)
26	BC	0.54	0/1775	0.86	0/2393
27	BD	0.72	2/2174 (0.1%)	1.19	12/2927 (0.4%)
28	BE	0.75	0/1611	1.16	13/2171 (0.6%)
29	BF	0.64	0/1660	1.03	4/2247 (0.2%)
30	BG	0.62	0/1507	1.06	4/2027 (0.2%)
31	BH	0.59	0/1354	0.99	4/1831 (0.2%)
32	BK	0.60	0/1170	1.02	4/1581 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	BL	0.61	0/1044	0.94	1/1415 (0.1%)
34	BM	0.77	1/1140 (0.1%)	1.16	8/1537 (0.5%)
35	BN	0.92	1/942 (0.1%)	1.31	10/1268 (0.8%)
36	BO	0.71	0/1123	1.12	5/1493 (0.3%)
37	BP	0.72	0/1100	1.19	8/1470 (0.5%)
38	BQ	0.70	0/974	1.06	2/1302 (0.2%)
39	BR	0.72	0/887	1.06	4/1180 (0.3%)
40	BS	0.85	0/990	1.31	9/1325 (0.7%)
41	BT	0.76	0/982	1.08	0/1306
42	BU	0.87	1/790 (0.1%)	1.28	9/1057 (0.9%)
43	BV	0.66	0/886	1.04	1/1189 (0.1%)
44	BW	0.57	0/756	0.93	0/1015
45	BX	0.54	0/857	1.04	2/1142 (0.2%)
46	BY	0.66	0/1467	1.11	7/1992 (0.4%)
47	BZ	0.65	0/679	1.04	1/902 (0.1%)
48	B1	0.59	0/569	0.88	0/751
49	B2	0.59	0/474	1.09	2/635 (0.3%)
50	B3	0.84	1/594 (0.2%)	1.31	8/795 (1.0%)
51	B4	0.71	0/459	1.16	3/621 (0.5%)
52	B5	0.85	1/433 (0.2%)	1.36	5/576 (0.9%)
53	B6	0.73	0/438	1.01	0/575
54	B7	0.60	0/523	1.14	5/690 (0.7%)
55	B8	0.59	0/310	1.08	1/407 (0.2%)
All	All	0.86	158/164854 (0.1%)	1.07	695/246484 (0.3%)

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	0	175
2	A1	0	3
3	AB	0	6
3	AC	0	8
3	AD	0	8
6	AG	0	1
8	AI	0	1
13	AN	0	1
15	AP	0	1
16	AQ	0	1
24	BA	0	463

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BB	0	18
26	BC	0	1
28	BE	0	1
34	BM	0	1
37	BP	0	1
40	BS	0	1
42	BU	0	1
50	B3	0	1
51	B4	0	1
All	All	0	694

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1203	G	O3'-P	-34.70	1.19	1.61
24	BA	2500	U	C4-O4	18.52	1.38	1.23
24	BA	2500	U	O3'-P	-15.17	1.43	1.61
24	BA	607	U	N3-C4	-14.53	1.25	1.38
24	BA	2448	A	O3'-P	-14.42	1.43	1.61

The worst 5 of 695 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1064	G	N1-C2-N2	-71.65	51.71	116.20
1	AA	1064	G	N3-C2-N2	57.72	160.30	119.90
24	BA	1203	G	P-O3'-C3'	27.70	152.94	119.70
24	BA	2448	A	C5'-C4'-O4'	-27.31	76.33	109.10
1	AA	1064	G	N1-C2-N3	-25.51	108.59	123.90

There are no chirality outliers.

5 of 694 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	31	G	Sidechain
1	AA	37	U	Sidechain
1	AA	45	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	32554	0	16431	6724	0
2	A1	1025	0	511	175	0
3	AB	1623	0	821	225	0
3	AC	1623	0	821	322	0
3	AD	1623	0	821	288	0
4	AE	1900	0	1951	1040	0
5	AF	1612	0	1677	721	0
6	AG	1703	0	1763	869	0
7	AH	1146	0	1207	588	0
8	AI	843	0	857	384	0
9	AJ	1257	0	1296	577	0
10	AK	1116	0	1177	735	0
11	AL	1010	0	1037	470	0
12	AM	794	0	840	358	0
13	AN	885	0	904	471	0
14	AO	970	0	1057	512	0
15	AP	997	0	1072	521	0
16	AQ	492	0	529	278	0
17	AR	734	0	771	332	0
18	AS	700	0	720	353	0
19	AT	857	0	930	450	0
20	AU	597	0	668	369	0
21	AV	647	0	673	312	0
22	AW	763	0	861	374	0
23	AX	208	0	221	83	0
24	BA	62218	0	31356	15296	0
25	BB	2641	0	1337	605	1
26	BC	1742	0	1796	739	0
27	BD	2124	0	2207	1491	0
28	BE	1578	0	1647	1084	0
29	BF	1625	0	1666	822	0
30	BG	1482	0	1546	898	0
31	BH	1328	0	1408	697	0
32	BK	1155	0	1244	502	0
33	BL	1025	0	1074	441	0
34	BM	1113	0	1183	782	0
35	BN	932	0	994	712	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BO	1106	0	1183	795	0
37	BP	1080	0	1127	752	0
38	BQ	960	0	1021	603	0
39	BR	877	0	938	517	0
40	BS	976	0	1033	636	0
41	BT	964	0	1022	742	0
42	BU	779	0	852	574	0
43	BV	876	0	941	459	0
44	BW	742	0	800	360	0
45	BX	844	0	930	421	0
46	BY	1435	0	1463	720	0
47	BZ	670	0	700	354	0
48	B1	567	0	621	312	0
49	B2	469	0	518	320	0
50	B3	581	0	577	397	0
51	B4	445	0	459	277	0
52	B5	426	0	452	279	0
53	B6	430	0	480	273	0
54	B7	515	0	587	396	0
55	B8	307	0	335	150	0
All	All	151691	0	103113	46416	1

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 183.

The worst 5 of 46416 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)
24:BA:2447:G:C8	24:BA:2500:U:H3'	1.23	1.61
24:BA:1202:C:C5	24:BA:1203:G:H1'	1.39	1.55
24:BA:1203:G:O6	24:BA:1240:U:C2	1.66	1.48
24:BA:2459:A:N3	24:BA:2460:U:H1'	1.38	1.38
24:BA:2596:U:H2'	27:BD:242:ARG:CZ	1.55	1.35

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BB:0:A:OP1	25:BB:0:A:OP1[15_545]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
4	AE	232/256 (91%)	114 (49%)	42 (18%)	76 (33%)	0	0
5	AF	204/239 (85%)	107 (52%)	46 (22%)	51 (25%)	0	1
6	AG	206/209 (99%)	96 (47%)	57 (28%)	53 (26%)	0	1
7	AH	148/162 (91%)	93 (63%)	38 (26%)	17 (12%)	0	5
8	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	1
9	AJ	153/156 (98%)	73 (48%)	45 (29%)	35 (23%)	0	1
10	AK	136/138 (99%)	68 (50%)	35 (26%)	33 (24%)	0	1
11	AL	125/128 (98%)	62 (50%)	33 (26%)	30 (24%)	0	1
12	AM	96/105 (91%)	52 (54%)	20 (21%)	24 (25%)	0	1
13	AN	117/129 (91%)	65 (56%)	29 (25%)	23 (20%)	0	2
14	AO	122/132 (92%)	50 (41%)	30 (25%)	42 (34%)	0	0
15	AP	123/126 (98%)	56 (46%)	34 (28%)	33 (27%)	0	0
16	AQ	58/61 (95%)	24 (41%)	16 (28%)	18 (31%)	0	0
17	AR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	2
18	AS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	2
19	AT	102/105 (97%)	62 (61%)	23 (22%)	17 (17%)	0	3
20	AU	71/88 (81%)	26 (37%)	26 (37%)	19 (27%)	0	0
21	AV	78/93 (84%)	32 (41%)	23 (30%)	23 (30%)	0	0
22	AW	97/106 (92%)	38 (39%)	32 (33%)	27 (28%)	0	0
23	AX	22/27 (82%)	9 (41%)	6 (27%)	7 (32%)	0	0
26	BC	226/229 (99%)	155 (69%)	41 (18%)	30 (13%)	0	4
27	BD	270/276 (98%)	125 (46%)	59 (22%)	86 (32%)	0	0
28	BE	204/206 (99%)	117 (57%)	31 (15%)	56 (28%)	0	0
29	BF	206/210 (98%)	109 (53%)	46 (22%)	51 (25%)	0	1
30	BG	180/182 (99%)	79 (44%)	47 (26%)	54 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	BH	172/180 (96%)	80 (46%)	46 (27%)	46 (27%)	0	0
32	BK	146/148 (99%)	91 (62%)	30 (20%)	25 (17%)	0	2
33	BL	136/147 (92%)	69 (51%)	38 (28%)	29 (21%)	0	2
34	BM	137/140 (98%)	64 (47%)	28 (20%)	45 (33%)	0	0
35	BN	120/122 (98%)	59 (49%)	23 (19%)	38 (32%)	0	0
36	BO	143/150 (95%)	57 (40%)	36 (25%)	50 (35%)	0	0
37	BP	134/141 (95%)	49 (37%)	33 (25%)	52 (39%)	0	0
38	BQ	115/118 (98%)	57 (50%)	39 (34%)	19 (16%)	0	3
39	BR	108/112 (96%)	48 (44%)	29 (27%)	31 (29%)	0	0
40	BS	115/146 (79%)	52 (45%)	26 (23%)	37 (32%)	0	0
41	BT	115/118 (98%)	35 (30%)	50 (44%)	30 (26%)	0	1
42	BU	99/101 (98%)	52 (52%)	19 (19%)	28 (28%)	0	0
43	BV	108/113 (96%)	63 (58%)	24 (22%)	21 (19%)	0	2
44	BW	92/96 (96%)	57 (62%)	16 (17%)	19 (21%)	0	2
45	BX	108/110 (98%)	43 (40%)	32 (30%)	33 (31%)	0	0
46	BY	178/206 (86%)	95 (53%)	44 (25%)	39 (22%)	0	1
47	BZ	83/85 (98%)	52 (63%)	21 (25%)	10 (12%)	0	4
48	B1	65/67 (97%)	36 (55%)	20 (31%)	9 (14%)	0	4
49	B2	57/60 (95%)	34 (60%)	8 (14%)	15 (26%)	0	1
50	B3	69/71 (97%)	23 (33%)	16 (23%)	30 (44%)	0	0
51	B4	55/60 (92%)	14 (26%)	19 (34%)	22 (40%)	0	0
52	B5	47/54 (87%)	14 (30%)	7 (15%)	26 (55%)	0	0
53	B6	47/49 (96%)	20 (43%)	12 (26%)	15 (32%)	0	0
54	B7	62/65 (95%)	23 (37%)	18 (29%)	21 (34%)	0	0
55	B8	35/37 (95%)	20 (57%)	5 (14%)	10 (29%)	0	0
All	All	5988/6337 (94%)	2955 (49%)	1476 (25%)	1557 (26%)	0	1

5 of 1557 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	AE	8	LYS
4	AE	11	LEU
4	AE	13	ALA

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Mol	Chain	Res	Type
4	AE	15	VAL
4	AE	16	HIS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
4	AE	202/220 (92%)	138 (68%)	64 (32%)	0	2
5	AF	160/188 (85%)	123 (77%)	37 (23%)	0	4
6	AG	180/181 (99%)	131 (73%)	49 (27%)	0	3
7	AH	115/123 (94%)	78 (68%)	37 (32%)	0	2
8	AI	90/90 (100%)	61 (68%)	29 (32%)	0	2
9	AJ	126/127 (99%)	93 (74%)	33 (26%)	0	3
10	AK	119/119 (100%)	86 (72%)	33 (28%)	0	2
11	AL	98/99 (99%)	73 (74%)	25 (26%)	0	3
12	AM	88/92 (96%)	67 (76%)	21 (24%)	0	4
13	AN	90/99 (91%)	74 (82%)	16 (18%)	1	8
14	AO	104/109 (95%)	81 (78%)	23 (22%)	1	5
15	AP	100/101 (99%)	75 (75%)	25 (25%)	0	3
16	AQ	49/50 (98%)	36 (74%)	13 (26%)	0	3
17	AR	79/80 (99%)	64 (81%)	15 (19%)	1	7
18	AS	72/74 (97%)	49 (68%)	23 (32%)	0	2
19	AT	96/97 (99%)	67 (70%)	29 (30%)	0	2
20	AU	64/77 (83%)	48 (75%)	16 (25%)	0	3
21	AV	71/80 (89%)	55 (78%)	16 (22%)	1	5
22	AW	76/82 (93%)	59 (78%)	17 (22%)	1	5
23	AX	19/22 (86%)	17 (90%)	2 (10%)	5	19
26	BC	180/181 (99%)	151 (84%)	29 (16%)	2	10
27	BD	215/218 (99%)	153 (71%)	62 (29%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	BE	166/166 (100%)	102 (61%)	64 (39%)	0	0
29	BF	164/166 (99%)	105 (64%)	59 (36%)	0	1
30	BG	156/156 (100%)	112 (72%)	44 (28%)	0	2
31	BH	143/148 (97%)	109 (76%)	34 (24%)	0	4
32	BK	124/124 (100%)	92 (74%)	32 (26%)	0	3
33	BL	105/111 (95%)	89 (85%)	16 (15%)	2	11
34	BM	118/119 (99%)	79 (67%)	39 (33%)	0	1
35	BN	100/100 (100%)	69 (69%)	31 (31%)	0	2
36	BO	111/116 (96%)	71 (64%)	40 (36%)	0	1
37	BP	106/111 (96%)	65 (61%)	41 (39%)	0	0
38	BQ	100/101 (99%)	71 (71%)	29 (29%)	0	2
39	BR	87/88 (99%)	63 (72%)	24 (28%)	0	2
40	BS	105/127 (83%)	68 (65%)	37 (35%)	0	1
41	BT	93/94 (99%)	64 (69%)	29 (31%)	0	2
42	BU	82/82 (100%)	57 (70%)	25 (30%)	0	2
43	BV	90/92 (98%)	64 (71%)	26 (29%)	0	2
44	BW	76/78 (97%)	57 (75%)	19 (25%)	0	3
45	BX	91/91 (100%)	72 (79%)	19 (21%)	1	6
46	BY	159/179 (89%)	120 (76%)	39 (24%)	0	3
47	BZ	67/67 (100%)	51 (76%)	16 (24%)	0	4
48	B1	62/62 (100%)	44 (71%)	18 (29%)	0	2
49	B2	51/52 (98%)	36 (71%)	15 (29%)	0	2
50	B3	63/63 (100%)	45 (71%)	18 (29%)	0	2
51	B4	50/52 (96%)	31 (62%)	19 (38%)	0	0
52	B5	48/52 (92%)	32 (67%)	16 (33%)	0	1
53	B6	42/42 (100%)	29 (69%)	13 (31%)	0	2
54	B7	54/55 (98%)	44 (82%)	10 (18%)	1	8
55	B8	34/34 (100%)	29 (85%)	5 (15%)	2	12
All	All	5040/5237 (96%)	3649 (72%)	1391 (28%)	0	2

5 of 1391 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	BN	82	ASN
42	BU	49	THR
36	BO	75	ILE
35	BN	78	ARG
38	BQ	105	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 180 such sidechains are listed below:

Mol	Chain	Res	Type
34	BM	38	HIS
43	BV	61	ASN
35	BN	90	GLN
38	BQ	31	HIS
45	BX	6	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	463 (30%)	137 (9%)
2	A1	49/50 (98%)	21 (42%)	4 (8%)
24	BA	2888/2916 (99%)	1204 (41%)	253 (8%)
25	BB	122/123 (99%)	46 (37%)	3 (2%)
3	AB	75/76 (98%)	32 (42%)	1 (1%)
3	AC	75/76 (98%)	23 (30%)	4 (5%)
3	AD	75/76 (98%)	23 (30%)	1 (1%)
All	All	4799/4839 (99%)	1812 (37%)	403 (8%)

5 of 1812 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	14	U
1	AA	19	C

5 of 403 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	973	A
24	BA	1603	A

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Mol	Chain	Res	Type
24	BA	2893	G
24	BA	1064	C
24	BA	1250	G

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 oligosaccharides 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
24	BA	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	2756:U	O3'	2757:A	P	1.77
1	BA	1203:G	O3'	1204:A	P	1.19

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1515/1522 (99%)	0.33	143 (9%) 15 16	145, 221, 302, 356	0
2	A1	50/50 (100%)	3.87	34 (68%) 0 1	200, 320, 348, 357	0
3	AB	76/76 (100%)	2.39	37 (48%) 0 2	288, 351, 370, 374	0
3	AC	76/76 (100%)	-0.07	2 (2%) 57 43	167, 214, 260, 284	0
3	AD	76/76 (100%)	0.36	6 (7%) 20 19	222, 271, 293, 316	0
4	AE	234/256 (91%)	1.96	76 (32%) 1 4	189, 226, 271, 304	0
5	AF	206/239 (86%)	2.13	83 (40%) 1 3	222, 244, 266, 277	0
6	AG	208/209 (99%)	1.39	57 (27%) 2 4	168, 215, 233, 242	0
7	AH	150/162 (92%)	2.35	62 (41%) 1 3	174, 210, 235, 257	0
8	AI	101/101 (100%)	2.87	56 (55%) 0 2	191, 223, 236, 261	0
9	AJ	155/156 (99%)	1.55	46 (29%) 1 4	210, 240, 256, 275	0
10	AK	138/138 (100%)	1.71	39 (28%) 1 4	186, 208, 225, 232	0
11	AL	127/128 (99%)	1.10	33 (25%) 2 5	222, 261, 276, 287	0
12	AM	98/105 (93%)	0.90	20 (20%) 3 6	230, 260, 274, 282	0
13	AN	119/129 (92%)	1.25	29 (24%) 2 5	193, 212, 245, 267	0
14	AO	124/132 (93%)	1.57	28 (22%) 3 6	179, 199, 233, 267	0
15	AP	125/126 (99%)	0.49	11 (8%) 17 17	223, 243, 272, 278	0
16	AQ	60/61 (98%)	0.66	8 (13%) 8 11	215, 248, 259, 263	0
17	AR	88/89 (98%)	1.50	29 (32%) 1 3	186, 207, 231, 238	0
18	AS	83/88 (94%)	0.58	11 (13%) 8 11	180, 201, 226, 249	0
19	AT	104/105 (99%)	0.86	20 (19%) 4 7	164, 193, 244, 277	0
20	AU	73/88 (82%)	3.00	37 (50%) 0 2	184, 209, 258, 287	0
21	AV	80/93 (86%)	0.54	10 (12%) 9 12	226, 252, 266, 270	0
22	AW	99/106 (93%)	1.02	18 (18%) 4 7	167, 195, 225, 241	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
23	AX	24/27 (88%)	-0.59	0 100 100	230, 249, 280, 288	0
24	BA	2889/2916 (99%)	0.52	429 (14%) 7 10	129, 215, 297, 342	0
25	BB	123/123 (100%)	-0.58	0 100 100	199, 259, 293, 316	0
26	BC	228/229 (99%)	1.55	68 (29%) 1 4	250, 281, 300, 313	0
27	BD	272/276 (98%)	0.84	42 (15%) 6 10	130, 199, 221, 259	0
28	BE	206/206 (100%)	1.83	80 (38%) 1 3	148, 186, 232, 269	0
29	BF	208/210 (99%)	1.87	70 (33%) 1 3	164, 238, 263, 276	0
30	BG	182/182 (100%)	0.53	20 (10%) 12 14	212, 246, 268, 276	0
31	BH	174/180 (96%)	1.56	56 (32%) 1 4	196, 241, 260, 271	0
32	BK	148/148 (100%)	1.78	53 (35%) 1 3	202, 227, 249, 257	0
33	BL	138/147 (93%)	2.55	69 (50%) 0 2	271, 298, 312, 327	0
34	BM	139/140 (99%)	1.00	26 (18%) 4 7	167, 198, 224, 235	0
35	BN	122/122 (100%)	1.37	28 (22%) 2 5	148, 177, 209, 221	0
36	BO	145/150 (96%)	0.60	23 (15%) 6 9	166, 247, 276, 315	0
37	BP	136/141 (96%)	1.13	32 (23%) 2 5	166, 208, 234, 241	0
38	BQ	117/118 (99%)	-0.00	5 (4%) 40 32	168, 192, 219, 226	0
39	BR	110/112 (98%)	-0.16	1 (0%) 81 67	186, 235, 263, 289	0
40	BS	117/146 (80%)	1.19	28 (23%) 2 5	164, 194, 227, 242	0
41	BT	117/118 (99%)	0.92	21 (17%) 4 8	183, 202, 220, 232	0
42	BU	101/101 (100%)	2.00	42 (41%) 1 3	168, 225, 246, 257	0
43	BV	110/113 (97%)	1.93	44 (40%) 1 3	180, 209, 237, 248	0
44	BW	94/96 (97%)	0.42	9 (9%) 15 15	212, 232, 280, 288	0
45	BX	110/110 (100%)	0.99	26 (23%) 2 5	221, 255, 287, 305	0
46	BY	180/206 (87%)	0.77	29 (16%) 5 9	208, 246, 268, 279	0
47	BZ	85/85 (100%)	0.22	9 (10%) 13 14	211, 229, 242, 271	0
48	B1	67/67 (100%)	0.31	2 (2%) 52 40	218, 243, 263, 268	0
49	B2	59/60 (98%)	0.65	8 (13%) 8 11	204, 224, 249, 259	0
50	B3	71/71 (100%)	1.99	26 (36%) 1 3	199, 223, 238, 246	0
51	B4	57/60 (95%)	1.49	21 (36%) 1 3	164, 209, 264, 289	0
52	B5	49/54 (90%)	0.78	8 (16%) 5 9	206, 232, 242, 252	0
53	B6	49/49 (100%)	0.36	6 (12%) 10 13	162, 209, 221, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	B7	64/65 (98%)	0.01	2 (3%) 51 39	164, 195, 225, 242	0
55	B8	37/37 (100%)	0.73	5 (13%) 8 11	205, 215, 224, 226	0
All	All	10893/11176 (97%)	0.93	2183 (20%) 3 7	129, 223, 295, 374	0

The worst 5 of 2183 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	AF	207	VAL	24.8
7	AH	154	GLY	23.7
20	AU	16	PRO	19.9
8	AI	101	ALA	18.4
4	AE	7	VAL	17.9

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.