



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2026 – 01:24 AM UTC

PDB ID : 4V4P / pdb_00004v4p
Title : Crystal structure of 70S ribosome with thrS operator and tRNAs.
Authors : Jenner, L.; Romby, P.; Rees, B.; Schulze-Briesse, C.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.; Yusupova, G.; Yusupov, M.
Deposited on : 2005-01-19
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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

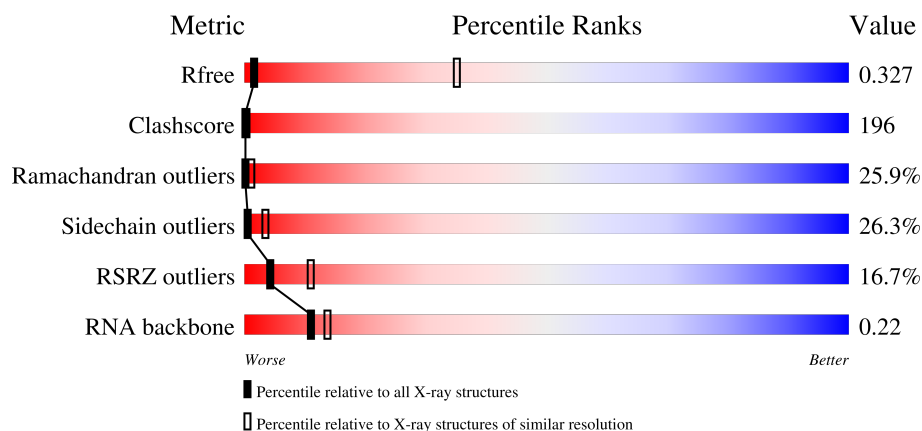
1 Overall quality at a glance

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}	180053	1088 (7.00-4.00)
Clashscore	190562	1147 (7.00-4.00)
Ramachandran outliers	187476	1012 (7.02-3.98)
Sidechain outliers	187428	1023 (7.04-3.96)
RSRZ outliers	180081	1081 (7.00-4.00)
RNA backbone	3983	1052 (7.80-3.10)

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	AB	123	54% 37% 9%
2	AA	2915	8% 40% 38% 21% •
3	AC	228	21% 7% 57% 28% 6% •
4	AD	178	47% 23% 44% 28% •

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Mol	Chain	Length	Quality of chain
5	AE	338	
6	AF	246	
7	AG	176	
8	AH	177	
9	AI	128	
9	AJ	128	
10	AK	149	
11	AL	141	
12	AM	145	
13	AN	122	
14	AO	164	
15	AP	138	
16	AQ	186	
17	AR	66	
18	AS	113	
19	AT	84	
20	AU	119	
21	AV	253	
22	AW	70	
23	AX	60	
24	A0	118	
25	A1	118	
26	A2	100	
27	A3	91	
28	A4	73	

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Mol	Chain	Length	Quality of chain
29	A5	60	
30	A6	82	
31	A7	47	
32	A8	64	
33	A9	36	
34	BA	1522	
35	BB	76	
35	BC	76	
36	B1	78	
37	BE	256	
38	BF	239	
39	BG	209	
40	BH	162	
41	BI	101	
42	BJ	156	
43	BK	138	
44	BL	128	
45	BM	105	
46	BN	129	
47	BO	135	
48	BP	126	
49	BQ	61	
50	BR	89	
51	BS	88	
52	BT	105	

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Mol	Chain	Length	Quality of chain
53	BU	88	30% 42% 26% 13% 17%
54	BV	93	15% 45% 30% 8% 14%
55	BW	106	13% 50% 36% 8% 7%
56	BX	27	48% 37% 11%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 148539 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 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	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
AB	-1	A	-	insertion	GB 48271
AB	120	U	-	insertion	GB 48271

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AA	2872	Total	C	N	O	P	0	0	0
			61847	27526	11556	19893	2872			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	494	G	-	insertion	GB 48268

- Molecule 3 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	221	Total	C	N	O	S	0	0	0
			1687	1066	306	312	3			

- Molecule 4 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	173	Total	C	N	O	S	0	0	0
			1308	820	246	236	6			

- Molecule 5 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	191	Total	C	N	O	S	0	0	0
			1507	940	290	273	4			

- Molecule 6 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	189	Total	C	N	O	S	0	0	0
			1430	872	255	302	1			

- Molecule 7 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	122	Total	C	N	O	S	0	0	0
			957	597	176	180	4			

- Molecule 8 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	164	Total	C	N	O	S	0	0	0
			1251	787	225	237	2			

- Molecule 9 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	128	Total	C	N	O	S	0	0	0
			945	599	152	193	1			
9	AJ	128	Total	C	N	O	S	0	0	0
			945	599	152	193	1			

- Molecule 10 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AK	148	Total	C	N	O	S	0	0	0
			1145	727	205	212	1			

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AL	133	Total	C	N	O	S	0	0	0
			999	642	169	182	6			

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	117	Total	C	N	O	S	0	0	0
			917	570	164	180	3			

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AN	122	Total	C	N	O	S	0	0	0
			937	585	180	169	3			

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AO	84	Total	C	N	O	0	0	0
			639	391	109	139			

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	138	Total	C	N	O	S	0	0	0
			1081	678	208	192	3			

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	113	Total	C	N	O	S	0	0	0
			866	536	165	164	1			

- Molecule 17 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AR	52	Total	C	N	O	S	0	0	0
			406	242	74	85	5			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AS	108	Total	C	N	O	0	0	0
			860	542	169	149			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AT	76	Total	C	N	O	S	0	0	0
			602	366	102	131	3			

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	110	Total	C	N	O		0	0	0
			879	531	166	182				

- Molecule 21 is a protein called 50S general stress protein CTC (L25).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AV	177	Total	C	N	O	S	0	0	0
			1360	859	238	257	6			

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AW	64	Total	C	N	O	S	0	0	0
			494	301	93	99	1			

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A0	105	Total	C	N	O		0	0	0
			855	536	174	145				

- Molecule 25 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A1	117	Total	C	N	O	S	0	0	0
			978	608	210	159	1			

- Molecule 26 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A2	100	Total	C	N	O	S	0	0	0
			787	495	146	145	1			

- Molecule 27 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A3	86	Total	C	N	O	S	0	0	0
			641	402	124	114	1			

- Molecule 28 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A4	73	Total	C	N	O	S	0	0	0
			604	382	110	108	4			

- Molecule 29 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A5	58	Total	C	N	O	S	0	0	0
			457	281	94	77	5			

- Molecule 30 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A6	53	Total	C	N	O	S	0	0	0
			431	274	80	76	1			

- Molecule 31 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A7	46	Total	C	N	O	S	0	0	0
			383	230	91	60	2			

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A8	63	Total	C	N	O	S	0	0	0
			496	312	101	78	5			

- Molecule 33 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A9	35	Total	C	N	O	S	0	0	0
			285	172	64	45	4			

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BA	1515	Total	C	N	O	P	0	0	0
			32554	14490	6022	10527	1515			

- Molecule 35 is a RNA chain called tRNA Phe (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BB	76	Total	C	N	O	P	0	0	0
			1626	725	293	532	76			
35	BC	76	Total	C	N	O	P	0	0	0
			1626	725	293	532	76			

- Molecule 36 is a RNA chain called thrS mRNA operator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B1	66	Total	C	N	O	P	0	0	0
			1405	629	247	463	66			

- Molecule 37 is a protein called 30S ribosomal protein S2.

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

- Molecule 38 is a protein called 30S ribosomal protein S3.

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

- Molecule 39 is a protein called 30S ribosomal protein S4.

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

- Molecule 40 is a protein called 30S ribosomal protein S5.

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

- Molecule 41 is a protein called 30S ribosomal protein S6.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S8.

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BK	25	ASP	GLU	conflict	UNP Q5SHQ2
BK	37	ARG	LYS	conflict	UNP Q5SHQ2
BK	52	ASP	GLU	conflict	UNP Q5SHQ2
BK	61	VAL	ILE	conflict	UNP Q5SHQ2
BK	62	TYR	HIS	conflict	UNP Q5SHQ2
BK	81	HIS	LYS	conflict	UNP Q5SHQ2
BK	88	LYS	ARG	conflict	UNP Q5SHQ2
BK	115	SER	PRO	conflict	UNP Q5SHQ2

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BL	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 45 is a protein called 30S ribosomal protein S10.

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

- Molecule 46 is a protein called 30S ribosomal protein S11.

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

- Molecule 47 is a protein called 30S ribosomal protein S12.

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

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

- Molecule 49 is a protein called 30S ribosomal protein S14.

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BT	96	GLN	GLU	conflict	UNP Q5SHP7

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	73	Total	C	N	O	S	0	0	0
			597	380	118	99				

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	41	VAL	ILE	conflict	UNP Q5SIH2

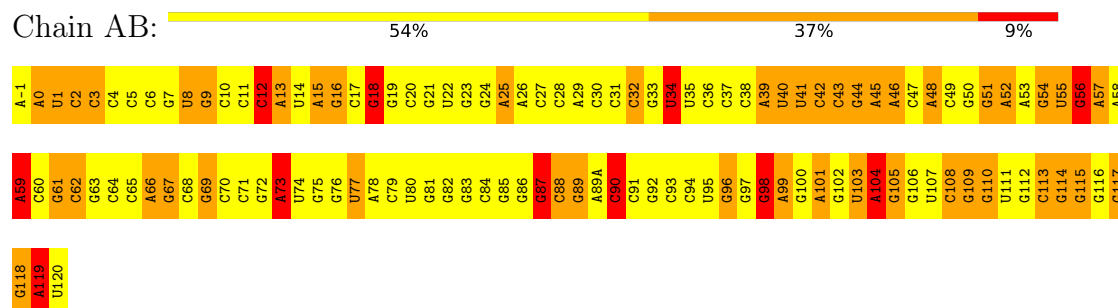
- Molecule 56 is a protein called 30S ribosomal protein Thx.

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

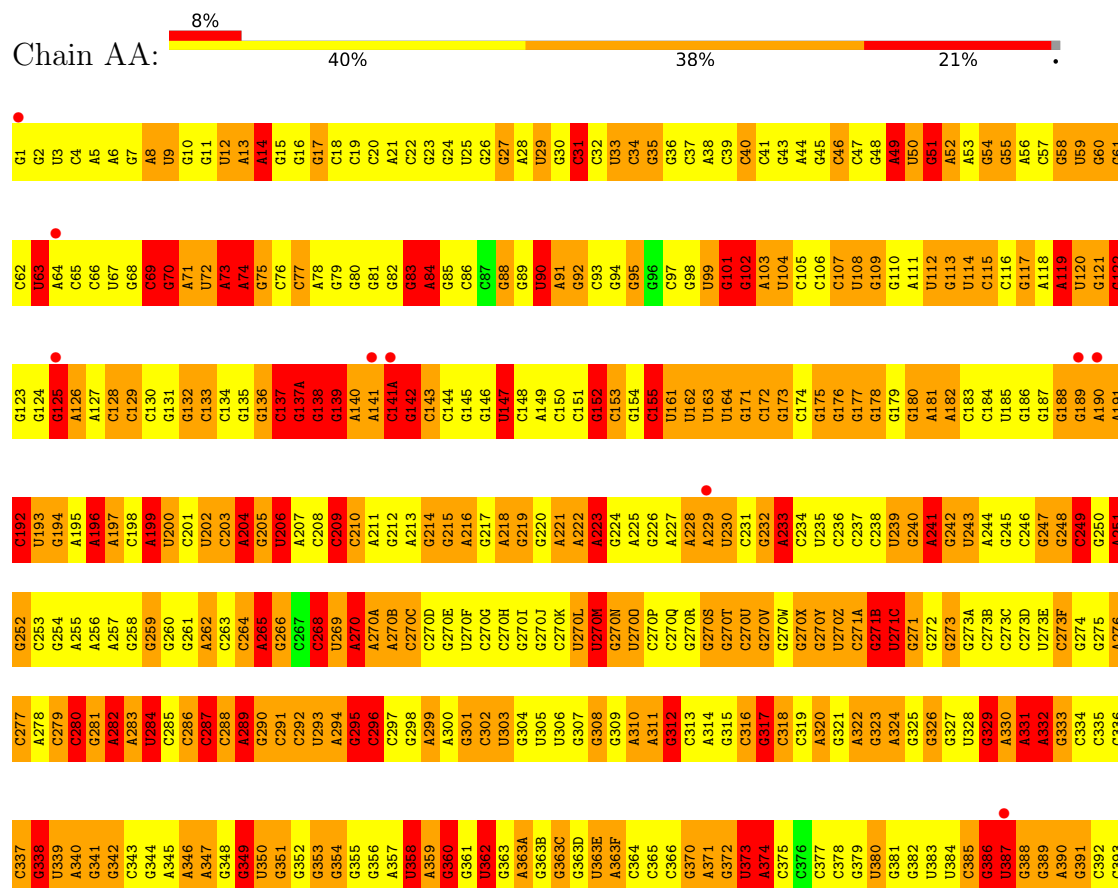
3 Residue-property plots

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: 5S ribosomal RNA



• Molecule 2: 23S ribosomal RNA



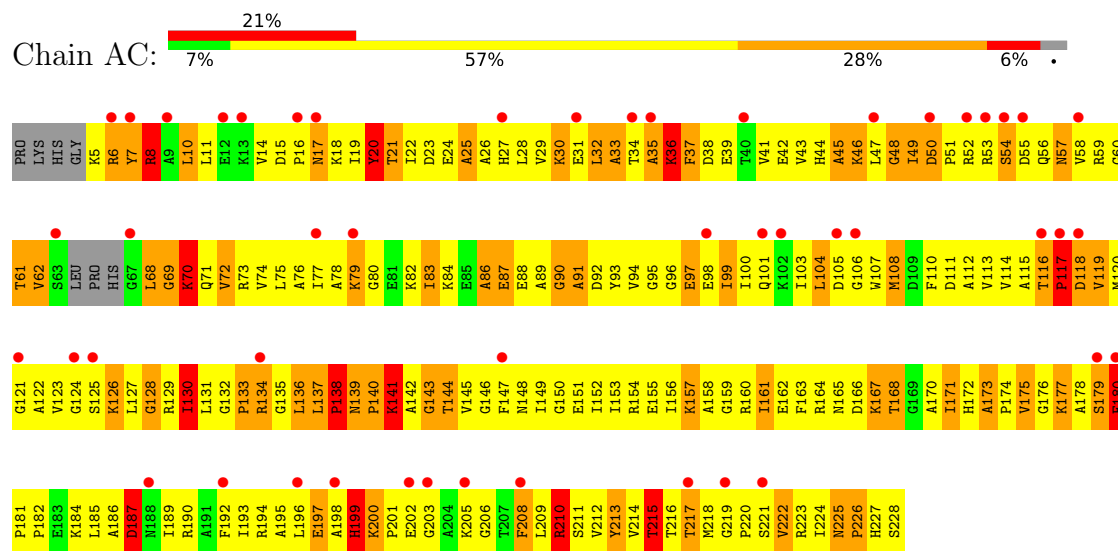
G1154	A1095	U1035	G975	C915	G854	G794	A734	G674	C635	G577	A515	A454	A394
A1155	A1096	G1036	C976	G916	G855	C995	A735	A675	G636	A578	C516	C455	U395
G1156	A1097	G1037	G977	A917	C856	C796	A736	A676	A637	A579	C517	C456	G396
A1157	A1098	G1038	G978	A918	C857	C797	A737	A677	G638	C580	G518	C457	G397
C1158	G1099	G1039	G979	A919	U858	G798	G738	C678	U639	C581	U519	G458	G398
U1159	A1100	C1040	A980	G920	G859	G799	G739	C679	G640	G582	G520	U459	G399
G1160	C1101	G1041	A981	G921	U860	A800	U740	G680	C641	G583	G521	A460	G400
C1161	C1102	G1042	A982	U922	A861	G801	G741	G681	G642	C584	G522	A461	A401
A1162	A1103	C1043	C983	G923	G862	A802	G742	G682	A643	C585	C523	C462	A402
G1163	C1104	G1044	A984	C924	A863	U803	G743	G683	A644	C586	U524	U463	U403
U1164	U1105	A1045	C985	G925	G864	A804	G744	G684	G645	C587	U525	U464	C404
U1165	G1106	A1046	C986	A926	C865	G805	G745	A685	A646	U588	A526	G465	U405
G1166	G1107	G1047	G987	G928	A866	G806	A746	G686	G647	C527	C527	A466	G406
U1167	U1108	A1048	A988	G929	C867	U807	U747	C887	G648	A590	A528	G467	G407
G1168	G989	C1049	G989	U930	U868	G808	G748	U688	G649	C591	A529	G468	G408
C1169	C1110	A1050	A990	G931	G869	G809	C749	A689	C	C	G530	G469	C409
A1170	A1111	G1051	C991	G932	A870	U810	A750	G690	G	G	C531	A470	C410
G1171	G1112	C1052	C992	A933	U871	U811	A751	C691	C	U594	A532	A471	C411
U1172	U1113	C1053	G993	G934	A872	C812	A752	C692	A	C595	G533	A472	A412
A1173	G1114	A1054	C994	C935	G873	U813	C753	C693	A	G	U534	G473	C413
U1174	G1115	G1055	C995	C936	G874	C814	C754	U694	G	U596	C535	G474	C414
G1175	C1116	A1056	A996	U937	G875	C815	C755	G695	C	C	A536	U475	A415
U1176	G1117	A1057	G997	G938	C876	C816	C756	G696	G	G	C537	G476	C416
C1177	C1118	G1058	G998	G939	U877	C817	U757	C697	G	G	G539	A477	C417
G1178	C1119	U1059	U999	G940	A878	G818	C758	C698	G	C601	G540	A478	G
U1179	G1120	U1060	A1000	A941	G879	A819	G759	A699	C	G602	C541	A479	C418
C1180	C1121	U1061	A1001	G942	G880	A820	G760	G700	C	A603	C542	A480	C419
G1181	G1122	G1062	A1002	U943	G881	A821	A761	G701	G	C	C543	G481	C420
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G1189	U1130	U1070	C951	C951	C889	A829	G769	U709	C	C611	G551	G489	A428
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G1191	A1132	C1072	U1012	A953	G892	G831	G771	G711	G	U613	U553	A492	G430
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G2017	C1957	G1897	G1828	U1768	U1692	A1632	A1572	C1513	C1451	C1393	U1273
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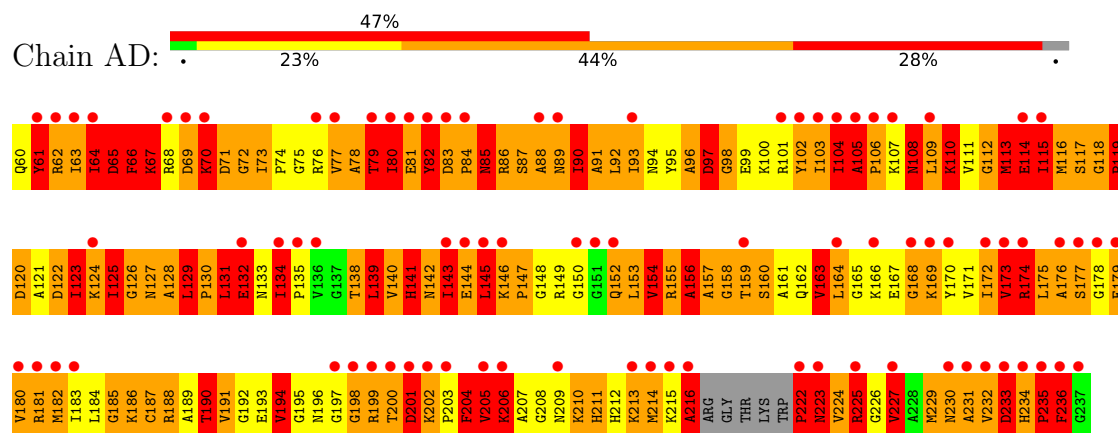




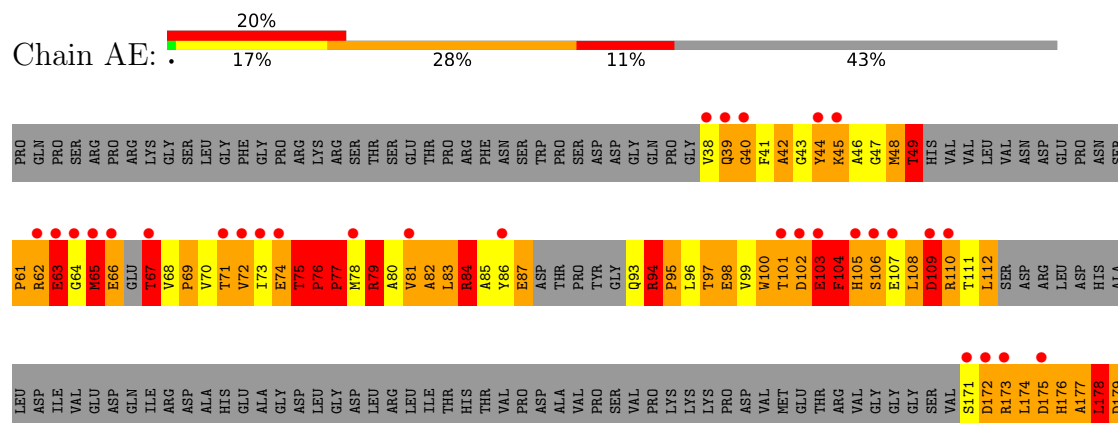
● Molecule 3: 50S ribosomal protein L1

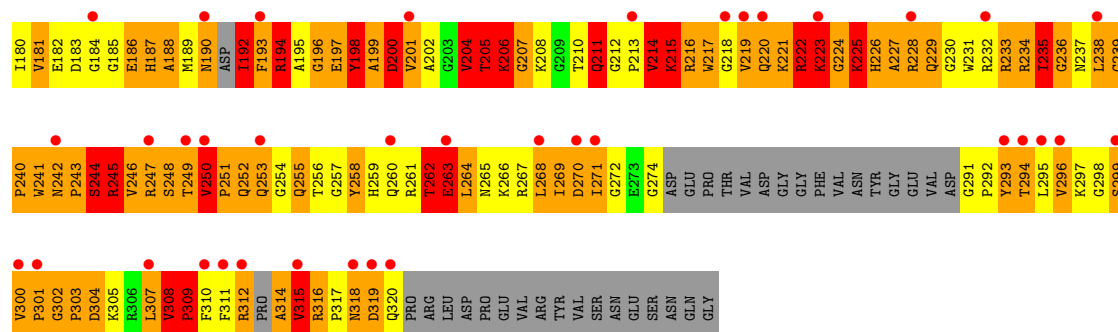


● Molecule 4: 50S ribosomal protein L2

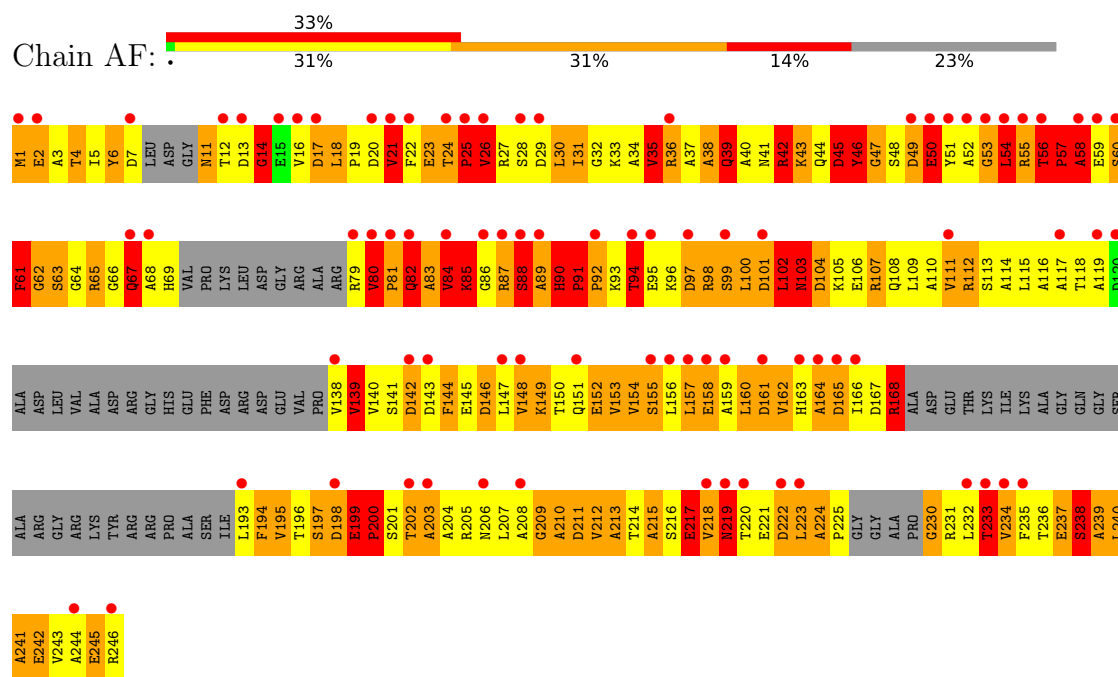


● Molecule 5: 50S ribosomal protein L3

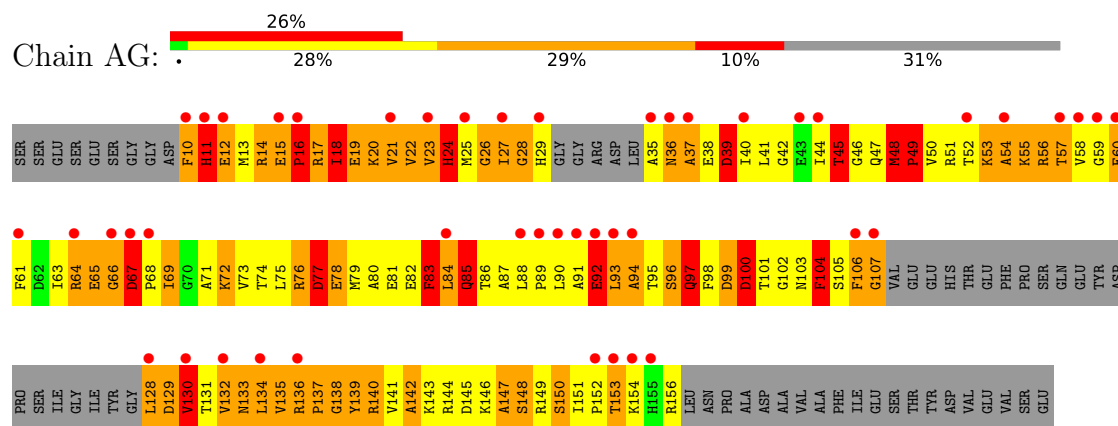




• Molecule 6: 50S ribosomal protein L4

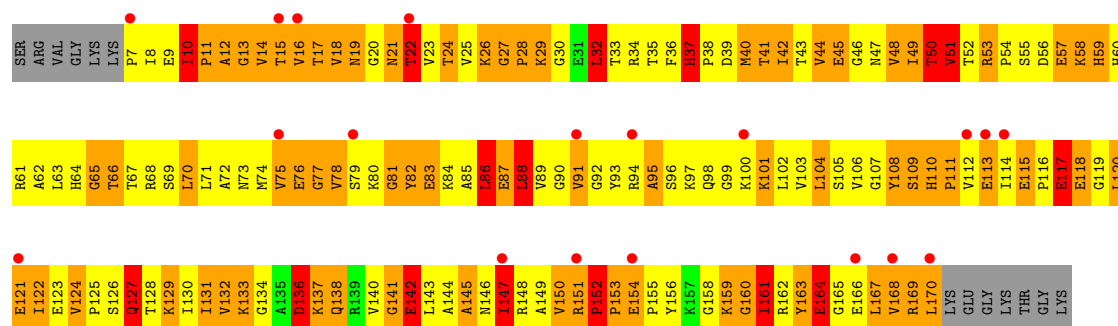


• Molecule 7: 50S ribosomal protein L5

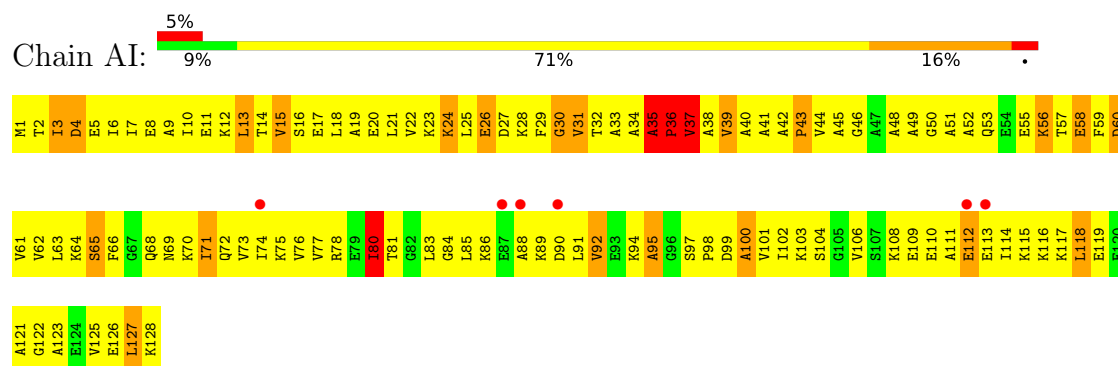


• Molecule 8: 50S ribosomal protein L6

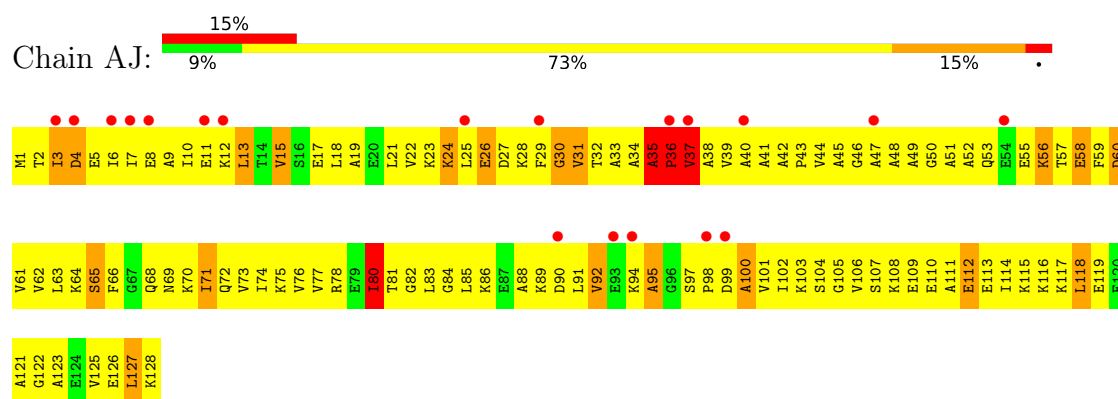




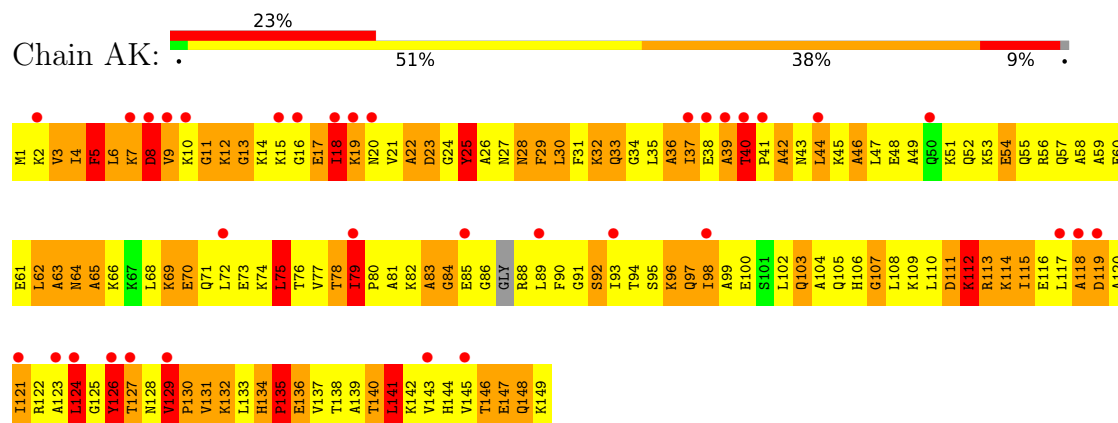
• Molecule 9: 50S ribosomal protein L7/L12



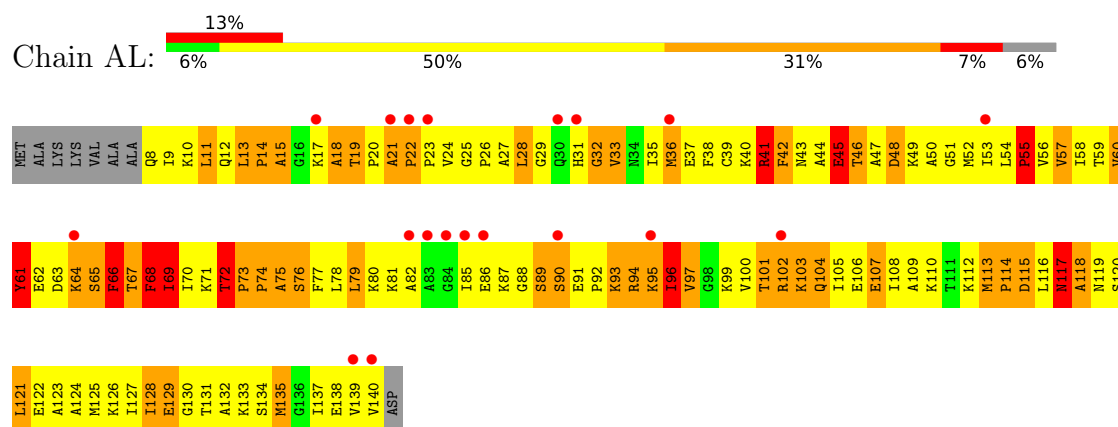
• Molecule 9: 50S ribosomal protein L7/L12



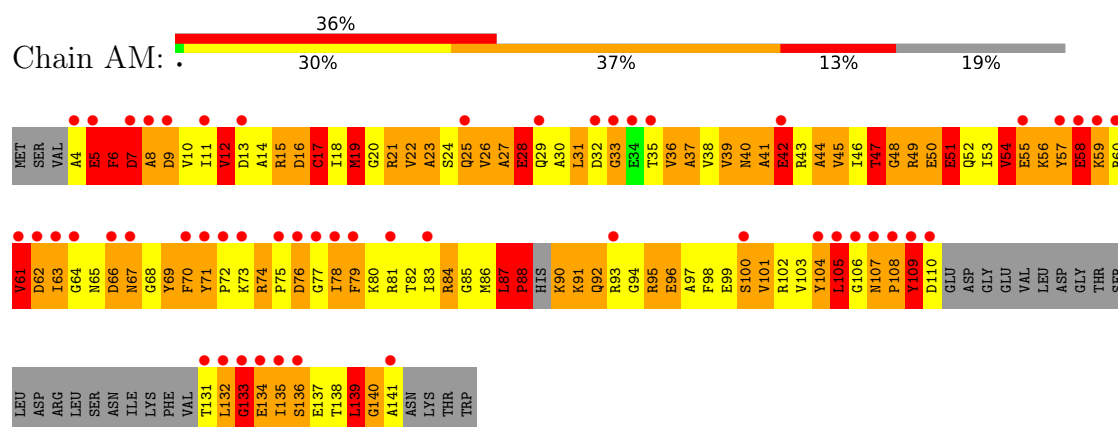
• Molecule 10: 50S ribosomal protein L9



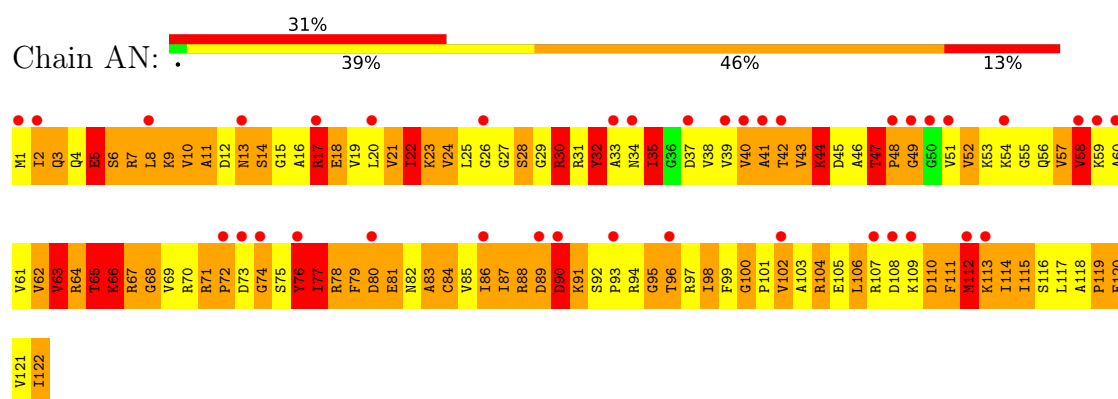
- Molecule 11: 50S ribosomal protein L11



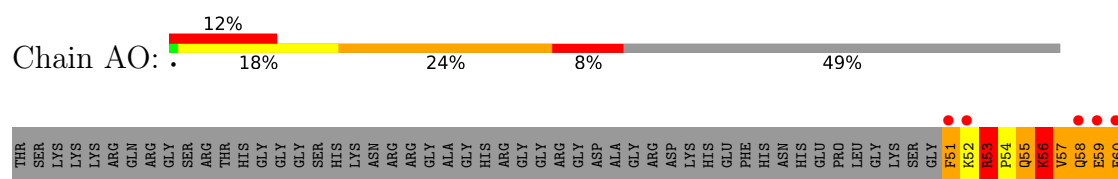
- Molecule 12: 50S ribosomal protein L13

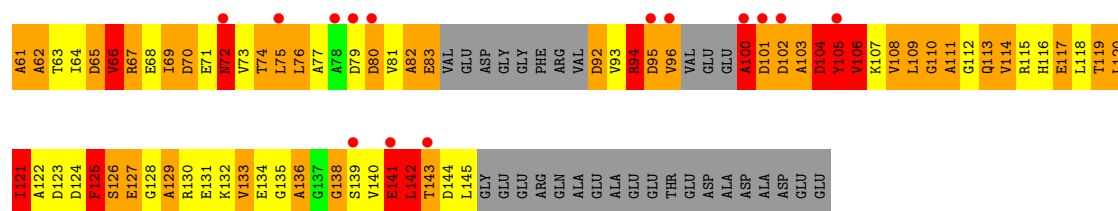


- Molecule 13: 50S ribosomal protein L14

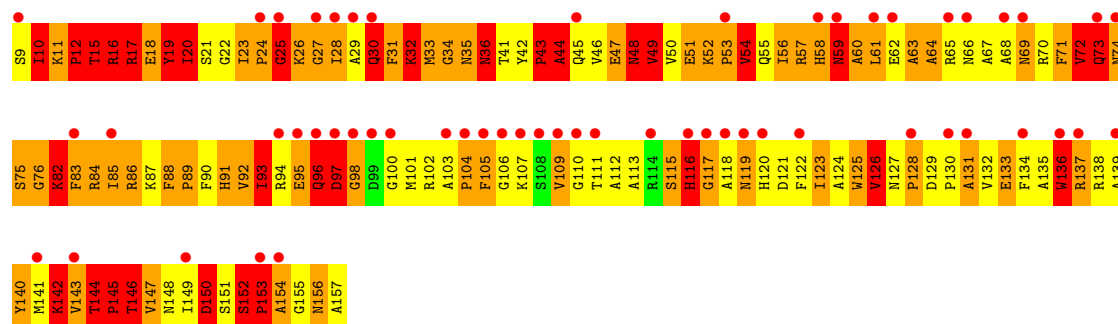


- Molecule 14: 50S ribosomal protein L15

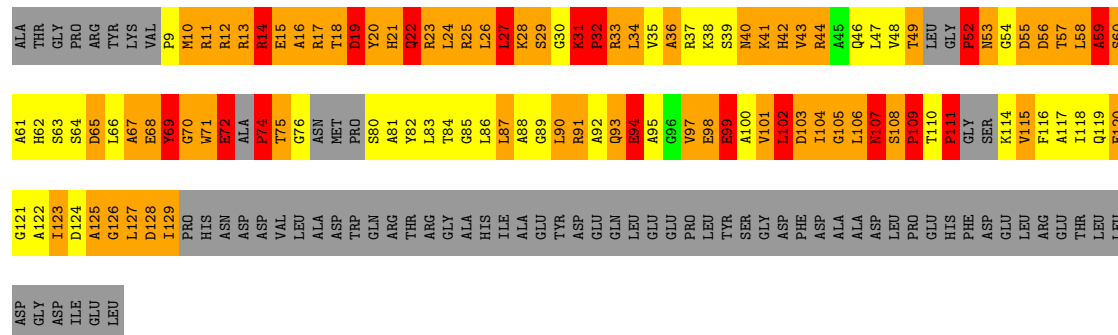
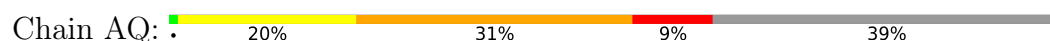




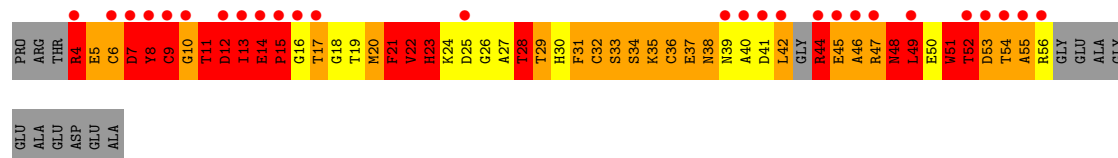
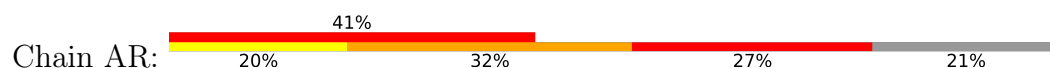
• Molecule 15: 50S ribosomal protein L16



• Molecule 16: 50S ribosomal protein L18

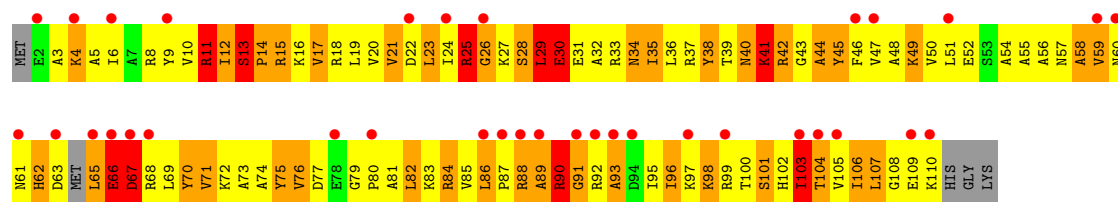


• Molecule 17: 50S ribosomal protein L19

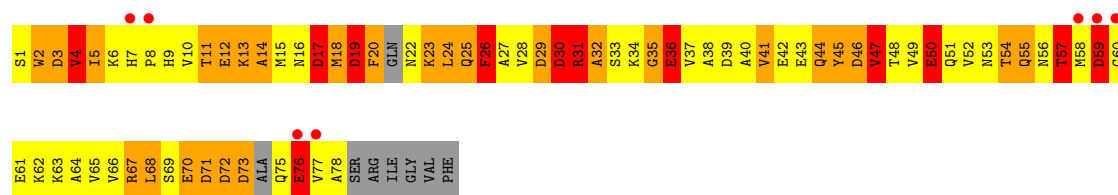


• Molecule 18: 50S ribosomal protein L22

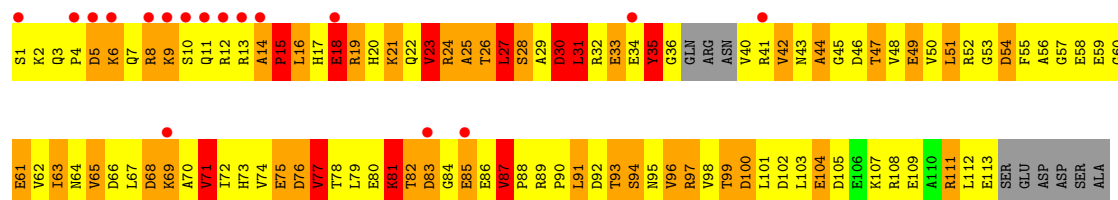




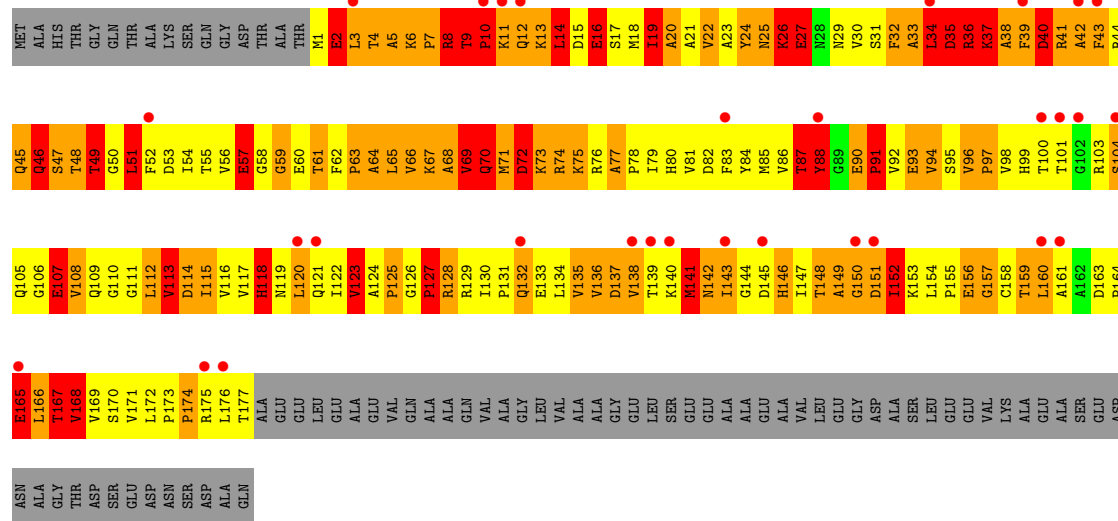
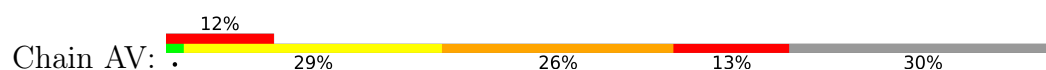
• Molecule 19: 50S ribosomal protein L23



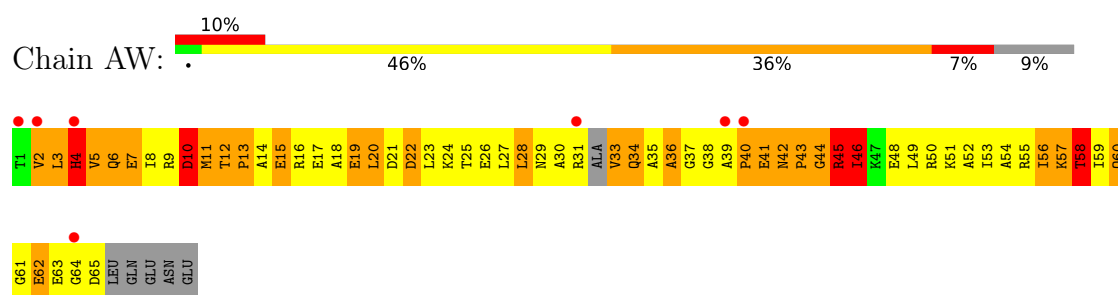
• Molecule 20: 50S ribosomal protein L24



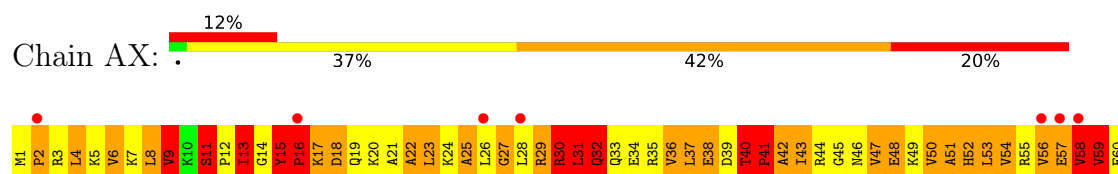
• Molecule 21: 50S general stress protein CTC (L25)



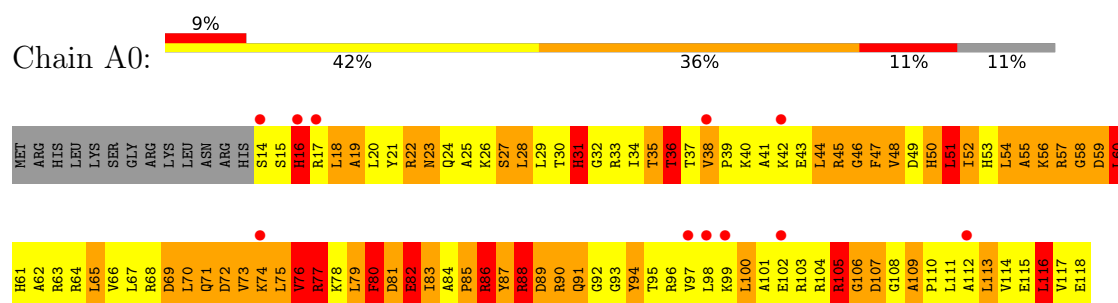
• Molecule 22: 50S ribosomal protein L29



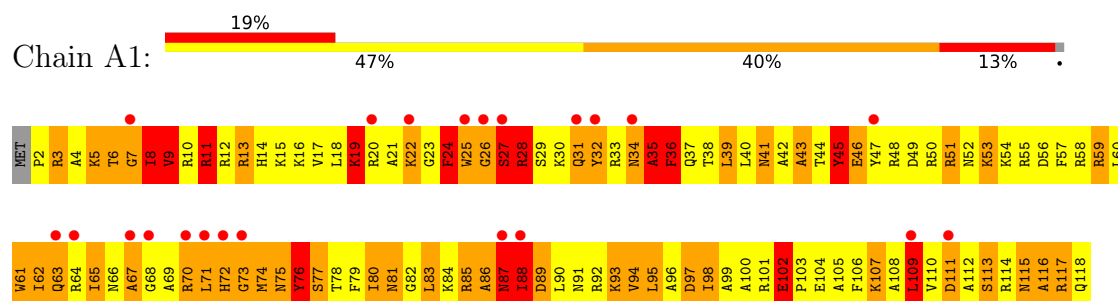
- Molecule 23: 50S ribosomal protein L30



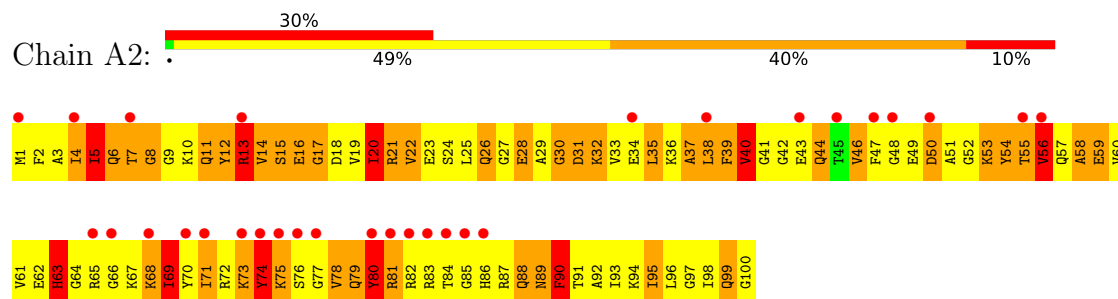
- Molecule 24: 50S ribosomal protein L17



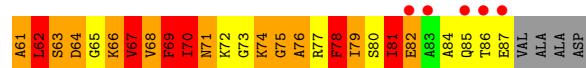
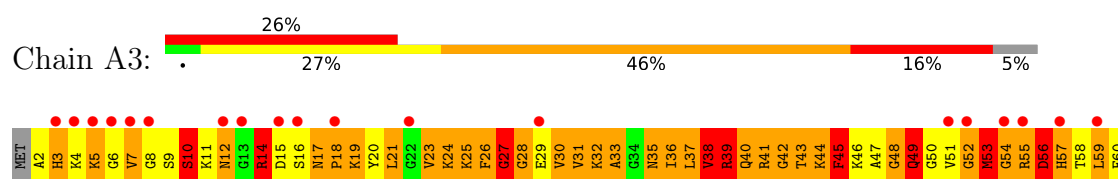
- Molecule 25: 50S ribosomal protein L20



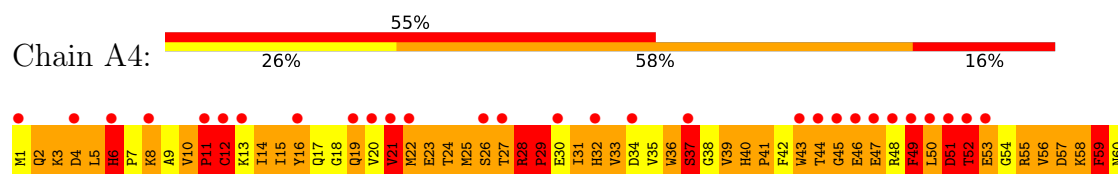
- Molecule 26: 50S ribosomal protein L21



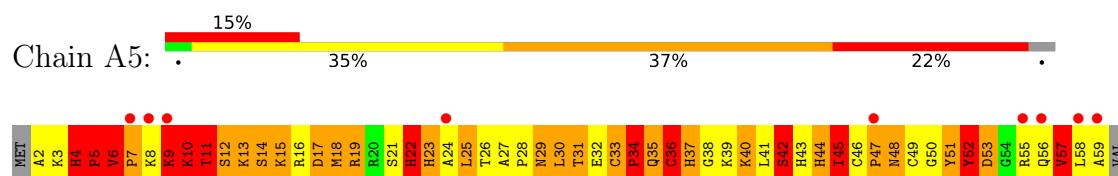
- Molecule 27: 50S ribosomal protein L27



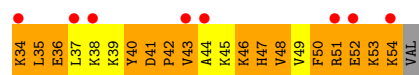
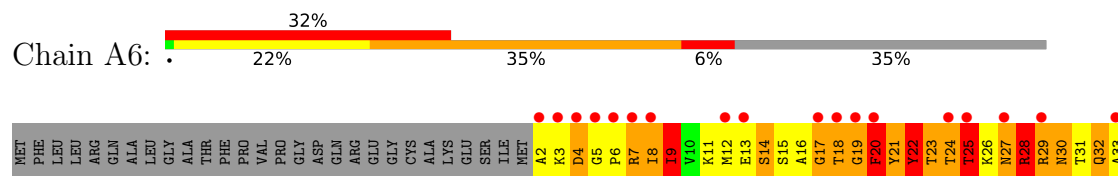
• Molecule 28: 50S ribosomal protein L31



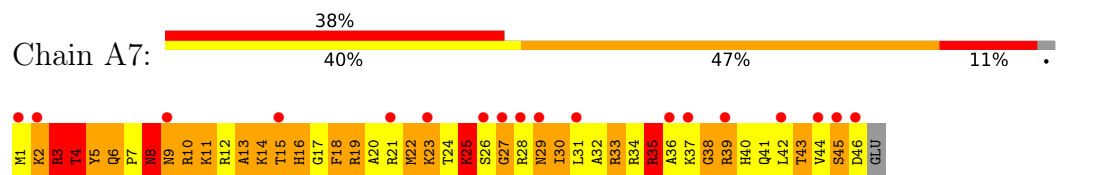
• Molecule 29: 50S ribosomal protein L32



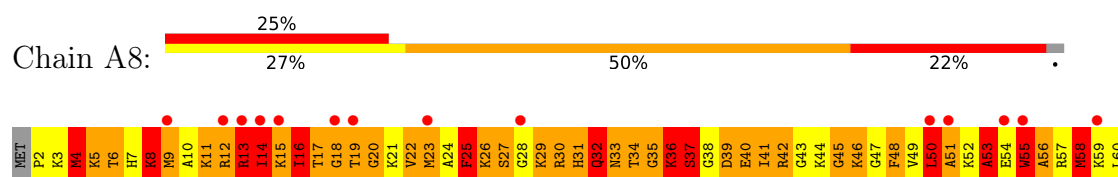
• Molecule 30: 50S ribosomal protein L33



• Molecule 31: 50S ribosomal protein L34



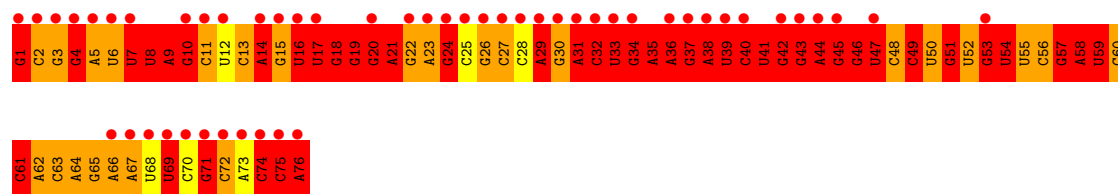
• Molecule 32: 50S ribosomal protein L35



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C1524	G1464	C1399	A1340	A1280	G1220	U1159	G1099	C1039	C984	C924	A854	G798	C738
G1525	C1465	C1400	U1341	U1281	G1221	G1160	C1100	U1040	C985	G925	A855	G799	C739
G1526	C1466	C1401	C1342	U1282	G1222	C1161	A1101	A1041	A986	G926	C866	G800	U740
C1527	G1467	C1402	G1343	G1283	C1223	C1162	C1102	G1042	G987	G927	C867	A801	G741
A1468	C1403	C1403	C1344	G1284	G1224	C1163	C1103	C1043	G988	G928	C868	A802	G742
G1469	U1345	C1404	U1346	A1285	A1225	G1164	G1104	A1044	C989	G929	G869	G803	U743
G1470	A1346	G1405	G1347	A1286	C1226	C1165	A1105	U1045	C990	C930	U870	U804	C744
U1471	G1347	U1406	U1348	A1287	C1227	G1166	G1106	A1046	U991	C931	U871	C805	C745
U1472	A1348	C1407	A1288	A1288	C1228	A1167	G1107	G1047	A992	C932	A872	C806	A746
A1473	A1349	A1408	A1289	A1289	C1229	A1168	G1108	G1048	G993	C933	A873	A807	C747
G1474	A1350	C1409	G1290	G1291	C1230	A1169	C1109	U1049	A994	C934	C874	C808	C748
G1475	U1351	G1410	U1351	G1291	G1231	C1171	A1110	G1050	C995	A935	C875	G809	C749
G1476	C1352	C1411	C1352	U1282	U1232	C1172	A1111	C1051	A996	C936	C876	C810	G750
C1477	G1353	C1412	G1353	G1293	C1233	G1173	C1112	U1052	U997	A937	C877	C811	U751
C1478	A1354	A1413	C1354	G1294	C1234	G1174	C1113	G1053	G998	A938	C878	C812	G752
C1479	G1355	G1414	G1355	G1295	U1235	A1175	C1114	C1054	C999	G939	C879	U813	A753
G1480	G1356	G1415	G1356	C1296	A1236	G1176	C1115	A1055	U1000	C940	C880	A814	A754
U1481	A1357	G1416	A1357	C1297	C1237	G1177	C1116	U1056	A1001	G941	C881	A815	G755
G1482	U1358	G1417	U1358	C1298	A1238	G1178	G1117	G1057	G1002	G942	C882	A816	C756
A1483	C1359	A1418	C1359	A1299	A1239	G1179	C1118	G1058	U1003	U943	C883	C817	U757
C1484	A1360	G1419	A1360	G1300	U1240	A1180	C1119	C1059	G3A	G944	U884	A818	A758
U1485	G1361	C1420	G1361	U1301	G1241	G1181	G1120	C1060	A1004	G945	C885	A819	G759
G1486	C361A	G1421	C361A	U1302	C1242	G1182	U1121	G1061	A946	U946	C886	U820	G760
G1487	C1362	G1422	C1362	U1303	C1243	A1183	U1122	U1062	C1006	G947	G887	G821	G761
G1488	A1363	G1423	A1363	G1304	C1244	G1184	A1123	C1063	C1007	C948	C888	C822	C762
G1489	U1364	C1424	U1364	G1305	A1245	G1185	G1124	G1064	U1008	A949	A889	G823	G763
C1490	G1365	U1425	G1365	A1306	C1246	G1186	U1125	U1065	G1009	U950	C889	C824	C764
G1491	C1366	C1426	C1366	U1307	U1247	G1187	U1126	C1066	G1010	G951	U891	G825	G765
A1492	C1367	U1427	C1367	U1308	A1248	A1188	G1127	A1067	G1011	U952	A892	C826	A766
A1493	G1368	A1428	G1368	G1309	C1249	C1189	C1128	G1068	C893	G953	C893	U827	A767
G1494	C1369	C1429	C1369	G1310	A1250	G1190	C1129	C1069	G1013	G954	C894	A828	A768
U1495	G1370	C1430	G1370	G1311	A1251	A1191	A1130	U1070	A1014	U955	C895	G829	G769
C1496	G1371	C1431	G1371	G1312	A1252	C1192	C1131	C1071	A1015	U956	C896	G830	C770
G1497	U1372	A1432	G1372	U1313	G1253	C1193	C1132	G1072	A1016	U957	C897	U831	G771
U1498	G1373	A1433	G1373	C1314	C1254	U1194	G1133	G1073	C898	A958	C898	C832	U772
A1499	A1374	A1434	A1374	U1315	G1255	C1195	G1134	G1074	C1018	A959	C899	U833	G773
A1500	U1375	G1435	U1375	G1316	A1256	U1196	U1135	C1075	C1019	U960	A900	C834	G774
C1501	U1376	U1436	U1376	G1317	U1257	G1197	U1136	C1076	U1020	U961	A901	U835	G775
A1502	A1377	C1437	A1377	A1318	G1258	G1198	C1137	G1077	G1021	C962	G902	C836	G776
G1503	C1378	G1438	C1378	A1319	C1259	U1199	G1138	U1078	G1022	G963	G903	C837	A777
G1504	G1379	C1439	G1379	C1320	C1260	C1200	G1139	G1079	G1023	A964	C904	U838	C778
G1505	U1380	G1440	U1380	C1321	A1261	A1201	C1140	A1080	U1025	G965	U905	U839	C779
U1506	U1381	C1441	U1381	C1322	C1262	G1202	C1141	G1081	G1026	C967	A907	C840	A780
A1507	C1382	G1442	C1382	G1323	C1263	C1203	G1142	G1082	C1027	C968	A907	U841	A781
G1508	C1383	G1443	C1383	A1324	C1264	A1204	G1143	U1083	C1028	A969	A908	C848	A782
C1509	C1384	A1446	C1384	C1325	G1265	U1205	G1144	G1084	A969	C970	A909	C849	C783
U1510	G1385	C1447	G1385	C1326	C1266	G1206	C1145	U1085	C1029	G971	C910	U850	C784
G1511	G1386	C1448	G1386	C1327	C1267	G1207	A1146	U1086	C1030	G971	U911	G851	G785
U1512	C1387	G1449	C1387	C1328	A1268	C1208	C1147	G1087	G30A	C972	C912	G852	G786
A1513	C1388	U1450	C1388	A1329	A1269	C1209	U1148	G1088	G30B	G973	A913	C853	A787
C1514	C1389	A1451	C1389	U1330	C1270	C1210	C1149	U1089	G30C	A974	A914	G854	U788
G1515	U1390	C1452	U1390	G1331	G1271	U1211	U1150	U1090	A30D	A975	A915	C855	U789
G1516	U1391	G1453	U1391	A1332	C1272	U1212	A1151	U1091	G1031	G976	G916	C856	A790
A1517	G1392	G1454	G1392	A1333	G1273	A1213	A1152	A1092	G1032	A977	G917	C857	G791
G1518	U1393	G1455	U1393	G1334	C1274	C1214	C1153	A1093	G1033	A978	A918	G858	A792
A1519	A1394	C1459	A1394	C1335	A1275	G1215	G1154	G1094	G1034	C979	A919	A859	U793
G1520	C1395	A1460	C1395	G1336	G1276	C1216	G1155	U1095	A1035	C980	A920	A860	A794
U1521	A1396	G1461	A1396	G1337	C1277	C1217	G1156	U1096	G1036	U981	U921	C861	C795
U1522	C1397	G1462	C1397	G1338	U1278	C1218	A1157	C1097	C1037	U982	G922	C862	C796

• Molecule 35: tRNA Phe (unmodified bases)

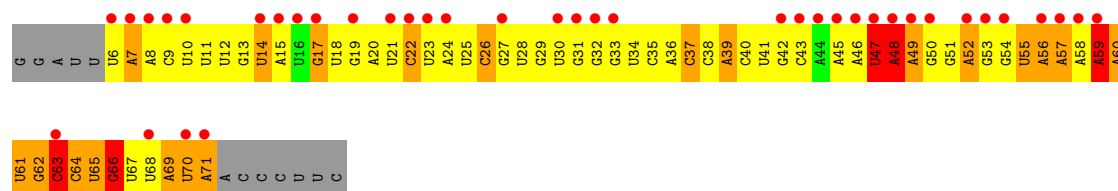




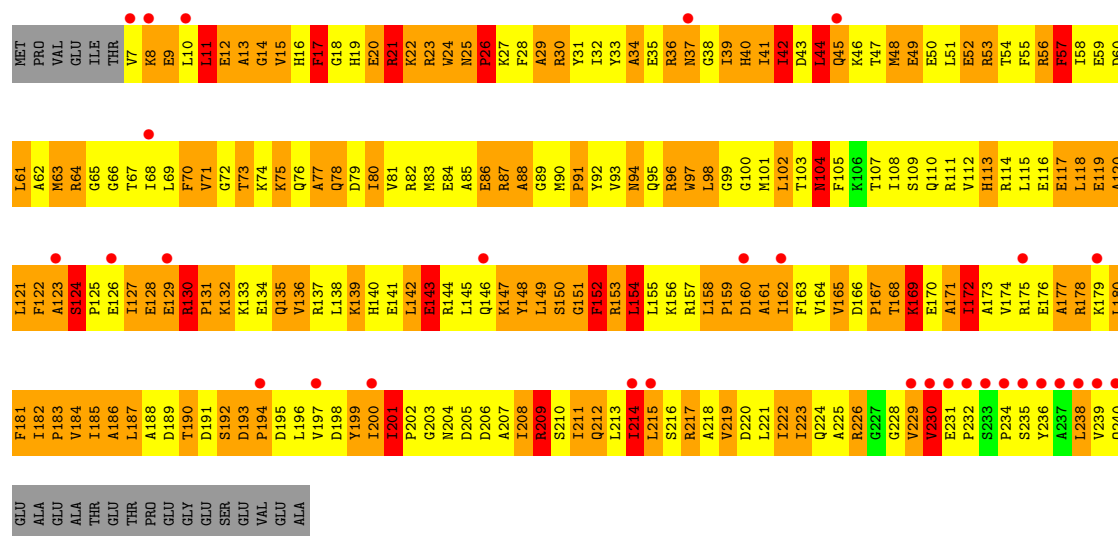
• Molecule 35: tRNA Phe (unmodified bases)



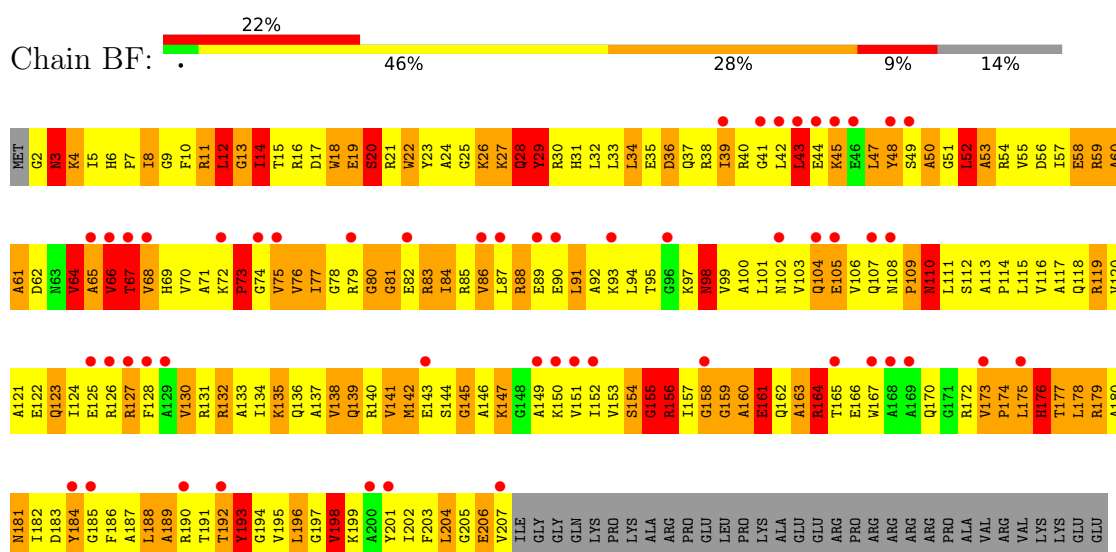
• Molecule 36: thrS mRNA operator



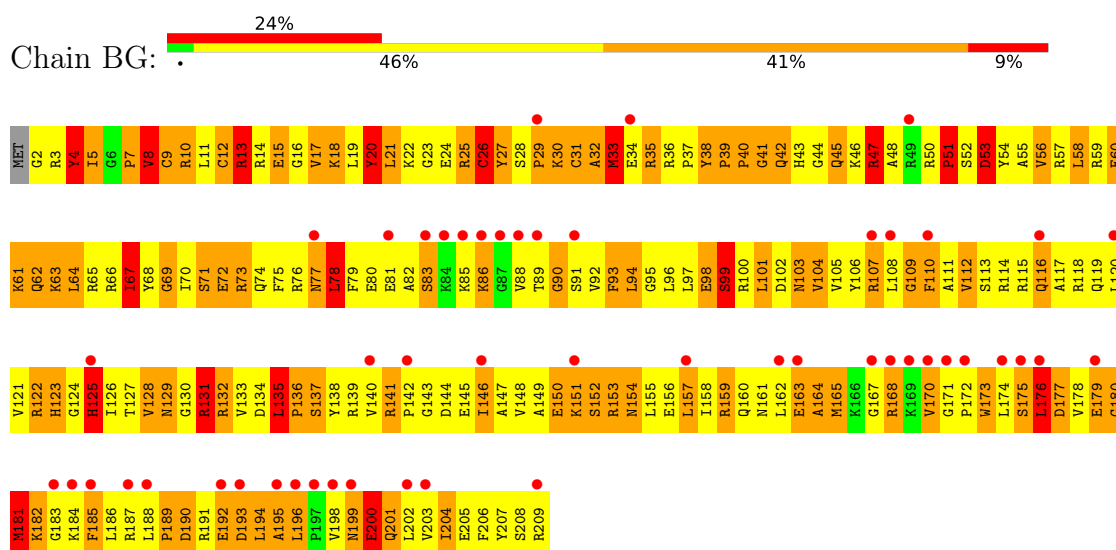
• Molecule 37: 30S ribosomal protein S2



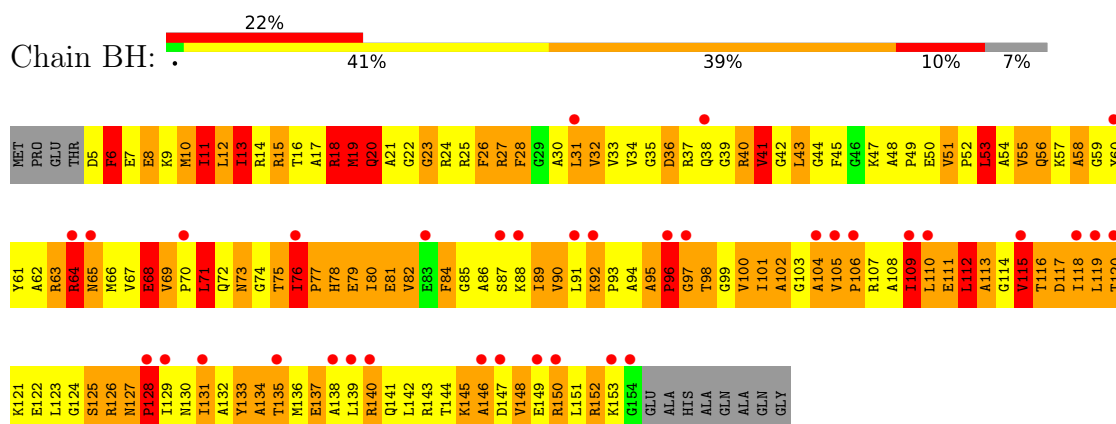
• Molecule 38: 30S ribosomal protein S3



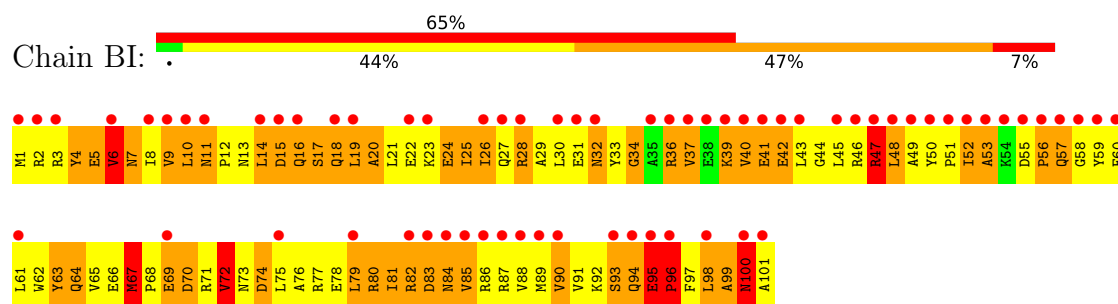
• Molecule 39: 30S ribosomal protein S4



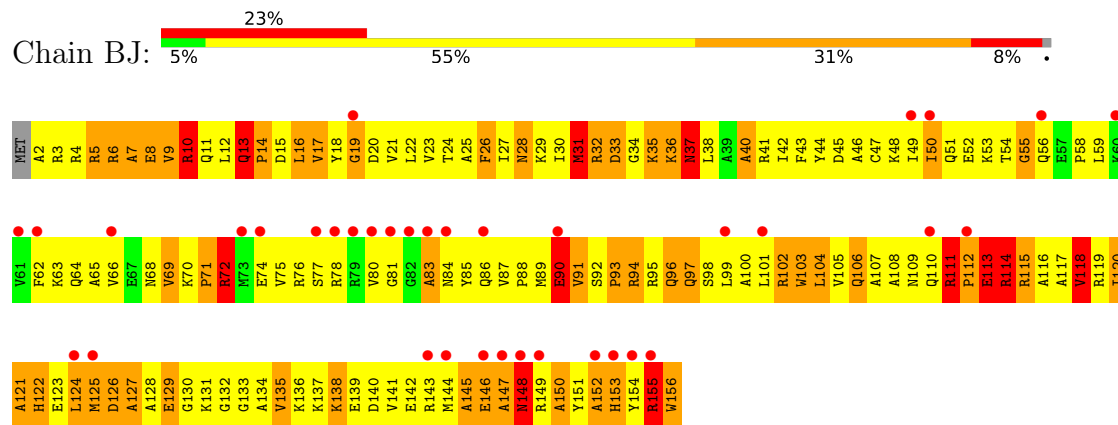
• Molecule 40: 30S ribosomal protein S5



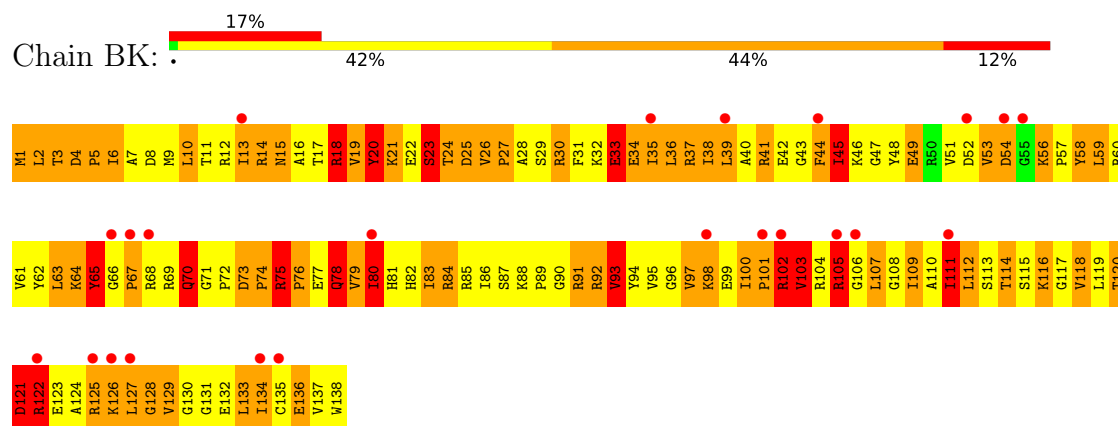
• Molecule 41: 30S ribosomal protein S6



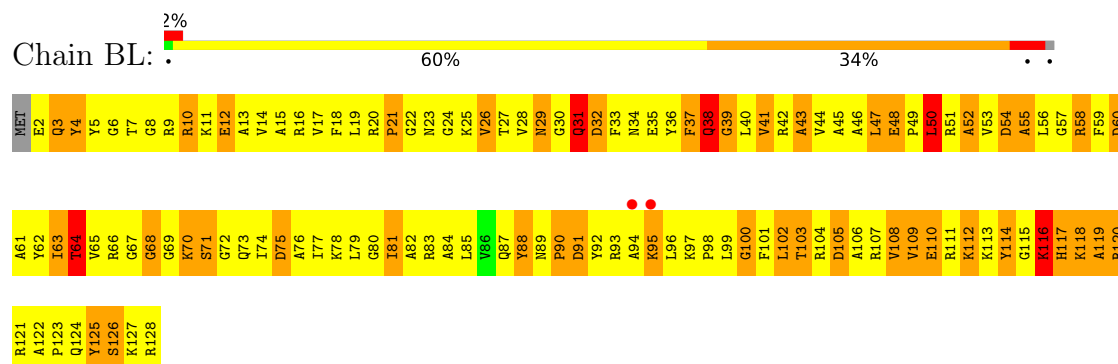
- Molecule 42: 30S ribosomal protein S7



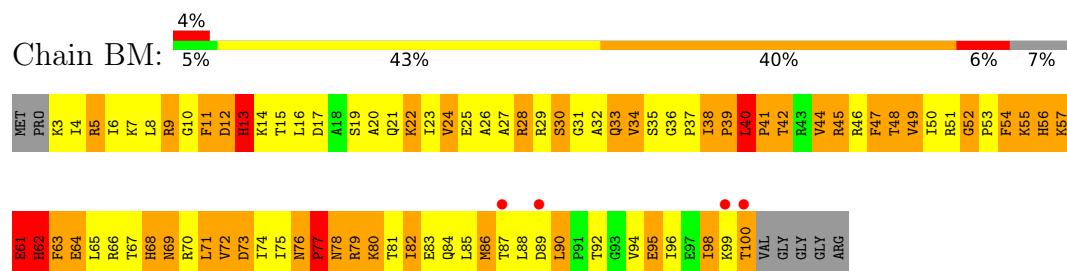
- Molecule 43: 30S ribosomal protein S8



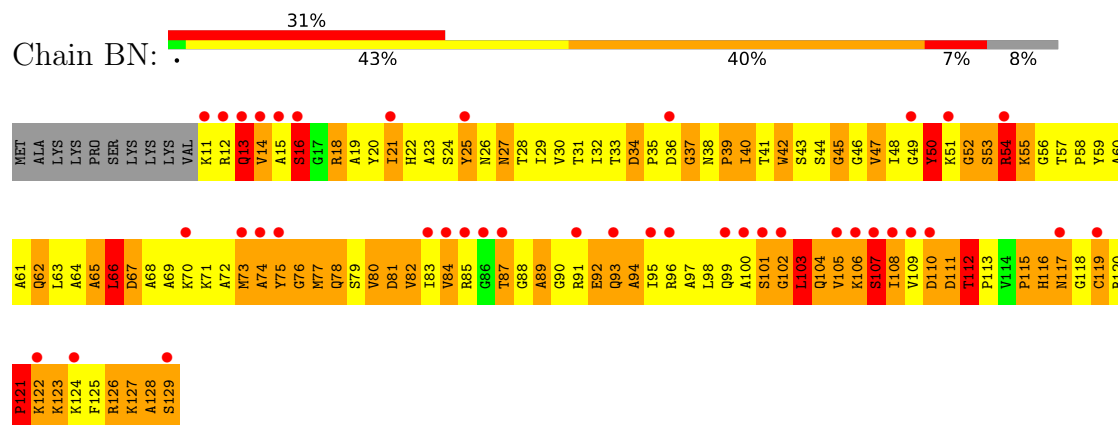
- Molecule 44: 30S ribosomal protein S9



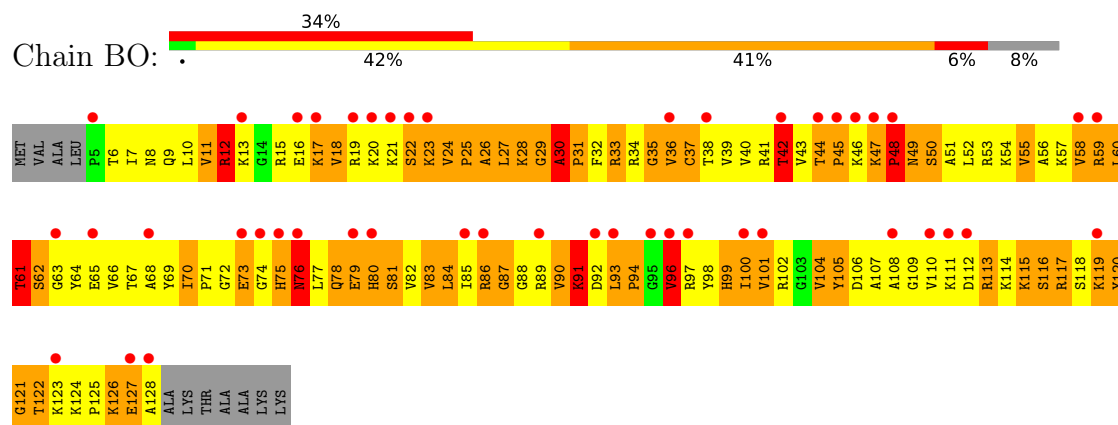
• Molecule 45: 30S ribosomal protein S10



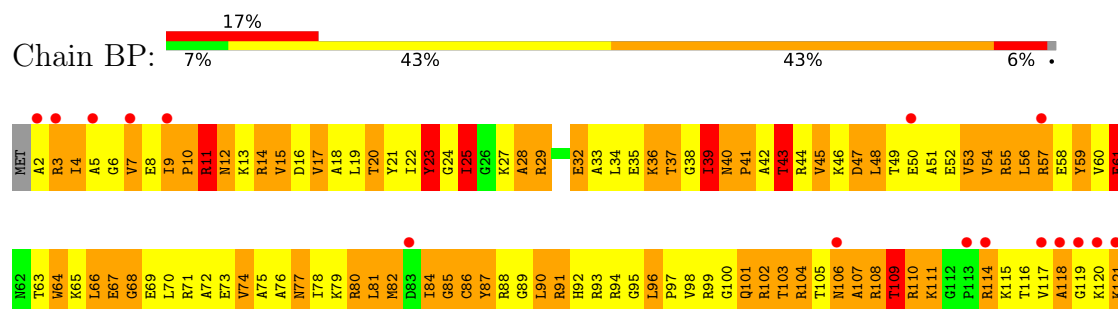
• Molecule 46: 30S ribosomal protein S11

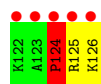


• Molecule 47: 30S ribosomal protein S12

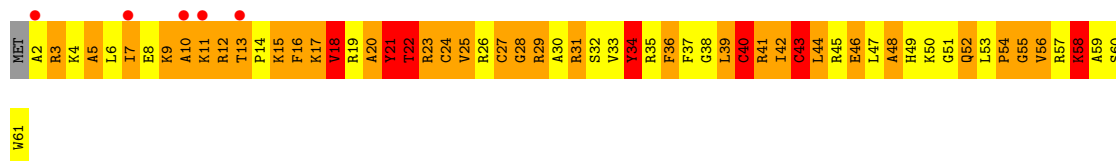


• Molecule 48: 30S ribosomal protein S13

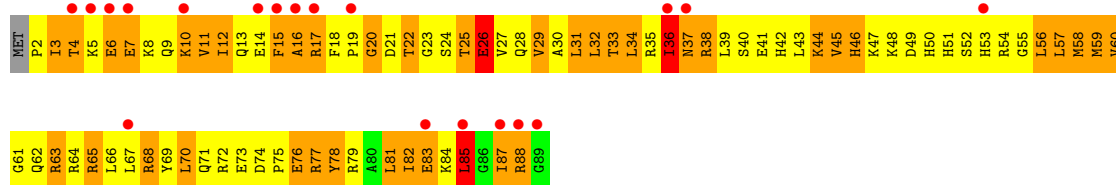




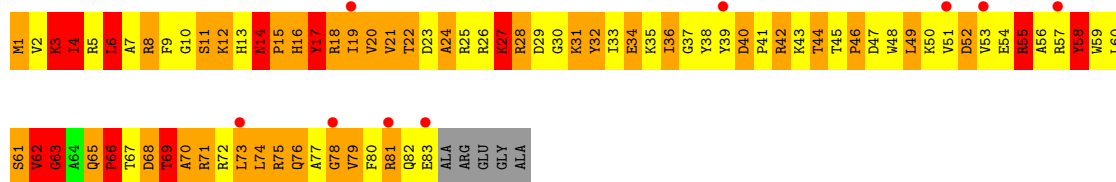
• Molecule 49: 30S ribosomal protein S14



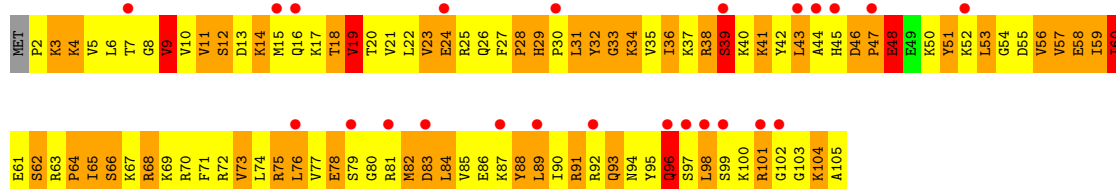
• Molecule 50: 30S ribosomal protein S15



• Molecule 51: 30S ribosomal protein S16

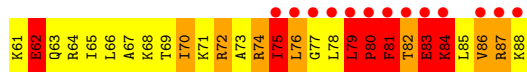


• Molecule 52: 30S ribosomal protein S17

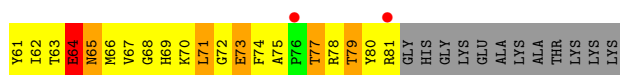
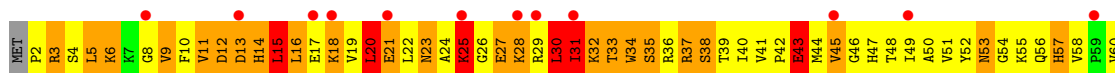


• Molecule 53: 30S ribosomal protein S18

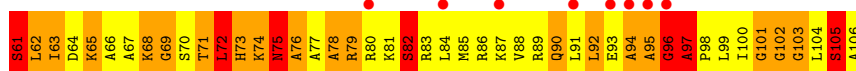
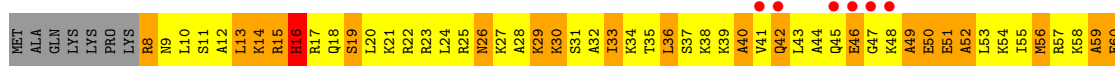




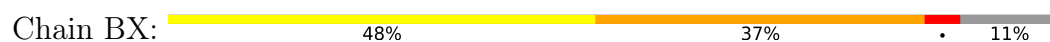
- Molecule 54: 30S ribosomal protein S19



- Molecule 55: 30S ribosomal protein S20



- Molecule 56: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	508.64Å 508.64Å 806.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 5.50 300.00 – 5.50	Depositor EDS
% Data completeness (in resolution range)	94.6 (300.00-5.50) 97.3 (300.00-5.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 5.42Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.307 , 0.356 0.283 , 0.327	Depositor DCC
R_{free} test set	7724 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	206.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 113.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	148539	wwPDB-VP
Average B, all atoms (Å ²)	338.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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	AB	0.66	0/2954	1.06	8/4606 (0.2%)
2	AA	0.78	30/69267 (0.0%)	1.22	747/108130 (0.7%)
3	AC	0.91	2/1715 (0.1%)	1.46	32/2310 (1.4%)
4	AD	1.48	16/1329 (1.2%)	2.24	84/1787 (4.7%)
5	AE	1.40	11/1542 (0.7%)	2.03	79/2084 (3.8%)
6	AF	1.13	4/1446 (0.3%)	1.97	68/1960 (3.5%)
7	AG	1.10	2/972 (0.2%)	1.83	30/1307 (2.3%)
8	AH	1.05	2/1272 (0.2%)	1.71	38/1721 (2.2%)
9	AI	0.72	2/950 (0.2%)	1.17	8/1275 (0.6%)
9	AJ	0.61	0/950	1.07	6/1275 (0.5%)
10	AK	1.03	0/1157	1.78	40/1547 (2.6%)
11	AL	0.71	0/1015	1.42	24/1366 (1.8%)
12	AM	1.36	4/928 (0.4%)	1.74	27/1248 (2.2%)
13	AN	1.41	4/946 (0.4%)	1.97	36/1269 (2.8%)
14	AO	1.01	0/643	1.98	30/870 (3.4%)
15	AP	1.46	9/1109 (0.8%)	2.12	51/1499 (3.4%)
16	AQ	1.00	0/880	1.68	25/1189 (2.1%)
17	AR	1.85	8/413 (1.9%)	2.98	47/557 (8.4%)
18	AS	1.15	3/869 (0.3%)	1.77	20/1166 (1.7%)
19	AT	1.02	1/609 (0.2%)	1.56	10/823 (1.2%)
20	AU	0.64	0/887	1.46	19/1195 (1.6%)
21	AV	1.02	3/1385 (0.2%)	1.62	34/1883 (1.8%)
22	AW	0.99	0/497	1.45	10/668 (1.5%)
23	AX	1.11	1/482 (0.2%)	1.73	15/646 (2.3%)
24	A0	1.20	0/867	1.72	22/1162 (1.9%)
25	A1	1.40	3/994 (0.3%)	1.85	26/1323 (2.0%)
26	A2	0.96	0/797	1.61	16/1061 (1.5%)
27	A3	0.99	1/649 (0.2%)	1.58	23/860 (2.7%)
28	A4	1.33	5/620 (0.8%)	1.69	17/831 (2.0%)
29	A5	1.06	1/469 (0.2%)	1.98	18/629 (2.9%)
30	A6	1.25	3/438 (0.7%)	1.91	13/583 (2.2%)
31	A7	1.09	1/387 (0.3%)	1.31	3/509 (0.6%)
32	A8	1.23	2/503 (0.4%)	2.15	22/657 (3.3%)
33	A9	1.66	5/286 (1.7%)	2.05	12/375 (3.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
34	BA	0.71	6/36438 (0.0%)	1.12	259/56869 (0.5%)
35	BB	1.44	17/1818 (0.9%)	2.13	128/2831 (4.5%)
35	BC	0.73	0/1818	1.13	12/2831 (0.4%)
36	B1	0.61	3/1571 (0.2%)	0.89	6/2445 (0.2%)
37	BE	1.02	2/1935 (0.1%)	1.53	40/2609 (1.5%)
38	BF	0.85	0/1636	1.47	32/2205 (1.5%)
39	BG	1.11	5/1733 (0.3%)	1.54	37/2318 (1.6%)
40	BH	1.20	4/1162 (0.3%)	1.66	30/1564 (1.9%)
41	BI	1.03	2/856 (0.2%)	1.48	18/1154 (1.6%)
42	BJ	0.91	1/1276 (0.1%)	1.38	19/1709 (1.1%)
43	BK	1.09	0/1136	1.57	24/1527 (1.6%)
44	BL	0.73	0/1029	1.23	8/1378 (0.6%)
45	BM	0.85	1/807 (0.1%)	1.41	15/1085 (1.4%)
46	BN	0.98	1/900 (0.1%)	1.50	21/1213 (1.7%)
47	BO	1.07	1/986 (0.1%)	1.79	38/1320 (2.9%)
48	BP	0.80	1/1008 (0.1%)	1.42	14/1347 (1.0%)
49	BQ	1.07	4/501 (0.8%)	1.40	8/664 (1.2%)
50	BR	1.04	0/745	1.44	9/992 (0.9%)
51	BS	1.07	1/716 (0.1%)	1.58	20/963 (2.1%)
52	BT	1.13	1/870 (0.1%)	1.51	16/1159 (1.4%)
53	BU	1.04	0/603	1.65	17/799 (2.1%)
54	BV	0.80	0/661	1.33	5/890 (0.6%)
55	BW	1.16	1/764 (0.1%)	1.42	11/1006 (1.1%)
56	BX	0.60	0/212	1.15	1/277 (0.4%)
All	All	0.88	174/161408 (0.1%)	1.34	2448/241526 (1.0%)

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	AB	0	14
2	AA	0	527
4	AD	0	1
5	AE	0	1
6	AF	0	1
7	AG	0	2
12	AM	0	2
13	AN	0	2
14	AO	0	2
16	AQ	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	AX	0	1
25	A1	0	3
26	A2	0	1
28	A4	0	1
30	A6	0	1
34	BA	0	220
35	BB	0	35
35	BC	0	12
36	B1	0	4
38	BF	0	1
39	BG	0	1
41	BI	0	1
43	BK	0	1
48	BP	0	1
51	BS	0	2
All	All	0	838

The worst 5 of 174 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AA	142	G	C5-C6	13.87	1.70	1.42
13	AN	84	CYS	CA-C	-13.20	1.41	1.53
36	B1	48	A	C5-C6	12.35	1.65	1.41
35	BB	36	A	C2'-C1'	11.92	1.71	1.53
17	AR	12	ASP	CA-C	11.80	1.67	1.52

The worst 5 of 2448 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	BA	1064	G	N1-C2-N2	-19.68	57.15	116.20
17	AR	31	PHE	N-CA-C	18.38	139.13	109.72
17	AR	14	GLU	CA-C-N	18.28	142.69	119.84
17	AR	14	GLU	C-N-CA	18.28	142.69	119.84
32	A8	55	TRP	N-CA-C	-16.93	90.79	111.11

There are no chirality outliers.

5 of 838 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AB	12	C	Sidechain
1	AB	18	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AB	34	U	Sidechain
1	AB	39	A	Sidechain
1	AB	44	G	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	AB	2641	0	1337	636	1
2	AA	61847	0	31165	17723	1
3	AC	1687	0	1737	748	0
4	AD	1308	0	1355	920	0
5	AE	1507	0	1494	1012	0
6	AF	1430	0	1386	857	0
7	AG	957	0	959	538	0
8	AH	1251	0	1298	625	0
9	AI	945	0	999	509	0
9	AJ	945	0	999	371	0
10	AK	1145	0	1227	645	0
11	AL	999	0	1071	508	0
12	AM	917	0	904	637	0
13	AN	937	0	1000	562	0
14	AO	639	0	615	385	0
15	AP	1081	0	1062	760	0
16	AQ	866	0	875	519	0
17	AR	406	0	361	169	0
18	AS	860	0	919	450	0
19	AT	602	0	563	351	0
20	AU	879	0	868	498	0
21	AV	1360	0	1390	804	0
22	AW	494	0	506	251	0
23	AX	477	0	529	324	0
24	A0	855	0	906	503	0
25	A1	978	0	1020	704	0
26	A2	787	0	804	586	0
27	A3	641	0	668	435	0
28	A4	604	0	595	377	0
29	A5	457	0	462	297	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	A6	431	0	456	228	0
31	A7	383	0	414	267	0
32	A8	496	0	549	300	0
33	A9	285	0	312	128	0
34	BA	32554	0	16429	7573	1
35	BB	1626	0	817	628	0
35	BC	1626	0	820	427	0
36	B1	1405	0	706	256	1
37	BE	1900	0	1951	974	0
38	BF	1612	0	1677	692	0
39	BG	1703	0	1763	747	0
40	BH	1146	0	1207	504	1
41	BI	843	0	857	419	0
42	BJ	1257	0	1296	547	0
43	BK	1116	0	1177	695	0
44	BL	1011	0	1043	462	0
45	BM	794	0	840	335	0
46	BN	885	0	904	420	0
47	BO	970	0	1057	470	0
48	BP	997	0	1072	512	0
49	BQ	492	0	529	269	0
50	BR	734	0	771	343	0
51	BS	700	0	720	328	0
52	BT	857	0	930	436	0
53	BU	597	0	668	347	0
54	BV	647	0	673	264	0
55	BW	762	0	859	374	0
56	BX	208	0	221	103	0
All	All	148539	0	99792	48424	3

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 196.

The worst 5 of 48424 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)
2:AA:2515:C:N4	2:AA:2569:G:H1	1.08	1.45
34:BA:144:G:H1	34:BA:178:C:N4	1.13	1.45
34:BA:292:G:H1	34:BA:308:C:N4	1.08	1.45
2:AA:447:A:H1'	2:AA:449:A:N6	1.28	1.44
33:A9:11:CYS:SG	33:A9:11:CYS:CB	2.06	1.44

All (3) 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)
1:AB:-1:A:O2'	1:AB:-1:A:O2'[15_545]	1.59	0.61
2:AA:2153:G:O2'	34:BA:423:G:OP2[3_655]	2.16	0.04
36:B1:29:G:O3'	40:BH:5:ASP:OD2[3_655]	2.17	0.03

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	
3	AC	217/228 (95%)	143 (66%)	36 (17%)	38 (18%)	0	2
4	AD	171/178 (96%)	71 (42%)	38 (22%)	62 (36%)	0	0
5	AE	187/338 (55%)	89 (48%)	41 (22%)	57 (30%)	0	0
6	AF	183/246 (74%)	83 (45%)	40 (22%)	60 (33%)	0	0
7	AG	118/176 (67%)	57 (48%)	29 (25%)	32 (27%)	0	0
8	AH	162/177 (92%)	89 (55%)	39 (24%)	34 (21%)	0	2
9	AI	126/128 (98%)	87 (69%)	24 (19%)	15 (12%)	0	4
9	AJ	126/128 (98%)	86 (68%)	25 (20%)	15 (12%)	0	4
10	AK	146/149 (98%)	83 (57%)	34 (23%)	29 (20%)	0	2
11	AL	131/141 (93%)	66 (50%)	33 (25%)	32 (24%)	0	1
12	AM	113/145 (78%)	48 (42%)	26 (23%)	39 (34%)	0	0
13	AN	120/122 (98%)	60 (50%)	33 (28%)	27 (22%)	0	1
14	AO	82/164 (50%)	40 (49%)	17 (21%)	25 (30%)	0	0
15	AP	136/138 (99%)	50 (37%)	43 (32%)	43 (32%)	0	0
16	AQ	111/186 (60%)	41 (37%)	32 (29%)	38 (34%)	0	0
17	AR	50/66 (76%)	19 (38%)	17 (34%)	14 (28%)	0	0
18	AS	104/113 (92%)	70 (67%)	18 (17%)	16 (15%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	74/84 (88%)	33 (45%)	17 (23%)	24 (32%)	0	0
20	AU	108/119 (91%)	60 (56%)	25 (23%)	23 (21%)	0	2
21	AV	175/253 (69%)	69 (39%)	46 (26%)	60 (34%)	0	0
22	AW	62/70 (89%)	21 (34%)	25 (40%)	16 (26%)	0	1
23	AX	58/60 (97%)	29 (50%)	13 (22%)	16 (28%)	0	0
24	A0	103/118 (87%)	50 (48%)	33 (32%)	20 (19%)	0	2
25	A1	115/118 (98%)	48 (42%)	40 (35%)	27 (24%)	0	1
26	A2	98/100 (98%)	54 (55%)	18 (18%)	26 (26%)	0	0
27	A3	84/91 (92%)	32 (38%)	16 (19%)	36 (43%)	0	0
28	A4	71/73 (97%)	21 (30%)	19 (27%)	31 (44%)	0	0
29	A5	56/60 (93%)	25 (45%)	11 (20%)	20 (36%)	0	0
30	A6	51/82 (62%)	26 (51%)	8 (16%)	17 (33%)	0	0
31	A7	44/47 (94%)	14 (32%)	12 (27%)	18 (41%)	0	0
32	A8	61/64 (95%)	24 (39%)	16 (26%)	21 (34%)	0	0
33	A9	33/36 (92%)	19 (58%)	8 (24%)	6 (18%)	0	2
37	BE	232/256 (91%)	107 (46%)	58 (25%)	67 (29%)	0	0
38	BF	204/239 (85%)	113 (55%)	46 (22%)	45 (22%)	0	1
39	BG	206/209 (99%)	97 (47%)	63 (31%)	46 (22%)	0	1
40	BH	148/162 (91%)	90 (61%)	38 (26%)	20 (14%)	0	3
41	BI	99/101 (98%)	55 (56%)	24 (24%)	20 (20%)	0	2
42	BJ	153/156 (98%)	63 (41%)	49 (32%)	41 (27%)	0	0
43	BK	136/138 (99%)	67 (49%)	39 (29%)	30 (22%)	0	1
44	BL	125/128 (98%)	64 (51%)	27 (22%)	34 (27%)	0	0
45	BM	96/105 (91%)	54 (56%)	19 (20%)	23 (24%)	0	1
46	BN	117/129 (91%)	54 (46%)	33 (28%)	30 (26%)	0	1
47	BO	122/135 (90%)	65 (53%)	28 (23%)	29 (24%)	0	1
48	BP	123/126 (98%)	59 (48%)	30 (24%)	34 (28%)	0	0
49	BQ	58/61 (95%)	22 (38%)	10 (17%)	26 (45%)	0	0
50	BR	86/89 (97%)	36 (42%)	35 (41%)	15 (17%)	0	2
51	BS	81/88 (92%)	42 (52%)	24 (30%)	15 (18%)	0	2
52	BT	102/105 (97%)	62 (61%)	20 (20%)	20 (20%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	BU	71/88 (81%)	29 (41%)	24 (34%)	18 (25%)	0	1
54	BV	78/93 (84%)	35 (45%)	17 (22%)	26 (33%)	0	0
55	BW	97/106 (92%)	27 (28%)	46 (47%)	24 (25%)	0	1
56	BX	22/27 (82%)	9 (41%)	5 (23%)	8 (36%)	0	0
All	All	5832/6739 (86%)	2857 (49%)	1467 (25%)	1508 (26%)	0	1

5 of 1508 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AC	17	ASN
3	AC	35	ALA
3	AC	54	SER
3	AC	68	LEU
3	AC	87	GLU

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	
3	AC	174/180 (97%)	142 (82%)	32 (18%)	1	9
4	AD	135/139 (97%)	84 (62%)	51 (38%)	0	1
5	AE	156/284 (55%)	113 (72%)	43 (28%)	0	3
6	AF	152/193 (79%)	120 (79%)	32 (21%)	1	6
7	AG	102/147 (69%)	74 (72%)	28 (28%)	0	3
8	AH	137/147 (93%)	94 (69%)	43 (31%)	0	2
9	AI	98/98 (100%)	87 (89%)	11 (11%)	6	19
9	AJ	98/98 (100%)	88 (90%)	10 (10%)	7	23
10	AK	119/119 (100%)	95 (80%)	24 (20%)	1	8
11	AL	108/113 (96%)	90 (83%)	18 (17%)	2	11
12	AM	95/121 (78%)	67 (70%)	28 (30%)	0	2
13	AN	101/101 (100%)	72 (71%)	29 (29%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	AO	67/126 (53%)	50 (75%)	17 (25%)	0	4
15	AP	110/110 (100%)	73 (66%)	37 (34%)	0	2
16	AQ	89/149 (60%)	58 (65%)	31 (35%)	0	1
17	AR	44/52 (85%)	26 (59%)	18 (41%)	0	0
18	AS	88/92 (96%)	63 (72%)	25 (28%)	0	3
19	AT	67/73 (92%)	50 (75%)	17 (25%)	0	4
20	AU	97/105 (92%)	77 (79%)	20 (21%)	1	7
21	AV	151/203 (74%)	106 (70%)	45 (30%)	0	2
22	AW	51/56 (91%)	39 (76%)	12 (24%)	1	5
23	AX	52/52 (100%)	31 (60%)	21 (40%)	0	1
24	A0	89/101 (88%)	58 (65%)	31 (35%)	0	1
25	A1	96/97 (99%)	69 (72%)	27 (28%)	0	3
26	A2	79/79 (100%)	61 (77%)	18 (23%)	1	6
27	A3	64/67 (96%)	46 (72%)	18 (28%)	0	3
28	A4	66/66 (100%)	48 (73%)	18 (27%)	0	3
29	A5	51/53 (96%)	35 (69%)	16 (31%)	0	2
30	A6	46/69 (67%)	35 (76%)	11 (24%)	1	5
31	A7	39/40 (98%)	29 (74%)	10 (26%)	0	4
32	A8	50/51 (98%)	32 (64%)	18 (36%)	0	1
33	A9	34/35 (97%)	29 (85%)	5 (15%)	3	13
37	BE	202/220 (92%)	153 (76%)	49 (24%)	1	4
38	BF	160/188 (85%)	124 (78%)	36 (22%)	1	6
39	BG	180/181 (99%)	135 (75%)	45 (25%)	0	4
40	BH	115/123 (94%)	64 (56%)	51 (44%)	0	0
41	BI	90/90 (100%)	65 (72%)	25 (28%)	0	3
42	BJ	126/127 (99%)	103 (82%)	23 (18%)	2	9
43	BK	119/119 (100%)	71 (60%)	48 (40%)	0	1
44	BL	98/99 (99%)	83 (85%)	15 (15%)	3	12
45	BM	88/92 (96%)	68 (77%)	20 (23%)	1	6
46	BN	90/99 (91%)	67 (74%)	23 (26%)	0	4
47	BO	104/111 (94%)	82 (79%)	22 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	BP	100/101 (99%)	75 (75%)	25 (25%)	0	4
49	BQ	49/50 (98%)	40 (82%)	9 (18%)	1	9
50	BR	79/80 (99%)	55 (70%)	24 (30%)	0	2
51	BS	72/74 (97%)	42 (58%)	30 (42%)	0	0
52	BT	96/97 (99%)	71 (74%)	25 (26%)	0	4
53	BU	64/77 (83%)	48 (75%)	16 (25%)	0	4
54	BV	71/80 (89%)	58 (82%)	13 (18%)	2	9
55	BW	76/82 (93%)	54 (71%)	22 (29%)	0	2
56	BX	19/22 (86%)	16 (84%)	3 (16%)	2	12
All	All	4903/5528 (89%)	3615 (74%)	1288 (26%)	0	3

5 of 1288 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	BH	82	VAL
49	BQ	21	TYR
41	BI	28	ARG
40	BH	81	GLU
43	BK	136	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 199 such sidechains are listed below:

Mol	Chain	Res	Type
37	BE	25	ASN
41	BI	13	ASN
37	BE	135	GLN
38	BF	136	GLN
42	BJ	11	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	122/123 (99%)	47 (38%)	5 (4%)
2	AA	2870/2915 (98%)	1233 (42%)	290 (10%)
34	BA	1515/1522 (99%)	455 (30%)	161 (10%)
35	BB	76/76 (100%)	35 (46%)	16 (21%)
35	BC	75/76 (98%)	31 (41%)	9 (12%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
36	B1	65/78 (83%)	24 (36%)	4 (6%)
All	All	4723/4790 (98%)	1825 (38%)	485 (10%)

5 of 1825 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	0	A
1	AB	1	U
1	AB	2	C
1	AB	3	C
1	AB	9	G

5 of 485 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	AA	2067	G
34	BA	1399	C
2	AA	2781	A
34	BA	1362	C
35	BC	9	A

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 ⓘ

There are no chain breaks in this entry.

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	AB	123/123 (100%)	-0.33	0	100	100	308, 357, 402, 412	0
2	AA	2872/2915 (98%)	0.35	220 (7%)	19	24	232, 307, 404, 474	0
3	AC	221/228 (96%)	1.10	49 (22%)	2	8	384, 428, 464, 467	0
4	AD	173/178 (97%)	2.96	83 (47%)	0	3	243, 279, 292, 298	0
5	AE	191/338 (56%)	1.77	67 (35%)	1	5	258, 311, 397, 403	0
6	AF	189/246 (76%)	2.02	82 (43%)	0	3	233, 399, 427, 434	0
7	AG	122/176 (69%)	1.80	46 (37%)	1	4	350, 366, 443, 447	0
8	AH	164/177 (92%)	0.71	19 (11%)	9	16	320, 351, 366, 370	0
9	AI	128/128 (100%)	0.38	6 (4%)	36	36	580, 591, 602, 603	0
9	AJ	128/128 (100%)	0.76	19 (14%)	5	13	569, 582, 594, 596	0
10	AK	148/149 (99%)	1.16	34 (22%)	2	7	305, 329, 353, 361	0
11	AL	133/141 (94%)	0.58	19 (14%)	6	13	455, 504, 541, 543	0
12	AM	117/145 (80%)	2.36	52 (44%)	0	3	286, 310, 364, 368	0
13	AN	122/122 (100%)	1.54	38 (31%)	1	5	245, 262, 277, 293	0
14	AO	84/164 (51%)	1.07	19 (22%)	2	8	330, 452, 471, 473	0
15	AP	138/138 (100%)	2.33	56 (40%)	0	3	283, 324, 364, 379	0
16	AQ	113/186 (60%)	-0.16	0	100	100	317, 367, 386, 390	0
17	AR	52/66 (78%)	2.67	27 (51%)	0	3	251, 267, 285, 288	0
18	AS	108/113 (95%)	1.39	35 (32%)	1	5	280, 311, 324, 332	0
19	AT	76/84 (90%)	0.30	7 (9%)	14	20	329, 344, 360, 363	0
20	AU	110/119 (92%)	1.20	17 (15%)	5	12	647, 661, 722, 724	0
21	AV	177/253 (69%)	0.85	30 (16%)	4	11	295, 365, 416, 424	0
22	AW	64/70 (91%)	0.39	7 (10%)	10	17	346, 364, 373, 375	0
23	AX	60/60 (100%)	0.59	7 (11%)	9	16	291, 306, 315, 316	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
24	A0	105/118 (88%)	0.28	11 (10%) 11 18	263, 281, 304, 308	0
25	A1	117/118 (99%)	1.03	22 (18%) 3 10	267, 297, 311, 317	0
26	A2	100/100 (100%)	1.58	30 (30%) 1 6	416, 430, 462, 470	0
27	A3	86/91 (94%)	1.72	24 (27%) 1 6	359, 389, 475, 486	0
28	A4	73/73 (100%)	3.02	40 (54%) 0 3	319, 354, 373, 378	0
29	A5	58/60 (96%)	1.00	9 (15%) 5 12	259, 314, 361, 373	0
30	A6	53/82 (64%)	2.50	26 (49%) 0 3	287, 316, 332, 340	0
31	A7	46/47 (97%)	2.15	18 (39%) 1 4	316, 339, 352, 357	0
32	A8	63/64 (98%)	1.25	16 (25%) 1 7	262, 282, 294, 306	0
33	A9	35/36 (97%)	0.42	4 (11%) 10 17	281, 303, 316, 319	0
34	BA	1515/1522 (99%)	-0.10	33 (2%) 62 52	251, 312, 419, 609	0
35	BB	76/76 (100%)	3.05	50 (65%) 0 2	631, 651, 667, 669	0
35	BC	76/76 (100%)	0.50	4 (5%) 32 33	273, 310, 328, 337	0
36	B1	66/78 (84%)	2.76	39 (59%) 0 2	337, 829, 918, 922	0
37	BE	234/256 (91%)	0.81	31 (13%) 7 14	293, 321, 364, 385	0
38	BF	206/239 (86%)	1.24	53 (25%) 1 7	301, 349, 377, 382	0
39	BG	208/209 (99%)	1.34	51 (24%) 2 7	276, 299, 318, 329	0
40	BH	150/162 (92%)	1.12	36 (24%) 2 7	277, 295, 315, 324	0
41	BI	101/101 (100%)	3.11	66 (65%) 0 2	299, 318, 330, 336	0
42	BJ	155/156 (99%)	1.35	36 (23%) 2 7	326, 357, 370, 373	0
43	BK	138/138 (100%)	0.60	23 (16%) 4 11	266, 284, 297, 306	0
44	BL	127/128 (99%)	-0.08	2 (1%) 70 58	385, 487, 499, 500	0
45	BM	98/105 (93%)	-0.15	4 (4%) 41 39	337, 394, 423, 424	0
46	BN	119/129 (92%)	1.51	40 (33%) 1 5	288, 307, 330, 334	0
47	BO	124/135 (91%)	1.85	46 (37%) 1 4	265, 282, 319, 328	0
48	BP	125/126 (99%)	0.91	21 (16%) 4 11	350, 370, 412, 415	0
49	BQ	60/61 (98%)	0.17	5 (8%) 17 23	322, 352, 360, 365	0
50	BR	88/89 (98%)	0.92	19 (21%) 2 8	277, 288, 315, 318	0
51	BS	83/88 (94%)	0.60	9 (10%) 11 17	271, 284, 303, 316	0
52	BT	104/105 (99%)	0.97	24 (23%) 2 7	249, 268, 323, 344	0
53	BU	73/88 (82%)	1.89	26 (35%) 1 4	259, 296, 323, 348	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	BV	80/93 (86%)	1.12	14 (17%) 4 10	353, 369, 395, 399	0
55	BW	99/106 (93%)	0.70	14 (14%) 6 13	264, 281, 292, 300	0
56	BX	24/27 (88%)	-0.65	0 100 100	475, 489, 493, 496	0
All	All	10678/11529 (92%)	0.80	1785 (16%) 4 11	232, 322, 533, 922	0

The worst 5 of 1785 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BE	237	ALA	25.2
37	BE	231	GLU	22.0
12	AM	72	PRO	19.7
4	AD	205	VAL	18.0
15	AP	29	ALA	18.0

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 oligosaccharides 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.