



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2017 – 07:57 PM EST

PDB ID : 4V4Z  
Title : 70S Thermus thermophilus ribosome functional complex with mRNA and E- and P-site tRNAs at 4.5Å.  
Authors : Jenner, L.; Yusupova, G.; Rees, B.; Moras, D.; Yusupov, M.  
Deposited on : unknown  
Resolution : 4.51 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

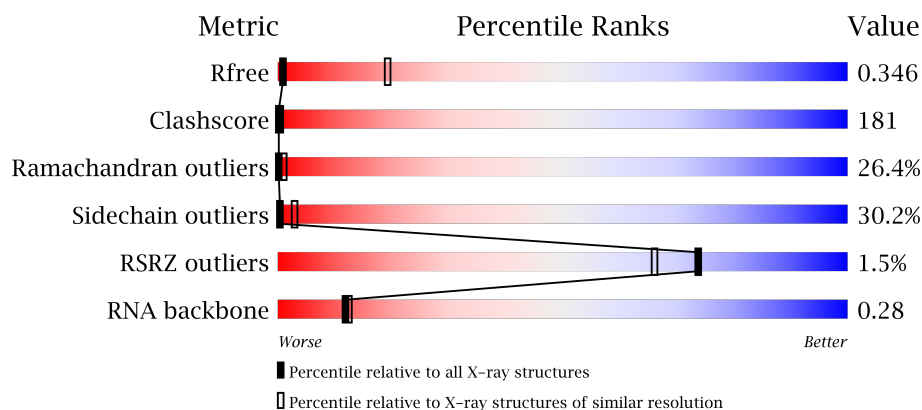
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.51 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))
$R_{free}$	100719	1008 (5.40-3.64)
Clashscore	112137	1029 (5.30-3.70)
Ramachandran outliers	110173	1025 (5.30-3.66)
Sidechain outliers	110143	1006 (5.30-3.66)
RSRZ outliers	101464	1016 (5.40-3.64)
RNA backbone	2435	1038 (6.00-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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>54%</div> <div>34%</div> <div>11%</div> </div>
2	AC	76	<div> <div>49%</div> <div>43%</div> <div>8%</div> </div>
3	AD	76	<div> <div>37%</div> <div>47%</div> <div>13%</div> </div>
4	A1	27	<div> <div>22%</div> <div>7%</div> <div>52%</div> <div>22%</div> <div>19%</div> </div>

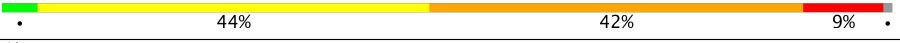

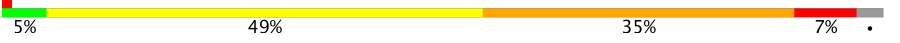
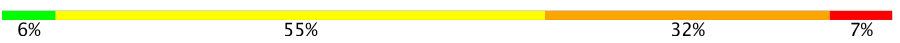








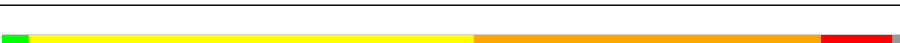
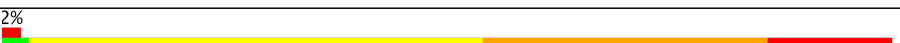
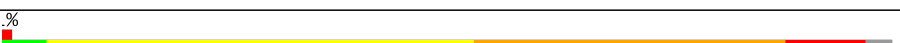

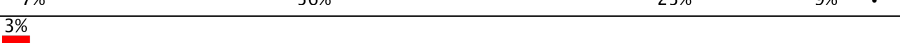
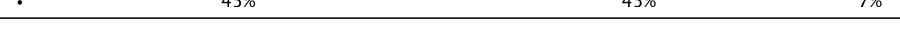






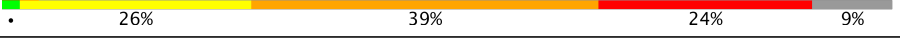
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Mol	Chain	Length	Quality of chain
5	AE	256	
6	AF	239	
7	AG	209	
8	AH	162	
9	AI	101	
10	AJ	156	
11	AK	138	
12	AL	128	
13	AM	105	
14	AN	129	
15	AO	132	
16	AP	126	
17	AQ	61	
18	AR	89	
19	AS	88	
20	AT	105	
21	AU	88	
22	AV	93	
23	AW	106	
24	AX	27	
25	BA	2916	
26	BB	123	
27	BC	229	
28	BD	276	
29	BE	206	

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Mol	Chain	Length	Quality of chain
30	BF	210	
31	BG	182	
32	BH	180	
33	BK	148	
34	BL	147	
35	BM	140	
36	BN	122	
37	BO	150	
38	BP	141	
39	BQ	118	
40	BR	112	
41	BS	146	
42	BT	118	
43	BU	101	
44	BV	113	
45	BW	96	
46	BX	110	
47	BY	206	
48	BZ	85	
49	B1	67	
50	B2	60	
51	B3	71	
52	B4	60	
53	B5	54	
54	B6	49	

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Mol	Chain	Length	Quality of chain
55	B7	65	<div><div></div><div>46%</div><div>43%</div><div>9%</div><div></div></div>
56	B8	37	<div><div>8%</div><div></div><div>46%</div><div></div><div>38%</div><div></div><div>8%</div></div>

## 2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 149640 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 rRNA.

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 tRNA fMET (unmodified bases).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	76	Total	C	N	O	P	0	0	0
			1624	723	295	530	76			

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

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

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A1	27	Total	C	N	O	P	0	0	0
			596	267	127	175	27			

- Molecule 5 is a protein called 30S ribosomal protein S2.

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

- Molecule 6 is a protein called 30S ribosomal protein S3.

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

- Molecule 7 is a protein called 30S ribosomal protein S4.

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

- Molecule 8 is a protein called 30S ribosomal protein S5.

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

- Molecule 9 is a protein called 30S ribosomal protein S6.

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

- Molecule 10 is a protein called 30S ribosomal protein S7.

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

- Molecule 11 is a protein called 30S ribosomal protein S8.

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

- Molecule 12 is a protein called 30S ribosomal protein S9.

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

- Molecule 13 is a protein called 30S ribosomal protein S10.

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

- Molecule 14 is a protein called 30S ribosomal protein S11.

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

- Molecule 15 is a protein called 30S ribosomal protein S12.

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

- Molecule 16 is a protein called 30S ribosomal protein S13.

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

- Molecule 17 is a protein called 30S ribosomal protein S14.

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

- Molecule 18 is a protein called 30S ribosomal protein S15.

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

- Molecule 19 is a protein called 30S ribosomal protein S16.

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

- Molecule 20 is a protein called 30S ribosomal protein S17.

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

- Molecule 21 is a protein called 30S ribosomal protein S18.



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

- Molecule 22 is a protein called 30S ribosomal protein S19.

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

- Molecule 23 is a protein called 30S ribosomal protein S20.

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

- Molecule 24 is a protein called 30S ribosomal protein Thx.

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

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	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 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	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 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L11.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

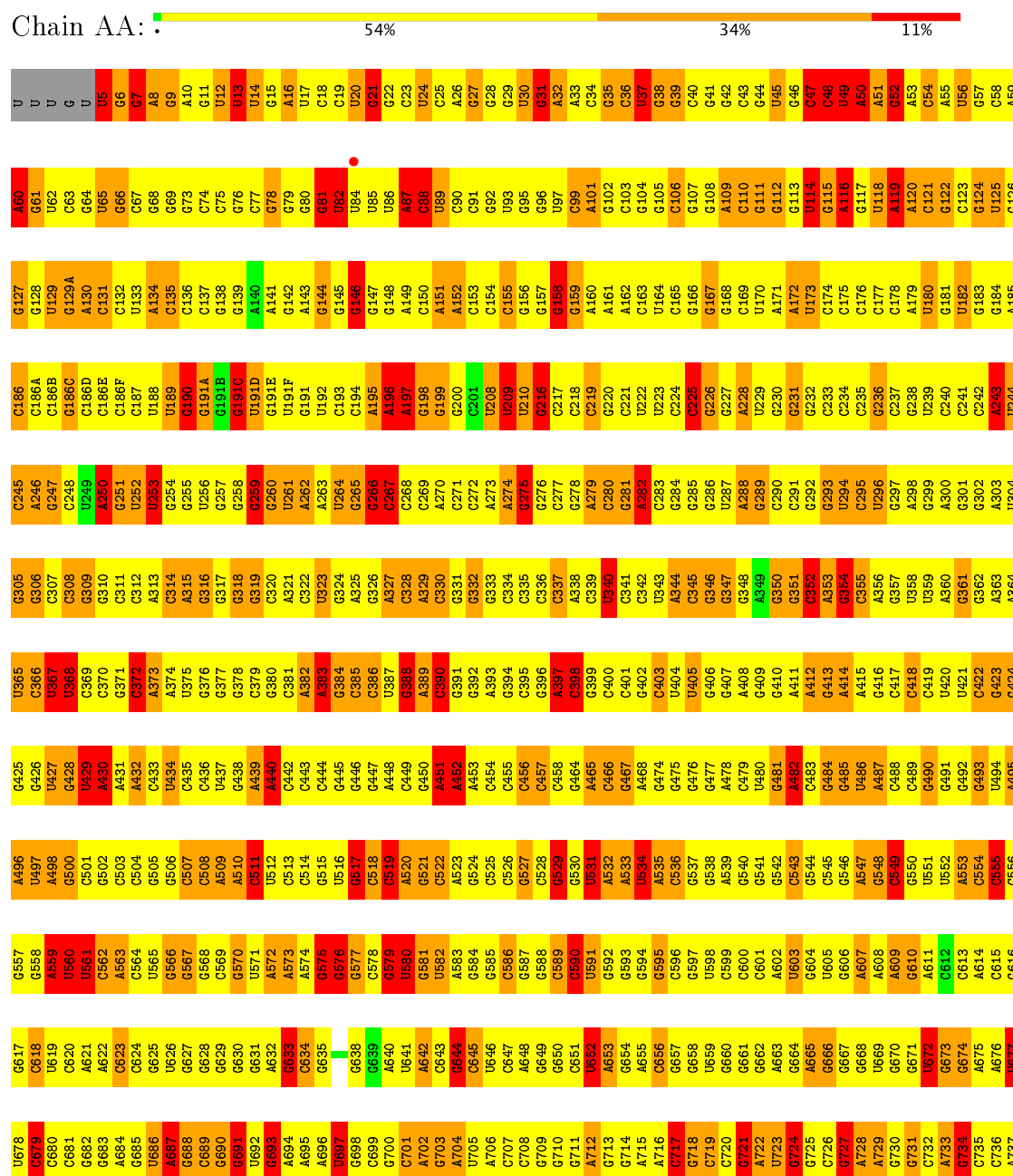
- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	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 and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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 rRNA



- Molecule 2: tRNA fMET (unmodified bases)

8%

C1	C2	C3	C4	C5	C6	C7	C8	C9	C10	C11	C12	C13	C14	C15	C16	C17	C18	C19	C20	C21	C22	C23	C24	C25	C26	C27	C28	C29	C30	C31	C32	C33	C34	C35	A35	U36	A37	A38	C39	C40	C41	C42	A43	A44	G45	G46	U47	C48	G49	U50	C51	C52	G53	U54	U55	C56	A57	A58	A59	U60	C61	C62	C63	C64	C65	C66	C67	C68	C69	C70	C71	C72	C73	C74	C75	C76	C77	C78	C79	C80	C81	C82	C83	C84	C85	C86	C87	C88	C89	C90	C91	C92	C93	C94	C95	C96	C97	C98	C99	C100	C101	C102	C103	C104	C105	C106	C107	C108	C109	C110	C111	C112	C113	C114	C115	C116	C117	C118	C119	C120	C121	C122	C123	C124	C125	C126	C127	C128	C129	C130	C131	C132	C133	C134	C135	C136	C137	C138	C139	C140	C141	C142	C143	C144	C145	C146	C147	C148	C149	C150	C151	C152	C153	C154	C155	C156	C157	C158	C159	C160	C161	C162	C163	C164	C165	C166	C167	C168	C169	C170	C171	C172	C173	C174	C175	C176	C177	C178	C179	C180	C181	C182	C183	C184	C185	C186	C187	C188	C189	C190	C191	C192	C193	C194	C195	C196	C197	C198	C199	C200	C201	C202	C203	C204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217	C218	C219	C220	C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	C250	C251	C252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000
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• Molecule 3: tRNA PHE (unmodified bases)

Chain AD: 37% 47% 13%



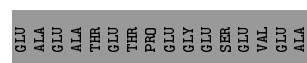
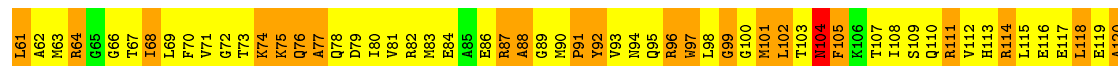
• Molecule 4: mRNA

Chain A1: 7% 52% 22% 19%



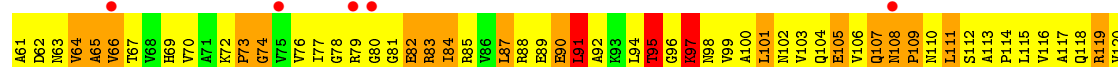
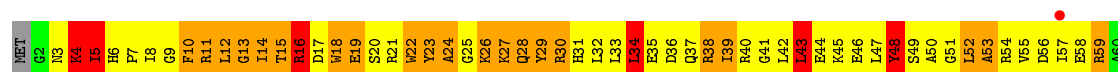
• Molecule 5: 30S ribosomal protein S2

Chain AE: 3% 45% 33% 11% 9%

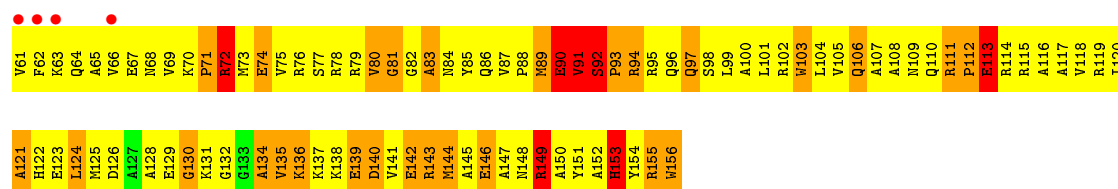


• Molecule 6: 30S ribosomal protein S3

Chain AF: 5% 51% 25% 5% 14%

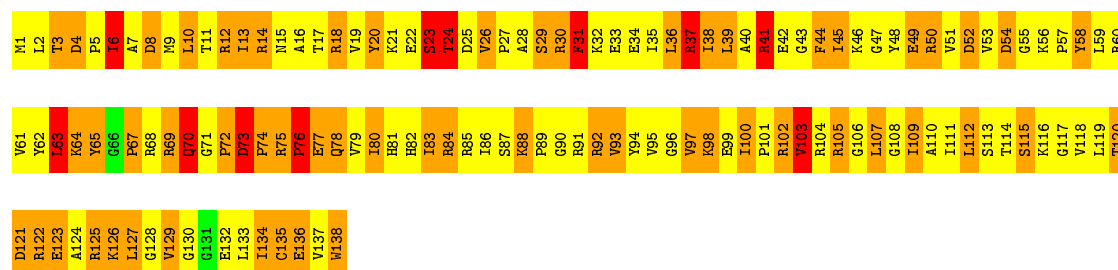






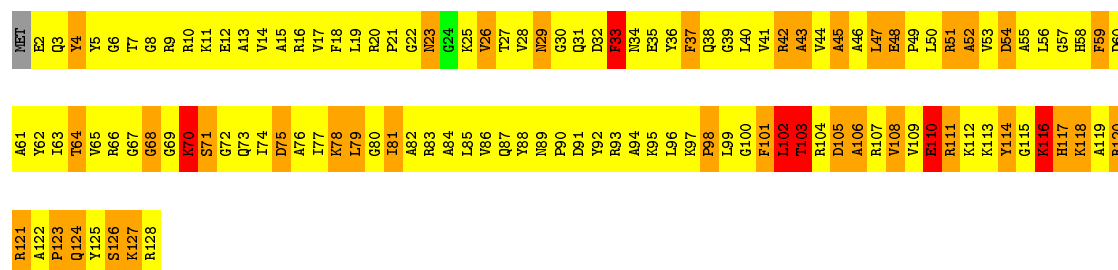
• Molecule 11: 30S ribosomal protein S8

Chain AK: . 49% 42% 8%



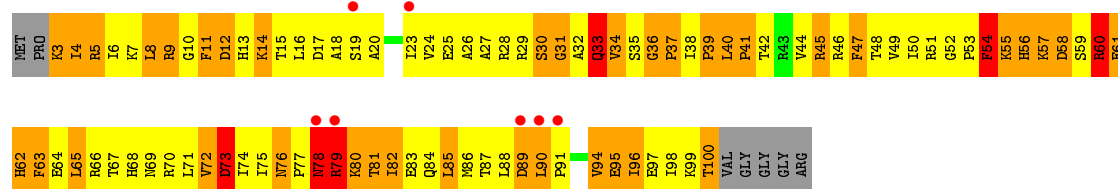
• Molecule 12: 30S ribosomal protein S9

Chain AL: . 66% 28% 5%



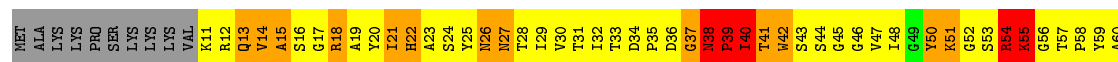
• Molecule 13: 30S ribosomal protein S10

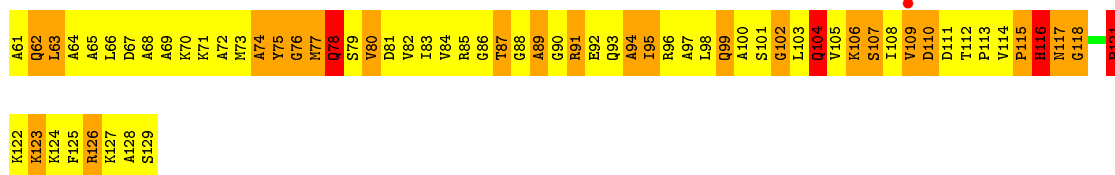
Chain AM: 7% 5% 47% 36% 6% 7%



• Molecule 14: 30S ribosomal protein S11

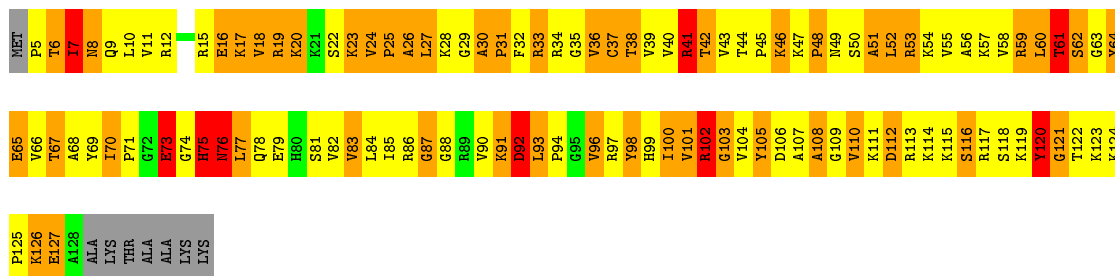
Chain AN: . 55% 28% 7% 8%





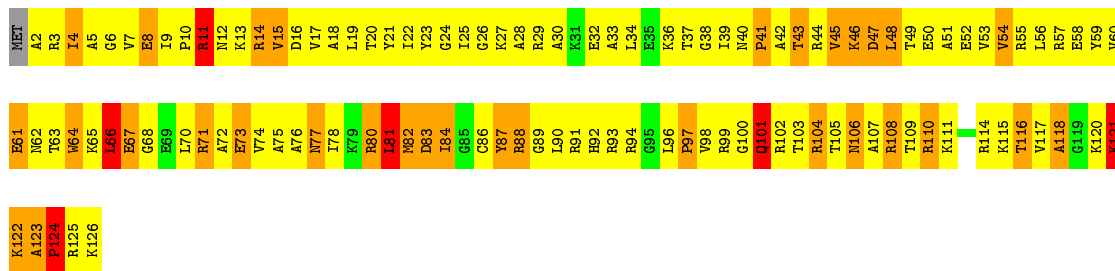
• Molecule 15: 30S ribosomal protein S12

Chain AO: 6% 44% 37% 7% 6%



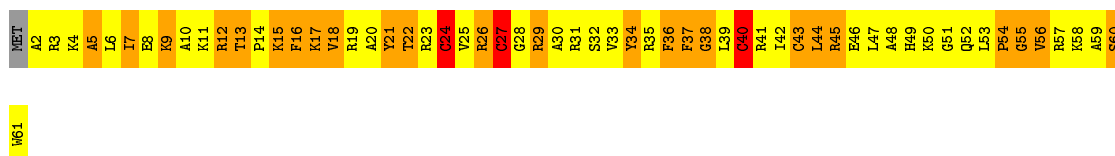
• Molecule 16: 30S ribosomal protein S13

Chain AP: 7% 62% 25% 5%



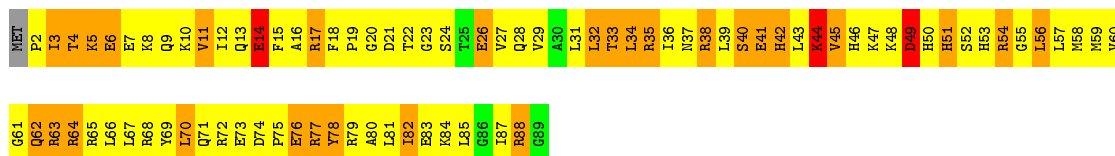
• Molecule 17: 30S ribosomal protein S14

Chain AQ: 54% 39% 5%



• Molecule 18: 30S ribosomal protein S15

Chain AR: 60% 31%





Chain AX:  56% 19% 11% 11%

WET	G2	G3	G4	D5	R6	R7	R8	R9	R10	G11	K12	I13	H14	G15	G16	T17	Y18	G19	K20	K25	LYS	LYS
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• Molecule 25: 23S rRNA

Chain BA:  42% 39% 18%

G733	A734	A735	C736	C737	C738	C739	U740	G741	G742	G743	G744	G745	A746	U747	G748	C749	A750	A751	A752	C753	C754	C755	C756	U757	C758	C759	A760	A761	U762	C763	A764	C765	C766	U767	C768	G769	G770	G771	C772	U773	A774	C775	U776	A777	C778	U779	G780	A781	A782	A783	G784	G785	C786	U787	A788	A789	C790	C791	C792																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
C673	G674	G675	C676	A677	C678	C679	G680	G681	C682	G683	G684	A685	C686	C687	U688	C689	G690	C691	A692	C693	C694	C695	C696	G697	C698	A699	G700	G701	U702	C703	A704	A705	C706	U707	C708	U709	G710	G711	C712	G713	U714	A715	C716	U717	A718	C719	C720	G721	A722	A723	G724	A725	C726	U727	A728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792																																																																																																																																																																																																																																																																																																																																																																																																												
A454	C455	C456	G457	G458	U459	U460	C461	C462	G463	U464	G465	A466	G467	U468	A469	C470	A471	A472	G473	C474	U475	G476	A477	A478	A479	A480	G481	C482	A483	U484	C485	C486	A487	G488	G489	A490	A491	A492	G493	G494	G495	G496	A497	G498	U499	G500	A501	A502	C503	U504	A505	U506	A507	G508	C509	A510	U511	C512	A513	A514	A515	C516	C517	G518	U519	G520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792																																																																																																																																																																																	
C337	C338	U339	U340	U341	U342	C343	C344	A345	A346	U347	G348	G349	U350	G351	G352	G353	G354	G355	G356	A357	U358	A359	G360	G361	U362	C363	A364	C365	U366	C367	C368	A369	C370	A371	G372	U373	C374	C375	C376	C377	C378	G379	U380	G381	U382	G383	A384	C385	U386	U387	G388	A389	C390	G391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792																																																												
C277	A278	C279	C280	G281	A282	C283	A284	C285	G286	C287	C288	A289	G290	C291	C292	U293	A294	C295	C296	U297	A298	C299	G300	G301	C302	U303	A304	C305	U306	C307	U308	C309	A310	A311	C312	G313	C314	G315	C316	G317	C318	C319	A320	G321	C322	C323	A324	G325	C326	C327	A328	G329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C525	C526	C527	C528	C529	C530	C531	C532	C533	C534	C535	C536	C537	C538	C539	C540	C541	C542	C543	C544	C545	C546	C547	C548	C549	C550	C551	C552	C553	C554	C555	C556	C557	C558	C559	C560	C561	C562	C563	C564	C565	C566	C567	C568	C569	C570	C571	C572	C573	C574	C575	C576	C577	C578	C579	C580	C581	C582	C583	C584	C585	C586	C587	C588	C589	C590	C591	C592	C593	C594	C595	C596	C597	C598	C599	C600	C601	C602	C603	C604	C605	C606	C607	C608	C609	C610	C611	C612	C613	C614	C615	C616	C617	C618	C619	C620	C621	C622	C623	C624	C625	C626	C627	C628	C629	C630	C631	C632	C633	C634	C635	C636	C637	C638	C639	C640	C641	C642	C643	C644	C645	C646	C647	C648	C649	C650	C651	C652	C653	C654	C655	C656	C657	C658	C659	C660	C661	C662	C663	C664	C665	C666	C667	C668	C669	C670	C671	C672	C673	C674	C675	C676	C677	C678	C679	C680	C681	C682	C683	C684	C685	C686	C687	C688	C689	C690	C691	C692	C693	C694	C695	C696	C697	C698	C699	C700	C701	C702	C703	C704	C705	C706	C707	C708	C709	C710	C711	C712	C713	C714	C715	C716	C717	C718	C719	C720	C721	C722	C723	C724	C725	C726	C727	C728	C729	C730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C743	C744	C745	C746	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792
G123	G124	G125	A126	A127	C128	C129	C130	G131	G132	C133	C134	C135	A136	G137	C138	A139	G140	C141	A142	C143	C144	G145	G146	C147	G148	C149	A150	C151	C152	G153	C154	C155	U156	A157	C158	A159	G160	C161	G162	C163	C164	G165	C166	C167	G168	C169	G170																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				

G1695	G1696	G1697	G1698	G1699	G1700	G1701	G1702	G1703	G1704	G1705	G1706	G1707	G1708	G1709	G1710	G1711	G1712	G1713	G1714	G1715	G1716	G1717	G1718	G1719	G1720	G1721	G1722	G1723	G1724	G1725	G1726	G1727	G1728	G1729	G1730	G1731	G1732	G1733	G1734	G1735	G1736	G1737	G1738	G1739	G1740	G1741	G1742	G1743	G1744	G1745	G1746	G1747	G1748	G1749	G1750	G1751	G1752	G1753	G1754	G1755	G1756	G1757	G1758	G1759	G1760	G1761	G1762	G1763	G1764	G1765	G1766	G1767	G1768	G1769	G1770																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
G1635	G1636	G1637	G1638	G1639	G1640	G1641	G1642	G1643	G1644	G1645	G1646	G1647	G1648	G1649	G1650	G1651	G1652	G1653	G1654	G1655	G1656	G1657	G1658	G1659	G1660	G1661	G1662	G1663	G1664	G1665	G1666	G1667	G1668	G1669	G1670	G1671	G1672	G1673	G1674	G1675	G1676	G1677	G1678	G1679	G1680	G1681	G1682	G1683	G1684	G1685	G1686	G1687	G1688	G1689	G1690	G1691	G1692	G1693	G1694	G1695	G1696	G1697	G1698	G1699	G1700																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C1575	C1576	C1577	C1578	C1579	C1580	C1581	C1582	C1583	C1584	C1585	C1586	C1587	C1588	C1589	C1590	C1591	C1592	C1593	C1594	C1595	C1596	C1597	C1598	C1599	C1600	C1601	C1602	C1603	C1604	C1605	C1606	C1607	C1608	C1609	C1610	C1611	C1612	C1613	C1614	C1615	C1616	C1617	C1618	C1619	C1620	C1621	C1622	C1623	C1624	C1625	C1626	C1627	C1628	C1629	C1630	C1631	C1632	C1633	C1634	C1635	C1636	C1637	C1638	C1639	C1640																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
G1455	G1456	G1457	G1458	G1459	G1460	G1461	G1462	G1463	G1464	G1465	G1466	G1467	G1468	G1469	G1470	G1471	G1472	G1473	G1474	G1475	G1476	G1477	G1478	G1479	G1480	G1481	G1482	G1483	G1484	G1485	G1486	G1487	G1488	G1489	G1490	G1491	G1492	G1493	G1494	G1495	G1496	G1497	G1498	G1499	G1500	G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	G1509	G1510	G1511	G1512	G1513	G1514	G1515	G1516	G1517	G1518	G1519	G1520																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
U1396	U1397	C1398	C1399	G1400	C1401	C1402	C1403	C1404	U1405	U1406	C1407	C1408	C1409	G1410	C1411	U1412	G1413	G1414	U1415	G1416	C1417	G1418	U1419	U1420	G1421	G1422	G1423	G1424	G1425	G1426	G1427	G1428	G1429	C1430	U1431	C1432	U1433	G1434	G1435	G1436	C1437	U1438	G1439	G1440	G1441	G1442	G1443	G1444	U1445	G1446	G1447	G1448	G1449	G1450	G1451	G1452	G1453	G1454	U1455	U1456	U1457	U1458	U1459	U1460																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
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G2762	C2825	C2885	C12	G73	
G2763	A2826	U2886	A13	A73	
A2764	C2827	U2887	U14	A74	
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C2767	G2830	G2891	C17	U77	
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C2774	G2837	U2898	G24	C84	
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G2777	C2840	C2901	C27	G87	
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G2795	G2857		A45	U103	
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A2801	G2861		U48	U107	
G2802	C2862		C49	C108	
C2803	G2863		G50	G109	
C2804	C2864		G51	G110	
G2805	U2865		A52	U111	
G2806	U2866		A53	G112	
G2807	G2867		G54	C113	
U2808	A2868		U55	G114	
A2809	G2869		G56	G115	
A2810	C2870		A57	G116	
G2811	C2871		A58	G117	

• Molecule 26: 5S rRNA

Chain BB: . 51% 37% 11%

A-1	A59	G118
A0	G60	A119
U1	G62	U120
C2	G63	
C3	G64	
C4	G65	
C5	A66	
C6	A67	
G7	A68	
U8	G69	
G9	G70	
C10	G71	
G11	G72	
C12	A73	
A13	U74	
U14	G75	
A15	G76	
G16	U77	
C17	A78	
G18	C79	
G19	U80	
C20	G81	
G21	G82	
U22	G83	
G23	C84	
G24	A25	
A26	G85	
C27	G86	
C28	G87	
C29	C88	
C30	G89	
C31	A89A	
C32	C90	
G33	C91	
U34	G92	
U35	C93	
C36	C94	
C37	U95	
C38	G96	
A39	G97	
U40	G98	
C41	A99	
C42	G100	
C43	A101	
G44	G102	
A45	U103	
A46	A104	
G105	G105	
C47	G106	
C48	U107	
C49	C108	
G50	G109	
G51	G110	
A52	U111	
A53	G112	
G54	C113	
U55	G114	
G56	G115	
A57	G116	
A58	G117	

• Molecule 27: 50S RIBOSOMAL PROTEIN L1

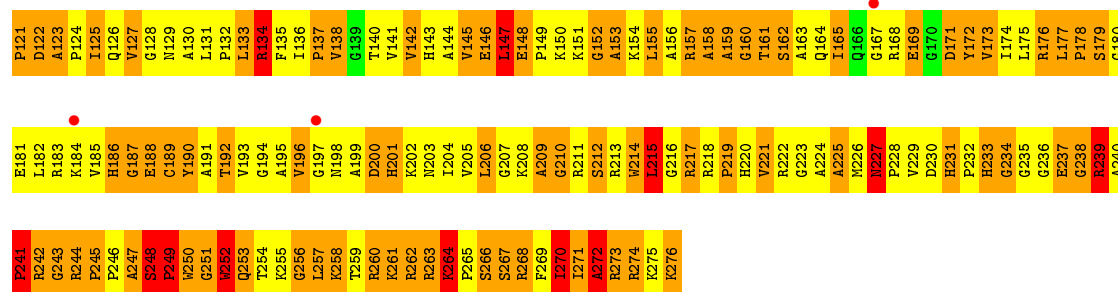
Chain BC: . 24% 6% 69% 23%

Met	G60	F180
P1	T61	P181
K2	V62	P182
H3	S63	E183
G4	L64	L184
K5	P65	K185
R6	H66	A186
Y7	G67	D187
R8	L68	N188
A9	G69	I189
L10	K70	R190
L11	Q71	A191
E12	W72	F192
K13	R73	I193
V14	V74	R194
D15	L75	A195
P16	A76	L196
N17	I77	E197
K18	A78	A198
I19	K79	H199
Y20	G80	K200
T21	E81	E202
D22	K82	G203
D23	L83	A204
D24	K84	G205
A25	E85	G206
A26	A86	G207
E27	E87	F207
L28	E88	F208
A29	A89	L209
K30	G90	R210
E31	A91	S211
L32	D92	E151
A33	Y93	I153
T34	V94	K154
A35	G95	R155
K36	G96	E156
F37	E97	I157
D38	F98	A158
E39	I99	G159
T40	R100	P160
V41	Q101	I161
E42	K102	E162
V43	L103	F163
H44	L104	R164
A45	D105	N165
K46	G106	D166
L47	W107	K167
G48	M108	T168
T49	D109	G169
D50	F110	A170
P51	D111	I171
R52	A112	I172
R53	V113	A173
S54	V114	P174
D55	V115	V175
Q56	T116	G176
N57	F117	K177
V58	A178	A178
R59	V119	S179

• Molecule 28: 50S RIBOSOMAL PROTEIN L2

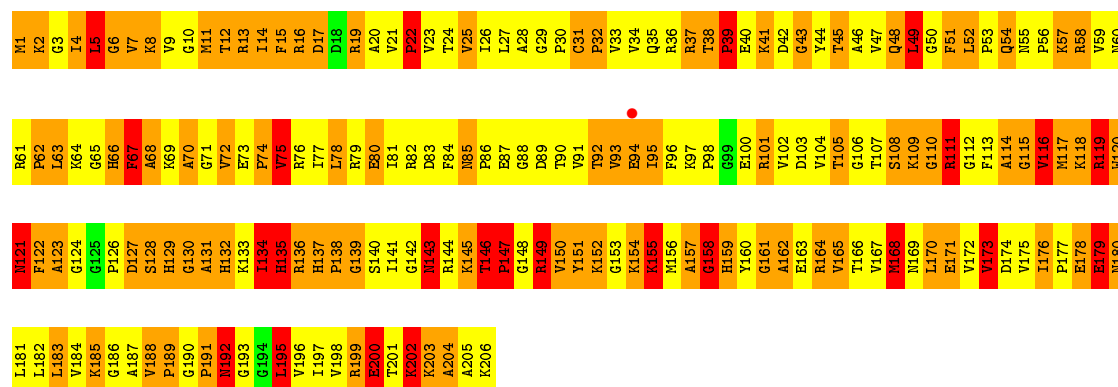
Chain BD: . 3% 44% 43% 11%

Met	L61	R69
ALA	T62	W70
VAL	R63	D71
LYS	I64	K72
K5	I65	S12
R6	D66	R13
K7	F67	F15
F8	K68	P16
Y9		T17
T10		K78
P11		V18
S12		A19
R13		D20
R14		F21
F15		S22
P16		E23
T17		T24
K78		D25
A19		K26
D20		T27
F21		E28
S22		P29
E23		E30
T24		K31
D25		S32
K26		L33
T27		V34
E28		K35
P29		P36
E30		L37
K31		K38
S32		K39
L33		T40
V34		G41
K35		G42
P36		R43
L37		I44
K38		N45
K39		Q46
T40		G47
G41		R48
G42		I49
R43		T50
I44		V51
N45		R52
Q46		F53
G47		V113
R48		R54
I49		G55
T50		G56
V51		V116
R52		V117
F53		V118
V113		A119
R54		K59
G55		R60
G56		
V116		
V117		
V118		
A119		
K59		
R60		



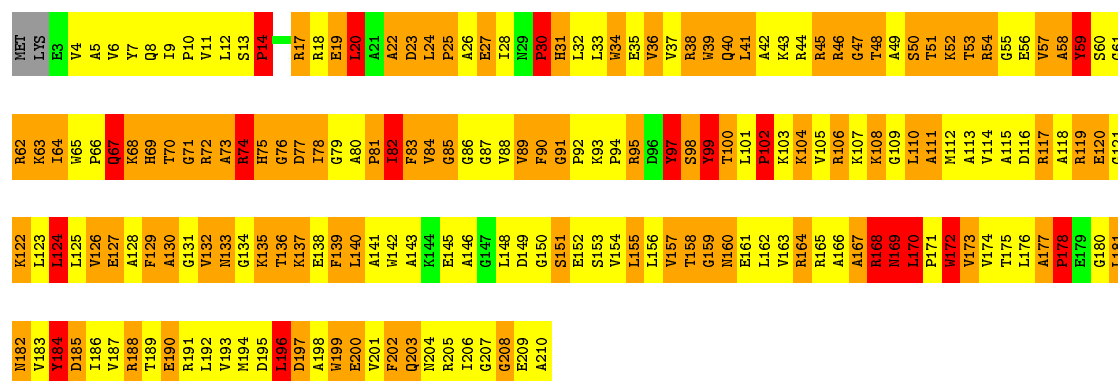
• Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain BE: . 43% 43% 12%



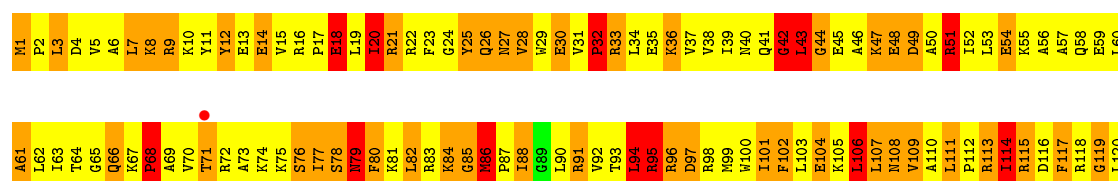
• Molecule 30: 50S RIBOSOMAL PROTEIN L4

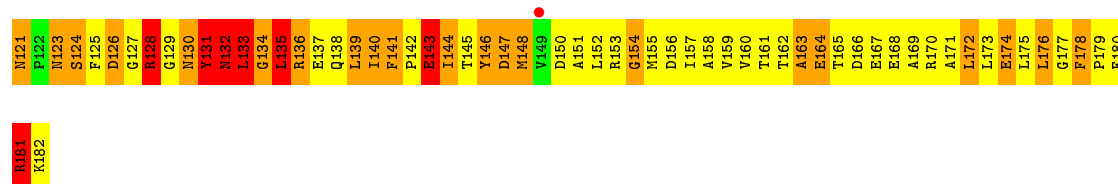
Chain BF: . 44% 42% 9%



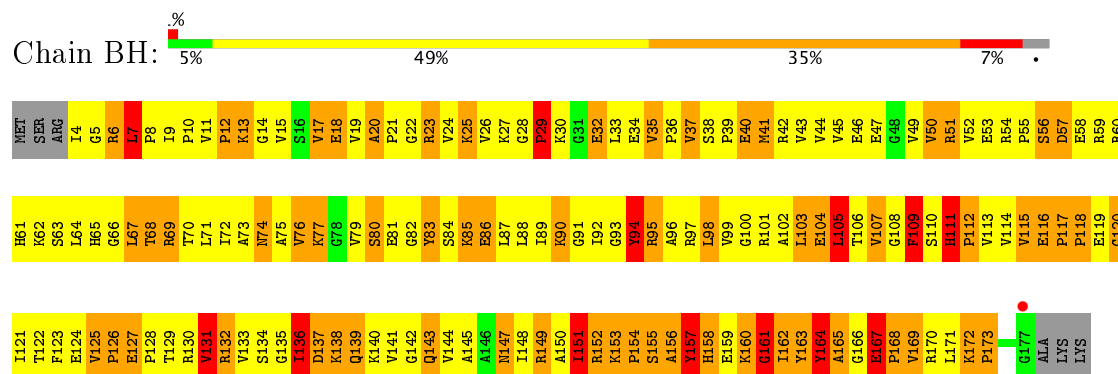
• Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain BG: . 51% 36% 11%

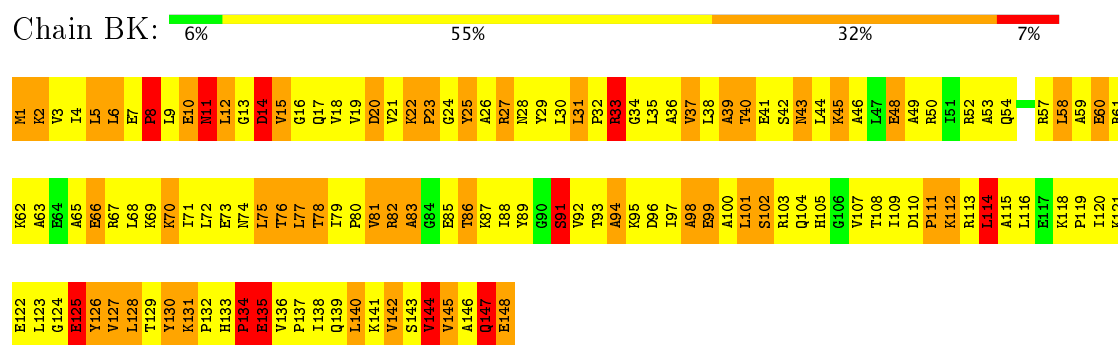




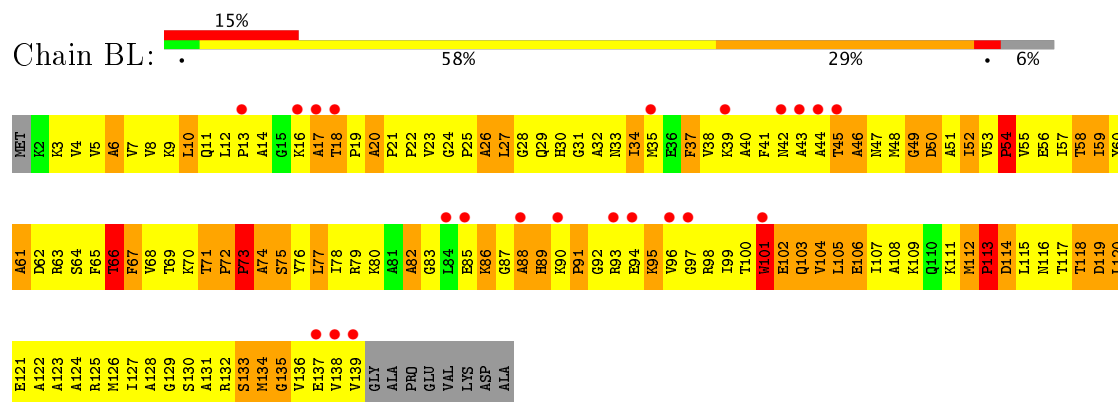
• Molecule 32: 50S RIBOSOMAL PROTEIN L6



• Molecule 33: 50S RIBOSOMAL PROTEIN L9

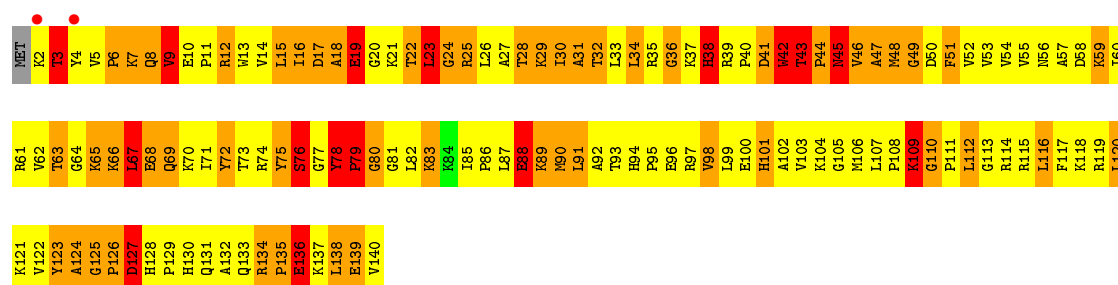


• Molecule 34: 50S RIBOSOMAL PROTEIN L11



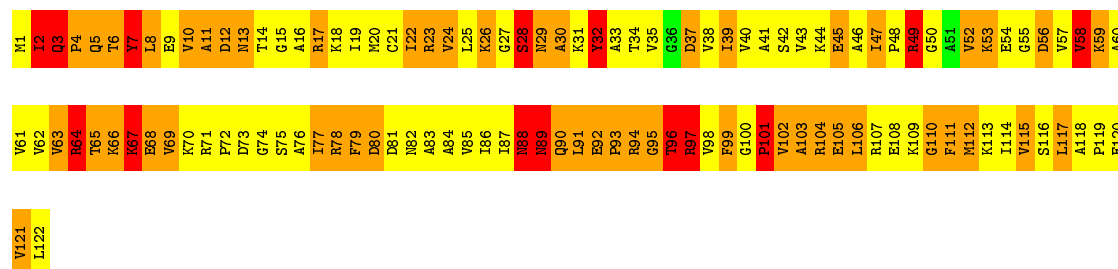
• Molecule 35: 50S RIBOSOMAL PROTEIN L13





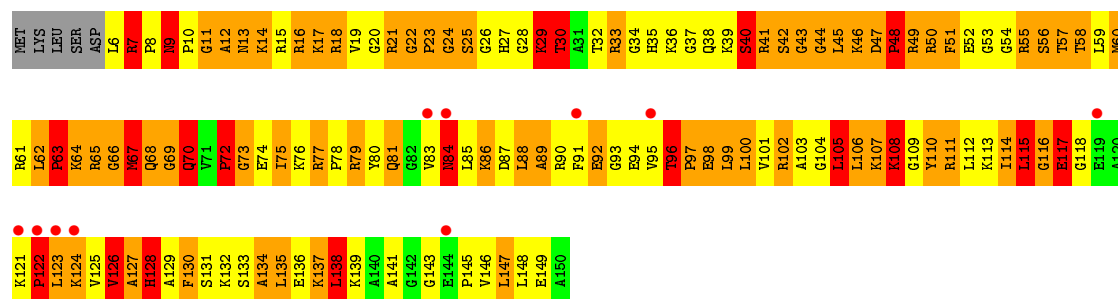
• Molecule 36: 50S RIBOSOMAL PROTEIN L14

Chain BN: . 46% 41% 11%



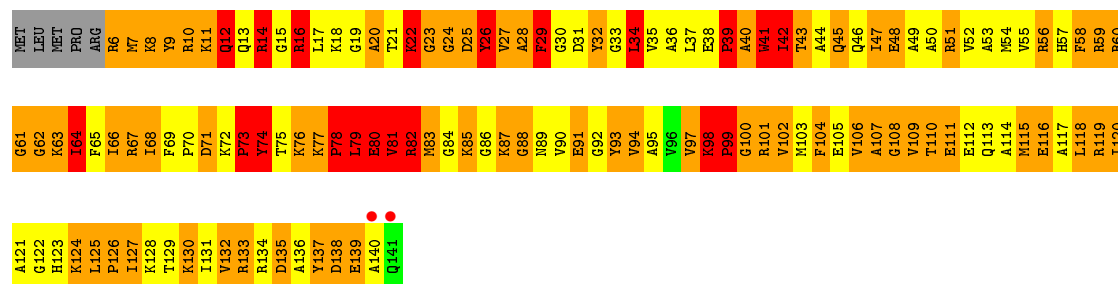
• Molecule 37: 50S RIBOSOMAL PROTEIN L15

Chain BO: 7% 6% 36% 41% 13% .



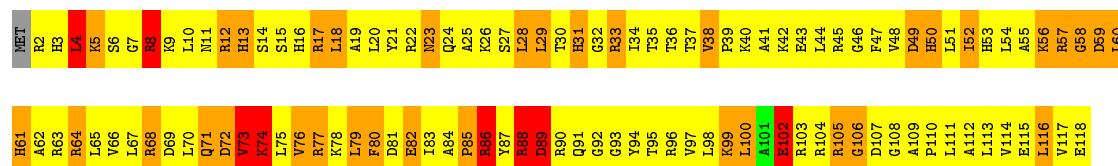
• Molecule 38: 50S RIBOSOMAL PROTEIN L16

Chain BP: . 34% 47% 14% .



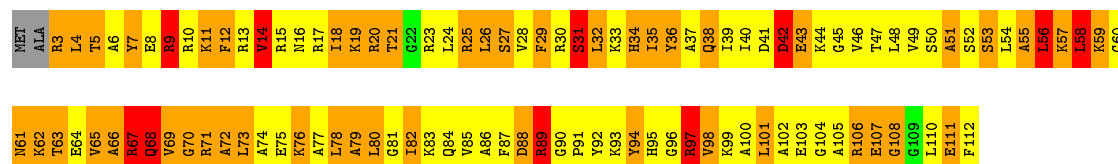
• Molecule 39: 50S RIBOSOMAL PROTEIN L17

Chain BQ: . 62% 30% 7% .



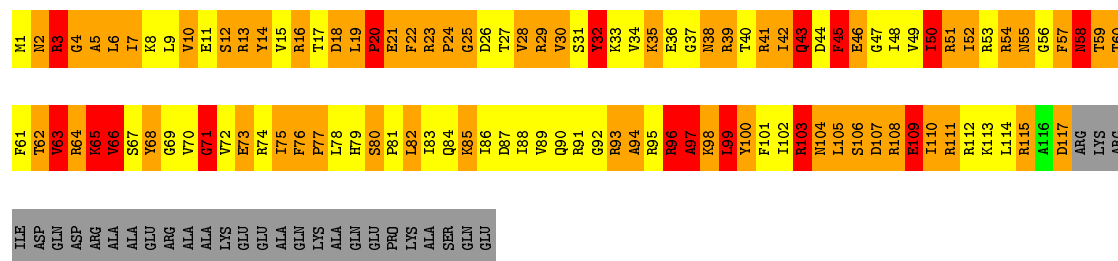
• Molecule 40: 50S RIBOSOMAL PROTEIN L18

Chain BR: . 45% 43% 9% .



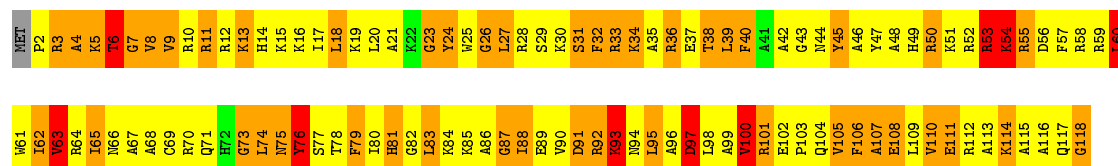
• Molecule 41: 50S RIBOSOMAL PROTEIN L19

Chain BS: . 30% 38% 11% 20%



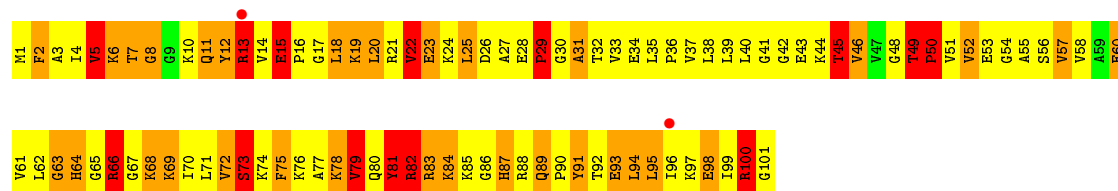
• Molecule 42: 50S RIBOSOMAL PROTEIN L20

Chain BT: . 50% 39% 8% .



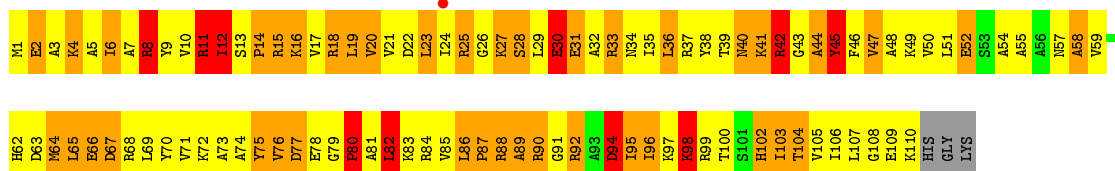
• Molecule 43: 50S RIBOSOMAL PROTEIN L21

Chain BU: . 2% 51% 32% 14%

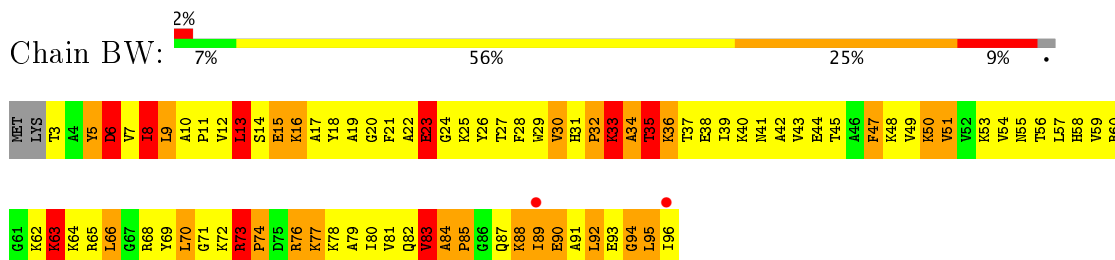


• Molecule 44: 50S RIBOSOMAL PROTEIN L22

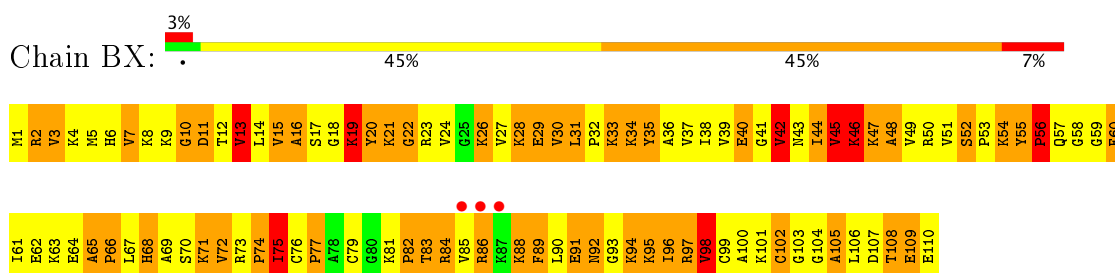
Chain BV: . 5% 48% 35% 9% .



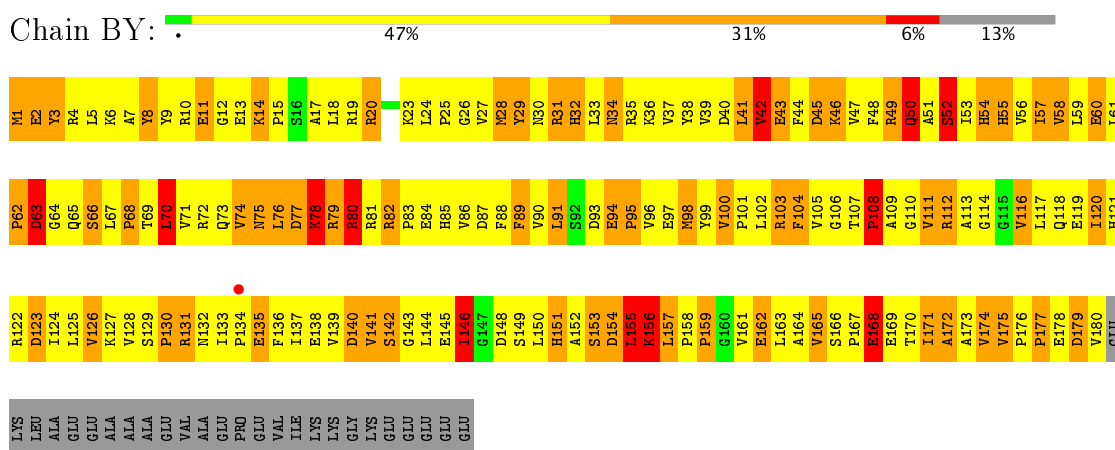
• Molecule 45: 50S RIBOSOMAL PROTEIN L23



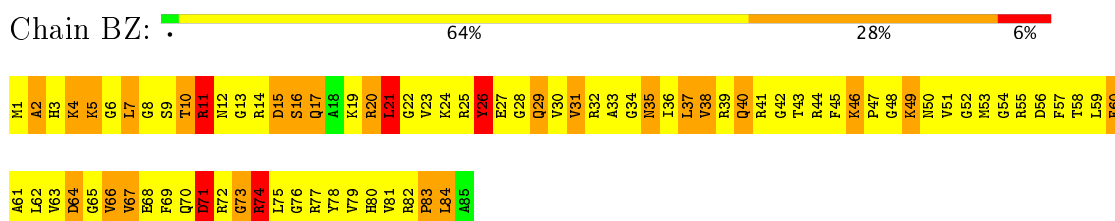
• Molecule 46: 50S RIBOSOMAL PROTEIN L24



• Molecule 47: 50S RIBOSOMAL PROTEIN L25

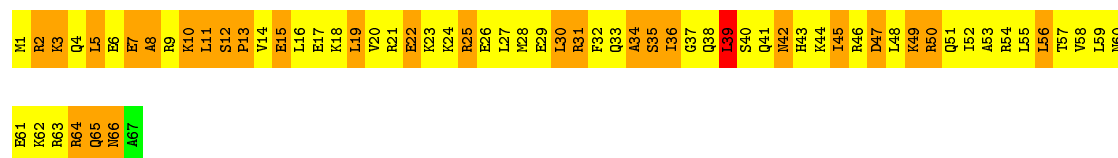


• Molecule 48: 50S RIBOSOMAL PROTEIN L27

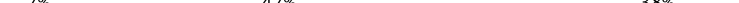


• Molecule 49: 50S RIBOSOMAL PROTEIN L29

Chain B1:  57% 40%



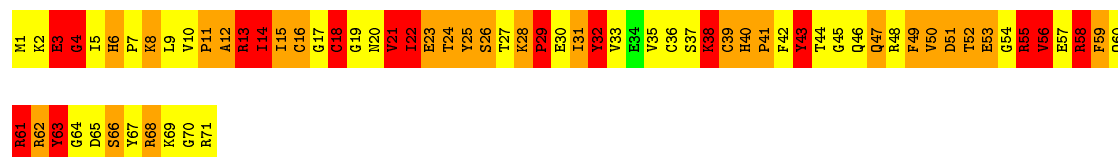
• Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain B2:  7% 47% 38% 7%



• Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain B3:  41% 35% 23%



- Molecule 52: 50S RIBOSOMAL PROTEIN L32

Chain B4:  27% 52% 15% 5%



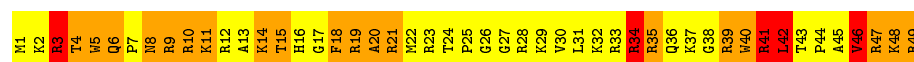
• Molecule 53: 50S RIBOSOMAL PROTEIN L33

Chain B5: 



- Molecule 54: 50S RIBOSOMAL PROTEIN L34

Chain B6:  51% 39% 10%



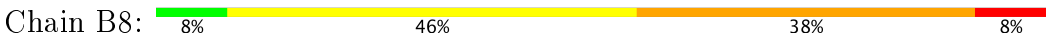
• Molecule 55: 50S RIBOSOMAL PROTEIN L35

Chain B7:  46% 43% 9%





● Molecule 56: 50S RIBOSOMAL PROTEIN L36





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	508.65Å 508.65Å 803.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	300.00 – 4.51 429.82 – 3.98	Depositor EDS
% Data completeness (in resolution range)	90.3 (300.00-4.51) 94.9 (429.82-3.98)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.00 (at 4.02Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.298 , 0.345 0.300 , 0.346	Depositor DCC
$R_{free}$ test set	14138 reflections (5.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	198.7	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.09 , 116.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.55$ , $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	149640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.62% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.93	38/36438 (0.1%)	1.05	172/56869 (0.3%)
2	AC	0.93	2/1814 (0.1%)	1.01	4/2825 (0.1%)
3	AD	1.47	34/1813 (1.9%)	1.27	21/2823 (0.7%)
4	A1	0.81	1/673 (0.1%)	1.07	3/1048 (0.3%)
5	AE	0.63	0/1935	1.01	4/2609 (0.2%)
6	AF	0.53	0/1636	0.93	4/2205 (0.2%)
7	AG	0.67	1/1733 (0.1%)	1.10	7/2318 (0.3%)
8	AH	0.70	0/1162	1.08	4/1564 (0.3%)
9	AI	0.69	0/856	1.03	3/1154 (0.3%)
10	AJ	0.54	0/1276	0.87	0/1709
11	AK	0.73	0/1136	1.08	3/1527 (0.2%)
12	AL	0.51	0/1029	0.84	1/1379 (0.1%)
13	AM	0.50	0/807	0.85	0/1085
14	AN	0.67	0/900	1.06	0/1213
15	AO	0.67	0/986	1.09	3/1320 (0.2%)
16	AP	0.51	0/1008	0.91	2/1347 (0.1%)
17	AQ	0.53	0/501	1.02	3/664 (0.5%)
18	AR	0.67	0/745	0.98	0/992
19	AS	0.72	0/716	1.04	4/963 (0.4%)
20	AT	0.67	0/870	1.05	2/1159 (0.2%)
21	AU	0.65	0/603	1.12	3/799 (0.4%)
22	AV	0.49	0/661	0.91	1/890 (0.1%)
23	AW	0.66	0/765	1.05	1/1007 (0.1%)
24	AX	0.47	0/212	0.82	0/277
25	BA	1.06	139/69685 (0.2%)	1.19	514/108786 (0.5%)
26	BB	0.80	2/2954 (0.1%)	1.00	4/4606 (0.1%)
27	BC	0.50	0/1775	0.89	2/2393 (0.1%)
28	BD	0.88	2/2174 (0.1%)	1.35	22/2927 (0.8%)
29	BE	0.87	0/1611	1.36	19/2171 (0.9%)
30	BF	0.74	0/1660	1.26	11/2247 (0.5%)
31	BG	0.60	0/1507	1.07	5/2027 (0.2%)
32	BH	0.64	0/1354	1.08	5/1831 (0.3%)
33	BK	0.68	0/1170	1.10	8/1581 (0.5%)
34	BL	0.50	0/1044	0.92	1/1415 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
35	BM	0.85	1/1140 (0.1%)	1.19	7/1537 (0.5%)
36	BN	1.07	4/942 (0.4%)	1.42	7/1268 (0.6%)
37	BO	0.75	0/1123	1.24	9/1493 (0.6%)
38	BP	0.86	1/1100 (0.1%)	1.23	9/1470 (0.6%)
39	BQ	0.70	0/974	1.07	2/1302 (0.2%)
40	BR	0.73	0/887	1.14	5/1180 (0.4%)
41	BS	0.98	0/990	1.52	16/1325 (1.2%)
42	BT	0.81	0/982	1.19	7/1306 (0.5%)
43	BU	0.94	1/790 (0.1%)	1.40	10/1057 (0.9%)
44	BV	0.73	0/886	1.21	7/1189 (0.6%)
45	BW	0.60	0/756	0.97	5/1015 (0.5%)
46	BX	0.61	0/857	1.10	3/1142 (0.3%)
47	BY	0.66	0/1467	1.11	5/1992 (0.3%)
48	BZ	0.67	0/679	1.02	1/902 (0.1%)
49	B1	0.60	0/569	0.89	1/751 (0.1%)
50	B2	0.71	1/474 (0.2%)	1.10	4/635 (0.6%)
51	B3	1.05	0/594	1.44	10/795 (1.3%)
52	B4	0.79	0/459	1.22	2/621 (0.3%)
53	B5	0.98	1/433 (0.2%)	1.49	6/576 (1.0%)
54	B6	0.84	1/438 (0.2%)	1.08	1/575 (0.2%)
55	B7	0.69	0/523	1.22	5/690 (0.7%)
56	B8	0.73	0/310	1.13	1/407 (0.2%)
All	All	0.94	229/162582 (0.1%)	1.13	959/242958 (0.4%)

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	241
2	AC	0	9
3	AD	0	12
4	A1	0	5
7	AG	0	1
8	AH	0	1
11	AK	0	2
14	AN	0	1
15	AO	0	1
20	AT	0	1
24	AX	0	1
25	BA	0	610

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	BB	0	20
28	BD	0	1
30	BF	0	1
32	BH	0	3
36	BN	0	2
38	BP	0	3
41	BS	0	2
42	BT	0	1
43	BU	0	2
44	BV	0	1
51	B3	0	2
52	B4	0	1
53	B5	0	1
56	B8	0	1
All	All	0	926

The worst 5 of 229 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1203	G	O3'-P	-34.71	1.19	1.61
25	BA	1202	C	O3'-P	29.90	1.97	1.61
25	BA	2447	G	O3'-P	-21.30	1.35	1.61
25	BA	2601	C	O3'-P	19.66	1.84	1.61
25	BA	2756	U	O3'-P	19.18	1.84	1.61

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BA	412	A	O5'-P-OP2	-28.87	76.06	110.70
25	BA	1203	G	P-O3'-C3'	27.73	152.97	119.70
25	BA	2448	A	C5'-C4'-O4'	-27.33	76.31	109.10
30	BF	20	LEU	O-C-N	-25.54	81.83	122.70
1	AA	37	U	N3-C4-O4	-25.04	101.87	119.40

There are no chirality outliers.

5 of 926 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	16	A	Sidechain
1	AA	21	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	24	U	Sidechain
1	AA	7	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	AA	32554	0	16429	6699	0
2	AC	1624	0	826	331	0
3	AD	1623	0	809	304	0
4	A1	596	0	296	65	0
5	AE	1900	0	1951	928	0
6	AF	1612	0	1677	661	0
7	AG	1703	0	1763	807	0
8	AH	1146	0	1207	482	0
9	AI	843	0	857	397	0
10	AJ	1257	0	1296	519	0
11	AK	1116	0	1177	666	0
12	AL	1010	0	1037	457	0
13	AM	794	0	840	327	0
14	AN	885	0	904	410	0
15	AO	970	0	1057	413	0
16	AP	997	0	1072	469	0
17	AQ	492	0	529	264	0
18	AR	734	0	771	353	0
19	AS	700	0	720	348	0
20	AT	857	0	930	385	0
21	AU	597	0	668	357	0
22	AV	647	0	673	241	0
23	AW	763	0	861	330	0
24	AX	208	0	221	87	0
25	BA	62218	0	31354	15682	0
26	BB	2641	0	1337	598	0
27	BC	1742	0	1796	761	0
28	BD	2124	0	2207	1434	0
29	BE	1578	0	1647	1120	0
30	BF	1625	0	1666	862	0
31	BG	1482	0	1546	838	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	BH	1328	0	1408	664	0
33	BK	1155	0	1244	574	0
34	BL	1025	0	1074	414	0
35	BM	1113	0	1183	722	0
36	BN	932	0	994	703	0
37	BO	1106	0	1183	801	0
38	BP	1080	0	1127	691	0
39	BQ	960	0	1021	505	0
40	BR	877	0	938	472	0
41	BS	976	0	1033	699	0
42	BT	964	0	1022	709	0
43	BU	779	0	852	626	0
44	BV	876	0	941	423	0
45	BW	742	0	800	336	0
46	BX	844	0	930	493	0
47	BY	1435	0	1463	683	0
48	BZ	670	0	700	365	0
49	B1	567	0	621	303	0
50	B2	469	0	518	302	0
51	B3	581	0	577	375	0
52	B4	445	0	459	271	0
53	B5	426	0	452	306	0
54	B6	430	0	480	275	0
55	B7	515	0	587	415	0
56	B8	307	0	335	126	0
All	All	149640	0	102066	45475	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 181.

The worst 5 of 45475 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:BA:1204:A:C2	30:BF:188:ARG:HA	1.17	1.61
25:BA:2459:A:N3	25:BA:2460:U:H1'	1.22	1.46
25:BA:1204:A:C2	30:BF:188:ARG:CA	1.98	1.45
25:BA:2745:C:N4	25:BA:2756:U:C5	1.85	1.45
25:BA:1475:G:H1	25:BA:1477:A:N6	1.11	1.44

There are no symmetry-related clashes.

## 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	
5	AE	232/256 (91%)	112 (48%)	47 (20%)	73 (32%)	0	0
6	AF	204/239 (85%)	115 (56%)	43 (21%)	46 (22%)	0	1
7	AG	206/209 (99%)	103 (50%)	61 (30%)	42 (20%)	0	2
8	AH	148/162 (91%)	92 (62%)	34 (23%)	22 (15%)	0	5
9	AI	99/101 (98%)	58 (59%)	19 (19%)	22 (22%)	0	2
10	AJ	153/156 (98%)	74 (48%)	40 (26%)	39 (26%)	0	1
11	AK	136/138 (99%)	71 (52%)	32 (24%)	33 (24%)	0	1
12	AL	125/128 (98%)	64 (51%)	33 (26%)	28 (22%)	0	1
13	AM	96/105 (91%)	55 (57%)	14 (15%)	27 (28%)	0	0
14	AN	117/129 (91%)	62 (53%)	30 (26%)	25 (21%)	0	2
15	AO	122/132 (92%)	62 (51%)	22 (18%)	38 (31%)	0	0
16	AP	123/126 (98%)	63 (51%)	36 (29%)	24 (20%)	0	3
17	AQ	58/61 (95%)	28 (48%)	14 (24%)	16 (28%)	0	0
18	AR	86/89 (97%)	40 (46%)	33 (38%)	13 (15%)	0	5
19	AS	81/88 (92%)	45 (56%)	21 (26%)	15 (18%)	0	3
20	AT	102/105 (97%)	63 (62%)	22 (22%)	17 (17%)	0	4
21	AU	71/88 (81%)	30 (42%)	18 (25%)	23 (32%)	0	0
22	AV	78/93 (84%)	32 (41%)	18 (23%)	28 (36%)	0	0
23	AW	97/106 (92%)	32 (33%)	36 (37%)	29 (30%)	0	0
24	AX	22/27 (82%)	9 (41%)	8 (36%)	5 (23%)	0	1
27	BC	226/229 (99%)	137 (61%)	52 (23%)	37 (16%)	0	4
28	BD	270/276 (98%)	129 (48%)	49 (18%)	92 (34%)	0	0
29	BE	204/206 (99%)	106 (52%)	39 (19%)	59 (29%)	0	0
30	BF	206/210 (98%)	100 (48%)	47 (23%)	59 (29%)	0	0
31	BG	180/182 (99%)	79 (44%)	42 (23%)	59 (33%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BH	172/180 (96%)	89 (52%)	41 (24%)	42 (24%)	0	1
33	BK	146/148 (99%)	88 (60%)	32 (22%)	26 (18%)	0	3
34	BL	136/147 (92%)	66 (48%)	32 (24%)	38 (28%)	0	0
35	BM	137/140 (98%)	66 (48%)	31 (23%)	40 (29%)	0	0
36	BN	120/122 (98%)	63 (52%)	21 (18%)	36 (30%)	0	0
37	BO	143/150 (95%)	60 (42%)	31 (22%)	52 (36%)	0	0
38	BP	134/141 (95%)	51 (38%)	35 (26%)	48 (36%)	0	0
39	BQ	115/118 (98%)	64 (56%)	33 (29%)	18 (16%)	0	4
40	BR	108/112 (96%)	45 (42%)	30 (28%)	33 (31%)	0	0
41	BS	115/146 (79%)	53 (46%)	26 (23%)	36 (31%)	0	0
42	BT	115/118 (98%)	49 (43%)	39 (34%)	27 (24%)	0	1
43	BU	99/101 (98%)	51 (52%)	22 (22%)	26 (26%)	0	1
44	BV	108/113 (96%)	69 (64%)	15 (14%)	24 (22%)	0	2
45	BW	92/96 (96%)	59 (64%)	14 (15%)	19 (21%)	0	2
46	BX	108/110 (98%)	41 (38%)	27 (25%)	40 (37%)	0	0
47	BY	178/206 (86%)	93 (52%)	48 (27%)	37 (21%)	0	2
48	BZ	83/85 (98%)	50 (60%)	14 (17%)	19 (23%)	0	1
49	B1	65/67 (97%)	27 (42%)	26 (40%)	12 (18%)	0	3
50	B2	57/60 (95%)	32 (56%)	16 (28%)	9 (16%)	0	4
51	B3	69/71 (97%)	26 (38%)	19 (28%)	24 (35%)	0	0
52	B4	55/60 (92%)	16 (29%)	12 (22%)	27 (49%)	0	0
53	B5	47/54 (87%)	13 (28%)	7 (15%)	27 (57%)	0	0
54	B6	47/49 (96%)	16 (34%)	16 (34%)	15 (32%)	0	0
55	B7	62/65 (95%)	29 (47%)	11 (18%)	22 (36%)	0	0
56	B8	35/37 (95%)	20 (57%)	4 (11%)	11 (31%)	0	0
All	All	5988/6337 (94%)	2997 (50%)	1412 (24%)	1579 (26%)	0	1

5 of 1579 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	AE	13	ALA
5	AE	15	VAL
5	AE	17	PHE

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Mol	Chain	Res	Type
5	AE	19	HIS
5	AE	20	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	
5	AE	202/220 (92%)	135 (67%)	67 (33%)	0	2
6	AF	160/188 (85%)	123 (77%)	37 (23%)	1	7
7	AG	180/181 (99%)	127 (71%)	53 (29%)	0	3
8	AH	115/123 (94%)	75 (65%)	40 (35%)	0	1
9	AI	90/90 (100%)	64 (71%)	26 (29%)	0	3
10	AJ	126/127 (99%)	95 (75%)	31 (25%)	1	6
11	AK	119/119 (100%)	76 (64%)	43 (36%)	0	1
12	AL	98/99 (99%)	76 (78%)	22 (22%)	1	8
13	AM	88/92 (96%)	65 (74%)	23 (26%)	0	5
14	AN	90/99 (91%)	62 (69%)	28 (31%)	0	2
15	AO	104/109 (95%)	77 (74%)	27 (26%)	0	5
16	AP	100/101 (99%)	79 (79%)	21 (21%)	1	9
17	AQ	49/50 (98%)	37 (76%)	12 (24%)	1	6
18	AR	79/80 (99%)	56 (71%)	23 (29%)	0	3
19	AS	72/74 (97%)	48 (67%)	24 (33%)	0	2
20	AT	96/97 (99%)	71 (74%)	25 (26%)	0	5
21	AU	64/77 (83%)	41 (64%)	23 (36%)	0	1
22	AV	71/80 (89%)	57 (80%)	14 (20%)	1	11
23	AW	76/82 (93%)	56 (74%)	20 (26%)	0	5
24	AX	19/22 (86%)	13 (68%)	6 (32%)	0	2
27	BC	180/181 (99%)	151 (84%)	29 (16%)	3	19
28	BD	215/218 (99%)	151 (70%)	64 (30%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BE	166/166 (100%)	102 (61%)	64 (39%)	0	0
30	BF	164/166 (99%)	104 (63%)	60 (37%)	0	1
31	BG	156/156 (100%)	112 (72%)	44 (28%)	0	3
32	BH	143/148 (97%)	97 (68%)	46 (32%)	0	2
33	BK	124/124 (100%)	87 (70%)	37 (30%)	0	3
34	BL	105/111 (95%)	85 (81%)	20 (19%)	2	12
35	BM	118/119 (99%)	80 (68%)	38 (32%)	0	2
36	BN	100/100 (100%)	65 (65%)	35 (35%)	0	1
37	BO	111/116 (96%)	64 (58%)	47 (42%)	0	0
38	BP	106/111 (96%)	55 (52%)	51 (48%)	0	0
39	BQ	100/101 (99%)	69 (69%)	31 (31%)	0	2
40	BR	87/88 (99%)	55 (63%)	32 (37%)	0	1
41	BS	105/127 (83%)	69 (66%)	36 (34%)	0	2
42	BT	93/94 (99%)	64 (69%)	29 (31%)	0	2
43	BU	82/82 (100%)	59 (72%)	23 (28%)	0	4
44	BV	90/92 (98%)	56 (62%)	34 (38%)	0	1
45	BW	76/78 (97%)	55 (72%)	21 (28%)	0	4
46	BX	91/91 (100%)	66 (72%)	25 (28%)	0	4
47	BY	159/179 (89%)	110 (69%)	49 (31%)	0	2
48	BZ	67/67 (100%)	52 (78%)	15 (22%)	1	8
49	B1	62/62 (100%)	46 (74%)	16 (26%)	0	5
50	B2	51/52 (98%)	34 (67%)	17 (33%)	0	2
51	B3	63/63 (100%)	42 (67%)	21 (33%)	0	2
52	B4	50/52 (96%)	30 (60%)	20 (40%)	0	0
53	B5	48/52 (92%)	32 (67%)	16 (33%)	0	2
54	B6	42/42 (100%)	30 (71%)	12 (29%)	0	3
55	B7	54/55 (98%)	40 (74%)	14 (26%)	0	5
56	B8	34/34 (100%)	25 (74%)	9 (26%)	0	5
All	All	5040/5237 (96%)	3520 (70%)	1520 (30%)	0	3

5 of 1520 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	BE	101	ARG
32	BH	103	LEU
49	B1	45	ILE
29	BE	155	LYS
30	BF	175	THR

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

Mol	Chain	Res	Type
22	AV	23	ASN
29	BE	129	HIS
51	B3	46	GLN
23	AW	45	GLN
28	BD	87	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1515/1522 (99%)	479 (31%)	151 (9%)
2	AC	75/76 (98%)	30 (40%)	7 (9%)
25	BA	2888/2916 (99%)	1241 (42%)	313 (10%)
26	BB	122/123 (99%)	46 (37%)	5 (4%)
3	AD	75/76 (98%)	27 (36%)	3 (4%)
4	A1	26/27 (96%)	11 (42%)	1 (3%)
All	All	4701/4740 (99%)	1834 (39%)	480 (10%)

5 of 1834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	14	U

5 of 480 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	BA	562	U
25	BA	974(A)	C
25	BA	2610	C

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Mol	Chain	Res	Type
25	BA	616	A
25	BA	783	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	6
1	AA	2

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1202:C	O3'	1203:G	P	1.97
1	AA	173:U	O3'	174:C	P	1.84
1	BA	2601:C	O3'	2602:A	P	1.84
1	BA	2756:U	O3'	2757:A	P	1.84
1	BA	2755:C	O3'	2756:U	P	1.75

## 6 Fit of model and data i

### 6.1 Protein, DNA and RNA chains i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AA	1515/1522 (99%)	-0.78	2 (0%) 95 94	188, 245, 349, 445	0
2	AC	76/76 (100%)	-0.93	0 100 100	213, 249, 283, 294	0
3	AD	76/76 (100%)	-0.82	0 100 100	301, 334, 358, 368	0
4	A1	27/27 (100%)	0.75	6 (22%) 1 3	225, 347, 415, 416	0
5	AE	234/256 (91%)	-0.26	7 (2%) 51 42	218, 248, 286, 307	0
6	AF	206/239 (86%)	0.23	12 (5%) 24 20	246, 269, 288, 296	0
7	AG	208/209 (99%)	-0.80	0 100 100	202, 233, 251, 265	0
8	AH	150/162 (92%)	-0.56	0 100 100	202, 220, 245, 262	0
9	AI	101/101 (100%)	0.32	4 (3%) 39 31	219, 237, 254, 271	0
10	AJ	155/156 (99%)	0.13	8 (5%) 28 24	250, 273, 285, 301	0
11	AK	138/138 (100%)	-0.80	0 100 100	203, 222, 236, 246	0
12	AL	127/128 (99%)	-0.50	0 100 100	247, 317, 349, 353	0
13	AM	98/105 (93%)	0.29	7 (7%) 17 15	256, 296, 311, 317	0
14	AN	119/129 (92%)	-0.24	1 (0%) 86 80	214, 234, 252, 279	0
15	AO	124/132 (93%)	-0.29	0 100 100	189, 217, 243, 263	0
16	AP	125/126 (99%)	-0.68	0 100 100	253, 281, 302, 306	0
17	AQ	60/61 (98%)	-0.43	0 100 100	243, 273, 286, 290	0
18	AR	88/89 (98%)	-1.04	0 100 100	199, 222, 244, 251	0
19	AS	83/88 (94%)	-0.89	0 100 100	192, 212, 232, 267	0
20	AT	104/105 (99%)	-1.08	0 100 100	192, 218, 252, 296	0
21	AU	73/88 (82%)	-0.46	3 (4%) 38 31	192, 228, 255, 277	0
22	AV	80/93 (86%)	0.29	2 (2%) 58 50	251, 287, 306, 310	0
23	AW	99/106 (93%)	-0.93	0 100 100	200, 228, 250, 254	0
24	AX	24/27 (88%)	-1.06	0 100 100	268, 289, 303, 306	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
25	BA	2889/2916 (99%)	-0.77	0 100 100	168, 241, 340, 398	0
26	BB	123/123 (100%)	-0.58	0 100 100	236, 293, 329, 343	0
27	BC	228/229 (99%)	0.98	54 (23%) 1 3	299, 326, 342, 347	0
28	BD	272/276 (98%)	-0.14	7 (2%) 56 48	184, 216, 235, 256	0
29	BE	206/206 (100%)	-0.61	1 (0%) 90 86	155, 205, 250, 276	0
30	BF	208/210 (99%)	-0.59	0 100 100	186, 255, 283, 288	0
31	BG	182/182 (100%)	-0.56	2 (1%) 80 73	247, 283, 306, 311	0
32	BH	174/180 (96%)	-0.40	1 (0%) 89 85	230, 260, 278, 284	0
33	BK	148/148 (100%)	-0.61	0 100 100	212, 241, 261, 265	0
34	BL	138/147 (93%)	0.62	22 (15%) 2 4	305, 358, 399, 403	0
35	BM	139/140 (99%)	-0.60	2 (1%) 75 67	187, 217, 245, 270	0
36	BN	122/122 (100%)	-0.66	0 100 100	172, 201, 228, 240	0
37	BO	145/150 (96%)	-0.20	10 (6%) 18 15	189, 271, 304, 346	0
38	BP	136/141 (96%)	-0.41	2 (1%) 74 66	199, 234, 257, 266	0
39	BQ	117/118 (99%)	-0.77	0 100 100	195, 214, 246, 256	0
40	BR	110/112 (98%)	-0.93	0 100 100	232, 266, 293, 300	0
41	BS	117/146 (80%)	-0.60	0 100 100	182, 205, 238, 244	0
42	BT	117/118 (99%)	-0.61	0 100 100	191, 221, 241, 250	0
43	BU	101/101 (100%)	-0.15	2 (1%) 65 58	190, 244, 272, 277	0
44	BV	110/113 (97%)	-0.43	1 (0%) 84 78	203, 226, 250, 260	0
45	BW	94/96 (97%)	-0.49	2 (2%) 64 56	237, 253, 304, 309	0
46	BX	110/110 (100%)	-0.31	3 (2%) 55 46	244, 282, 303, 312	0
47	BY	180/206 (87%)	-0.11	1 (0%) 89 85	235, 267, 281, 287	0
48	BZ	85/85 (100%)	-0.99	0 100 100	236, 259, 272, 289	0
49	B1	67/67 (100%)	-0.62	0 100 100	251, 264, 276, 281	0
50	B2	59/60 (98%)	-0.57	0 100 100	208, 244, 261, 268	0
51	B3	71/71 (100%)	-0.93	0 100 100	212, 239, 259, 276	0
52	B4	57/60 (95%)	-0.61	0 100 100	200, 227, 276, 299	0
53	B5	49/54 (90%)	-0.37	2 (4%) 38 31	211, 247, 269, 277	0
54	B6	49/49 (100%)	-0.89	0 100 100	189, 228, 244, 250	0
55	B7	64/65 (98%)	-0.80	0 100 100	201, 220, 235, 247	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
56	B8	37/37 (100%)	-1.11	0	100	100	212, 230, 240, 244	0
All	All	10794/11077 (97%)	-0.55	164 (1%)	74	66	155, 245, 336, 445	0

The worst 5 of 164 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
37	BO	123	LEU	12.3
27	BC	126	LYS	9.8
4	A1	1	G	9.5
27	BC	125	SER	9.3
27	BC	121	GLY	8.4

## 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 carbohydrates 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.