



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:49 PM BST

PDB ID : 4V9I  
Title : Crystal structure of thermus thermophilus 70S in complex with tRNAs and mRNA containing a pseudouridine in a stop codon  
Authors : Fernandez, I.S.; Ng, C.L.; Kelley, A.C.; Guowei, W.; Yu, Y.T.; Ramakrishnan, V.  
Deposited on : 2013-04-04  
Resolution : 3.30 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

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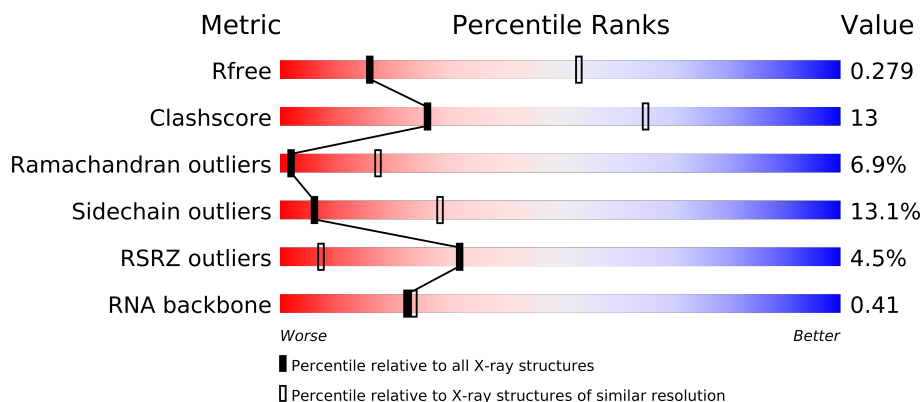
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable23397  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23397

# 1 Overall quality at a glance

The reported resolution of this entry is 3.30 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))
$R_{free}$	66092	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1504	
1	CA	1504	
2	AB	234	
2	CB	234	
3	AC	206	
3	CC	206	
4	AD	208	
4	CD	208	
5	AE	150	
5	CE	150	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	155	
7	CG	155	
8	AH	138	
8	CH	138	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	119	
11	CK	119	
12	AL	124	
12	CL	124	
13	AM	124	
13	CM	124	
14	AN	60	
14	CN	60	
15	AO	88	
15	CO	88	
16	AP	83	
16	CP	83	
17	AQ	99	
17	CQ	99	
18	AR	70	
18	CR	70	
19	AS	78	
19	CS	78	
20	AT	99	
20	CT	99	
21	AU	24	
21	CU	24	
22	AV	77	
22	CV	77	
23	AW	76	
23	CW	76	
24	AY	75	
24	CY	75	
25	AX	7	
26	BA	2915	
26	DA	2915	
27	BB	119	
27	DB	119	
28	BC	206	







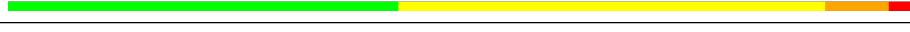


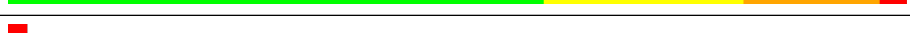
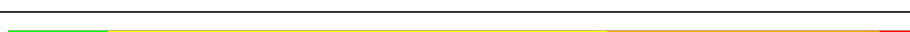
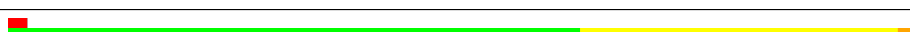

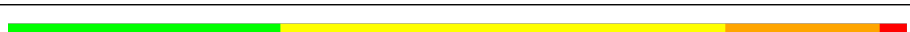
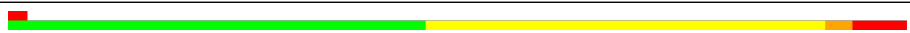
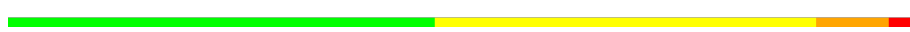




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Mol	Chain	Length	Quality of chain
29	BD	271	
29	DD	271	
30	BE	204	
30	DE	204	
31	BF	207	
31	DF	207	
32	BG	181	
32	DG	181	
33	BH	159	
33	DH	159	
34	BI	145	
34	DI	145	
35	BJ	130	
35	DJ	130	
36	BN	138	
36	DN	138	
37	BO	122	
37	DO	122	
38	BP	146	
38	DP	146	
39	BQ	141	
39	DQ	141	
40	BR	117	
40	DR	117	
41	BS	98	
41	DS	98	
42	BT	137	
42	DT	137	
43	BU	117	
43	DU	117	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	92	
46	DX	92	
47	BY	100	
47	DY	100	
48	BZ	176	
48	DZ	176	
49	B0	84	
49	D0	84	

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Mol	Chain	Length	Quality of chain
50	B1	93	
50	D1	93	
51	B2	71	
51	D2	71	
52	B3	59	
52	D3	59	
53	B4	30	
53	D4	30	
54	B5	59	
54	D5	59	
55	B6	44	
55	D6	44	
56	B7	48	
56	D7	48	
57	B8	63	
57	D8	63	
58	B9	36	
58	D9	36	
59	CX	4	
60	DC	196	

## 2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 295724 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S Ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			
2	CB	234	Total	C	N	O	S	0	0	0
			1901	1213	341	342	5			

- Molecule 3 is a protein called 30S Ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			
3	CC	206	Total	C	N	O	S	0	0	0
			1613	1016	314	282	1			

- Molecule 4 is a protein called 30S Ribosomal protein S4.

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

- Molecule 5 is a protein called 30S Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			
5	CE	150	Total	C	N	O	S	0	0	0
			1147	724	217	202	4			

- Molecule 6 is a protein called 30S Ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S Ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S Ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S Ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	CONFLICT	UNP P80374
CI	58	ARG	HIS	CONFLICT	UNP P80374

- Molecule 10 is a protein called 30S Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			
10	CJ	98	Total	C	N	O	S	0	0	0
			795	499	156	139	1			

- Molecule 11 is a protein called 30S Ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S Ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			
12	CL	124	Total	C	N	O	S	0	0	0
			971	611	195	164	1			

- Molecule 13 is a protein called 30S Ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			
13	CM	124	Total	C	N	O	S	0	0	0
			988	611	205	170	2			

- Molecule 14 is a protein called 30S Ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S Ribosomal protein S15.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S Ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			
16	CP	83	Total	C	N	O	S	0	0	0
			701	443	139	118	1			

- Molecule 17 is a protein called 30S Ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			
17	CQ	99	Total	C	N	O	S	0	0	0
			824	528	151	143	2			

- Molecule 18 is a protein called 30S Ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S Ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			
19	CS	78	Total	C	N	O	S	0	0	0
			630	403	114	111	2			

- Molecule 20 is a protein called 30S Ribosomal protein S20.

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

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

- Molecule 21 is a protein called 30S Ribosomal protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	24	Total	C	N	O	0	0	0
			209	128	50	31			
21	CU	24	Total	C	N	O	0	0	0
			209	128	50	31			

- Molecule 22 is a RNA chain called P-SITE tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
22	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 23 is a RNA chain called E-SITE tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 24 is a RNA chain called A-SITE tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	75	Total	C	N	O	P	0	0	0
			1619	722	309	514	74			
24	CY	75	Total	C	N	O	P	0	0	0
			1619	722	309	514	74			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	?	-	C	DELETION	GB 443419838
CY	?	-	C	DELETION	GB 443419838

- Molecule 25 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AX	7	Total	C	N	O	P	0	0	0
			151	68	29	47	7			

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			
26	DA	2807	Total	C	N	O	P	0	0	0
			60459	26907	11311	19435	2806			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BA	1151	A	G	CONFLICT	GB 55771382
DA	1151	A	G	CONFLICT	GB 55771382

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
27	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 28 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BC	190	Total	C	N	O		0	0	0
			1157	706	220	231				

- Molecule 29 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			
29	DD	271	Total	C	N	O	S	0	0	0
			2105	1329	416	357	3			

- Molecule 30 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			
30	DE	204	Total	C	N	O	S	0	0	0
			1564	988	299	271	6			

- Molecule 31 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BF	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			
31	DF	207	Total	C	N	O	S	0	0	0
			1624	1035	303	283	3			

- Molecule 32 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
32	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 33 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			
33	DH	159	Total	C	N	O	S	0	0	0
			1223	773	228	221	1			

- Molecule 34 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			
34	DI	145	Total	C	N	O	S	0	0	0
			1132	723	200	208	1			

- Molecule 35 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
35	DJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BN	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			
36	DN	138	Total	C	N	O	S	0	0	0
			1105	712	206	183	4			

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
37	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
38	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
39	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	BR	117	Total	C	N	O	0	0	0
			960	599	202	159			
40	DR	117	Total	C	N	O	0	0	0
			960	599	202	159			

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	BS	98	Total	C	N	O	0	0	0
			771	486	154	131			
41	DS	98	Total	C	N	O	0	0	0
			771	486	154	131			

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			
42	DT	137	Total	C	N	O	S	0	0	0
			1142	710	234	197	1			

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
43	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BU	32	ALA	PHE	CONFLICT	UNP P60491
DU	32	ALA	PHE	CONFLICT	UNP P60491

- Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
44	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BW	113	ALA	LYS	CONFLICT	UNP Q5SHP3
DW	113	ALA	LYS	CONFLICT	UNP Q5SHP3

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BX	92	Total	C	N	O		0	0	0
			726	471	131	124				
46	DX	92	Total	C	N	O		0	0	0
			726	471	131	124				

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			
47	DY	100	Total	C	N	O	S	0	0	0
			776	500	148	124	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			
48	DZ	176	Total	C	N	O	S	0	0	0
			1404	897	252	253	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
49	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 50 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			
50	D1	93	Total	C	N	O	S	0	0	0
			734	460	147	126	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B1	81	ARG	LYS	CONFLICT	UNP P60494
D1	81	ARG	LYS	CONFLICT	UNP P60494

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
51	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			
52	D3	59	Total	C	N	O	S	0	0	0
			468	298	90	79	1			

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			
53	D4	30	Total	C	N	O	S	0	0	0
			226	142	36	44	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			



- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			
55	D6	44	Total	C	N	O	S	0	0	0
			381	235	77	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			
56	D7	48	Total	C	N	O	S	0	0	0
			419	257	104	56	2			

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			
57	D8	63	Total	C	N	O	S	0	0	0
			508	326	101	79	2			

- Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
58	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 59 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	4	Total	C	N	O	P	0	0	0
			85	38	14	29	4			

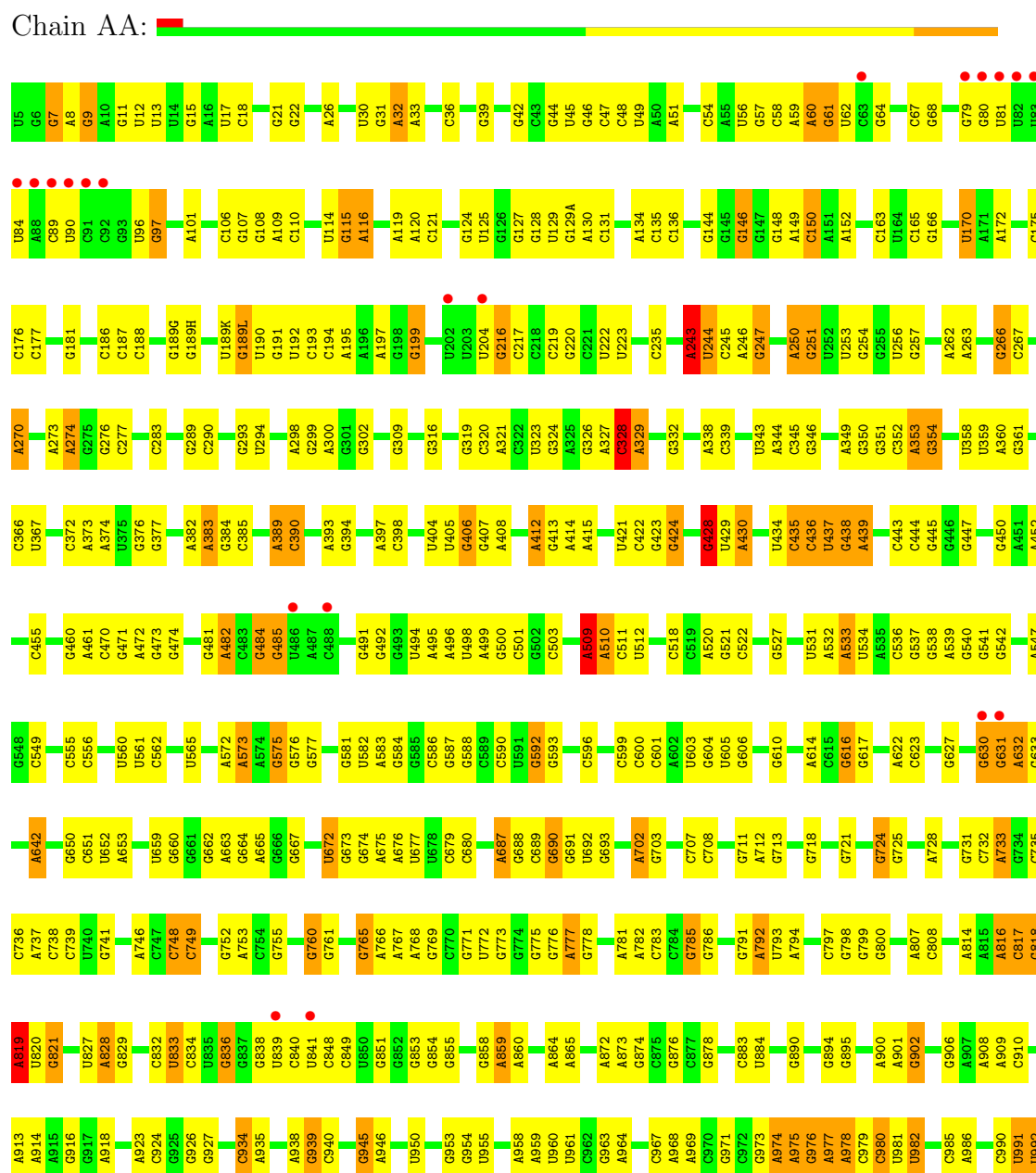
- Molecule 60 is a protein called 50S Ribosomal protein L1.

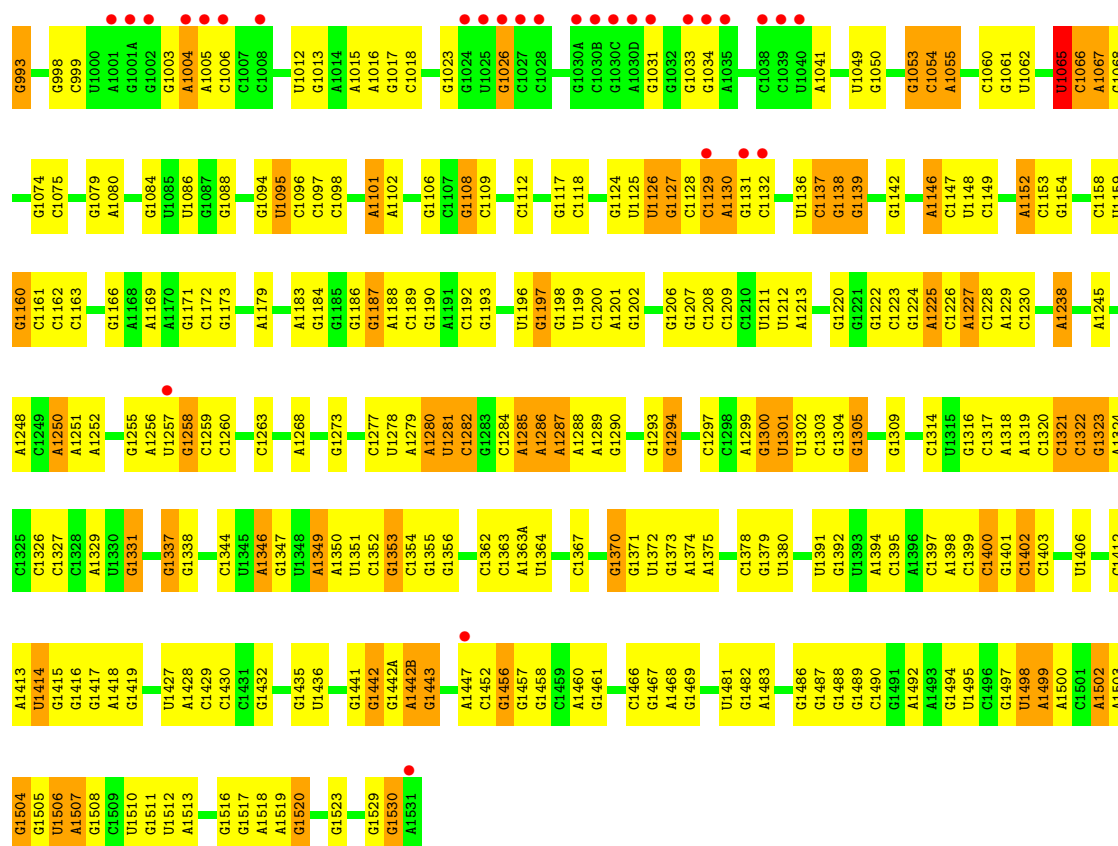
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
60	DC	190	Total	C	N	O	0	0	0
			1157	706	220	231			

### 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 errors 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 ( $\text{RSRZ} > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

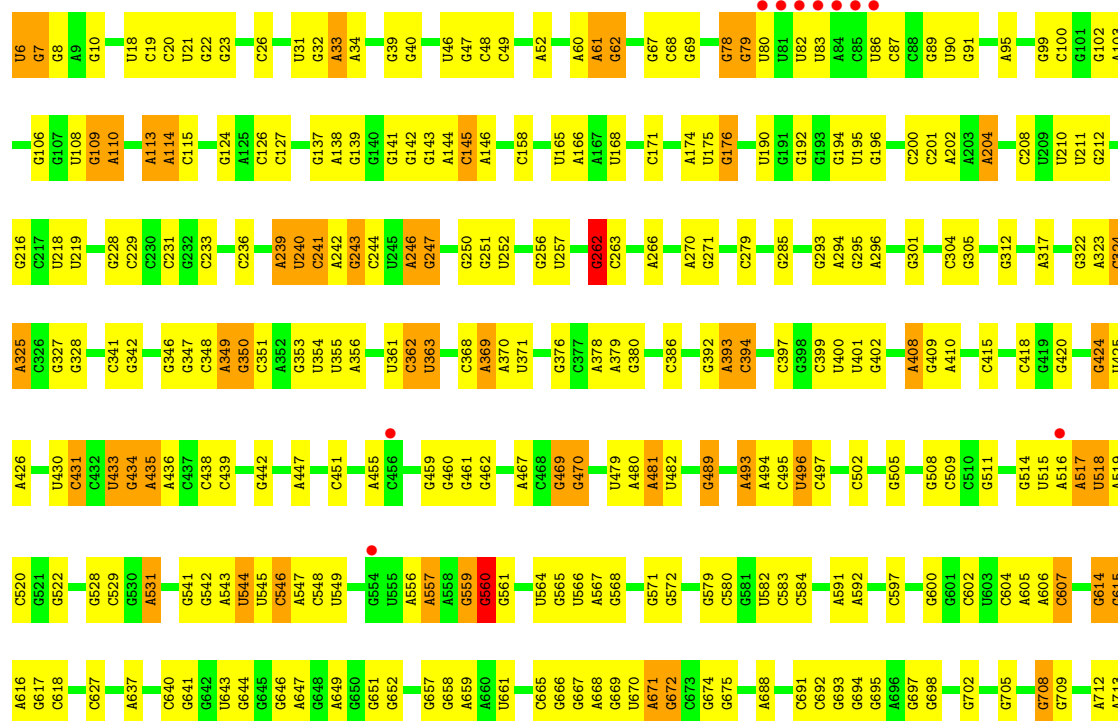
#### • Molecule 1: 16S ribosomal RNA





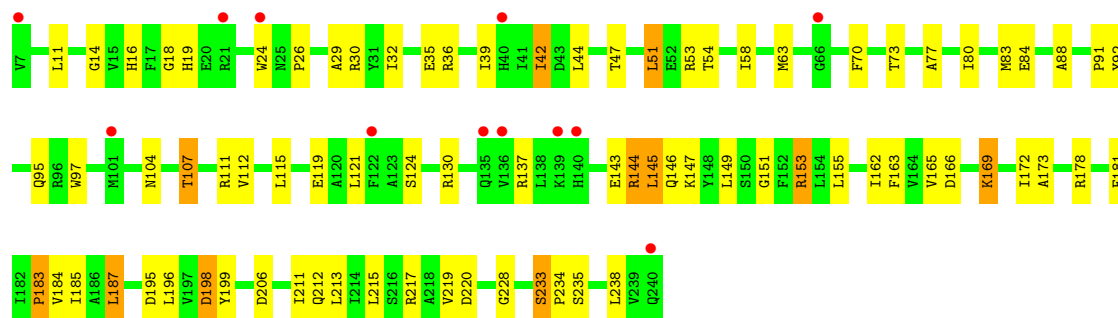
• Molecule 1: 16S ribosomal RNA

Chain CA:



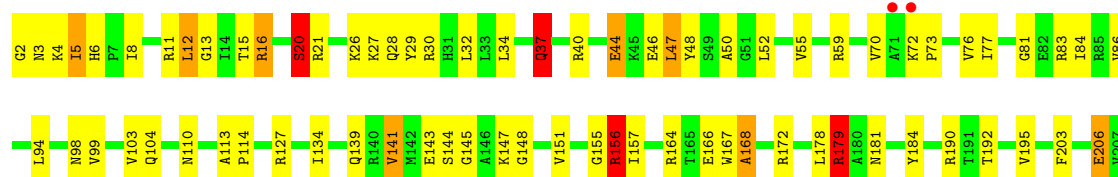


Chain CB:



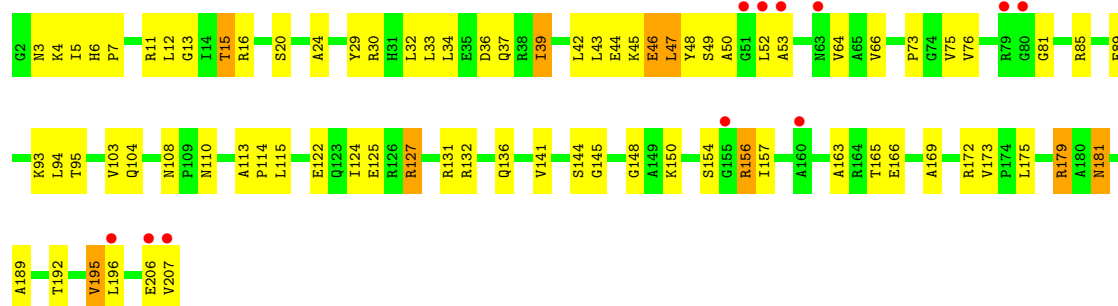
- Molecule 3: 30S Ribosomal protein S3

Chain AC:



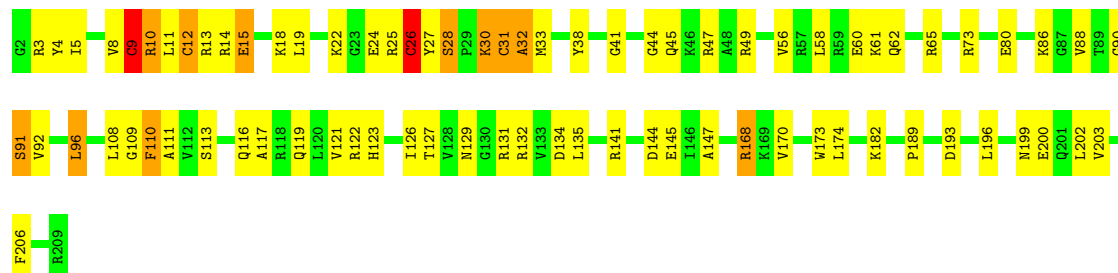
- Molecule 3: 30S Ribosomal protein S3

Chain CC:



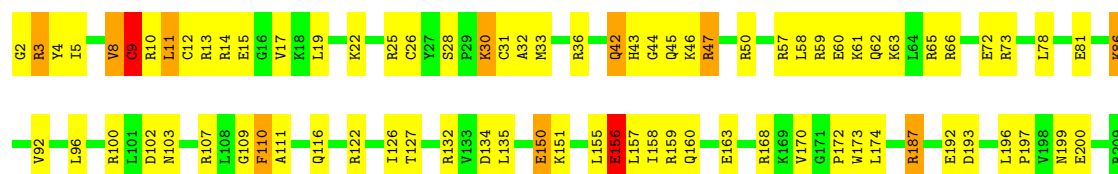
- Molecule 4: 30S Ribosomal protein S4

Chain AD:



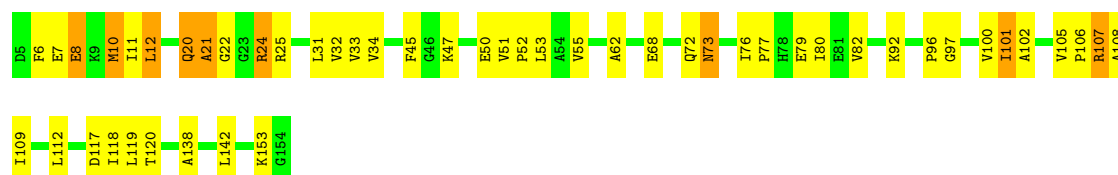
- Molecule 4: 30S Ribosomal protein S4

Chain CD:



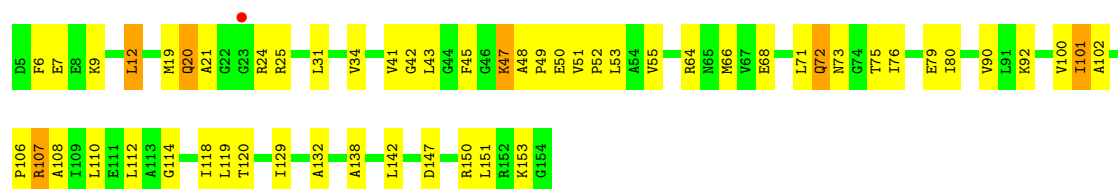
• Molecule 5: 30S Ribosomal protein S5

Chain AE:



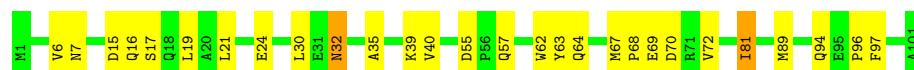
• Molecule 5: 30S Ribosomal protein S5

Chain CE:



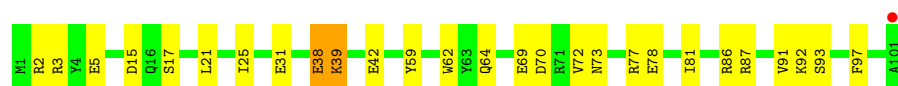
• Molecule 6: 30S Ribosomal protein S6

Chain AF:



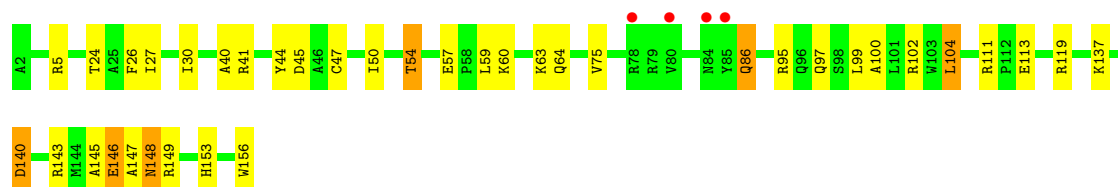
• Molecule 6: 30S Ribosomal protein S6

Chain CF:



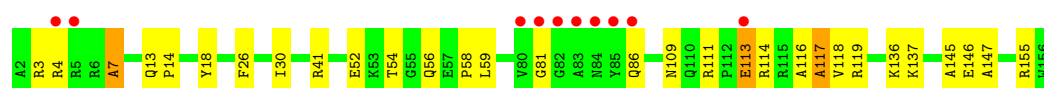
• Molecule 7: 30S Ribosomal protein S7

Chain AG:



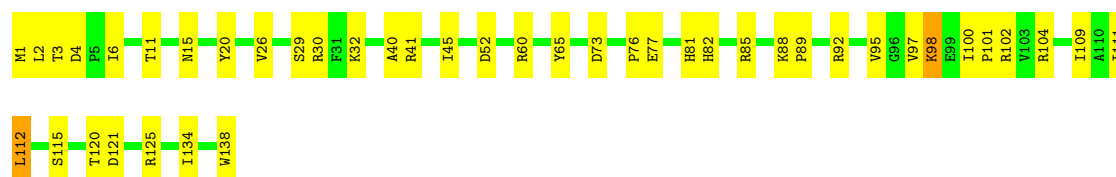
• Molecule 7: 30S Ribosomal protein S7

Chain CG:



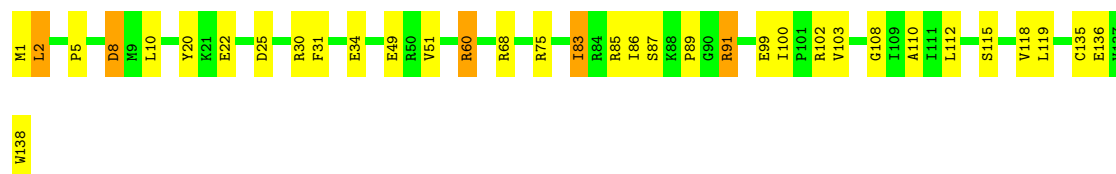
• Molecule 8: 30S Ribosomal protein S8

Chain AH:



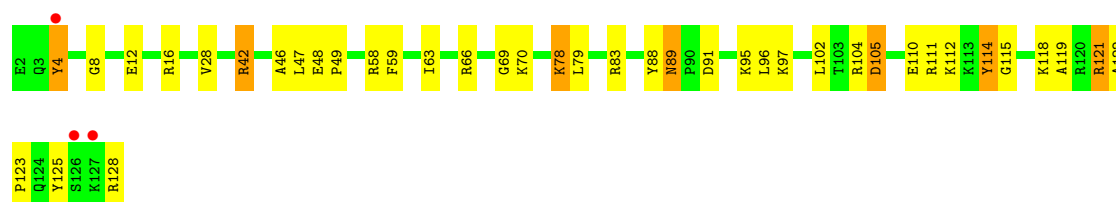
• Molecule 8: 30S Ribosomal protein S8

Chain CH:



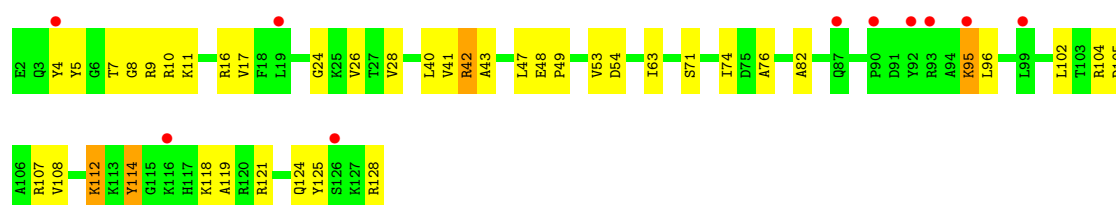
• Molecule 9: 30S Ribosomal protein S9

Chain AI:



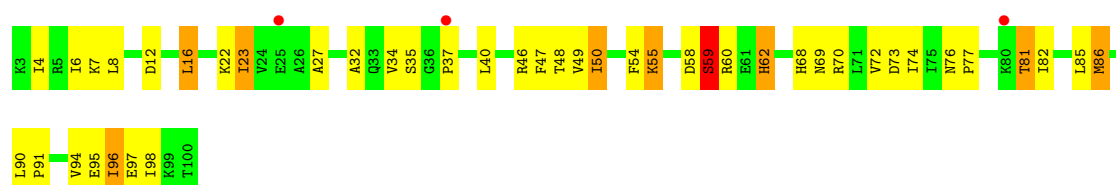
• Molecule 9: 30S Ribosomal protein S9

Chain CI:

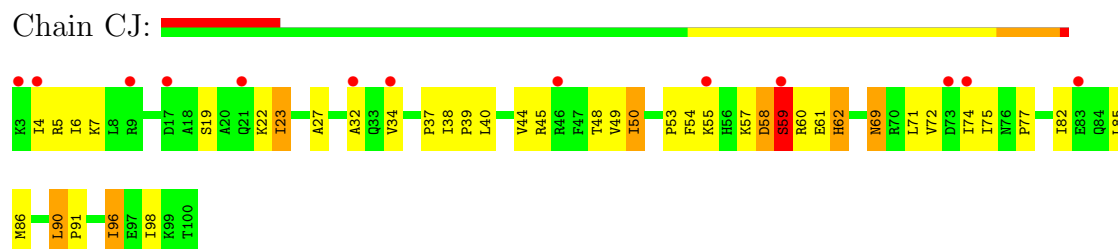


• Molecule 10: 30S Ribosomal protein S10

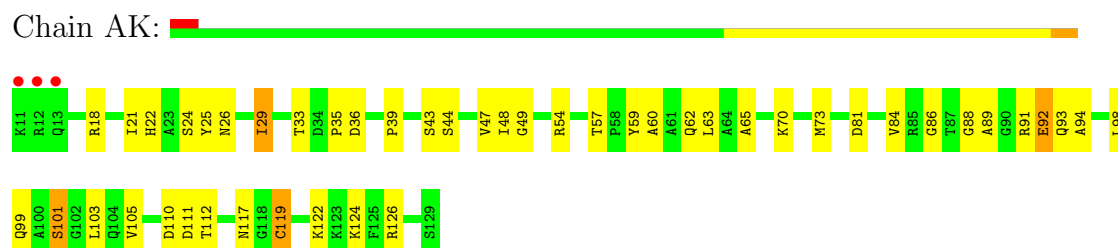
Chain AJ:



- Molecule 10: 30S Ribosomal protein S10



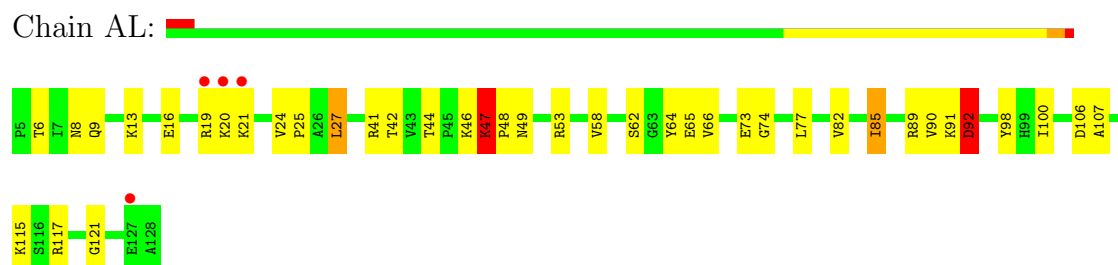
- Molecule 11: 30S Ribosomal protein S11



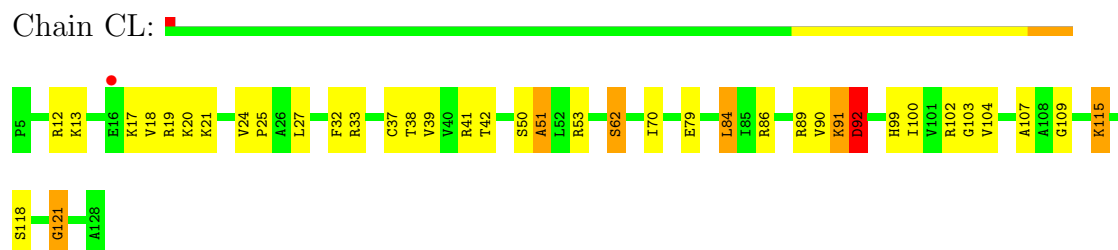
- Molecule 11: 30S Ribosomal protein S11



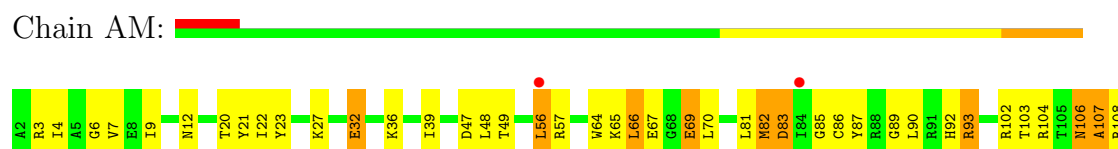
- Molecule 12: 30S Ribosomal protein S12



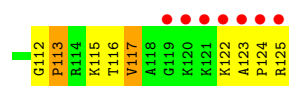
- Molecule 12: 30S Ribosomal protein S12



- Molecule 13: 30S Ribosomal protein S13

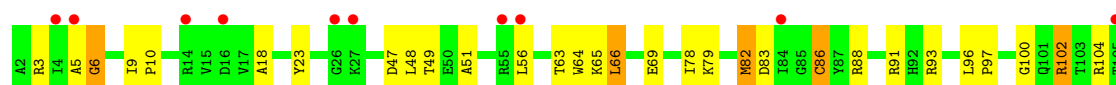






- Molecule 13: 30S Ribosomal protein S13

Chain CM:



- Molecule 14: 30S Ribosomal protein S14

Chain AN:



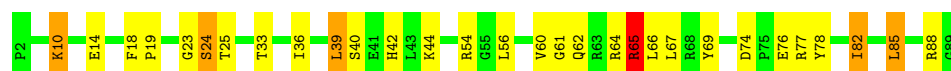
- Molecule 14: 30S Ribosomal protein S14

Chain CN:



- Molecule 15: 30S Ribosomal protein S15

Chain AO:



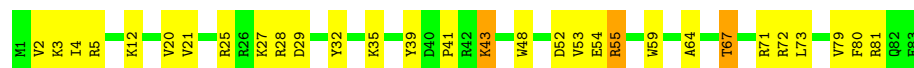
- Molecule 15: 30S Ribosomal protein S15

Chain CO:



- Molecule 16: 30S Ribosomal protein S16

Chain AP:



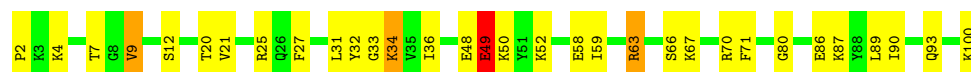
- Molecule 16: 30S Ribosomal protein S16

Chain CP:



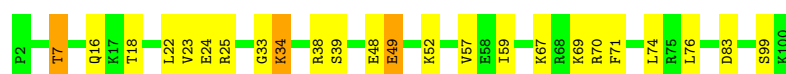
- Molecule 17: 30S Ribosomal protein S17

Chain AQ:



- Molecule 17: 30S Ribosomal protein S17

Chain CQ:



- Molecule 18: 30S Ribosomal protein S18

Chain AR:



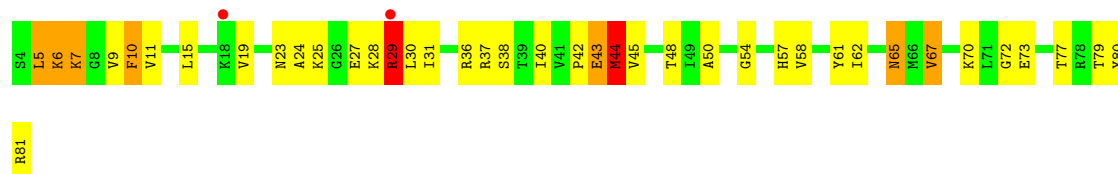
- Molecule 18: 30S Ribosomal protein S18

Chain CR:



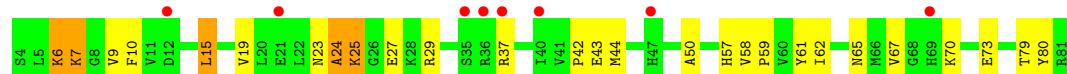
- Molecule 19: 30S Ribosomal protein S19

Chain AS:



- Molecule 19: 30S Ribosomal protein S19

Chain CS:



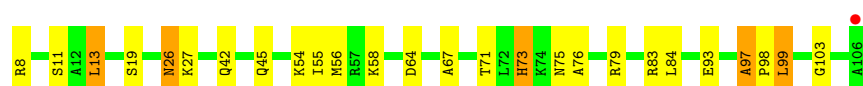
- Molecule 20: 30S Ribosomal protein S20

Chain AT:



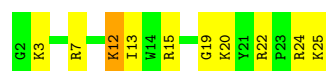
- Molecule 20: 30S Ribosomal protein S20

Chain CT:



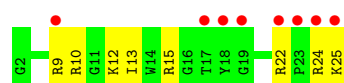
- Molecule 21: 30S Ribosomal protein THX

Chain AU:



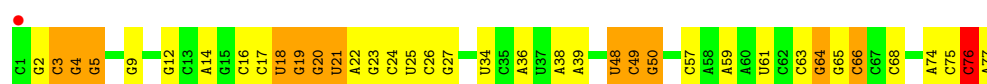
- Molecule 21: 30S Ribosomal protein THX

Chain CU:



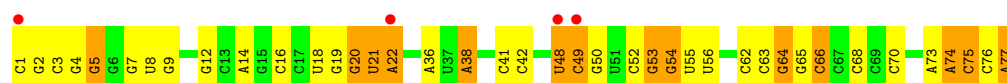
- Molecule 22: P-SITE tRNA

Chain AV:



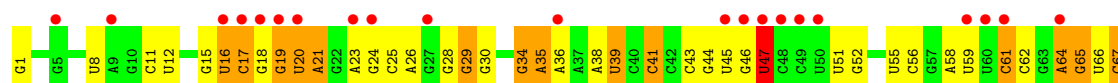
- Molecule 22: P-SITE tRNA

Chain CV:



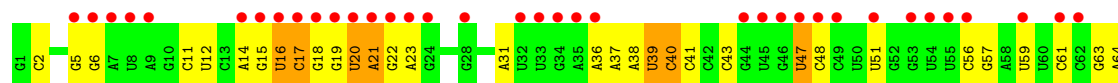
- Molecule 23: E-SITE tRNA

Chain AW:



- Molecule 23: E-SITE tRNA

Chain CW:

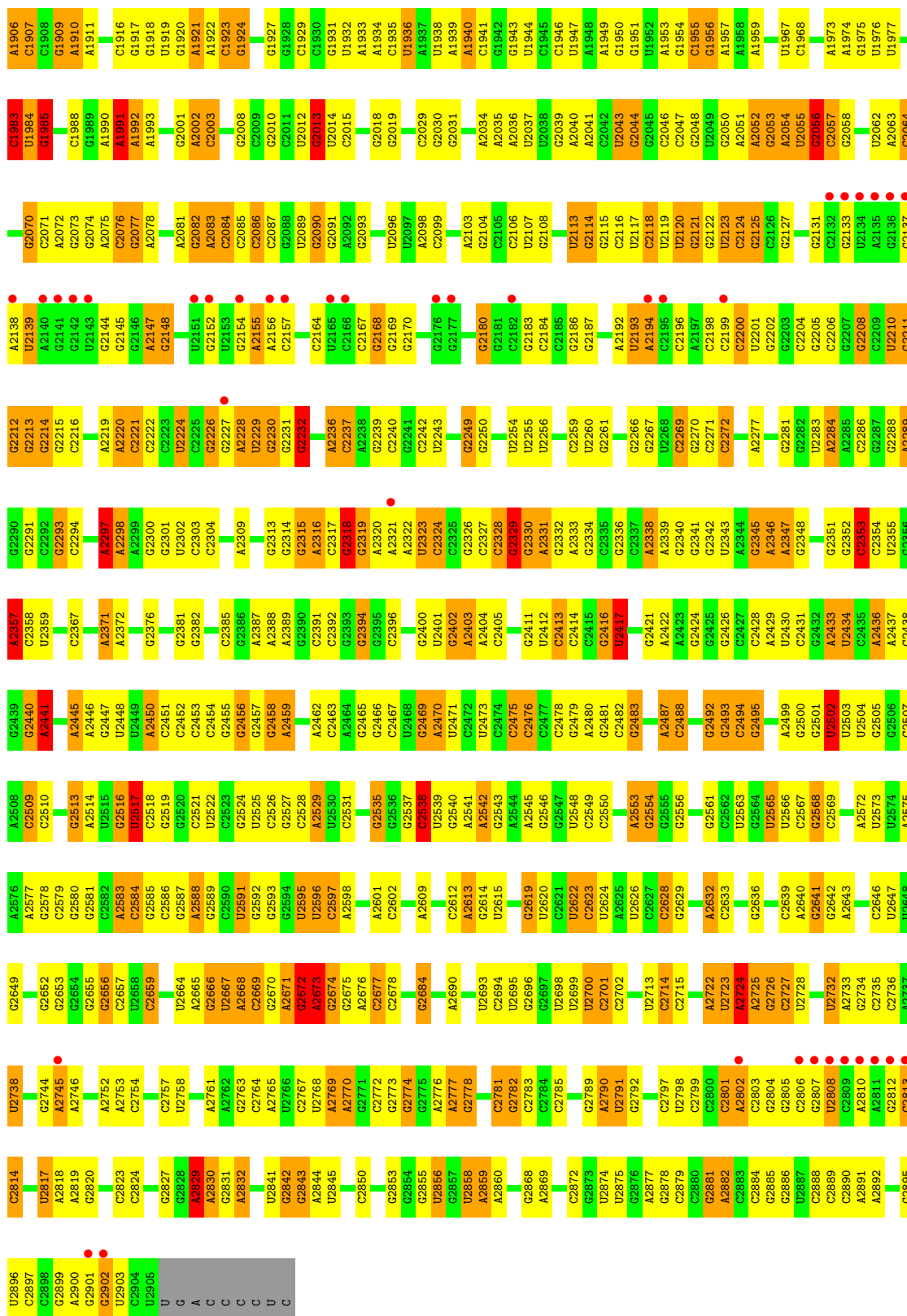


- Molecule 24: A-SITE tRNA

Chain AY:



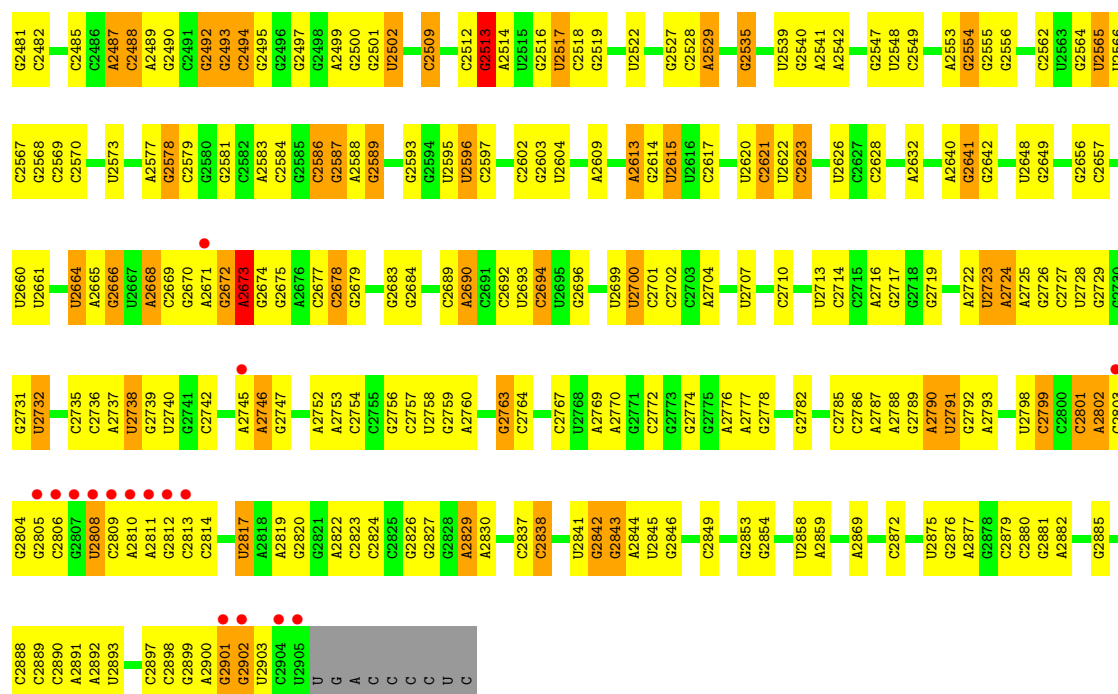
U1828	G1741	U1847	G1570	A1404	A1320	A1248	G1167	G	C1037	A955	A875	C799	G712	G647
G1829	G1742	A1843	A1574	A1405	A1323	U1249	G1170	U	G1038	A956	G876	C800	U713	C648
C1830	G1743	C1849	G1575	G1406	G1324	C1252	A1171	U	C1039	G877	G877	C801	G714	G649
G1831	A1744	C1850	C1497	G1576	G1325	C1253	A1172	U	C1040	C960	G878	C802	G715	U650
A1832	G1745	G1851	C1577	A1410	G1326	A1254	A1173	C	A1041	C961	U879	G806	G716	A651
A1833	A1746	A1499	C1578	A1412	U1329	U1255	A1174	U	U1044	A962	C880	G807	G717	G652
A1839	G1747	U1500	C1578	G1413	A1330	G1256	U1175	U	A1045	U967	U885	U808	C718	G653
A1842	G1748	A1854	G1579	G1414	G1331	G1257	U1176	A	A1046	C968	C886	G809	C719	G654
G1843	G1749	C1855	U	C1415	A1332	C1261	A1177	G	G1047	C969	C887	A810	G720	A655
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G1845	U1764	C1857	C	G1505	G1421	A1264	C1179	A	C1051	A971	U893	G814	G728	A661
G1846	C1858	A1861	G	A1506	G1422	C1265	G1180	G	C1052	U894	U894	U894	C729	G662
G1847	A1766	A1863	G	A1423	U1337	G1266	G1181	C	C1053	G973	C894	G817	C730	U663
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G1852	C1771	A1868	A1517	G1430	U1346	A1271	U1186	A	U1057	G978	U904	G822	C735	C669
G1853	C1772	C1869	A1518	C1431	A1347	G1272	A1187	U	C1058	G979	U905	G823	C736	A670
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G1856	G1775	A1872	A1521	U1438	C1352	G1280	C1197	C	U1061	A982	U908	G826	A746	G673
G1857	G1776	G1873	G1522	A1440	A1353	G1281	C1198	U	A1062	A983	A907	A827	G747	C674
G1858	G1777	C1874	G1523	U1441	G1354	A1282	C1199	A	A1063	U987	U909	A828	G748	G675
G1859	A1778	C1875	G1524	U1442	G1355	G1283	G1200	C	G1064	G988	U910	A829	G749	C676
A1860	G1779	G1876	G1525	C1443	U1356	G1284	A1201	A	U1065	A989	A911	G831	G750	A
A1861	G1780	C1877	U1526	C1444	U1357	G1285	U1202	G	U1066	G990	A912	C832	A751	A
A1862	G1781	C1878	G1527	C1445	U1358	A1286	G1203	A	G1067	G991	A913	U833	A752	G
G1863	C1782	C1879	G1528	C1446	U1359	A1287	C1204	U	G1068	G992	A914	A834	G753	G
G1864	U1783	A1880	G1529	C1447	C1360	U1288	U1205	C	U1069	G993	U915	A835	C754	C
G1865	G1784	C1881	G1530	U1448	U1361	U1289	U1206	A	U1070	G994	U916	A836	U755	G
G1866	A1785	C1882	G1531	C1449	C1362	G1290	G1207	U	A1071	G995	U917	C837	G756	G
G1867	G1786	U1883	A1532	U1450	G1363	A1291	G1208	C	A1072	G996	U918	U923	U757	G
G1868	G1787	A1884	A1533	U1451	G1364	A1292	U1209	U	A1073	G997	U919	A924	G758	G
G1869	G1788	C1885	G1534	U1452	G1365	G1293	U1210	C	U1074	G998	A920	G925	G759	C
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G1871	G1790	G1887	A1536	U1454	U1367	U1295	G1212	A	U1076	G999	A922	G927	C761	G
G1872	A1791	C1888	G1537	U1455	U1368	G1296	G1213	C	U1077	G999	A923	G928	A762	G
G1873	C1792	C1889	C1538	G1456	A1369	U1297	U1214	U	U1078	G999	U924	C941	C763	C
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G1876	C1795	C1892	G1541	U1459	C1372	U1300	G1217	U	G1081	G999	U927	C943	G766	G
G1877	A1796	C1893	C1542	U1460	A1373	U1301	A1218	A	C1082	G999	U928	C944	G767	C
G1878	G1797	C1894	G1543	U1461	G1374	G1302	U1219	G	G1083	G999	U929	U940	A768	G
G1879	U1798	C1895	C1544	C1462	A1375	C1303	U1220	C	U1084	G999	U930	U941	C769	G
G1880	C1799	C1896	G1545	U1463	G1376	U1304	G1221	U	G1085	G999	U931	U942	C770	C
G1881	G1800	C1897	C1546	U1464	U1377	G1305	G1222	C	C1086	G999	U932	C943	G771	A
G1882	G1801	C1898	U1547	U1465	G1378	C1306	C1223	A	G1087	G999	U933	U944	G772	C
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G1893	G1812	C1909	C1558	U1476	G1389	U1317	G1234	A	A1098	G999	U944	U955	C783	C
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G1896	G1815	C1912	C1561	U1479	G1392	U1320	G1237	C	G1101	G999	U947	U958	C786	C
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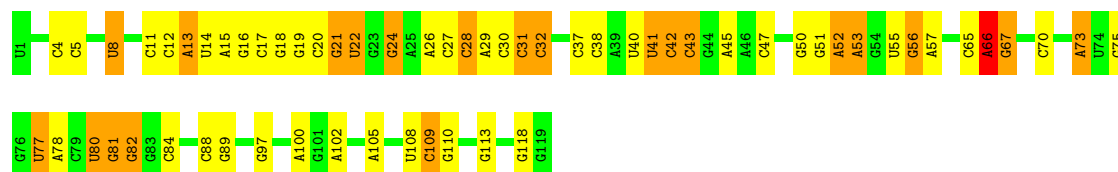
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G2174	G2175	G2176	G2177	G2178	A2179	G2180	G2181	G2182	G2183	G2184	G2189	A2190	A2191	U2192	A2193	U2194	U2195	G2196	G2197	G2198	G2199	G2200	U2201	G2202	G2203	C2206	C2207	G2208	C2209	G2210	G2211	C2212	G2213	G2214	G2215	G2216	U2217	U2218	A2219	C2220	C2221	C2222	C2223	C2224	C2225	G2226	C2227	A2228	U2229	G2230	G2231	G2232	G2233	G2234	G2235	G2236	G2237																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
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G2018	G2019	G2020	G2021	C2027	C2028	G2029	G2030	G2031	G2032	G2033	A2034	A2035	U2037	A2041	G2042	U2043	G2044	C2047	G2048	A2052	G2053	A2054	U2055	G2056	C2057	G2058	G2059	C2060	C2061	U2062	A2063	C2064	C2071	A2072	G2076	G2077	A2078	G2079	A2080	A2081	G2082	A2083	C2084	C2085	C2086	C2087	G2088	U2089	U2090	G2091	C2094																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U1936	A1937	G1943	G1944	G1945	G1946	G1947	G1948	G1949	G1950	G1951	C1955	G1956	A1957	G1958	A1959	U1960	U1961	C1962	C1963	U1967	G1968	A1973	A1974	G1975	U1976	C1983	U1984	G1985	C1986	A1987	G1988	G1989	C1990	C1991	A1905	G1906	C1907	C1908	C1909	A1910	A1911	A1912	C1913	G1914	C1915	A1916	G1917	G1920	A1921	C1922	C1923	G1927	U1950	G1958	C1959	A1961	C1962	C1963	G1965	U1966	U1967	G1968	A1969	C1970	C1971	C1972	C1973	G1974	G1975	G1976	G1977	G1978	C1979	C1980	C1981	C1982	C1983	C1984	C1985	C1986	C1987	C1988	C1989	C1990	C1991	C1992	C1993	C1994	C1995	C1996	C1997	C1998	C1999	C2000	C2001	C2002	C2003	C2004	C2005	C2006	C2007	C2008	C2009	C2010	C2011	C2012	C2013	C2014	C2015	C2016	C2017	C2018	C2019	C2020	C2021	C2022	C2023	C2024	C2025	C2026	C2027	C2028	C2029	C2030	C2031	C2032	C2033	C2034	C2035	C2036	C2037	C2038	C2039	C2040	C2041	C2042	C2043	C2044	C2045	C2046	C2047	C2048	C2049	C2050	C2051	C2052	C2053	C2054	C2055	C2056	C2057	C2058	C2059	C2060	C2061	C2062	C2063	C2064	C2065	C2066	C2067	C2068	C2069	C2070	C2071	C2072	C2073	C2074	C2075	C2076	C2077	C2078	C2079	C2080	C2081	C2082	C2083	C2084	C2085	C2086	C2087	C2088	C2089	C2090	C2091	C2092	C2093	C2094	C2095	C2096	C2097	C2098	C2099	C2100	C2101	C2102	C2103	C2104	C2105	C2106	C2107	C2108	C2109	C2110	C2111	C2112	C2113	C2114	C2115	C2116	C2117	C2118	C2119	C2120	C2121	C2122	C2123	C2124	C2125	C2126	C2127	C2128	C2129	C2130	C2131	C2132	C2133	C2134	C2135	C2136	C2137	C2138	C2139	C2140	C2141	C2142	C2143	C2144	C2145	C2146	C2147	C2148	C2149	C2150	C2151	C2152	C2153	C2154	C2155	C2156	C2157	C2158	C2159	C2160	C2161	C2162	C2163	C2164	C2165	C2166	C2167	C2168	C2169	C2170	C2171	C2172	C2173	C2174	C2175	C2176	C2177	C2178	C2179	C2180	C2181	C2182	C2183	C2184	C2185	C2186	C2187	C2188	C2189	C2190	C2191	C2192	C2193	C2194	C2195	C2196	C2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	C2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	C2366	C2367	C2368	C2369	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389	C2390	C2391	C2392	C2393	C2394	C2395	C2396	C2397	C2398	C2399	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	C2446	C2447	C2448	C2449	C2450	C2451	C2452	C2453	C2454	C2455	C2456	C2457	C2458	C2459	C2460	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	C2479	C2480	C2481	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550	C2551	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625	C2626	C2627	C2628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	C2712	C2713	C2714	C2715	C2716	C2717	C2718	C2719	C2720	C2721	C2722	C2723	C2724	C2725	C2726	C2727	C2728	C2729	C2730	C2731	C2732	C2733	C2734	C2735	C2736	C2737	C2738	C2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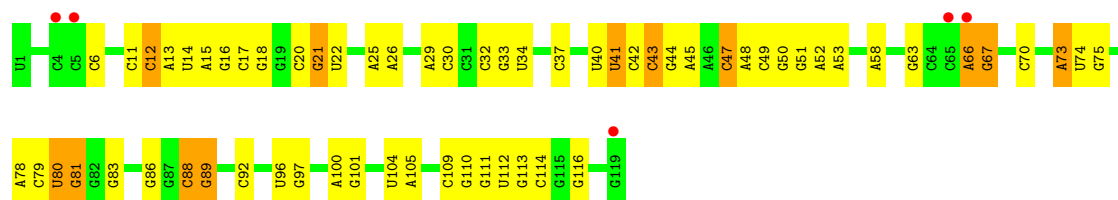
• Molecule 27: 5S ribosomal RNA

Chain BB:



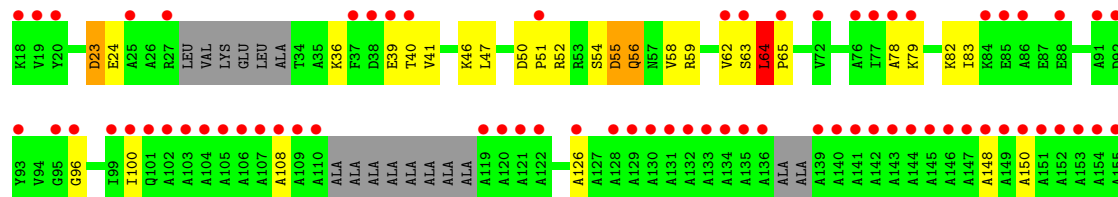
• Molecule 27: 5S ribosomal RNA

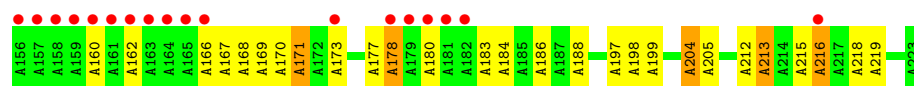
Chain DB:



• Molecule 28: 50S ribosomal protein L1

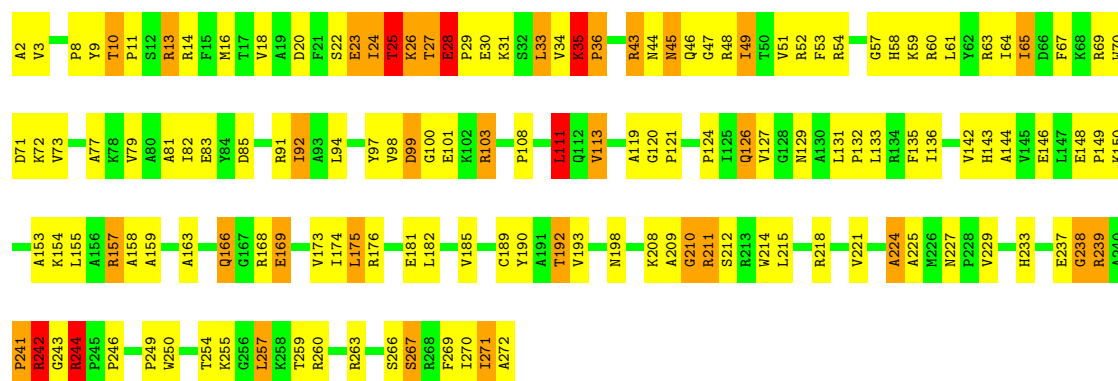
Chain BC:





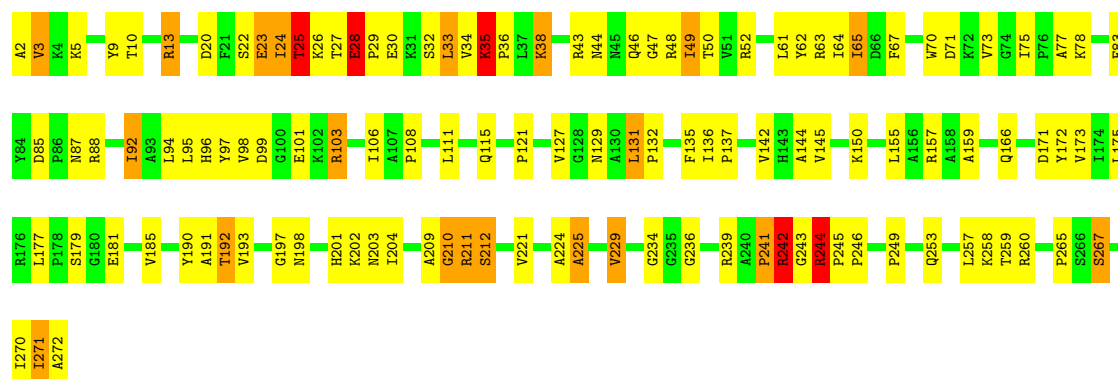
• Molecule 29: 50S ribosomal protein L2

Chain BD:



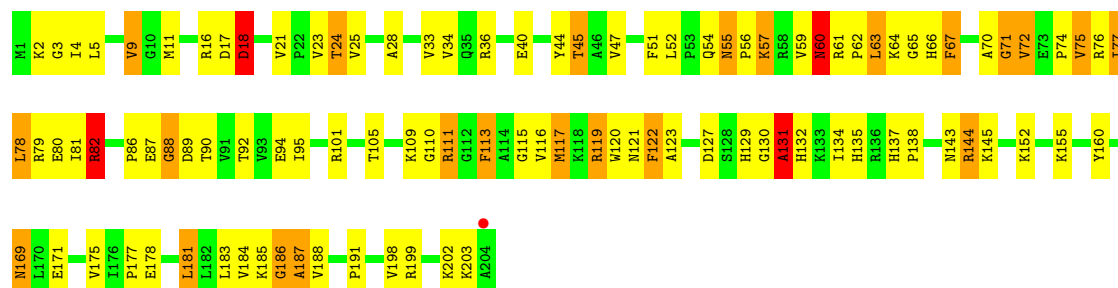
• Molecule 29: 50S ribosomal protein L2

Chain DD:



• Molecule 30: 50S ribosomal protein L3

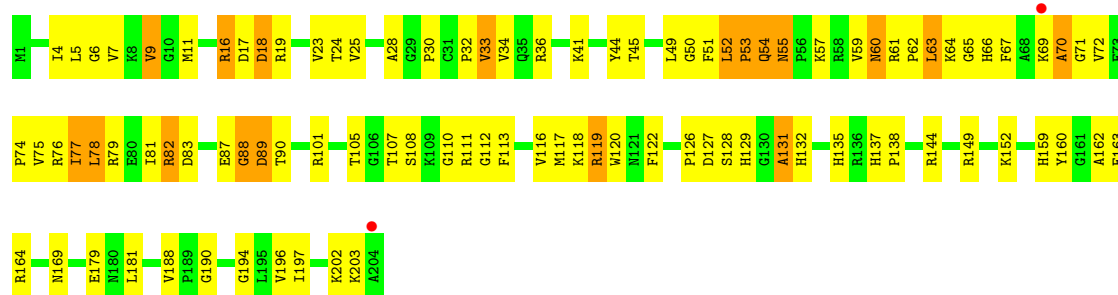
Chain BE:



• Molecule 30: 50S ribosomal protein L3

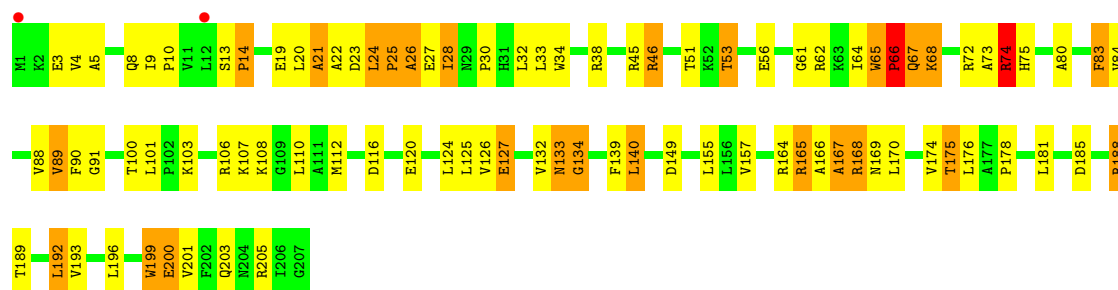
Chain DE:





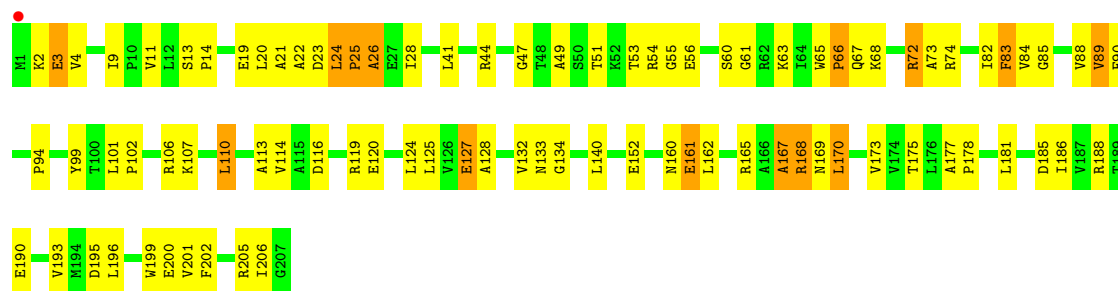
- Molecule 31: 50S ribosomal protein L4

Chain BF:



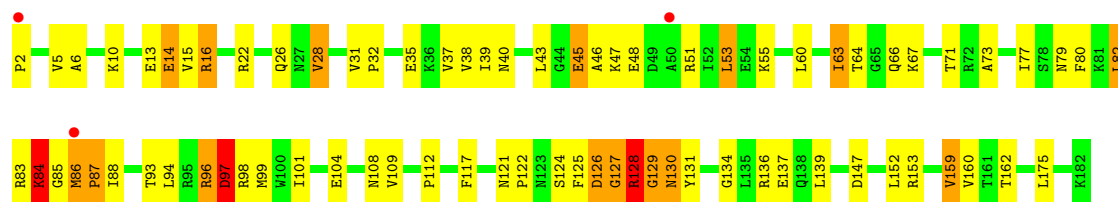
- Molecule 31: 50S ribosomal protein L4

Chain DF:



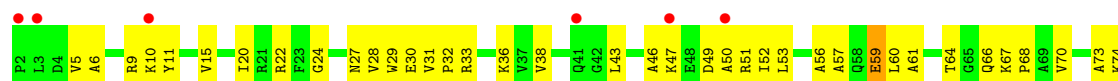
- Molecule 32: 50S ribosomal protein L5

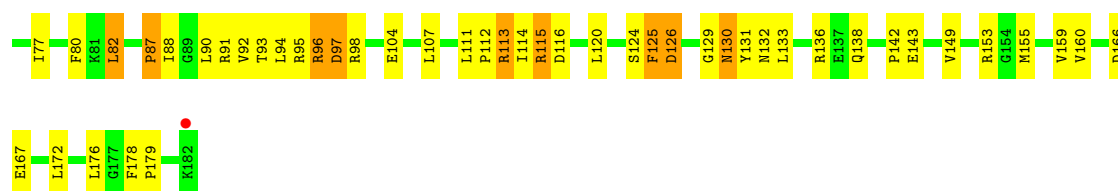
Chain BG:



- Molecule 32: 50S ribosomal protein L5

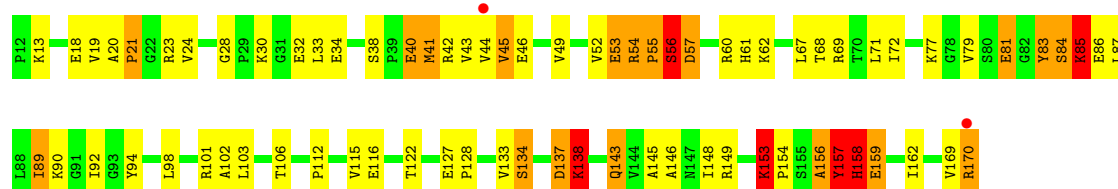
Chain DG:





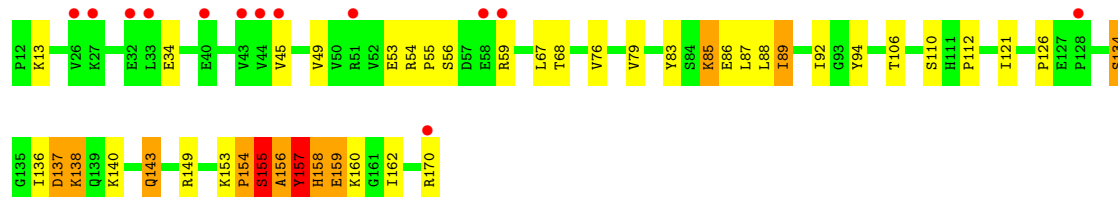
- Molecule 33: 50S ribosomal protein L6

Chain BH:



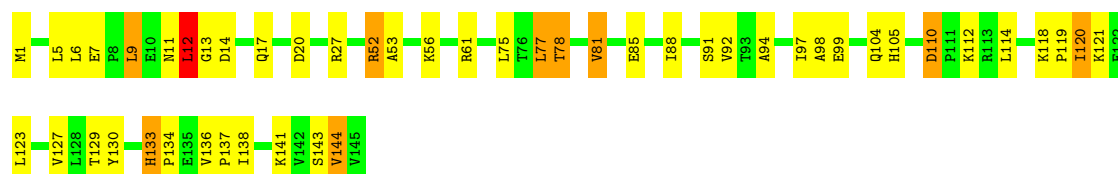
- Molecule 33: 50S ribosomal protein L6

Chain DH:



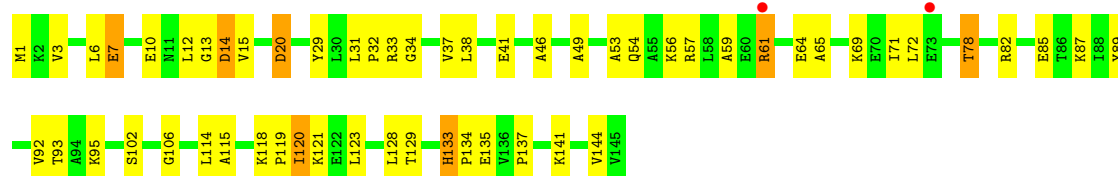
- Molecule 34: 50S ribosomal protein L9

Chain BI:



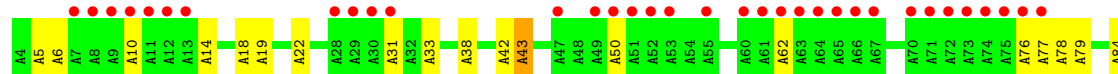
- Molecule 34: 50S ribosomal protein L9

Chain DI:



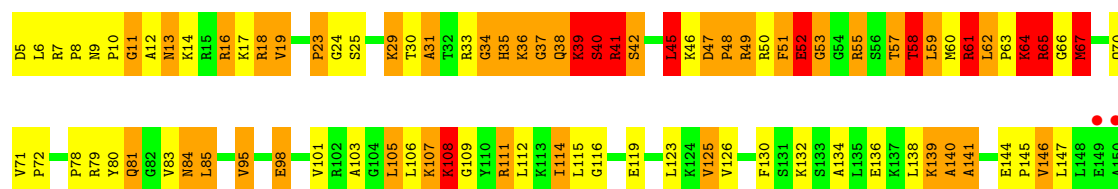
- Molecule 35: 50S ribosomal protein L10

Chain BJ:



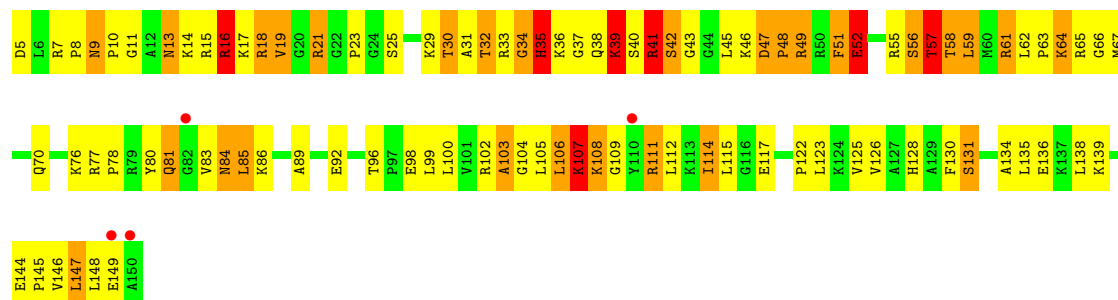


Chain BP:



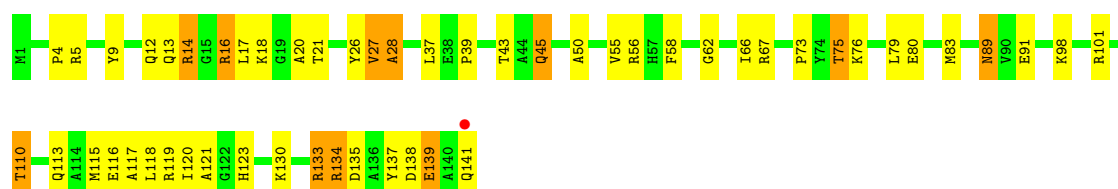
- Molecule 38: 50S ribosomal protein L15

Chain DP:



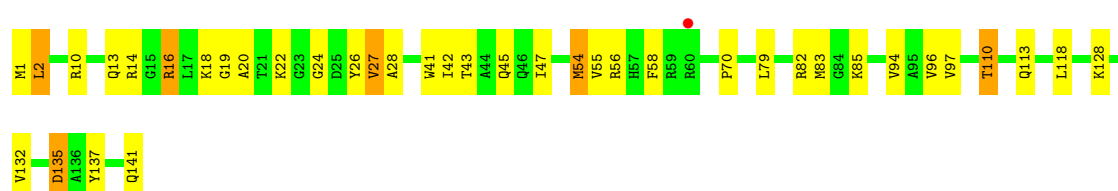
- Molecule 39: 50S ribosomal protein L16

Chain BQ:



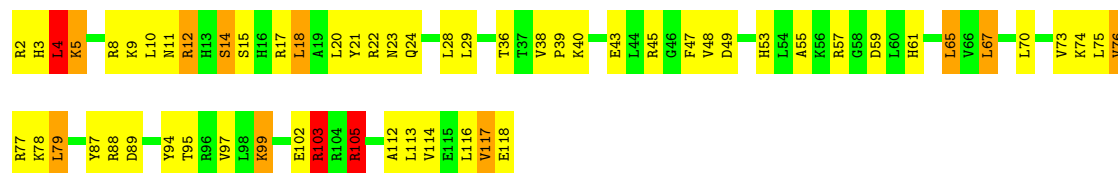
- Molecule 39: 50S ribosomal protein L16

Chain DQ:



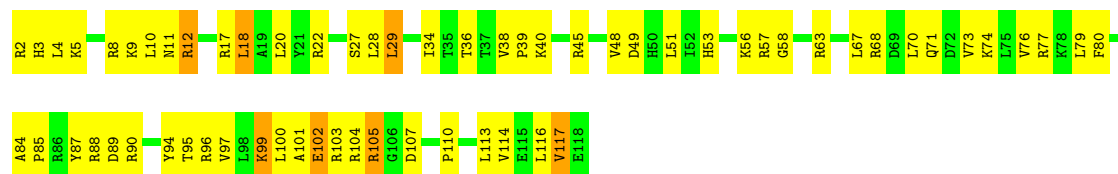
- Molecule 40: 50S ribosomal protein L17

Chain BR:



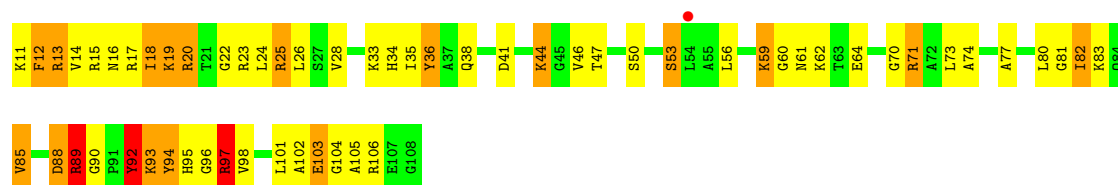
- Molecule 40: 50S ribosomal protein L17

Chain DR:



- Molecule 41: 50S ribosomal protein L18

Chain BS:



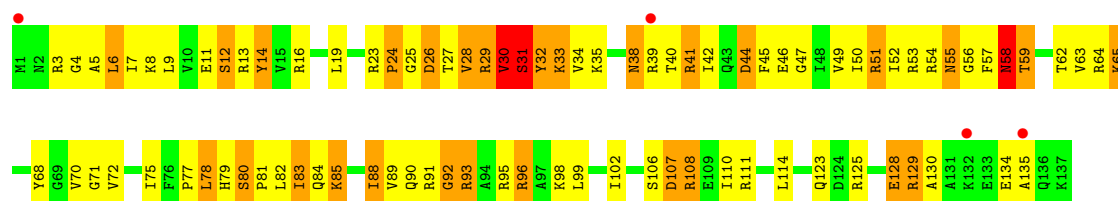
- Molecule 41: 50S ribosomal protein L18

Chain DS:



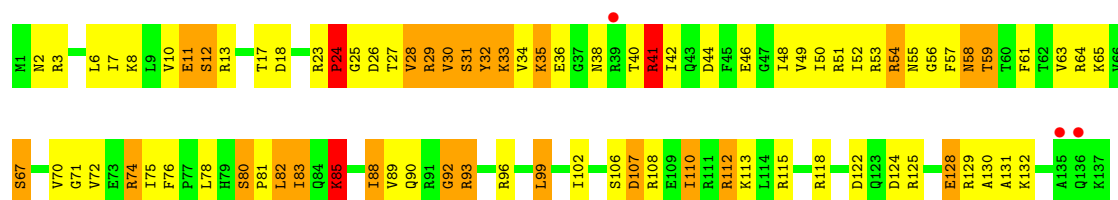
- Molecule 42: 50S ribosomal protein L19

Chain BT:



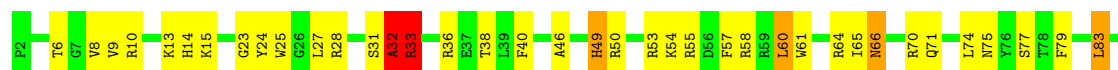
- Molecule 42: 50S ribosomal protein L19

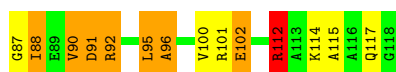
Chain DT:



- Molecule 43: 50S ribosomal protein L20

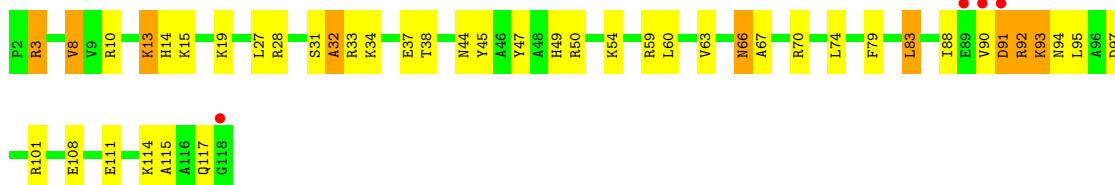
Chain BU:





- Molecule 43: 50S ribosomal protein L20

Chain DU:



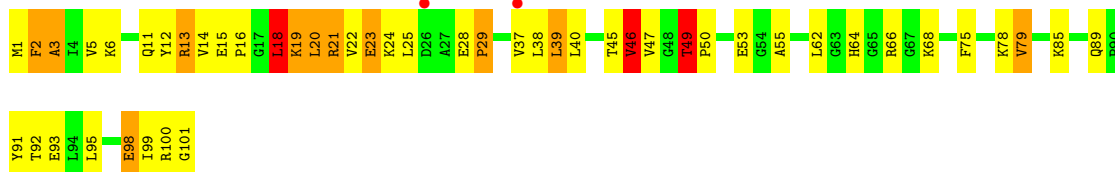
- Molecule 44: 50S ribosomal protein L21

Chain BV:



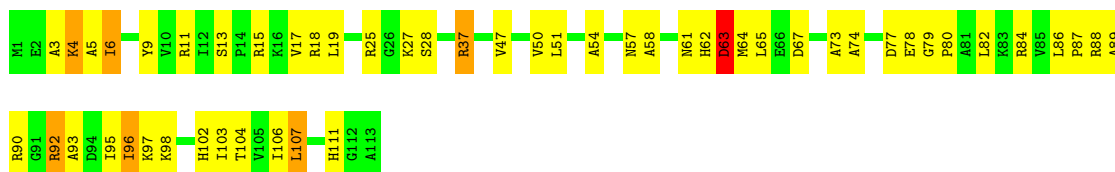
- Molecule 44: 50S ribosomal protein L21

Chain DV:



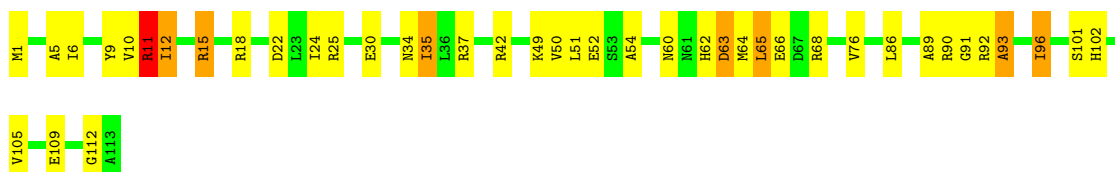
- Molecule 45: 50S ribosomal protein L22

Chain BW:



- Molecule 45: 50S ribosomal protein L22

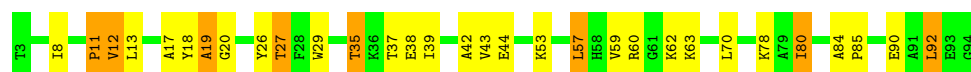
Chain DW:



- Molecule 46: 50S ribosomal protein L23

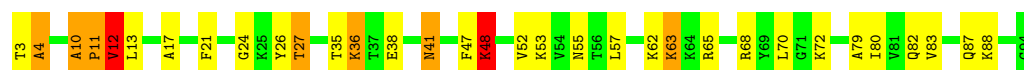


Chain BX:



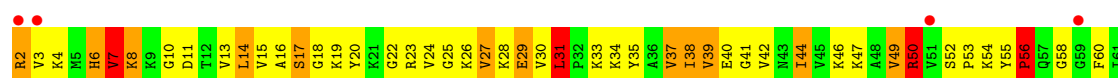
- Molecule 46: 50S ribosomal protein L23

Chain DX:



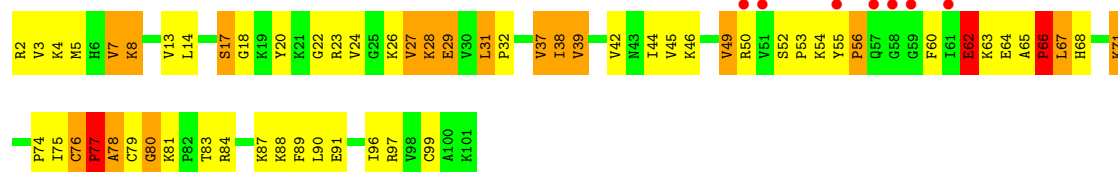
- Molecule 47: 50S ribosomal protein L24

Chain BY:



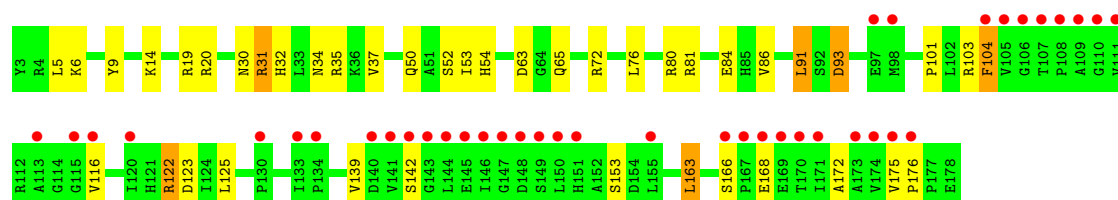
- Molecule 47: 50S ribosomal protein L24

Chain DY:



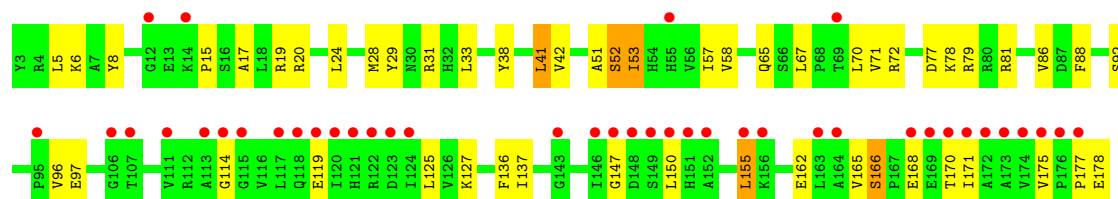
- Molecule 48: 50S ribosomal protein L25

Chain BZ:



- Molecule 48: 50S ribosomal protein L25

Chain DZ:



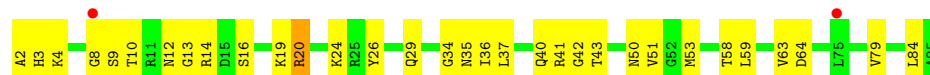
- Molecule 49: 50S ribosomal protein L27

Chain B0: 



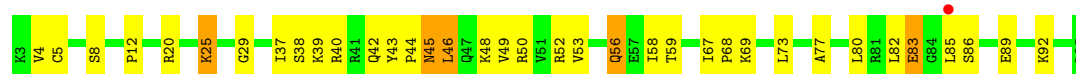
- Molecule 49: 50S ribosomal protein L27

Chain D0: 



- Molecule 50: 50S ribosomal protein L28

Chain B1: 



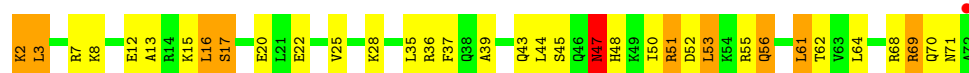
- Molecule 50: 50S ribosomal protein L28

Chain D1: 



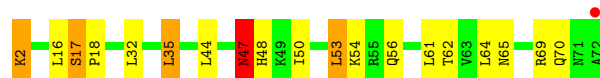
- Molecule 51: 50S ribosomal protein L29

Chain B2: 



- Molecule 51: 50S ribosomal protein L29

Chain D2: 



- Molecule 52: 50S ribosomal protein L30

Chain B3: 



- Molecule 52: 50S ribosomal protein L30

Chain D3: 



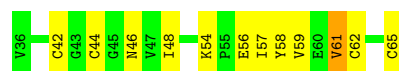
- Molecule 53: 50S ribosomal protein L31

Chain B4: 



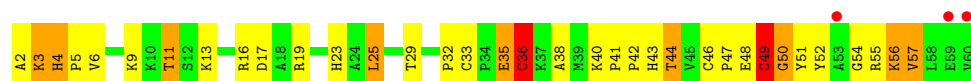
- Molecule 53: 50S ribosomal protein L31

Chain D4: 



- Molecule 54: 50S ribosomal protein L32

Chain B5: 



- Molecule 54: 50S ribosomal protein L32

Chain D5: 



- Molecule 55: 50S ribosomal protein L33

Chain B6: 



- Molecule 55: 50S ribosomal protein L33

Chain D6: 



- Molecule 56: 50S ribosomal protein L34

Chain B7: 



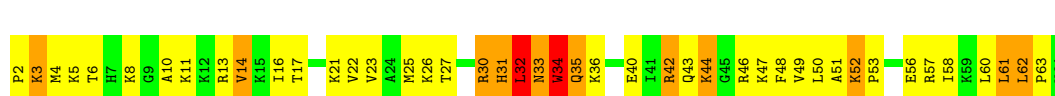
- Molecule 56: 50S ribosomal protein L34

Chain D7: 



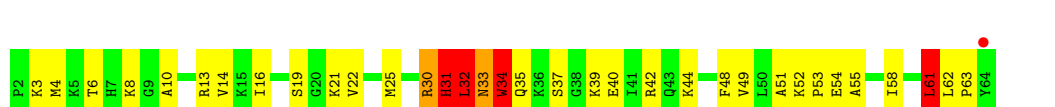
- Molecule 57: 50S ribosomal protein L35

Chain B8:



- Molecule 57: 50S ribosomal protein L35

Chain D8:



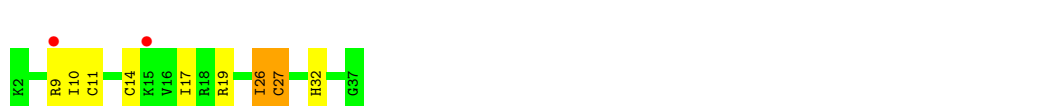
- Molecule 58: 50S ribosomal protein L36

Chain B9:



- Molecule 58: 50S ribosomal protein L36

Chain D9:



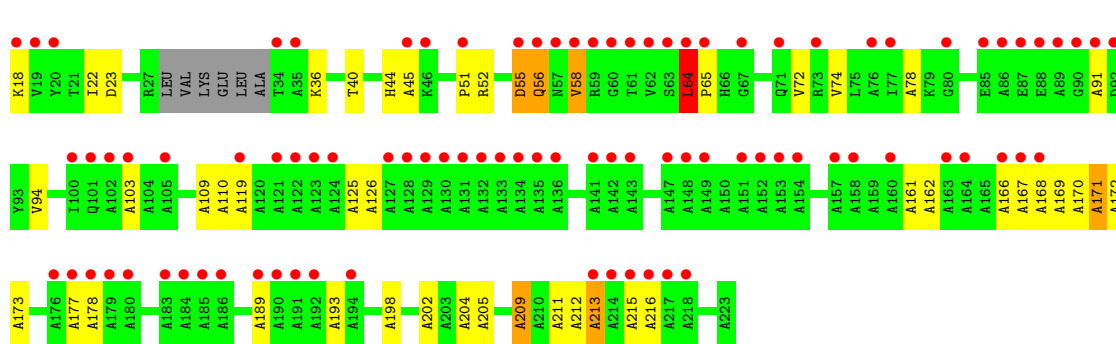
- Molecule 59: mRNA

Chain CX:



- Molecule 60: 50S Ribosomal protein L1

Chain DC:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.92Å 449.90Å 624.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.57 – 3.30 39.57 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.6 (39.57-3.30) 95.6 (39.57-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.8.0031	Depositor
R, $R_{free}$	0.225 , 0.279 0.230 , 0.279	Depositor DCC
$R_{free}$ test set	41956 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	63.7	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 839115 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	295724	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: PSU

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	0.42	4/36190 (0.0%)	0.75	26/56486 (0.0%)
1	CA	0.40	1/36190 (0.0%)	0.73	17/56486 (0.0%)
2	AB	0.43	0/1936	0.67	0/2609
2	CB	0.44	0/1936	0.64	0/2609
3	AC	0.49	0/1637	0.71	0/2205
3	CC	0.44	0/1637	0.67	0/2205
4	AD	0.54	0/1733	0.84	4/2318 (0.2%)
4	CD	0.52	0/1733	0.77	1/2318 (0.0%)
5	AE	0.45	0/1163	0.76	0/1564
5	CE	0.46	0/1163	0.72	0/1564
6	AF	0.49	0/856	0.77	1/1154 (0.1%)
6	CF	0.48	0/856	0.75	0/1154
7	AG	0.43	0/1276	0.65	0/1709
7	CG	0.40	0/1276	0.64	0/1709
8	AH	0.47	0/1136	0.72	0/1527
8	CH	0.45	0/1136	0.69	0/1527
9	AI	0.48	0/1029	0.71	0/1378
9	CI	0.42	0/1029	0.68	0/1378
10	AJ	0.47	0/808	0.76	0/1085
10	CJ	0.46	0/808	0.68	0/1085
11	AK	0.49	0/900	0.71	0/1213
11	CK	0.45	0/900	0.70	0/1213
12	AL	0.55	0/987	0.81	0/1320
12	CL	0.50	0/987	0.77	0/1320
13	AM	0.45	0/999	0.78	0/1336
13	CM	0.43	0/999	0.68	0/1336
14	AN	0.50	0/501	0.88	1/664 (0.2%)
14	CN	0.46	0/501	0.74	0/664
15	AO	0.46	0/745	0.70	0/992
15	CO	0.40	0/745	0.64	0/992
16	AP	0.47	0/717	0.74	0/963
16	CP	0.50	0/717	0.78	1/963 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.44	0/837	0.70	0/1117
17	CQ	0.46	0/837	0.72	0/1117
18	AR	0.47	0/579	0.79	0/768
18	CR	0.47	0/579	0.69	0/768
19	AS	0.47	0/643	0.68	0/865
19	CS	0.43	0/643	0.61	0/865
20	AT	0.45	0/765	0.70	0/1007
20	CT	0.43	0/765	0.71	0/1007
21	AU	0.52	0/213	0.71	0/277
21	CU	0.53	0/213	0.68	0/277
22	AV	0.40	0/1832	0.75	1/2855 (0.0%)
22	CV	0.38	0/1832	0.72	0/2855
23	AW	0.29	0/1809	0.68	2/2819 (0.1%)
23	CW	0.27	0/1809	0.70	1/2819 (0.0%)
24	AY	0.86	17/1815 (0.9%)	0.94	1/2833 (0.0%)
24	CY	0.86	17/1815 (0.9%)	0.94	1/2833 (0.0%)
25	AX	0.31	0/147	0.72	0/227
26	BA	0.57	22/67709 (0.0%)	0.91	196/105690 (0.2%)
26	DA	0.45	5/67709 (0.0%)	0.80	93/105690 (0.1%)
27	BB	0.45	0/2853	0.81	3/4451 (0.1%)
27	DB	0.35	0/2853	0.72	0/4451
28	BC	0.46	0/1160	0.59	0/1584
29	BD	0.71	0/2155	0.95	1/2905 (0.0%)
29	DD	0.60	0/2155	0.85	0/2905
30	BE	0.70	1/1597 (0.1%)	0.91	1/2153 (0.0%)
30	DE	0.56	1/1597 (0.1%)	0.83	2/2153 (0.1%)
31	BF	0.68	0/1659	0.88	1/2244 (0.0%)
31	DF	0.52	0/1659	0.75	0/2244
32	BG	0.49	0/1499	0.74	0/2016
32	DG	0.44	0/1499	0.67	0/2016
33	BH	0.64	1/1246 (0.1%)	0.88	2/1682 (0.1%)
33	DH	0.47	0/1246	0.67	1/1682 (0.1%)
34	BI	0.48	0/1147	0.75	1/1551 (0.1%)
34	DI	0.47	0/1147	0.72	0/1551
35	BJ	0.51	0/650	0.55	0/907
35	DJ	0.44	0/650	0.53	0/907
36	BN	0.70	0/1132	0.96	0/1525
36	DN	0.49	0/1132	0.77	0/1525
37	BO	0.57	0/943	0.81	0/1269
37	DO	0.53	0/943	0.78	0/1269
38	BP	0.71	0/1131	1.09	3/1504 (0.2%)
38	DP	0.57	0/1131	0.98	2/1504 (0.1%)
39	BQ	0.58	0/1143	0.85	1/1527 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DQ	0.46	0/1143	0.68	0/1527
40	BR	0.70	0/974	0.98	1/1302 (0.1%)
40	DR	0.54	0/974	0.87	0/1302
41	BS	0.60	0/779	0.98	0/1036
41	DS	0.48	0/779	0.79	0/1036
42	BT	0.59	0/1156	0.97	1/1542 (0.1%)
42	DT	0.58	0/1156	0.95	0/1542
43	BU	0.76	0/975	0.98	1/1297 (0.1%)
43	DU	0.50	0/975	0.75	0/1297
44	BV	0.69	0/790	1.03	4/1057 (0.4%)
44	DV	0.47	0/790	0.76	0/1057
45	BW	0.65	0/907	0.95	1/1216 (0.1%)
45	DW	0.52	0/907	0.77	0/1216
46	BX	0.67	0/740	0.94	1/993 (0.1%)
46	DX	0.52	0/740	0.74	0/993
47	BY	0.68	0/789	0.99	3/1051 (0.3%)
47	DY	0.53	0/789	0.83	0/1051
48	BZ	0.49	0/1436	0.72	0/1949
48	DZ	0.44	0/1436	0.66	0/1949
49	B0	0.61	0/671	0.85	0/892
49	D0	0.51	0/671	0.76	0/892
50	B1	0.62	0/741	0.84	0/984
50	D1	0.53	0/741	0.84	1/984 (0.1%)
51	B2	0.57	0/600	0.86	0/793
51	D2	0.48	0/600	0.79	0/793
52	B3	0.55	0/473	0.87	0/634
52	D3	0.44	0/473	0.70	0/634
53	B4	0.53	0/229	0.79	0/309
53	D4	0.49	0/229	0.75	0/309
54	B5	0.73	0/473	1.08	0/639
54	D5	0.57	0/473	0.88	0/639
55	B6	0.96	1/388 (0.3%)	2.06	4/518 (0.8%)
55	D6	0.83	0/388	1.06	2/518 (0.4%)
56	B7	0.73	0/427	0.96	0/561
56	D7	0.58	0/427	0.85	0/561
57	B8	0.75	0/516	1.12	2/679 (0.3%)
57	D8	0.54	0/516	0.88	1/679 (0.1%)
58	B9	0.69	0/302	1.00	2/397 (0.5%)
58	D9	0.45	0/302	0.73	0/397
59	CX	0.52	0/94	0.72	0/144
60	DC	0.48	0/1160	0.55	0/1584
All	All	0.50	70/321233 (0.0%)	0.81	388/480213 (0.1%)



Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	0
1	CA	1	0
2	AB	0	1
13	AM	0	1
13	CM	0	1
23	AW	1	0
23	CW	1	0
26	BA	22	0
26	DA	20	0
29	BD	0	3
29	DD	0	2
30	BE	0	2
30	DE	0	1
33	BH	0	1
38	BP	0	10
38	DP	0	4
40	BR	0	2
40	DR	0	1
41	BS	0	1
42	BT	0	3
43	BU	0	3
44	BV	0	2
47	BY	0	1
55	B6	0	1
55	D6	0	1
57	B8	0	1
All	All	46	42

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	B6	47	THR	C-N	8.32	1.53	1.34
24	AY	50	G	C1'-N9	-6.96	1.37	1.46
24	CY	50	G	C1'-N9	-6.95	1.37	1.46
26	BA	1816	A	O3'-P	6.86	1.69	1.61
24	CY	66	G	C1'-N9	-6.73	1.37	1.46

The worst 5 of 388 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	B6	45	LYS	O-C-N	-30.98	73.14	122.70
55	B6	45	LYS	CA-C-N	22.24	166.13	117.20
26	BA	2513	G	O5'-P-OP1	-13.46	93.59	105.70
26	BA	1850	U	O5'-P-OP1	-12.67	94.30	105.70
26	BA	1955	C	C2'-C3'-O3'	12.16	136.24	109.50

5 of 46 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	412	A	C1'
23	AW	47	U	C1'
26	BA	98	G	C1'
26	BA	497	A	C3'
26	BA	715	G	C4',C3',C1'

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	AB	23	ARG	Peptide
13	AM	69	GLU	Peptide
29	BD	224	ALA	Peptide
29	BD	244	ARG	Peptide
29	BD	36	PRO	Peptide

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	494	1
1	CA	32329	0	16318	469	0
2	AB	1901	0	1951	42	0
2	CB	1901	0	1951	43	0
3	AC	1613	0	1677	43	0
3	CC	1613	0	1677	46	0
4	AD	1703	0	1763	64	0
4	CD	1703	0	1763	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	AE	1147	0	1207	44	0
5	CE	1147	0	1207	35	0
6	AF	843	0	857	14	0
6	CF	843	0	857	18	0
7	AG	1257	0	1296	20	0
7	CG	1257	0	1296	12	0
8	AH	1116	0	1177	28	0
8	CH	1116	0	1177	17	0
9	AI	1011	0	1043	31	0
9	CI	1011	0	1043	27	0
10	AJ	795	0	840	36	0
10	CJ	795	0	840	36	0
11	AK	885	0	904	31	0
11	CK	885	0	904	17	0
12	AL	971	0	1057	16	0
12	CL	971	0	1057	19	0
13	AM	988	0	1059	35	0
13	CM	988	0	1059	26	0
14	AN	492	0	529	14	0
14	CN	492	0	529	21	0
15	AO	734	0	771	17	0
15	CO	734	0	771	21	0
16	AP	701	0	720	22	0
16	CP	701	0	720	17	0
17	AQ	824	0	891	23	0
17	CQ	824	0	891	13	0
18	AR	574	0	644	16	0
18	CR	574	0	644	16	0
19	AS	630	0	652	30	0
19	CS	630	0	652	12	0
20	AT	763	0	861	26	0
20	CT	763	0	861	14	0
21	AU	209	0	221	4	0
21	CU	209	0	221	3	0
22	AV	1640	0	837	29	0
22	CV	1640	0	837	27	0
23	AW	1619	0	822	58	0
23	CW	1619	0	822	21	0
24	AY	1619	0	792	222	0
24	CY	1619	0	792	241	0
25	AX	151	0	76	15	0
26	BA	60459	0	30488	1163	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	DA	60459	0	30487	1024	0
27	BB	2551	0	1295	38	0
27	DB	2551	0	1295	35	0
28	BC	1157	0	1160	27	0
29	BD	2105	0	2182	126	0
29	DD	2105	0	2182	89	0
30	BE	1564	0	1629	97	0
30	DE	1564	0	1629	66	0
31	BF	1624	0	1677	72	0
31	DF	1624	0	1677	63	0
32	BG	1474	0	1535	53	0
32	DG	1474	0	1535	49	0
33	BH	1223	0	1282	48	0
33	DH	1223	0	1282	22	0
34	BI	1132	0	1218	30	0
34	DI	1132	0	1218	29	1
35	BJ	651	0	649	10	0
35	DJ	651	0	649	14	0
36	BN	1105	0	1180	62	0
36	DN	1105	0	1180	42	0
37	BO	933	0	996	33	0
37	DO	933	0	996	30	0
38	BP	1114	0	1187	141	0
38	DP	1114	0	1187	82	0
39	BQ	1122	0	1179	35	0
39	DQ	1122	0	1179	31	0
40	BR	960	0	1021	47	0
40	DR	960	0	1021	46	0
41	BS	771	0	832	46	0
41	DS	771	0	832	33	0
42	BT	1142	0	1202	92	0
42	DT	1142	0	1202	72	0
43	BU	958	0	1018	57	0
43	DU	958	0	1018	52	0
44	BV	779	0	852	54	0
44	DV	779	0	852	39	0
45	BW	896	0	956	40	0
45	DW	896	0	956	23	0
46	BX	726	0	778	26	0
46	DX	726	0	778	20	0
47	BY	776	0	868	79	0
47	DY	776	0	870	45	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	BZ	1404	0	1432	20	0
48	DZ	1404	0	1432	34	0
49	B0	662	0	688	18	0
49	D0	662	0	688	20	0
50	B1	734	0	808	22	0
50	D1	734	0	808	21	0
51	B2	598	0	653	24	0
51	D2	598	0	653	13	0
52	B3	468	0	523	20	0
52	D3	468	0	523	12	0
53	B4	226	0	229	8	0
53	D4	226	0	229	4	0
54	B5	459	0	477	48	0
54	D5	459	0	478	21	0
55	B6	381	0	390	52	0
55	D6	381	0	391	30	0
56	B7	419	0	467	12	0
56	D7	419	0	467	15	0
57	B8	508	0	576	58	0
57	D8	508	0	576	33	0
58	B9	299	0	324	19	0
58	D9	299	0	324	7	0
59	CX	85	0	43	7	0
60	DC	1157	0	1160	22	0
All	All	295724	0	201402	6566	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

The worst 5 of 6566 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:AY:10:C:H41	24:AY:45:G:N2	1.03	1.51
24:CY:7:A:N1	24:CY:66:G:N2	1.61	1.48
24:AY:7:A:N1	24:AY:66:G:N2	1.61	1.46
24:CY:10:C:H41	24:CY:45:G:N2	1.03	1.46
24:CY:9:G:H21	24:CY:11:C:N4	1.02	1.45

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:358:U:OP1	34:DI:87:LYS:NZ[4_455]	2.03	0.17

## 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	
2	AB	232/234 (99%)	170 (73%)	51 (22%)	11 (5%)	4	30
2	CB	232/234 (99%)	181 (78%)	41 (18%)	10 (4%)	4	34
3	AC	204/206 (99%)	150 (74%)	40 (20%)	14 (7%)	2	17
3	CC	204/206 (99%)	159 (78%)	32 (16%)	13 (6%)	2	20
4	AD	206/208 (99%)	155 (75%)	37 (18%)	14 (7%)	2	18
4	CD	206/208 (99%)	160 (78%)	36 (18%)	10 (5%)	3	29
5	AE	148/150 (99%)	129 (87%)	15 (10%)	4 (3%)	8	49
5	CE	148/150 (99%)	130 (88%)	16 (11%)	2 (1%)	16	67
6	AF	99/101 (98%)	89 (90%)	7 (7%)	3 (3%)	7	46
6	CF	99/101 (98%)	88 (89%)	9 (9%)	2 (2%)	11	58
7	AG	153/155 (99%)	133 (87%)	18 (12%)	2 (1%)	18	69
7	CG	153/155 (99%)	130 (85%)	18 (12%)	5 (3%)	6	43
8	AH	136/138 (99%)	119 (88%)	14 (10%)	3 (2%)	10	55
8	CH	136/138 (99%)	115 (85%)	18 (13%)	3 (2%)	10	55
9	AI	125/127 (98%)	96 (77%)	25 (20%)	4 (3%)	6	43
9	CI	125/127 (98%)	101 (81%)	21 (17%)	3 (2%)	9	53
10	AJ	96/98 (98%)	76 (79%)	17 (18%)	3 (3%)	7	45
10	CJ	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	3	27
11	AK	117/119 (98%)	96 (82%)	19 (16%)	2 (2%)	14	62
11	CK	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	8	50
12	AL	122/124 (98%)	95 (78%)	18 (15%)	9 (7%)	2	15
12	CL	122/124 (98%)	95 (78%)	20 (16%)	7 (6%)	3	24
13	AM	122/124 (98%)	87 (71%)	23 (19%)	12 (10%)	1	8
13	CM	122/124 (98%)	90 (74%)	23 (19%)	9 (7%)	2	15
14	AN	58/60 (97%)	43 (74%)	11 (19%)	4 (7%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/60 (97%)	46 (79%)	8 (14%)	4 (7%)	2	17
15	AO	86/88 (98%)	62 (72%)	19 (22%)	5 (6%)	3	23
15	CO	86/88 (98%)	71 (83%)	10 (12%)	5 (6%)	3	23
16	AP	81/83 (98%)	68 (84%)	13 (16%)	0	100	100
16	CP	81/83 (98%)	64 (79%)	12 (15%)	5 (6%)	2	21
17	AQ	97/99 (98%)	85 (88%)	8 (8%)	4 (4%)	4	35
17	CQ	97/99 (98%)	89 (92%)	5 (5%)	3 (3%)	7	45
18	AR	68/70 (97%)	55 (81%)	8 (12%)	5 (7%)	2	15
18	CR	68/70 (97%)	58 (85%)	6 (9%)	4 (6%)	2	23
19	AS	76/78 (97%)	57 (75%)	11 (14%)	8 (10%)	1	6
19	CS	76/78 (97%)	64 (84%)	8 (10%)	4 (5%)	3	26
20	AT	97/99 (98%)	71 (73%)	22 (23%)	4 (4%)	4	35
20	CT	97/99 (98%)	72 (74%)	21 (22%)	4 (4%)	4	35
21	AU	22/24 (92%)	13 (59%)	7 (32%)	2 (9%)	1	10
21	CU	22/24 (92%)	17 (77%)	4 (18%)	1 (4%)	4	32
28	BC	182/206 (88%)	111 (61%)	50 (28%)	21 (12%)	1	5
29	BD	269/271 (99%)	214 (80%)	34 (13%)	21 (8%)	1	14
29	DD	269/271 (99%)	217 (81%)	31 (12%)	21 (8%)	1	14
30	BE	202/204 (99%)	138 (68%)	47 (23%)	17 (8%)	1	12
30	DE	202/204 (99%)	152 (75%)	35 (17%)	15 (7%)	2	15
31	BF	205/207 (99%)	163 (80%)	28 (14%)	14 (7%)	2	18
31	DF	205/207 (99%)	163 (80%)	28 (14%)	14 (7%)	2	18
32	BG	179/181 (99%)	140 (78%)	27 (15%)	12 (7%)	2	18
32	DG	179/181 (99%)	137 (76%)	31 (17%)	11 (6%)	2	22
33	BH	157/159 (99%)	113 (72%)	24 (15%)	20 (13%)	0	3
33	DH	157/159 (99%)	116 (74%)	25 (16%)	16 (10%)	1	7
34	BI	143/145 (99%)	107 (75%)	29 (20%)	7 (5%)	3	29
34	DI	143/145 (99%)	110 (77%)	25 (18%)	8 (6%)	3	25
35	BJ	128/130 (98%)	70 (55%)	42 (33%)	16 (12%)	1	4
35	DJ	128/130 (98%)	72 (56%)	42 (33%)	14 (11%)	1	6
36	BN	136/138 (99%)	100 (74%)	25 (18%)	11 (8%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	DN	136/138 (99%)	108 (79%)	15 (11%)	13 (10%)	1	9
37	BO	120/122 (98%)	106 (88%)	12 (10%)	2 (2%)	14	62
37	DO	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	27	78
38	BP	144/146 (99%)	82 (57%)	37 (26%)	25 (17%)	0	1
38	DP	144/146 (99%)	87 (60%)	28 (19%)	29 (20%)	0	1
39	BQ	139/141 (99%)	109 (78%)	25 (18%)	5 (4%)	5	40
39	DQ	139/141 (99%)	116 (84%)	19 (14%)	4 (3%)	7	47
40	BR	115/117 (98%)	93 (81%)	16 (14%)	6 (5%)	3	27
40	DR	115/117 (98%)	92 (80%)	17 (15%)	6 (5%)	3	27
41	BS	96/98 (98%)	58 (60%)	22 (23%)	16 (17%)	0	1
41	DS	96/98 (98%)	63 (66%)	20 (21%)	13 (14%)	0	3
42	BT	135/137 (98%)	95 (70%)	23 (17%)	17 (13%)	0	3
42	DT	135/137 (98%)	89 (66%)	30 (22%)	16 (12%)	1	4
43	BU	115/117 (98%)	90 (78%)	19 (16%)	6 (5%)	3	27
43	DU	115/117 (98%)	92 (80%)	19 (16%)	4 (4%)	6	41
44	BV	99/101 (98%)	74 (75%)	14 (14%)	11 (11%)	1	5
44	DV	99/101 (98%)	72 (73%)	17 (17%)	10 (10%)	1	8
45	BW	111/113 (98%)	92 (83%)	16 (14%)	3 (3%)	8	49
45	DW	111/113 (98%)	96 (86%)	7 (6%)	8 (7%)	2	16
46	BX	90/92 (98%)	80 (89%)	7 (8%)	3 (3%)	6	43
46	DX	90/92 (98%)	75 (83%)	8 (9%)	7 (8%)	1	14
47	BY	98/100 (98%)	53 (54%)	22 (22%)	23 (24%)	0	0
47	DY	98/100 (98%)	60 (61%)	19 (19%)	19 (19%)	0	1
48	BZ	174/176 (99%)	141 (81%)	26 (15%)	7 (4%)	5	36
48	DZ	174/176 (99%)	130 (75%)	33 (19%)	11 (6%)	2	20
49	B0	82/84 (98%)	75 (92%)	6 (7%)	1 (1%)	19	71
49	D0	82/84 (98%)	72 (88%)	9 (11%)	1 (1%)	19	71
50	B1	91/93 (98%)	76 (84%)	12 (13%)	3 (3%)	6	43
50	D1	91/93 (98%)	74 (81%)	10 (11%)	7 (8%)	1	14
51	B2	69/71 (97%)	53 (77%)	10 (14%)	6 (9%)	1	11
51	D2	69/71 (97%)	54 (78%)	11 (16%)	4 (6%)	3	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	B3	57/59 (97%)	51 (90%)	5 (9%)	1 (2%)	13	61
52	D3	57/59 (97%)	53 (93%)	3 (5%)	1 (2%)	13	61
53	B4	28/30 (93%)	21 (75%)	4 (14%)	3 (11%)	1	6
53	D4	28/30 (93%)	20 (71%)	5 (18%)	3 (11%)	1	6
54	B5	57/59 (97%)	43 (75%)	9 (16%)	5 (9%)	1	11
54	D5	57/59 (97%)	48 (84%)	4 (7%)	5 (9%)	1	11
55	B6	42/44 (96%)	21 (50%)	8 (19%)	13 (31%)	0	0
55	D6	42/44 (96%)	23 (55%)	7 (17%)	12 (29%)	0	0
56	B7	46/48 (96%)	45 (98%)	1 (2%)	0	100	100
56	D7	46/48 (96%)	45 (98%)	0	1 (2%)	10	55
57	B8	61/63 (97%)	44 (72%)	10 (16%)	7 (12%)	1	5
57	D8	61/63 (97%)	47 (77%)	8 (13%)	6 (10%)	1	8
58	B9	34/36 (94%)	32 (94%)	2 (6%)	0	100	100
58	D9	34/36 (94%)	33 (97%)	1 (3%)	0	100	100
60	DC	182/196 (93%)	115 (63%)	47 (26%)	20 (11%)	1	6
All	All	11898/12136 (98%)	9181 (77%)	1900 (16%)	817 (7%)	2	17

5 of 817 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	106	LYS
2	AB	165	VAL
3	AC	12	LEU
3	AC	20	SER
3	AC	47	LEU

### 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	
2	AB	202/202 (100%)	185 (92%)	17 (8%)	16	55
2	CB	202/202 (100%)	181 (90%)	21 (10%)	10	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AC	160/160 (100%)	142 (89%)	18 (11%)	9	36
3	CC	160/160 (100%)	145 (91%)	15 (9%)	13	47
4	AD	180/180 (100%)	160 (89%)	20 (11%)	9	37
4	CD	180/180 (100%)	160 (89%)	20 (11%)	9	37
5	AE	115/115 (100%)	104 (90%)	11 (10%)	12	46
5	CE	115/115 (100%)	101 (88%)	14 (12%)	7	32
6	AF	90/90 (100%)	82 (91%)	8 (9%)	14	51
6	CF	90/90 (100%)	85 (94%)	5 (6%)	30	75
7	AG	126/126 (100%)	115 (91%)	11 (9%)	15	53
7	CG	126/126 (100%)	115 (91%)	11 (9%)	15	53
8	AH	119/119 (100%)	108 (91%)	11 (9%)	13	48
8	CH	119/119 (100%)	107 (90%)	12 (10%)	11	42
9	AI	98/98 (100%)	88 (90%)	10 (10%)	11	42
9	CI	98/98 (100%)	89 (91%)	9 (9%)	13	48
10	AJ	88/88 (100%)	76 (86%)	12 (14%)	5	26
10	CJ	88/88 (100%)	79 (90%)	9 (10%)	11	42
11	AK	90/90 (100%)	82 (91%)	8 (9%)	14	51
11	CK	90/90 (100%)	84 (93%)	6 (7%)	23	67
12	AL	104/104 (100%)	88 (85%)	16 (15%)	4	20
12	CL	104/104 (100%)	90 (86%)	14 (14%)	6	27
13	AM	99/99 (100%)	88 (89%)	11 (11%)	9	37
13	CM	99/99 (100%)	88 (89%)	11 (11%)	9	37
14	AN	49/49 (100%)	43 (88%)	6 (12%)	7	32
14	CN	49/49 (100%)	44 (90%)	5 (10%)	11	42
15	AO	79/79 (100%)	73 (92%)	6 (8%)	19	61
15	CO	79/79 (100%)	76 (96%)	3 (4%)	44	84
16	AP	72/72 (100%)	65 (90%)	7 (10%)	12	45
16	CP	72/72 (100%)	62 (86%)	10 (14%)	5	25
17	AQ	94/94 (100%)	88 (94%)	6 (6%)	25	69
17	CQ	94/94 (100%)	89 (95%)	5 (5%)	32	76
18	AR	61/61 (100%)	54 (88%)	7 (12%)	8	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	CR	61/61 (100%)	59 (97%)	2 (3%)	50	87
19	AS	69/69 (100%)	56 (81%)	13 (19%)	2	11
19	CS	69/69 (100%)	58 (84%)	11 (16%)	4	18
20	AT	76/76 (100%)	68 (90%)	8 (10%)	10	40
20	CT	76/76 (100%)	67 (88%)	9 (12%)	8	34
21	AU	19/19 (100%)	15 (79%)	4 (21%)	1	7
21	CU	19/19 (100%)	17 (90%)	2 (10%)	10	40
28	BC	61/66 (92%)	55 (90%)	6 (10%)	12	45
29	BD	213/213 (100%)	180 (84%)	33 (16%)	4	19
29	DD	213/213 (100%)	176 (83%)	37 (17%)	3	14
30	BE	165/165 (100%)	134 (81%)	31 (19%)	2	11
30	DE	165/165 (100%)	139 (84%)	26 (16%)	4	18
31	BF	165/165 (100%)	138 (84%)	27 (16%)	3	16
31	DF	165/165 (100%)	149 (90%)	16 (10%)	12	45
32	BG	155/155 (100%)	128 (83%)	27 (17%)	3	14
32	DG	155/155 (100%)	137 (88%)	18 (12%)	8	35
33	BH	132/132 (100%)	106 (80%)	26 (20%)	2	9
33	DH	132/132 (100%)	120 (91%)	12 (9%)	14	49
34	BI	122/122 (100%)	110 (90%)	12 (10%)	12	45
34	DI	122/122 (100%)	111 (91%)	11 (9%)	14	50
36	BN	117/117 (100%)	90 (77%)	27 (23%)	1	5
36	DN	117/117 (100%)	94 (80%)	23 (20%)	2	9
37	BO	100/100 (100%)	92 (92%)	8 (8%)	17	58
37	DO	100/100 (100%)	93 (93%)	7 (7%)	21	66
38	BP	112/112 (100%)	83 (74%)	29 (26%)	1	3
38	DP	112/112 (100%)	86 (77%)	26 (23%)	1	5
39	BQ	111/111 (100%)	97 (87%)	14 (13%)	7	31
39	DQ	111/111 (100%)	101 (91%)	10 (9%)	14	50
40	BR	100/100 (100%)	85 (85%)	15 (15%)	4	21
40	DR	100/100 (100%)	85 (85%)	15 (15%)	4	21
41	BS	77/77 (100%)	60 (78%)	17 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DS	77/77 (100%)	67 (87%)	10 (13%)	6	29
42	BT	120/120 (100%)	98 (82%)	22 (18%)	2	12
42	DT	120/120 (100%)	93 (78%)	27 (22%)	1	6
43	BU	92/92 (100%)	78 (85%)	14 (15%)	4	20
43	DU	92/92 (100%)	82 (89%)	10 (11%)	9	38
44	BV	82/82 (100%)	60 (73%)	22 (27%)	1	2
44	DV	82/82 (100%)	65 (79%)	17 (21%)	2	8
45	BW	91/91 (100%)	81 (89%)	10 (11%)	9	38
45	DW	91/91 (100%)	80 (88%)	11 (12%)	7	33
46	BX	74/74 (100%)	67 (90%)	7 (10%)	12	46
46	DX	74/74 (100%)	65 (88%)	9 (12%)	7	32
47	BY	84/84 (100%)	65 (77%)	19 (23%)	1	5
47	DY	84/84 (100%)	67 (80%)	17 (20%)	2	8
48	BZ	155/155 (100%)	141 (91%)	14 (9%)	14	50
48	DZ	155/155 (100%)	148 (96%)	7 (4%)	38	81
49	B0	66/66 (100%)	55 (83%)	11 (17%)	3	16
49	D0	66/66 (100%)	60 (91%)	6 (9%)	14	49
50	B1	78/78 (100%)	68 (87%)	10 (13%)	6	29
50	D1	78/78 (100%)	62 (80%)	16 (20%)	2	8
51	B2	66/66 (100%)	51 (77%)	15 (23%)	1	5
51	D2	66/66 (100%)	60 (91%)	6 (9%)	14	49
52	B3	51/51 (100%)	47 (92%)	4 (8%)	18	60
52	D3	51/51 (100%)	48 (94%)	3 (6%)	28	73
53	B4	27/27 (100%)	22 (82%)	5 (18%)	2	11
53	D4	27/27 (100%)	24 (89%)	3 (11%)	9	37
54	B5	51/51 (100%)	39 (76%)	12 (24%)	1	4
54	D5	51/51 (100%)	41 (80%)	10 (20%)	2	9
55	B6	43/43 (100%)	33 (77%)	10 (23%)	1	5
55	D6	43/43 (100%)	36 (84%)	7 (16%)	3	17
56	B7	41/41 (100%)	35 (85%)	6 (15%)	5	23
56	D7	41/41 (100%)	32 (78%)	9 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
57	B8	53/53 (100%)	41 (77%)	12 (23%)	<b>1</b> <b>5</b>
57	D8	53/53 (100%)	43 (81%)	10 (19%)	<b>2</b> <b>11</b>
58	B9	33/33 (100%)	26 (79%)	7 (21%)	<b>1</b> <b>7</b>
58	D9	33/33 (100%)	30 (91%)	3 (9%)	<b>14</b> 49
60	DC	61/66 (92%)	56 (92%)	5 (8%)	<b>17</b> 57
All	All	9654/9664 (100%)	8391 (87%)	1263 (13%)	<b>6</b> <b>28</b>

5 of 1263 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	BY	79	CYS
3	CC	34	LEU
47	DY	8	LYS
48	BZ	125	LEU
54	B5	35	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 167 such sidechains are listed below:

Mol	Chain	Res	Type
42	BT	38	ASN
56	B7	8	ASN
46	DX	41	ASN
42	BT	84	GLN
48	BZ	73	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	300 (19%)	43 (2%)
1	CA	1504/1504 (100%)	296 (19%)	53 (3%)
22	AV	76/77 (98%)	18 (23%)	4 (5%)
22	CV	76/77 (98%)	22 (28%)	1 (1%)
23	AW	75/76 (98%)	22 (29%)	2 (2%)
23	CW	75/76 (98%)	19 (25%)	2 (2%)
24	AY	74/75 (98%)	38 (51%)	4 (5%)
24	CY	74/75 (98%)	38 (51%)	4 (5%)
25	AX	6/7 (85%)	3 (50%)	1 (16%)
26	BA	2800/2915 (96%)	779 (27%)	151 (5%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
26	DA	2799/2915 (96%)	754 (26%)	122 (4%)
27	BB	118/119 (99%)	36 (30%)	4 (3%)
27	DB	118/119 (99%)	27 (22%)	4 (3%)
59	CX	3/4 (75%)	2 (66%)	0
All	All	9301/9543 (97%)	2354 (25%)	395 (4%)

5 of 2354 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	G
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	22	G

5 of 395 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	BA	2416	G
1	CA	262	G
26	DA	2236	A
26	BA	2469	G
26	BA	2812	G

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
25	PSU	AX	19	24,25	19,21,22	1.59	3 (15%)	23,30,33	0.99	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical

component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PSU	AX	19	24,25	-	0/8/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	AX	19	PSU	C5-C1'	-5.41	1.47	1.52
25	AX	19	PSU	P-OP1	2.57	1.49	1.46
25	AX	19	PSU	C2-N1	2.04	1.43	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	AX	19	PSU	C6-C5-C4	2.01	121.03	116.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
60	DC	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DC	110:ALA	C	119:ALA	N	13.98
1	DC	136:ALA	C	139:ALA	N	11.93



## 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, 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	1504/1504 (100%)	-0.06	49 (3%) 44 10	23, 77, 165, 393	0
1	CA	1504/1504 (100%)	0.07	67 (4%) 32 7	38, 86, 188, 312	0
2	AB	234/234 (100%)	0.11	2 (0%) 81 37	66, 113, 158, 196	0
2	CB	234/234 (100%)	0.37	12 (5%) 27 6	85, 139, 177, 216	0
3	AC	206/206 (100%)	-0.08	2 (0%) 79 33	64, 96, 134, 183	0
3	CC	206/206 (100%)	0.45	11 (5%) 25 6	90, 130, 182, 221	0
4	AD	208/208 (100%)	0.04	0 100 100	55, 91, 126, 174	0
4	CD	208/208 (100%)	-0.07	0 100 100	49, 79, 108, 139	0
5	AE	150/150 (100%)	-0.07	0 100 100	47, 76, 104, 125	0
5	CE	150/150 (100%)	0.04	1 (0%) 84 42	58, 88, 126, 148	0
6	AF	101/101 (100%)	-0.16	0 100 100	52, 80, 108, 124	0
6	CF	101/101 (100%)	-0.08	1 (0%) 79 33	52, 82, 116, 139	0
7	AG	155/155 (100%)	0.00	4 (2%) 53 13	61, 97, 137, 156	0
7	CG	155/155 (100%)	0.34	10 (6%) 18 5	82, 119, 157, 175	0
8	AH	138/138 (100%)	-0.15	0 100 100	50, 81, 105, 135	0
8	CH	138/138 (100%)	-0.04	0 100 100	59, 95, 119, 146	0
9	AI	127/127 (100%)	0.22	3 (2%) 56 15	58, 112, 146, 230	0
9	CI	127/127 (100%)	0.72	10 (7%) 13 4	94, 136, 180, 235	0
10	AJ	98/98 (100%)	0.41	3 (3%) 47 11	67, 119, 160, 187	0
10	CJ	98/98 (100%)	0.84	13 (13%) 4 2	94, 158, 190, 226	0
11	AK	119/119 (100%)	-0.03	3 (2%) 54 14	45, 79, 108, 165	0
11	CK	119/119 (100%)	0.28	8 (6%) 17 4	55, 95, 132, 161	0
12	AL	124/124 (100%)	0.04	4 (3%) 45 11	47, 71, 105, 155	0
12	CL	124/124 (100%)	0.12	1 (0%) 83 39	50, 81, 115, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	124/124 (100%)	0.49	9 (7%) 15 4	68, 112, 153, 231	0
13	CM	124/124 (100%)	1.01	17 (13%) 4 1	101, 153, 200, 218	0
14	AN	60/60 (100%)	-0.01	0 100 100	55, 85, 135, 155	0
14	CN	60/60 (100%)	0.57	4 (6%) 17 4	104, 137, 160, 182	0
15	AO	88/88 (100%)	-0.00	0 100 100	48, 80, 111, 130	0
15	CO	88/88 (100%)	-0.03	0 100 100	55, 87, 117, 139	0
16	AP	83/83 (100%)	0.11	0 100 100	65, 92, 125, 149	0
16	CP	83/83 (100%)	-0.10	0 100 100	51, 73, 112, 139	0
17	AQ	99/99 (100%)	0.07	0 100 100	51, 90, 112, 117	0
17	CQ	99/99 (100%)	0.03	0 100 100	63, 87, 115, 126	0
18	AR	70/70 (100%)	-0.01	1 (1%) 72 25	48, 76, 108, 138	0
18	CR	70/70 (100%)	0.09	0 100 100	61, 91, 126, 149	0
19	AS	78/78 (100%)	0.24	2 (2%) 53 13	72, 114, 165, 189	0
19	CS	78/78 (100%)	0.94	8 (10%) 7 2	111, 160, 209, 221	0
20	AT	99/99 (100%)	0.19	2 (2%) 62 19	67, 102, 150, 169	0
20	CT	99/99 (100%)	0.05	1 (1%) 79 33	49, 96, 135, 150	0
21	AU	24/24 (100%)	0.37	0 100 100	74, 92, 117, 119	0
21	CU	24/24 (100%)	1.84	8 (33%) 1 0	105, 141, 205, 253	0
22	AV	77/77 (100%)	-0.26	1 (1%) 74 27	34, 78, 122, 187	0
22	CV	77/77 (100%)	0.13	4 (5%) 26 6	41, 107, 162, 175	0
23	AW	76/76 (100%)	1.49	21 (27%) 1 1	37, 183, 225, 269	0
23	CW	76/76 (100%)	2.07	37 (48%) 1 0	59, 192, 268, 296	0
24	AY	75/75 (100%)	1.43	23 (30%) 1 1	37, 107, 188, 213	0
24	CY	75/75 (100%)	2.13	30 (40%) 1 0	37, 107, 188, 213	0
25	AX	7/7 (100%)	-0.02	0 100 100	50, 53, 106, 116	0
26	BA	2807/2915 (96%)	-0.35	52 (1%) 64 20	9, 38, 151, 312	0
26	DA	2807/2915 (96%)	-0.16	78 (2%) 50 12	24, 64, 168, 297	0
27	BB	119/119 (100%)	-0.38	0 100 100	32, 60, 91, 118	0
27	DB	119/119 (100%)	0.23	5 (4%) 35 8	71, 112, 151, 191	0
28	BC	190/206 (92%)	2.13	88 (46%) 1 0	108, 181, 242, 295	0
29	BD	271/271 (100%)	-0.31	0 100 100	18, 36, 76, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	DD	271/271 (100%)	-0.18	0 100 100	23, 56, 91, 127	0
30	BE	204/204 (100%)	-0.23	1 (0%) 88 51	18, 48, 92, 134	0
30	DE	204/204 (100%)	-0.12	2 (0%) 79 33	28, 65, 120, 165	0
31	BF	207/207 (100%)	-0.23	2 (0%) 79 33	17, 48, 133, 191	0
31	DF	207/207 (100%)	0.00	1 (0%) 88 51	31, 87, 149, 214	0
32	BG	181/181 (100%)	-0.01	3 (1%) 67 21	56, 82, 129, 172	0
32	DG	181/181 (100%)	0.29	7 (3%) 37 8	82, 128, 167, 210	0
33	BH	159/159 (100%)	-0.06	2 (1%) 74 27	32, 68, 118, 181	0
33	DH	159/159 (100%)	0.58	13 (8%) 12 3	70, 128, 180, 235	0
34	BI	145/145 (100%)	-0.03	0 100 100	44, 95, 123, 159	0
34	DI	145/145 (100%)	0.12	2 (1%) 72 25	48, 101, 137, 159	0
35	BJ	130/130 (100%)	1.73	42 (32%) 1 1	120, 164, 275, 373	0
35	DJ	130/130 (100%)	2.13	60 (46%) 1 0	122, 193, 233, 284	0
36	BN	138/138 (100%)	-0.24	0 100 100	24, 46, 95, 129	0
36	DN	138/138 (100%)	-0.01	1 (0%) 84 42	54, 90, 120, 133	0
37	BO	122/122 (100%)	-0.34	0 100 100	26, 49, 75, 91	0
37	DO	122/122 (100%)	-0.25	0 100 100	39, 64, 85, 92	0
38	BP	146/146 (100%)	-0.07	2 (1%) 72 25	21, 65, 115, 159	0
38	DP	146/146 (100%)	0.19	4 (2%) 52 13	39, 92, 134, 174	0
39	BQ	141/141 (100%)	-0.25	1 (0%) 84 42	27, 51, 85, 188	0
39	DQ	141/141 (100%)	0.09	1 (0%) 84 42	58, 92, 125, 161	0
40	BR	117/117 (100%)	-0.27	0 100 100	21, 42, 78, 93	0
40	DR	117/117 (100%)	-0.12	0 100 100	40, 65, 100, 131	0
41	BS	98/98 (100%)	-0.07	1 (1%) 79 33	35, 64, 105, 136	0
41	DS	98/98 (100%)	0.25	1 (1%) 79 33	72, 110, 151, 181	0
42	BT	137/137 (100%)	-0.09	4 (2%) 49 12	34, 64, 139, 181	0
42	DT	137/137 (100%)	0.00	3 (2%) 59 16	43, 77, 135, 170	0
43	BU	117/117 (100%)	-0.32	0 100 100	15, 37, 73, 98	0
43	DU	117/117 (100%)	0.02	4 (3%) 43 10	40, 80, 135, 155	0
44	BV	101/101 (100%)	-0.24	0 100 100	24, 51, 85, 119	0
44	DV	101/101 (100%)	0.30	2 (1%) 62 19	61, 110, 143, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	BW	113/113 (100%)	-0.25	0 100 100	25, 37, 75, 137	0
45	DW	113/113 (100%)	-0.01	0 100 100	49, 66, 103, 147	0
46	BX	92/92 (100%)	-0.32	0 100 100	25, 44, 73, 82	0
46	DX	92/92 (100%)	-0.06	0 100 100	43, 77, 98, 114	0
47	BY	100/100 (100%)	0.10	5 (5%) 28 6	34, 66, 163, 201	0
47	DY	100/100 (100%)	0.38	7 (7%) 16 4	56, 100, 175, 209	0
48	BZ	176/176 (100%)	1.06	40 (22%) 1 1	43, 119, 275, 309	0
48	DZ	176/176 (100%)	1.34	41 (23%) 1 1	92, 149, 299, 353	0
49	B0	84/84 (100%)	-0.10	0 100 100	25, 43, 78, 110	0
49	D0	84/84 (100%)	0.34	2 (2%) 56 15	58, 84, 105, 128	0
50	B1	93/93 (100%)	-0.14	1 (1%) 77 30	26, 48, 94, 131	0
50	D1	93/93 (100%)	-0.04	2 (2%) 59 16	39, 63, 111, 153	0
51	B2	71/71 (100%)	-0.03	1 (1%) 72 25	34, 61, 101, 164	0
51	D2	71/71 (100%)	-0.04	1 (1%) 72 25	60, 90, 131, 150	0
52	B3	59/59 (100%)	-0.09	1 (1%) 67 21	29, 48, 92, 149	0
52	D3	59/59 (100%)	0.43	2 (3%) 43 10	65, 101, 135, 253	0
53	B4	30/30 (100%)	-0.01	0 100 100	69, 116, 141, 154	0
53	D4	30/30 (100%)	0.38	0 100 100	121, 142, 163, 173	0
54	B5	59/59 (100%)	-0.03	3 (5%) 27 6	21, 42, 139, 213	0
54	D5	59/59 (100%)	-0.07	2 (3%) 43 10	42, 67, 130, 179	0
55	B6	44/44 (100%)	0.02	1 (2%) 57 15	30, 60, 93, 118	0
55	D6	44/44 (100%)	0.34	0 100 100	51, 90, 113, 121	0
56	B7	48/48 (100%)	-0.19	1 (2%) 60 17	20, 30, 63, 124	0
56	D7	48/48 (100%)	-0.13	0 100 100	31, 49, 80, 98	0
57	B8	63/63 (100%)	-0.20	0 100 100	30, 44, 64, 129	0
57	D8	63/63 (100%)	-0.02	1 (1%) 68 22	50, 77, 112, 154	0
58	B9	36/36 (100%)	0.03	0 100 100	34, 49, 63, 78	0
58	D9	36/36 (100%)	0.50	2 (5%) 24 5	63, 91, 115, 125	0
59	CX	4/4 (100%)	0.30	1 (25%) 1 1	70, 87, 90, 158	0
60	DC	190/196 (96%)	2.34	91 (47%) 1 0	109, 188, 240, 265	0
All	All	21441/21679 (98%)	0.07	959 (4%) 32 7	9, 77, 180, 393	0

The worst 5 of 959 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
26	DA	2812	G	16.8
1	AA	88	A	15.0
1	AA	84	U	14.2
35	BJ	52	ALA	13.5
1	CA	82	U	13.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
25	PSU	AX	19	20/21	0.17	-	83,95,104,110	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.