



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:43 PM BST

PDB ID : 4V8A
Title : The structure of thermorubin in complex with the 70S ribosome from *Thermus thermophilus*.
Authors : Bulkley, D.; Johnson, F.A.; Steitz, T.A.
Deposited on : 2011-12-05
Resolution : 3.20 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

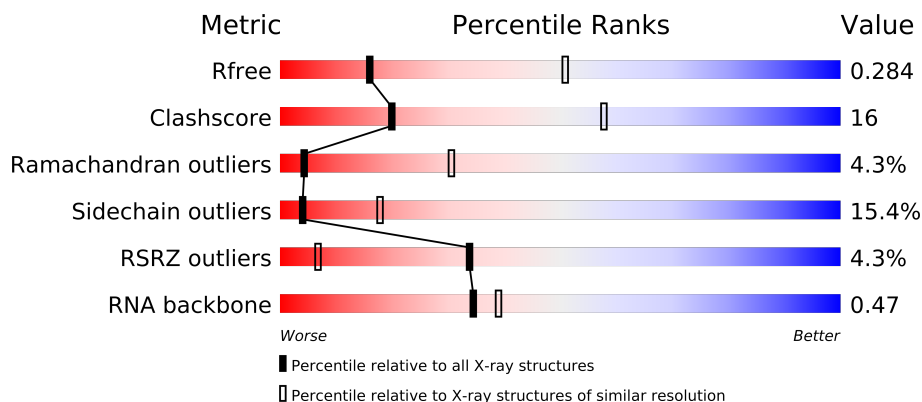
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 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	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)
RNA backbone	1838	1002 (3.72-2.68)

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 ≥ 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	2915	
1	BA	2915	
2	AB	122	
2	BB	122	
3	AD	276	
3	BD	276	
4	AE	206	
4	BE	206	
5	AF	205	
5	BF	205	
6	AG	182	
6	BG	182	

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Mol	Chain	Length	Quality of chain
7	AH	180	
7	BH	180	
8	AI	148	
8	BI	148	
9	AN	140	
9	BN	140	
10	AO	122	
10	BO	122	
11	AP	150	
11	BP	150	
12	AQ	141	
12	BQ	141	
13	AR	118	
13	BR	118	
14	AS	112	
14	BS	112	
15	AT	146	
15	BT	146	
16	AU	118	
16	BU	118	
17	AV	101	
17	BV	101	
18	AW	113	
18	BW	113	
19	AX	96	
19	BX	96	
20	AY	110	
20	BY	110	
21	AZ	206	
21	BZ	206	
22	A0	85	
22	B0	85	
23	A1	98	
23	B1	98	
24	A2	72	
24	B2	72	
25	A3	60	
25	B3	60	
26	A4	71	
26	B4	71	
27	A5	60	
27	B5	60	

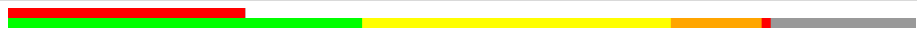
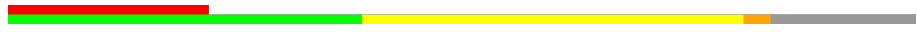




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Mol	Chain	Length	Quality of chain
28	A6	54	
28	B6	54	
29	A7	49	
29	B7	49	
30	A8	65	
30	B8	65	
31	CA	1521	
31	DA	1521	
32	CB	256	
32	DB	256	
33	CC	239	
33	DC	239	
34	CD	209	
34	DD	209	
35	CE	162	
35	DE	162	
36	CF	101	
36	DF	101	
37	CG	156	
37	DG	156	
38	CH	138	
38	DH	138	
39	CI	128	
39	DI	128	
40	CJ	105	
40	DJ	105	
41	CK	129	
41	DK	129	
42	CL	132	
42	DL	132	
43	CM	126	
43	DM	126	
44	CN	61	
44	DN	61	
45	CO	89	
45	DO	89	
46	CP	88	
46	DP	88	
47	CQ	105	
47	DQ	105	
48	CR	88	
48	DR	88	

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Mol	Chain	Length	Quality of chain
49	CS	93	
49	DS	93	
50	CT	106	
50	DT	106	
51	CU	27	
51	DU	27	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 279316 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			
1	BA	2827	Total	C	N	O	P	0	0	0
			60900	27102	11403	19569	2826			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	272A	G	U	CONFLICT	GB AP008226.1
BA	272A	G	U	CONFLICT	GB AP008226.1

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			
2	BB	120	Total	C	N	O	P	0	0	0
			2574	1146	476	833	119			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AB	120	G	A	CONFLICT	GB AP008226.1
BB	120	G	A	CONFLICT	GB AP008226.1

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			
3	BD	275	Total	C	N	O	S	0	0	0
			2136	1349	423	361	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			
4	BE	204	Total	C	N	O	S	0	0	0
			1555	982	297	270	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			
5	BF	203	Total	C	N	O	S	0	0	1
			1576	1005	297	272	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			
6	BG	181	Total	C	N	O	S	0	0	0
			1368	879	242	244	3			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			
7	BH	174	Total	C	N	O	S	0	0	0
			1317	837	243	236	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			
8	BI	145	Total	C	N	O	S	0	0	0
			1046	674	180	191	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

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Chain	Residue	Modelled	Actual	Comment	Reference
BI	110	GLU	ASP	CONFLICT	UNP Q5SLQ1

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			
9	BN	140	Total	C	N	O	S	0	0	0
			1112	717	207	184	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			
10	BO	122	Total	C	N	O	S	0	0	0
			923	583	168	168	4			

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			
11	BP	147	Total	C	N	O	S	0	0	0
			1119	695	227	194	3			

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			
13	BR	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	AS	110	Total	C	N	O	0	0	0
			865	544	172	149			
14	BS	110	Total	C	N	O	0	0	0
			865	544	172	149			

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			
15	BT	131	Total	C	N	O	S	0	0	0
			1063	666	213	183	1			

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			
16	BU	116	Total	C	N	O	S	0	0	0
			959	608	201	149	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			
17	BV	101	Total	C	N	O	S	0	0	0
			771	495	140	135	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			
18	BW	112	Total	C	N	O	S	0	0	0
			881	554	172	153	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			
19	BX	95	Total	C	N	O	S	0	0	0
			742	483	134	124	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			
20	BY	107	Total	C	N	O	S	0	0	0
			785	503	145	131	6			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			
21	BZ	198	Total	C	N	O	S	0	0	0
			1522	972	269	279	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	A0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			
22	B0	76	Total	C	N	O	S	0	0	0
			594	368	125	100	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	A1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			
23	B1	97	Total	C	N	O	S	0	0	0
			745	469	144	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	A2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	70	Total	C	N	O	S	0	0	0
			588	365	118	103	2			

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	A3	59	Total	C	N	O	S	0	0	0
			458	293	87	78				
25	B3	59	Total	C	N	O	S	0	0	0
			458	293	87	78				

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	A4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			
26	B4	46	Total	C	N	O	S	0	0	0
			349	223	57	64	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			
27	B5	59	Total	C	N	O	S	0	0	0
			455	286	90	74	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	A6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			
28	B6	53	Total	C	N	O	S	0	0	0
			449	278	90	77	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			
29	B7	48	Total	C	N	O	S	0	0	0
			418	257	104	55	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			
30	B8	64	Total	C	N	O	S	0	0	0
			509	326	99	82	2			

- Molecule 31 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			
31	DA	1498	Total	C	N	O	P	0	0	0
			32208	14334	5974	10402	1498			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CA	?	-	U	DELETION	GB AP008226.1
DA	?	-	U	DELETION	GB AP008226.1

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			
32	DB	229	Total	C	N	O	S	0	0	0
			1777	1134	318	320	5			

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			
33	DC	206	Total	C	N	O	S	0	0	0
			1450	906	279	264	1			

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	DD	208	Total	C	N	O	S	0	0	0
			1520	960	283	272	5			

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			
35	DE	148	Total	C	N	O	S	0	0	0
			1105	699	204	198	4			

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			
36	DF	100	Total	C	N	O	S	0	0	0
			781	495	137	146	3			

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CG	155	Total	C	N	O	S	0	0	0
			1167	727	224	210	6			
37	DG	155	Total	C	N	O	S	0	0	0
			1167	727	224	210	6			

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			
38	DH	138	Total	C	N	O	S	0	0	0
			1045	665	188	190	2			

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	CI	125	Total	C	N	O	0	0	0
			852	533	163	156			
39	DI	125	Total	C	N	O	0	0	0
			852	533	163	156			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	CJ	96	Total	C	N	O	0	0	0
			659	408	131	120			
40	DJ	96	Total	C	N	O	0	0	0
			659	408	131	120			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7
DJ	75	LEU	ILE	CONFLICT	UNP Q5SHN7

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	CK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			
41	DK	114	Total	C	N	O	S	0	0	0
			828	516	155	154	3			

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			
42	DL	122	Total	C	N	O	S	0	0	0
			909	570	179	159	1			

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			
43	DM	114	Total	C	N	O	S	0	0	0
			801	494	164	142	1			

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			
44	DN	60	Total	C	N	O	S	0	0	0
			478	303	99	72	4			

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			
45	DO	88	Total	C	N	O	S	0	0	0
			724	453	143	126	2			

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			
46	DP	82	Total	C	N	O	S	0	0	0
			651	416	123	111	1			

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			
47	DQ	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	CR	68	Total	C	N	O	0	0	0
			514	329	98	87			
48	DR	68	Total	C	N	O	0	0	0
			514	329	98	87			

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CS	78	Total	C	N	O	S	0	0	0
			544	342	105	95	2			
49	DS	78	Total	C	N	O	S	0	0	0
			544	342	105	95	2			

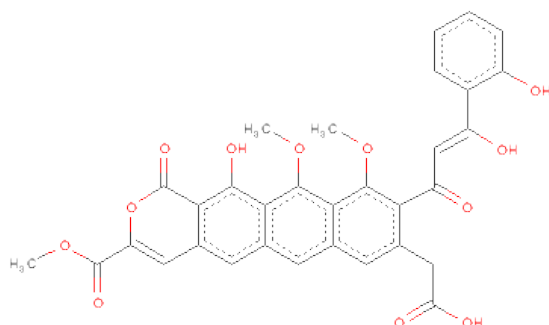
- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CT	96	Total	C	N	O	S	0	0	0
			708	435	151	120	2			
50	DT	96	Total	C	N	O	S	0	0	0
			708	435	151	120	2			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
51	CU	23	Total	C	N	O	0	0	0
			199	122	48	29			
51	DU	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 52 is Thermorubin (three-letter code: T8B) (formula: $C_{32}H_{24}O_{12}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
52	AA	1	Total	C	O	0	0
			44	32	12		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
52	BA	1	Total	C	O	0	0
			44	32	12		

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

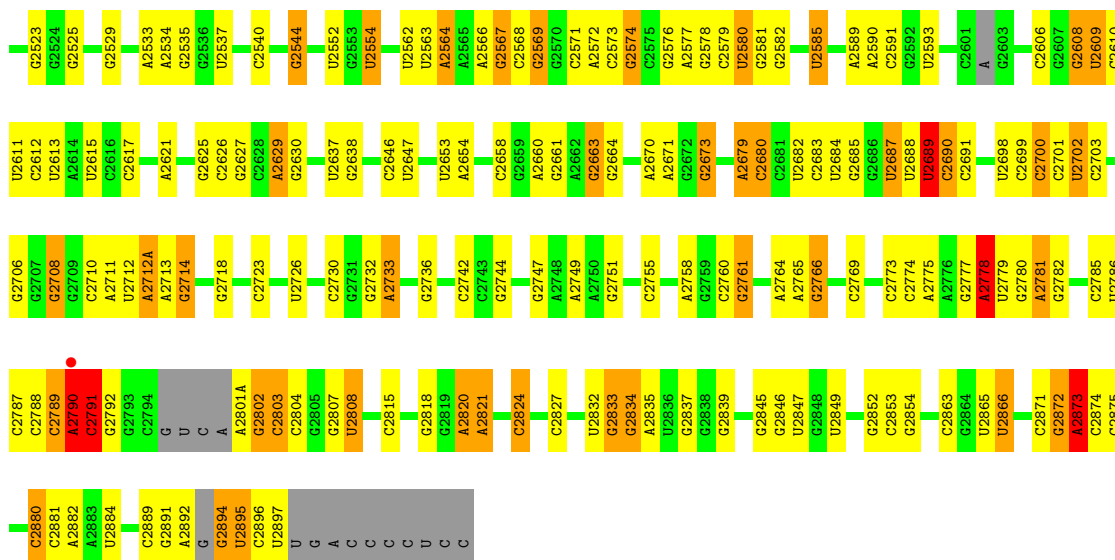
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AA	2	Total	Mg	0	0
			2	2		
53	BA	2	Total	Mg	0	0
			2	2		

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C1711	C1712	U1639	A1545	C1403	U1249	C1180	G	A1046	G975A	C903	C837	G770
A1815	C1546	C1640	C1404	G1404	G1250	G1183	G1107	G1047	C976	C904	C838	
G1817	C1547	C1644	U1405	U1405	C1320	G1184	U1108	A1048	G977	U905	U839	U773
U1818	G1482	G1645	U1406	U1406	A1252	C1185	C1109	C1049	A880	G906	C840	A774
A1819	U1722	C1646	C1407	G1484	A1253	G1186	G1110	A1050		U907	A841	G775
U1820	A1739	G1647	C1408	G1485	G1261	G1187	A1111	G1051		C908	G842	G776
G1823	G1742	G1651	G1409	A1486	C1267	U1188	U1112	G1052		A909		A777
G1826	C1743	A1652	U1410	G1487	G1268	A1189	G1113	C	A883	A910	G845	G778
C1827		A1653	A1412	U1489	G1269	G1191	G1114	G	A884	A911		U779
A1828		A1654	G1413	A1490	C1261	G1192	C1116	G		A912	G848	G780
U1833		G1655	G1416	U1491	A1265	G1193	G1120	G		A913	A849	A781
U1834		A1656	C1417	G1492	U1266	U1198	C1121	G		A916	G854	A783
G1835		C1657	G1418	C1493	U1267	U1199	G1122	U		A917	G855	A784
C1836		C1657	A1419	G1494	U1273	G1200	G1123	G		A918	C856	G786
C1837			U1420	G1495	A1274	G1201	G1124	U		G919	C857	U787
C1838			U1421	U1496	A1275	C1202	G1125	G		G920	U858	A788
G1839			G1422	U1497	A1278	C1203	U1130	C		G921	G859	
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C1844			A1427	G1500		U1205	A1132	A		C923	A861	A793
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G1848			G1429	U1502		U1210	G1136	G			A864	C795
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G1858			A1434	U1507			U1142	C			A870	A804
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			A1445			A1226	G1154	U			C879	C814
			G1448			G1227	A1155	A			G880	C815
			U1449			U1228	A1156	A			C881	C816
			G1450			G1229	U1159	G			G882	C817
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						G1231	C1161	G			C884	A819
						G1232	G1162	A			C885	A820
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						A1237	C1166	C			A887	U822
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						U1240		A			A890	C825
						A1241	G1171	A			C892	U826
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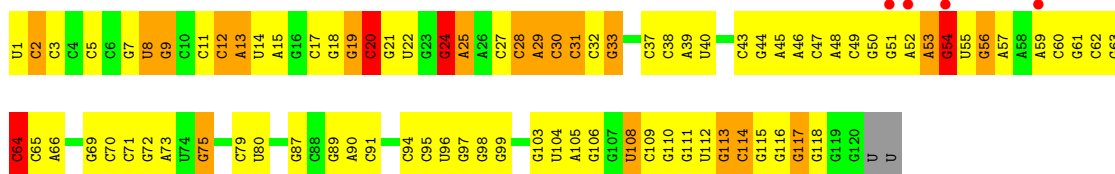


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G2447	A2289	A2136	A2062	A1972	G1889	C1796	G1687	U1608	C1505	G1418	G1330	G1253
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U2473	U2312	A2157	U2098	A2020	A1918	G1824	U1746	A1641	U1540	G1449	A1360	A1275
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A2425	G2341	G2181	G2121	A2049	U1959	G1882	A1786	C1675	G1581	G1491	U1405	C1314
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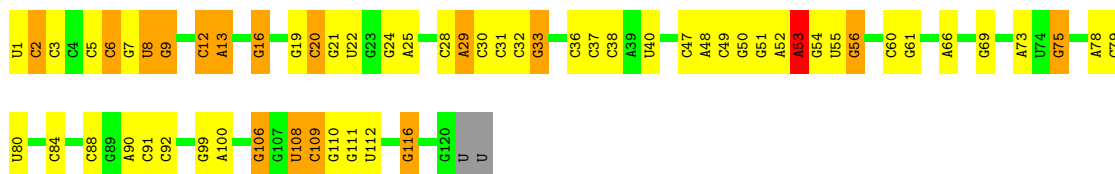
• Molecule 2: 5S ribosomal RNA

Chain AB:



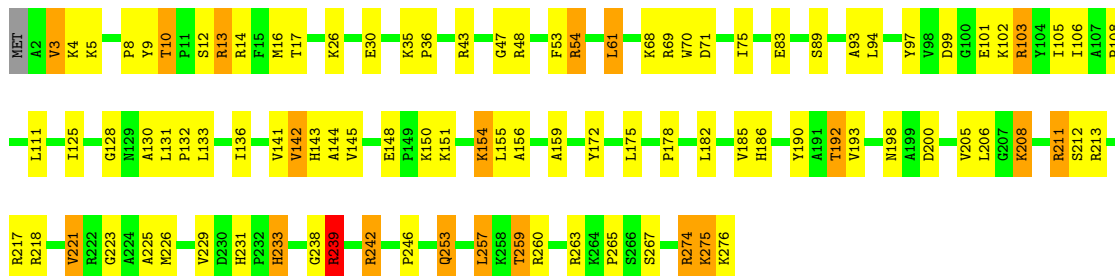
• Molecule 2: 5S ribosomal RNA

Chain BB:



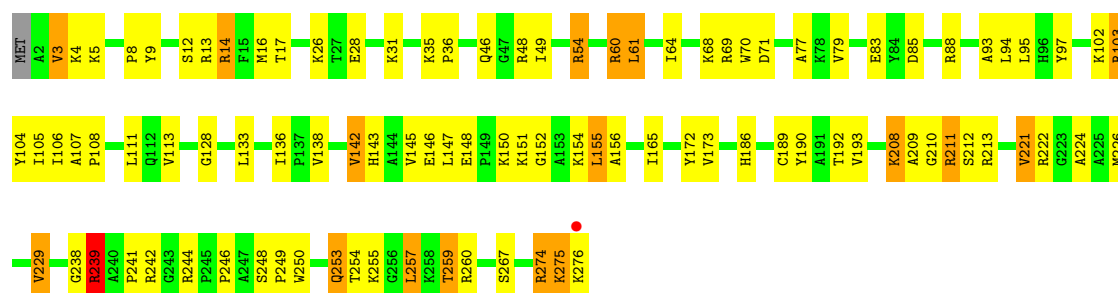
• Molecule 3: 50S ribosomal protein L2

Chain AD:



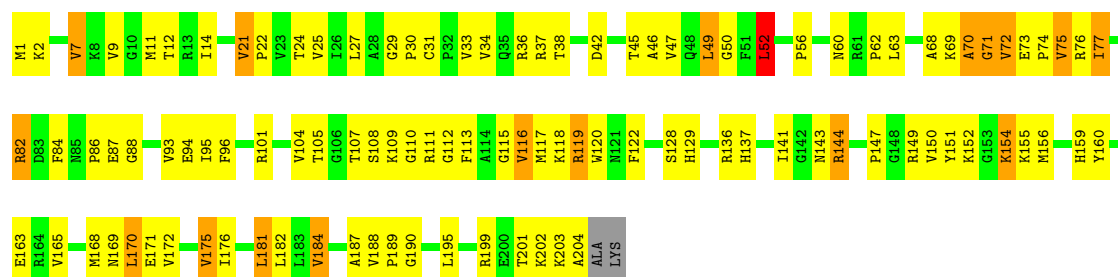
• Molecule 3: 50S ribosomal protein L2

Chain BD:



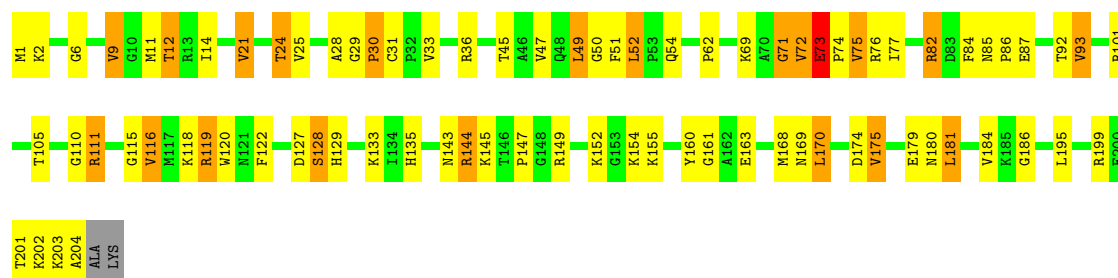
• Molecule 4: 50S ribosomal protein L3

Chain AE:



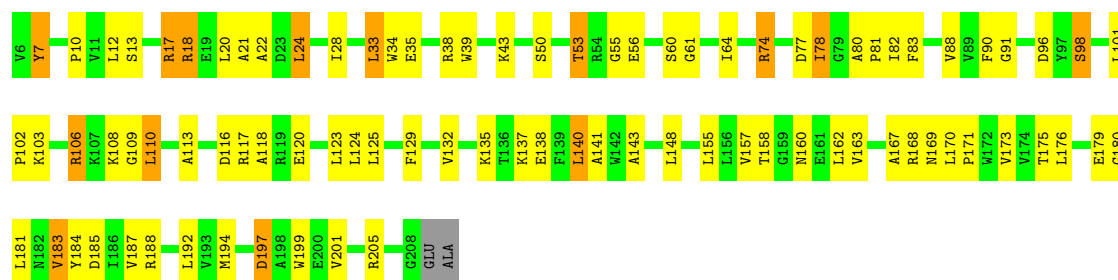
• Molecule 4: 50S ribosomal protein L3

Chain BE:



• Molecule 5: 50S ribosomal protein L4

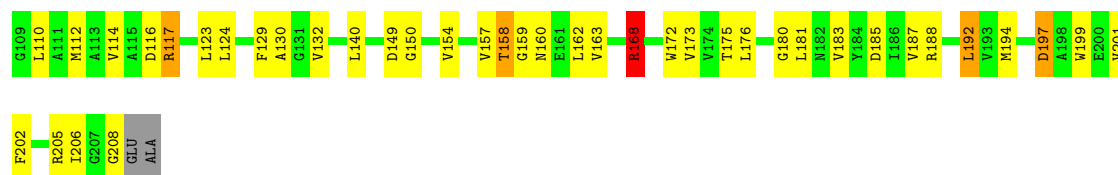
Chain AF:



• Molecule 5: 50S ribosomal protein L4

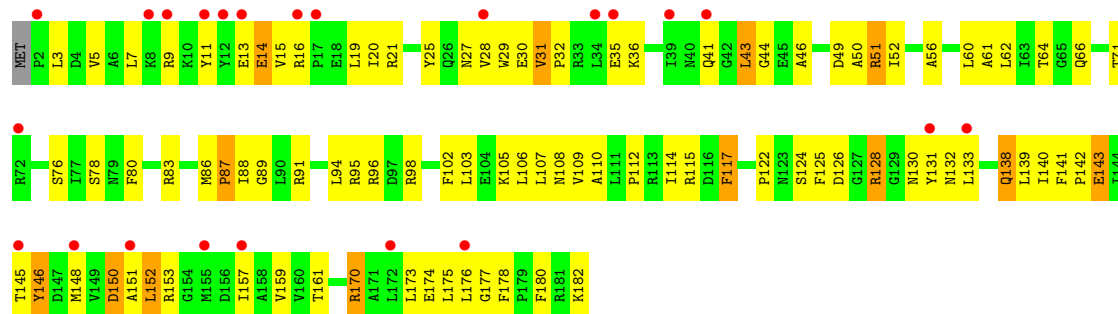
Chain BF:





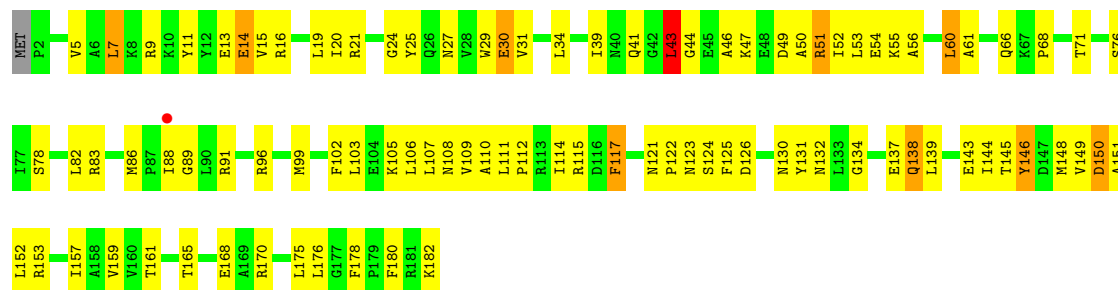
- Molecule 6: 50S ribosomal protein L5

Chain AG:



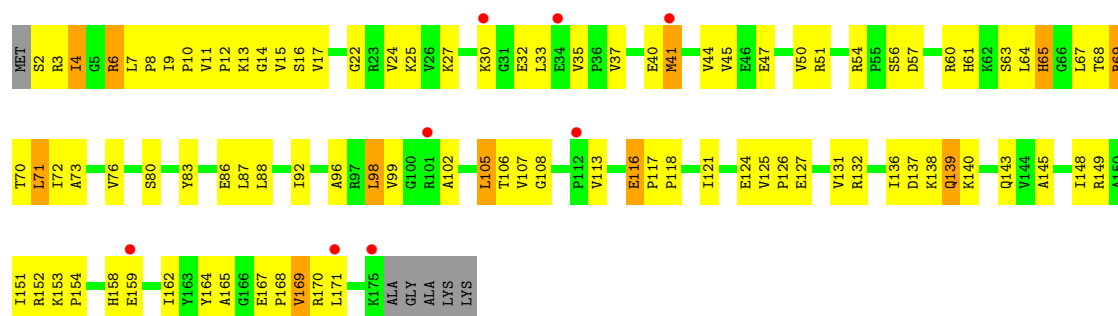
- Molecule 6: 50S ribosomal protein L5

Chain BG:



- Molecule 7: 50S ribosomal protein L6

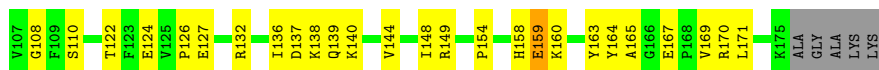
Chain AH:



- Molecule 7: 50S ribosomal protein L6

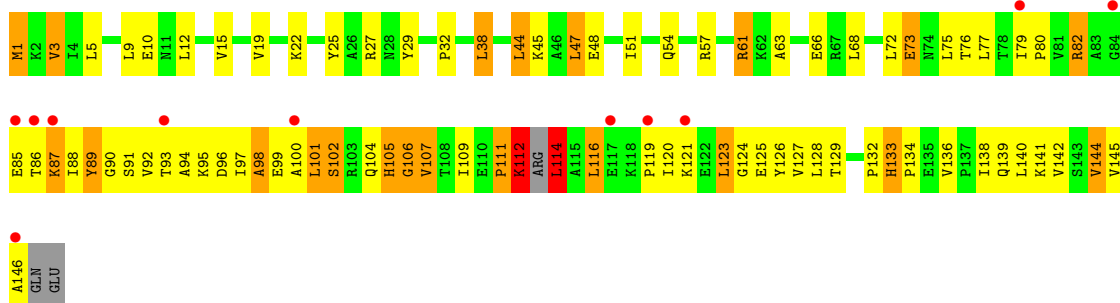
Chain BH:





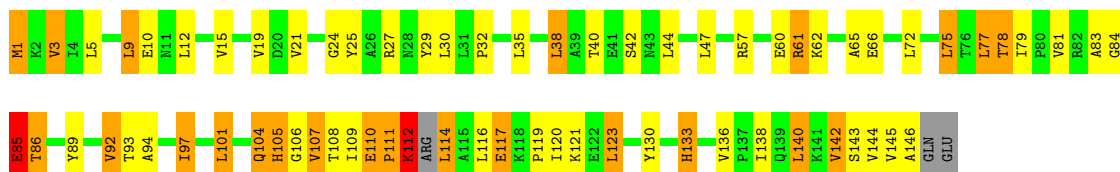
• Molecule 8: 50S ribosomal protein L9

Chain AI:



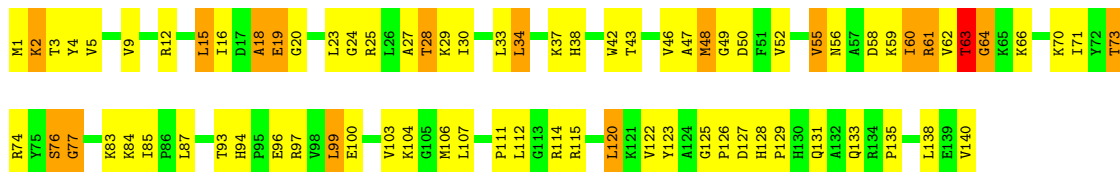
• Molecule 8: 50S ribosomal protein L9

Chain BI:



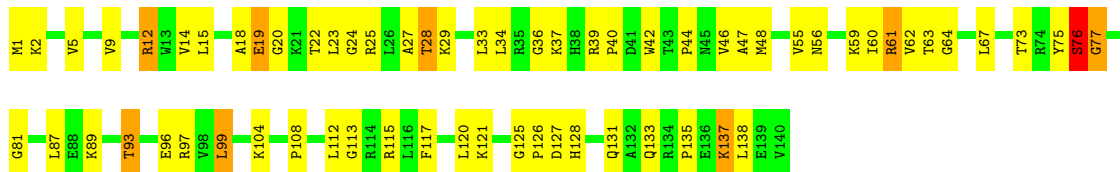
• Molecule 9: 50S ribosomal protein L13

Chain AN:



• Molecule 9: 50S ribosomal protein L13

Chain BN:



• Molecule 10: 50S ribosomal protein L14

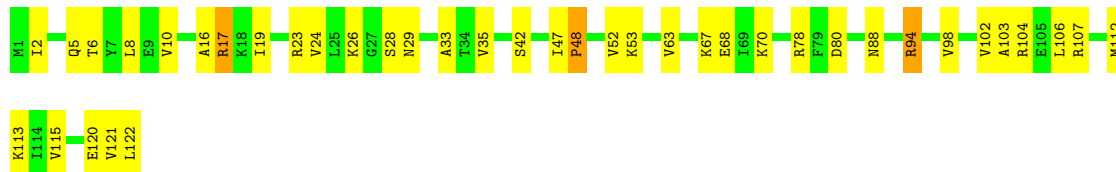
Chain AO:





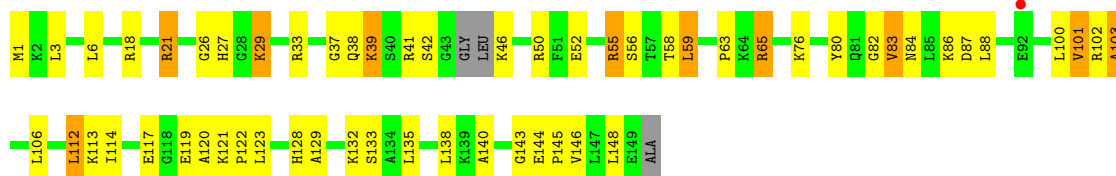
- Molecule 10: 50S ribosomal protein L14

Chain BO:



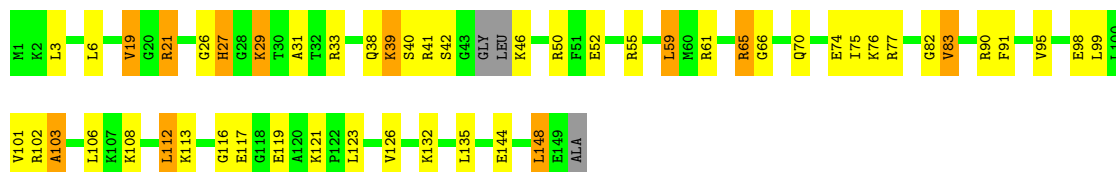
- Molecule 11: 50S ribosomal protein L15

Chain AP:



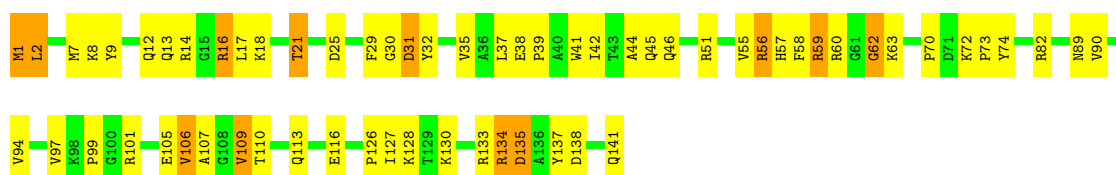
- Molecule 11: 50S ribosomal protein L15

Chain BP:



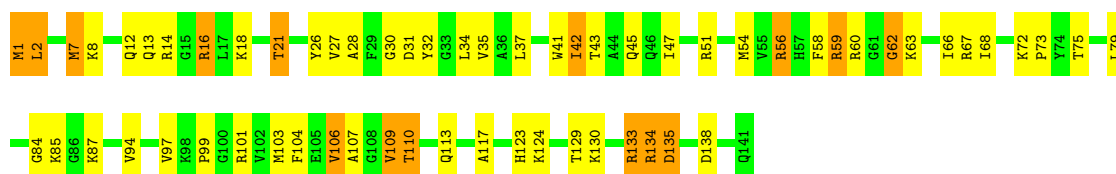
- Molecule 12: 50S ribosomal protein L16

Chain AQ:



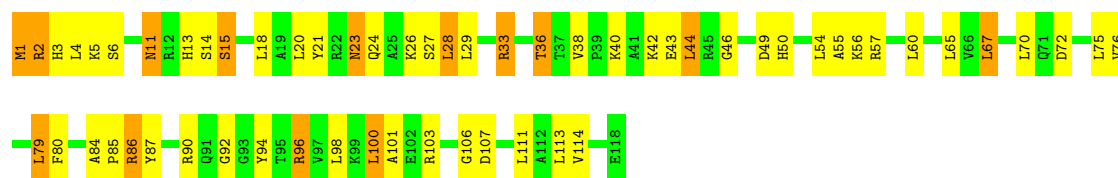
- Molecule 12: 50S ribosomal protein L16

Chain BQ:



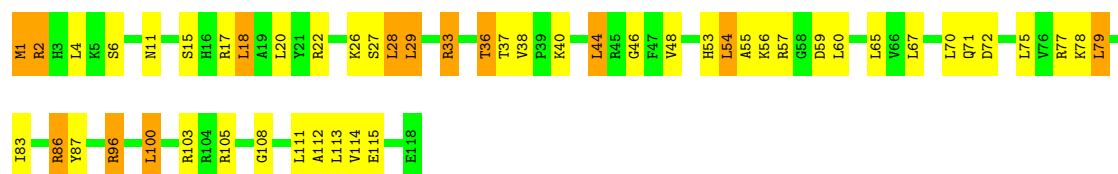
- Molecule 13: 50S ribosomal protein L17

Chain AR:



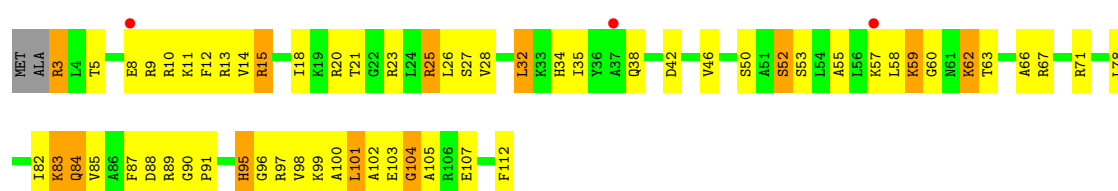
- Molecule 13: 50S ribosomal protein L17

Chain BR:



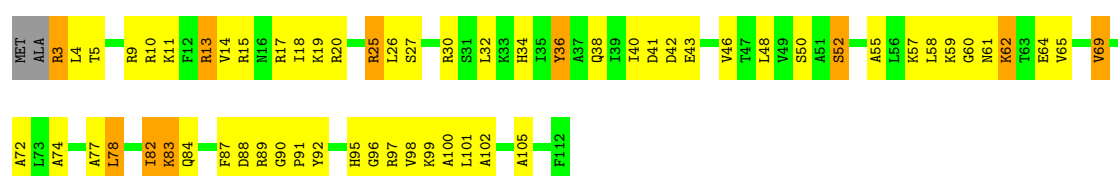
- Molecule 14: 50S ribosomal protein L18

Chain AS:



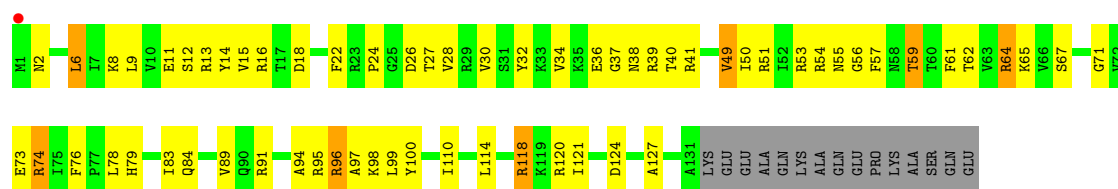
- Molecule 14: 50S ribosomal protein L18

Chain BS:



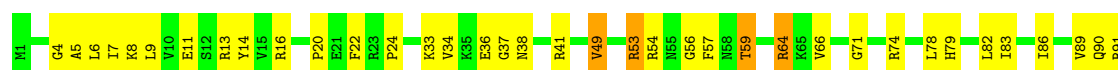
- Molecule 15: 50S ribosomal protein L19

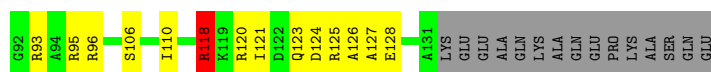
Chain AT:



- Molecule 15: 50S ribosomal protein L19

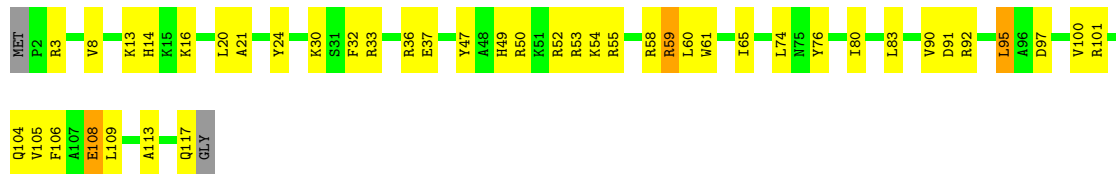
Chain BT:





- Molecule 16: 50S ribosomal protein L20

Chain AU:



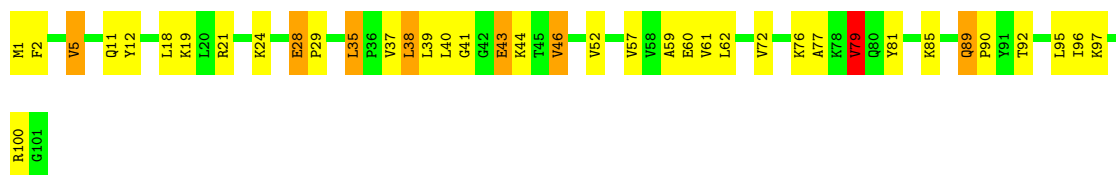
- Molecule 16: 50S ribosomal protein L20

Chain BU:



- Molecule 17: 50S ribosomal protein L21

Chain AV:



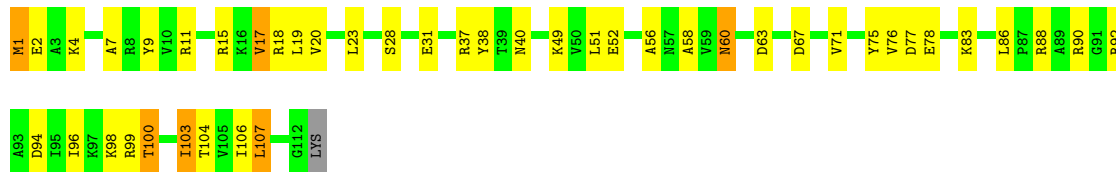
- Molecule 17: 50S ribosomal protein L21

Chain BV:



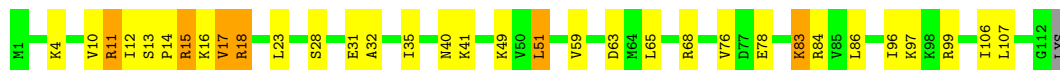
- Molecule 18: 50S ribosomal protein L22

Chain AW:



- Molecule 18: 50S ribosomal protein L22

Chain BW:



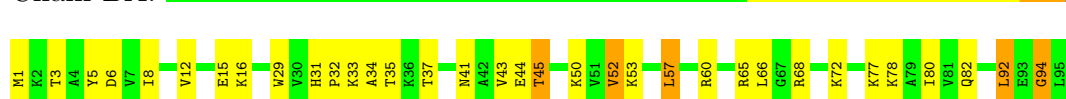
- Molecule 19: 50S ribosomal protein L23

Chain AX:



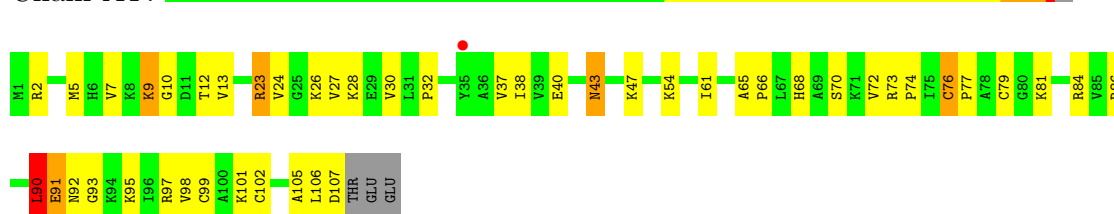
- Molecule 19: 50S ribosomal protein L23

Chain BX:



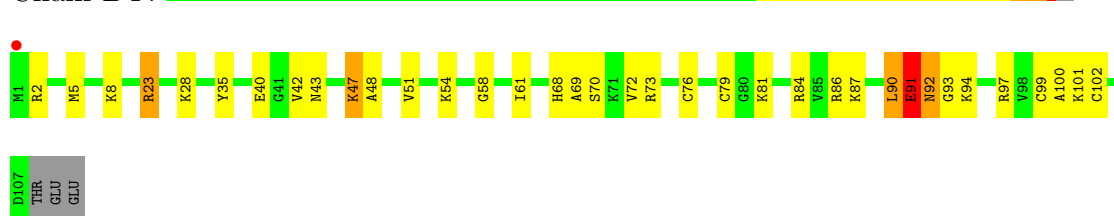
- Molecule 20: 50S ribosomal protein L24

Chain AY:



- Molecule 20: 50S ribosomal protein L24

Chain BY:



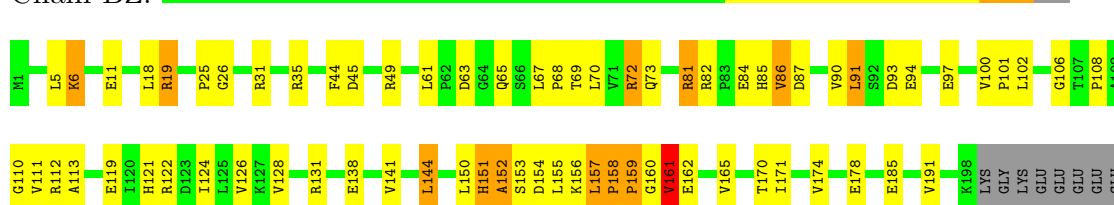
- Molecule 21: 50S ribosomal protein L25

Chain AZ:



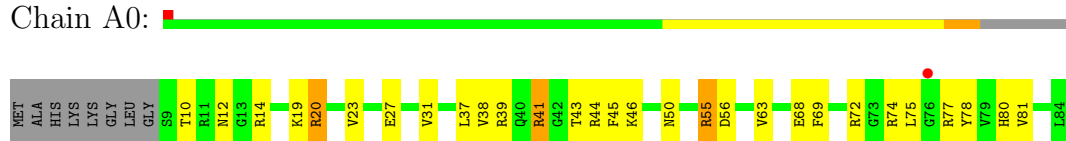
- Molecule 21: 50S ribosomal protein L25

Chain BZ:



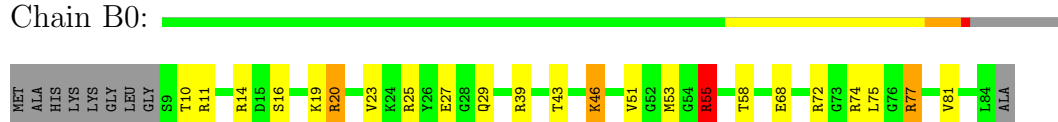
- Molecule 22: 50S ribosomal protein L27

Chain A0:



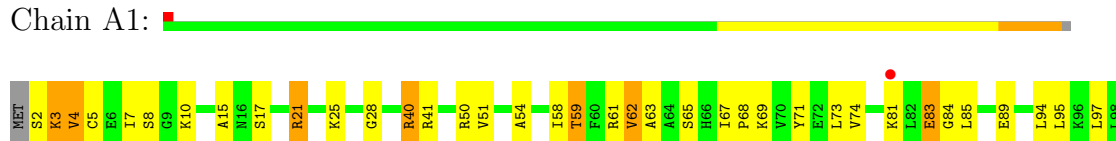
- Molecule 22: 50S ribosomal protein L27

Chain B0:



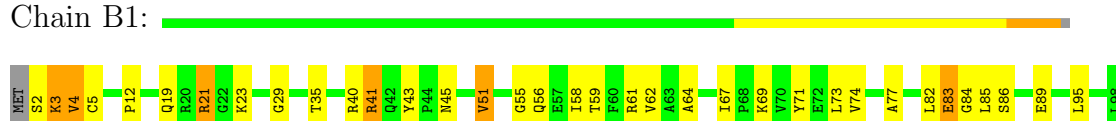
- Molecule 23: 50S ribosomal protein L28

Chain A1:



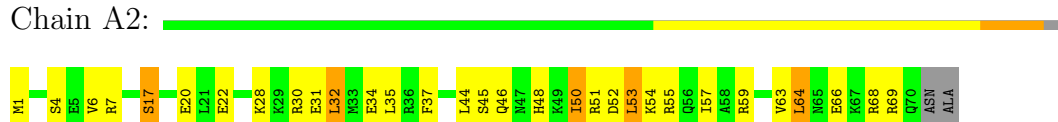
- Molecule 23: 50S ribosomal protein L28

Chain B1:



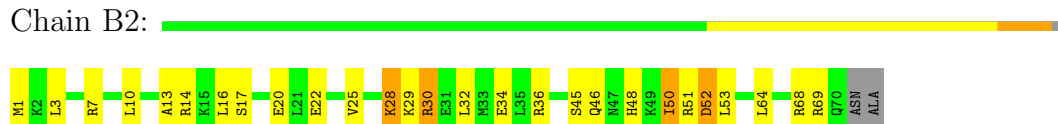
- Molecule 24: 50S ribosomal protein L29

Chain A2:



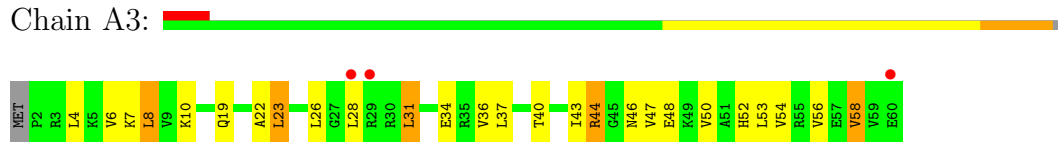
- Molecule 24: 50S ribosomal protein L29

Chain B2:



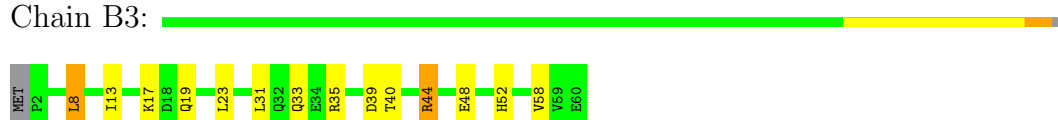
- Molecule 25: 50S ribosomal protein L30

Chain A3:



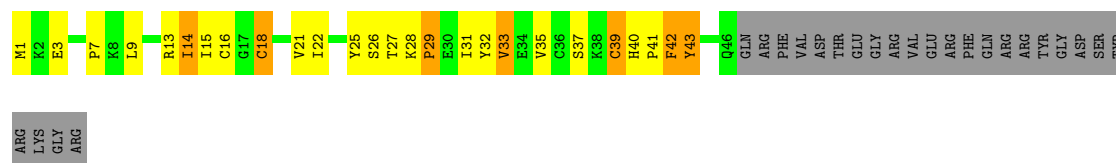
- Molecule 25: 50S ribosomal protein L30

Chain B3:



- Molecule 26: 50S ribosomal protein L31

Chain A4:



- Molecule 26: 50S ribosomal protein L31

Chain B4:



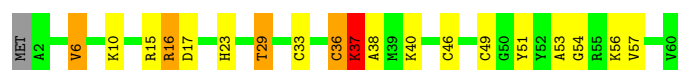
- Molecule 27: 50S ribosomal protein L32

Chain A5:



- Molecule 27: 50S ribosomal protein L32

Chain B5:



- Molecule 28: 50S ribosomal protein L33

Chain A6:



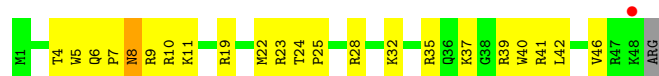
- Molecule 28: 50S ribosomal protein L33

Chain B6:



- Molecule 29: 50S ribosomal protein L34

Chain A7:



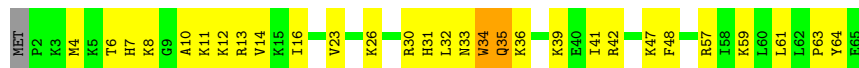
- Molecule 29: 50S ribosomal protein L34

Chain B7:



- Molecule 30: 50S ribosomal protein L35

Chain A8:



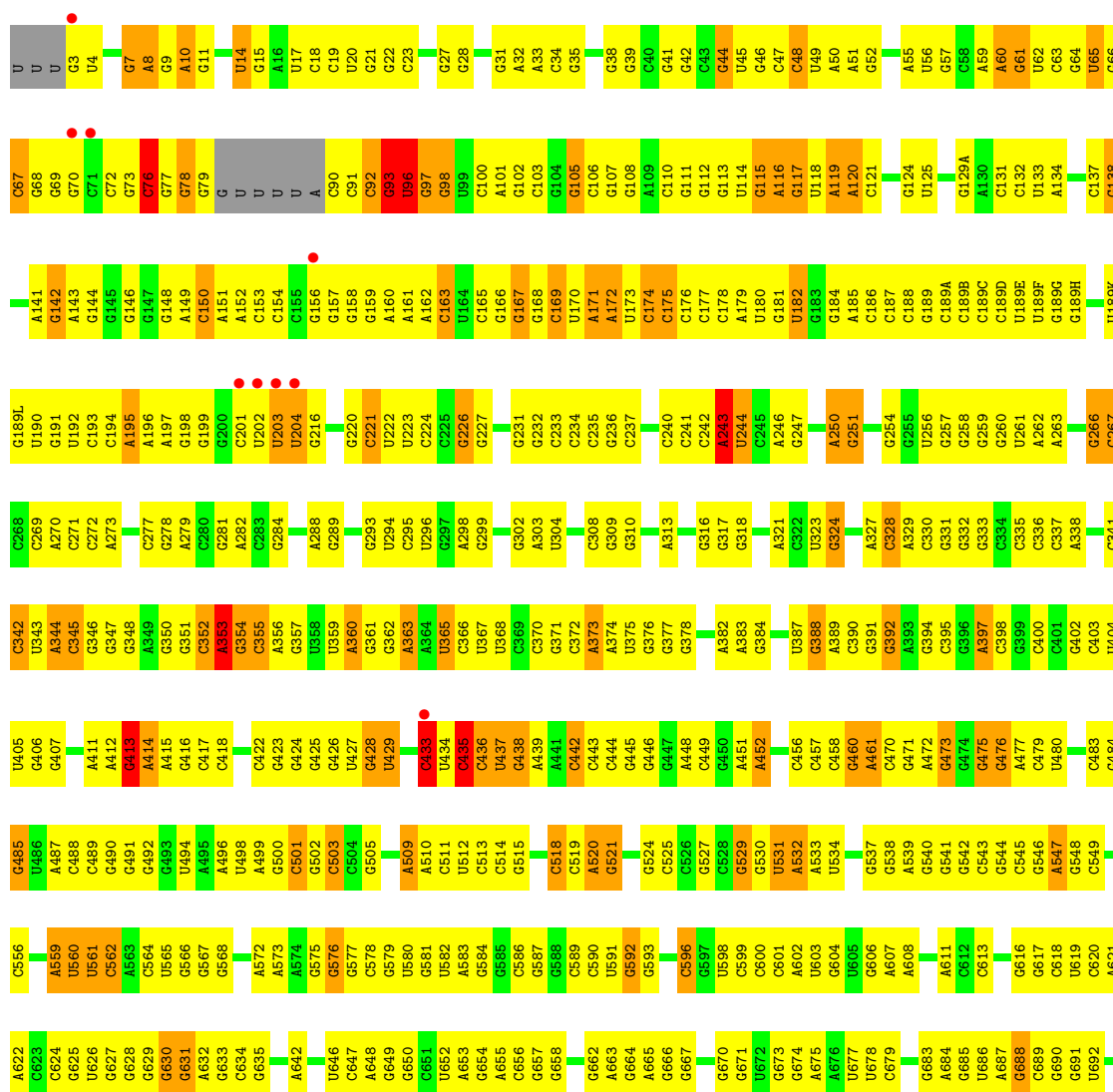
- Molecule 30: 50S ribosomal protein L35

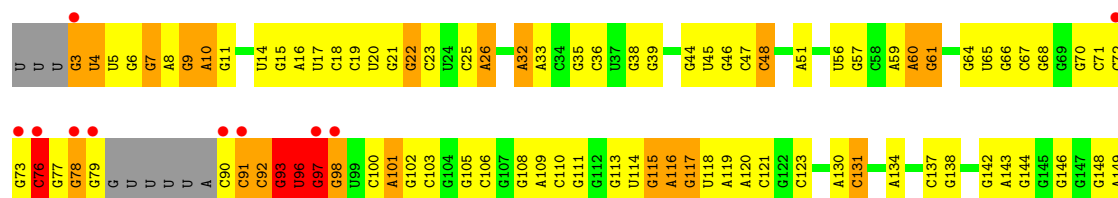
Chain B8:

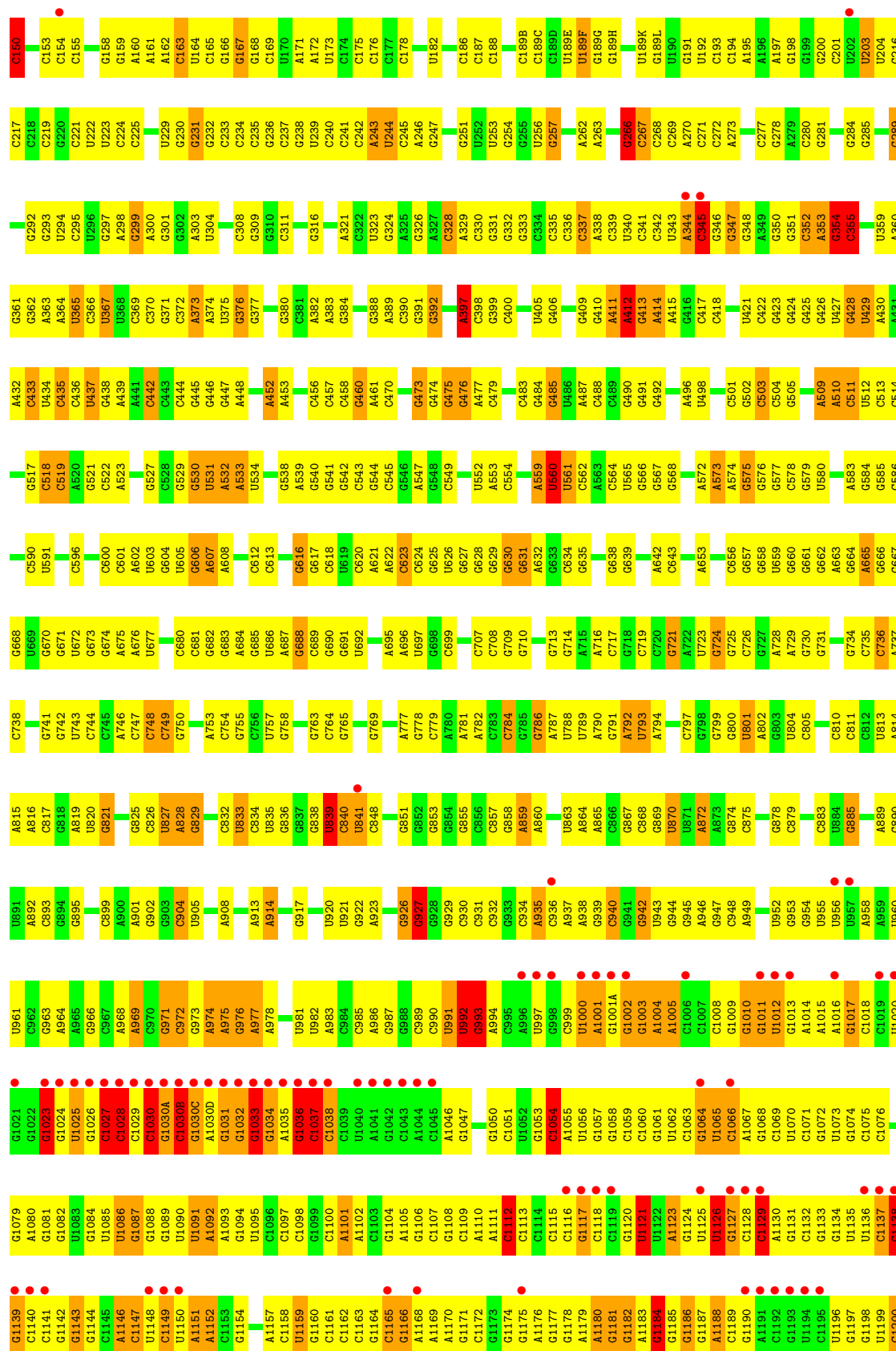


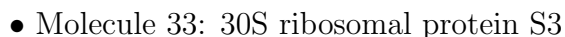
- Molecule 31: 16S ribosomal RNA

Chain CA:



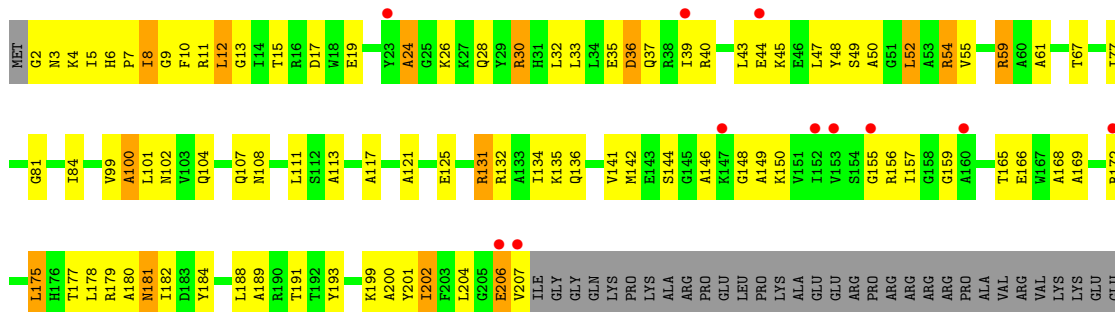




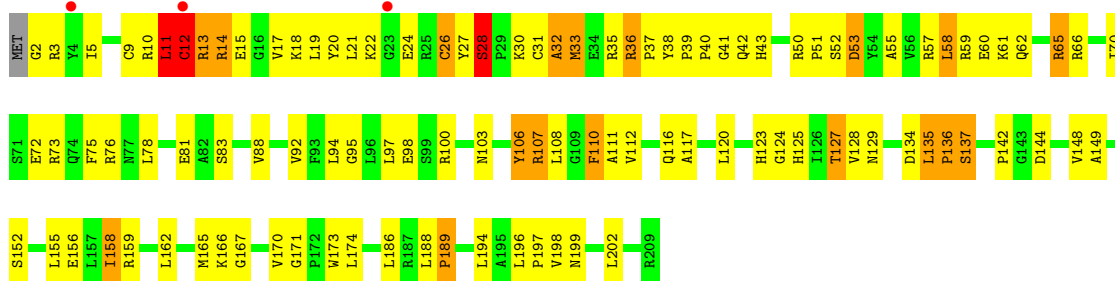


R190	T191	T192	T193	G194	V195	L196	K199	A200	V201	I202	E206	V207	ILE	GLY	GLY	GLN	LYS	PRO	LYS	ALA	ARG	PRO	GLU	LEU	PRO	LYS	ALA	ARG	ARG	ARG	ARG	VAL	ARG	VAL	LYS	GLU
R190	T191	T192	T193	G194	V195	L196	K199	A200	V201	I202	E206	V207	ILE	GLY	GLY	GLN	LYS	PRO	LYS	ALA	ARG	PRO	GLU	LEU	PRO	LYS	ALA	ARG	ARG	ARG	VAL	ARG	VAL	LYS	GLU	
					</																															

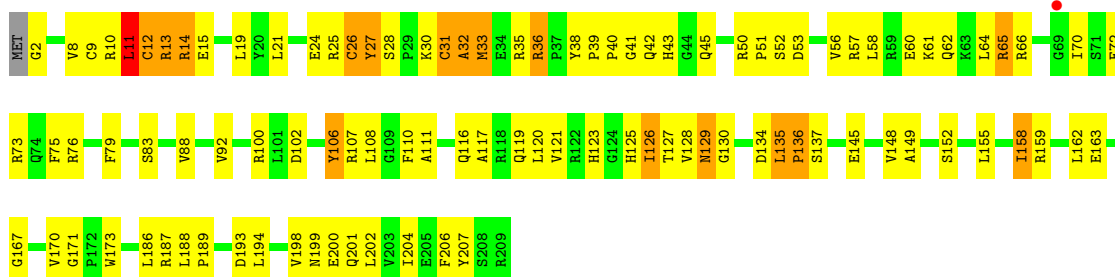
- Chain DC:



- Chain CD:

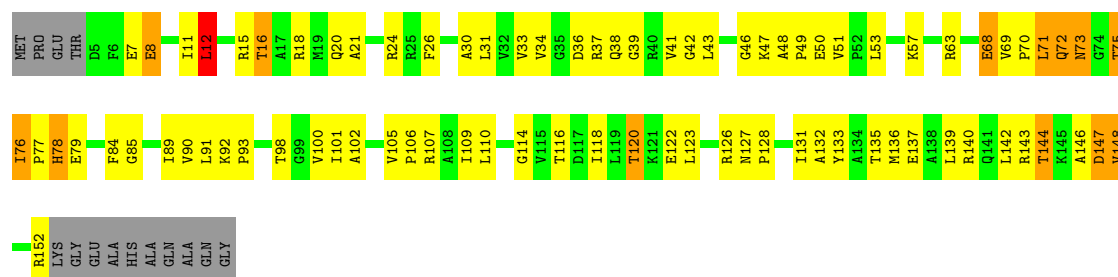


- Chain DD:



- Molecule 35: 30S ribosomal protein S5

Chain CE:



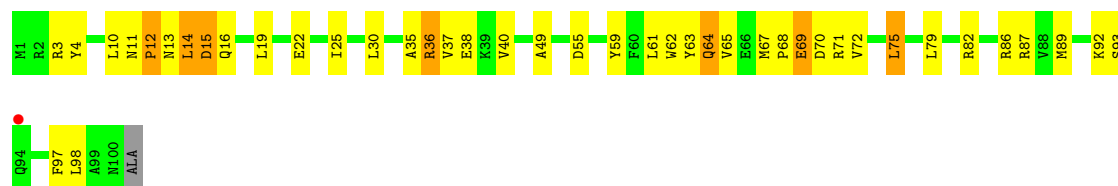
- Molecule 35: 30S ribosomal protein S5

Chain DE:



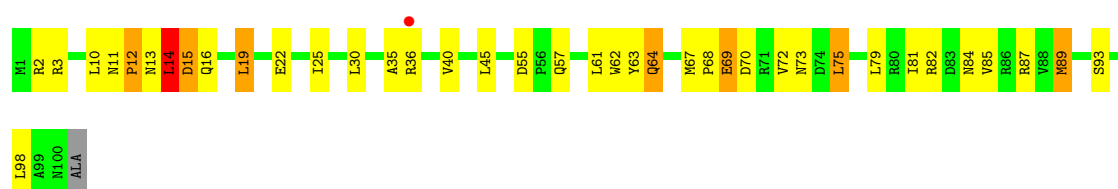
- Molecule 36: 30S ribosomal protein S6

Chain CF:



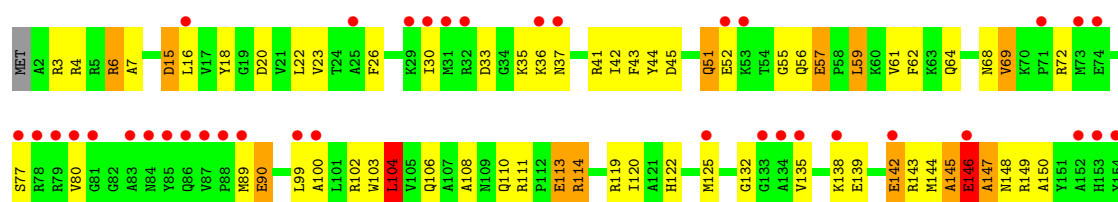
- Molecule 36: 30S ribosomal protein S6

Chain DF:



- Molecule 37: 30S ribosomal protein S7

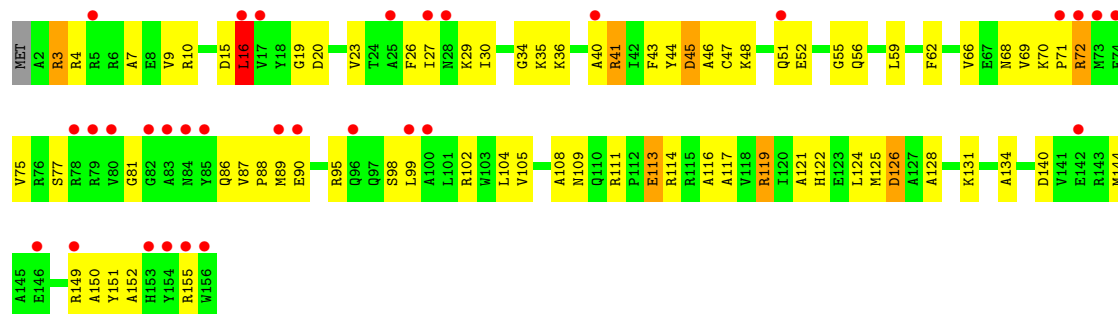
Chain CG:





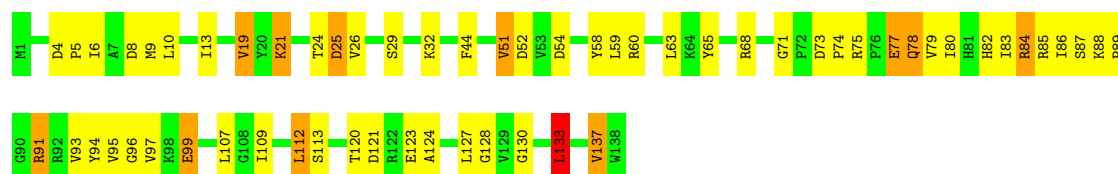
• Molecule 37: 30S ribosomal protein S7

Chain DG:



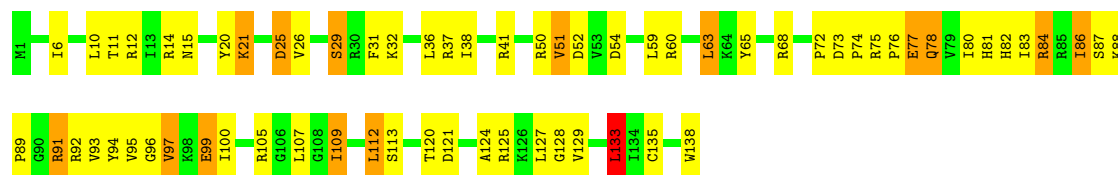
• Molecule 38: 30S ribosomal protein S8

Chain CH:



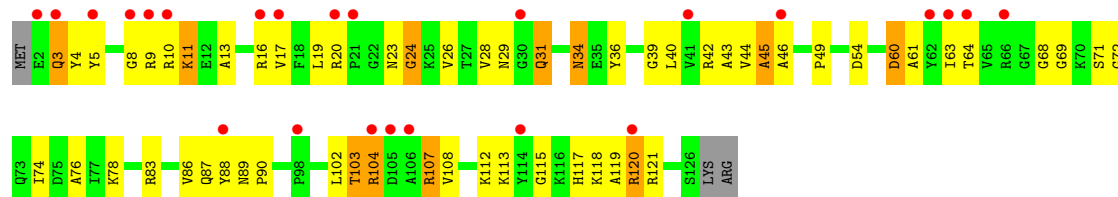
• Molecule 38: 30S ribosomal protein S8

Chain DH:



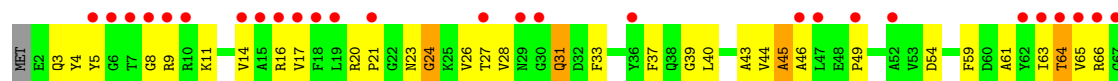
• Molecule 39: 30S ribosomal protein S9

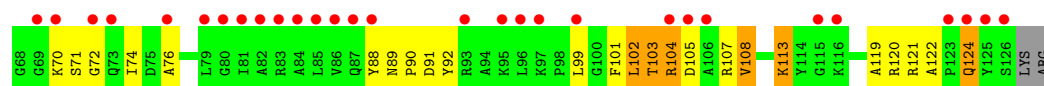
Chain CI:



• Molecule 39: 30S ribosomal protein S9

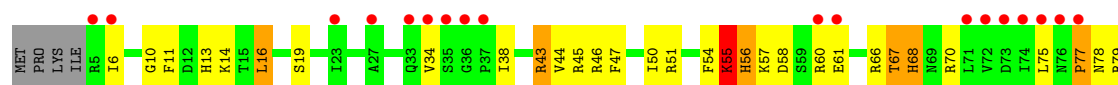
Chain DI:





- Molecule 40: 30S ribosomal protein S10

Chain CJ:



- Molecule 40: 30S ribosomal protein S10

Chain DJ:



- Molecule 41: 30S ribosomal protein S11

Chain CK:



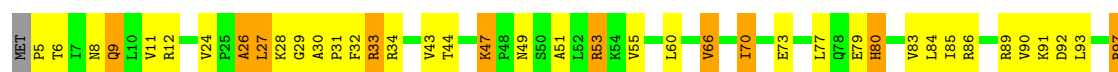
- Molecule 41: 30S ribosomal protein S11

Chain DK:



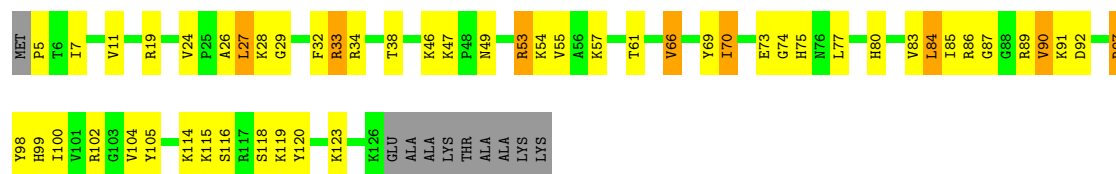
- Molecule 42: 30S ribosomal protein S12

Chain CL:



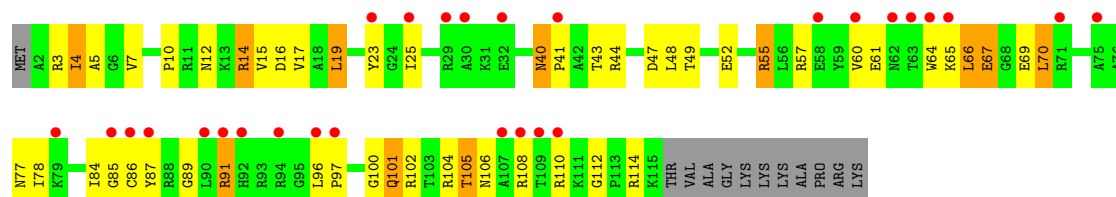
- Molecule 42: 30S ribosomal protein S12

Chain DL:



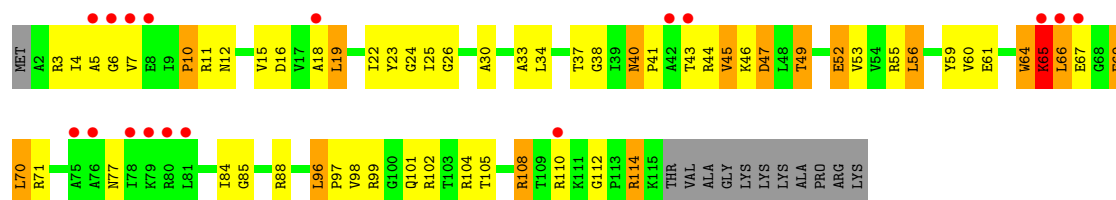
- Molecule 43: 30S ribosomal protein S13

Chain CM:



- Molecule 43: 30S ribosomal protein S13

Chain DM:



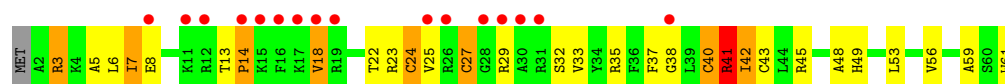
- Molecule 44: 30S ribosomal protein S14

Chain CN:



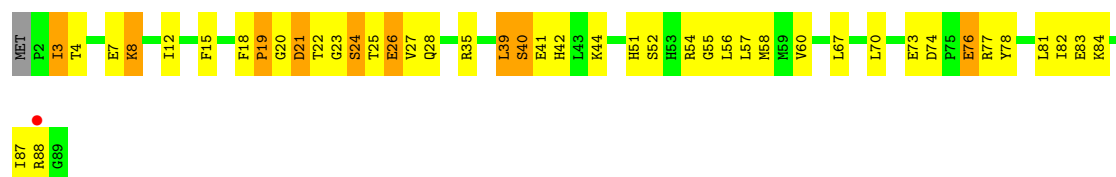
- Molecule 44: 30S ribosomal protein S14

Chain DN:



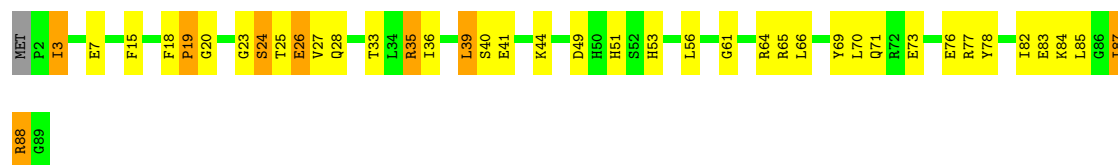
- Molecule 45: 30S ribosomal protein S15

Chain CO:



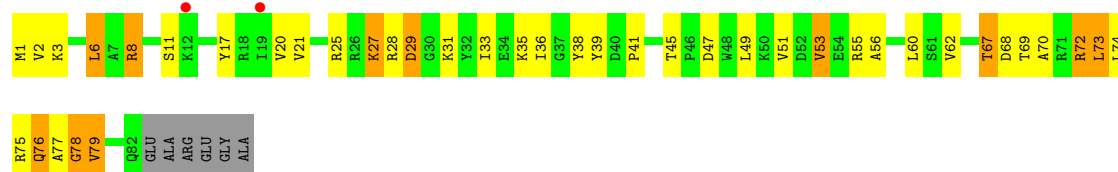
- Molecule 45: 30S ribosomal protein S15

Chain DO: 



- Molecule 46: 30S ribosomal protein S16

Chain CP: 



- Molecule 46: 30S ribosomal protein S16

Chain DP: 



- Molecule 47: 30S ribosomal protein S17

Chain CQ: 



- Molecule 47: 30S ribosomal protein S17

Chain DQ: 



- Molecule 48: 30S ribosomal protein S18

Chain CR: 

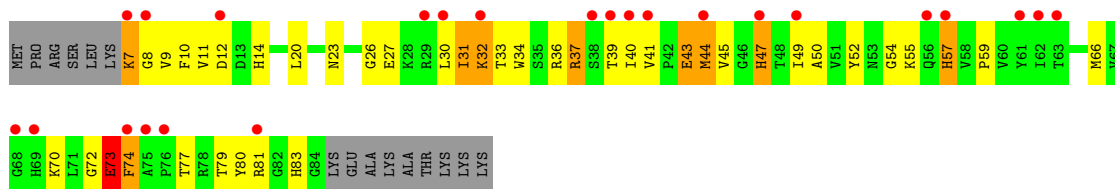


LYS

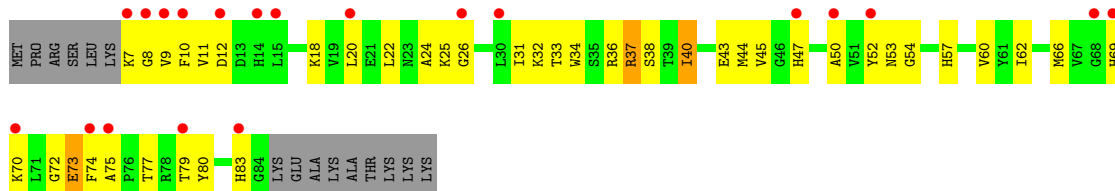
- Molecule 48: 30S ribosomal protein S18

Chain DR: 

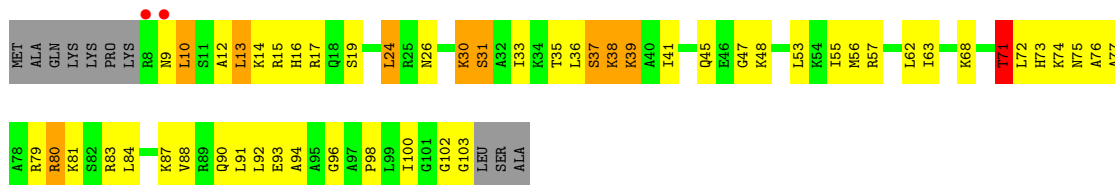
- Molecule 49: 30S ribosomal protein S19

Chain CS: 

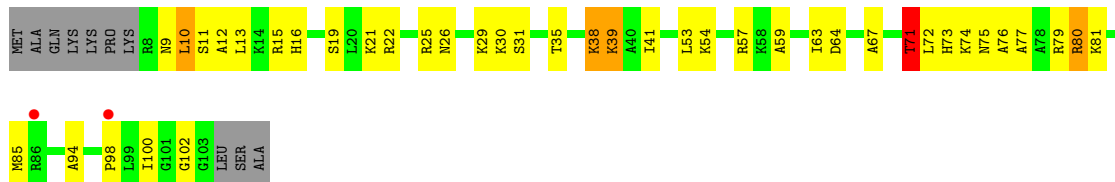
- Molecule 49: 30S ribosomal protein S19

Chain DS: 

- Molecule 50: 30S ribosomal protein S20

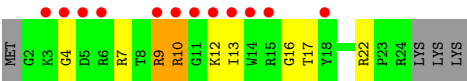
Chain CT: 

- Molecule 50: 30S ribosomal protein S20

Chain DT: 

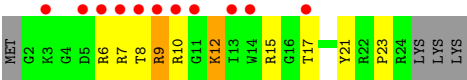
- Molecule 51: 30S ribosomal protein THX

Chain CU: 



● Molecule 51: 30S ribosomal protein THX

Chain DU:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.37Å 445.46Å 619.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.29 – 3.20 49.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.29-3.20) 99.7 (49.43-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.228 , 0.273 0.246 , 0.284	Depositor DCC
R_{free} test set	63137 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 36.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 1261811 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	279316	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, T8B

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	0.82	17/68203 (0.0%)	1.30	624/106459 (0.6%)
1	BA	1.20	70/68203 (0.1%)	1.37	800/106459 (0.8%)
2	AB	0.94	0/2879	1.25	21/4492 (0.5%)
2	BB	0.88	0/2879	1.26	21/4492 (0.5%)
3	AD	0.54	0/2186	0.75	2/2944 (0.1%)
3	BD	0.67	0/2186	0.81	4/2944 (0.1%)
4	AE	0.55	0/1588	0.76	0/2145
4	BE	0.72	0/1588	0.83	1/2145 (0.0%)
5	AF	0.51	0/1609	0.70	0/2177
5	BF	0.73	0/1609	0.77	0/2177
6	AG	0.61	0/1393	0.66	0/1892
6	BG	0.46	0/1393	0.64	0/1892
7	AH	0.58	0/1343	0.68	1/1820 (0.1%)
7	BH	0.59	0/1343	0.70	0/1820
8	AI	0.63	1/1061 (0.1%)	0.78	0/1451
8	BI	0.50	0/1061	0.74	0/1451
9	AN	0.52	0/1139	0.72	0/1538
9	BN	0.74	0/1139	0.78	0/1538
10	AO	0.50	0/933	0.72	1/1257 (0.1%)
10	BO	0.67	0/933	0.74	0/1257
11	AP	0.50	0/1135	0.75	1/1510 (0.1%)
11	BP	0.64	0/1135	0.81	2/1510 (0.1%)
12	AQ	0.53	0/1143	0.74	0/1527
12	BQ	0.64	0/1143	0.74	0/1527
13	AR	0.51	0/982	0.74	0/1312
13	BR	0.69	0/982	0.82	1/1312 (0.1%)
14	AS	0.64	0/875	0.79	0/1168
14	BS	0.53	0/875	0.79	1/1168 (0.1%)
15	AT	0.52	0/1077	0.73	0/1444
15	BT	0.61	0/1077	0.79	1/1444 (0.1%)
16	AU	0.56	0/977	0.69	0/1301
16	BU	0.88	1/977 (0.1%)	0.81	1/1301 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AV	0.58	0/782	0.67	0/1049
17	BV	0.70	0/782	0.77	0/1049
18	AW	0.56	0/891	0.75	0/1197
18	BW	0.82	0/891	0.80	0/1197
19	AX	0.55	0/756	0.77	1/1016 (0.1%)
19	BX	0.66	0/756	0.76	1/1016 (0.1%)
20	AY	0.50	0/798	0.77	0/1073
20	BY	0.61	0/798	0.80	1/1073 (0.1%)
21	AZ	0.57	0/1555	0.68	0/2118
21	BZ	0.49	0/1555	0.71	0/2118
22	A0	0.50	0/602	0.69	0/804
22	B0	0.66	0/602	0.77	0/804
23	A1	0.51	0/752	0.72	0/1003
23	B1	0.62	0/752	0.76	0/1003
24	A2	0.59	0/590	0.68	0/781
24	B2	0.60	0/590	0.74	0/781
25	A3	0.45	0/463	0.69	0/623
25	B3	0.65	0/463	0.74	0/623
26	A4	0.65	0/358	0.74	0/487
26	B4	0.56	0/358	0.74	1/487 (0.2%)
27	A5	0.67	1/469 (0.2%)	0.83	2/634 (0.3%)
27	B5	0.79	0/469	0.88	0/634
28	A6	0.59	0/456	0.70	0/609
28	B6	0.68	0/456	0.74	0/609
29	A7	0.57	0/426	0.75	0/561
29	B7	0.78	0/426	0.84	0/561
30	A8	0.50	0/516	0.73	0/679
30	B8	0.70	0/516	0.82	0/679
31	CA	0.80	10/36054 (0.0%)	1.18	176/56272 (0.3%)
31	DA	0.77	7/36054 (0.0%)	1.19	211/56272 (0.4%)
32	CB	0.51	0/1811	0.69	0/2452
32	DB	0.56	0/1811	0.69	0/2452
33	CC	0.56	0/1474	0.65	0/2003
33	DC	0.58	0/1474	0.65	0/2003
34	CD	0.53	0/1550	0.72	3/2106 (0.1%)
34	DD	0.84	2/1550 (0.1%)	0.78	4/2106 (0.2%)
35	CE	0.49	0/1121	0.70	1/1517 (0.1%)
35	DE	0.52	0/1121	0.72	1/1517 (0.1%)
36	CF	0.49	0/794	0.64	0/1082
36	DF	0.49	0/794	0.67	1/1082 (0.1%)
37	CG	0.57	0/1186	0.65	0/1603
37	DG	0.56	0/1186	0.62	0/1603
38	CH	0.44	0/1065	0.67	0/1445

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DH	0.44	0/1065	0.64	0/1445
39	CI	0.62	0/867	0.71	0/1180
39	DI	0.62	0/867	0.69	0/1180
40	CJ	0.60	0/672	0.74	1/919 (0.1%)
40	DJ	0.60	0/672	0.70	1/919 (0.1%)
41	CK	0.47	0/843	0.71	0/1144
41	DK	0.47	0/843	0.67	0/1144
42	CL	0.44	0/925	0.67	0/1251
42	DL	0.46	0/925	0.69	0/1251
43	CM	0.67	0/811	0.72	0/1103
43	DM	0.63	0/811	0.73	1/1103 (0.1%)
44	CN	0.60	0/487	0.68	0/649
44	DN	0.59	0/487	0.74	0/649
45	CO	0.49	0/735	0.64	0/981
45	DO	0.47	0/735	0.61	0/981
46	CP	0.51	0/667	0.70	0/905
46	DP	0.43	0/667	0.65	0/905
47	CQ	0.46	0/836	0.68	0/1117
47	DQ	0.47	0/836	0.66	0/1117
48	CR	0.43	0/519	0.64	0/699
48	DR	0.50	0/519	0.67	0/699
49	CS	0.69	0/558	0.88	1/759 (0.1%)
49	DS	0.76	1/558 (0.2%)	0.87	3/759 (0.4%)
50	CT	0.47	0/710	0.72	0/940
50	DT	0.42	0/710	0.68	0/940
51	CU	0.64	0/203	0.67	0/266
51	DU	0.59	0/203	0.70	0/266
All	All	0.86	110/303650 (0.0%)	1.16	1892/454928 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
26	A4	0	1
34	CD	0	1
34	DD	0	1
42	CL	0	1
42	DL	0	1
All	All	0	5

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	DD	12	CYS	CB-SG	19.94	2.16	1.82
34	DD	26	CYS	CB-SG	15.79	2.09	1.82
31	DA	1492	A	C6-N6	-12.21	1.24	1.33
31	CA	1492	A	C2-N3	12.12	1.44	1.33
31	CA	1493	A	N9-C4	-11.96	1.30	1.37

The worst 5 of 1892 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	DA	1492	A	C6-N1-C2	-28.45	101.53	118.60
31	DA	1492	A	C5-C6-N1	26.41	130.90	117.70
31	CA	1492	A	C8-N9-C4	-21.05	97.38	105.80
1	BA	1332	G	C2-N3-C4	-19.65	102.08	111.90
1	BA	1332	G	N3-C4-C5	17.99	137.59	128.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	A4	42	PHE	Peptide
34	CD	11	LEU	Peptide
42	CL	26	ALA	Peptide
34	DD	11	LEU	Peptide
42	DL	26	ALA	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	60900	0	30712	1406	0
1	BA	60900	0	30712	1060	0
2	AB	2574	0	1306	87	0
2	BB	2574	0	1306	35	0
3	AD	2136	0	2218	77	0
3	BD	2136	0	2218	81	0
4	AE	1555	0	1607	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	BE	1555	0	1607	54	0
5	AF	1576	0	1616	57	0
5	BF	1576	0	1616	59	0
6	AG	1368	0	1324	70	0
6	BG	1368	0	1324	61	0
7	AH	1317	0	1376	66	0
7	BH	1317	0	1376	33	0
8	AI	1046	0	1067	55	2
8	BI	1046	0	1067	47	0
9	AN	1112	0	1180	60	0
9	BN	1112	0	1180	34	0
10	AO	923	0	981	28	0
10	BO	923	0	981	23	0
11	AP	1119	0	1186	38	0
11	BP	1119	0	1186	40	0
12	AQ	1122	0	1179	43	0
12	BQ	1122	0	1179	47	0
13	AR	968	0	1033	43	0
13	BR	968	0	1033	33	0
14	AS	865	0	905	62	0
14	BS	865	0	905	54	0
15	AT	1063	0	1103	48	0
15	BT	1063	0	1103	37	0
16	AU	959	0	1019	31	0
16	BU	959	0	1019	20	0
17	AV	771	0	830	22	0
17	BV	771	0	830	15	0
18	AW	881	0	935	25	0
18	BW	881	0	935	24	0
19	AX	742	0	799	22	0
19	BX	742	0	799	23	0
20	AY	785	0	832	36	0
20	BY	785	0	832	30	0
21	AZ	1522	0	1511	56	0
21	BZ	1522	0	1511	47	0
22	A0	594	0	604	27	0
22	B0	594	0	604	21	0
23	A1	745	0	804	26	0
23	B1	745	0	804	26	0
24	A2	588	0	643	31	0
24	B2	588	0	643	18	0
25	A3	458	0	503	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	B3	458	0	503	6	0
26	A4	349	0	340	22	0
26	B4	349	0	340	16	0
27	A5	455	0	476	25	0
27	B5	455	0	476	18	0
28	A6	449	0	464	19	0
28	B6	449	0	466	17	0
29	A7	418	0	467	18	0
29	B7	418	0	467	14	0
30	A8	509	0	565	23	0
30	B8	509	0	565	20	0
31	CA	32208	0	16256	921	2
31	DA	32208	0	16254	923	0
32	CB	1777	0	1747	100	0
32	DB	1777	0	1747	95	0
33	CC	1450	0	1314	45	0
33	DC	1450	0	1314	58	0
34	CD	1520	0	1407	73	0
34	DD	1520	0	1406	85	0
35	CE	1105	0	1130	48	0
35	DE	1105	0	1130	54	0
36	CF	781	0	741	25	0
36	DF	781	0	741	29	0
37	CG	1167	0	1108	39	0
37	DG	1167	0	1108	46	0
38	CH	1045	0	1033	45	0
38	DH	1045	0	1033	53	0
39	CI	852	0	742	43	0
39	DI	852	0	742	52	0
40	CJ	659	0	552	31	0
40	DJ	659	0	552	37	0
41	CK	828	0	822	24	0
41	DK	828	0	822	32	0
42	CL	909	0	927	43	0
42	DL	909	0	927	38	0
43	CM	801	0	743	33	0
43	DM	801	0	743	37	0
44	CN	478	0	498	33	0
44	DN	478	0	497	30	0
45	CO	724	0	749	32	0
45	DO	724	0	749	27	0
46	CP	651	0	638	33	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	DP	651	0	638	28	0
47	CQ	823	0	891	33	0
47	DQ	823	0	891	22	0
48	CR	514	0	530	19	0
48	DR	514	0	530	17	0
49	CS	544	0	457	21	0
49	DS	544	0	457	26	0
50	CT	708	0	764	37	0
50	DT	708	0	764	26	0
51	CU	199	0	208	8	0
51	DU	199	0	208	6	0
52	AA	44	0	20	31	0
52	BA	44	0	20	23	0
53	AA	2	0	0	0	0
53	BA	2	0	0	0	0
All	All	279316	0	185722	7170	2

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 16.

The worst 5 of 7170 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
52:AA:3001:T8B:C13	31:DA:1492:A:H5''	1.47	1.41
34:DD:26:CYS:SG	34:DD:26:CYS:CB	2.09	1.41
34:DD:12:CYS:SG	34:DD:12:CYS:CB	2.16	1.34
52:AA:3001:T8B:H13	52:AA:3001:T8B:C22	1.58	1.33
52:BA:3001:T8B:H13	52:BA:3001:T8B:C22	1.58	1.32

All (2) 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)
8:AI:89:TYR:O	31:CA:357:G:O2'[2_654]	2.11	0.09
8:AI:91:SER:OG	31:CA:368:U:OP2[2_654]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AD	273/276 (99%)	240 (88%)	27 (10%)	6 (2%)	10	53
3	BD	273/276 (99%)	246 (90%)	23 (8%)	4 (2%)	15	64
4	AE	202/206 (98%)	177 (88%)	18 (9%)	7 (4%)	6	37
4	BE	202/206 (98%)	174 (86%)	21 (10%)	7 (4%)	6	37
5	AF	198/205 (97%)	168 (85%)	25 (13%)	5 (2%)	9	49
5	BF	198/205 (97%)	170 (86%)	21 (11%)	7 (4%)	6	37
6	AG	179/182 (98%)	136 (76%)	33 (18%)	10 (6%)	3	23
6	BG	179/182 (98%)	135 (75%)	30 (17%)	14 (8%)	1	11
7	AH	172/180 (96%)	143 (83%)	21 (12%)	8 (5%)	4	27
7	BH	172/180 (96%)	144 (84%)	22 (13%)	6 (4%)	6	37
8	AI	143/148 (97%)	103 (72%)	28 (20%)	12 (8%)	1	9
8	BI	143/148 (97%)	109 (76%)	24 (17%)	10 (7%)	2	13
9	AN	138/140 (99%)	113 (82%)	16 (12%)	9 (6%)	2	17
9	BN	138/140 (99%)	119 (86%)	13 (9%)	6 (4%)	4	30
10	AO	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	6	38
10	BO	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	6	38
11	AP	143/150 (95%)	117 (82%)	18 (13%)	8 (6%)	3	23
11	BP	143/150 (95%)	126 (88%)	12 (8%)	5 (4%)	6	37
12	AQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	7	43
12	BQ	139/141 (99%)	126 (91%)	9 (6%)	4 (3%)	7	43
13	AR	116/118 (98%)	95 (82%)	16 (14%)	5 (4%)	4	30
13	BR	116/118 (98%)	108 (93%)	7 (6%)	1 (1%)	25	76
14	AS	108/112 (96%)	84 (78%)	21 (19%)	3 (3%)	8	44
14	BS	108/112 (96%)	93 (86%)	12 (11%)	3 (3%)	8	44
15	AT	129/146 (88%)	109 (84%)	16 (12%)	4 (3%)	7	41
15	BT	129/146 (88%)	116 (90%)	12 (9%)	1 (1%)	27	77
16	AU	114/118 (97%)	104 (91%)	10 (9%)	0	100	100
16	BU	114/118 (97%)	111 (97%)	3 (3%)	0	100	100
17	AV	99/101 (98%)	89 (90%)	8 (8%)	2 (2%)	11	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	BV	99/101 (98%)	89 (90%)	9 (9%)	1 (1%)	22	74
18	AW	110/113 (97%)	101 (92%)	8 (7%)	1 (1%)	25	76
18	BW	110/113 (97%)	104 (94%)	6 (6%)	0	100	100
19	AX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	10	53
19	BX	93/96 (97%)	82 (88%)	9 (10%)	2 (2%)	10	53
20	AY	105/110 (96%)	90 (86%)	10 (10%)	5 (5%)	4	27
20	BY	105/110 (96%)	88 (84%)	13 (12%)	4 (4%)	5	34
21	AZ	196/206 (95%)	153 (78%)	32 (16%)	11 (6%)	3	23
21	BZ	196/206 (95%)	158 (81%)	31 (16%)	7 (4%)	5	36
22	A0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	16	66
22	B0	74/85 (87%)	67 (90%)	6 (8%)	1 (1%)	16	66
23	A1	95/98 (97%)	88 (93%)	5 (5%)	2 (2%)	11	55
23	B1	95/98 (97%)	86 (90%)	6 (6%)	3 (3%)	6	39
24	A2	68/72 (94%)	59 (87%)	8 (12%)	1 (2%)	15	64
24	B2	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
25	A3	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
25	B3	57/60 (95%)	54 (95%)	2 (4%)	1 (2%)	13	60
26	A4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	8
26	B4	44/71 (62%)	30 (68%)	10 (23%)	4 (9%)	1	8
27	A5	57/60 (95%)	50 (88%)	6 (10%)	1 (2%)	13	60
27	B5	57/60 (95%)	49 (86%)	6 (10%)	2 (4%)	6	37
28	A6	51/54 (94%)	46 (90%)	4 (8%)	1 (2%)	11	56
28	B6	51/54 (94%)	47 (92%)	4 (8%)	0	100	100
29	A7	46/49 (94%)	41 (89%)	4 (9%)	1 (2%)	10	53
29	B7	46/49 (94%)	42 (91%)	3 (6%)	1 (2%)	10	53
30	A8	62/65 (95%)	48 (77%)	13 (21%)	1 (2%)	14	63
30	B8	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
32	CB	227/256 (89%)	171 (75%)	36 (16%)	20 (9%)	1	8
32	DB	227/256 (89%)	173 (76%)	39 (17%)	15 (7%)	2	16
33	CC	204/239 (85%)	163 (80%)	30 (15%)	11 (5%)	3	24
33	DC	204/239 (85%)	144 (71%)	42 (21%)	18 (9%)	1	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	CD	206/209 (99%)	154 (75%)	40 (19%)	12 (6%)	3	21
34	DD	206/209 (99%)	152 (74%)	47 (23%)	7 (3%)	6	38
35	CE	146/162 (90%)	112 (77%)	23 (16%)	11 (8%)	2	12
35	DE	146/162 (90%)	116 (80%)	25 (17%)	5 (3%)	6	38
36	CF	98/101 (97%)	87 (89%)	8 (8%)	3 (3%)	7	41
36	DF	98/101 (97%)	85 (87%)	9 (9%)	4 (4%)	4	32
37	CG	153/156 (98%)	127 (83%)	16 (10%)	10 (6%)	2	17
37	DG	153/156 (98%)	129 (84%)	18 (12%)	6 (4%)	5	33
38	CH	136/138 (99%)	116 (85%)	18 (13%)	2 (2%)	15	64
38	DH	136/138 (99%)	118 (87%)	13 (10%)	5 (4%)	5	34
39	CI	123/128 (96%)	93 (76%)	20 (16%)	10 (8%)	1	10
39	DI	123/128 (96%)	94 (76%)	21 (17%)	8 (6%)	2	17
40	CJ	94/105 (90%)	66 (70%)	19 (20%)	9 (10%)	1	7
40	DJ	94/105 (90%)	74 (79%)	14 (15%)	6 (6%)	2	17
41	CK	112/129 (87%)	96 (86%)	12 (11%)	4 (4%)	5	36
41	DK	112/129 (87%)	90 (80%)	19 (17%)	3 (3%)	8	46
42	CL	120/132 (91%)	98 (82%)	17 (14%)	5 (4%)	4	31
42	DL	120/132 (91%)	100 (83%)	15 (12%)	5 (4%)	4	31
43	CM	112/126 (89%)	84 (75%)	18 (16%)	10 (9%)	1	8
43	DM	112/126 (89%)	80 (71%)	20 (18%)	12 (11%)	1	5
44	CN	58/61 (95%)	43 (74%)	10 (17%)	5 (9%)	1	8
44	DN	58/61 (95%)	48 (83%)	7 (12%)	3 (5%)	3	25
45	CO	86/89 (97%)	71 (83%)	12 (14%)	3 (4%)	6	37
45	DO	86/89 (97%)	68 (79%)	16 (19%)	2 (2%)	10	52
46	CP	80/88 (91%)	50 (62%)	23 (29%)	7 (9%)	1	8
46	DP	80/88 (91%)	52 (65%)	25 (31%)	3 (4%)	5	34
47	CQ	97/105 (92%)	84 (87%)	8 (8%)	5 (5%)	3	25
47	DQ	97/105 (92%)	81 (84%)	13 (13%)	3 (3%)	7	41
48	CR	66/88 (75%)	55 (83%)	10 (15%)	1 (2%)	15	64
48	DR	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
49	CS	76/93 (82%)	48 (63%)	17 (22%)	11 (14%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DS	76/93 (82%)	54 (71%)	17 (22%)	5 (7%)	2	16
50	CT	94/106 (89%)	73 (78%)	13 (14%)	8 (8%)	1	9
50	DT	94/106 (89%)	72 (77%)	15 (16%)	7 (7%)	2	12
51	CU	21/27 (78%)	18 (86%)	3 (14%)	0	100	100
51	DU	21/27 (78%)	16 (76%)	3 (14%)	2 (10%)	1	7
All	All	11280/12044 (94%)	9338 (83%)	1460 (13%)	482 (4%)	4	30

5 of 482 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AD	239	ARG
3	AD	275	LYS
5	AF	60	SER
6	AG	14	GLU
6	AG	78	SER

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AD	215/218 (99%)	185 (86%)	30 (14%)	5	23
3	BD	215/218 (99%)	189 (88%)	26 (12%)	7	32
4	AE	163/166 (98%)	139 (85%)	24 (15%)	4	21
4	BE	163/166 (98%)	134 (82%)	29 (18%)	2	13
5	AF	158/162 (98%)	133 (84%)	25 (16%)	4	16
5	BF	158/162 (98%)	138 (87%)	20 (13%)	6	29
6	AG	128/156 (82%)	110 (86%)	18 (14%)	5	23
6	BG	128/156 (82%)	114 (89%)	14 (11%)	9	37
7	AH	141/148 (95%)	125 (89%)	16 (11%)	9	36
7	BH	141/148 (95%)	124 (88%)	17 (12%)	7	32
8	AI	102/124 (82%)	76 (74%)	26 (26%)	1	3
8	BI	102/124 (82%)	76 (74%)	26 (26%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AN	117/119 (98%)	94 (80%)	23 (20%)	2	10
9	BN	117/119 (98%)	91 (78%)	26 (22%)	1	6
10	AO	98/100 (98%)	89 (91%)	9 (9%)	13	47
10	BO	98/100 (98%)	89 (91%)	9 (9%)	13	47
11	AP	113/116 (97%)	96 (85%)	17 (15%)	4	19
11	BP	113/116 (97%)	97 (86%)	16 (14%)	5	22
12	AQ	111/111 (100%)	94 (85%)	17 (15%)	4	18
12	BQ	111/111 (100%)	94 (85%)	17 (15%)	4	18
13	AR	101/101 (100%)	80 (79%)	21 (21%)	2	8
13	BR	101/101 (100%)	79 (78%)	22 (22%)	1	7
14	AS	84/88 (96%)	67 (80%)	17 (20%)	2	9
14	BS	84/88 (96%)	72 (86%)	12 (14%)	5	22
15	AT	110/127 (87%)	99 (90%)	11 (10%)	11	41
15	BT	110/127 (87%)	100 (91%)	10 (9%)	14	47
16	AU	93/94 (99%)	83 (89%)	10 (11%)	9	37
16	BU	93/94 (99%)	77 (83%)	16 (17%)	3	14
17	AV	80/82 (98%)	63 (79%)	17 (21%)	1	7
17	BV	80/82 (98%)	63 (79%)	17 (21%)	1	7
18	AW	89/92 (97%)	75 (84%)	14 (16%)	4	17
18	BW	89/92 (97%)	78 (88%)	11 (12%)	7	30
19	AX	75/78 (96%)	67 (89%)	8 (11%)	10	38
19	BX	75/78 (96%)	66 (88%)	9 (12%)	7	32
20	AY	80/91 (88%)	70 (88%)	10 (12%)	7	30
20	BY	80/91 (88%)	72 (90%)	8 (10%)	11	41
21	AZ	159/179 (89%)	139 (87%)	20 (13%)	7	30
21	BZ	159/179 (89%)	137 (86%)	22 (14%)	5	24
22	A0	59/67 (88%)	52 (88%)	7 (12%)	8	33
22	B0	59/67 (88%)	52 (88%)	7 (12%)	8	33
23	A1	78/83 (94%)	68 (87%)	10 (13%)	6	28
23	B1	78/83 (94%)	70 (90%)	8 (10%)	10	40
24	A2	65/67 (97%)	56 (86%)	9 (14%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	B2	65/67 (97%)	57 (88%)	8 (12%)	7	31
25	A3	49/52 (94%)	43 (88%)	6 (12%)	7	31
25	B3	49/52 (94%)	43 (88%)	6 (12%)	7	31
26	A4	39/63 (62%)	32 (82%)	7 (18%)	2	12
26	B4	39/63 (62%)	30 (77%)	9 (23%)	1	5
27	A5	50/52 (96%)	43 (86%)	7 (14%)	5	23
27	B5	50/52 (96%)	43 (86%)	7 (14%)	5	23
28	A6	50/52 (96%)	40 (80%)	10 (20%)	2	9
28	B6	50/52 (96%)	41 (82%)	9 (18%)	2	12
29	A7	41/42 (98%)	35 (85%)	6 (15%)	5	21
29	B7	41/42 (98%)	32 (78%)	9 (22%)	1	7
30	A8	52/55 (94%)	45 (86%)	7 (14%)	6	26
30	B8	52/55 (94%)	47 (90%)	5 (10%)	12	44
32	CB	177/220 (80%)	141 (80%)	36 (20%)	2	9
32	DB	177/220 (80%)	142 (80%)	35 (20%)	2	9
33	CC	114/188 (61%)	95 (83%)	19 (17%)	3	14
33	DC	114/188 (61%)	96 (84%)	18 (16%)	4	16
34	CD	139/181 (77%)	117 (84%)	22 (16%)	4	16
34	DD	139/181 (77%)	120 (86%)	19 (14%)	5	25
35	CE	108/123 (88%)	86 (80%)	22 (20%)	2	8
35	DE	108/123 (88%)	88 (82%)	20 (18%)	2	11
36	CF	77/90 (86%)	65 (84%)	12 (16%)	4	17
36	DF	77/90 (86%)	65 (84%)	12 (16%)	4	17
37	CG	104/127 (82%)	86 (83%)	18 (17%)	3	13
37	DG	104/127 (82%)	88 (85%)	16 (15%)	4	18
38	CH	103/119 (87%)	85 (82%)	18 (18%)	3	13
38	DH	103/119 (87%)	84 (82%)	19 (18%)	2	11
39	CI	62/99 (63%)	53 (86%)	9 (14%)	5	22
39	DI	62/99 (63%)	54 (87%)	8 (13%)	6	28
40	CJ	52/92 (56%)	42 (81%)	10 (19%)	2	10
40	DJ	52/92 (56%)	41 (79%)	11 (21%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	CK	81/99 (82%)	69 (85%)	12 (15%)	4	20
41	DK	81/99 (82%)	71 (88%)	10 (12%)	7	31
42	CL	92/109 (84%)	81 (88%)	11 (12%)	7	32
42	DL	92/109 (84%)	83 (90%)	9 (10%)	12	43
43	CM	63/101 (62%)	49 (78%)	14 (22%)	1	6
43	DM	63/101 (62%)	49 (78%)	14 (22%)	1	6
44	CN	46/50 (92%)	35 (76%)	11 (24%)	1	4
44	DN	46/50 (92%)	33 (72%)	13 (28%)	0	2
45	CO	77/80 (96%)	65 (84%)	12 (16%)	4	17
45	DO	77/80 (96%)	66 (86%)	11 (14%)	5	22
46	CP	63/74 (85%)	49 (78%)	14 (22%)	1	6
46	DP	63/74 (85%)	53 (84%)	10 (16%)	4	16
47	CQ	94/97 (97%)	90 (96%)	4 (4%)	40	81
47	DQ	94/97 (97%)	84 (89%)	10 (11%)	10	38
48	CR	49/77 (64%)	44 (90%)	5 (10%)	11	40
48	DR	49/77 (64%)	46 (94%)	3 (6%)	26	71
49	CS	42/80 (52%)	25 (60%)	17 (40%)	0	0
49	DS	42/80 (52%)	36 (86%)	6 (14%)	5	22
50	CT	65/82 (79%)	53 (82%)	12 (18%)	2	11
50	DT	65/82 (79%)	57 (88%)	8 (12%)	7	31
51	CU	18/22 (82%)	16 (89%)	2 (11%)	9	36
51	DU	18/22 (82%)	14 (78%)	4 (22%)	1	6
All	All	8652/9990 (87%)	7319 (85%)	1333 (15%)	4	18

5 of 1333 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	BR	6	SER
24	B2	34	GLU
40	DJ	72	VAL
13	BR	96	ARG
17	BV	85	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
13	BR	13	HIS
35	CE	78	HIS
43	DM	106	ASN
19	BX	31	HIS
30	B8	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	2819/2915 (96%)	581 (20%)	59 (2%)
1	BA	2819/2915 (96%)	586 (20%)	60 (2%)
2	AB	119/122 (97%)	25 (21%)	0
2	BB	119/122 (97%)	21 (17%)	0
31	CA	1496/1521 (98%)	339 (22%)	31 (2%)
31	DA	1496/1521 (98%)	341 (22%)	27 (1%)
All	All	8868/9116 (97%)	1893 (21%)	177 (1%)

5 of 1893 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	10	G
1	AA	14	A
1	AA	15	G
1	AA	34	C
1	AA	45	C

5 of 177 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	BA	1047	G
1	BA	1819	A
31	DA	560	U
1	BA	1106	A
1	BA	1301	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
52	T8B	AA	3001	53	48,48,48	1.81	5 (10%)	68,71,71	49.73	9 (13%)
52	T8B	BA	3001	53	48,48,48	1.81	5 (10%)	68,71,71	49.55	9 (13%)

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
52	T8B	AA	3001	53	-	0/24/26/26	0/5/5/5
52	T8B	BA	3001	53	-	0/24/26/26	0/5/5/5

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AA	3001	T8B	O5-C14	8.21	1.37	1.33
52	BA	3001	T8B	O5-C14	8.16	1.37	1.33
52	AA	3001	T8B	C14-C15	5.12	1.49	1.37
52	BA	3001	T8B	C14-C15	5.10	1.48	1.37
52	AA	3001	T8B	O5-C11	4.72	1.40	1.35

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	AA	3001	T8B	O5-C11-C12	409.99	117.33	112.43
52	BA	3001	T8B	O5-C11-C12	408.48	117.32	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	BA	3001	T8B	O5-C11-C10	4.05	124.04	119.36
52	AA	3001	T8B	O5-C11-C10	4.02	124.01	119.36
52	BA	3001	T8B	C21-C23-C24	-3.49	120.19	125.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	2827/2915 (96%)	-0.16	93 (3%) 44 9	46, 70, 113, 128	0
1	BA	2827/2915 (96%)	-0.10	55 (1%) 64 18	27, 56, 110, 126	0
2	AB	120/122 (98%)	-0.09	4 (3%) 44 9	68, 95, 108, 111	0
2	BB	120/122 (98%)	-0.38	0 100 100	46, 80, 95, 103	0
3	AD	275/276 (99%)	-0.10	0 100 100	45, 67, 83, 103	0
3	BD	275/276 (99%)	-0.15	1 (0%) 90 51	36, 59, 78, 103	0
4	AE	204/206 (99%)	-0.13	0 100 100	47, 72, 87, 98	0
4	BE	204/206 (99%)	-0.19	0 100 100	33, 60, 81, 96	0
5	AF	203/205 (99%)	-0.26	0 100 100	44, 77, 95, 112	0
5	BF	203/205 (99%)	-0.21	0 100 100	27, 64, 90, 110	0
6	AG	181/182 (99%)	0.77	23 (12%) 4 1	89, 106, 114, 116	0
6	BG	181/182 (99%)	0.00	1 (0%) 86 41	81, 101, 110, 118	0
7	AH	174/180 (96%)	0.50	8 (4%) 31 6	80, 93, 101, 108	0
7	BH	174/180 (96%)	-0.15	0 100 100	63, 78, 91, 98	0
8	AI	145/148 (97%)	0.34	11 (7%) 14 3	72, 104, 116, 123	0
8	BI	145/148 (97%)	-0.11	0 100 100	68, 90, 98, 100	0
9	AN	140/140 (100%)	-0.11	0 100 100	59, 73, 90, 94	0
9	BN	140/140 (100%)	-0.20	0 100 100	38, 57, 82, 85	0
10	AO	122/122 (100%)	-0.26	0 100 100	56, 73, 85, 91	0
10	BO	122/122 (100%)	-0.22	0 100 100	43, 64, 82, 89	0
11	AP	147/150 (98%)	-0.02	1 (0%) 84 38	47, 81, 96, 105	0
11	BP	147/150 (98%)	-0.17	0 100 100	28, 68, 91, 100	0
12	AQ	141/141 (100%)	-0.00	0 100 100	60, 78, 91, 97	0
12	BQ	141/141 (100%)	-0.13	0 100 100	44, 65, 78, 88	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AR	118/118 (100%)	-0.13	0 100 100	47, 66, 78, 88	0
13	BR	118/118 (100%)	-0.19	0 100 100	35, 53, 69, 86	0
14	AS	110/112 (98%)	0.34	3 (2%) 52 11	74, 91, 102, 109	0
14	BS	110/112 (98%)	-0.11	0 100 100	58, 79, 93, 100	0
15	AT	131/146 (89%)	-0.14	1 (0%) 83 35	66, 76, 99, 109	0
15	BT	131/146 (89%)	-0.24	0 100 100	55, 68, 91, 102	0
16	AU	116/118 (98%)	-0.07	0 100 100	53, 70, 84, 89	0
16	BU	116/118 (98%)	-0.16	0 100 100	34, 50, 70, 84	0
17	AV	101/101 (100%)	-0.16	0 100 100	48, 79, 93, 103	0
17	BV	101/101 (100%)	-0.28	0 100 100	31, 61, 81, 95	0
18	AW	112/113 (99%)	-0.22	0 100 100	50, 59, 80, 104	0
18	BW	112/113 (99%)	-0.27	0 100 100	36, 45, 75, 106	0
19	AX	95/96 (98%)	-0.08	0 100 100	54, 71, 89, 93	0
19	BX	95/96 (98%)	-0.16	0 100 100	33, 59, 83, 91	0
20	AY	107/110 (97%)	0.09	1 (0%) 81 32	71, 81, 94, 105	0
20	BY	107/110 (97%)	-0.17	1 (0%) 81 32	56, 71, 89, 103	0
21	AZ	198/206 (96%)	-0.02	2 (1%) 79 29	80, 92, 103, 108	0
21	BZ	198/206 (96%)	-0.26	0 100 100	64, 82, 97, 103	0
22	A0	76/85 (89%)	0.12	1 (1%) 74 24	59, 74, 84, 89	0
22	B0	76/85 (89%)	-0.18	0 100 100	46, 60, 74, 82	0
23	A1	97/98 (98%)	0.05	1 (1%) 79 29	54, 71, 94, 99	0
23	B1	97/98 (98%)	-0.13	0 100 100	42, 65, 91, 95	0
24	A2	70/72 (97%)	-0.07	0 100 100	65, 81, 92, 101	0
24	B2	70/72 (97%)	-0.11	0 100 100	52, 70, 85, 102	0
25	A3	59/60 (98%)	0.28	3 (5%) 27 5	63, 74, 92, 101	0
25	B3	59/60 (98%)	-0.17	0 100 100	43, 56, 84, 94	0
26	A4	46/71 (64%)	0.18	0 100 100	101, 109, 113, 119	0
26	B4	46/71 (64%)	0.14	1 (2%) 59 14	98, 107, 113, 118	0
27	A5	59/60 (98%)	-0.24	0 100 100	46, 64, 78, 91	0
27	B5	59/60 (98%)	-0.21	0 100 100	28, 52, 71, 89	0
28	A6	53/54 (98%)	0.03	1 (1%) 64 18	62, 77, 87, 89	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B6	53/54 (98%)	-0.18	0 100 100	52, 66, 77, 85	0
29	A7	48/49 (97%)	0.09	1 (2%) 60 15	43, 54, 79, 99	0
29	B7	48/49 (97%)	-0.01	0 100 100	29, 44, 73, 89	0
30	A8	64/65 (98%)	0.10	0 100 100	60, 68, 76, 85	0
30	B8	64/65 (98%)	0.05	0 100 100	45, 56, 65, 79	0
31	CA	1498/1521 (98%)	0.33	147 (9%) 8 2	59, 99, 120, 126	0
31	DA	1498/1521 (98%)	0.29	131 (8%) 10 3	65, 99, 120, 128	0
32	CB	229/256 (89%)	0.01	4 (1%) 67 19	93, 103, 111, 117	0
32	DB	229/256 (89%)	0.31	9 (3%) 37 7	95, 105, 112, 115	0
33	CC	206/239 (86%)	0.55	19 (9%) 9 2	92, 106, 112, 115	0
33	DC	206/239 (86%)	0.51	11 (5%) 25 5	97, 108, 115, 120	0
34	CD	208/209 (99%)	-0.00	3 (1%) 72 22	85, 98, 108, 114	0
34	DD	208/209 (99%)	-0.03	1 (0%) 88 46	87, 97, 107, 123	0
35	CE	148/162 (91%)	-0.17	0 100 100	74, 93, 103, 110	0
35	DE	148/162 (91%)	0.03	0 100 100	84, 96, 104, 110	0
36	CF	100/101 (99%)	-0.10	1 (1%) 79 29	80, 92, 101, 107	0
36	DF	100/101 (99%)	-0.10	1 (1%) 79 29	84, 93, 103, 110	0
37	CG	155/156 (99%)	1.35	39 (25%) 1 1	99, 109, 115, 120	0
37	DG	155/156 (99%)	1.16	31 (20%) 2 1	97, 109, 115, 119	0
38	CH	138/138 (100%)	-0.01	0 100 100	82, 94, 101, 104	0
38	DH	138/138 (100%)	-0.07	0 100 100	86, 96, 102, 106	0
39	CI	125/128 (97%)	1.12	24 (19%) 2 1	97, 111, 117, 120	0
39	DI	125/128 (97%)	1.95	56 (44%) 1 0	100, 112, 118, 120	0
40	CJ	96/105 (91%)	1.20	20 (20%) 1 1	100, 109, 115, 117	0
40	DJ	96/105 (91%)	1.14	14 (14%) 3 1	97, 110, 115, 119	0
41	CK	114/129 (88%)	-0.12	0 100 100	72, 93, 101, 105	0
41	DK	114/129 (88%)	0.02	0 100 100	75, 95, 103, 107	0
42	CL	122/132 (92%)	-0.17	0 100 100	72, 85, 96, 100	0
42	DL	122/132 (92%)	-0.07	0 100 100	77, 87, 96, 105	0
43	CM	114/126 (90%)	1.35	28 (24%) 1 1	102, 111, 118, 126	0
43	DM	114/126 (90%)	1.12	17 (14%) 3 1	101, 109, 115, 117	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CN	60/61 (98%)	0.68	7 (11%) 5 2	99, 108, 116, 118	0
44	DN	60/61 (98%)	1.10	16 (26%) 1 1	103, 111, 116, 122	0
45	CO	88/89 (98%)	0.00	1 (1%) 77 27	72, 91, 101, 107	0
45	DO	88/89 (98%)	0.12	0 100 100	81, 93, 103, 107	0
46	CP	82/88 (93%)	0.29	2 (2%) 56 13	88, 96, 106, 112	0
46	DP	82/88 (93%)	0.30	0 100 100	86, 94, 103, 111	0
47	CQ	99/105 (94%)	0.05	0 100 100	78, 90, 98, 102	0
47	DQ	99/105 (94%)	0.04	1 (1%) 79 29	79, 92, 100, 103	0
48	CR	68/88 (77%)	0.03	2 (2%) 49 10	80, 91, 102, 103	0
48	DR	68/88 (77%)	0.18	0 100 100	85, 93, 104, 106	0
49	CS	78/93 (83%)	1.60	24 (30%) 1 1	107, 111, 117, 123	0
49	DS	78/93 (83%)	1.54	20 (25%) 1 1	91, 112, 117, 119	0
50	CT	96/106 (90%)	0.11	2 (2%) 60 15	84, 93, 99, 102	0
50	DT	96/106 (90%)	0.40	2 (2%) 60 15	82, 92, 100, 101	0
51	CU	23/27 (85%)	2.31	12 (52%) 0 0	106, 112, 117, 119	0
51	DU	23/27 (85%)	2.06	11 (47%) 1 0	104, 109, 112, 113	0
All	All	20372/21160 (96%)	0.09	869 (4%) 34 7	27, 84, 115, 128	0

The worst 5 of 869 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
31	CA	1286	A	10.1
31	CA	1353	G	9.7
31	DA	1149	C	9.4
31	DA	1286	A	8.6
49	CS	40	ILE	7.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 95th 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 ²)	Q<0.9
53	MG	BA	3003	1/1	0.15	-	30,30,30,30	0
52	T8B	BA	3001	44/44	0.32	-	20,20,20,20	0
53	MG	BA	3002	1/1	0.15	-	30,30,30,30	0
53	MG	AA	3002	1/1	0.19	-	30,30,30,30	0
52	T8B	AA	3001	44/44	0.26	-	20,20,20,20	0
53	MG	AA	3003	1/1	0.16	-	30,30,30,30	0

6.5 Other polymers

There are no such residues in this entry.