



# wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 08:43 PM BST

PDB ID : 4V5G  
Title : The crystal structure of the 70S ribosome bound to EF-Tu and tRNA  
Authors : Schmeing, T.M.; Voorhees, R.M.; Ramakrishnan, V.  
Deposited on : 2009-09-01  
Resolution : 3.60 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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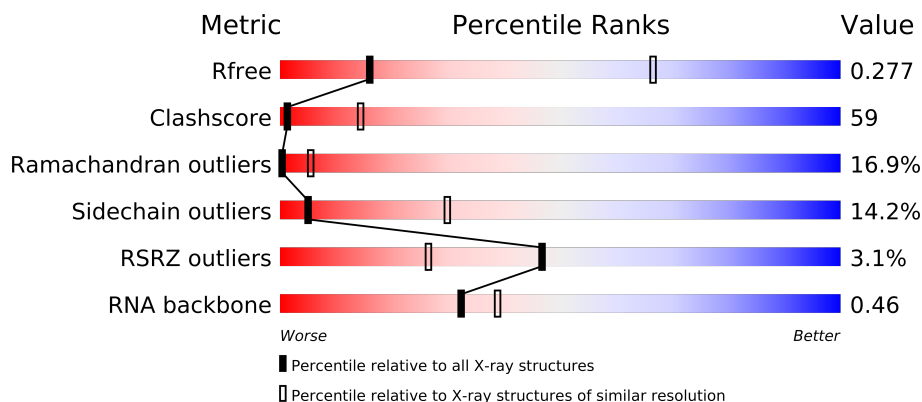
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.60 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	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)
RNA backbone	1838	1012 (4.40-2.76)

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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	

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Mol	Chain	Length	Quality of chain
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	135	
12	CL	135	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	27	
23	CX	27	
24	AY	77	
24	CY	77	
25	AZ	406	
25	CZ	406	
26	B0	85	
26	D0	85	

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Mol	Chain	Length	Quality of chain
27	B1	98	
27	D1	98	
28	B2	72	
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2915	
36	DA	2915	
37	BB	122	
37	DB	122	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BJ	173	
44	DJ	173	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	

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Mol	Chain	Length	Quality of chain
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 306876 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	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	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	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	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
			1010	639	197	174				
9	CI	127	Total	C	N	O		0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	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	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	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	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	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			
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	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE.

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

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	13	Total	C	N	O	P	0	0	0
			272	124	50	86	12			
23	CX	13	Total	C	N	O	P	0	0	0
			272	124	50	86	12			

- Molecule 24 is a RNA chain called A-SITE TRNA THR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	77	Total	C	N	O	P	0	0	0
			1650	741	292	541	76			
24	CY	77	Total	C	N	O	P	0	0	0
			1650	741	292	541	76			

- Molecule 25 is a protein called ELONGATION FACTOR TU-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AZ	374	Total	C	N	O	S	0	0	0
			2900	1832	508	548	12			
25	CZ	374	Total	C	N	O	S	0	0	0
			2900	1832	508	548	12			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
27	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
29	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			
30	D4	45	Total	C	N	O	S	0	0	1
			341	218	58	61	4			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
33	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
34	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			
36	DA	2901	Total	C	N	O	P	0	0	0
			62474	27806	11681	20087	2900			

- Molecule 37 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			
38	DC	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			
39	DD	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
40	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
41	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
43	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BJ	131	Total	C	N	O		0	0	1
			651	390	131	130				
44	DJ	131	Total	C	N	O		0	0	1
			651	390	131	130				

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	141	Total	C	N	O		0	0	1
			701	420	141	140				
45	DK	141	Total	C	N	O		0	0	1
			701	420	141	140				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
46	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
51	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
52	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

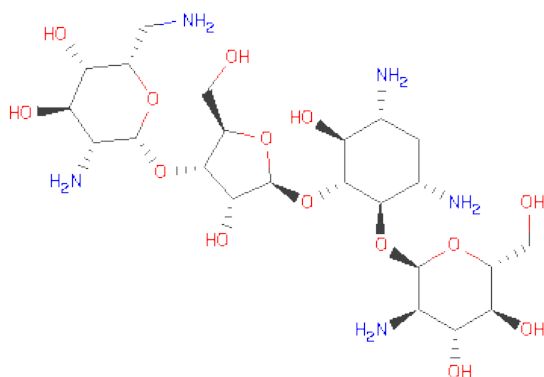
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
57	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			
58	DZ	176	Total	C	N	O	S	0	0	0
			1403	897	252	252	2			

- Molecule 59 is PAROMOMYCIN (three-letter code: PAR) (formula:  $C_{23}H_{45}N_5O_{14}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
59	AA	1	Total	C	N	O	0	0
			42	23	5	14		
59	CA	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	B4	1	Total	Zn	0	0
			1	1		
60	CN	1	Total	Zn	0	0
			1	1		
60	AN	1	Total	Zn	0	0
			1	1		
60	B9	1	Total	Zn	0	0
			1	1		
60	D9	1	Total	Zn	0	0
			1	1		
60	D4	1	Total	Zn	0	0
			1	1		

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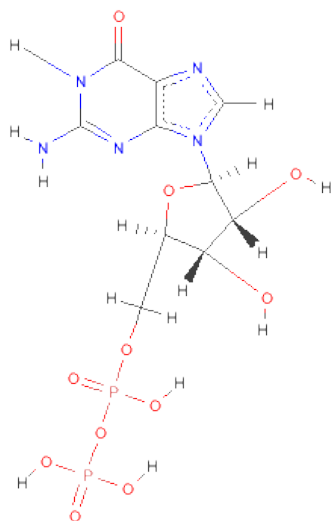
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CD	1	Total	Zn	0	0
			1	1		
60	AD	1	Total	Zn	0	0
			1	1		

- Molecule 61 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

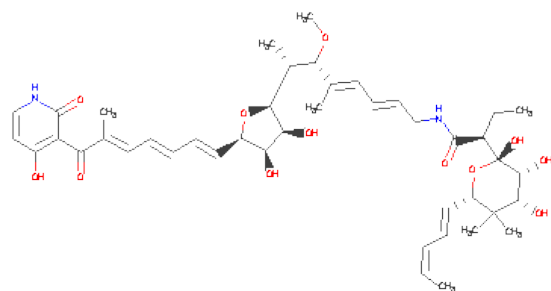
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	AY	1	Total	Mg	0	0
			1	1		
61	CY	1	Total	Mg	0	0
			1	1		

- Molecule 62 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
62	AZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
62	CZ	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 63 is KIRROMYCIN (three-letter code: KIR) (formula:  $C_{43}H_{60}N_2O_{12}$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
63	AZ	1	Total	C	N	O	0	0
			57	43	2	12		
63	CZ	1	Total	C	N	O	0	0
			57	43	2	12		



WORLDWIDE  
**PDB**  
PROTEIN DATA BANK

G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021	G1022		G1023	G1024	G1025	G1026	G1027	G1028	G1029	G1030	G1030A	G1030B	G1031	G1032	G1033	G1034	G1035	G1036		G1037	G1038	G1039	G1040	G1041	G1042	G1043	G1044	G1045	G1046	G1047	G1048	G1049	G1050	G1051	G1052	G1053	G1054	G1055	G1056	G1057	G1058	G1059	G1060	G1061	G1062	G1063	G1064	G1065	G1066	G1067	G1068																																																																																																																																																																																																																																																																																																																																																																																																																																				
G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000	G1001A	G1001B	G1002	G1003	G1004	G1005	G1006	G1007	G1008	G1009	G1010	G1011	G1012	G1013	G1014	G1015	G1016	G1017	G1018	G1019	G1020	G1021																																																																																																																																																																																																																																																																																																																																																																																																																											
G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999																																																																																																																																																																																																																																																																																																																																																																																					
C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999																																																																																																																																																																																																																																																																																																																			
C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999																																																																																																																																																																																																																																																							
G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999
C131	C132	C133	C134	C135	C136	C137	C138	C139	C140	C141	C142	C143	C144	C145	C146	C147	C148	C149	C150	C151	C152	C153	C154	C155	C156	C157	C158	C159	C160	C161	C162	C163	C164	C165	C166	C167	C168	C169	C170	C171	C172	C173	C174	C175	C176	C177	C178	C179	C180	C181	C182	C183	C184	C185	C186	C187	C188	C189	C190	C191	C192	C193	C194	C195	C196	C197	C198	C199	C200	C201	C202	C203	C204	C205	C206	C207	C208	C209	C210	C211	C212	C213	C214	C215	C216	C217	C218	C219	C220	C221	C222	C223	C224	C225	C226	C227	C228	C229	C230	C231	C232	C233	C234	C235	C236	C237	C238	C239	C240	C241	C242	C243	C244	C245	C246	C247	C248	C249	C250	C251	C252	C253	C254	C255	C256	C257	C258	C259	C260	C261	C262	C263	C264	C265	C266	C267	C268	C269	C270	C271	C272	C273	C274	C275	C276	C277	C278	C279	C280	C281	C282	C283	C284	C285	C286	C287	C288	C289	C290	C291	C292	C293	C294	C295	C296	C297	C298	C299	C300	C301	C302	C303	C304	C305	C306	C307	C308	C309	C310	C311	C312	C313	C314	C315	C316	C317	C318	C319	C320	C321	C322	C323	C324	C325	C326	C327	C328	C329	C330	C331	C332	C333	C334	C335	C336	C337	C338	C339	C340	C341	C342	C343	C344	C345	C346	C347	C348	C349	C350	C351	C352	C353	C354	C355	C356	C357	C358	C359	C360	C361	C362	C363	C364	C365	C366	C367	C368	C369	C370	C371	C372	C373	C374	C375	C376	C377	C378	C379	C380	C381	C382	C383	C384	C385	C386	C387	C388	C389	C390	C391	C392	C393	C394	C395	C396	C397	C398	C399	C400	C401	C402	C403	C404	C405	C406	C407	C408	C409	C410	C411	C412	C413	C414	C415	C416	C417	C418	C419	C420	C421	C422	C423	C424	C425	C426	C427	C428	C429	C430	C431	C432	C433	C434	C435	C436	C437	C438	C439	C440	C441	C442	C443	C444	C445	C446	C447	C448	C449	C450	C451	C452	C453	C454	C455	C456	C457	C458	C459	C460	C461	C462	C463	C464	C465	C466	C467	C468	C469	C470	C471	C472	C473	C474	C475	C476	C477	C478	C479	C480	C481	C482	C483	C484	C485	C486	C487	C488	C489	C490	C491	C492	C493	C494	C495	C496	C497	C498	C499	C500	C501	C502	C503	C504	C505	C506	C507	C508	C509	C510	C511	C512	C513	C514	C515	C516	C517	C518	C519	C520	C521	C522	C523	C524	C52																																																																																								

G1069	G1129	G1190	G1250	A1318	G1378	C1439	G1504
U1070	A1130	A1191	A1251	A1319	G1379	C1440	G1505
C1071	G1131	C1192	A1252	C1320	U1380	G1441	U1506
G1072	G1132	G1193	G1253	C1321	U1381	G1442	A1507
G1073	G1133	G1194	G1254	C1322	C1382	A1442A	G1508
U1074	G1134	C1195	G1255	G1323	C1383	G1443	C1509
C1075	U1135	U1196	A1256	A1324	C1384	G1444	U1510
G1076	U1136	G1197	U1257	C1325	G1385	G1445	G1511
G1077	C1137	G1198	G1258	G1326	G1386	G1446	U1512
U1078	G1138	U1199	C1259	C1327	G1387	A1447	A1513
G1079	G1139	C1200	C1260	C1328	C1388	G1448	G1514
A1080	C1140	A1201	A1261	A1329	C1389	G1452	C1515
G1081	C1141	G1202	C1262	U1330	U1390	G1456	G1516
G1082	G1142	C1203		G1331	U1391	G1457	G1517
U1083	G1143	A1204	A1269	A1332	G1392	G1458	A1518
G1084	G1144	U1205	C1270	A1333	U1393	G1459	A1519
U1085	C1145	G1206	G1271	G1334	A1394	A1460	G1520
U1086	A1146	G1207	G1272	C1335	C1395	G1461	G1521
G1087	C1147	C1208	G1273	G1336	A1396	G1462	U1522
G1088	U1148	C1209	G1274	G1337	C1397	G1463	G1523
G1089	U1149	C1210	A1275	G1338	A1398	G1464	G1524
U1090	U1150	U1211	G1276	C1339	C1399	C1465	G1525
U1091	A1151	U1212	C1277	A1339	C1400	G1466	G1526
A1092	A1152	A1213	U1278	G1401	G1402	G1467	C1527
A1093	C1153	C1214	A1279	G1342	C1403	A1468	U1528
G1094	G1154	G1215	A1280	C1343		G1469	G1529
U1095	G1155	G1216	U1281	U1345	U1406	G1470	G1530
C1096	G1156	C1217	C1282	A1346	G1407	G1471	A1531
C1097	A1157	G1218	G1283	G1347	C1408	U1472	U
G1098	C1158	C1219	G1284	U1348	A1408	A1473	C
G1099	U1159	G1220	A1285	A1349	C1409	G1474	A
C1100	G1160	G1221	A1286	A1350	G1410	G1475	C
A1101	C1161	G1222	U1287	U1351	C1411	G1476	C
A1102	C1162	C1223	A1288	C1352	C1412	C1477	U
C1103	C1163	G1224	A1289	G1353	A1413	C1478	C
G1104	G1164	A1225	G1290	C1354	U1414	G1479	C
A1105	C1165	C1226	G1291	G1355	G1415	G1480	U
U1106	G1166	A1227	U1292	G1356	G1416	U1481	U
C1107	A1168	C1228	G1293	U1357	G1417	G1482	C
G1108	A1169	A1229		U1358	A1418	C1483	U
C1109	U1170	C1230	C1298	C1359	G1419	G1484	
G1110	G1171	G1231	A1299	A1360	C1420	U1485	
A1111	C1172	U1232	U1300	G1361	G1421	G1486	
C1112	G1173	G1233	U1301	C1362	G1422	G1487	
C1113	G1174	C1234	U1302	C1363	G1423	G1488	
G1114	G1175	U1235	C1303	A1363A	C1424	G1489	
C1115	A1176	A1236	G1304	U1364	U1425	C1490	
G1116	C1177	C1237	G1305	G1365	C1426	G1491	
G1117	G1178	A1238	A1306	C1366	U1427	A1492	
C1118	A1179	U1239	U1307	C1367	A1428	A1493	
G1119	A1180	U1240	U1308	G1368	C1429	G1494	
G1120	G1181	G1241	G1309	C1369	C1430	U1495	
U1121	G1182	C1242	G1310	G1370	C1431	G1496	
U1122	A1183	C1243	G1311	G1371	G1432	C1497	
G1123	G1184	C1244	U1312	U1372	A1433	U1498	
A1124	G1185	A1245	G1313	G1373	A1434	A1499	
U1125	G1186	C1246	C1314	A1374	G1435	A1500	
U1126	G1187	U1247	C1315	U1375	U1436	C1501	
G1127	A1188	A1248	G1316	U1376	C1437	A1502	
C1128	C1189	C1249	C1317	A1377	G1438	A1503	

• Molecule 2: 30S RIBOSOMAL PROTEIN S2

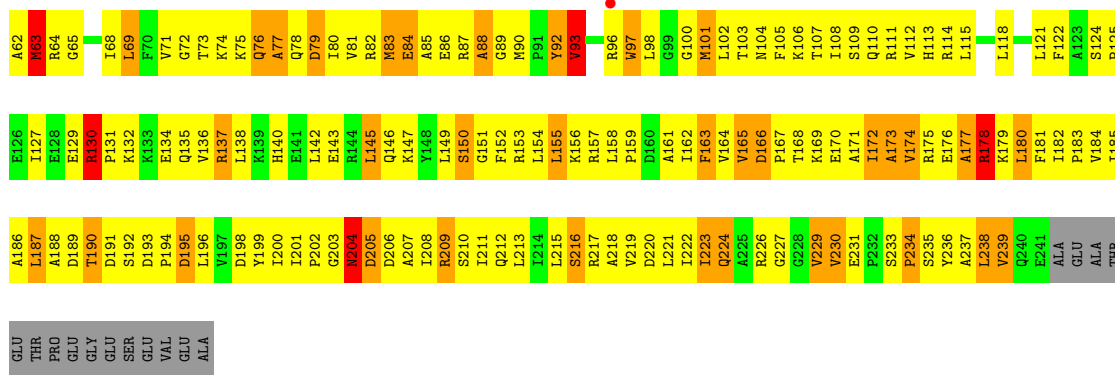
Chain AB:

MET	A62	P125	I185	THR
PRO	M63	E126	A186	GLU
VAL	R64	E127	I187	THR
GLU	G65	E128	A188	PRO
ILE		E129	D189	GLU
THR	I68	R130	T190	GLY
V7	L69	P131	D191	GLU
K8	F70	K132	S192	SER
E9	V71	K133	D193	GLU
L10	G72	E134	P194	VAL
L11	T73	Q135	D195	GLU
E12	K74	V136	L196	ALA
A13	K75	R137	V197	
G14	Q76	L138	D198	
V15	A77	K139	Y199	
H16	Q78	H140	I200	
F17	D79	E141	T201	
G18	I80	L142	P202	
H19	V81	E143	G203	
R20	R82	R144	N204	
R21	M83	L145	D205	
E22	E84	K146	A206	
R23	A85	K147	D207	
W24	E86	Y148	I208	
N25	R87	L149	R209	
P26	A88	S150	S210	
K27	G89	G151	I211	
F28	M90	F152	Q212	
A29	P91	R153	L213	
R30	Y92	L154	L214	
Y31	R93	L155	L215	
I32	N94	K156	S216	
Y33	Q95	R157	R217	
A34	R96	L158	A218	
E35	W97	P159	V219	
R36	L98	D160	D220	
G99	G99	A161	L221	
G100	M101	I162	I222	
L102	L102	F163	I223	
T103	T103	V164	Q224	
N104	N104	V165	A225	
D43	F105	D166	R226	
L44	K106	P167	G227	
Q45	T107	T168	G228	
K46	I108	K169	V229	
T47	S109	E170	V230	
N48	Q110	A171	E231	
R111	R111	I172	P232	
V112	V112	A173	S233	
H113	H113	V174	P234	
R114	R114	R175	S235	
L115	L115	E176	Y236	
L118	L118	A177	A237	
L121	L121	R178	L238	
F122	F122	K179	V239	
D60	D60	L180	Q240	
L61	S124	F181	E241	
		I182	ALA	
		P183	GLU	
		D60	ALA	

• Molecule 2: 30S RIBOSOMAL PROTEIN S2

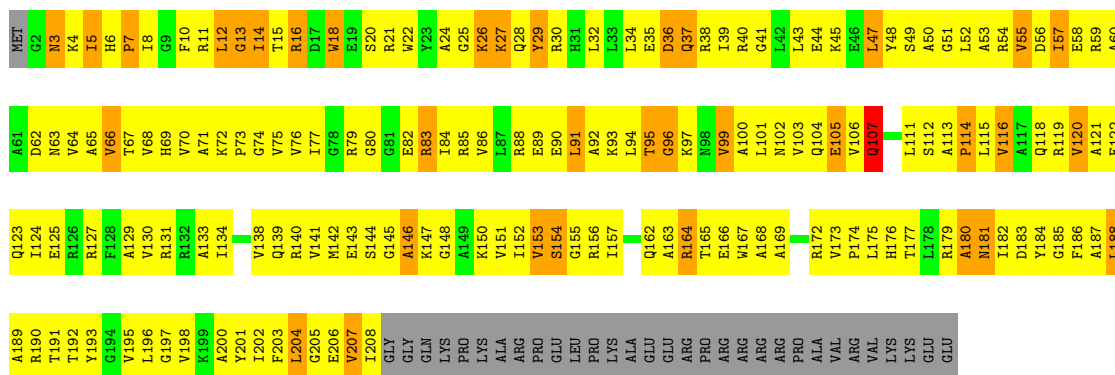
Chain CB:

MET	L51
PRO	E52
VAL	R53
GLU	T54
ILE	F55
THR	R56
V7	F57
K8	I58
E9	E59
L10	I182
L11	P183
E12	D60
A13	L61
G14	
V15	
H16	
F17	
G18	
H19	
E20	
R21	
K22	
R23	
W24	
N25	
P26	
K27	
F28	
A29	
R30	
Y31	
I32	
Y33	
A34	
E35	
R36	
N37	
G38	
I39	
H40	
I41	
I42	
D43	
L44	
Q45	
K46	
T47	
M48	
L51	
E52	
R53	
T54	
F55	
R56	
F57	
I58	
E59	
I182	
P183	
D60	
L61	



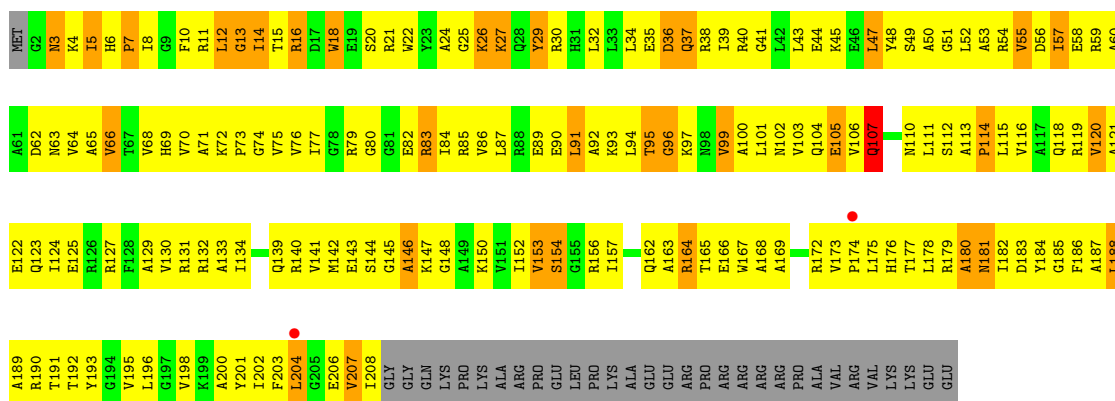
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



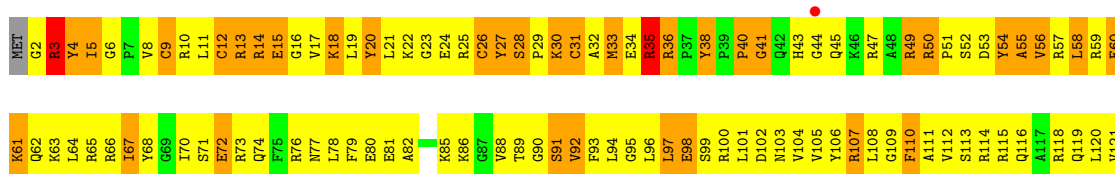
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:

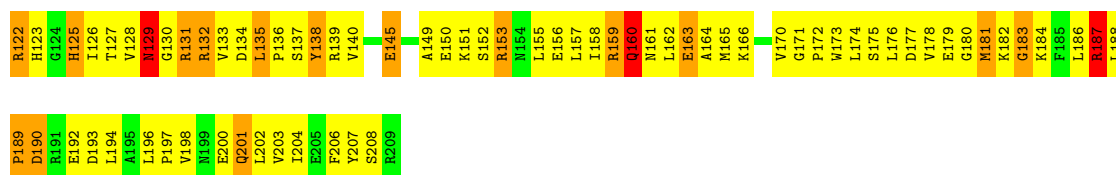


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain AD:

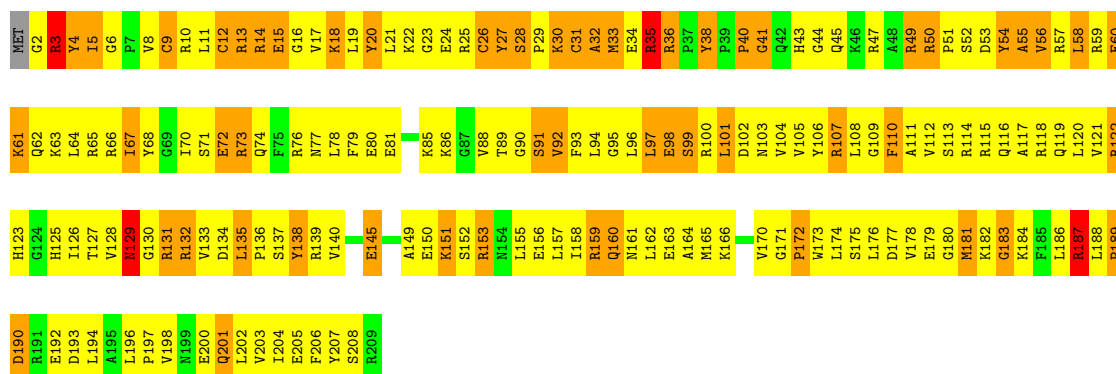






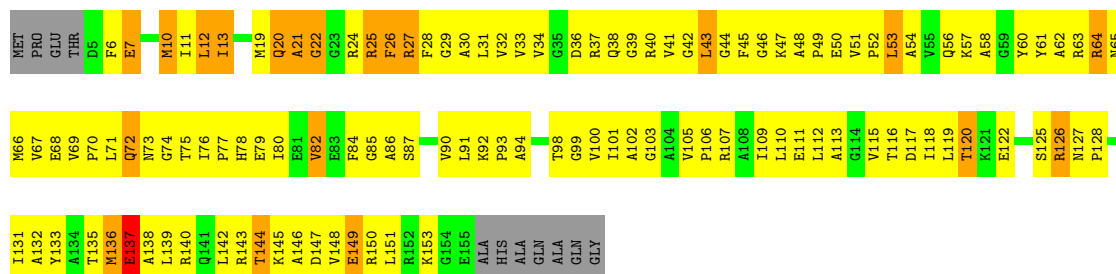
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain CD:



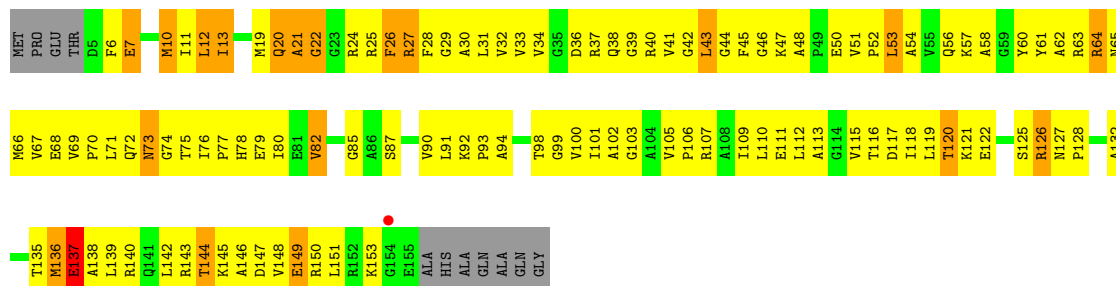
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



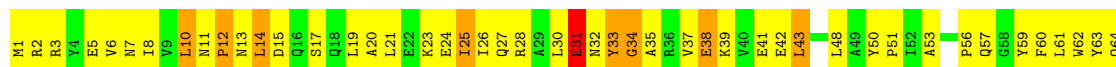
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

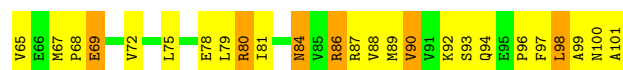
Chain CE:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

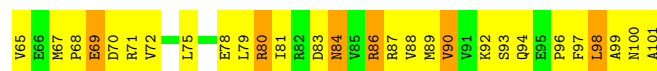
Chain AF:





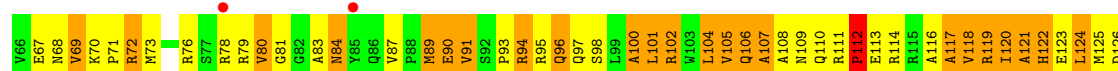
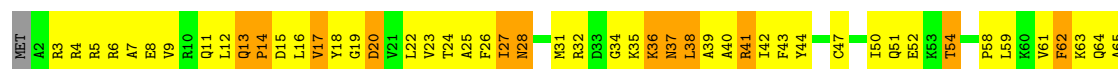
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain CF:



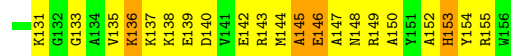
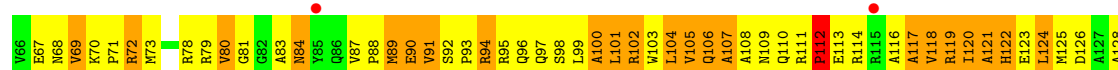
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



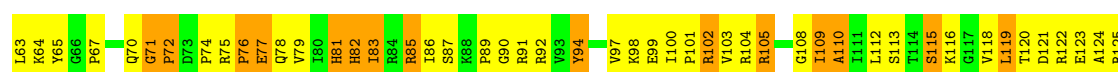
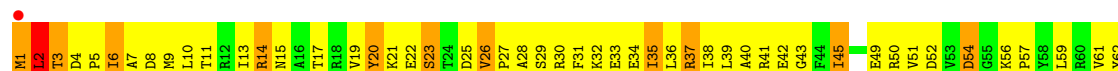
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



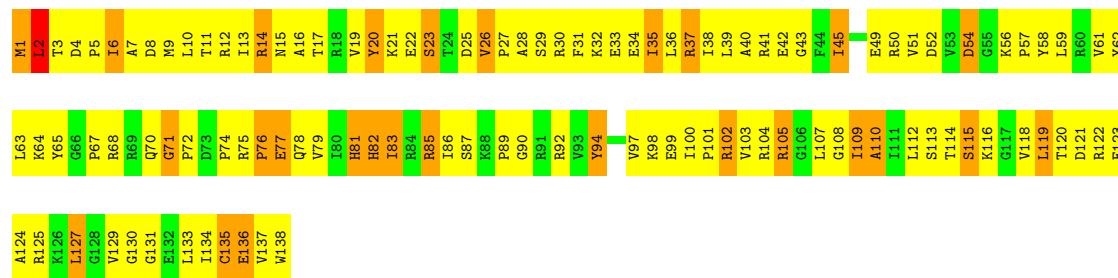
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



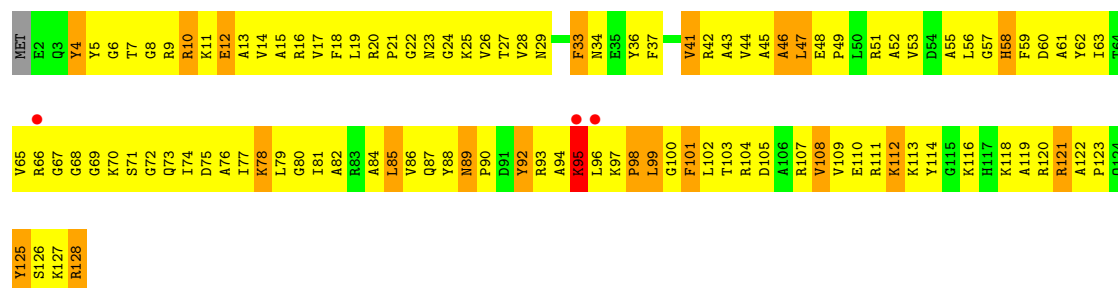
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain CH:



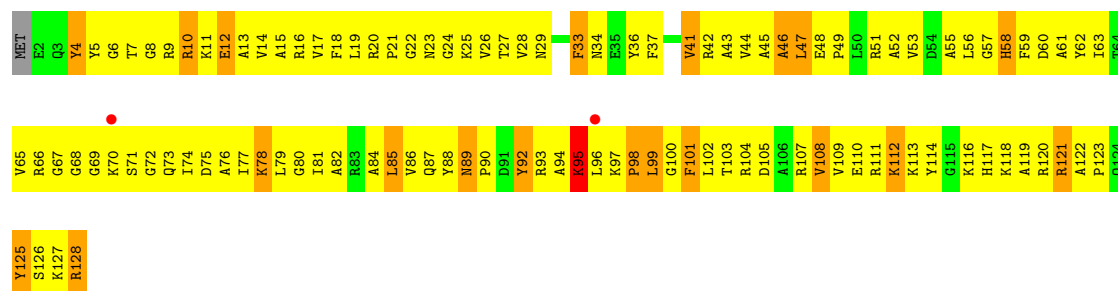
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



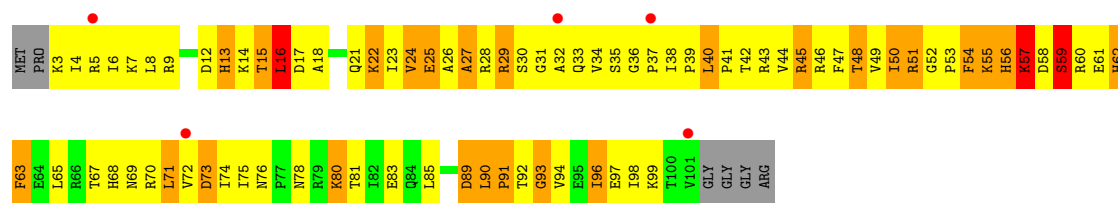
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



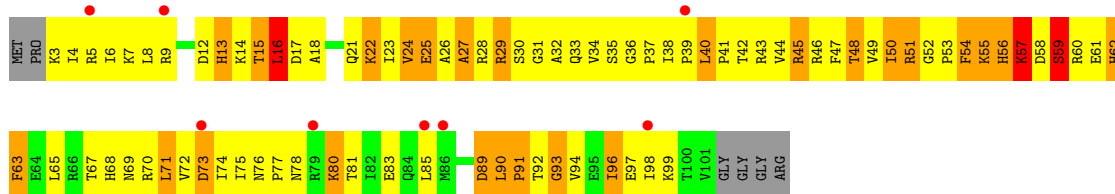
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



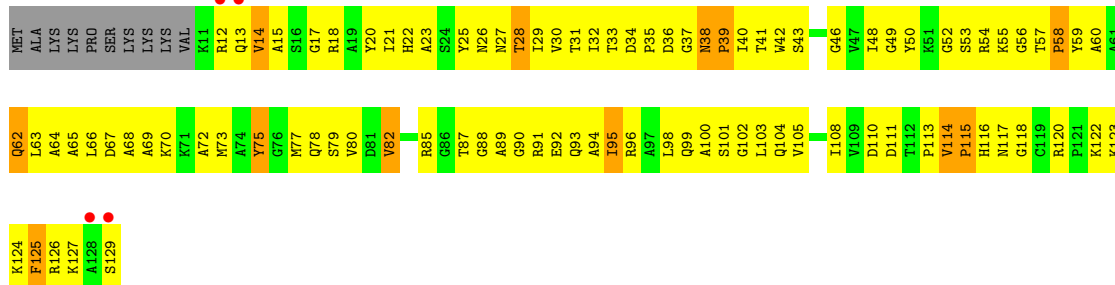
- Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain CJ:



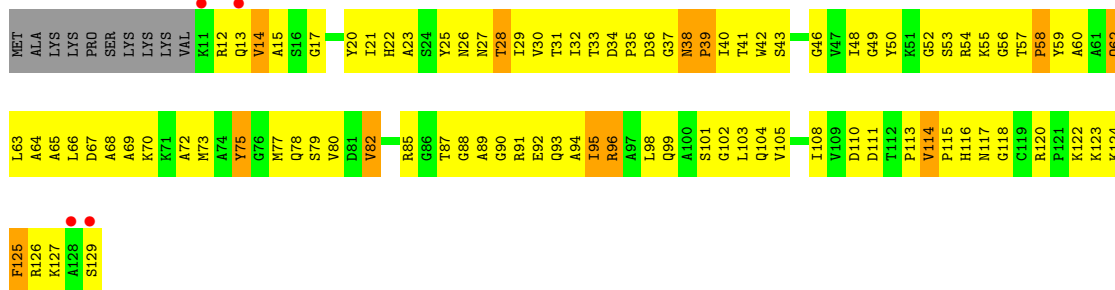
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain AK:



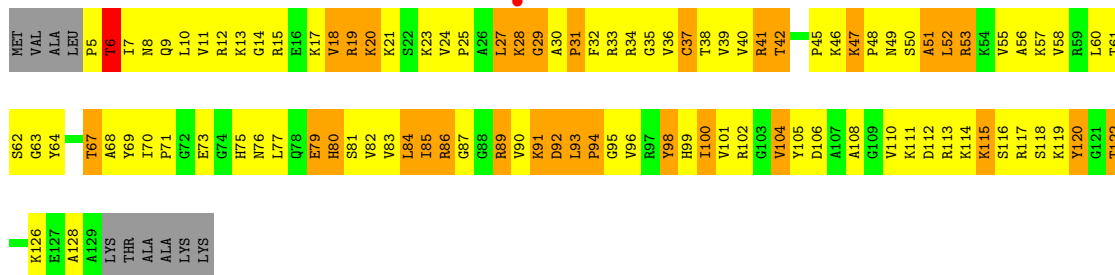
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

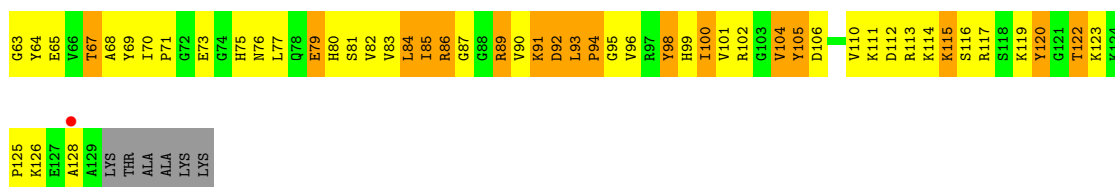
Chain AL:



• Molecule 12: 30S RIBOSOMAL PROTEIN S12

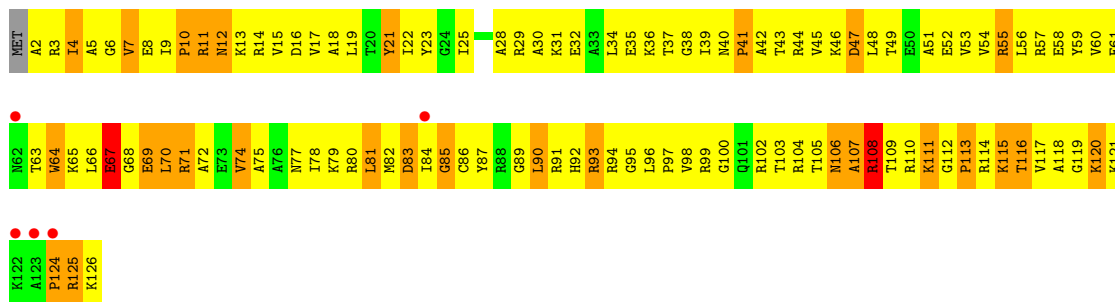
Chain CL:





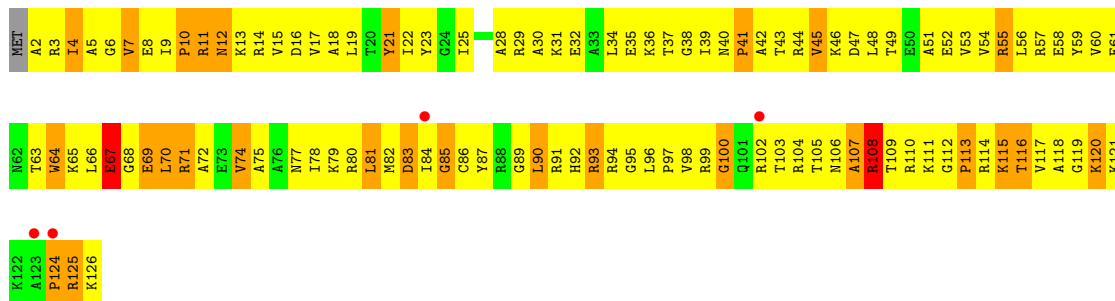
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain AM:



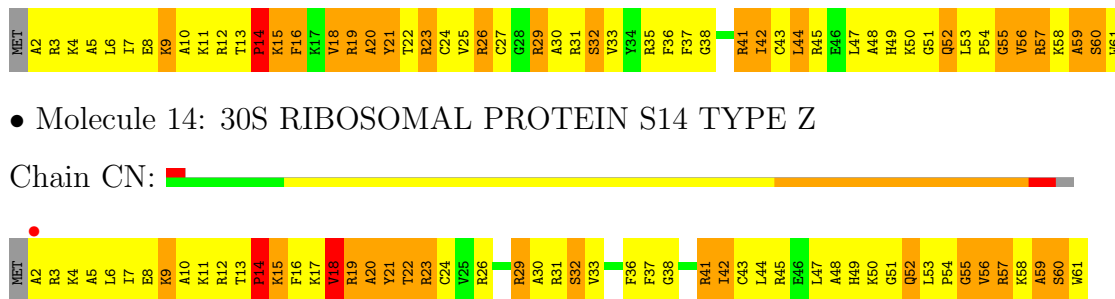
• Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain CM:



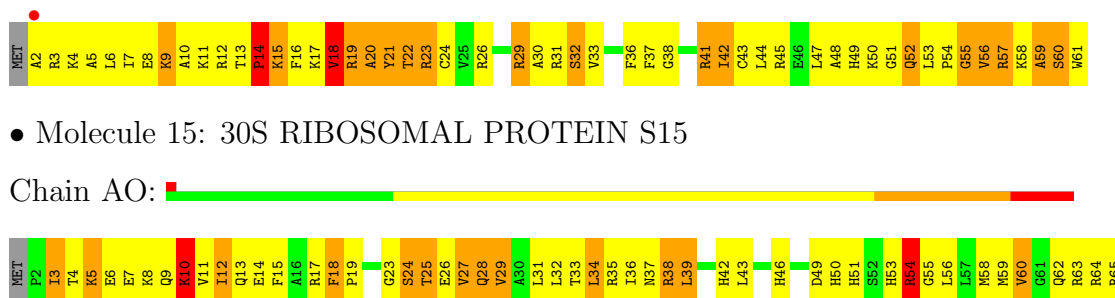
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



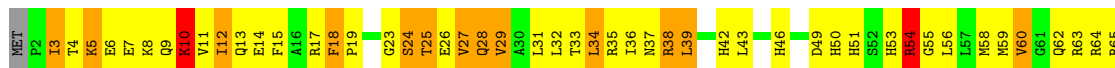
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



• Molecule 15: 30S RIBOSOMAL PROTEIN S15

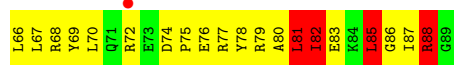
Chain AO:





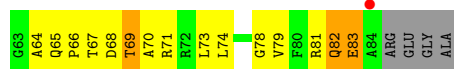
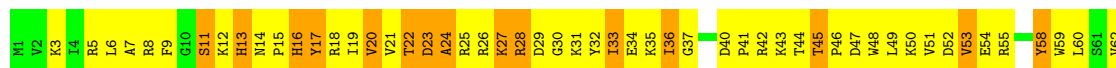
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



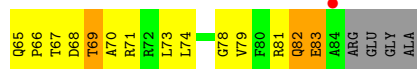
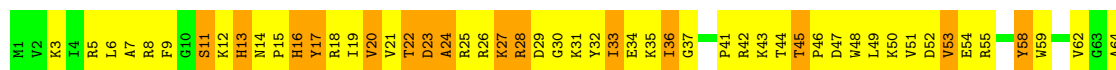
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



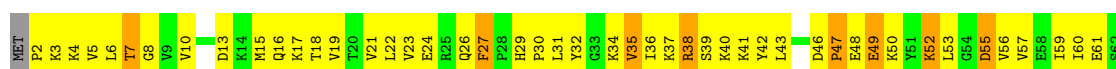
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



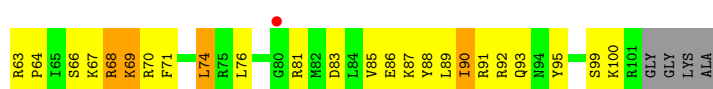
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



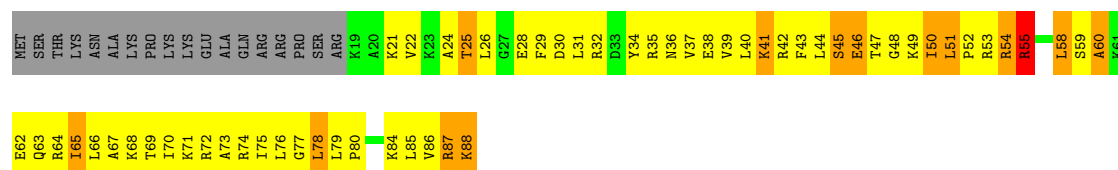
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



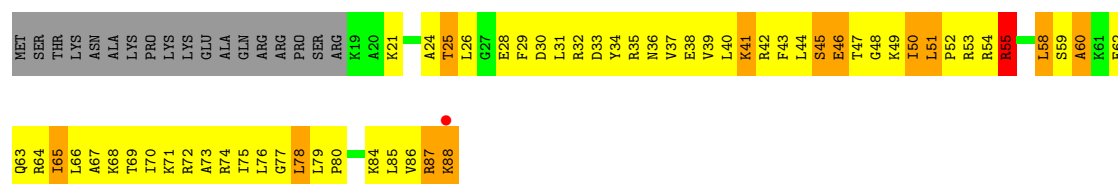
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



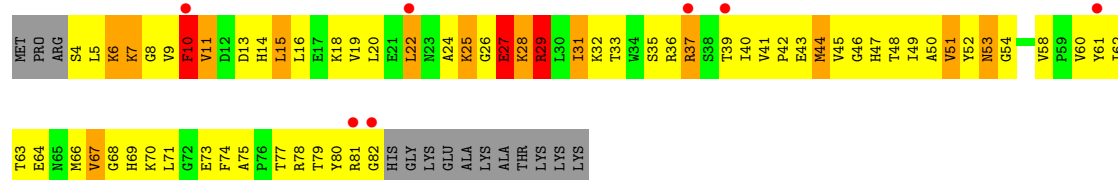
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



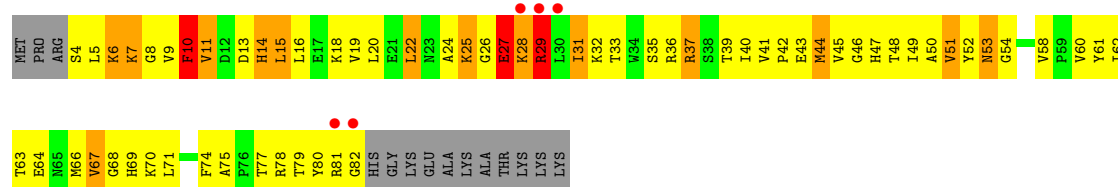
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS:



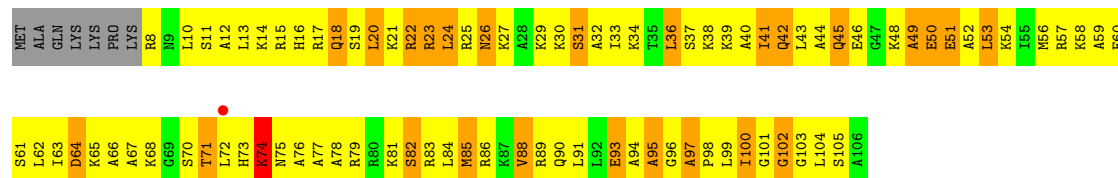
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS:



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

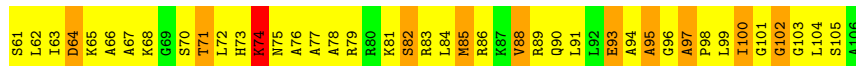
Chain AT:



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain CT:





- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain AU:



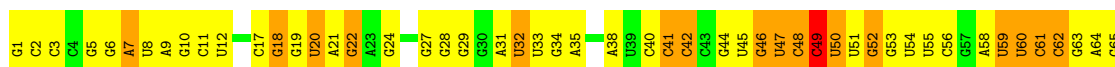
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain CU:



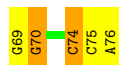
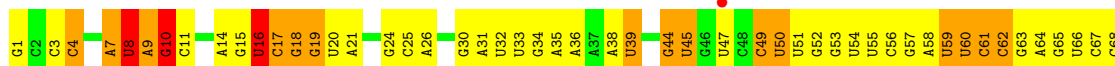
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AV:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

Chain AW:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

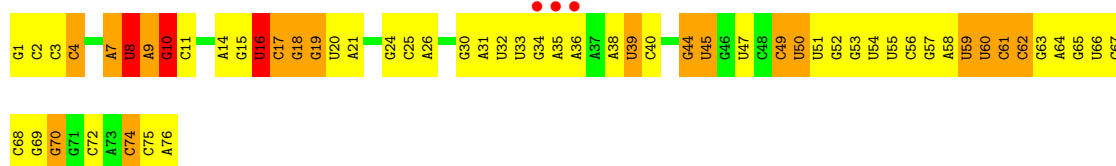
Chain CV:



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE

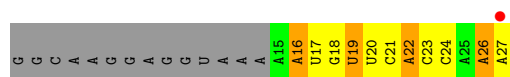
Chain CW:





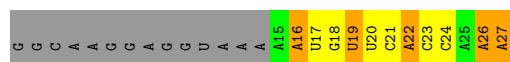
- Molecule 23: MRNA

Chain AX:



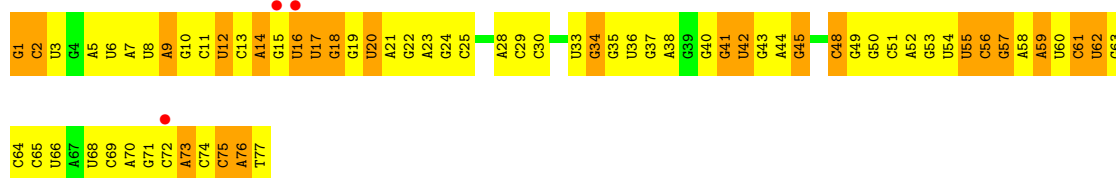
- Molecule 23: MRNA

Chain CX:



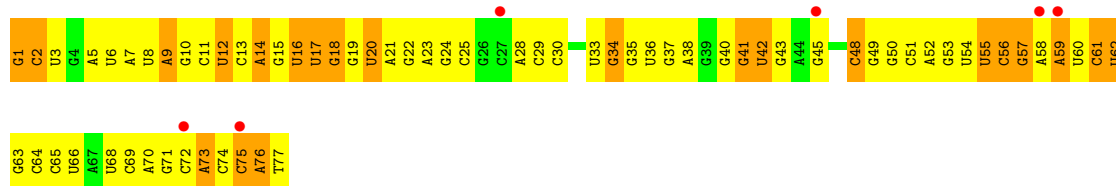
- Molecule 24: A-SITE TRNA THR

Chain AY:



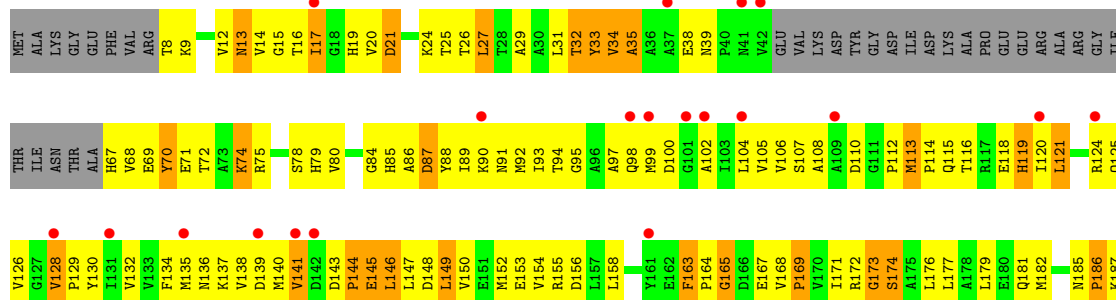
- Molecule 24: A-SITE TRNA THR

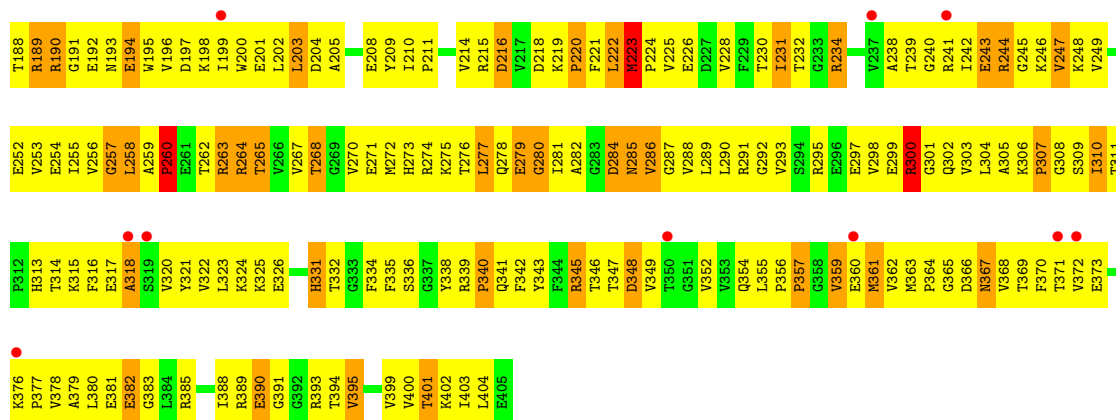
Chain CY:



- Molecule 25: ELONGATION FACTOR TU-A

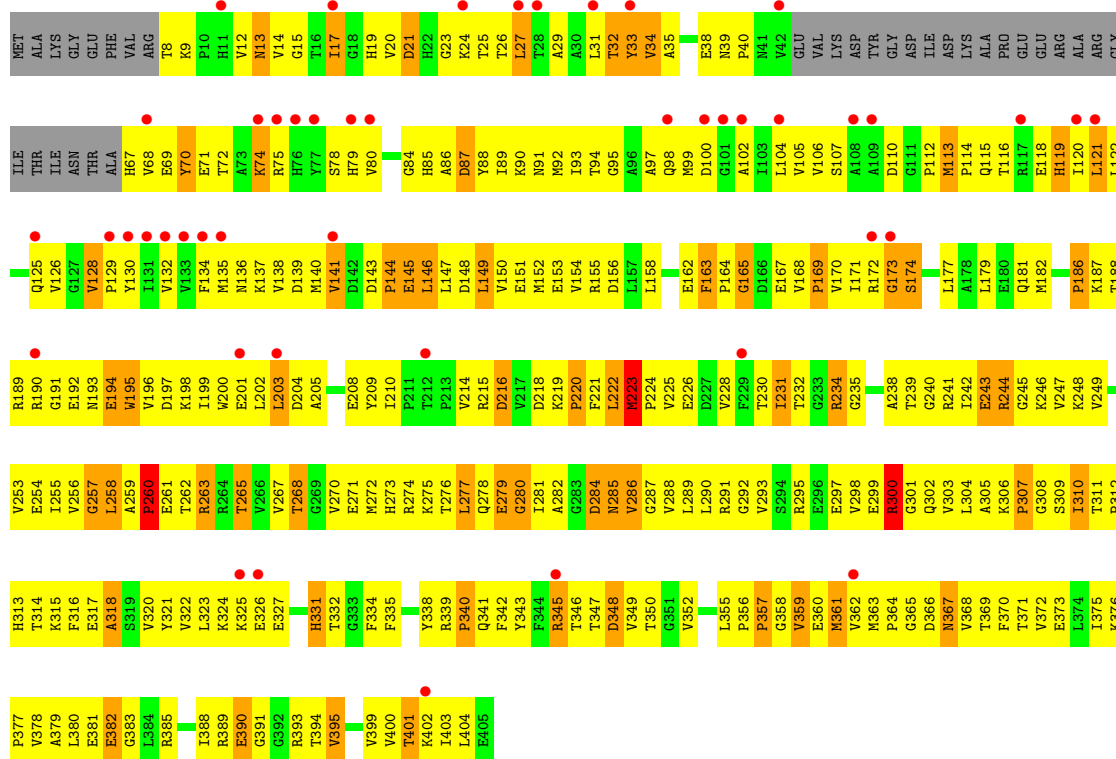
Chain AZ:





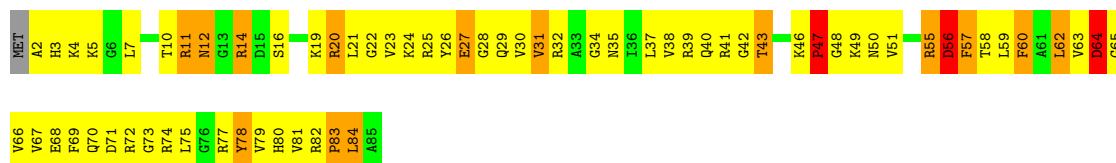
### • Molecule 25: ELONGATION FACTOR TU-A

Chain CZ:



### • Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



### • Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain D0:

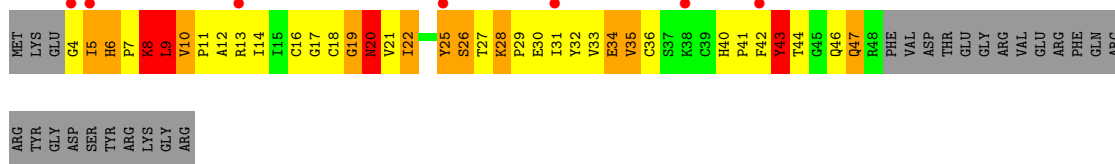


Chain D3: 



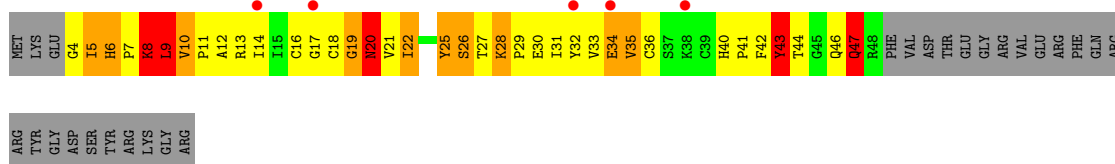
- Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4: 



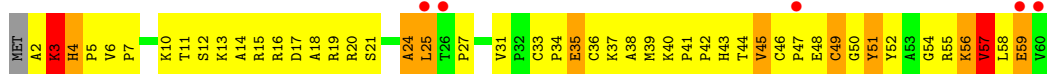
- Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4: 



- Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5: 



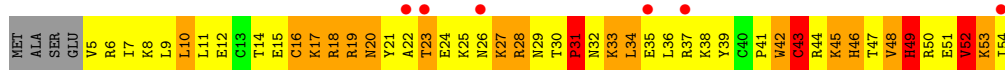
- Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain D5: 



- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6: 



- Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6: 



- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:



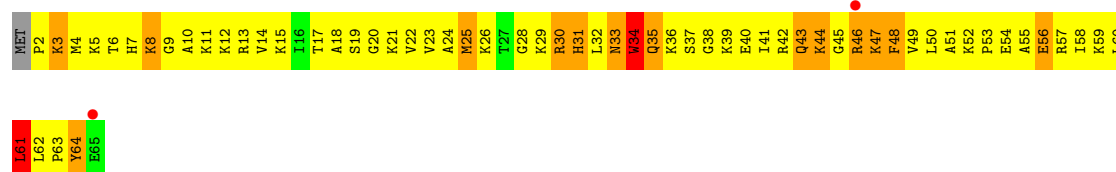
- Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:



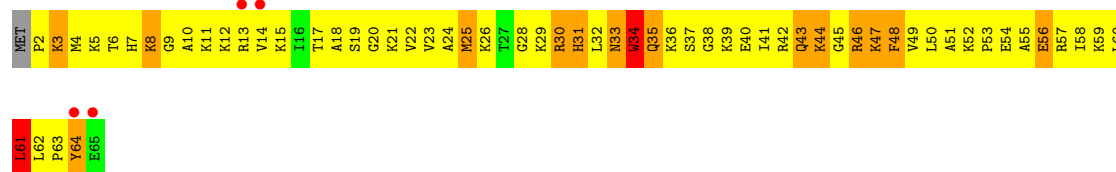
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



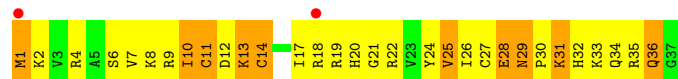
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8:



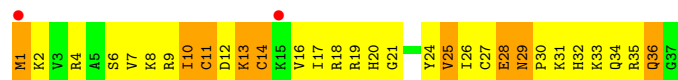
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



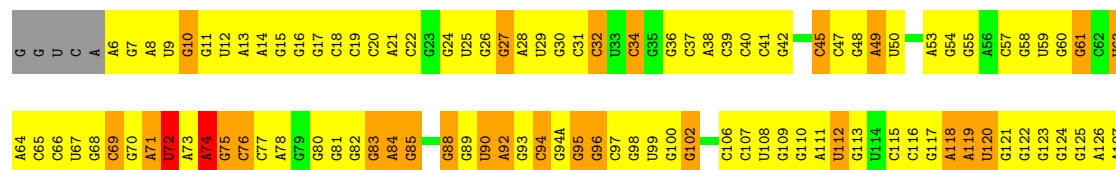
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9:



- Molecule 36: 23S RIBOSOMAL RNA

Chain BA:



C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
G942	U943	G944	A945	G946	G947	G948	C949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	A980	A981	A982	A983	A984	C985	C986	C987	A988	A989	A990	C991	C992	C993	C994	C995	A996	G997	C998	C1005																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
C876	C877	A878	G879	G880	G881	G882	G883	G884	G885	G886	G887	C888	C889	A890	G891	C892	C893	C894	C895	C896	C897	C898	C899	A899	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	A918	A919	C920	C921	C922	C923	C924	C925	A926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
G942	U943	G944	A945	G946	G947	G948	C949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	A980	A981	A982	A983	A984	C985	C986	C987	A988	A989	A990	C991	C992	C993	C994	C995	A996	G997	C998	C1005																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
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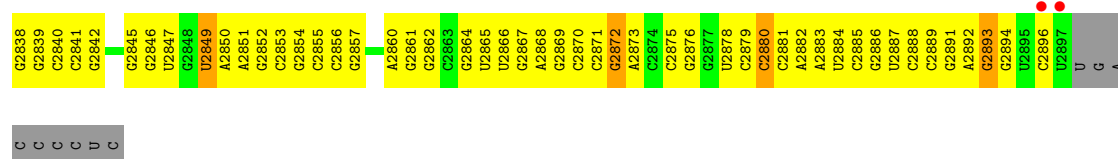




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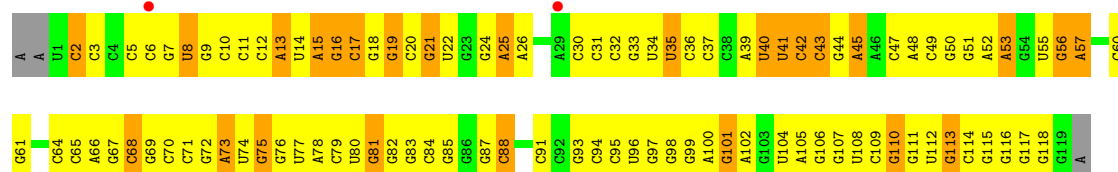
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U1833	C1773	U1693	G1568	U1503	G1440	G1380	C1320	G1254	G1192	U1130	G1062	A997	G938
U1834	C1774	C1694	A1569	U1504	G1441	G1381	A1321	U1255	G1193	G1131	G1063	C998	G939
G1835	U1775	G1695	A1570	C1505	G1442	C1382	A1322	G1256	A1194	U1132	C1064	U999	G940
C1836	G1776	G1696	A1571	C1506		C1383	U1323	C1257	G1195	U1133	U1065		A941
C1837	U1777	G1697	A1572		A1445	A1384	G1324	C1258	G1196	C1135	U1066	C1005	G942
C1838	U1778	A1698	G1573	C1509	G1446	C1385	G1325	G1259	G1197	G1136	A1067	C1006	U943
C1839	U1779	G1699	A1509A	U1509	G1447	C1386	U1326	G1260	U1198	G1137	G1068	C1007	U944
G1840	A1780	C1699	G1575	A1509B	G1448	C1387	C1327	A1261	U1199	G1138	A1069	G1008	A945
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G1842	G1782	G1702	C1511	C1511		C1389	U1329	U1263	C1201	C1140	G1071	A1010	G947
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A1849	A1788	C1708	G1517	G1517	G1455	A1395	U1335	A1269	C1207	C1146		C1018	G954
	U1789	U1709	U1518	U1518	G1458	U1396	A1336	C1270	C1208	C1147		U1019	G955
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	G1823	C1761	G1623	A1558	C1493	G1430	C1370	G1309	G1243	C1181		C1052	C987
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U1898	G1826	G1764	G1626	G1561	A1496	U1433	A1373	U1313	A1247	C1185		G1055	A990
G1899	C1827	C1765	G1627	A1562	U1497	A1434	G1374	C1314	G1248	G1186		G1056	C991
A1900	G1828		G1628	G1563	U1498	G1435	C1375	C1315	U1249	G1187		A1057	C992
A1901	A1829	G1769	C1499	C1564	G1499	U1316	C1376	U1316	G1250	U1188		A1126	G993
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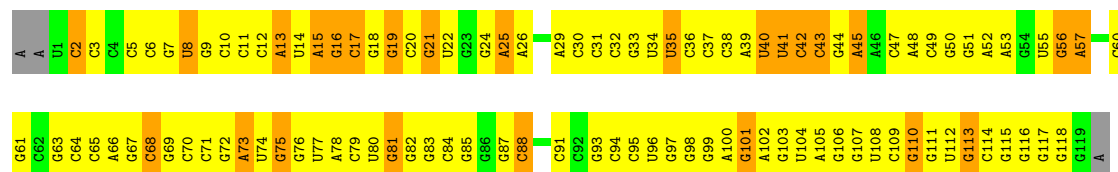
• Molecule 37: 5S RIBOSOMAL RNA

Chain BB:



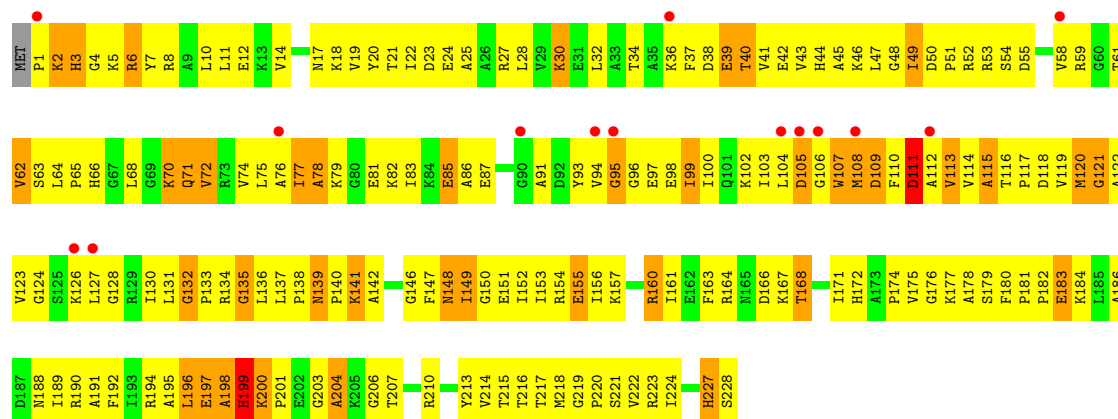
• Molecule 37: 5S RIBOSOMAL RNA

Chain DB:



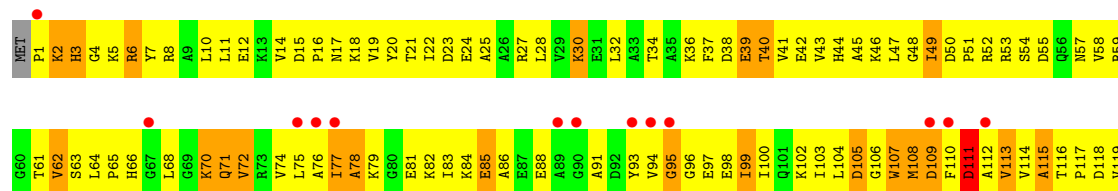
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

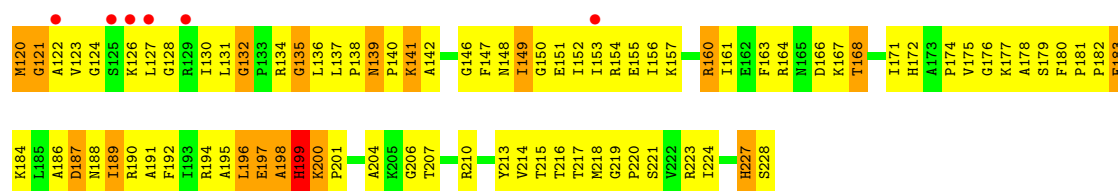
Chain BC:



• Molecule 38: 50S RIBOSOMAL PROTEIN L1

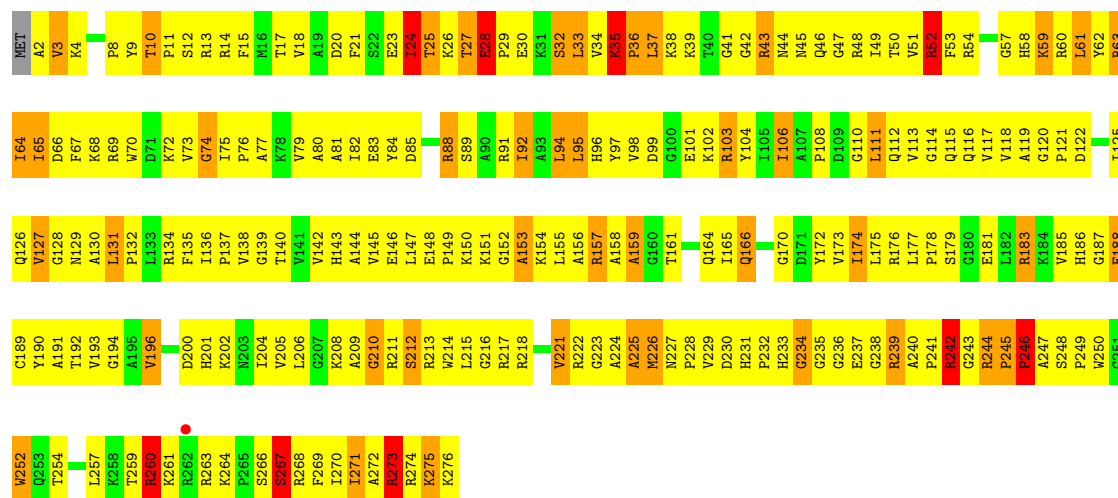
Chain DC:





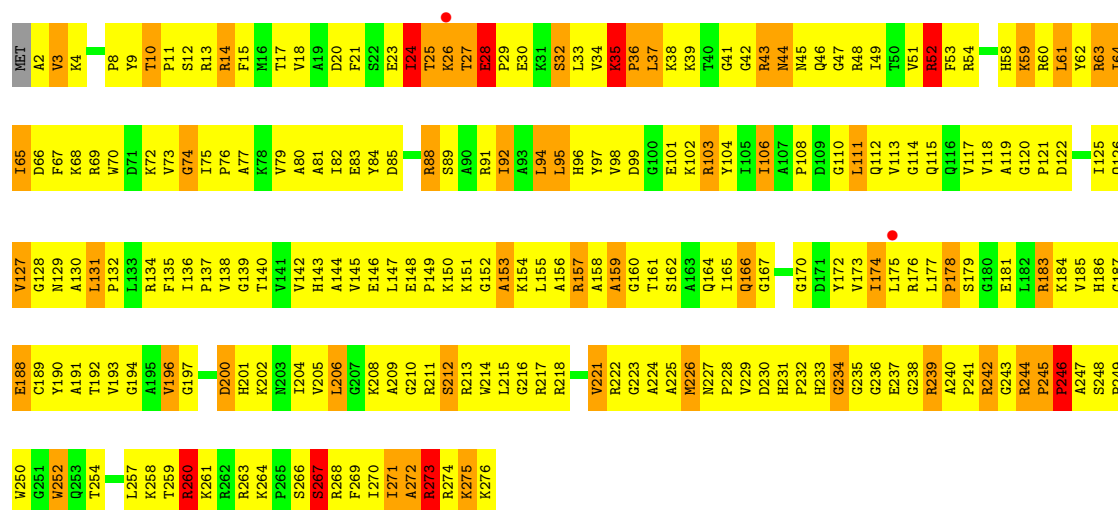
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain BD:



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

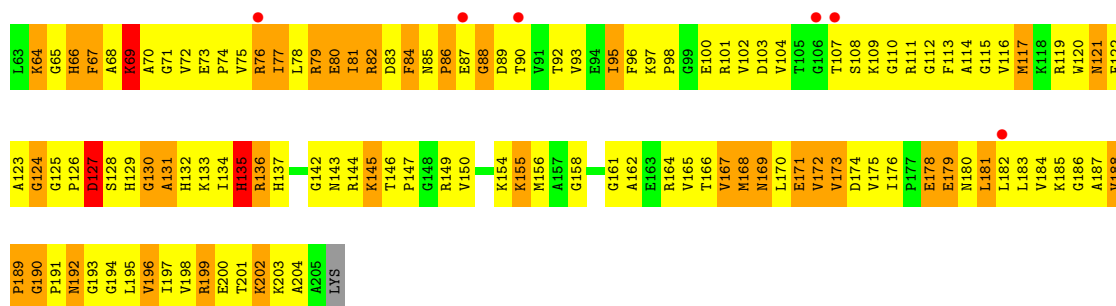
Chain DD:



• Molecule 40: 50S RIBOSOMAL PROTEIN L3

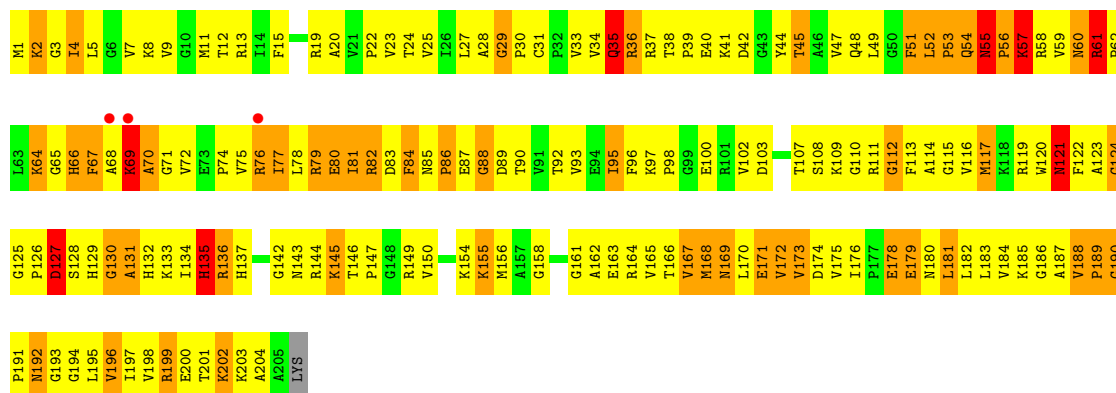
Chain BE:





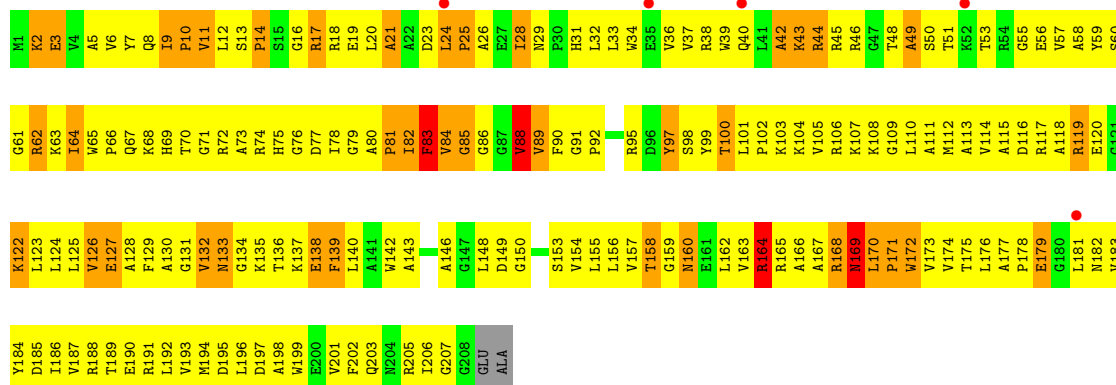
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain DE:



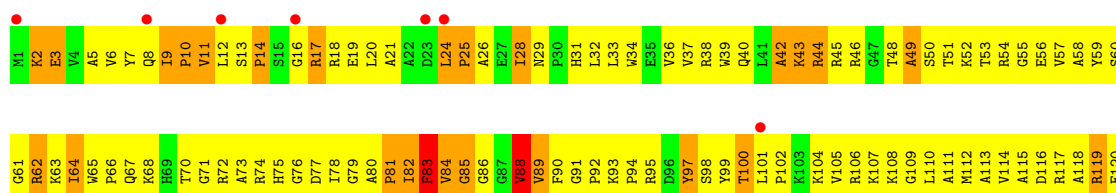
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

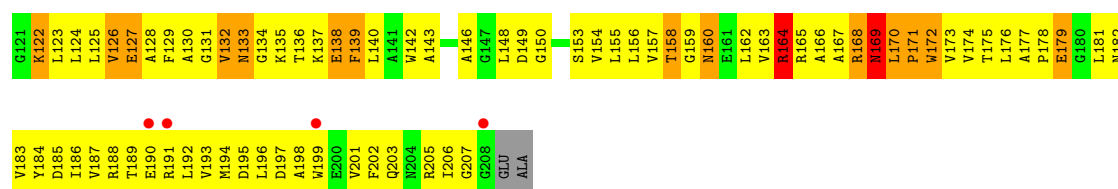
Chain BF:



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

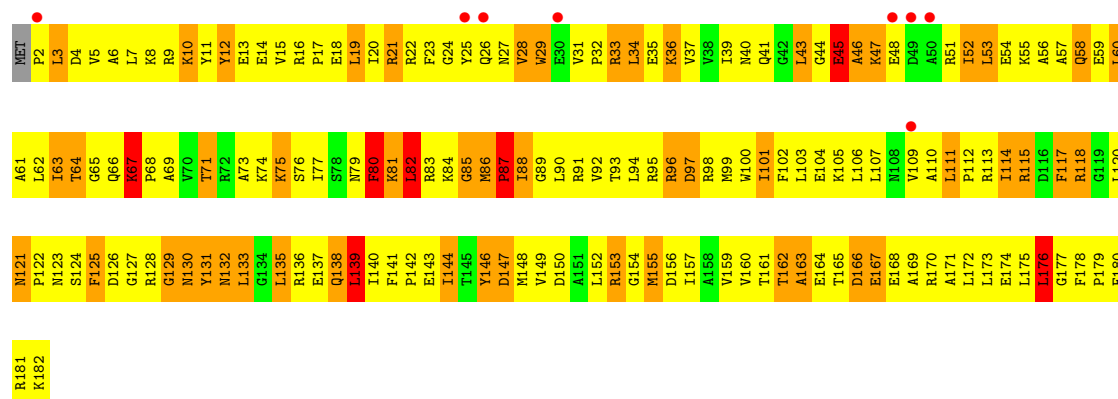
Chain DF:





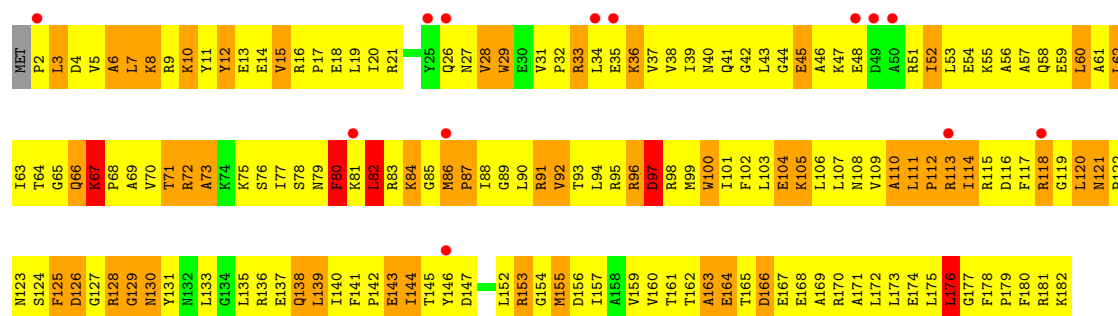
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

Chain BG:



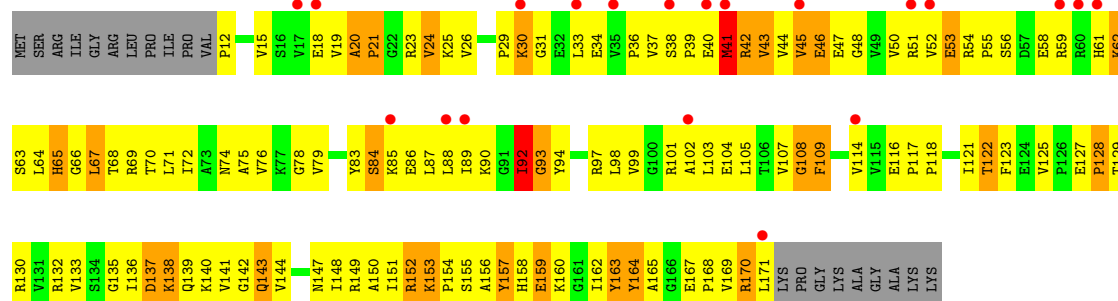
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

Chain DG:



• Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain BH:

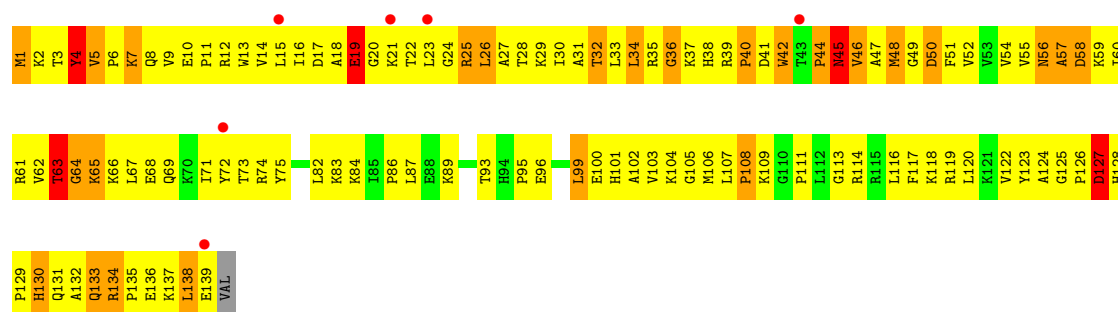


• Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain DH:

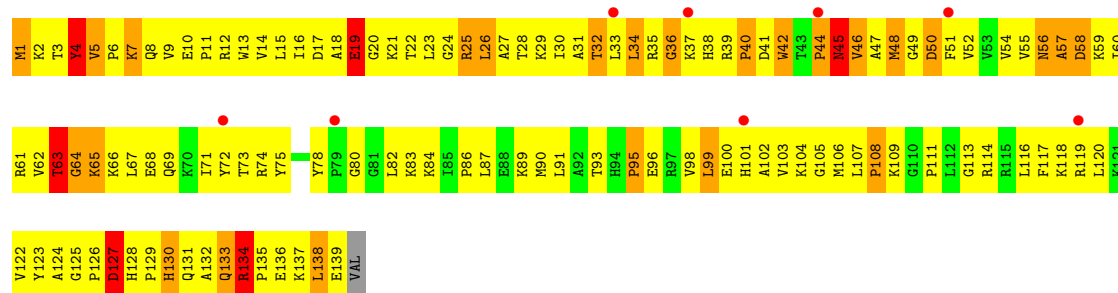






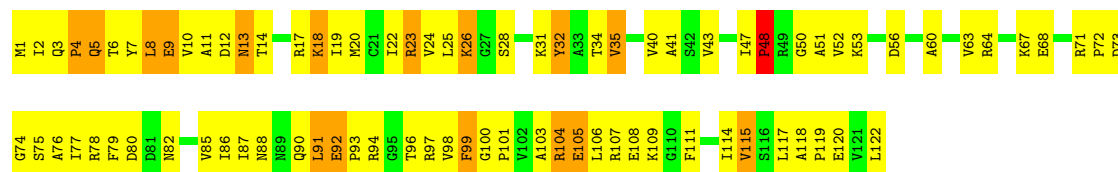
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



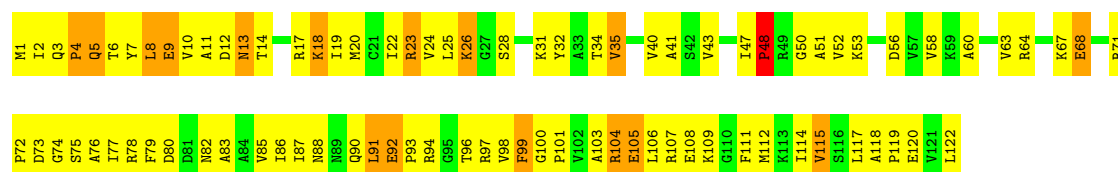
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



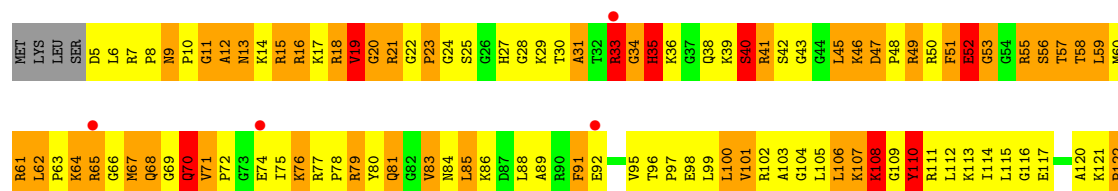
• Molecule 47: 50S RIBOSOMAL PROTEIN L14

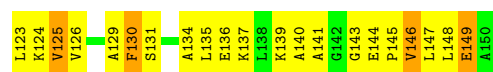
Chain DO:



• Molecule 48: 50S RIBOSOMAL PROTEIN L15

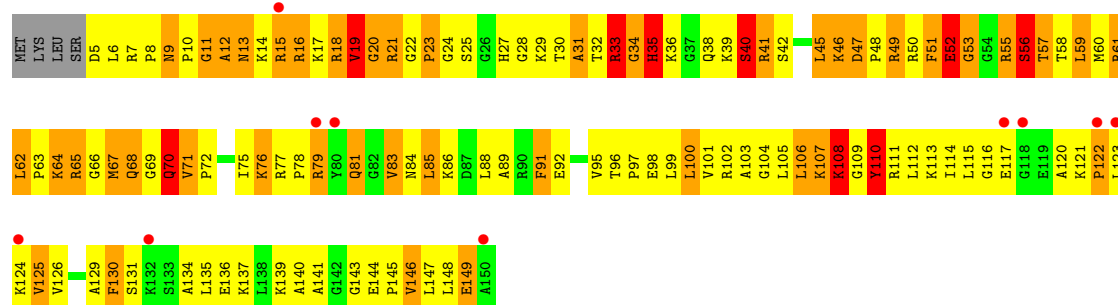
Chain BP:





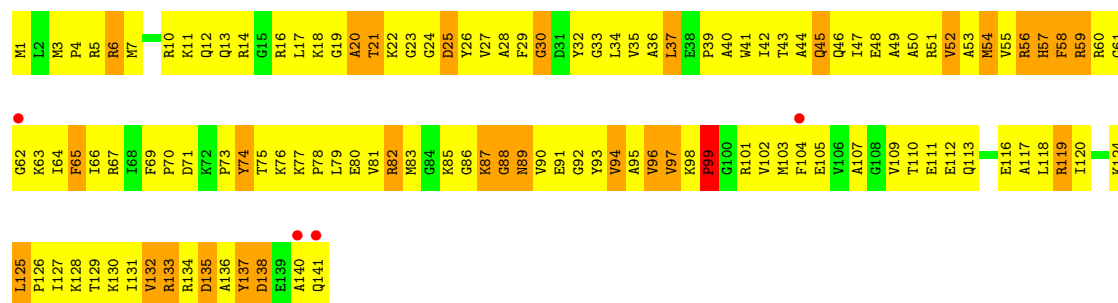
• Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



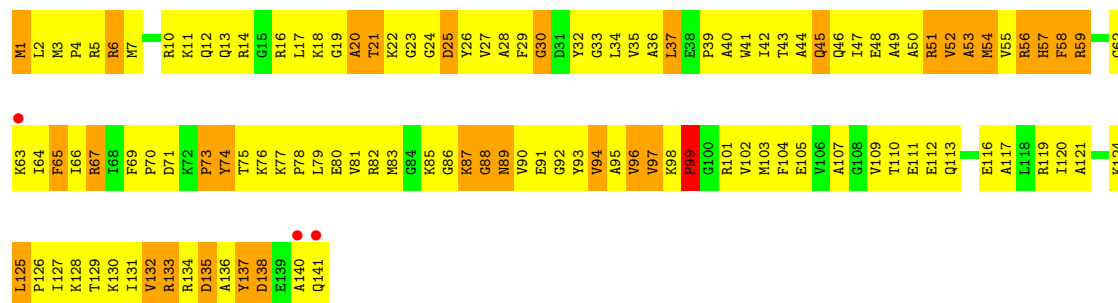
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ:



• Molecule 50: 50S RIBOSOMAL PROTEIN L17

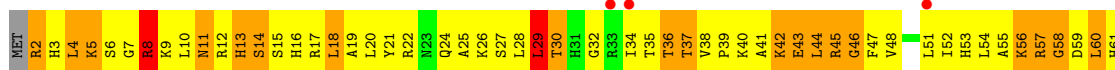
Chain BR:





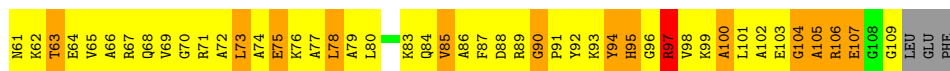
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR:



• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS:



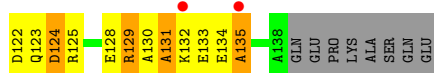
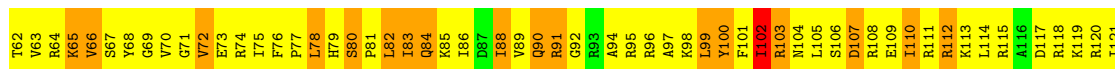
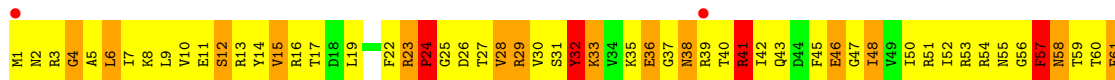
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain DS:



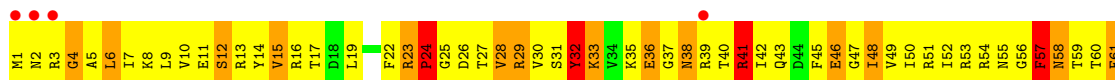
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

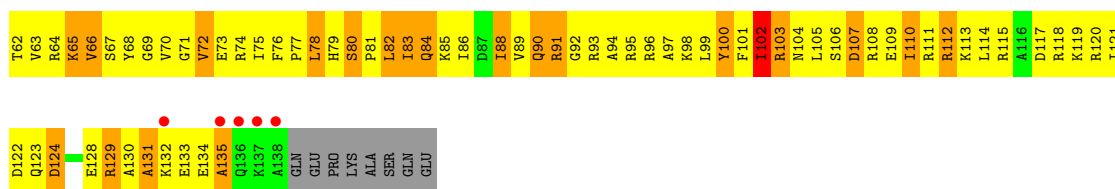
Chain BT:



• Molecule 52: 50S RIBOSOMAL PROTEIN L19

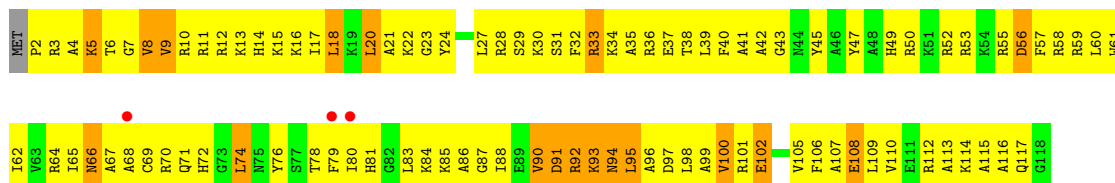
Chain DT:





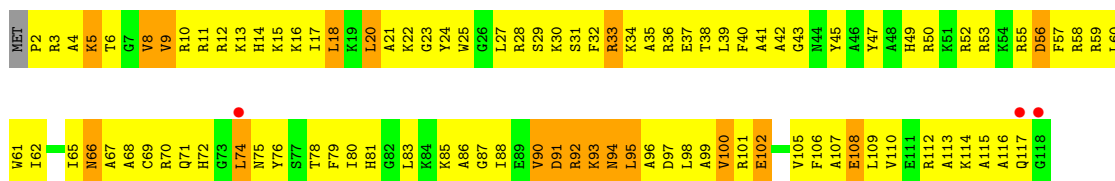
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



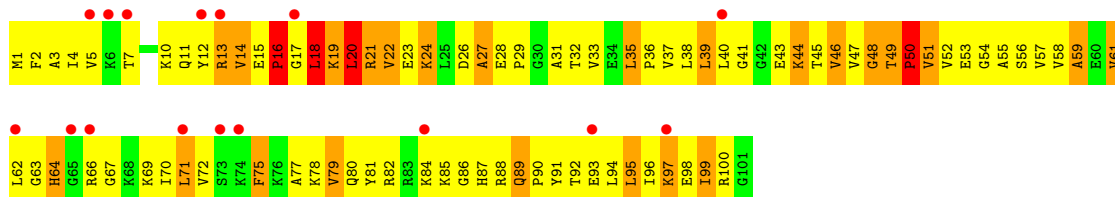
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



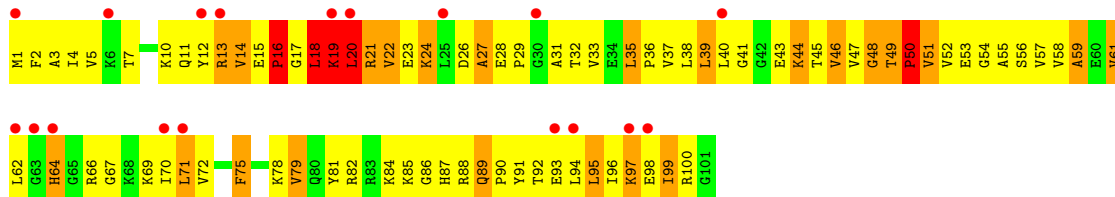
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



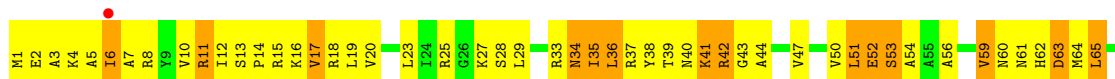
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

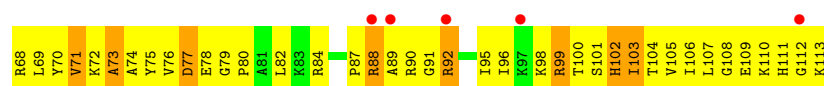
Chain DV:



• Molecule 55: 50S RIBOSOMAL PROTEIN L22

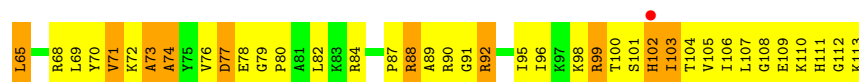
Chain BW:





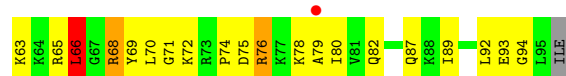
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



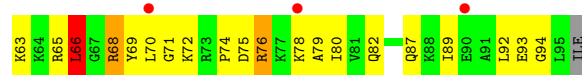
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



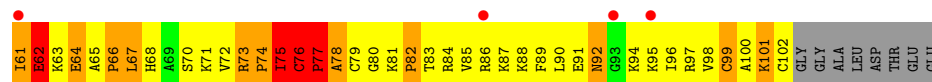
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain DX:



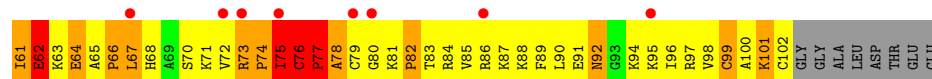
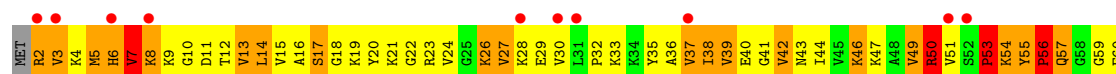
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



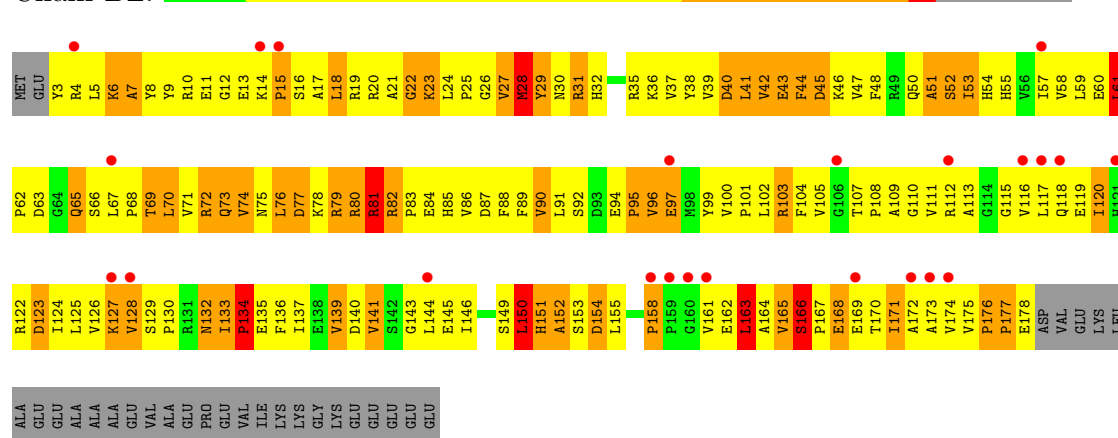
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY:



## ● Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



## ● Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	289.57Å 268.36Å 403.88Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	50.00 – 3.60 49.91 – 3.48	Depositor EDS
% Data completeness (in resolution range)	93.6 (50.00-3.60) 87.3 (49.91-3.48)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.281 , 0.315 0.261 , 0.277	Depositor DCC
$R_{free}$ test set	35772 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.0	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 62.0	EDS
Estimated twinning fraction	0.098 for h,-k,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.37$ , $\langle L^2 \rangle = 0.19$	Xtriage
Outliers	0 of 714740 reflections	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	306876	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.21% 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: 5MU, GDP, PAR, H2U, MG, ZN, YG, KIR, 7MG, 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	0.64	1/36190 (0.0%)	0.78	23/56486 (0.0%)
1	CA	0.64	0/36190	0.77	20/56486 (0.0%)
2	AB	0.44	0/1936	0.71	0/2611
2	CB	0.44	0/1936	0.72	0/2611
3	AC	0.46	0/1637	0.73	1/2207 (0.0%)
3	CC	0.47	0/1637	0.73	0/2207
4	AD	0.46	0/1733	0.75	1/2318 (0.0%)
4	CD	0.44	0/1733	0.73	2/2318 (0.1%)
5	AE	0.57	0/1163	0.79	1/1566 (0.1%)
5	CE	0.56	0/1163	0.78	0/1566
6	AF	0.42	0/856	0.67	0/1154
6	CF	0.42	0/856	0.67	0/1154
7	AG	0.41	0/1276	0.66	0/1709
7	CG	0.42	0/1276	0.66	0/1709
8	AH	0.51	0/1136	0.72	0/1527
8	CH	0.49	0/1136	0.74	0/1527
9	AI	0.39	0/1029	0.65	0/1379
9	CI	0.39	0/1029	0.65	0/1379
10	AJ	0.46	0/808	0.71	1/1087 (0.1%)
10	CJ	0.48	0/808	0.71	1/1087 (0.1%)
11	AK	0.48	0/900	0.73	0/1213
11	CK	0.48	0/900	0.73	0/1213
12	AL	0.52	0/987	0.81	0/1322
12	CL	0.54	0/987	0.81	0/1322
13	AM	0.43	0/999	0.75	0/1338
13	CM	0.43	0/999	0.74	0/1338
14	AN	0.52	0/501	0.73	0/664
14	CN	0.51	0/501	0.74	0/664
15	AO	0.45	0/745	0.73	0/992
15	CO	0.44	0/745	0.73	0/992
16	AP	0.48	0/717	0.72	0/965
16	CP	0.46	0/717	0.72	0/965



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AQ	0.46	0/837	0.74	0/1119
17	CQ	0.48	0/837	0.74	0/1119
18	AR	0.50	0/579	0.75	1/768 (0.1%)
18	CR	0.49	0/579	0.75	1/768 (0.1%)
19	AS	0.47	0/643	0.67	0/867
19	CS	0.45	0/643	0.67	0/867
20	AT	0.38	0/765	0.70	0/1007
20	CT	0.36	0/765	0.70	0/1007
21	AU	0.55	0/213	0.63	0/279
21	CU	0.56	0/213	0.64	0/279
22	AV	0.53	0/1809	0.76	0/2819
22	AW	0.45	0/1809	0.73	0/2819
22	CV	0.49	0/1809	0.76	0/2819
22	CW	0.45	0/1809	0.72	0/2819
23	AX	0.71	0/304	0.83	0/471
23	CX	0.72	0/304	0.81	0/471
24	AY	0.50	1/1660 (0.1%)	0.72	1/2583 (0.0%)
24	CY	0.51	1/1660 (0.1%)	0.72	1/2583 (0.0%)
25	AZ	0.38	0/2957	0.65	0/4015
25	CZ	0.38	0/2957	0.65	0/4015
26	B0	0.40	0/671	0.67	0/892
26	D0	0.40	0/671	0.66	0/892
27	B1	0.57	0/739	0.91	0/983
27	D1	0.60	0/739	0.92	1/983 (0.1%)
28	B2	0.44	0/600	0.87	2/793 (0.3%)
28	D2	0.43	0/600	0.80	1/793 (0.1%)
29	B3	0.44	0/473	0.74	0/636
29	D3	0.42	0/473	0.75	0/636
30	B4	0.71	0/350	0.79	0/476
30	D4	0.73	1/350 (0.3%)	0.75	0/476
31	B5	0.44	0/473	0.72	0/639
31	D5	0.43	0/473	0.71	0/639
32	B6	0.53	0/440	0.91	0/586
32	D6	0.56	0/440	0.93	0/586
33	B7	0.50	0/427	0.75	0/563
33	D7	0.50	0/427	0.74	0/563
34	B8	0.51	0/516	0.78	0/681
34	D8	0.51	0/516	0.77	0/681
35	B9	0.42	0/310	0.66	0/407
35	D9	0.44	0/310	0.67	0/407
36	BA	0.61	2/69972 (0.0%)	0.76	36/109237 (0.0%)
36	DA	0.61	2/69972 (0.0%)	0.77	37/109237 (0.0%)
37	BB	0.46	0/2853	0.72	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
37	DB	0.45	0/2853	0.72	0/4451
38	BC	0.45	2/1774 (0.1%)	0.69	0/2391
38	DC	0.44	2/1774 (0.1%)	0.69	0/2391
39	BD	0.59	0/2195	0.86	1/2955 (0.0%)
39	DD	0.57	0/2195	0.86	0/2955
40	BE	0.48	0/1597	0.75	0/2155
40	DE	0.47	0/1597	0.75	0/2155
41	BF	0.45	0/1659	0.73	0/2246
41	DF	0.43	0/1659	0.72	0/2246
42	BG	0.46	0/1499	0.81	3/2016 (0.1%)
42	DG	0.50	1/1499 (0.1%)	0.77	0/2016
43	BH	0.37	0/1246	0.70	0/1684
43	DH	0.36	0/1246	0.70	0/1684
46	BN	0.42	0/1132	0.75	1/1527 (0.1%)
46	DN	0.43	0/1132	0.75	1/1527 (0.1%)
47	BO	0.49	0/943	0.79	0/1269
47	DO	0.52	0/943	0.78	0/1269
48	BP	0.49	0/1131	1.00	7/1504 (0.5%)
48	DP	0.48	0/1131	0.99	6/1504 (0.4%)
49	BQ	0.44	0/1143	0.71	0/1527
49	DQ	0.43	0/1143	0.72	0/1527
50	BR	0.41	0/974	0.74	0/1302
50	DR	0.39	0/974	0.74	0/1302
51	BS	0.41	0/779	0.72	0/1038
51	DS	0.41	0/779	0.72	0/1038
52	BT	0.47	0/1156	0.75	0/1544
52	DT	0.44	0/1156	0.75	0/1544
53	BU	0.43	0/975	0.74	0/1297
53	DU	0.45	0/975	0.75	0/1297
54	BV	0.39	0/790	0.73	0/1057
54	DV	0.40	0/790	0.73	0/1057
55	BW	0.44	0/907	0.71	0/1216
55	DW	0.42	0/907	0.72	0/1216
56	BX	0.47	0/740	0.71	0/995
56	DX	0.45	0/740	0.71	0/995
57	BY	0.44	0/789	0.81	1/1053 (0.1%)
57	DY	0.43	0/789	0.81	1/1053 (0.1%)
58	BZ	0.43	0/1435	0.77	0/1949
58	DZ	0.45	0/1435	0.78	0/1949
All	All	0.57	13/329754 (0.0%)	0.76	152/492708 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is

detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	68
1	CA	0	63
22	AV	0	2
22	AW	0	3
22	CV	0	2
22	CW	0	3
23	AX	0	1
23	CX	0	1
30	B4	0	1
30	D4	0	1
36	BA	2	84
36	DA	1	84
46	BN	0	1
46	DN	0	1
All	All	4	315

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	1	G	OP3-P	-7.09	1.52	1.61
24	AY	1	G	OP3-P	-7.06	1.52	1.61
30	D4	47	GLN	C-N	-6.41	1.19	1.34
38	BC	218	MET	CG-SD	6.21	1.97	1.81
36	DA	2551	C	N1-C2	6.07	1.46	1.40

The worst 5 of 152 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	1498	U	C2'-C3'-O3'	11.14	134.01	109.50
1	AA	1050	G	N9-C1'-C2'	-9.97	101.03	112.00
1	CA	1050	G	N9-C1'-C2'	-9.73	101.29	112.00
1	AA	961	U	N1-C1'-C2'	-9.15	101.93	112.00
1	CA	961	U	N1-C1'-C2'	-9.06	102.03	112.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	1498	U	C3'
36	BA	1799	G	C3'
36	BA	1819	A	C3'

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Mol	Chain	Res	Type	Atom
36	DA	1819	A	C3'

5 of 315 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	109	A	Sidechain
1	AA	189(H)	G	Sidechain
1	AA	24	U	Sidechain
1	AA	37	U	Sidechain
1	AA	7	G	Sidechain

## 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	2214	0
1	CA	32329	0	16318	2217	0
2	AB	1901	0	1951	376	1
2	CB	1901	0	1951	383	1
3	AC	1613	0	1677	265	0
3	CC	1613	0	1677	260	0
4	AD	1703	0	1764	296	0
4	CD	1703	0	1765	305	0
5	AE	1147	0	1207	196	0
5	CE	1147	0	1207	198	0
6	AF	843	0	857	86	0
6	CF	843	0	857	101	0
7	AG	1257	0	1296	187	0
7	CG	1257	0	1296	187	0
8	AH	1116	0	1177	192	0
8	CH	1116	0	1177	204	0
9	AI	1010	0	1037	165	0
9	CI	1010	0	1037	168	0
10	AJ	795	0	840	197	0
10	CJ	795	0	840	209	0
11	AK	885	0	904	130	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	124	0
12	AL	971	0	1057	156	0
12	CL	971	0	1057	149	0
13	AM	988	0	1059	215	0
13	CM	988	0	1059	208	0
14	AN	492	0	529	130	0
14	CN	492	0	529	129	0
15	AO	734	0	771	94	0
15	CO	734	0	771	97	0
16	AP	701	0	720	116	0
16	CP	701	0	720	114	0
17	AQ	824	0	891	88	0
17	CQ	824	0	891	89	0
18	AR	574	0	644	97	0
18	CR	574	0	644	95	0
19	AS	630	0	652	129	0
19	CS	630	0	652	129	0
20	AT	763	0	861	148	0
20	CT	763	0	861	141	0
21	AU	209	0	221	30	0
21	CU	209	0	221	33	0
22	AV	1619	0	822	101	0
22	AW	1619	0	822	82	0
22	CV	1619	0	822	89	0
22	CW	1619	0	822	90	0
23	AX	272	0	142	23	0
23	CX	272	0	142	21	0
24	AY	1650	0	851	118	0
24	CY	1650	0	851	115	0
25	AZ	2900	0	2907	491	0
25	CZ	2900	0	2907	478	0
26	B0	662	0	688	112	0
26	D0	662	0	688	112	0
27	B1	732	0	808	156	0
27	D1	732	0	808	158	0
28	B2	598	0	653	166	0
28	D2	598	0	653	153	0
29	B3	468	0	523	74	0
29	D3	468	0	523	76	0
30	B4	341	0	337	72	0
30	D4	341	0	337	63	0
31	B5	459	0	480	98	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	D5	459	0	480	100	0
32	B6	433	0	461	157	0
32	D6	433	0	461	162	0
33	B7	419	0	467	71	0
33	D7	419	0	467	76	0
34	B8	508	0	576	141	0
34	D8	508	0	576	147	0
35	B9	307	0	335	74	0
35	D9	307	0	337	78	0
36	BA	62474	0	31497	4312	0
36	DA	62474	0	31497	4327	0
37	BB	2551	0	1295	152	0
37	DB	2551	0	1295	162	0
38	BC	1742	0	1800	269	1
38	DC	1742	0	1800	272	1
39	BD	2145	0	2234	441	0
39	DD	2145	0	2234	438	0
40	BE	1564	0	1629	331	0
40	DE	1564	0	1629	327	0
41	BF	1624	0	1677	362	0
41	DF	1624	0	1677	351	0
42	BG	1474	0	1535	396	0
42	DG	1474	0	1535	365	0
43	BH	1223	0	1282	214	0
43	DH	1223	0	1282	215	0
44	BJ	651	0	136	11	0
44	DJ	651	0	136	9	0
45	BK	701	0	157	35	0
45	DK	701	0	157	34	0
46	BN	1105	0	1180	233	0
46	DN	1105	0	1180	232	0
47	BO	933	0	996	121	0
47	DO	933	0	996	120	0
48	BP	1114	0	1187	309	0
48	DP	1114	0	1187	308	0
49	BQ	1122	0	1179	240	0
49	DQ	1122	0	1179	226	0
50	BR	960	0	1021	198	0
50	DR	960	0	1021	197	0
51	BS	771	0	832	195	0
51	DS	771	0	832	189	0
52	BT	1142	0	1202	274	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	DT	1142	0	1202	274	0
53	BU	958	0	1015	223	0
53	DU	958	0	1015	223	0
54	BV	779	0	852	167	0
54	DV	779	0	852	169	0
55	BW	896	0	953	153	0
55	DW	896	0	953	160	0
56	BX	726	0	778	118	0
56	DX	726	0	778	115	0
57	BY	776	0	870	208	0
57	DY	776	0	870	203	0
58	BZ	1403	0	1432	320	0
58	DZ	1403	0	1432	293	0
59	AA	42	0	45	4	0
59	CA	42	0	45	3	0
60	AD	1	0	0	1	0
60	AN	1	0	0	0	0
60	B4	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	0	0
60	CN	1	0	0	0	0
60	D4	1	0	0	0	0
60	D9	1	0	0	2	0
61	AY	1	0	0	0	0
61	CY	1	0	0	0	0
62	AZ	28	0	12	15	0
62	CZ	28	0	12	15	0
63	AZ	57	0	58	4	0
63	CZ	57	0	59	8	0
All	All	306876	0	208322	30320	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 59.

The worst 5 of 30320 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
25:AZ:356:PRO:O	25:AZ:359:VAL:CG2	1.74	1.32
27:B1:41:ARG:NH2	36:BA:1365:A:H5''	1.53	1.24
25:CZ:356:PRO:O	25:CZ:359:VAL:HG22	1.38	1.20
24:CY:41:G:H2'	24:CY:42:U:H5''	1.24	1.19
32:B6:45:LYS:H	32:B6:45:LYS:CD	1.48	1.19

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)
2:AB:65:GLY:O	38:BC:27:ARG:NH2[2_445]	1.63	0.57
2:CB:65:GLY:O	38:DC:27:ARG:NH2[2_646]	1.66	0.54

## 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	233/256 (91%)	116 (50%)	72 (31%)	45 (19%)	0	3
2	CB	233/256 (91%)	115 (49%)	74 (32%)	44 (19%)	0	3
3	AC	205/239 (86%)	117 (57%)	52 (25%)	36 (18%)	0	4
3	CC	205/239 (86%)	113 (55%)	57 (28%)	35 (17%)	0	5
4	AD	206/209 (99%)	123 (60%)	49 (24%)	34 (16%)	0	6
4	CD	206/209 (99%)	122 (59%)	48 (23%)	36 (18%)	0	4
5	AE	149/162 (92%)	101 (68%)	33 (22%)	15 (10%)	1	17
5	CE	149/162 (92%)	98 (66%)	37 (25%)	14 (9%)	1	20
6	AF	99/101 (98%)	70 (71%)	20 (20%)	9 (9%)	1	21
6	CF	99/101 (98%)	69 (70%)	21 (21%)	9 (9%)	1	21
7	AG	153/156 (98%)	86 (56%)	35 (23%)	32 (21%)	0	3
7	CG	153/156 (98%)	86 (56%)	37 (24%)	30 (20%)	0	3
8	AH	136/138 (99%)	88 (65%)	34 (25%)	14 (10%)	1	16
8	CH	136/138 (99%)	89 (65%)	35 (26%)	12 (9%)	1	22
9	AI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	8
9	CI	125/128 (98%)	80 (64%)	27 (22%)	18 (14%)	0	8
10	AJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	8
10	CJ	97/105 (92%)	63 (65%)	20 (21%)	14 (14%)	0	8
11	AK	117/129 (91%)	80 (68%)	29 (25%)	8 (7%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	CK	117/129 (91%)	77 (66%)	32 (27%)	8 (7%)	2	30
12	AL	123/135 (91%)	71 (58%)	32 (26%)	20 (16%)	0	6
12	CL	123/135 (91%)	73 (59%)	31 (25%)	19 (15%)	0	6
13	AM	123/126 (98%)	58 (47%)	39 (32%)	26 (21%)	0	3
13	CM	123/126 (98%)	58 (47%)	39 (32%)	26 (21%)	0	3
14	AN	58/61 (95%)	28 (48%)	17 (29%)	13 (22%)	0	2
14	CN	58/61 (95%)	29 (50%)	14 (24%)	15 (26%)	0	1
15	AO	86/89 (97%)	54 (63%)	16 (19%)	16 (19%)	0	4
15	CO	86/89 (97%)	55 (64%)	15 (17%)	16 (19%)	0	4
16	AP	82/88 (93%)	50 (61%)	18 (22%)	14 (17%)	0	5
16	CP	82/88 (93%)	50 (61%)	18 (22%)	14 (17%)	0	5
17	AQ	98/105 (93%)	70 (71%)	21 (21%)	7 (7%)	2	29
17	CQ	98/105 (93%)	69 (70%)	21 (21%)	8 (8%)	1	24
18	AR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	4
18	CR	68/88 (77%)	39 (57%)	17 (25%)	12 (18%)	0	4
19	AS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	8
19	CS	77/93 (83%)	39 (51%)	27 (35%)	11 (14%)	0	8
20	AT	97/106 (92%)	49 (50%)	30 (31%)	18 (19%)	0	4
20	CT	97/106 (92%)	50 (52%)	29 (30%)	18 (19%)	0	4
21	AU	23/27 (85%)	10 (44%)	7 (30%)	6 (26%)	0	1
21	CU	23/27 (85%)	10 (44%)	8 (35%)	5 (22%)	0	2
25	AZ	370/406 (91%)	254 (69%)	77 (21%)	39 (10%)	1	15
25	CZ	370/406 (91%)	252 (68%)	81 (22%)	37 (10%)	1	17
26	B0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	1	18
26	D0	82/85 (96%)	54 (66%)	20 (24%)	8 (10%)	1	18
27	B1	92/98 (94%)	55 (60%)	22 (24%)	15 (16%)	0	6
27	D1	92/98 (94%)	54 (59%)	25 (27%)	13 (14%)	0	9
28	B2	69/72 (96%)	43 (62%)	10 (14%)	16 (23%)	0	2
28	D2	69/72 (96%)	44 (64%)	14 (20%)	11 (16%)	0	6
29	B3	58/60 (97%)	28 (48%)	15 (26%)	15 (26%)	0	1
29	D3	58/60 (97%)	28 (48%)	16 (28%)	14 (24%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	B4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	4
30	D4	43/71 (61%)	20 (46%)	15 (35%)	8 (19%)	0	4
31	B5	57/60 (95%)	33 (58%)	13 (23%)	11 (19%)	0	3
31	D5	57/60 (95%)	32 (56%)	14 (25%)	11 (19%)	0	3
32	B6	48/54 (89%)	17 (35%)	14 (29%)	17 (35%)	0	0
32	D6	48/54 (89%)	18 (38%)	14 (29%)	16 (33%)	0	0
33	B7	47/49 (96%)	27 (57%)	12 (26%)	8 (17%)	0	5
33	D7	47/49 (96%)	27 (57%)	12 (26%)	8 (17%)	0	5
34	B8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	3
34	D8	62/65 (95%)	34 (55%)	16 (26%)	12 (19%)	0	3
35	B9	35/37 (95%)	18 (51%)	9 (26%)	8 (23%)	0	2
35	D9	35/37 (95%)	18 (51%)	10 (29%)	7 (20%)	0	3
38	BC	226/229 (99%)	143 (63%)	53 (24%)	30 (13%)	0	10
38	DC	226/229 (99%)	141 (62%)	55 (24%)	30 (13%)	0	10
39	BD	273/276 (99%)	176 (64%)	63 (23%)	34 (12%)	1	12
39	DD	273/276 (99%)	172 (63%)	66 (24%)	35 (13%)	0	11
40	BE	203/206 (98%)	109 (54%)	45 (22%)	49 (24%)	0	1
40	DE	203/206 (98%)	108 (53%)	46 (23%)	49 (24%)	0	1
41	BF	206/210 (98%)	120 (58%)	47 (23%)	39 (19%)	0	3
41	DF	206/210 (98%)	121 (59%)	46 (22%)	39 (19%)	0	3
42	BG	179/182 (98%)	86 (48%)	52 (29%)	41 (23%)	0	2
42	DG	179/182 (98%)	96 (54%)	45 (25%)	38 (21%)	0	3
43	BH	158/180 (88%)	98 (62%)	36 (23%)	24 (15%)	0	7
43	DH	158/180 (88%)	99 (63%)	35 (22%)	24 (15%)	0	7
46	BN	137/140 (98%)	75 (55%)	39 (28%)	23 (17%)	0	5
46	DN	137/140 (98%)	74 (54%)	40 (29%)	23 (17%)	0	5
47	BO	120/122 (98%)	91 (76%)	17 (14%)	12 (10%)	1	17
47	DO	120/122 (98%)	93 (78%)	15 (12%)	12 (10%)	1	17
48	BP	144/150 (96%)	72 (50%)	35 (24%)	37 (26%)	0	1
48	DP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	1
49	BQ	139/141 (99%)	77 (55%)	46 (33%)	16 (12%)	1	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	DQ	139/141 (99%)	81 (58%)	39 (28%)	19 (14%)	0	9
50	BR	115/118 (98%)	68 (59%)	25 (22%)	22 (19%)	0	3
50	DR	115/118 (98%)	70 (61%)	23 (20%)	22 (19%)	0	3
51	BS	97/112 (87%)	37 (38%)	35 (36%)	25 (26%)	0	1
51	DS	97/112 (87%)	36 (37%)	37 (38%)	24 (25%)	0	1
52	BT	136/146 (93%)	63 (46%)	40 (29%)	33 (24%)	0	1
52	DT	136/146 (93%)	63 (46%)	40 (29%)	33 (24%)	0	1
53	BU	115/118 (98%)	69 (60%)	34 (30%)	12 (10%)	1	16
53	DU	115/118 (98%)	66 (57%)	37 (32%)	12 (10%)	1	16
54	BV	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	3
54	DV	99/101 (98%)	61 (62%)	18 (18%)	20 (20%)	0	3
55	BW	111/113 (98%)	73 (66%)	24 (22%)	14 (13%)	0	11
55	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	11
56	BX	91/96 (95%)	55 (60%)	20 (22%)	16 (18%)	0	4
56	DX	91/96 (95%)	54 (59%)	22 (24%)	15 (16%)	0	6
57	BY	99/110 (90%)	37 (37%)	29 (29%)	33 (33%)	0	0
57	DY	99/110 (90%)	38 (38%)	28 (28%)	33 (33%)	0	0
58	BZ	174/206 (84%)	87 (50%)	47 (27%)	40 (23%)	0	2
58	DZ	174/206 (84%)	96 (55%)	41 (24%)	37 (21%)	0	2
All	All	12280/13108 (94%)	7151 (58%)	3059 (25%)	2070 (17%)	0	5

5 of 2070 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	19	HIS
2	AB	76	GLN
2	AB	77	ALA
2	AB	93	VAL

### 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	202/220 (92%)	178 (88%)	24 (12%)	8	39
2	CB	202/220 (92%)	179 (89%)	23 (11%)	8	41
3	AC	160/188 (85%)	148 (92%)	12 (8%)	19	67
3	CC	160/188 (85%)	148 (92%)	12 (8%)	19	67
4	AD	180/181 (99%)	147 (82%)	33 (18%)	2	16
4	CD	180/181 (99%)	146 (81%)	34 (19%)	2	14
5	AE	115/123 (94%)	103 (90%)	12 (10%)	10	48
5	CE	115/123 (94%)	103 (90%)	12 (10%)	10	48
6	AF	90/90 (100%)	79 (88%)	11 (12%)	7	37
6	CF	90/90 (100%)	78 (87%)	12 (13%)	6	33
7	AG	126/127 (99%)	113 (90%)	13 (10%)	10	48
7	CG	126/127 (99%)	113 (90%)	13 (10%)	10	48
8	AH	119/119 (100%)	100 (84%)	19 (16%)	3	24
8	CH	119/119 (100%)	101 (85%)	18 (15%)	4	27
9	AI	98/99 (99%)	86 (88%)	12 (12%)	7	37
9	CI	98/99 (99%)	86 (88%)	12 (12%)	7	37
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	2	13
10	CJ	88/92 (96%)	71 (81%)	17 (19%)	2	13
11	AK	90/99 (91%)	81 (90%)	9 (10%)	11	50
11	CK	90/99 (91%)	82 (91%)	8 (9%)	14	58
12	AL	104/111 (94%)	82 (79%)	22 (21%)	1	10
12	CL	104/111 (94%)	82 (79%)	22 (21%)	1	10
13	AM	99/101 (98%)	88 (89%)	11 (11%)	9	43
13	CM	99/101 (98%)	88 (89%)	11 (11%)	9	43
14	AN	49/50 (98%)	40 (82%)	9 (18%)	2	15
14	CN	49/50 (98%)	40 (82%)	9 (18%)	2	15
15	AO	79/80 (99%)	69 (87%)	10 (13%)	6	35
15	CO	79/80 (99%)	68 (86%)	11 (14%)	5	31
16	AP	72/74 (97%)	65 (90%)	7 (10%)	12	51
16	CP	72/74 (97%)	65 (90%)	7 (10%)	12	51
17	AQ	94/97 (97%)	88 (94%)	6 (6%)	25	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	CQ	94/97 (97%)	87 (93%)	7 (7%)	20	67
18	AR	61/77 (79%)	56 (92%)	5 (8%)	17	62
18	CR	61/77 (79%)	56 (92%)	5 (8%)	17	62
19	AS	69/80 (86%)	59 (86%)	10 (14%)	5	28
19	CS	69/80 (86%)	59 (86%)	10 (14%)	5	28
20	AT	76/82 (93%)	63 (83%)	13 (17%)	3	20
20	CT	76/82 (93%)	63 (83%)	13 (17%)	3	20
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	47
21	CU	19/22 (86%)	17 (90%)	2 (10%)	10	47
25	AZ	314/339 (93%)	272 (87%)	42 (13%)	6	32
25	CZ	314/339 (93%)	273 (87%)	41 (13%)	6	33
26	B0	66/67 (98%)	52 (79%)	14 (21%)	1	10
26	D0	66/67 (98%)	51 (77%)	15 (23%)	1	8
27	B1	78/83 (94%)	59 (76%)	19 (24%)	1	7
27	D1	78/83 (94%)	59 (76%)	19 (24%)	1	7
28	B2	66/67 (98%)	49 (74%)	17 (26%)	1	6
28	D2	66/67 (98%)	56 (85%)	10 (15%)	4	26
29	B3	51/52 (98%)	44 (86%)	7 (14%)	5	31
29	D3	51/52 (98%)	44 (86%)	7 (14%)	5	31
30	B4	39/63 (62%)	26 (67%)	13 (33%)	0	3
30	D4	39/63 (62%)	26 (67%)	13 (33%)	0	3
31	B5	51/52 (98%)	47 (92%)	4 (8%)	18	65
31	D5	51/52 (98%)	47 (92%)	4 (8%)	18	65
32	B6	49/52 (94%)	41 (84%)	8 (16%)	3	22
32	D6	49/52 (94%)	40 (82%)	9 (18%)	2	15
33	B7	41/42 (98%)	32 (78%)	9 (22%)	1	9
33	D7	41/42 (98%)	33 (80%)	8 (20%)	2	13
34	B8	53/55 (96%)	45 (85%)	8 (15%)	4	27
34	D8	53/55 (96%)	45 (85%)	8 (15%)	4	27
35	B9	34/34 (100%)	30 (88%)	4 (12%)	8	39
35	D9	34/34 (100%)	30 (88%)	4 (12%)	8	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BC	180/181 (99%)	157 (87%)	23 (13%)	6	35
38	DC	180/181 (99%)	157 (87%)	23 (13%)	6	35
39	BD	217/218 (100%)	180 (83%)	37 (17%)	3	20
39	DD	217/218 (100%)	178 (82%)	39 (18%)	2	16
40	BE	165/166 (99%)	142 (86%)	23 (14%)	5	31
40	DE	165/166 (99%)	143 (87%)	22 (13%)	6	33
41	BF	165/166 (99%)	152 (92%)	13 (8%)	18	64
41	DF	165/166 (99%)	152 (92%)	13 (8%)	18	64
42	BG	155/156 (99%)	130 (84%)	25 (16%)	3	23
42	DG	155/156 (99%)	129 (83%)	26 (17%)	3	21
43	BH	132/148 (89%)	118 (89%)	14 (11%)	10	46
43	DH	132/148 (89%)	119 (90%)	13 (10%)	12	51
46	BN	117/119 (98%)	103 (88%)	14 (12%)	7	38
46	DN	117/119 (98%)	102 (87%)	15 (13%)	6	35
47	BO	100/100 (100%)	90 (90%)	10 (10%)	11	50
47	DO	100/100 (100%)	90 (90%)	10 (10%)	11	50
48	BP	112/116 (97%)	88 (79%)	24 (21%)	1	10
48	DP	112/116 (97%)	89 (80%)	23 (20%)	2	11
49	BQ	111/111 (100%)	91 (82%)	20 (18%)	2	16
49	DQ	111/111 (100%)	91 (82%)	20 (18%)	2	16
50	BR	100/101 (99%)	86 (86%)	14 (14%)	5	30
50	DR	100/101 (99%)	82 (82%)	18 (18%)	2	16
51	BS	77/88 (88%)	66 (86%)	11 (14%)	5	29
51	DS	77/88 (88%)	66 (86%)	11 (14%)	5	29
52	BT	120/127 (94%)	99 (82%)	21 (18%)	3	18
52	DT	120/127 (94%)	100 (83%)	20 (17%)	3	21
53	BU	92/94 (98%)	84 (91%)	8 (9%)	15	59
53	DU	92/94 (98%)	84 (91%)	8 (9%)	15	59
54	BV	82/82 (100%)	66 (80%)	16 (20%)	2	13
54	DV	82/82 (100%)	66 (80%)	16 (20%)	2	13
55	BW	91/92 (99%)	79 (87%)	12 (13%)	6	33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	DW	91/92 (99%)	79 (87%)	12 (13%)	6	33
56	BX	74/78 (95%)	67 (90%)	7 (10%)	12	52
56	DX	74/78 (95%)	67 (90%)	7 (10%)	12	52
57	BY	84/91 (92%)	68 (81%)	16 (19%)	2	14
57	DY	84/91 (92%)	68 (81%)	16 (19%)	2	14
58	BZ	155/179 (87%)	127 (82%)	28 (18%)	2	16
58	DZ	155/179 (87%)	131 (84%)	24 (16%)	4	25
All	All	10322/10862 (95%)	8852 (86%)	1470 (14%)	5	30

5 of 1470 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
54	BV	20	LEU
6	CF	31	GLU
51	DS	15	ARG
55	BW	92	ARG
2	CB	63	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 331 such sidechains are listed below:

Mol	Chain	Res	Type
54	BV	11	GLN
5	CE	73	ASN
50	DR	23	ASN
56	BX	41	ASN
2	CB	146	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	288 (19%)	59 (3%)
1	CA	1503/1522 (98%)	284 (18%)	59 (3%)
22	AV	75/76 (98%)	20 (26%)	0
22	AW	75/76 (98%)	21 (28%)	2 (2%)
22	CV	75/76 (98%)	20 (26%)	0
22	CW	75/76 (98%)	21 (28%)	2 (2%)
23	AX	12/27 (44%)	4 (33%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	CX	12/27 (44%)	4 (33%)	0
24	AY	75/77 (97%)	29 (38%)	0
24	CY	75/77 (97%)	28 (37%)	0
36	BA	2900/2915 (99%)	647 (22%)	55 (1%)
36	DA	2900/2915 (99%)	653 (22%)	55 (1%)
37	BB	118/122 (96%)	29 (24%)	1 (0%)
37	DB	118/122 (96%)	29 (24%)	1 (0%)
All	All	9516/9630 (98%)	2077 (21%)	234 (2%)

5 of 2077 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G

5 of 234 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2126	A
1	CA	266	G
36	DA	1819	A
36	BA	2282	G
1	CA	30	U

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

14 non-standard protein/DNA/RNA residues are 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$
24	H2U	AY	16	24	19,21,22	1.11	3 (15%)	27,30,33	1.82	6 (22%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	H2U	AY	17	24	19,21,22	1.03	1 (5%)	27,30,33	1.86	5 (18%)
24	H2U	AY	20	24	19,21,22	1.03	1 (5%)	27,30,33	1.69	4 (14%)
24	YG	AY	37	24	40,42,43	1.46	4 (10%)	50,62,65	4.13	14 (28%)
24	7MG	AY	46	24	24,26,27	2.29	4 (16%)	34,39,42	2.33	6 (17%)
24	5MU	AY	54	24	20,22,23	1.04	2 (10%)	25,32,35	1.33	2 (8%)
24	PSU	AY	55	24	19,21,22	1.49	3 (15%)	23,30,33	1.39	3 (13%)
24	H2U	CY	16	24	19,21,22	1.11	3 (15%)	27,30,33	1.83	6 (22%)
24	H2U	CY	17	24	19,21,22	1.10	1 (5%)	27,30,33	1.85	5 (18%)
24	H2U	CY	20	24	19,21,22	0.99	0	27,30,33	1.70	4 (14%)
24	YG	CY	37	24	40,42,43	1.45	5 (12%)	50,62,65	4.32	14 (28%)
24	7MG	CY	46	24	24,26,27	2.33	3 (12%)	34,39,42	2.31	6 (17%)
24	5MU	CY	54	24	20,22,23	1.07	2 (10%)	25,32,35	1.37	2 (8%)
24	PSU	CY	55	24	19,21,22	1.49	3 (15%)	23,30,33	1.41	3 (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
24	H2U	AY	16	24	-	0/8/38/39	0/2/2/2
24	H2U	AY	17	24	-	0/8/38/39	0/2/2/2
24	H2U	AY	20	24	-	0/8/38/39	0/2/2/2
24	YG	AY	37	24	-	0/25/42/43	0/4/4/4
24	7MG	AY	46	24	-	1/8/37/38	0/3/3/3
24	5MU	AY	54	24	-	0/6/25/26	0/2/2/2
24	PSU	AY	55	24	-	0/8/25/26	0/2/2/2
24	H2U	CY	16	24	-	0/8/38/39	0/2/2/2
24	H2U	CY	17	24	-	0/8/38/39	0/2/2/2
24	H2U	CY	20	24	-	0/8/38/39	0/2/2/2
24	YG	CY	37	24	-	0/25/42/43	0/4/4/4
24	7MG	CY	46	24	-	1/8/37/38	0/3/3/3
24	5MU	CY	54	24	-	0/6/25/26	0/2/2/2
24	PSU	CY	55	24	-	0/8/25/26	0/2/2/2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	CY	46	7MG	C8-N9	-10.20	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AY	46	7MG	C8-N9	-9.97	1.38	1.46
24	AY	37	YG	C2-N2	-5.09	1.29	1.36
24	CY	37	YG	C2-N2	-4.89	1.30	1.36
24	AY	37	YG	C12-N1	4.77	1.43	1.39

The worst 5 of 80 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	CY	37	YG	C6-C5-N7	-26.61	132.82	134.24
24	AY	37	YG	C6-C5-N7	-25.16	132.90	134.24
24	AY	46	7MG	C6-N1-C2	8.92	125.24	120.20
24	CY	46	7MG	C6-N1-C2	8.85	125.20	120.20
24	AY	46	7MG	N7-C8-N9	7.52	113.11	103.13

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	AY	46	7MG	OP2-P-O5'-C5'
24	CY	46	7MG	OP2-P-O5'-C5'

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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
59	PAR	AA	1601	-	45,45,45	1.37	5 (11%)	67,67,67	1.45	8 (11%)
62	GDP	AZ	501	-	30,30,30	1.39	5 (16%)	45,47,47	1.94	8 (17%)
63	KIR	AZ	502	-	59,59,59	3.59	22 (37%)	82,84,84	1.69	18 (21%)
59	PAR	CA	1601	-	45,45,45	1.35	4 (8%)	67,67,67	1.38	9 (13%)
62	GDP	CZ	501	-	30,30,30	1.42	5 (16%)	45,47,47	1.75	7 (15%)
63	KIR	CZ	502	-	59,59,59	3.62	27 (45%)	82,84,84	1.71	17 (20%)

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
59	PAR	AA	1601	-	-	0/18/94/94	0/4/4/4
62	GDP	AZ	501	-	-	0/16/32/32	0/3/3/3
63	KIR	AZ	502	-	-	0/54/98/98	0/3/3/3
59	PAR	CA	1601	-	-	0/18/94/94	0/4/4/4
62	GDP	CZ	501	-	-	0/16/32/32	0/3/3/3
63	KIR	CZ	502	-	-	0/54/98/98	0/3/3/3

The worst 5 of 68 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	AZ	502	KIR	O18-C17	-13.72	1.22	1.44
63	CZ	502	KIR	O18-C17	-13.62	1.22	1.44
63	CZ	502	KIR	O30-C30	-11.60	1.18	1.42
63	AZ	502	KIR	O30-C30	-11.52	1.18	1.42
63	AZ	502	KIR	O34-C33	-11.22	1.29	1.44

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	AZ	501	GDP	C6-C5-N7	-6.81	133.22	134.14
62	AZ	501	GDP	C2-N3-C4	5.00	121.30	115.30
63	CZ	502	KIR	C45-C28-C27	5.00	113.29	108.38
62	CZ	501	GDP	C2-N3-C4	4.91	121.19	115.30
62	CZ	501	GDP	C5-C4-N3	-4.90	120.42	126.07

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, 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	1504/1522 (98%)	-0.06	10 (0%) 84 63	29, 82, 163, 200	0
1	CA	1504/1522 (98%)	-0.15	13 (0%) 81 57	28, 83, 163, 200	0
2	AB	235/256 (91%)	0.18	1 (0%) 90 76	63, 102, 151, 161	0
2	CB	235/256 (91%)	0.11	2 (0%) 81 57	63, 102, 151, 162	0
3	AC	207/239 (86%)	0.06	0 100 100	54, 91, 111, 117	0
3	CC	207/239 (86%)	0.08	2 (0%) 79 53	59, 91, 111, 117	0
4	AD	208/209 (99%)	0.05	1 (0%) 88 71	60, 91, 116, 122	0
4	CD	208/209 (99%)	0.12	0 100 100	61, 92, 117, 123	0
5	AE	151/162 (93%)	-0.02	0 100 100	44, 72, 90, 108	0
5	CE	151/162 (93%)	0.02	1 (0%) 84 63	43, 73, 91, 109	0
6	AF	101/101 (100%)	0.07	0 100 100	91, 102, 110, 118	0
6	CF	101/101 (100%)	0.21	1 (0%) 79 53	92, 103, 111, 118	0
7	AG	155/156 (99%)	0.17	2 (1%) 74 47	79, 104, 134, 141	0
7	CG	155/156 (99%)	0.13	4 (2%) 53 30	81, 104, 134, 141	0
8	AH	138/138 (100%)	0.20	1 (0%) 84 63	62, 80, 97, 116	0
8	CH	138/138 (100%)	0.12	0 100 100	61, 82, 97, 115	0
9	AI	127/128 (99%)	0.30	3 (2%) 56 32	73, 126, 153, 158	0
9	CI	127/128 (99%)	0.33	2 (1%) 68 41	74, 126, 154, 159	0
10	AJ	99/105 (94%)	0.53	5 (5%) 27 15	79, 121, 149, 154	0
10	CJ	99/105 (94%)	0.56	8 (8%) 12 8	80, 121, 148, 153	0
11	AK	119/129 (92%)	0.12	4 (3%) 43 24	63, 84, 125, 150	0
11	CK	119/129 (92%)	0.19	4 (3%) 43 24	65, 85, 126, 151	0
12	AL	125/135 (92%)	0.04	1 (0%) 83 60	47, 70, 100, 125	0
12	CL	125/135 (92%)	0.16	1 (0%) 83 60	52, 71, 101, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AM	125/126 (99%)	0.33	5 (4%) 36 20	79, 119, 143, 159	0
13	CM	125/126 (99%)	0.32	4 (3%) 45 25	81, 118, 143, 159	0
14	AN	60/61 (98%)	0.06	0 100 100	60, 77, 96, 101	0
14	CN	60/61 (98%)	0.14	1 (1%) 67 40	61, 77, 95, 103	0
15	AO	88/89 (98%)	0.19	1 (1%) 77 50	69, 92, 109, 112	0
15	CO	88/89 (98%)	0.23	1 (1%) 77 50	72, 91, 109, 112	0
16	AP	84/88 (95%)	0.19	1 (1%) 75 49	76, 89, 119, 137	0
16	CP	84/88 (95%)	0.21	1 (1%) 75 49	74, 89, 118, 137	0
17	AQ	100/105 (95%)	0.19	0 100 100	65, 92, 115, 121	0
17	CQ	100/105 (95%)	0.25	2 (2%) 62 36	67, 93, 115, 121	0
18	AR	70/88 (79%)	0.08	0 100 100	55, 86, 114, 121	0
18	CR	70/88 (79%)	0.07	1 (1%) 72 45	57, 87, 115, 121	0
19	AS	79/93 (84%)	0.55	7 (8%) 10 7	82, 120, 143, 146	0
19	CS	79/93 (84%)	0.46	5 (6%) 19 11	83, 120, 144, 146	0
20	AT	99/106 (93%)	0.11	1 (1%) 79 53	94, 109, 129, 132	0
20	CT	99/106 (93%)	0.10	0 100 100	93, 109, 129, 132	0
21	AU	25/27 (92%)	0.83	3 (12%) 5 5	104, 116, 137, 139	0
21	CU	25/27 (92%)	0.52	1 (4%) 36 20	104, 116, 136, 138	0
22	AV	76/76 (100%)	-0.13	0 100 100	54, 120, 170, 179	0
22	AW	76/76 (100%)	-0.03	1 (1%) 74 47	82, 147, 186, 199	0
22	CV	76/76 (100%)	-0.17	0 100 100	54, 121, 170, 179	0
22	CW	76/76 (100%)	0.09	3 (3%) 37 21	84, 148, 185, 199	0
23	AX	13/27 (48%)	0.31	1 (7%) 13 8	45, 63, 136, 154	0
23	CX	13/27 (48%)	0.19	0 100 100	47, 63, 136, 154	0
24	AY	77/77 (100%)	0.27	3 (3%) 37 21	74, 156, 198, 200	0
24	CY	77/77 (100%)	0.50	6 (7%) 13 8	76, 156, 198, 200	0
25	AZ	374/406 (92%)	0.58	30 (8%) 12 8	97, 139, 158, 177	0
25	CZ	374/406 (92%)	0.79	46 (12%) 5 4	98, 139, 158, 176	0
26	B0	84/85 (98%)	0.36	0 100 100	104, 116, 128, 137	0
26	D0	84/85 (98%)	0.44	1 (1%) 75 49	104, 116, 129, 137	0
27	B1	94/98 (95%)	0.06	3 (3%) 45 25	41, 71, 107, 111	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
27	D1	94/98 (95%)	0.07	1 (1%) 77 50	63, 85, 115, 122	0
28	B2	71/72 (98%)	0.04	0 100 100	84, 115, 128, 130	0
28	D2	71/72 (98%)	0.34	3 (4%) 35 19	104, 125, 144, 163	0
29	B3	60/60 (100%)	0.87	4 (6%) 17 10	106, 122, 132, 148	0
29	D3	60/60 (100%)	0.59	4 (6%) 17 10	107, 122, 132, 148	0
30	B4	45/71 (63%)	0.81	7 (15%) 3 3	107, 169, 196, 198	0
30	D4	45/71 (63%)	0.71	5 (11%) 6 6	107, 170, 195, 197	0
31	B5	59/60 (98%)	0.70	5 (8%) 11 7	89, 116, 175, 187	0
31	D5	59/60 (98%)	0.56	4 (6%) 17 10	90, 115, 175, 186	0
32	B6	50/54 (92%)	0.59	6 (12%) 5 5	78, 119, 146, 152	0
32	D6	50/54 (92%)	0.60	5 (10%) 8 6	79, 119, 147, 152	0
33	B7	49/49 (100%)	0.09	0 100 100	59, 77, 144, 152	0
33	D7	49/49 (100%)	-0.09	0 100 100	60, 78, 145, 152	0
34	B8	64/65 (98%)	0.36	2 (3%) 47 26	80, 104, 124, 138	0
34	D8	64/65 (98%)	0.43	4 (6%) 19 11	83, 104, 125, 138	0
35	B9	37/37 (100%)	0.43	2 (5%) 25 13	104, 117, 124, 128	0
35	D9	37/37 (100%)	0.80	2 (5%) 25 13	103, 118, 125, 126	0
36	BA	2901/2915 (99%)	-0.03	47 (1%) 68 41	31, 100, 192, 200	0
36	DA	2901/2915 (99%)	-0.04	57 (1%) 62 36	31, 101, 192, 200	0
37	BB	119/122 (97%)	0.05	2 (1%) 67 40	103, 142, 169, 175	0
37	DB	119/122 (97%)	-0.11	0 100 100	102, 142, 168, 174	0
38	BC	228/229 (99%)	0.50	14 (6%) 21 11	92, 122, 168, 178	0
38	DC	228/229 (99%)	0.62	19 (8%) 11 8	92, 122, 167, 179	0
39	BD	275/276 (99%)	0.12	1 (0%) 90 76	30, 67, 96, 110	0
39	DD	275/276 (99%)	0.09	2 (0%) 84 63	38, 68, 96, 109	0
40	BE	205/206 (99%)	0.36	7 (3%) 43 24	67, 106, 143, 154	0
40	DE	205/206 (99%)	0.31	3 (1%) 70 43	67, 106, 143, 153	0
41	BF	208/210 (99%)	0.33	5 (2%) 56 32	61, 123, 160, 167	0
41	DF	208/210 (99%)	0.47	11 (5%) 25 14	62, 123, 160, 166	0
42	BG	181/182 (99%)	0.29	8 (4%) 33 18	103, 128, 146, 163	0
42	DG	181/182 (99%)	0.51	13 (7%) 15 9	111, 133, 151, 159	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
43	BH	160/180 (88%)	0.74	20 (12%) 5 4	131, 155, 174, 176	0
43	DH	160/180 (88%)	0.94	23 (14%) 3 3	131, 155, 174, 176	0
44	BJ	0/173	-	-	-	-
44	DJ	0/173	-	-	-	-
45	BK	0/147	-	-	-	-
45	DK	0/147	-	-	-	-
46	BN	139/140 (99%)	0.39	6 (4%) 34 19	103, 123, 148, 155	0
46	DN	139/140 (99%)	0.41	8 (5%) 22 12	103, 123, 148, 155	0
47	BO	122/122 (100%)	0.11	0 100 100	60, 80, 96, 105	0
47	DO	122/122 (100%)	0.17	0 100 100	61, 80, 96, 106	0
48	BP	146/150 (97%)	0.25	4 (2%) 52 29	71, 113, 133, 140	0
48	DP	146/150 (97%)	0.49	10 (6%) 17 10	70, 114, 133, 139	0
49	BQ	141/141 (100%)	0.30	4 (2%) 50 29	73, 106, 130, 159	0
49	DQ	141/141 (100%)	0.36	3 (2%) 60 35	73, 105, 129, 159	0
50	BR	117/118 (99%)	0.33	4 (3%) 43 24	81, 105, 123, 143	0
50	DR	117/118 (99%)	0.38	5 (4%) 34 19	82, 105, 124, 143	0
51	BS	99/112 (88%)	0.40	2 (2%) 62 36	96, 133, 155, 162	0
51	DS	99/112 (88%)	0.49	6 (6%) 21 11	97, 133, 156, 162	0
52	BT	138/146 (94%)	0.31	4 (2%) 49 28	72, 112, 166, 181	0
52	DT	138/146 (94%)	0.39	9 (6%) 18 11	73, 111, 166, 181	0
53	BU	117/118 (99%)	0.35	3 (2%) 53 30	87, 120, 141, 147	0
53	DU	117/118 (99%)	0.18	3 (2%) 53 30	88, 119, 141, 148	0
54	BV	101/101 (100%)	0.83	16 (15%) 3 3	105, 144, 159, 164	0
54	DV	101/101 (100%)	0.83	18 (17%) 2 2	106, 145, 159, 165	0
55	BW	113/113 (100%)	0.34	6 (5%) 25 14	81, 109, 132, 136	0
55	DW	113/113 (100%)	0.35	1 (0%) 81 57	81, 109, 131, 136	0
56	BX	93/96 (96%)	0.26	1 (1%) 77 50	96, 108, 124, 128	0
56	DX	93/96 (96%)	0.35	4 (4%) 34 19	97, 109, 125, 130	0
57	BY	101/110 (91%)	0.73	10 (9%) 8 6	124, 145, 165, 170	0
57	DY	101/110 (91%)	1.14	18 (17%) 2 2	123, 145, 163, 170	0
58	BZ	176/206 (85%)	0.77	23 (13%) 4 4	107, 133, 161, 164	0
58	DZ	176/206 (85%)	0.98	35 (19%) 2 2	109, 139, 168, 171	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	22016/23378 (94%)	0.18	683 (3%) 47 26	28, 105, 164, 200	0

The worst 5 of 683 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	DQ	140	ALA	13.2
31	B5	60	VAL	10.8
1	AA	89	C	10.5
36	DA	654(I)	C	10.1
36	DA	654(G)	C	9.7

## 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
24	PSU	AY	55	20/21	0.19	-	171,180,181,182	0
24	H2U	AY	17	20/21	0.39	-	195,199,199,200	0
24	7MG	AY	46	24/25	0.23	-	186,189,190,190	0
24	H2U	AY	20	20/21	0.21	-	196,198,200,200	0
24	H2U	AY	16	20/21	0.66	-	198,199,200,200	0
24	7MG	CY	46	24/25	0.24	-	186,189,190,190	0
24	YG	CY	37	39/40	0.27	-	77,108,122,122	0
24	H2U	CY	16	20/21	0.47	-	199,199,200,200	0
24	5MU	AY	54	21/22	0.23	-	164,166,168,171	0
24	YG	AY	37	39/40	0.30	-	77,108,121,122	0
24	PSU	CY	55	20/21	0.31	-	172,180,180,180	0
24	H2U	CY	20	20/21	0.18	-	195,198,200,200	0
24	H2U	CY	17	20/21	0.50	-	196,199,200,200	0
24	5MU	CY	54	21/22	0.36	-	165,167,168,171	0

## 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, 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
60	ZN	D4	101	1/1	0.12	-	133,133,133,133	0
60	ZN	D9	101	1/1	0.08	-	126,126,126,126	0
61	MG	AY	101	1/1	0.24	-	109,109,109,109	0
60	ZN	CD	301	1/1	0.28	-	56,56,56,56	0
63	KIR	CZ	502	57/57	0.43	-	99,106,116,117	0
63	KIR	AZ	502	57/57	0.46	-	98,106,116,117	0
59	PAR	CA	1601	42/42	0.20	-	41,46,64,65	0
61	MG	CY	101	1/1	1.91	-	181,181,181,181	0
60	ZN	AN	101	1/1	0.16	-	45,45,45,45	0
60	ZN	B4	101	1/1	0.15	-	97,97,97,97	0
60	ZN	CN	101	1/1	0.19	-	100,100,100,100	0
62	GDP	CZ	501	28/28	0.18	-	117,126,128,128	0
62	GDP	AZ	501	28/28	0.20	-	117,124,126,126	0
60	ZN	AD	301	1/1	0.27	-	52,52,52,52	0
60	ZN	B9	101	1/1	0.18	-	113,113,113,113	0
59	PAR	AA	1601	42/42	0.20	-	40,44,48,49	0

## 6.5 Other polymers

There are no such residues in this entry.