



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:13 PM BST

PDB ID : 4V9D
Title : Structures of the bacterial ribosome in classical and hybrid states of tRNA binding
Authors : Dunkle, J.A.; Wang, L.; Feldman, M.B.; Pulk, A.; Chen, V.B.; Kapral, G.J.; Noeske, J.; Richardson, J.S.; Blanchard, S.C.; Cate, J.H.D.
Deposited on : 2012-07-31
Resolution : 3.00 Å(reported)

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

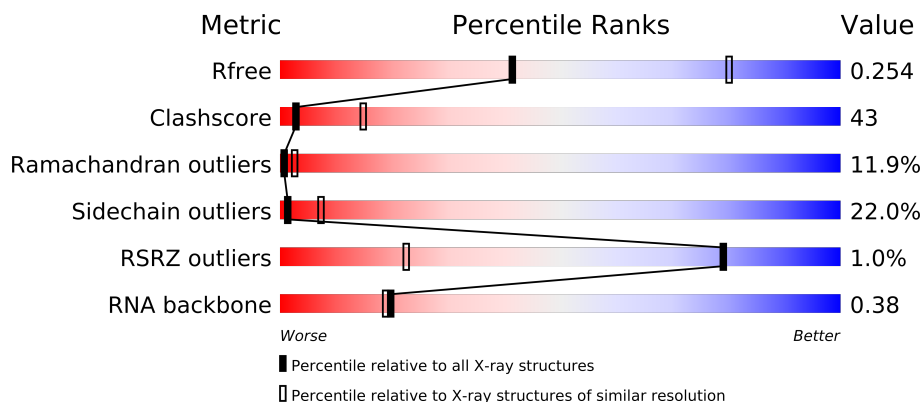
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)
RNA backbone	1838	1070 (3.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	AA	1539	
1	BA	1539	
2	AB	218	
2	BB	218	
3	AC	206	
3	BC	206	
4	AD	205	
4	BD	205	
5	AE	150	
5	BE	150	
6	AF	100	
6	BF	100	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
7	AG	151	
7	BG	151	
8	AH	129	
8	BH	129	
9	AI	127	
9	BI	127	
10	AJ	98	
10	BJ	98	
11	AK	117	
11	BK	117	
12	AL	123	
12	BL	123	
13	AM	114	
13	BM	114	
14	AN	100	
14	BN	100	
15	AO	88	
15	BO	88	
16	AP	82	
16	BP	82	
17	AQ	80	
17	BQ	80	
18	AR	55	
18	BR	55	
19	AS	79	
19	BS	79	
20	AT	85	
20	BT	85	
21	AU	51	
21	BU	51	
22	AV	76	
22	BV	76	
23	AX	16	
23	BX	16	
24	AY	183	
25	CA	2903	
25	DA	2903	
26	CB	119	
27	CC	271	
27	DC	271	
28	CD	209	
28	DD	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	CE	201	
29	DE	201	
30	CF	177	
30	DF	177	
31	CG	176	
31	DG	176	
32	CH	149	
32	DH	149	
33	CI	141	
33	DI	141	
34	CJ	142	
34	DJ	142	
35	CK	122	
35	DK	122	
36	CL	143	
36	DL	143	
37	CM	136	
37	DM	136	
38	CN	120	
38	DN	120	
39	CO	116	
39	DO	116	
40	CP	114	
40	DP	114	
41	CQ	117	
41	DQ	117	
42	CR	103	
42	DR	103	
43	CS	110	
43	DS	110	
44	CT	93	
44	DT	93	
45	CU	102	
45	DU	102	
46	CV	94	
46	DV	94	
47	CW	76	
48	CX	77	
48	DX	77	
49	CY	63	
49	DY	63	
50	CZ	58	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
50	DZ	58	
51	C0	56	
51	D0	56	
52	C1	50	
52	D1	50	
53	C2	46	
53	D2	46	
54	C3	64	
54	D3	64	
55	C4	38	
55	D4	38	
56	DB	118	
57	DW	75	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
58	MG	AA	1604	-	X
58	MG	AA	1608	-	X
58	MG	AA	1619	-	X
58	MG	AA	1622	-	X
58	MG	AA	1631	-	X
58	MG	AA	1640	-	X
58	MG	AA	1643	-	X
58	MG	AA	1644	-	X
58	MG	AA	1645	-	X
58	MG	AA	1646	-	X
58	MG	AA	1647	-	X
58	MG	AA	1649	-	X
58	MG	AA	1651	-	X
58	MG	AA	1653	-	X
58	MG	AA	1655	-	X
58	MG	AA	1657	-	X
58	MG	AA	1658	-	X
58	MG	AA	1661	-	X
58	MG	AA	1666	-	X
58	MG	AA	1667	-	X
58	MG	AA	1670	-	X
58	MG	AA	1672	-	X
58	MG	BA	1608	-	X
58	MG	BA	1615	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
58	MG	BA	1618	-	X
58	MG	BA	1637	-	X
58	MG	BA	1642	-	X
58	MG	BA	1648	-	X
58	MG	BA	1649	-	X
58	MG	BA	1650	-	X
58	MG	BA	1656	-	X
58	MG	CA	3018	-	X
58	MG	CA	3031	-	X
58	MG	CA	3066	-	X
58	MG	CA	3095	-	X
58	MG	CA	3110	-	X
58	MG	CA	3116	-	X
58	MG	CA	3132	-	X
58	MG	CA	3141	-	X
58	MG	CA	3142	-	X
58	MG	CA	3143	-	X
58	MG	CA	3144	-	X
58	MG	CA	3147	-	X
58	MG	CA	3149	-	X
58	MG	CA	3151	-	X
58	MG	CA	3153	-	X
58	MG	CA	3154	-	X
58	MG	CA	3155	-	X
58	MG	CA	3157	-	X
58	MG	CA	3158	-	X
58	MG	CA	3159	-	X
58	MG	CA	3163	-	X
58	MG	CA	3164	-	X
58	MG	CA	3165	-	X
58	MG	CA	3166	-	X
58	MG	CA	3167	-	X
58	MG	CA	3169	-	X
58	MG	CA	3173	-	X
58	MG	CA	3174	-	X
58	MG	CA	3182	-	X
58	MG	CA	3183	-	X
58	MG	CA	3184	-	X
58	MG	CA	3185	-	X
58	MG	CA	3186	-	X
58	MG	CA	3188	-	X
58	MG	CA	3190	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
58	MG	CA	3191	-	X
58	MG	CA	3194	-	X
58	MG	CB	204	-	X
58	MG	DA	3007	-	X
58	MG	DA	3015	-	X
58	MG	DA	3025	-	X
58	MG	DA	3037	-	X
58	MG	DA	3061	-	X
58	MG	DA	3083	-	X
58	MG	DA	3085	-	X
58	MG	DA	3091	-	X
58	MG	DA	3092	-	X
58	MG	DA	3098	-	X
58	MG	DA	3115	-	X
58	MG	DA	3116	-	X
58	MG	DA	3119	-	X
58	MG	DA	3131	-	X
58	MG	DA	3133	-	X
58	MG	DA	3137	-	X
58	MG	DA	3139	-	X
58	MG	DA	3140	-	X
58	MG	DA	3141	-	X
58	MG	DA	3142	-	X
58	MG	DA	3143	-	X
58	MG	DA	3146	-	X
58	MG	DA	3147	-	X
58	MG	DA	3148	-	X
58	MG	DA	3149	-	X
58	MG	DA	3150	-	X
58	MG	DA	3152	-	X
58	MG	DA	3154	-	X
58	MG	DA	3156	-	X
58	MG	DA	3157	-	X
58	MG	DA	3159	-	X
58	MG	DA	3165	-	X
58	MG	DA	3166	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 292354 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	BA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	BB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	BC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
4	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	BE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	BF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	BG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
8	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
9	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	BJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
11	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
12	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	BM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
14	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- 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
			714	439	144	130	1			
15	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	BQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	BR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- 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	0
			638	408	120	108	2			
19	BS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
20	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	BU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called phenylalanine specific transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			
22	BV	76	Total	C	N	O	P	0	0	0
			1623	723	290	534	76			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	15	Total	C	N	O	P	0	0	0
			324	145	61	103	15			
23	BX	16	Total	C	N	O	P	0	0	0
			346	155	66	109	16			

- Molecule 24 is a protein called ribosome recycling factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	183	Total	C	N	O	S	0	0	0
			1419	871	260	283	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	2	GLY	-	EXPRESSION TAG	UNP P0A805

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	CA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
25	DA	2896	Total	C	N	O	P	0	0	0
			62173	27735	11441	20101	2896			

- Molecule 26 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	CB	119	Total	C	N	O	P	0	0	0
			2548	1135	466	829	118			

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	CC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
27	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
28	DD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
29	DE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	CF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
30	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
31	DG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	CH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
32	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
33	DI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
34	DJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	CK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
35	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
36	DL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
37	DM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	CN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
38	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	CO	116	Total	C	N	O	0	0	0
			892	552	178	162			
39	DO	116	Total	C	N	O	0	0	0
			892	552	178	162			

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
40	DP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	CQ	117	Total	C	N	O	0	0	0
			947	604	192	151			
41	DQ	117	Total	C	N	O	0	0	0
			947	604	192	151			

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
43	DS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	CT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
44	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	CU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				
45	DU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
46	DV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	CW	76	Total	C	N	O	S	0	0	0
			575	356	117	101	1			

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
48	DX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
49	DY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
50	DZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
51	D0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
52	C1	50	Total	C	N	O	0	0	0
			410	263	75	72			
52	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
54	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
55	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 56 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 57 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	DW	75	Total	C	N	O	S	0	0	0
			564	350	113	100	1			

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	BA	56	Total	Mg	0	0
			56	56		
58	CA	194	Total	Mg	0	0
			194	194		
58	DQ	1	Total	Mg	0	0
			1	1		
58	CB	4	Total	Mg	0	0
			4	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	DL	1	Total 1	Mg 1	0	0
58	AA	72	Total 72	Mg 72	0	0
58	CQ	1	Total 1	Mg 1	0	0
58	DA	166	Total 166	Mg 166	0	0
58	DB	3	Total 3	Mg 3	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	D4	1	Total 1	Zn 1	0	0
59	C4	1	Total 1	Zn 1	0	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	197	Total 197	O 197	0	0
60	AN	4	Total 4	O 4	0	0
60	AT	1	Total 1	O 1	0	0
60	AU	1	Total 1	O 1	0	0
60	BA	190	Total 190	O 190	0	0
60	BL	1	Total 1	O 1	0	0
60	BN	5	Total 5	O 5	0	0
60	BT	1	Total 1	O 1	0	0
60	BU	1	Total 1	O 1	0	0
60	CA	625	Total 625	O 625	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CB	13	Total 13	O 13	0	0
60	CC	8	Total 8	O 8	0	0
60	CD	2	Total 2	O 2	0	0
60	CE	2	Total 2	O 2	0	0
60	CF	1	Total 1	O 1	0	0
60	CJ	1	Total 1	O 1	0	0
60	CL	6	Total 6	O 6	0	0
60	CN	4	Total 4	O 4	0	0
60	CS	1	Total 1	O 1	0	0
60	CV	1	Total 1	O 1	0	0
60	C2	1	Total 1	O 1	0	0
60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	622	Total 622	O 622	0	0
60	DB	14	Total 14	O 14	0	0
60	DC	4	Total 4	O 4	0	0
60	DD	5	Total 5	O 5	0	0
60	DE	2	Total 2	O 2	0	0
60	DJ	1	Total 1	O 1	0	0
60	DL	4	Total 4	O 4	0	0
60	DN	1	Total 1	O 1	0	0

Continued on next page...

Continued from previous page...

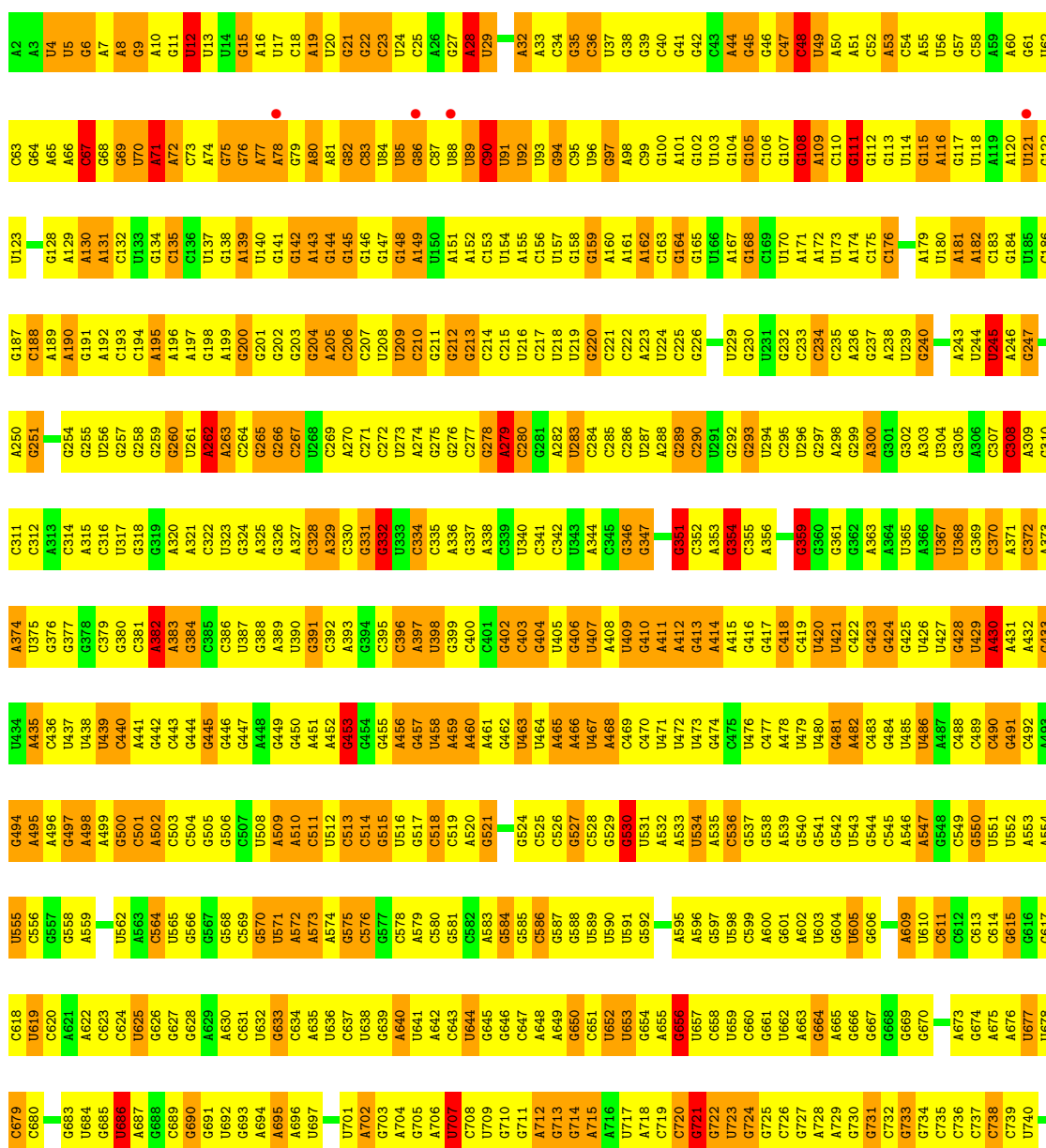
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DR	1	Total 1	O 1	0	0
60	D2	1	Total 1	O 1	0	0
60	D3	2	Total 2	O 2	0	0
60	D4	1	Total 1	O 1	0	0

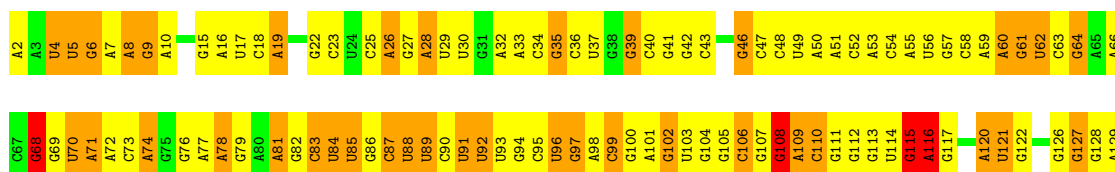
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

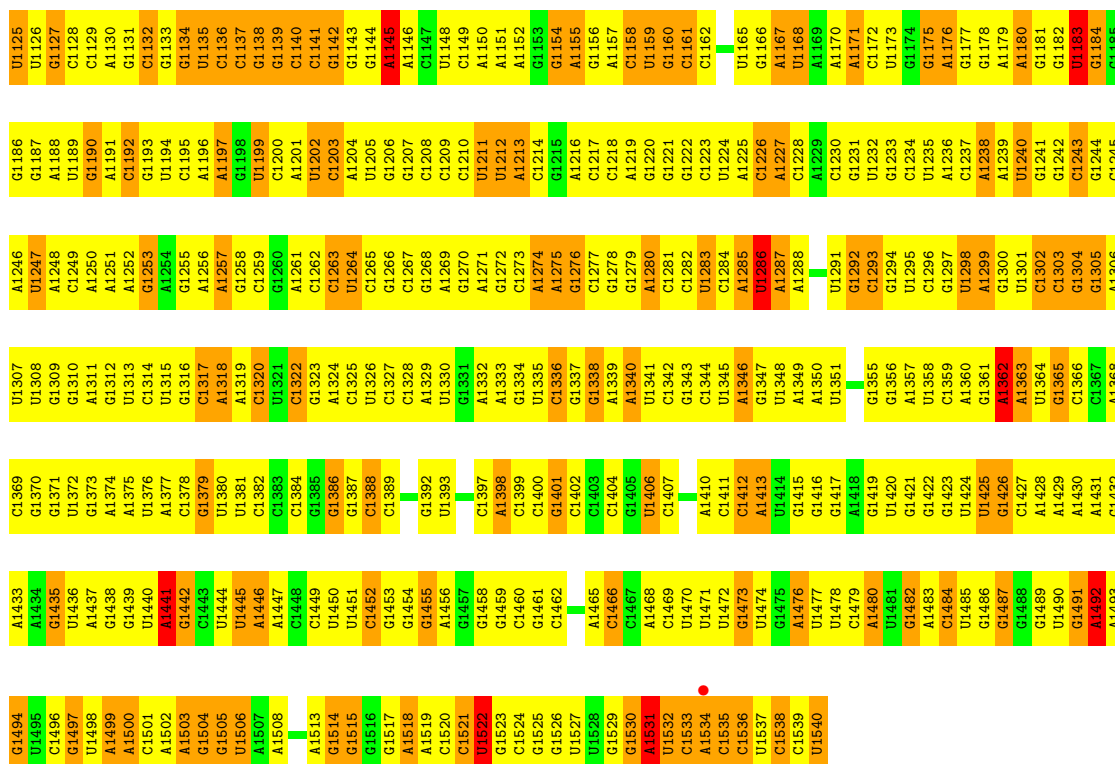
• Molecule 1: 16S rRNA

Chain AA: 



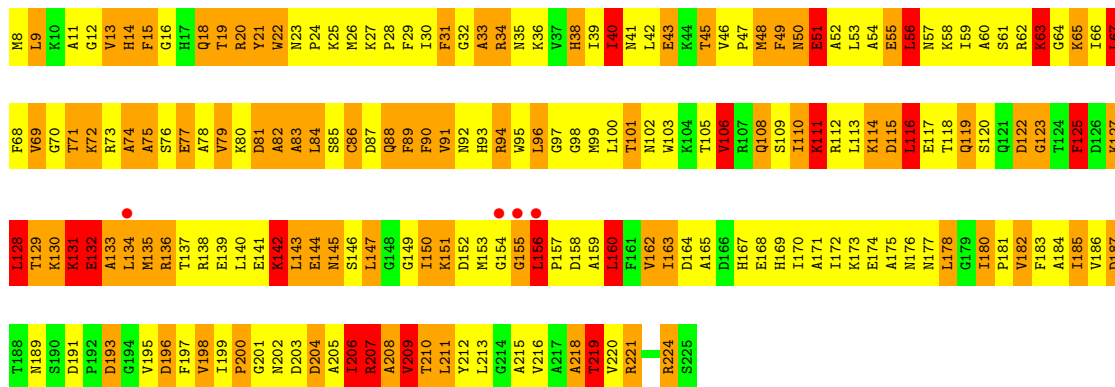


U1065	C1066	A1067	G1068	C1069	U1070	C1071	G1072	U1073	G1013	U1013	A1014	G1015	U1016	C1017	U1078	G1079	A1080	C1081	A1082	U1083	G1084	U1085	C1086	G1087	U1088	C1089	U1090	U1091	A1092	C1093	G1094	U1095	C1096	C1097	U1098	G1099	C1100	A1101	C1102	C1103	G1104	A1105	C1106	G1107	C1108	C1109	A1110	C1111	C1112	C1113	C1114	U1115	U1116	A1117	U1118	C1119	C1120	U1121	U1122	U1123	G1124																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
G877	A878	C879	C880	G881	A882	C883	U884	G885	A889	G890	U891	A892	C893	G894	U895	A896	C897	G898	U899	A900	C901	G902	U903	A904	C905	U906	A907	C908	U909	A910	C911	U912	A913	C914	U915	A916	C917	U918	A919	C920	U921	A922	C923	U924	A925	C926	U927	G928	C929	U930	A931	C932	U933	G934	A935	C936	U937	A938	C939	U940	A941	C942	U943	A944	C945	U946	A947	C948	U949	A950	C951	U952	A953	C954	U955	A956	C957	U958	A959	C960	U961	A962	C963	U964	A965	C966	U967	A968	C969	U970	A971	C972	U973	A974	C975	U976	A977	C978	U979	A980	C981	U982	A983	C984	U985	A986	C987	U988	A989	C990	U991	A992	C993	U994	A995	C996	U997	A998	C999	U1000	C1001	U1002	G1003	U1004																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
G828	A829	C830	U831	G832	U833	C834	A835	U836	G837	A838	C839	U840	G841	A842	C843	U844	G845	A846	C847	U848	G849	A850	C851	U852	G853	A854	C855	U856	G857	A858	C859	U860	G861	A862	C863	U864	G865	A866	C867	U868	G869	A870	C871	U872	G873	A874	C875	U876	G877	A878	C879	U880	G881	A882	C883	U884	G885	A886	C887	U888	G889	A890	C891	U892	G893	A894	C895	U896	G897	A898	C899	U900	G901	A902	C903	U904	G905	A906	C907	U908	G909	A910	C911	U912	G913	A914	C915	U916	G917	A918	C919	U920	G921	A922	C923	U924	G925	A926	C927	U928	G929	A930	C931	U932	G933	A934	C935	U936	G937	A938	C939	U940	G941	A942	C943	U944	G945	A946	C947	U948	G949	A950	C951	U952	G953	A954	C955	U956	G957	A958	C959	U960	G961	A962	C963	U964	G965	A966	C967	U968	G969	A970	C971	U972	G973	A974	C975	U976	G977	A978	C979	U980	G981	A982	C983	U984	G985	A986	C987	U988	G989	A990	C991	U992	G993	A994	C995	U996	G997	A998	C999	U1000	G1001	A1002	C1003	U1004																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G566	C567	U568	A569	C570	U571	A572	C573	U574	A575	C576	U577	A578	C579	U580	A581	C582	U583	A584	C585	U586	A587	C588	U589	A590	C591	U592	A593	C594	U595	A596	C597	U598	A599	C600	U601	A602	C603	U604	A605	C606	U607	A608	C609	U610	A611	C612	U613	A614	C615	U616	A617	C618	U619	A620	C621	U622	A623	C624	U625	A626	C627	U628	A629	C630	U631	A632	C633	U634	A635	C636	U637	A638	C639	U640	A641	C642	U643	A644	C645	U646	A647	C648	U649	A650	C651	U652	A653	C654	U655	A656	C657	U658	A659	C660	U661	A662	C663	U664	A665	C666	U667	A668	C669	U670	A671	C672	U673	A674	C675	U676	A677	C678	U679	A680	C681	U682	A683	C684	U685	A686	C687	U688	A689	C690	U691	A692	C693	U694	A695	C696	U697	A698	C699	U700	A701	C702	U703	A704	C705	U706	A707	C708	U709	A710	C711	U712	A713	C714	U715	A716	C717	U718	A719	C720	U721	A722	C723	U724	A725	C726	U727	A728	C729	U730	A731	C732	U733	A734	C735	U736	A737	C738	U739	A740	C741	U742	A743	C744	U745	A746	C747	U748	A749	C750	U751	A752	C753	U754	A755	C756	U757	A758	C759	U760	A761	C762	U763	A764	C765	U766	A767	C768	U769	A770	C771	U772	A773	C774	U775	A776	C777	U778	A779	C780	U781	A782	C783	U784	A785	C786	U787	A788	C789	U790	A791	C792	U793	A794	C795	U796	A797	C798	U799	A800	C801	U802	A803	C804	U805	A806	C807	U808	A809	C810	U811	A812	C813	U814	A815	C816	U817	A818	C819	U820	A821	C822	U823	A824	C825	U826	A827	C828	U829	A830	C831	U832	A833	C834	U835	A836	C837	U838	A839	C840	U841	A842	C843	U844	A845	C846	U847	A848	C849	U850	A851	C852	U853	A854	C855	U856	A857	C858	U859	A860	C861	U862	A863	C864	U865	A866	C867	U868	A869	C870	U871	A872	C873	U874	A875	C876	U877	A878	C879	U880	A881	C882	U883	A884	C885	U886	A887	C888	U889	A890	C891	U892	A893	C894	U895	A896	C897	U898	A899	C900	U901	A902	C903	U904	A905	C906	U907	A908	C909	U910	A911	C912	U913	A914	C915	U916	A917	C918	U919	A920	C921	U922	A923	C924	U925	A926	C927	U928	A929	C930	U931	A932	C933	U934	A935	C936	U937	A938	C939	U940	A941	C942	U943	A944	C945	U946	A947	C948	U949	A950	C951	U952	A953	C954	U955	A956	C957	U958	A959	C960	U961	A962	C963	U964	A965	C966	U967	A968	C969	U970	A971	C972	U973	A974	C975	U976	A977	C978	U979	A980	C981	U982	A983	C984	U985	A986	C987	U988	A989	C990	U991	A992	C993	U994	A995	C996	U997	A998	C999	U1000	G1001	A1002	C1003	U1004																																																																																																																																																																																																																										
G191	A192	C193	U194	G195	A196	C197	U198	A199	G200	C201	U202	A203	C204	U205	A206	C207	U208	A209	C210	U211	A212	C213	U214	A215	C216	U217	A218	C219	U220	A221	C222	U223	A224	C225	U226	A227	C228	U229	A230	C231	U232	A233	C234	U235	A236	C237	U238	A239	C240	U241	A242	C243	U244	A245	C246	U247	A248	C249	U250	A251	C252	U253	A254	C255	U256	A257	C258	U259	A260	C261	U262	A263	C264	U265	A266	C267	U268	A269	C270	U271	A272	C273	U274	A275	C276	U277	A278	C279	U280	A281	C282	U283	A284	C285	U286	A287	C288	U289	A289	C290	U291	A292	C293	U294	A295	C296	U297	A298	C299	U300	A301	C302	U303	A304	C305	U306	A307	C308	U309	A310	C311	U312	A313	C314	U315	A316	C317	U318	A319	C320	U321	A322	C323	U324	A325	C326	U327	A328	C329	U330	A331	C332	U333	A334	C335	U336	A337	C338	U339	A340	C341	U342	A343	C344	U345	A346	C347	U348	A349	C350	U351	A352	C353	U354	A355	C356	U357	A358	C359	U360	A361	C362	U363	A364	C365	U366	A367	C368	U369	A370	C371	U372	A373	C374	U375	A376	C377	U378	A379	C380	U381	A382	C383	U384	A385	C386	U387	A388	C389	U390	A391	C392	U393	A394	C395	U396	A397	C398	U399	A400	C401	U402	A403	C404	U405	A406	C407	U408	A409	C410	U411	A412	C413	U414	A415	C416	U417	A418	C419	U420	A421	C422	U423	A424	C425	U426	A427	C428	U429	A430	C431	U432	A433	C434	U435	A436	C437	U438	A439	C440	U441	A442	C443	U444	A445	C446	U447	A448	C449	U450	A451	C452	U453	A454	C455	U456	A457	C458	U459	A460	C461	U462	A463	C464	U465	A466	C467	U468	A469	C470	U471	A472	C473	U474	A475	C476	U477	A478	C479	U480	A481	C482	U483	A484	C485	U486	A487	C488	U489	A490	C491	U492	A493	C494	U495	A496	C497	U498	A499	C500	U501	A502	C503	U504	A505	C506	U507	A508	C509	U510	A511	C512	U513	A514	C515	U516	A517	C518	U519	A520	C521	U522	A523	C524	U525	A526	C527	U528	A529	C530	U531	A532	U533	A534	C535	U536	A537	C538	U539	A540	C541	U542	A543	C544	U545	A546	C547	U548	A549	C550	U551	A552	C553	U554	A555	C556	U557	A558	C559	U560	A561	C562	U563	A564	C565	U566	A567	C568	U569	A570	C571	U572	A573	C574	U575	A576	C577	U578	A579	C580	U581	A582	C583	U584	A585	C586	U587	A588	C589	U590	A591	C592	U593	A594	C595	U596	A597	C598	U599	A600	C601	U602	A603	C604	U605	A606	C607	U608	A609	C610	U611	A612	C613	U614	A615	C616	U617	A618	C619	U620	A621	C622	U623	A624	C625	U626	A627	C628	U629	A630	C631	U632	A633	C634	U635	A636	C637	U638	A639	C640	U641	A642	C643	U644	A645	C646	U647	A648	C649	U650	A651	C652	U653	A654	C655	U656	A657	C658	U659	A660	C661	U662	A663	C664	U665	A666	C667	U668	A669	C670	U671	A672	C673	U674	A675	C676	U677	A678	C679	U680	A681	C682	U683	A684	C685	U686	A687	C688	U689	A690	C691	U692	A693	C694	U695	A696	C697	U698	A699	C700	U701	A702	C703	U704	A705	C706	U707	A708	C709	U710	A711	C712	U713	A714	C715	U716	A717	C718	U719	A720	C721	U722	A723	C724	U725	A726	C727	U728	A729	C730	U731	A732	C733	U734	A735	C736	U737	A738	C739	U740	A741	C742	U743	A744	C745	U746	A747	C748	U749	A750	C751	U752	A753	C754	U755	A756	C757	U758	A759	C760	U761	A762	C763	U764	A765	C766	U767	A768	C769	U770	A771	C772	U773	A774	C775	U776	A777	C778	U779	A780	C781	U782	A783	C784	U785	A786	C787	U788	A789	C790	U791	A792	C793	U794	A795	C796	U797	A798	C799	U800	A801	C802	U803	A804	C805	U806	A807	C808	U809	A810	C811	U812	A813	C814	U815	A816	C817	U818	A819	C820	U821	A822	C823	U824	A825	C826	U827	A828	C829	U830	A831	C832	U833	A834	C835	U836	A837	C838	U839	A840	C841	U842	A843	C844	U845	A846



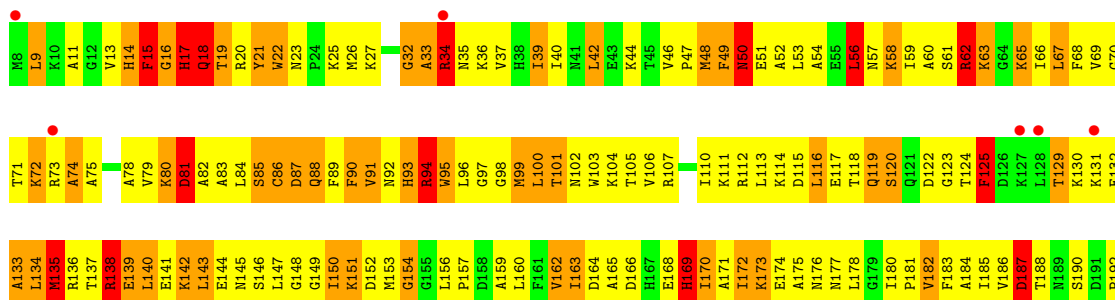
• Molecule 2: 30S ribosomal protein S2

Chain AB:



• Molecule 2: 30S ribosomal protein S2

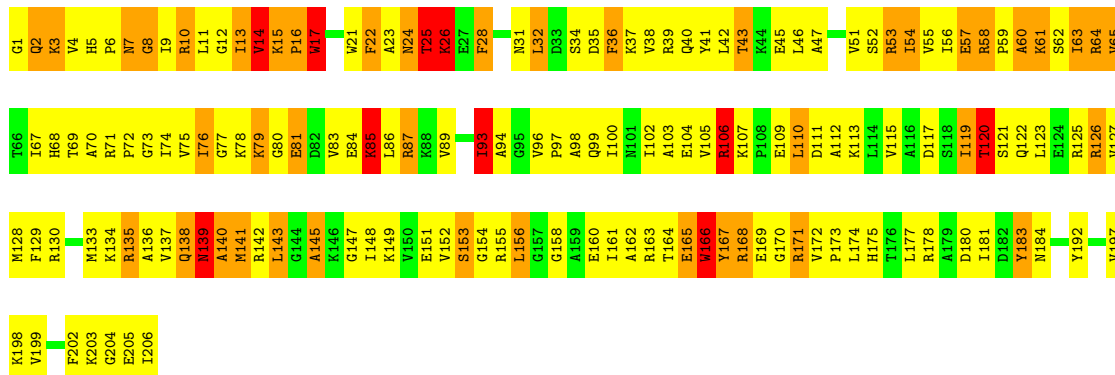
Chain BB:





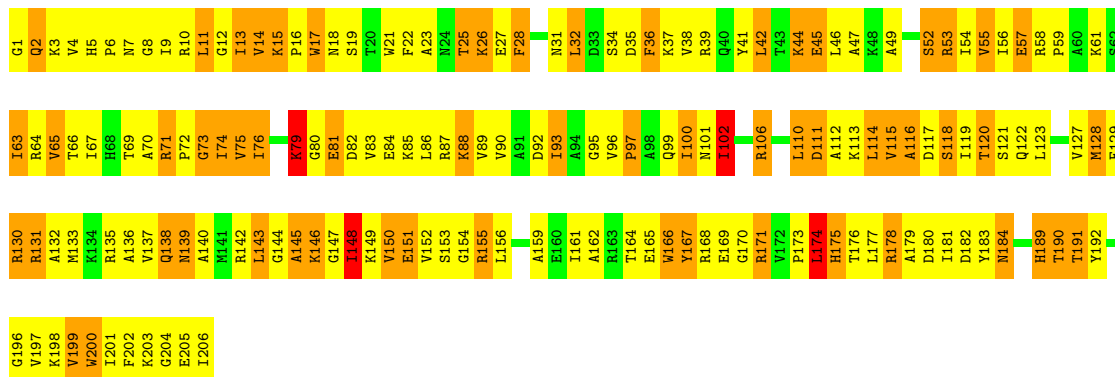
• Molecule 3: 30S ribosomal protein S3

Chain AC:



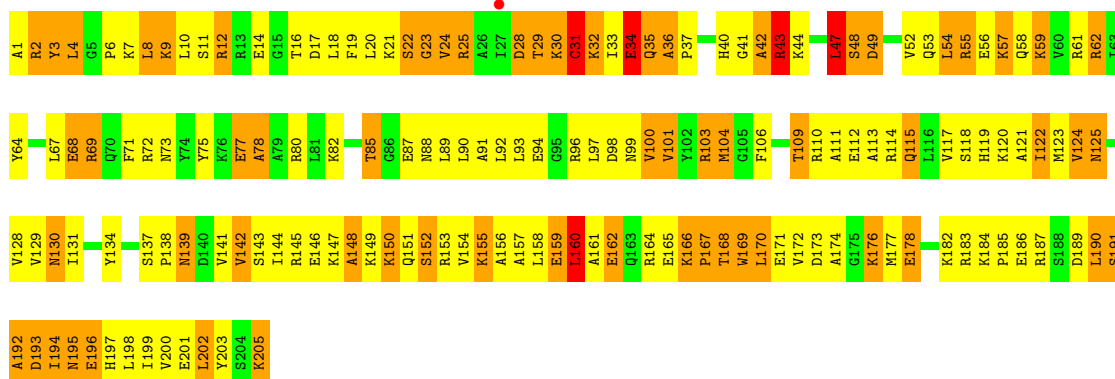
• Molecule 3: 30S ribosomal protein S3

Chain BC:



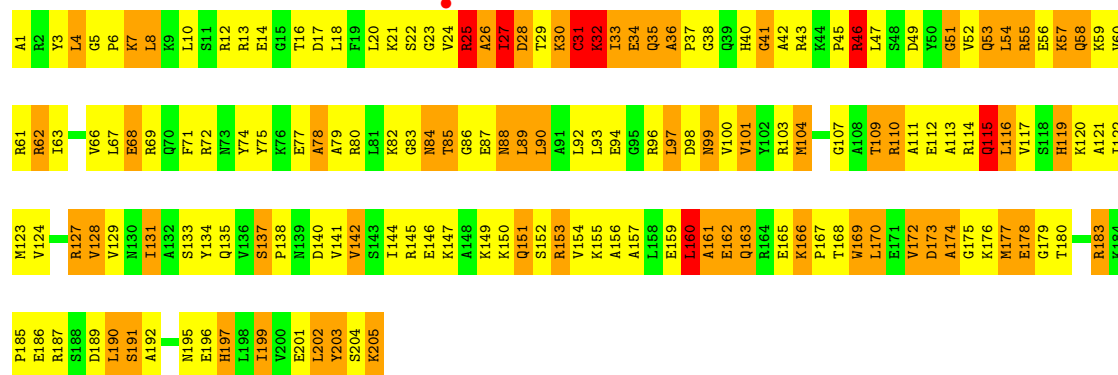
• Molecule 4: 30S ribosomal protein S4

Chain AD:



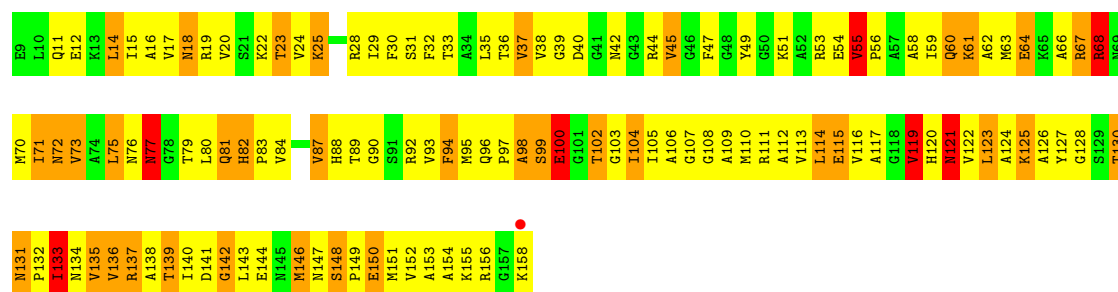
• Molecule 4: 30S ribosomal protein S4

Chain BD:



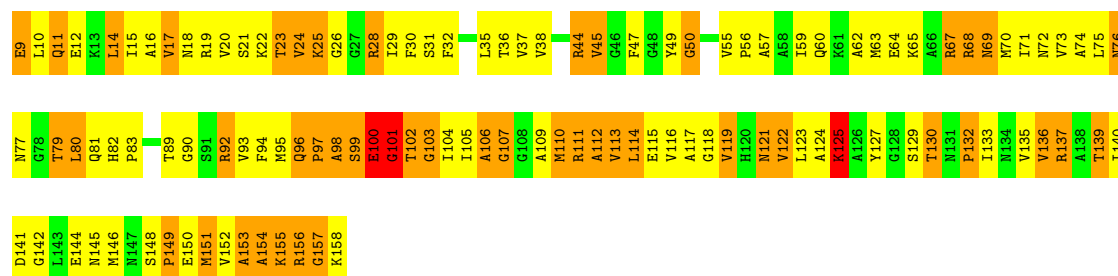
• Molecule 5: 30S ribosomal protein S5

Chain AE:



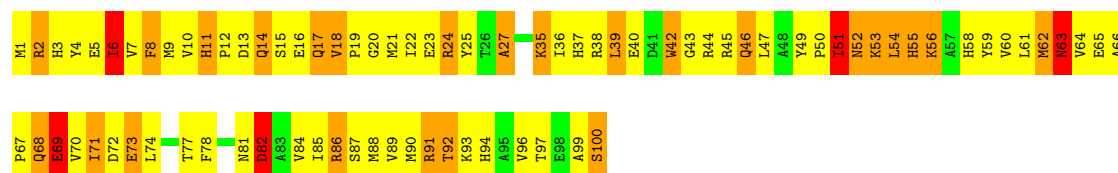
• Molecule 5: 30S ribosomal protein S5

Chain BE:



• Molecule 6: 30S ribosomal protein S6

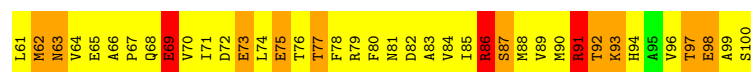
Chain AF:



• Molecule 6: 30S ribosomal protein S6

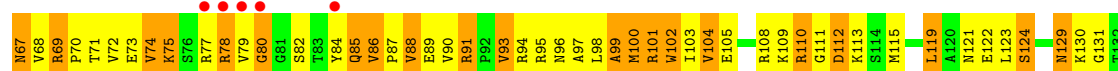
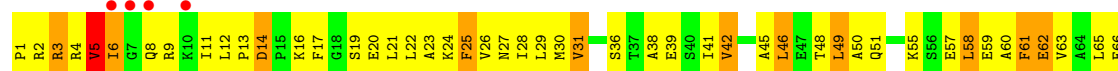
Chain BF:





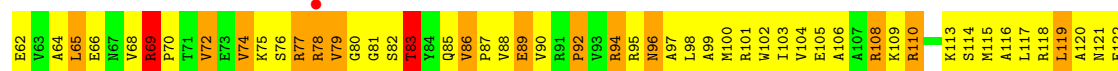
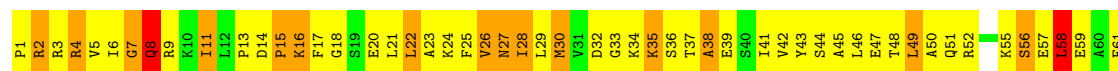
• Molecule 7: 30S ribosomal protein S7

Chain AG:



• Molecule 7: 30S ribosomal protein S7

Chain BG:



• Molecule 8: 30S ribosomal protein S8

Chain AH:



• Molecule 8: 30S ribosomal protein S8

Chain BH:



• Molecule 9: 30S ribosomal protein S9

- Molecule 9: 30S ribosomal protein S9

- Molecule 10: 30S ribosomal protein S10

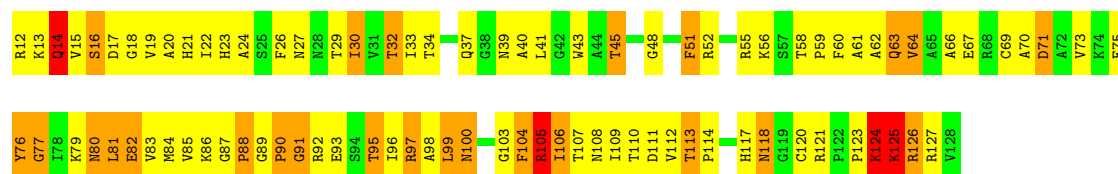
- Molecule 10: 30S ribosomal protein S10

- Molecule 11: 30S ribosomal protein S11



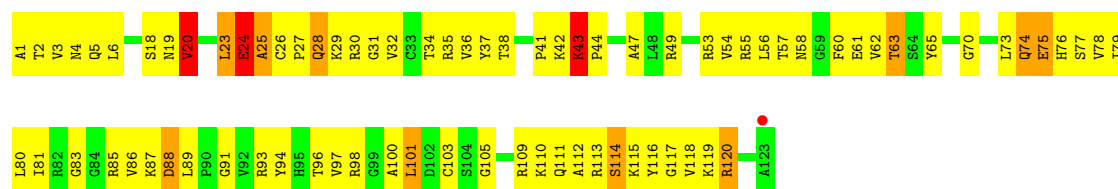
- Molecule 11: 30S ribosomal protein S11

Chain BK:



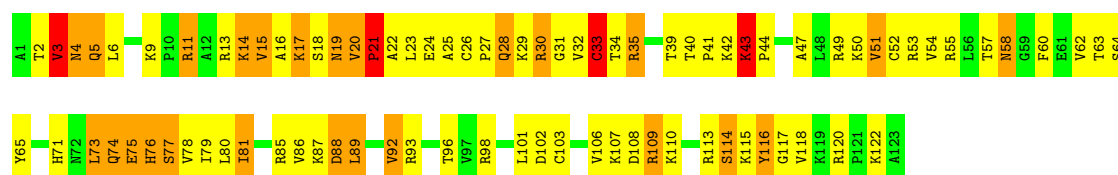
- Molecule 12: 30S ribosomal protein S12

Chain AL:



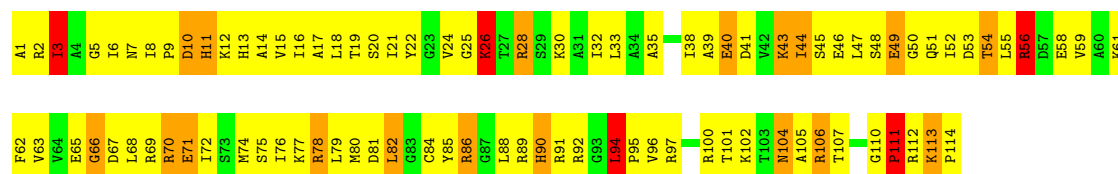
- Molecule 12: 30S ribosomal protein S12

Chain BL:



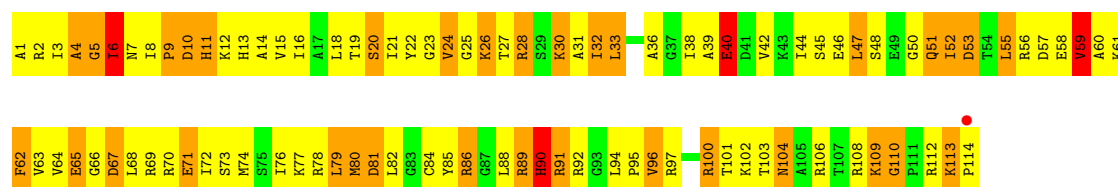
- Molecule 13: 30S ribosomal protein S13

Chain AM:



- Molecule 13: 30S ribosomal protein S13

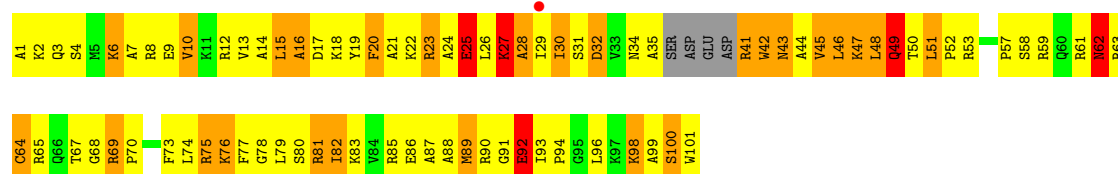
Chain BM:



- Molecule 14: 30S ribosomal protein S14

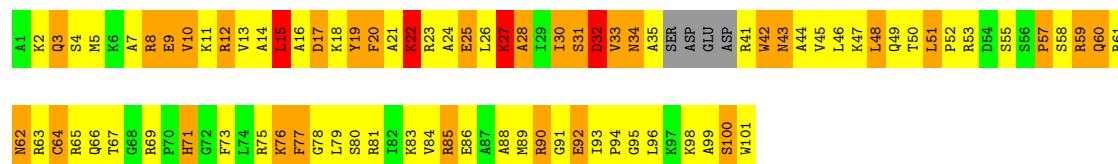
Chain AN:





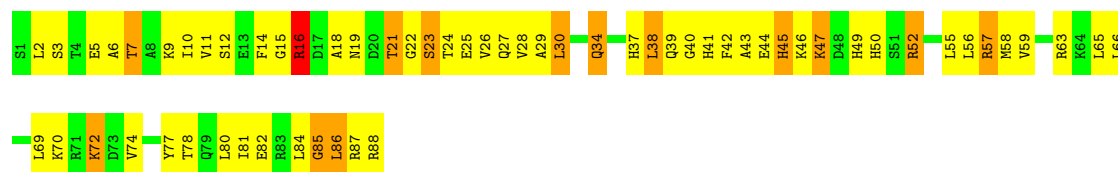
- Molecule 14: 30S ribosomal protein S14

Chain BN:



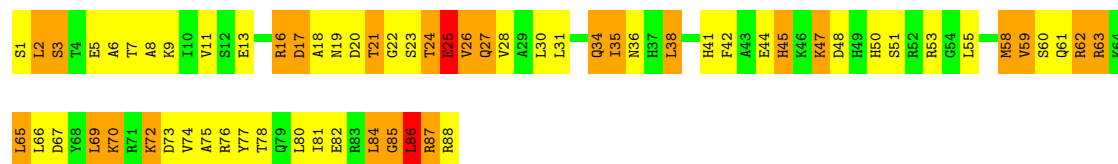
- Molecule 15: 30S ribosomal protein S15

Chain AO:



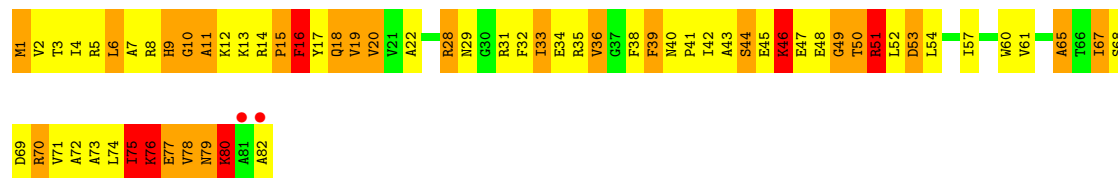
- Molecule 15: 30S ribosomal protein S15

Chain BO:



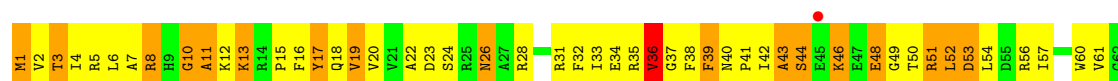
- Molecule 16: 30S ribosomal protein S16

Chain AP:



- Molecule 16: 30S ribosomal protein S16

Chain BP:





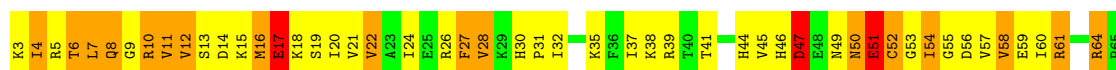
- Molecule 17: 30S ribosomal protein S17

Chain AQ:



- Molecule 17: 30S ribosomal protein S17

Chain BQ:



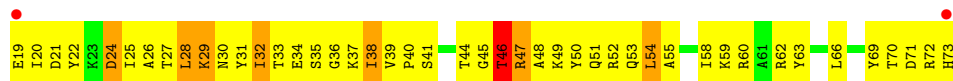
- Molecule 18: 30S ribosomal protein S18

Chain AR:



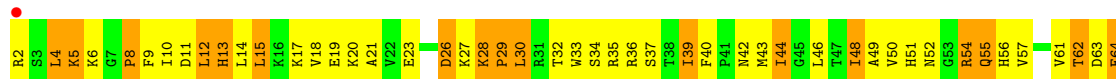
- Molecule 18: 30S ribosomal protein S18

Chain BR:



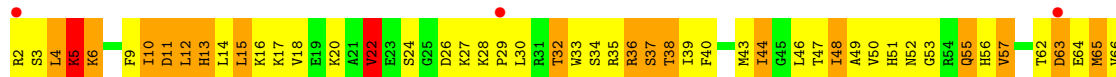
- Molecule 19: 30S ribosomal protein S19

Chain AS:



- Molecule 19: 30S ribosomal protein S19

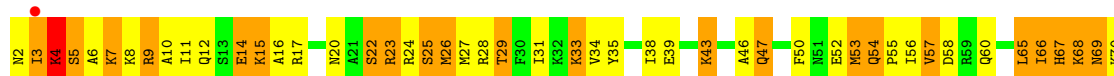
Chain BS:





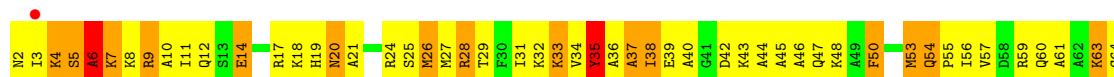
- Molecule 20: 30S ribosomal protein S20

Chain AT:



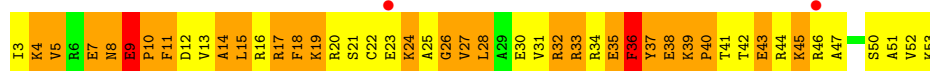
- Molecule 20: 30S ribosomal protein S20

Chain BT:



- Molecule 21: 30S ribosomal protein S21

Chain AU:



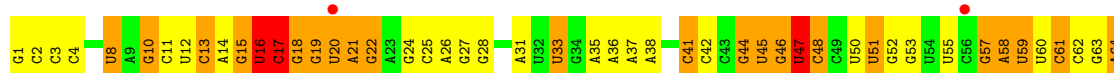
- Molecule 21: 30S ribosomal protein S21

Chain BU:



- Molecule 22: phenylalanine specific transfer RNA

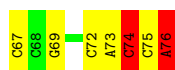
Chain AV:



- Molecule 22: phenylalanine specific transfer RNA

Chain BV:





- Molecule 23: messenger RNA

Chain AX:



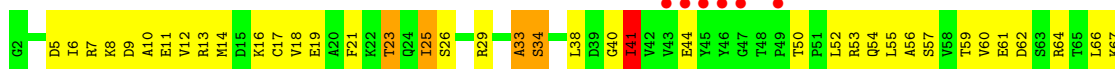
- Molecule 23: messenger RNA

Chain BX:



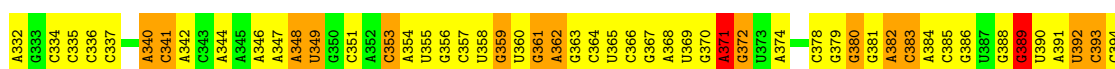
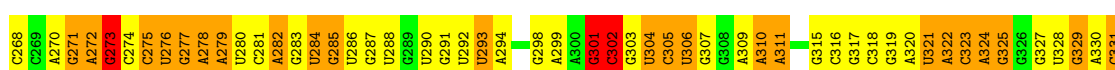
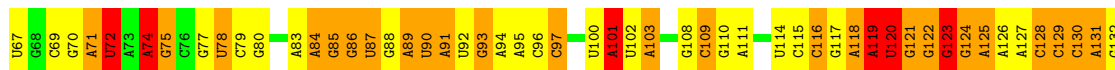
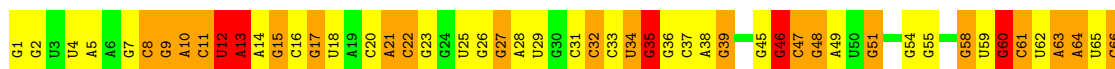
- Molecule 24: ribosome recycling factor

Chain AY:



- Molecule 25: 23S rRNA

Chain CA:



G1332	G1270	C1208	U1441	U1081	A1021	A959	U895	A833	U773	G712	C650	A586	A526	A460	U395
G1335	G1271	U1209	A1442	U1082	G1022	A960	A896	G834	G774	G713	U653	C587	C527	C461	G396
A1336	A1272	U1273	A1443	U1083	U1023	C961	C897	C835	G775	U714	U654	U588	A528	C462	U397
G1339	A1274	G1212	C1445	A1085	G1025	G962	A899	G836	G776	A715	A655	U589	A529	G463	C398
U1340		G1213		A1086	G1026	A900	A900	C837	G777	A716	A656	U590	G530	G468	A401
G1341	G1277	A1214	U1148	G1087	A1027	C901	C901	U839	G778	A717	A657	A592	A532	G469	A402
G1342	G1278	G1215	G1149	A1088	A1028	C902	C902	C840	G779	A718	U658	U593	U533	G470	U403
G1343	G1279	C1150	G1150	A1089	A1029	C968	A905	G841	A781	C719	U659	U594	G534	A471	A404
U1344	G1280	U1217	A1151	A1090	C1030	G969	U906	U842	A782	A721	C660	U594	G535	G472	U405
G1344	G1281	G1091		G1091	G1031	U970	U970	G843	A783	A722	A661	C595	G536	G473	G406
G1345	U1282	G1218		G1092	A1032	G971	C907	A844	G784	G723	G662	U598	G537	G474	G407
G1348	G1283	G1220	A1155	G1093	U1033	A972	C908	A845	G785	U724	G663	A599	G538	C475	G408
A1349	A1284	G1221	A1156	U1094	G1034	A973	A909	U846	G786	G725	G664	G600	G539	C476	G409
C1350	A1285	U1222	G1157	A1095	U1035	G974	A910	U847	C787	G726	U665	A601	C540	A477	G410
C1351	A1286	G1223	C1158	A1096	G1036	A975	A911	U848	A788	A727	U666	A602	G541	A478	G411
G1352	A1287	U1224		U1097	G1037	G976	C912	A849	A789	G728	U667	A603	C542	A479	A412
U1353	G1288	G1225	C1161	A1098	G1038	G977	U913	U850	U790	G729	U668	G604	G543	A480	C413
C1353	C1289	A1226	G1162	G1099	A1039	G978	C914	C851	C791	A730	G669	G605	C544	G481	C414
A1354	C1290	G1227	G1163	C1100	A1040	A979	C915	U852	A792	C731	A670	U606	U545	A482	A415
G1355	C1291	U1228	C1164	U1101	G1041	A980	G916	C853	A793	G732	C671	C611	U546	A483	U416
G1356	G1292		A1165	C1102	G1042	A981	A917	C854	A794	A733	C672	G612	A547	C484	C417
C1357	C1293	U1231	G1166	A1103	C1043	C982	A918	G855	C795	A734	C673	G613	G548	C485	C418
G1358	U1294	G1232	C1167	C1104	C1044	A983	U919	G856	C796	A735	G674	A614	G549	C486	U419
A1359	C1295	C1233	G1168	U1105	C1045	A984	A920	G857	G797	A736	A675	G614	C550	C487	C420
G1360	G1296	U1234	A1169	G1106	A1046	C985	C921	G858	G798	C737	A676	U615	G551	G488	
G1361	C1297	G1235	C1170	U1107	G1047	C986	C922	G859	G799	G738	A677	U616	U552	C489	A423
C1362	A1298	G1236	G1171	U1108	A1048	C987	G923	U860	A800	A739	C678	G617	G553	C490	G424
A1363	G1299	C1237	C1172	C1109	C1049	A988	G924	A861	G801	C740	C679	G618	U554	C491	G425
G1365	C1300	G1238	U1173	G1110	A1050	G989	A925	G862	A802	U741	C680	G619	G555	A492	
A1366	A1301	G1239	U1174	A1111	G1051	A990	G926	A863	U803	A742	G681	G620	A556	C493	A428
A1367	A1302	U1240	A1175	G1112	C1052	C991	A927	G864	A804	A743	G682	A621	C557	C494	
G1368	G1303	A1241	U1176	U1113	C1053	C992	A928	C865	G805	U744	U683	G622	U558	G495	A429
C1369		U1242	C1177	G1114	A1054	G993	U929	A866	C806	G745	G684	C623	G559	G496	A430
G1370	C1306	C1243	G1178	C1115	G1055	C994	G930	C867	U807	U746	A685	G624	C560	A497	U431
A1371	A1307	A1244	U1179	G1116	G1056	C995	U931	U868	G808	U747	U686	G625	G561	G498	
U1372	A1308	G1245	A1180	C1117	A1057	A996	U932	G869	G809	G748	U687	A626	U562	U499	U434
A1373	G1309	A1246	U1181	C1118	U1058	C997	A933	U870	U810	A749	U688	A627	A563	C435	C436
G1374	C1310	U1247	G1182	U1119	G1059	C998	U934	U871	U811	A750	A689	G628	C564	A501	U437
U1375	G1311	A1248	U1183	G1120	U1060	U999	C936	U872	C812	A751	G690	G629	C565	A502	G438
C1376	C1312	U1249	U1184	C1121	U1061	A1000	A936	C873	U813	A752	C691	G630	U566	A503	A439
G1377	U1313	G1250	G1185	G1122	G1062	A1001	C937		C814	A753	C692	A631	U567	A504	C440
A1378	C1314	C1251	G1186	C1123	G1063	A1002	G938		C815	U754	A693	A632	U568	A505	U441
U1379	C1315	G1252	G1187	G1124	C1064	G1003	G939	A877	C816		U694	A633	U569	C442	
G1380	U1316	A1253	U1188	G1125	U1065	U1004	G940	A878	C817	G757		C634	G570	A508	A443
C1381	G1317	A1254	A1189	U1066	U1066	G879	G941	G880	C818	C758	G697	C635	U571	C509	C444
G1382	U1318	U1255	G1190	A1127	A1067	C1005	G942	C881	A819	G759	C698	C636	A572	C510	C445
A1383	C1319	G1256	G1191	G1128	G1068	C1007	A943	G882	A820	G760	A699	A637	U573	U511	G446
A1384	C1320	C1257		A1129	A1069	C1008	C944	G883	A821	A761	G700	G638	A574	G512	
A1385	A1321	U1258	G1195	U1130	A1070	A1009	A945	U884	G822	U762	G701	U639	A575	A513	A449
C1386	A1322	G1259		G1131	A1071	C946	C946	C885	C823	G763	U702	C640	U576	A514	G450
A1387	C1323	A1260	G1196	U1132	C1072	A947	A947	A	U824	A764	U703	U641	G577	A515	U451
G1388	G1324	C1261	G1197	A1133	A1073	U1011	C948	U	A825	C765	G704	U642	G578	C516	G452
G1389	U1325	A1262	U1198	A1134	G1074	C	G949	C	U826	U766	A705	A643	G579	C517	A453
A1390	U1326		U1199	C1135	C1075	C		C	U827	U767	A706	A644	U580	G518	A454
U1391	A1327	A1265	G1136	G1136	C1076	G952	G952		U828	G768	G707	C645	C581	G519	C455
A1392	A1328	G1266	G1137	G1137	A1077	G1017		G	A829	U769	G708	U646	A582	A522	C456
U1393	U1329	U1267	U1138	G1138	U1078	A892	G956	A892	G830	G770	U709	G647	G583	C523	A457
A1394	C1330	A1268	C1139	C1079	U1019	C893	C957	C893	G831	G771	U710	G648	G524	C584	G458
A1395	G1331	A1269	A1205	C1140	A1080	U894	U958	U894	U832	C772	G711	U649	G585	U525	U459

A2333	G2271	U2210	G2148	U2086	C2025	A1960	G1897	G1835	U1769	G1708	G1645	A1583	U1458	U1396
U2334	U2272	A2211	U2149	G2087	U2026	C1961	U1898	C1836	G1770	U1709	C1646	U1584	G1459	G1436
A2335	A2273	A2212	A2088	A2089	G2027	G1965	A1900	C1838	A1772	G1711	U1647	C1585	C1461	C1399
G2337	G2275	C2214	G2152	A2090	G2029	A1966	A1901	G1839	A1773	A1710	U1648	A1586	C1460	G1402
G2338	G2276	C2215	G2153	C2091	A2030	C1967	C1902	G1840	C1774	A1712	A1650	G1588	C1463	A1403
C2339	G2277	G2216	A2154	U2092	A2031	G1968	G1903	U1841	U1775	A1713	G1651	U1589	C1404	C1404
A2340	A2278	G2217	U2155	C2093	G2032	A1969	G1904	C1842	G1776	G1714	A1652	G1527	G1464	U1405
G2341	G2279	A2203	G2156	A2094	C2033	A1970	G1907	C1843	U1779	U1716	G1653	U1529	U1466	U1406
U2342	G2280	U2219	G2157	A2095	U2034	C1971	C1908	C1844	A1717	A1718	U1654	C1592	U1467	G1407
G2343	A2281	U2220	A2158	C2096	G2035	G1972	G1909	G1846	G1845	G1718	A1655	A1593	U1468	G1408
U2344	G2282	G2221	G2159	U2037	C2036	G1975	C1910	U1847	U1782	G1721	U1657	U1594	A1470	U1410
G2345	C2283	G2222	C2160	A2037	U2038	U1976	U1911	A1848	A1783	A1722	C1658	A1596	G1471	U1411
A2346	A2284	G2223	C2161	G2038	G2039	A1977	A1912	U1851	A1784	G1723	G1659	G1535	C1472	U1412
C2347	C2285	G2224	A2162	U2040	C2041	A1978	A1913	U1852	A1785	G1724	G1660	C1536	G1473	A1413
U2348	G2286	A2225	A2163	C2103	G2042	U1979	A1914	U1853	A1786	U1725	G1661	G1537	U1474	C1414
G2349	A2287	C2226	C2164	C2104	U2041	U1979	C1915	A1854	A1787	G1726	U1662	G1538	G1475	U1415
C2350	A2288	G2227	C2165	U2105	A2042	G1980	U1915	U1855	C1788	C1727	G1663	U1602	U1476	G1416
G2351	G2289	G2228	U2166	U2106	C2043	A1981	A1916	U1856	A1789	G1728	A1664	A1603	A1477	C1417
A2352	U2290	U2229	U2167	G2107	C2044	U1982	U1917	U1857	C1790	U1729	U1665	C1604	G1478	G1418
G2353	U2291	G2230	C2168	A2108	C2045	U1983	A1918	C1856	A1791	C1730	G1666	C1605	G1479	A1419
C2354	U2292	U2231	A2169	U2109	G2046	G1984	A1919	C1857	G1792	G1731	G1667	C1606	C1480	A1420
G2355	G2293	C2232	A2170	C2110	C2047	C1985	C1920	C1858	C1793	G1732	G1668	C1607	U1481	G1421
U2356	G2294	U2233	A2171	U2111	G2048	G1986	G1921	U1859	A1794	G1733	A1669	A1608	G1482	G1422
G2357	U2295	G2234	U2172	G2112	C2049	G1988	G1922	U1860	C1795	G1734	C1670	A1609	G1483	G1423
U2296	U2296	G2235	A2173	U2113	C2050	C1989	U1923	G1861	C1796	A1735	A1548	A1610	G1484	G1424
A2297	A2297	U2236	C2174	A2114	A2051	C1990	C1924	C1862	U1796	U1736	A1549	C1550	U1485	G1425
G2359	G2298	G2237	C2175	G2115	A2052	U1991	C1925	G1863	G1797	C1737	A1551	C1551	U1486	G1426
C2360	U2299	U2238	A2176	C2116	G2053	G1992	U1926	U1864	U1798	G1738	U1559	A1494	U1487	G1427
G2361	G2299	C2239	C2177	A2117	A2054	U1993	A1927	U1865	C1799	G1739	A1553	A1553	G1428	G1428
U2362	C2301	U2240	C2178	U2118	C2055	C1994	A1928	C1866	C1800	A1740	U1554	A1490	G1430	G1429
G2363	U2241	A2241	C2179	A2119	G2056	C1997	G1928	C1867	A1801	C1741	U1555	G1491	A1431	A1431
A2365	G2242	G2242	U2180	G2120	G2057	A1998	G1930	C1868	A1802	G1742	C1556	G1492	C1432	G1432
C2367	U2243	U2243	U2181	G2121	A2058	C1999	U1931	C1869	A1803	U1743	C1557	C1493	A1433	A1433
U2371	U2244	U2244	U2182	U2122	A2059	G1999	A1932	C1870	C1804	A1744	U1563	G1501	A1434	A1434
G2372	U2245	U2245	A2183	G2123	A2060	C2001	G1933	C1871	A1805	A1745	C1564	A1502	U1440	U1440
U2373	G2246	G2246	A2184	G2124	G2061	C2002	C1941	C1872	C1806	U1746	C1565	A1503	U1441	U1441
G2375	A2247	A2247	U2185	G2125	A2062	G2002	U1936	C1873	G1807	U1746	G1566	A1504	U1442	U1442
A2376	C2248	C2248	G2186	A2126	C2063	A2003	A1937	C1874	A1808	U1747	C1567	A1505	U1443	U1443
A2377	U2249	U2249	U2187	G2127	C2064	G2004	A1938	C1875	A1809	C1748	U1562	G1500	G1444	G1444
G2378	G2250	G2250	U2188	G2128	C2065	A2005	U1939	A1876	A1810	A1749	C1563	A1506	C1507	C1507
C2379	G2251	C2251	U2189	C2129	C2066	C2006	U1940	A1877	G1811	G1750	C1564	C1507	G1445	G1445
C2380	G2252	G2252	C2190	U2130	G2067	U2007	C1941	C1878	A1626	U1751	C1565	A1507	C1446	C1446
A2381	C2253	G2253	A2191	U2131	U2068	C2008	C1942	C1879	G1816	C1752	A1566	A1508	C1447	C1447
G2382	C2254	C2254	U2192	U2132	G2069	A2009	U1943	U1880	G1817	G1753	G1567	A1509	G1448	G1448
C2383	G2255	G2255	G2193	G2133	A2070	G2010	U1944	C1881	A1818	A1754	C1568	A1505	U1512	U1512
U2384	G2256	A2071	U2194	A2134	C2071	G2011	G1945	U1882	A1819	A1755	A1569	U1506	G1450	G1450
G2385	U2257	C2072	G2195	A2135	C2072	G2012	U1946	U1883	U1820	G1756	A1570	C1507	G1451	G1451
U2386	C2073	C2073	U2196	A2136	C2072	G2013	U1946	C1884	A1632	A1571	C1571	A1508	G1452	G1452
A2388	U2075	U2075	U2197	U2137	U2075	A2014	C1947	G1885	G1824	U1758	C1694	A1509	A1515	A1515
G2389	U2076	U2076	G2138	G2138	A2015	G1950	G1950	U1888	U1825	A1759	G1685	G1510	C1454	C1454
U2390	A2077	A2077	U2139	U2139	U2016	U1951	U1951	G1889	G1826	C1760	C1686	G1511	G1455	G1455
G2391	C2078	C2078	G2140	G2140	U2017	A1952	A1952	A1889	U1827	C1761	G1699	U1513	G1519	G1519
A2392	U2079	U2079	G2141	G2141	G2018	A1953	A1953	A1890	G1828	A1762	A1700	C1512	U1520	U1520
C2393	A2080	A2080	A2142	A2142	A2019	G1954	G1954	A1891	A1829	G1763	A1701	C1513	G1456	G1456
U2394	U2081	U2081	C2143	C2143	A2020	U1955	U1955	C1892	C1830	U1764	G1702	A1514	G1457	G1457
G2395	A2082	A2082	G2144	G2144	C2021	U1956	U1956	C1893	G1831	U1765	G1703	A1515	C1458	C1458
C2396	G2083	G2083	C2145	C2145	U2022	C1957	C1957	C1894	C1832	G1766	C1704	A1580	G1459	G1459
U2397	C2084	C2084	U2146	U2146	C2023	C1958	C1958	C1895	C1833	G1767	G1642	G1581	G1460	G1460
G2397	U2085	U2085	A2147	A2147	G2024	G1959	G1959	G1896	U1834	C1768	G1707	C1644	U1520	U1520

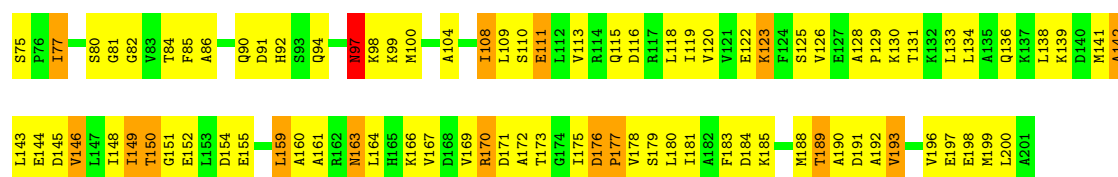


C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438												
U1326	A1327	U1328	U1329	C1330	G1331	G1332	G1333	G1334	C1335	A1336	G1337	G1338	G1339	U1340	G1341	A1342	G1343	U1344	C1345	C1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	A1354	C1355	C1356	C1357	C1358	C1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	C1371	U1372	A1373	A1374	U1375	C1376	C1377	A1378	U1379	G1380	G1381	C1382	A1383	C1384	C1385					
C1257	U1258	C1259	A1260	C1261	A1262	U1263	A1264	U1203	A1265	C1266	U1267	A1268	C1269	G1270	A1271	C1272	A1273	A1274	C1275	A1276	C1277	C1278	G1281	U1282	C1283	A1284	C1285	A1286	A1287	C1288	U1289	C1290	C1291	C1292	A1293	C1294	C1295	C1296	C1297	C1298	C1299	G1300	A1301	C1302	G1303	G1310	C1311	U1312	C1313	C1314	C1315	C1316	G1317	C1318	C1319	C1320	A1321	A1322	C1323	C1324	C1325	U1326		
A1194	G1195	C1196	G1197	U1198	U1199	C1200	U1203	A1204	A1205	G1206	C1207	C1208	G1212	A1213	A1214	G1215	G1216	U1217	G1218	U1219	G1220	C1221	U1222	G1223	U1224	G1225	A1226	G1227	C1228	A1229	C1230	U1231	G1232	C1233	U1234	G1235	A1236	C1237	G1238	G1239	U1240	A1241	U1242	C1243	A1244	C1245	A1246	A1247	G1248	U1249	C1250	C1251	U1252	A1253	U1254	C1255	C1256							
A1133	A1134	C1135	G1136	G1137	G1138	G1139	U1140	U1141	A1142	A1143	C1144	C1145	C1146	U1149	C1150	A1151	C1152	C1153	G1154	A1155	G1156	C1157	C1158	U1159	G1160	C1161	G1162	C1163	C1164	A1165	C1166	C1167	G1168	A1169	C1170	C1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	U1184	G1185	U1186	G1187	U1188	A1189	C1190	G1191	C1192	G1193						
A1073	C1074	C1075	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	A1094	A1095	A1096	U1097	A1098	U1099	C1100	U1101	C1102	A1103	C1104	U1105	A1046	C985	C986	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	U1003	U1004	U1005	A1006	C1007	A1008	U1009	A1010					
A1011	C1012	C1013	A1014	U1015	G1016	G1017	U1018	U1019	A1020	C1021	G1022	U1023	G1024	G1025	C964	U967	C968	C969	U970	A973	G974	A975	C976	G977	C978	C979	C980	A981	A982	C983	C984	C985	C986	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	U1003	U1004	U1005	A1006	C1007	A1008	U1009	A1010							
G1011	U1012	C1013	A1014	U1015	G1016	G1017	U1018	U1019	A1020	C1021	G1022	U1023	G1024	G1025	C964	U967	C968	C969	U970	A973	G974	A975	C976	G977	C978	C979	C980	A981	A982	C983	C984	C985	C986	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	U1003	U1004	U1005	A1006	C1007	A1008	U1009	A1010							
A1073	C1074	C1075	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	A1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	G1093	A1094	A1095	A1096	U1097	A1098	U1099	C1100	U1101	C1102	A1103	C1104	U1105	A1046	C985	C986	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002	U1003	U1004	U1005	A1006	C1007	A1008	U1009	A1010					
A1133	A1134	C1135	G1136	G1137	G1138	G1139	U1140	U1141	A1142	A1143	C1144	C1145	C1146	U1149	C1150	A1151	C1152	C1153	G1154	A1155	G1156	C1157	C1158	U1159	G1160	C1161	G1162	C1163	C1164	A1165	C1166	C1167	G1168	A1169	C1170	C1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	U1184	G1185	U1186	G1187	U1188	A1189	C1190	G1191	C1192	G1193						
A1194	G1195	C1196	G1197	U1198	U1199	C1200	U1203	A1204	A1205	G1206	C1207	C1208	G1212	A1213	A1214	G1215	G1216	U1217	G1218	U1219	G1220	C1221	U1222	G1223	U1224	G1225	A1226	G1227	C1228	A1229	C1230	U1231	G1232	C1233	U1234	G1235	A1236	C1237	G1238	G1239	U1240	A1241	U1242	C1243	A1244	C1245	A1246	A1247	G1248	U1249	C1250	C1251	U1252	A1253	U1254	C1255	C1256							
C1257	U1258	C1259	A1260	C1261	A1262	U1263	A1264	U1203	A1265	C1266	U1267	A1268	C1269	G1270	A1271	C1272	A1273	A1274	C1275	A1276	C1277	C1278	G1281	U1282	C1283	A1284	C1285	A1286	A1287	C1288	U1289	C1290	C1291	C1292	A1293	C1294	C1295	C1296	C1297	C1298	C1299	G1300	A1301	C1302	G1303	G1310	C1311	U1312	C1313	C1314	C1315	C1316	G1317	C1318	C1319	C1320	A1321	A1322	C1323	C1324	C1325	U1326		
U1326	A1327	U1328	U1329	C1330	G1331	G1332	G1333	G1334	C1335	A1336	G1337	G1338	G1339	U1340	G1341	A1342	G1343	U1344	C1345	C1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	A1354	C1355	C1356	C1357	C1358	C1359	G1360	G1361	C1362	C1363	G1364	A1365	A1366	A1367	G1368	G1369	C1370	C1371	U1372	A1373	A1374	U1375	C1376	C1377	A1378	U1379	G1380	G1381	C1382	A1383	C1384	C1385					
C1386	C1387	C1388	C1389	C1390	C1391	C1392	C1393	C1394	C1395	C1396	C1397	C1398	C1399	C1400	C1401	C1402	C1403	C1404	C1405	C1406	C1407	C1408	C1409	C1410	C1411	C1412	C1413	C1414	C1415	C1416	C1417	C1418	C1419	C1420	C1421	C1422	C1423	C1424	C1425	C1426	C1427	C1428	C1429	C1430	C1431	C1432	C1433	C1434	C1435	C1436	C1437	C1438												
C435	C436	C437	C438	G442	A443	G446	A447	U448	A449	G450	A453	A454	C455	G458	U459	A460	C461	C462	C463	U464	C465	A466	C467	C468	C469	C470	A471	A472	C475	C476	A477	A478	A479	A480	C481	A482	A483	C484	C485	C486	C487	C488	C489	C490	G491	A492	C493	C494	A497	C498	U499	A500												
A502	A503	A504	A505	A506	A507	A508	C509	C510	U511	C512	A515	C516	C517	C518	C519	C520	U521	A522	C523	C524	A525	C526	C527	A528	A529	C530	C531	A532	C533	U534	C535	A536	C537	C538	C539	C540	A541	C542	C543	C544	U545	U546	A547	C548	C549	C550	C551	C552	C553	C554														
U566	U567	U568	U569	C570	U571	A572	U573	A574	U575	C576	G579	U580	C581	A582	C583	C584	C585	A586	C587	U588	U589	C590	U591	A592	A593	C594	C595	U596	A597	C600	C601	A602	A603	C604	C605	U606	U607	A608	C609	C610	C611	C612	A613	A614	U615	A616	C617	C618	C619	C620	A621	C622	C623	C624	C625	A626	C627	C628						
C629	C630	A631	A632	A633	C634	C635	C636	A637	C638	U639	C640	U641	U642	A643	A644	C645	U646	C647	C648	C649	C650	A654	A655	C656	U657	C658	C659	C660	A661	C664	U665	A666	U667	C668	C669	C670	C671	C672	C673	C674	A675	C676	A677	C678	C679	C680	C681	C682	U683	C684	C685	C686	C687	C688	C689	C690	C691							
C692	A693	U694	C695	C696	G701	U702	U703	G704	A705	A706	U709	U710	G711	G712	C713	U714	A715	A716	C717	A718	C719	U720	A721	A722	C723	U724	C725	C726	A727	C728	C729	A730	C731	C732	C733	A734	C735	C736	C737	C738	A739	C740	U741	A742	A743	U744	C745	C746	U747	C748	C749	C750	C751	C752	C753	C754								
A756	C757	C760	U761	U762	C763	A764	C765	U769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	A780	C781	A782	C783	C784	C785	C786	C787	C788	C789	A790	C791	A792	C793	A794	C795	C796	C797	C798	C799	A800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818							
A819	A820	A821	C822	C823	U824	A825	U826	U827	C828	A829	C830	C831	U832	A833	C834	C835	C836	U837	C838	U839	C840	C841	C842	C843	A844	A845	U846	U847	C848	A849	U850	C851	C852	C853	C854	C855	C856	C857	C858	C859	U860	A861	C862	A863	C864	C865	C866	C867	C868	C869	U870	U871	U872	C873	C874	C875	C876	A877	A878	C879	C880			
C881	C882	C883	C884	C885	A	U	C	C	C	C	A892	C893	U894	C895	C896	C897	C898	C899	A900	C901	C902	C903	C904	A905	U906	C907	C908	A909	C910	A911	C912	C913	C914	C915	C916	C917	A918	C919	A920	C921	A922	A923	A924	U925	U926	U927	U928	U929	U930	U931	U932	U933	U934	C935	A936	C937	C938	C939	C940	C941	C942	A943	C944	C945
C946	A947	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	A1000	A1001	G1002	U1003	U1004	U1005	A1006	C1007	A1008	U1009	A1010
G1011	U1012	C1013	A1014	U1015	G1016	G1017	U1018	U1019	A1020	C1021	G1022	U1023	G1024	G1025	C964	U967	C968	C969	U970	A973	G974	A975	C976	G977	C978	C979	C980	A981	A982	C983	C984	C985	C986	C987	A988	G989	A990	C991	C992	G993	C994	C995	A996	G997	C998	U999	A1000	A1001	G1002															

C2332	G2271	A2015	G1948	U1886	A1821	A1757	G1696	A1630	G1567	U1506	G1446
A2333	U2272	U2016	G1949	C1887	C1822	U1758	G1697	G1631	G1568	C1507	C1447
A2334	A2273	U2017	G1950	G1888	G1823	A1759		A1632	A1569	A1508	G1448
A2335	G2208	G2018	U1951		G1824	C1760	A1700	A1633	A1570	A1509	G1449
A2336	U2210	A2019	A1952	G1891	U1825	C1761	A1701	A1634	A1571	G1510	G1450
G2337	U2081	A2020	A1953	C1892	G1826	A1762	G1702	A1635	A1572	G1511	C1451
C2338		C2021	G1954	C1893	U1827	G1763	G1703	U1636	G1573	G1512	G1452
C2339	U2085	U2022	U1955	C1895	G1828	C1764	C1704	A1637	C1574	C1513	A1453
A2340	U2086	C2023	U1956	G1896	G1830	C1768		C1638	C1575	G1514	A1454
G2341	G2087	G2024	C1957	G1897	G1831	U1769	G1707	A1639	U1576	A1515	G1455
G2342		G2025	C1958	G1898	C1832	G1770	G1706		C1577	G1516	G1456
U2343	U2091	G2026		U1899	C1833	C1771	U1708	G1643	U1578	G1517	U1457
G2344	G2092	G2027	C1961	A1899	C1834	U1772	U1709	G1644	A1579	C1518	U1458
G2345	G2093	U2028	C1962	A1900	U1834	A1773	G1710	G1645	A1580	G1519	G1459
A2346	A2094	G2029	U1963	A1901	G1835	U1773	A1711	C1646	G1581	U1520	U1460
G2347	A2095	G2030	G1964	U1902	C1836	C1774	U1712	U1647	C1582	G1521	C1461
U2348	C2096	A2031	C1965	G1903	C1837	U1775	A1713	U1648	A1583	A1522	C1462
G2349	C2097	G2032	A1966	G1904	C1838	G1776	U1714	G1649	U1584	U1523	C1463
G2350	U2098	A2033	C1967	C1905		U1777	G1715	A1650	C1585	G1524	G1464
G2351	U2099	U2034	G1968	G1906	G1842	U1778	U1716	G1651	A1586	A1525	G1465
A2352	G2100	G2035	A1969	U1907	C1843	U1779	U1717	A1652	G1587	C1526	U1466
G2353	A2101	C2036	A1970	C1908	C1844	U1780	G1718	G1653	G1588	G1527	U1467
G2354	G2102	A2037	U1971	U1911	G1845	U1781	G1719	A1654	U1589	A1528	U1468
G2355	U2093	G2038	G1972	G1910	G1846	U1782	U1720	A1655	A1590	A1469	A1469
G2356	U2098	U2039	G1973	G1911	A	A1783	G1721	C1656	A1591	G1530	A1470
U2356	C2104	G2040	C1974	A1912	A1848	U1784	A1722	U1657	C1592	C1531	G1471
A2170	U2105	U2041	G1975	A1913	A1853	A1785	G1723	C1658	A1593	A1532	C1472
A2171	G2106	A2042	U1976	C1914	A1854	A1786	G1724	C1659	A1594	C1533	G1473
U2172	U2107	C2043	G1980	U1915	A1855	A1787	U1725	C1660	C1595	U1534	U1474
A2173	U2108	C2044	A1981	A1916	A1856	C1788	G1726	A1596	A1535	A1475	G1475
A2176	U2109	G2045	U1982	U1917	U1857	A1789	G1727	A1597	U1536	U1476	U1476
C2177	U2111	G2046	G1983	A1918	G1857	C1790	C1728	A1598	G1537	A1477	A1477
C2178	U2112	C2047	U1984	A1919	A1858	U1791	U1729	U1599	G1538	G1478	A1478
C2179	G2113	G2048	C1985	C1920	G1859	G1792	G1730	C1600	U1539	G1479	G1479
U2180	U2114	G2049	C1986	U1923	G1860	C1793	G1731	A1668	G1601	G1540	C1480
U2181	A2115	C2050	U1987	C1924	G1861	A1794	C1732	C1670	A1602	C1541	U1481
G2115	G2116	A2051		U1925	G1862	C1795	G1733	A1603	U1542	G1482	G1482
A2117	A2117	A2052	C1990	C1926	G1863	U1796	G1734	C1604	G1543	G1483	G1483
G2118	U2118	G2053	U1991	U1926	U1864	G1797	A1735	U1672	A1544	U1484	U1484
A2119	A2119	A2054	G1992	A1927	U1865	U1798	U1736	G1673	A1545	A1485	A1485
G2120	G2120	C2055	U1993	A1928	A1866	G1799	G1737	C1607	G1546	U1486	U1486
G2121	G2121	G2056	C1994	G1929	G1867	C1800	G1738	C1675	C1547	U1487	U1487
		G2057	U1995	G1930	C1868	A1801	A1739	A1676	A1609	A1548	
		A2058	C1996	U1931	G1869	A1802	G1740	A1677	A1610	C1488	C1488
		A2059	C1997	A1932	C1870		C1741	A1678	C1611	A1490	A1490
		A2060	A1998	G1933	A1871		U1742	A1679	C1612	A1551	A1551
		G2061	C1999	C1934	A1872		G1743	U1680	G1613	A1552	G1491
		A2062		G1935	G1873		A1744	G1681	A1614	A1553	G1492
		C2064	G2002	A1936	C1874	A1809	A1745	G1682	C1615	U1554	C1493
		C2065	A2003	A1937	G1875	A1810	A1746	U1683	A1616	G1555	A1494
		C2066	G2004	A1938	A1876	G1811	U1747	G1684	C1617	C1557	A1495
			A2005	U1939	A1877	A1812	C1748	C1685	A1619	C1558	A1496
			C2006	C2006	G1878	G1813	G1749	C1686		U1559	U1497
			G2069	U1940	C1879	G1814	A1750	G1687	U1621	U1560	C1498
			C2008	C1941	U1880	A1815	U1751	U1688	U1622	G1561	C1499
			A2071	U1943	C1881	C1816	G1752		G1623	C1562	G1500
			A2070	U1944	U1882	G1817	G1753			U1563	G1501
			U2011	G1945	U1883	A1818	A1754		A1626	U1564	A1502
			G2012	A2013	G1884	A1819	A1755			C1565	A1503
			A2014	C1947	A1885		G1756			A1566	A1504

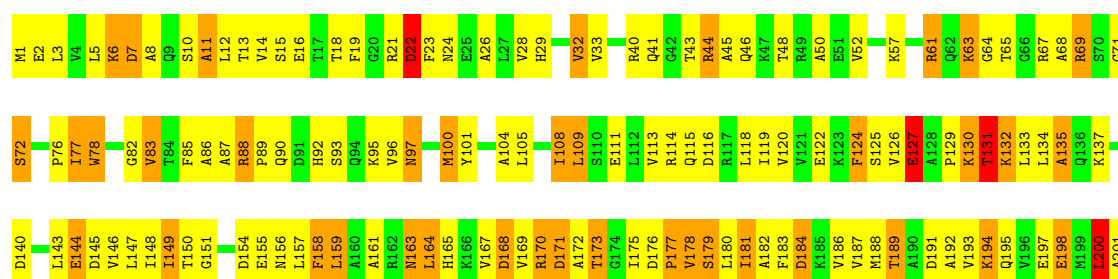






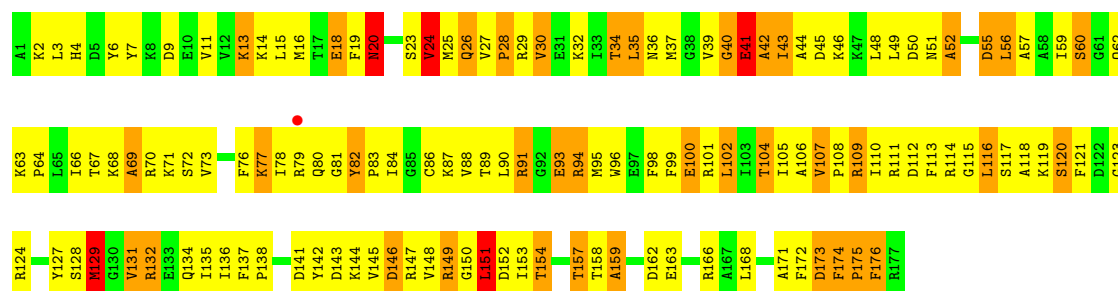
• Molecule 29: 50S ribosomal protein L4

Chain DE:



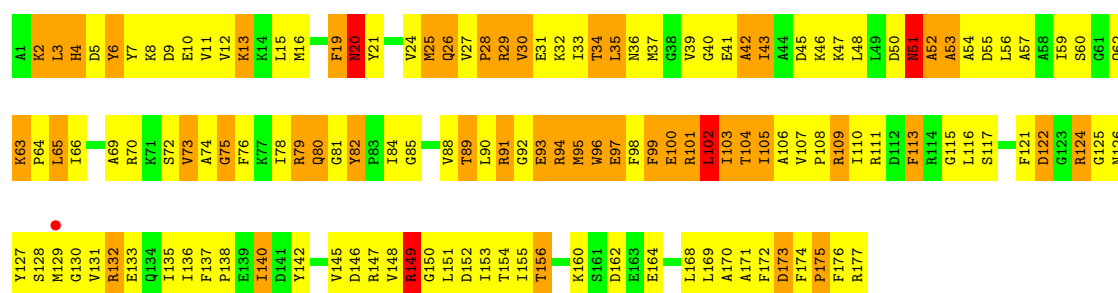
• Molecule 30: 50S ribosomal protein L5

Chain CF:



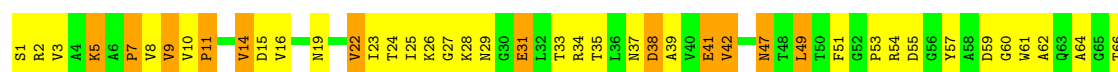
• Molecule 30: 50S ribosomal protein L5

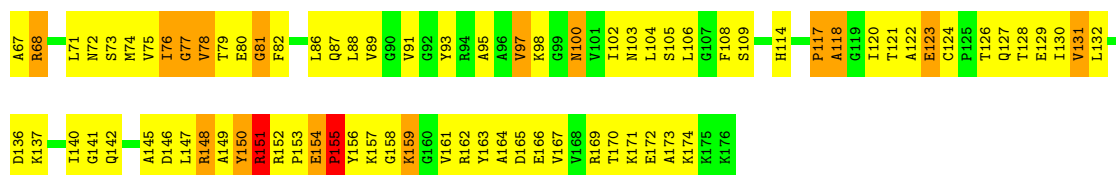
Chain DF:



• Molecule 31: 50S ribosomal protein L6

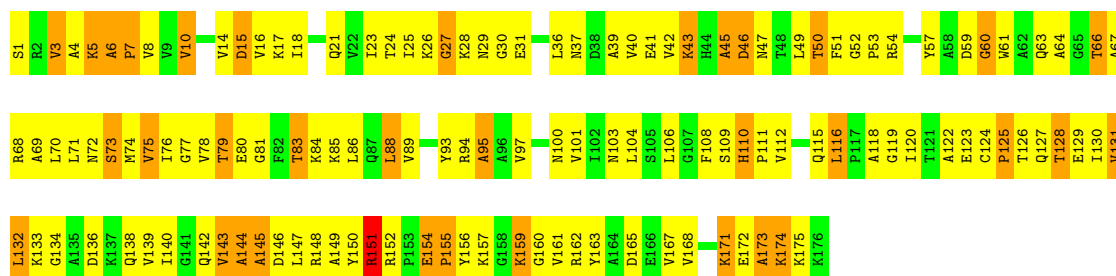
Chain CG:





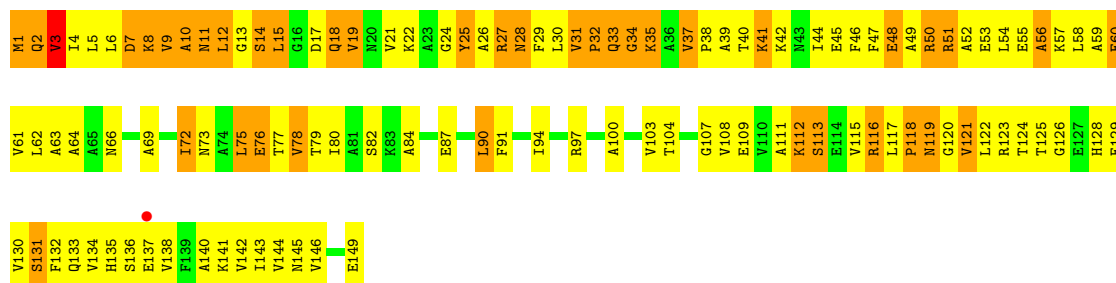
• Molecule 31: 50S ribosomal protein L6

Chain DG:



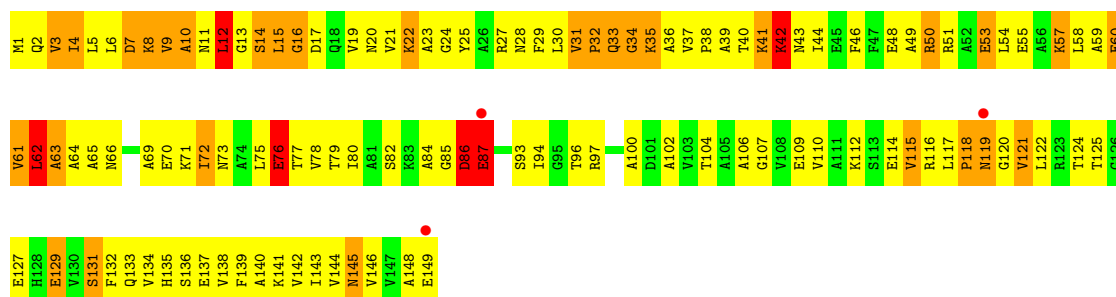
• Molecule 32: 50S ribosomal protein L9

Chain CH:



• Molecule 32: 50S ribosomal protein L9

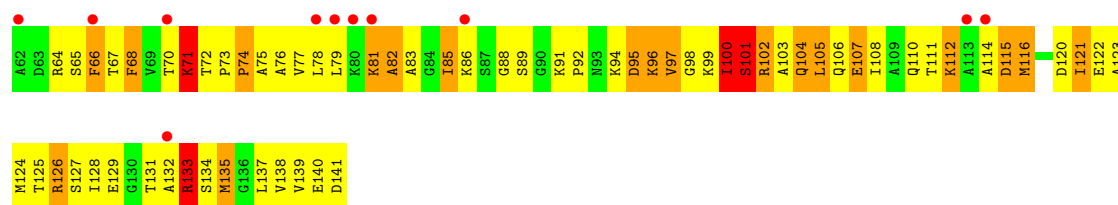
Chain DH:



• Molecule 33: 50S ribosomal protein L11

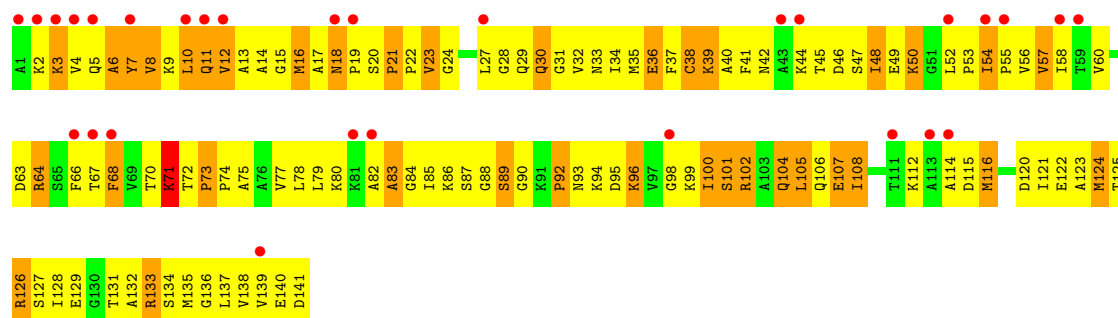
Chain CI:





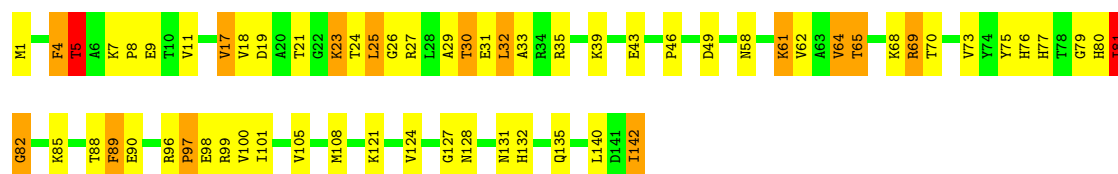
• Molecule 33: 50S ribosomal protein L11

Chain DI:



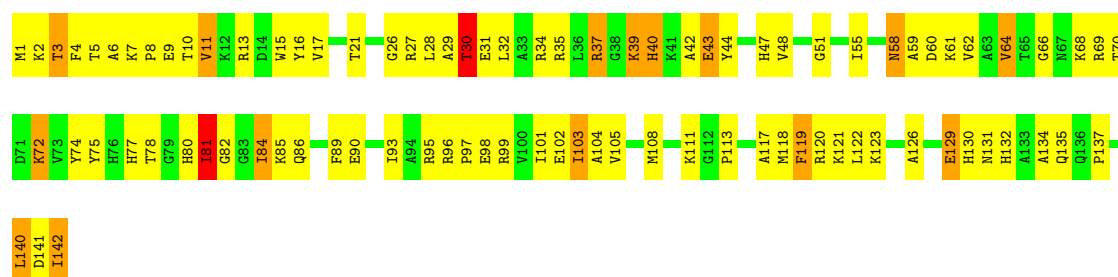
• Molecule 34: 50S ribosomal protein L13

Chain CJ:



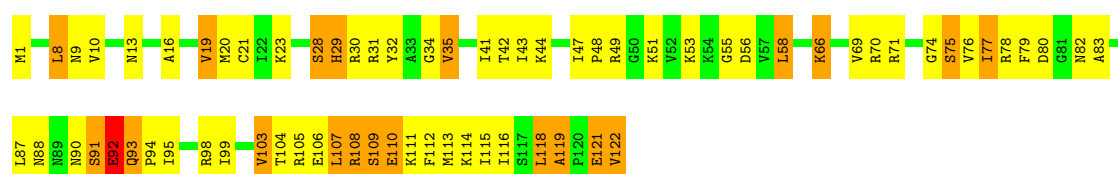
• Molecule 34: 50S ribosomal protein L13

Chain DJ:



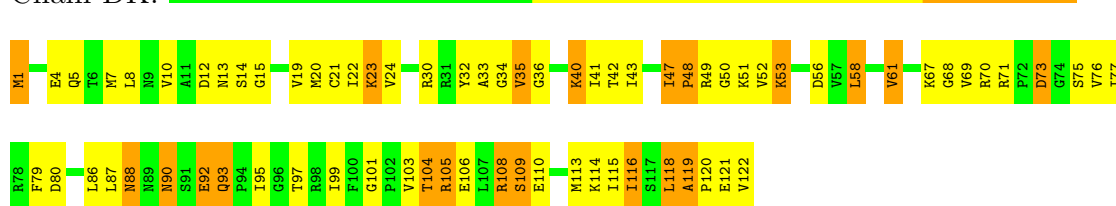
• Molecule 35: 50S ribosomal protein L14

Chain CK:



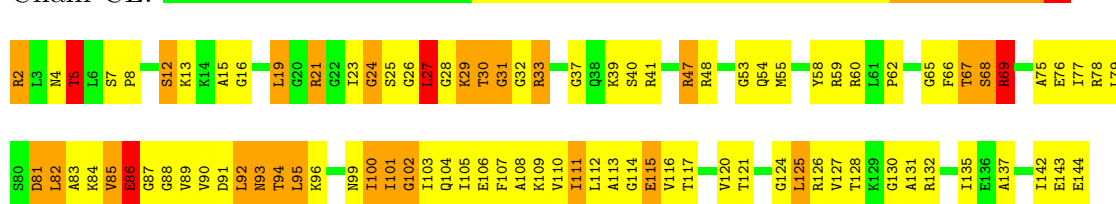
• Molecule 35: 50S ribosomal protein L14

Chain DK:



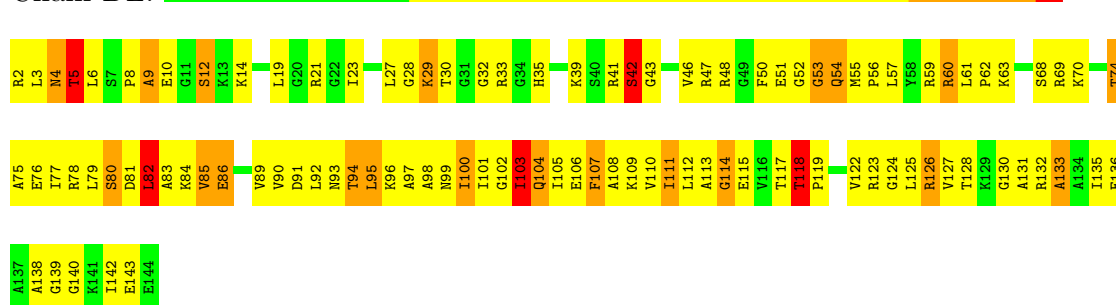
- Molecule 36: 50S ribosomal protein L15

Chain CL:



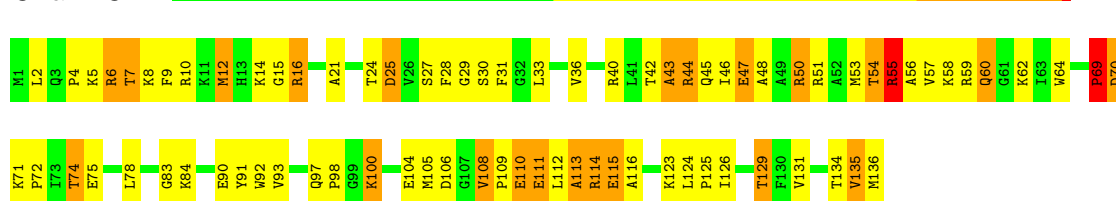
- Molecule 36: 50S ribosomal protein L15

Chain DL:



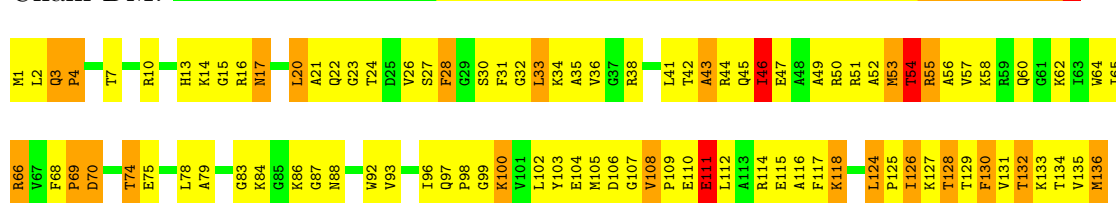
- Molecule 37: 50S ribosomal protein L16

Chain CM:



- Molecule 37: 50S ribosomal protein L16

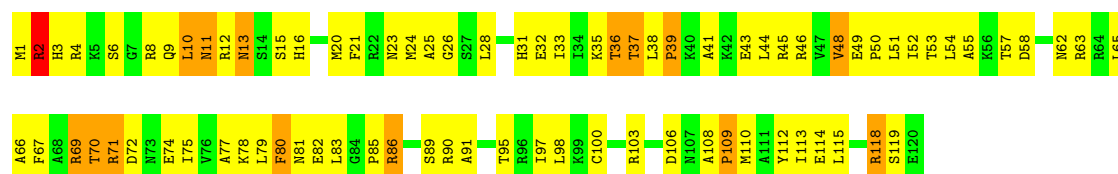
Chain DM:



- Molecule 38: 50S ribosomal protein L17

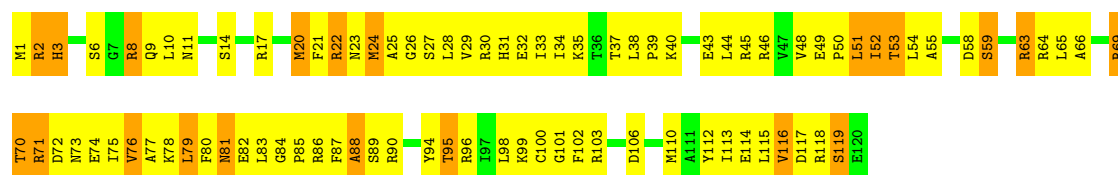
Chain CN:





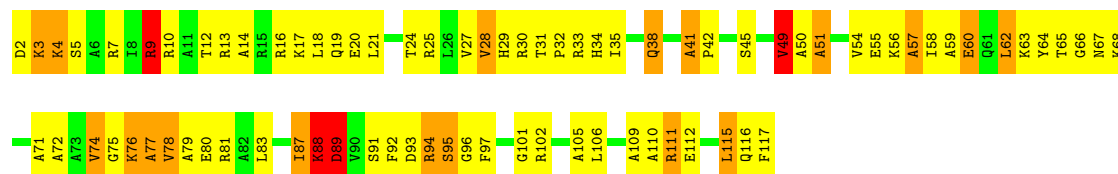
• Molecule 38: 50S ribosomal protein L17

Chain DN:



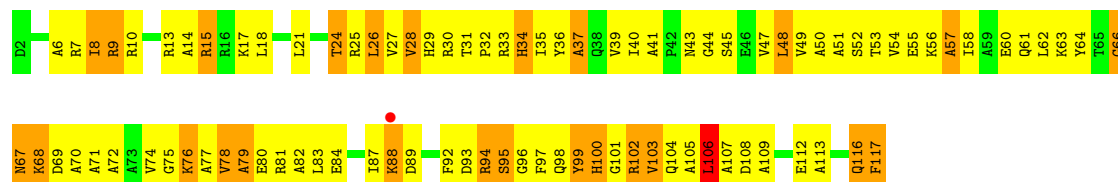
• Molecule 39: 50S ribosomal protein L18

Chain CO:



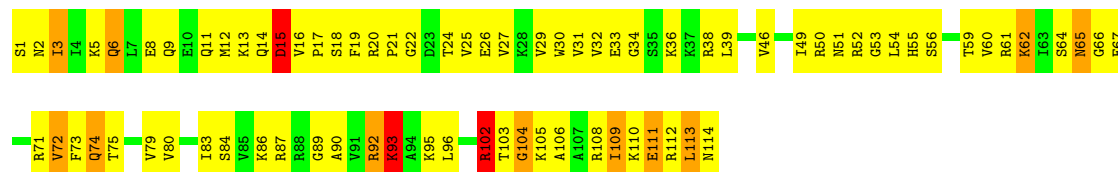
• Molecule 39: 50S ribosomal protein L18

Chain DO:



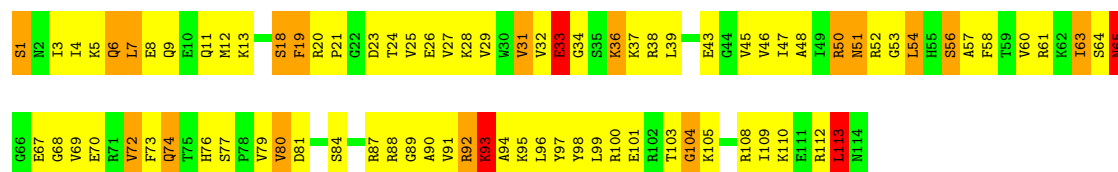
• Molecule 40: 50S ribosomal protein L19

Chain CP:

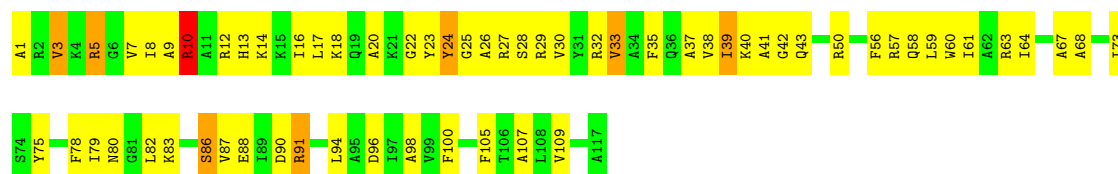


• Molecule 40: 50S ribosomal protein L19

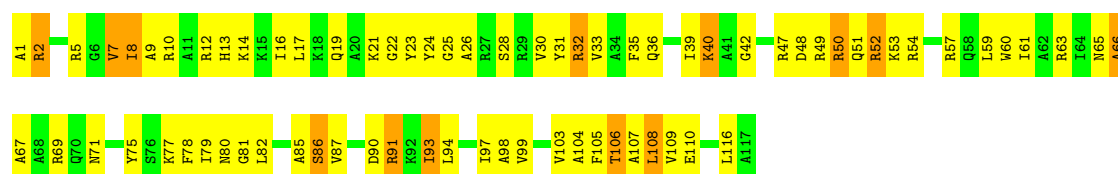
Chain DP:



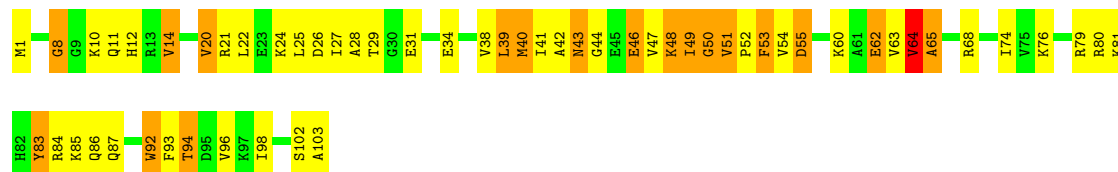
- Chain CQ:



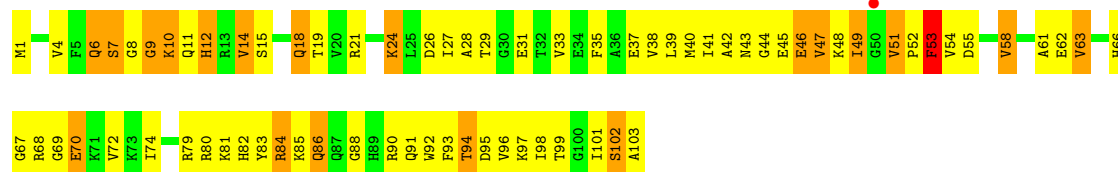
- Chain DQ:



- Chain CR:



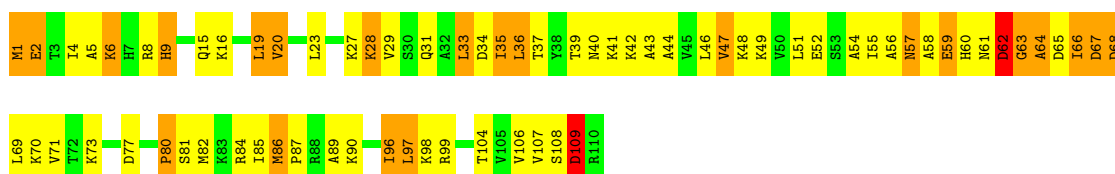
- Chain DR:



- Chain CS: 

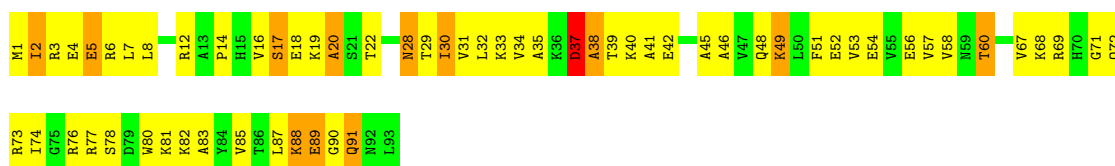


- Chain DS:



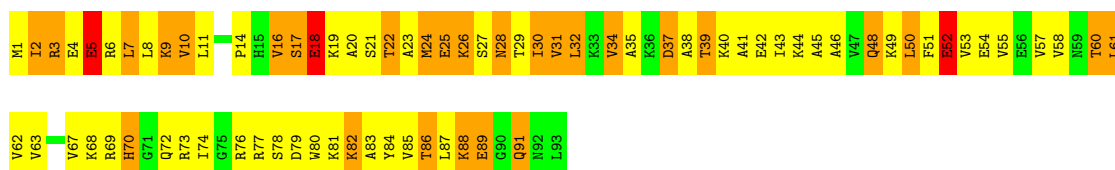
• Molecule 44: 50S ribosomal protein L23

Chain CT:



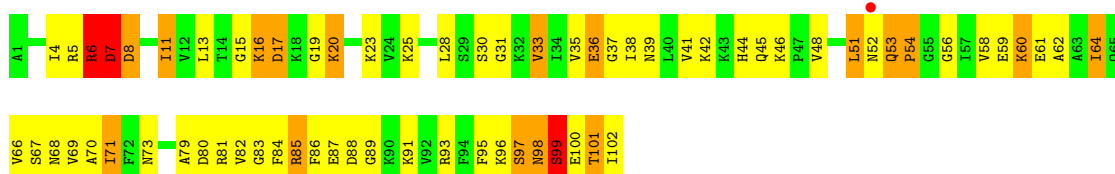
• Molecule 44: 50S ribosomal protein L23

Chain DT:



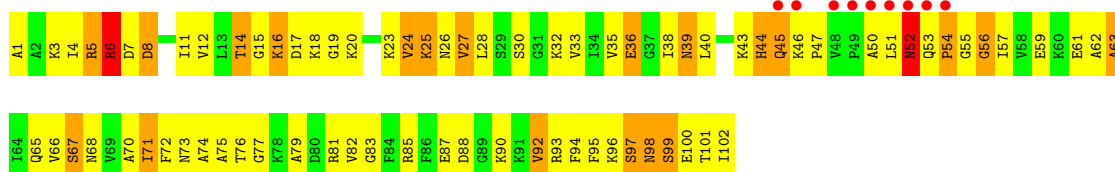
• Molecule 45: 50S ribosomal protein L24

Chain CU:



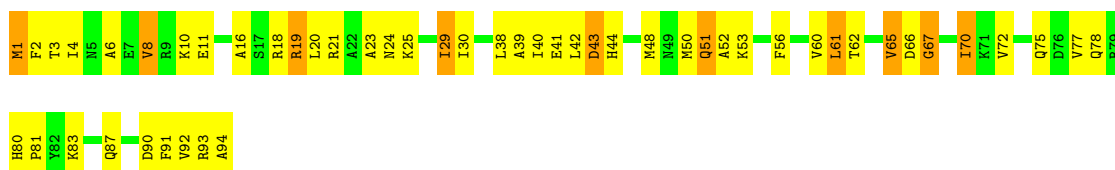
• Molecule 45: 50S ribosomal protein L24

Chain DU:



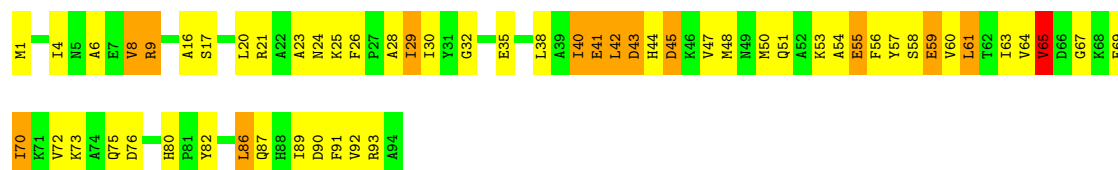
• Molecule 46: 50S ribosomal protein L25

Chain CV:



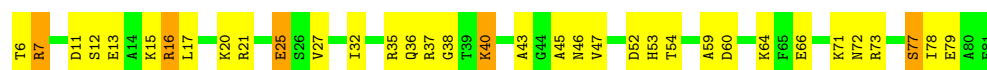
- Molecule 46: 50S ribosomal protein L25

Chain DV: 



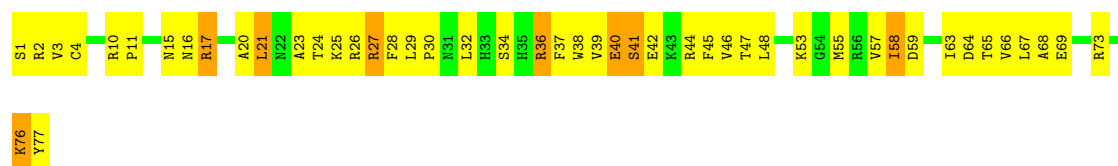
- Molecule 47: 50S ribosomal protein L27

Chain CW: 



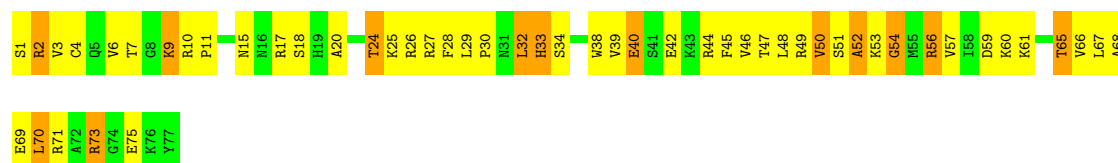
- Molecule 48: 50S ribosomal protein L28

Chain CX: 



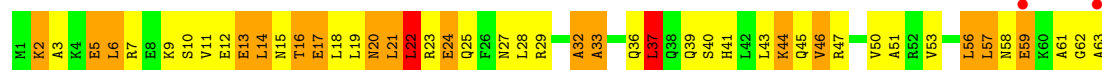
- Molecule 48: 50S ribosomal protein L28

Chain DX: 



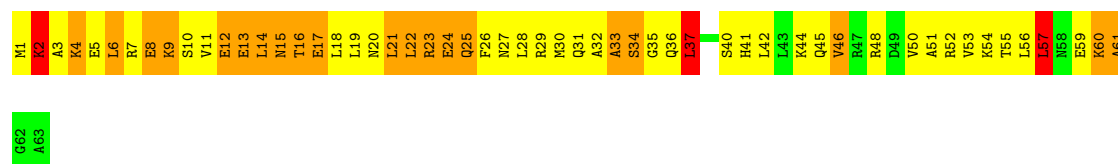
- Molecule 49: 50S ribosomal protein L29

Chain CY: 



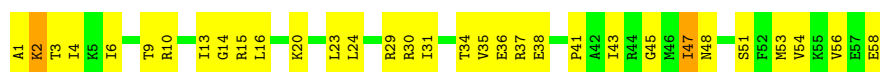
- Molecule 49: 50S ribosomal protein L29

Chain DY: 



- Molecule 50: 50S ribosomal protein L30

Chain CZ: 



- Molecule 50: 50S ribosomal protein L30

Chain DZ:



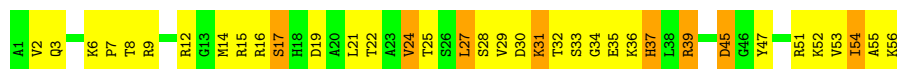
- Molecule 51: 50S ribosomal protein L32

Chain C0:



- Molecule 51: 50S ribosomal protein L32

Chain D0:



- Molecule 52: 50S ribosomal protein L33

Chain C1:



- Molecule 52: 50S ribosomal protein L33

Chain D1:



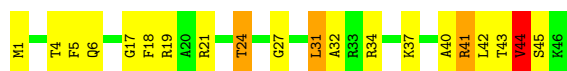
- Molecule 53: 50S ribosomal protein L34

Chain C2:



- Molecule 53: 50S ribosomal protein L34

Chain D2:



- Molecule 54: 50S ribosomal protein L35

Chain C3:

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.67Å 438.07Å 613.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 69.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 83.5 (69.21-3.00)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.202 , 0.260 0.197 , 0.254	Depositor DCC
R_{free} test set	19022 reflections (2.07%)	DCC
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , -10.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 938380 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	292354	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.87	8/36944 (0.0%)	1.28	318/57632 (0.6%)
1	BA	0.86	8/36966 (0.0%)	1.30	335/57666 (0.6%)
2	AB	0.60	0/1736	0.79	0/2338
2	BB	0.54	0/1736	0.72	0/2338
3	AC	0.56	0/1652	0.72	0/2225
3	BC	0.51	0/1652	0.72	1/2225 (0.0%)
4	AD	0.59	0/1665	0.74	1/2227 (0.0%)
4	BD	0.65	0/1665	0.80	1/2227 (0.0%)
5	AE	0.62	0/1119	0.85	0/1504
5	BE	0.62	0/1119	0.85	0/1504
6	AF	0.65	0/836	0.82	1/1128 (0.1%)
6	BF	0.55	0/836	0.80	1/1128 (0.1%)
7	AG	0.50	0/1196	0.67	0/1602
7	BG	0.48	0/1196	0.67	0/1602
8	AH	0.60	0/989	0.77	0/1326
8	BH	0.58	0/989	0.74	0/1326
9	AI	0.48	0/1034	0.71	0/1375
9	BI	0.53	0/1034	0.75	0/1375
10	AJ	0.57	0/797	0.74	0/1077
10	BJ	0.52	0/797	0.76	1/1077 (0.1%)
11	AK	0.67	0/893	0.82	0/1205
11	BK	0.59	0/893	0.75	0/1205
12	AL	0.61	0/969	0.81	0/1300
12	BL	0.72	0/969	0.92	0/1300
13	AM	0.52	0/893	0.74	0/1193
13	BM	0.50	0/893	0.71	0/1193
14	AN	0.55	0/785	0.76	0/1043
14	BN	0.51	0/785	0.65	0/1043
15	AO	0.55	0/722	0.73	0/964
15	BO	0.53	0/722	0.73	0/964
16	AP	0.54	0/659	0.82	1/884 (0.1%)
16	BP	0.61	0/659	0.79	1/884 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.57	0/658	0.74	0/881
17	BQ	0.62	0/658	0.76	0/881
18	AR	0.61	0/463	0.69	0/621
18	BR	0.54	0/463	0.68	0/621
19	AS	0.48	0/653	0.73	0/877
19	BS	0.55	0/653	0.67	0/877
20	AT	0.54	0/671	0.69	0/888
20	BT	0.57	0/671	0.73	0/888
21	AU	0.93	0/431	0.96	0/570
21	BU	0.78	0/431	0.85	0/570
22	AV	0.76	1/1813 (0.1%)	1.22	14/2823 (0.5%)
22	BV	0.74	1/1813 (0.1%)	1.22	10/2823 (0.4%)
23	AX	0.86	0/363	1.11	0/564
23	BX	0.73	0/388	1.09	0/603
24	AY	0.65	0/1430	0.74	0/1924
25	CA	1.60	600/69659 (0.9%)	1.67	2062/108672 (1.9%)
25	DA	1.07	82/69633 (0.1%)	1.48	1284/108629 (1.2%)
26	CB	1.33	5/2847 (0.2%)	1.58	77/4440 (1.7%)
27	CC	0.80	0/2122	0.90	1/2852 (0.0%)
27	DC	0.68	1/2122 (0.0%)	0.86	1/2852 (0.0%)
28	CD	0.96	0/1586	0.92	1/2134 (0.0%)
28	DD	0.70	0/1586	0.87	2/2134 (0.1%)
29	CE	0.91	0/1571	0.89	1/2113 (0.0%)
29	DE	0.67	0/1571	0.81	0/2113
30	CF	0.64	0/1435	0.74	0/1926
30	DF	0.51	0/1435	0.67	0/1926
31	CG	0.75	0/1343	0.85	1/1816 (0.1%)
31	DG	0.51	0/1343	0.69	0/1816
32	CH	0.68	1/1121 (0.1%)	0.77	0/1515
32	DH	0.66	1/1121 (0.1%)	0.80	1/1515 (0.1%)
33	CI	0.72	0/1046	0.74	0/1410
33	DI	0.67	0/1046	0.72	0/1410
34	CJ	1.01	0/1152	0.84	1/1551 (0.1%)
34	DJ	0.77	0/1152	0.82	0/1551
35	CK	0.91	3/948 (0.3%)	0.94	1/1268 (0.1%)
35	DK	0.68	0/948	0.84	0/1268
36	CL	0.94	0/1054	1.01	0/1403
36	DL	0.65	0/1054	0.85	0/1403
37	CM	0.94	0/1093	0.96	0/1460
37	DM	0.64	0/1093	0.80	0/1460
38	CN	0.91	0/974	0.96	1/1301 (0.1%)
38	DN	0.67	0/974	0.82	0/1301
39	CO	0.76	0/902	0.87	1/1209 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	DO	0.50	0/902	0.66	0/1209
40	CP	0.89	0/929	0.88	1/1242 (0.1%)
40	DP	0.71	0/929	0.82	0/1242
41	CQ	1.14	0/960	0.96	1/1278 (0.1%)
41	DQ	0.80	0/960	0.79	0/1278
42	CR	1.01	1/829 (0.1%)	0.98	0/1107
42	DR	0.79	0/829	0.90	1/1107 (0.1%)
43	CS	1.08	1/864 (0.1%)	0.97	1/1156 (0.1%)
43	DS	0.71	0/864	0.89	1/1156 (0.1%)
44	CT	0.82	0/745	0.86	0/994
44	DT	0.59	0/745	0.74	0/994
45	CU	0.91	0/788	0.90	0/1051
45	DU	0.66	0/788	0.76	0/1051
46	CV	0.79	0/766	0.81	0/1025
46	DV	0.53	0/766	0.69	0/1025
47	CW	1.02	0/582	0.97	0/769
48	CX	0.78	0/635	0.84	0/848
48	DX	0.61	0/635	0.77	0/848
49	CY	0.76	0/510	0.96	1/677 (0.1%)
49	DY	0.56	0/510	0.77	0/677
50	CZ	1.04	0/453	0.94	0/605
50	DZ	0.58	0/453	0.78	0/605
51	C0	0.95	0/450	0.98	2/599 (0.3%)
51	D0	0.71	0/450	0.89	1/599 (0.2%)
52	C1	0.74	0/417	0.76	0/554
52	D1	0.50	0/417	0.66	0/554
53	C2	1.03	0/380	0.99	2/498 (0.4%)
53	D2	0.70	0/380	0.84	0/498
54	C3	0.94	0/513	0.85	0/676
54	D3	0.60	0/513	0.78	1/676 (0.1%)
55	C4	0.92	0/303	0.99	0/397
55	D4	0.68	0/303	0.76	0/397
56	DB	0.75	0/2828	1.23	18/4410 (0.4%)
57	DW	0.60	0/571	0.72	0/755
All	All	1.08	713/315257 (0.2%)	1.34	4150/471496 (0.9%)

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
4	AD	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
4	BD	0	1
5	AE	0	1
5	BE	0	2
6	BF	0	1
9	AI	0	1
11	AK	0	1
11	BK	0	2
12	BL	0	2
13	AM	0	1
14	AN	0	1
20	BT	0	1
21	AU	0	2
21	BU	0	1
27	CC	0	1
27	DC	0	1
28	CD	0	2
28	DD	0	1
32	DH	0	2
33	CI	0	1
34	DJ	0	1
39	DO	0	1
42	CR	0	1
45	CU	0	1
50	CZ	0	1
All	All	0	31

The worst 5 of 713 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	CA	1142	A	N9-C4	-18.22	1.26	1.37
25	CA	984	A	N9-C4	-13.29	1.29	1.37
25	DA	984	A	N9-C4	-10.51	1.31	1.37
25	CA	984	A	C5-C6	-10.44	1.31	1.41
25	CA	528	A	N7-C5	-10.29	1.33	1.39

The worst 5 of 4150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	984	A	C2-N3-C4	-18.86	101.17	110.60
25	CA	2250	G	N3-C4-C5	17.23	137.22	128.60
25	CA	1638	C	N1-C2-O2	-16.64	108.92	118.90
25	CA	1142	A	C2-N3-C4	-16.61	102.29	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	CA	1142	A	N3-C4-C5	16.11	138.07	126.80

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	AD	47	LEU	Peptide
5	AE	100	GLU	Peptide
9	AI	5	TYR	Peptide
11	AK	125	LYS	Peptide
13	AM	111	PRO	Peptide

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	2052	0
1	BA	33015	0	16617	2194	0
2	AB	1705	0	1732	374	0
2	BB	1705	0	1732	298	0
3	AC	1625	0	1699	235	0
3	BC	1625	0	1699	237	0
4	AD	1643	0	1710	291	0
4	BD	1643	0	1710	228	0
5	AE	1106	0	1148	214	0
5	BE	1106	0	1148	211	0
6	AF	818	0	808	116	0
6	BF	818	0	808	156	0
7	AG	1182	0	1240	116	0
7	BG	1182	0	1240	166	0
8	AH	979	0	1034	161	0
8	BH	979	0	1034	119	0
9	AI	1022	0	1070	189	0
9	BI	1022	0	1070	186	0
10	AJ	787	0	828	178	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	BJ	787	0	828	142	0
11	AK	877	0	887	160	0
11	BK	877	0	887	136	0
12	AL	955	0	1019	94	0
12	BL	955	0	1019	118	0
13	AM	884	0	944	163	0
13	BM	884	0	944	144	0
14	AN	774	0	827	130	0
14	BN	774	0	827	131	0
15	AO	714	0	737	61	0
15	BO	714	0	737	87	0
16	AP	649	0	666	106	0
16	BP	649	0	666	87	0
17	AQ	649	0	691	118	0
17	BQ	649	0	691	103	0
18	AR	456	0	478	46	0
18	BR	456	0	478	57	0
19	AS	638	0	665	88	0
19	BS	638	0	665	96	0
20	AT	665	0	714	84	0
20	BT	665	0	714	129	0
21	AU	426	0	449	139	0
21	BU	426	0	449	119	0
22	AV	1623	0	821	88	0
22	BV	1623	0	821	47	0
23	AX	324	0	162	19	0
23	BX	346	0	173	24	0
24	AY	1419	0	1467	97	0
25	CA	62195	0	31271	2445	0
25	DA	62173	0	31270	3398	0
26	CB	2548	0	1292	98	0
27	CC	2083	0	2157	227	0
27	DC	2083	0	2157	213	0
28	CD	1565	0	1616	129	0
28	DD	1565	0	1616	114	0
29	CE	1552	0	1619	143	0
29	DE	1552	0	1619	163	0
30	CF	1411	0	1447	202	0
30	DF	1411	0	1447	197	0
31	CG	1323	0	1374	146	0
31	DG	1323	0	1374	177	0
32	CH	1110	0	1148	145	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	DH	1110	0	1148	210	0
33	CI	1032	0	1088	246	0
33	DI	1032	0	1088	180	0
34	CJ	1129	0	1162	57	0
34	DJ	1129	0	1162	96	0
35	CK	939	0	1012	75	0
35	DK	939	0	1012	79	0
36	CL	1045	0	1117	130	0
36	DL	1045	0	1117	168	0
37	CM	1074	0	1157	96	0
37	DM	1074	0	1157	127	0
38	CN	961	0	1000	94	0
38	DN	961	0	1000	124	0
39	CO	892	0	923	84	0
39	DO	892	0	923	141	0
40	CP	917	0	965	93	0
40	DP	917	0	965	107	0
41	CQ	947	0	1022	63	0
41	DQ	947	0	1022	83	0
42	CR	816	0	839	84	0
42	DR	816	0	839	99	0
43	CS	857	0	922	42	0
43	DS	857	0	922	82	0
44	CT	739	0	807	71	0
44	DT	739	0	807	114	0
45	CU	780	0	834	66	0
45	DU	780	0	834	111	0
46	CV	753	0	780	59	0
46	DV	753	0	780	71	0
47	CW	575	0	589	27	0
48	CX	625	0	655	41	0
48	DX	625	0	655	58	0
49	CY	509	0	543	88	0
49	DY	509	0	543	109	0
50	CZ	449	0	491	26	0
50	DZ	449	0	491	47	0
51	C0	444	0	461	35	0
51	D0	444	0	461	41	0
52	C1	410	0	440	37	0
52	D1	410	0	440	45	0
53	C2	377	0	418	26	0
53	D2	377	0	418	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	C3	504	0	574	40	0
54	D3	504	0	574	42	0
55	C4	302	0	340	23	0
55	D4	302	0	340	34	0
56	DB	2529	0	1281	163	0
57	DW	564	0	576	36	0
58	AA	72	0	0	0	0
58	BA	56	0	0	0	0
58	CA	194	0	0	0	0
58	CB	4	0	0	0	0
58	CQ	1	0	0	0	0
58	DA	166	0	0	0	0
58	DB	3	0	0	0	0
58	DL	1	0	0	0	0
58	DQ	1	0	0	0	0
59	C4	1	0	0	0	0
59	D4	1	0	0	0	0
60	AA	197	0	0	11	0
60	AN	4	0	0	0	0
60	AT	1	0	0	0	0
60	AU	1	0	0	0	0
60	BA	190	0	0	12	0
60	BL	1	0	0	0	0
60	BN	5	0	0	1	0
60	BT	1	0	0	0	0
60	BU	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	625	0	0	62	0
60	CB	13	0	0	0	0
60	CC	8	0	0	0	0
60	CD	2	0	0	0	0
60	CE	2	0	0	0	0
60	CF	1	0	0	0	0
60	CJ	1	0	0	0	0
60	CL	6	0	0	2	0
60	CN	4	0	0	0	0
60	CS	1	0	0	0	0
60	CV	1	0	0	0	0
60	D2	1	0	0	0	0
60	D3	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	D4	1	0	0	0	0
60	DA	622	0	0	70	0
60	DB	14	0	0	0	0
60	DC	4	0	0	0	0
60	DD	5	0	0	2	0
60	DE	2	0	0	0	0
60	DJ	1	0	0	0	0
60	DL	4	0	0	1	0
60	DN	1	0	0	0	0
60	DR	1	0	0	0	0
All	All	292354	0	195461	20868	0

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 43.

The worst 5 of 20868 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
32:DH:93:SER:OG	32:DH:121:VAL:HG12	1.46	1.15
1:BA:1053:G:H4'	1:BA:1054:C:H5'	1.29	1.11
32:DH:93:SER:OG	32:DH:121:VAL:CG1	2.03	1.06
25:DA:1153:C:OP2	60:DA:3363:HOH:O	1.78	1.01
12:BL:33:CYS:HA	12:BL:54:VAL:HA	1.44	0.99

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	AB	216/218 (99%)	109 (50%)	49 (23%)	58 (27%)	0 0
2	BB	216/218 (99%)	112 (52%)	49 (23%)	55 (26%)	0 0
3	AC	204/206 (99%)	125 (61%)	49 (24%)	30 (15%)	0 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	BC	204/206 (99%)	126 (62%)	47 (23%)	31 (15%)	0	1
4	AD	203/205 (99%)	123 (61%)	41 (20%)	39 (19%)	0	0
4	BD	203/205 (99%)	136 (67%)	36 (18%)	31 (15%)	0	1
5	AE	148/150 (99%)	87 (59%)	38 (26%)	23 (16%)	0	1
5	BE	148/150 (99%)	90 (61%)	31 (21%)	27 (18%)	0	1
6	AF	98/100 (98%)	62 (63%)	21 (21%)	15 (15%)	0	1
6	BF	98/100 (98%)	54 (55%)	23 (24%)	21 (21%)	0	0
7	AG	149/151 (99%)	86 (58%)	41 (28%)	22 (15%)	0	1
7	BG	149/151 (99%)	79 (53%)	46 (31%)	24 (16%)	0	1
8	AH	127/129 (98%)	79 (62%)	37 (29%)	11 (9%)	1	5
8	BH	127/129 (98%)	82 (65%)	32 (25%)	13 (10%)	1	4
9	AI	125/127 (98%)	76 (61%)	34 (27%)	15 (12%)	1	2
9	BI	125/127 (98%)	77 (62%)	33 (26%)	15 (12%)	1	2
10	AJ	96/98 (98%)	60 (62%)	14 (15%)	22 (23%)	0	0
10	BJ	96/98 (98%)	64 (67%)	14 (15%)	18 (19%)	0	1
11	AK	115/117 (98%)	84 (73%)	17 (15%)	14 (12%)	1	2
11	BK	115/117 (98%)	81 (70%)	19 (16%)	15 (13%)	0	2
12	AL	121/123 (98%)	85 (70%)	29 (24%)	7 (6%)	3	15
12	BL	121/123 (98%)	91 (75%)	16 (13%)	14 (12%)	1	3
13	AM	112/114 (98%)	78 (70%)	22 (20%)	12 (11%)	1	3
13	BM	112/114 (98%)	65 (58%)	24 (21%)	23 (20%)	0	0
14	AN	92/100 (92%)	47 (51%)	27 (29%)	18 (20%)	0	0
14	BN	92/100 (92%)	39 (42%)	30 (33%)	23 (25%)	0	0
15	AO	86/88 (98%)	57 (66%)	22 (26%)	7 (8%)	1	7
15	BO	86/88 (98%)	52 (60%)	17 (20%)	17 (20%)	0	0
16	AP	80/82 (98%)	48 (60%)	11 (14%)	21 (26%)	0	0
16	BP	80/82 (98%)	47 (59%)	22 (28%)	11 (14%)	0	2
17	AQ	78/80 (98%)	47 (60%)	18 (23%)	13 (17%)	0	1
17	BQ	78/80 (98%)	48 (62%)	18 (23%)	12 (15%)	0	1
18	AR	53/55 (96%)	34 (64%)	13 (24%)	6 (11%)	1	3
18	BR	53/55 (96%)	31 (58%)	19 (36%)	3 (6%)	3	16

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AS	77/79 (98%)	36 (47%)	29 (38%)	12 (16%)	0	1
19	BS	77/79 (98%)	56 (73%)	14 (18%)	7 (9%)	1	5
20	AT	83/85 (98%)	37 (45%)	31 (37%)	15 (18%)	0	1
20	BT	83/85 (98%)	46 (55%)	23 (28%)	14 (17%)	0	1
21	AU	49/51 (96%)	20 (41%)	15 (31%)	14 (29%)	0	0
21	BU	49/51 (96%)	22 (45%)	10 (20%)	17 (35%)	0	0
24	AY	181/183 (99%)	135 (75%)	35 (19%)	11 (6%)	2	14
27	CC	269/271 (99%)	216 (80%)	32 (12%)	21 (8%)	1	7
27	DC	269/271 (99%)	198 (74%)	43 (16%)	28 (10%)	1	4
28	CD	207/209 (99%)	166 (80%)	30 (14%)	11 (5%)	3	18
28	DD	207/209 (99%)	162 (78%)	35 (17%)	10 (5%)	4	20
29	CE	199/201 (99%)	158 (79%)	32 (16%)	9 (4%)	4	22
29	DE	199/201 (99%)	142 (71%)	38 (19%)	19 (10%)	1	4
30	CF	175/177 (99%)	118 (67%)	38 (22%)	19 (11%)	1	3
30	DF	175/177 (99%)	113 (65%)	34 (19%)	28 (16%)	0	1
31	CG	174/176 (99%)	129 (74%)	30 (17%)	15 (9%)	1	5
31	DG	174/176 (99%)	106 (61%)	43 (25%)	25 (14%)	0	1
32	CH	147/149 (99%)	95 (65%)	29 (20%)	23 (16%)	0	1
32	DH	147/149 (99%)	95 (65%)	27 (18%)	25 (17%)	0	1
33	CI	139/141 (99%)	65 (47%)	47 (34%)	27 (19%)	0	0
33	DI	139/141 (99%)	71 (51%)	46 (33%)	22 (16%)	0	1
34	CJ	140/142 (99%)	123 (88%)	11 (8%)	6 (4%)	4	23
34	DJ	140/142 (99%)	112 (80%)	24 (17%)	4 (3%)	7	35
35	CK	120/122 (98%)	88 (73%)	24 (20%)	8 (7%)	2	10
35	DK	120/122 (98%)	87 (72%)	21 (18%)	12 (10%)	1	4
36	CL	141/143 (99%)	99 (70%)	21 (15%)	21 (15%)	0	1
36	DL	141/143 (99%)	88 (62%)	36 (26%)	17 (12%)	1	2
37	CM	134/136 (98%)	110 (82%)	15 (11%)	9 (7%)	2	10
37	DM	134/136 (98%)	97 (72%)	23 (17%)	14 (10%)	1	4
38	CN	118/120 (98%)	91 (77%)	21 (18%)	6 (5%)	3	18
38	DN	118/120 (98%)	82 (70%)	28 (24%)	8 (7%)	2	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	CO	114/116 (98%)	83 (73%)	17 (15%)	14 (12%)	1	2
39	DO	114/116 (98%)	77 (68%)	25 (22%)	12 (10%)	1	3
40	CP	112/114 (98%)	96 (86%)	12 (11%)	4 (4%)	5	29
40	DP	112/114 (98%)	86 (77%)	19 (17%)	7 (6%)	2	12
41	CQ	115/117 (98%)	100 (87%)	13 (11%)	2 (2%)	14	54
41	DQ	115/117 (98%)	95 (83%)	18 (16%)	2 (2%)	14	54
42	CR	101/103 (98%)	84 (83%)	9 (9%)	8 (8%)	1	7
42	DR	101/103 (98%)	78 (77%)	14 (14%)	9 (9%)	1	5
43	CS	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	3	16
43	DS	108/110 (98%)	78 (72%)	19 (18%)	11 (10%)	1	4
44	CT	91/93 (98%)	67 (74%)	13 (14%)	11 (12%)	1	2
44	DT	91/93 (98%)	59 (65%)	20 (22%)	12 (13%)	0	2
45	CU	100/102 (98%)	74 (74%)	14 (14%)	12 (12%)	1	2
45	DU	100/102 (98%)	73 (73%)	14 (14%)	13 (13%)	0	2
46	CV	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	10	45
46	DV	92/94 (98%)	71 (77%)	15 (16%)	6 (6%)	2	11
47	CW	74/76 (97%)	68 (92%)	4 (5%)	2 (3%)	8	38
48	CX	75/77 (97%)	64 (85%)	9 (12%)	2 (3%)	8	38
48	DX	75/77 (97%)	54 (72%)	15 (20%)	6 (8%)	1	7
49	CY	61/63 (97%)	34 (56%)	13 (21%)	14 (23%)	0	0
49	DY	61/63 (97%)	28 (46%)	16 (26%)	17 (28%)	0	0
50	CZ	56/58 (97%)	50 (89%)	6 (11%)	0	100	100
50	DZ	56/58 (97%)	50 (89%)	4 (7%)	2 (4%)	5	29
51	C0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	5	28
51	D0	54/56 (96%)	39 (72%)	10 (18%)	5 (9%)	1	5
52	C1	48/50 (96%)	32 (67%)	12 (25%)	4 (8%)	1	6
52	D1	48/50 (96%)	36 (75%)	10 (21%)	2 (4%)	4	24
53	C2	44/46 (96%)	37 (84%)	6 (14%)	1 (2%)	10	43
53	D2	44/46 (96%)	31 (70%)	8 (18%)	5 (11%)	1	3
54	C3	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
54	D3	62/64 (97%)	49 (79%)	11 (18%)	2 (3%)	6	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
55	C4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	8	37
55	D4	36/38 (95%)	31 (86%)	4 (11%)	1 (3%)	8	37
57	DW	73/75 (97%)	57 (78%)	12 (16%)	4 (6%)	3	16
All	All	11416/11626 (98%)	7804 (68%)	2248 (20%)	1364 (12%)	1	2

5 of 1364 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	PHE
2	AB	21	TYR
2	AB	33	ALA
2	AB	63	LYS
2	AB	67	LEU

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	114 (63%)	66 (37%)	0	1
2	BB	180/180 (100%)	131 (73%)	49 (27%)	0	3
3	AC	170/170 (100%)	127 (75%)	43 (25%)	1	4
3	BC	170/170 (100%)	123 (72%)	47 (28%)	0	3
4	AD	172/172 (100%)	132 (77%)	40 (23%)	1	6
4	BD	172/172 (100%)	123 (72%)	49 (28%)	0	3
5	AE	113/113 (100%)	80 (71%)	33 (29%)	0	2
5	BE	113/113 (100%)	87 (77%)	26 (23%)	1	6
6	AF	87/87 (100%)	60 (69%)	27 (31%)	0	2
6	BF	87/87 (100%)	61 (70%)	26 (30%)	0	2
7	AG	124/124 (100%)	90 (73%)	34 (27%)	0	3
7	BG	124/124 (100%)	85 (68%)	39 (32%)	0	2
8	AH	104/104 (100%)	78 (75%)	26 (25%)	1	4
8	BH	104/104 (100%)	78 (75%)	26 (25%)	1	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	AI	105/105 (100%)	74 (70%)	31 (30%)	0	2
9	BI	105/105 (100%)	67 (64%)	38 (36%)	0	1
10	AJ	86/86 (100%)	63 (73%)	23 (27%)	1	4
10	BJ	86/86 (100%)	61 (71%)	25 (29%)	0	2
11	AK	90/90 (100%)	66 (73%)	24 (27%)	1	4
11	BK	90/90 (100%)	67 (74%)	23 (26%)	1	4
12	AL	103/103 (100%)	86 (84%)	17 (16%)	3	16
12	BL	103/103 (100%)	75 (73%)	28 (27%)	0	3
13	AM	92/92 (100%)	73 (79%)	19 (21%)	2	8
13	BM	92/92 (100%)	71 (77%)	21 (23%)	1	6
14	AN	79/83 (95%)	56 (71%)	23 (29%)	0	2
14	BN	79/83 (95%)	60 (76%)	19 (24%)	1	5
15	AO	76/76 (100%)	61 (80%)	15 (20%)	2	11
15	BO	76/76 (100%)	60 (79%)	16 (21%)	1	8
16	AP	65/65 (100%)	45 (69%)	20 (31%)	0	2
16	BP	65/65 (100%)	48 (74%)	17 (26%)	1	4
17	AQ	74/74 (100%)	54 (73%)	20 (27%)	1	3
17	BQ	74/74 (100%)	47 (64%)	27 (36%)	0	1
18	AR	48/48 (100%)	40 (83%)	8 (17%)	3	16
18	BR	48/48 (100%)	40 (83%)	8 (17%)	3	16
19	AS	70/70 (100%)	56 (80%)	14 (20%)	2	10
19	BS	70/70 (100%)	53 (76%)	17 (24%)	1	5
20	AT	65/65 (100%)	45 (69%)	20 (31%)	0	2
20	BT	65/65 (100%)	47 (72%)	18 (28%)	0	3
21	AU	44/44 (100%)	23 (52%)	21 (48%)	0	0
21	BU	44/44 (100%)	26 (59%)	18 (41%)	0	0
24	AY	157/157 (100%)	139 (88%)	18 (12%)	8	32
27	CC	216/216 (100%)	182 (84%)	34 (16%)	4	18
27	DC	216/216 (100%)	173 (80%)	43 (20%)	2	10
28	CD	164/164 (100%)	143 (87%)	21 (13%)	6	27
28	DD	164/164 (100%)	135 (82%)	29 (18%)	3	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	CE	165/165 (100%)	143 (87%)	22 (13%)	6	25
29	DE	165/165 (100%)	126 (76%)	39 (24%)	1	5
30	CF	148/148 (100%)	112 (76%)	36 (24%)	1	5
30	DF	148/148 (100%)	114 (77%)	34 (23%)	1	6
31	CG	137/137 (100%)	114 (83%)	23 (17%)	3	15
31	DG	137/137 (100%)	119 (87%)	18 (13%)	6	25
32	CH	114/114 (100%)	89 (78%)	25 (22%)	1	7
32	DH	114/114 (100%)	92 (81%)	22 (19%)	2	12
33	CI	109/109 (100%)	78 (72%)	31 (28%)	0	3
33	DI	109/109 (100%)	83 (76%)	26 (24%)	1	5
34	CJ	116/116 (100%)	97 (84%)	19 (16%)	3	16
34	DJ	116/116 (100%)	95 (82%)	21 (18%)	2	13
35	CK	103/103 (100%)	85 (82%)	18 (18%)	3	14
35	DK	103/103 (100%)	85 (82%)	18 (18%)	3	14
36	CL	102/102 (100%)	81 (79%)	21 (21%)	2	9
36	DL	102/102 (100%)	81 (79%)	21 (21%)	2	9
37	CM	109/109 (100%)	87 (80%)	22 (20%)	2	10
37	DM	109/109 (100%)	87 (80%)	22 (20%)	2	10
38	CN	100/100 (100%)	83 (83%)	17 (17%)	3	15
38	DN	100/100 (100%)	80 (80%)	20 (20%)	2	10
39	CO	86/86 (100%)	68 (79%)	18 (21%)	1	8
39	DO	86/86 (100%)	66 (77%)	20 (23%)	1	6
40	CP	99/99 (100%)	78 (79%)	21 (21%)	1	8
40	DP	99/99 (100%)	76 (77%)	23 (23%)	1	6
41	CQ	89/89 (100%)	76 (85%)	13 (15%)	5	21
41	DQ	89/89 (100%)	74 (83%)	15 (17%)	3	15
42	CR	84/84 (100%)	70 (83%)	14 (17%)	3	16
42	DR	84/84 (100%)	66 (79%)	18 (21%)	1	8
43	CS	93/93 (100%)	83 (89%)	10 (11%)	9	35
43	DS	93/93 (100%)	71 (76%)	22 (24%)	1	5
44	CT	80/80 (100%)	69 (86%)	11 (14%)	5	24

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	DT	80/80 (100%)	57 (71%)	23 (29%)	0	3
45	CU	83/83 (100%)	64 (77%)	19 (23%)	1	6
45	DU	83/83 (100%)	63 (76%)	20 (24%)	1	5
46	CV	78/78 (100%)	63 (81%)	15 (19%)	2	12
46	DV	78/78 (100%)	63 (81%)	15 (19%)	2	12
47	CW	56/58 (97%)	50 (89%)	6 (11%)	10	35
48	CX	67/67 (100%)	56 (84%)	11 (16%)	3	16
48	DX	67/67 (100%)	56 (84%)	11 (16%)	3	16
49	CY	55/55 (100%)	46 (84%)	9 (16%)	3	16
49	DY	55/55 (100%)	43 (78%)	12 (22%)	1	8
50	CZ	48/48 (100%)	40 (83%)	8 (17%)	3	16
50	DZ	48/48 (100%)	38 (79%)	10 (21%)	2	8
51	C0	47/47 (100%)	41 (87%)	6 (13%)	6	27
51	D0	47/47 (100%)	41 (87%)	6 (13%)	6	27
52	C1	45/45 (100%)	38 (84%)	7 (16%)	4	18
52	D1	45/45 (100%)	37 (82%)	8 (18%)	2	14
53	C2	38/38 (100%)	32 (84%)	6 (16%)	4	18
53	D2	38/38 (100%)	33 (87%)	5 (13%)	6	25
54	C3	51/51 (100%)	48 (94%)	3 (6%)	28	70
54	D3	51/51 (100%)	48 (94%)	3 (6%)	28	70
55	C4	34/34 (100%)	28 (82%)	6 (18%)	3	14
55	D4	34/34 (100%)	27 (79%)	7 (21%)	2	9
57	DW	55/57 (96%)	47 (86%)	8 (14%)	5	22
All	All	9482/9494 (100%)	7392 (78%)	2090 (22%)	1	7

5 of 2090 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	BN	25	GLU
30	CF	55	ASP
42	DR	48	LYS
15	BO	87	ARG
21	BU	4	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 211 such sidechains are listed below:

Mol	Chain	Res	Type
27	CC	116	GLN
34	CJ	58	ASN
45	DU	26	ASN
28	CD	67	HIS
30	CF	62	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	441 (28%)	28 (1%)
1	BA	1538/1539 (99%)	445 (28%)	20 (1%)
22	AV	75/76 (98%)	29 (38%)	1 (1%)
22	BV	75/76 (98%)	15 (20%)	1 (1%)
23	AX	14/16 (87%)	5 (35%)	0
23	BX	15/16 (93%)	4 (26%)	0
25	CA	2895/2903 (99%)	747 (25%)	53 (1%)
25	DA	2893/2903 (99%)	764 (26%)	48 (1%)
26	CB	118/119 (99%)	24 (20%)	1 (0%)
56	DB	117/118 (99%)	34 (29%)	3 (2%)
All	All	9277/9305 (99%)	2508 (27%)	155 (1%)

5 of 2508 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	5	U
1	AA	6	G
1	AA	7	A
1	AA	9	G
1	AA	12	U

5 of 155 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	CA	1046	A
25	CA	1800	C
25	DA	2311	A
25	CA	1133	A
25	CA	1301	A

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 500 ligands modelled in this entry, 500 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.70	8 (0%) 88 36	0, 31, 105, 170	0
1	BA	1539/1539 (100%)	-0.65	6 (0%) 90 41	0, 33, 101, 147	0
2	AB	218/218 (100%)	0.21	4 (1%) 65 14	12, 52, 84, 115	0
2	BB	218/218 (100%)	0.19	6 (2%) 50 10	19, 59, 88, 113	0
3	AC	206/206 (100%)	-0.23	0 100 100	0, 35, 69, 93	0
3	BC	206/206 (100%)	0.13	0 100 100	9, 46, 75, 92	0
4	AD	205/205 (100%)	0.02	1 (0%) 88 36	14, 42, 73, 98	0
4	BD	205/205 (100%)	-0.16	1 (0%) 88 36	0, 24, 64, 82	0
5	AE	150/150 (100%)	-0.08	1 (0%) 84 28	0, 32, 68, 105	0
5	BE	150/150 (100%)	-0.27	0 100 100	0, 31, 68, 98	0
6	AF	100/100 (100%)	-0.27	0 100 100	0, 33, 68, 86	0
6	BF	100/100 (100%)	-0.04	0 100 100	17, 54, 80, 93	0
7	AG	151/151 (100%)	0.28	9 (5%) 21 5	12, 56, 86, 111	0
7	BG	151/151 (100%)	-0.06	1 (0%) 84 28	20, 54, 81, 94	0
8	AH	129/129 (100%)	-0.32	0 100 100	0, 32, 60, 71	0
8	BH	129/129 (100%)	-0.17	0 100 100	4, 34, 58, 82	0
9	AI	127/127 (100%)	0.11	1 (0%) 83 26	6, 54, 79, 108	0
9	BI	127/127 (100%)	0.25	2 (1%) 68 16	20, 55, 85, 117	0
10	AJ	98/98 (100%)	0.21	1 (1%) 79 22	8, 55, 89, 104	0
10	BJ	98/98 (100%)	0.22	0 100 100	25, 58, 82, 113	0
11	AK	117/117 (100%)	-0.25	1 (0%) 81 24	0, 19, 50, 87	0
11	BK	117/117 (100%)	-0.17	0 100 100	0, 32, 66, 79	0
12	AL	123/123 (100%)	-0.20	1 (0%) 83 26	0, 22, 67, 93	0
12	BL	123/123 (100%)	-0.19	0 100 100	0, 17, 58, 93	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	-0.03	0 100 100	9, 53, 87, 100	0
13	BM	114/114 (100%)	0.48	1 (0%) 81 24	26, 63, 87, 97	0
14	AN	96/100 (96%)	-0.03	1 (1%) 79 22	12, 45, 84, 107	0
14	BN	96/100 (96%)	0.16	0 100 100	10, 56, 84, 98	0
15	AO	88/88 (100%)	-0.29	0 100 100	0, 28, 55, 93	0
15	BO	88/88 (100%)	-0.08	0 100 100	1, 33, 66, 89	0
16	AP	82/82 (100%)	0.09	2 (2%) 56 11	5, 30, 73, 86	0
16	BP	82/82 (100%)	-0.06	3 (3%) 39 8	0, 24, 67, 91	0
17	AQ	80/80 (100%)	-0.04	1 (1%) 74 19	8, 42, 75, 96	0
17	BQ	80/80 (100%)	-0.09	0 100 100	7, 44, 79, 94	0
18	AR	55/55 (100%)	-0.25	0 100 100	0, 25, 59, 93	0
18	BR	55/55 (100%)	-0.02	2 (3%) 41 8	5, 38, 80, 101	0
19	AS	79/79 (100%)	0.23	1 (1%) 74 19	21, 52, 83, 98	0
19	BS	79/79 (100%)	0.46	3 (3%) 38 7	37, 65, 83, 95	0
20	AT	85/85 (100%)	0.19	1 (1%) 75 20	7, 37, 67, 80	0
20	BT	85/85 (100%)	0.15	1 (1%) 75 20	8, 38, 69, 96	0
21	AU	51/51 (100%)	0.19	2 (3%) 37 7	7, 39, 74, 77	0
21	BU	51/51 (100%)	0.24	1 (1%) 62 12	8, 47, 74, 80	0
22	AV	76/76 (100%)	-0.40	2 (2%) 53 10	0, 70, 127, 154	0
22	BV	76/76 (100%)	-0.43	0 100 100	22, 43, 72, 119	0
23	AX	15/16 (93%)	0.37	1 (6%) 17 4	6, 76, 115, 133	0
23	BX	16/16 (100%)	0.22	1 (6%) 19 5	16, 77, 102, 124	0
24	AY	183/183 (100%)	0.27	10 (5%) 24 5	0, 50, 96, 117	0
25	CA	2897/2903 (99%)	-0.59	28 (0%) 79 22	0, 0, 103, 162	0
25	DA	2896/2903 (99%)	-0.66	23 (0%) 83 26	0, 15, 109, 162	0
26	CB	119/119 (100%)	-0.88	0 100 100	0, 7, 32, 85	0
27	CC	271/271 (100%)	-0.42	0 100 100	0, 1, 29, 56	0
27	DC	271/271 (100%)	-0.33	0 100 100	0, 19, 47, 77	0
28	CD	209/209 (100%)	-0.42	0 100 100	0, 0, 19, 61	0
28	DD	209/209 (100%)	-0.37	0 100 100	0, 10, 52, 66	0
29	CE	201/201 (100%)	-0.39	0 100 100	0, 0, 39, 84	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	DE	201/201 (100%)	-0.30	0 100 100	0, 21, 60, 89	0
30	CF	177/177 (100%)	0.03	1 (0%) 86 32	0, 35, 82, 91	0
30	DF	177/177 (100%)	0.20	1 (0%) 86 32	12, 58, 84, 95	0
31	CG	176/176 (100%)	-0.25	0 100 100	0, 15, 48, 88	0
31	DG	176/176 (100%)	0.08	0 100 100	15, 48, 73, 93	0
32	CH	149/149 (100%)	0.03	1 (0%) 84 28	0, 52, 87, 100	0
32	DH	149/149 (100%)	0.33	3 (2%) 62 12	8, 58, 92, 107	0
33	CI	141/141 (100%)	1.43	31 (21%) 1 1	44, 79, 102, 124	0
33	DI	141/141 (100%)	1.37	29 (20%) 1 1	54, 82, 104, 118	0
34	CJ	142/142 (100%)	-0.41	0 100 100	0, 0, 21, 56	0
34	DJ	142/142 (100%)	-0.31	0 100 100	0, 8, 37, 65	0
35	CK	122/122 (100%)	-0.42	0 100 100	0, 0, 27, 73	0
35	DK	122/122 (100%)	-0.28	0 100 100	0, 15, 50, 71	0
36	CL	143/143 (100%)	-0.36	0 100 100	0, 0, 27, 68	0
36	DL	143/143 (100%)	-0.17	0 100 100	0, 18, 56, 82	0
37	CM	136/136 (100%)	-0.41	0 100 100	0, 0, 21, 83	0
37	DM	136/136 (100%)	-0.12	0 100 100	0, 21, 55, 88	0
38	CN	120/120 (100%)	-0.36	0 100 100	0, 0, 14, 68	0
38	DN	120/120 (100%)	-0.33	0 100 100	0, 12, 44, 78	0
39	CO	116/116 (100%)	-0.39	0 100 100	0, 11, 39, 49	0
39	DO	116/116 (100%)	0.13	1 (0%) 81 24	5, 49, 78, 98	0
40	CP	114/114 (100%)	-0.41	0 100 100	0, 0, 47, 70	0
40	DP	114/114 (100%)	-0.30	0 100 100	0, 21, 51, 81	0
41	CQ	117/117 (100%)	-0.41	0 100 100	0, 0, 7, 63	0
41	DQ	117/117 (100%)	-0.46	0 100 100	0, 2, 27, 45	0
42	CR	103/103 (100%)	-0.39	0 100 100	0, 0, 35, 57	0
42	DR	103/103 (100%)	-0.40	1 (0%) 79 22	0, 10, 46, 78	0
43	CS	110/110 (100%)	-0.31	1 (0%) 81 24	0, 0, 22, 98	0
43	DS	110/110 (100%)	-0.39	0 100 100	0, 8, 40, 77	0
44	CT	93/93 (100%)	-0.18	0 100 100	0, 6, 68, 78	0
44	DT	93/93 (100%)	0.13	0 100 100	0, 35, 71, 96	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
45	CU	102/102 (100%)	-0.35	1 (0%) 79 22	0, 5, 42, 79	0
45	DU	102/102 (100%)	0.24	9 (8%) 10 3	0, 34, 74, 100	0
46	CV	94/94 (100%)	-0.36	0 100 100	0, 6, 42, 62	0
46	DV	94/94 (100%)	-0.12	0 100 100	11, 43, 68, 82	0
47	CW	76/76 (100%)	-0.33	0 100 100	0, 1, 31, 69	0
48	CX	77/77 (100%)	-0.27	0 100 100	0, 1, 47, 74	0
48	DX	77/77 (100%)	-0.21	0 100 100	0, 23, 55, 67	0
49	CY	63/63 (100%)	-0.20	2 (3%) 45 9	0, 14, 56, 97	0
49	DY	63/63 (100%)	-0.14	0 100 100	8, 43, 70, 111	0
50	CZ	58/58 (100%)	-0.36	0 100 100	0, 0, 13, 50	0
50	DZ	58/58 (100%)	-0.30	0 100 100	0, 20, 52, 72	0
51	C0	56/56 (100%)	-0.39	0 100 100	0, 0, 25, 69	0
51	D0	56/56 (100%)	-0.38	0 100 100	0, 10, 53, 94	0
52	C1	50/50 (100%)	-0.08	1 (2%) 62 12	0, 8, 51, 93	0
52	D1	50/50 (100%)	0.22	1 (2%) 62 12	21, 38, 70, 88	0
53	C2	46/46 (100%)	-0.33	1 (2%) 59 12	0, 0, 15, 101	0
53	D2	46/46 (100%)	-0.41	0 100 100	0, 10, 26, 94	0
54	C3	64/64 (100%)	-0.43	0 100 100	0, 0, 11, 38	0
54	D3	64/64 (100%)	-0.26	0 100 100	0, 15, 35, 52	0
55	C4	38/38 (100%)	-0.29	0 100 100	0, 1, 32, 72	0
55	D4	38/38 (100%)	-0.07	0 100 100	3, 26, 59, 65	0
56	DB	118/118 (100%)	-0.75	0 100 100	6, 58, 86, 106	0
57	DW	75/75 (100%)	-0.08	0 100 100	0, 27, 54, 94	0
All	All	20908/20931 (99%)	-0.34	211 (1%) 79 22	0, 23, 86, 170	0

The worst 5 of 211 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
33	CI	52	LEU	8.4
33	DI	2	LYS	7.6
25	CA	2145	C	6.9
33	CI	2	LYS	6.7
33	CI	48	ILE	5.9

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
58	MG	DA	3098	1/1	0.55	849.00	49,49,49,49	0
58	MG	DA	3137	1/1	0.46	43.61	0,0,0,0	0
58	MG	DA	3131	1/1	0.64	39.35	55,55,55,55	0
58	MG	CA	3149	1/1	0.32	35.02	0,0,0,0	0
58	MG	CB	204	1/1	0.40	31.48	0,0,0,0	0
58	MG	CA	3158	1/1	0.34	31.46	0,0,0,0	0
58	MG	CA	3142	1/1	0.39	29.04	0,0,0,0	0
58	MG	DA	3141	1/1	0.23	25.10	0,0,0,0	0
58	MG	CA	3141	1/1	0.27	23.72	0,0,0,0	0
58	MG	CA	3132	1/1	0.40	21.59	24,24,24,24	0
58	MG	CA	3167	1/1	0.33	19.44	0,0,0,0	0
58	MG	AA	1647	1/1	0.23	19.15	1,1,1,1	0
58	MG	CA	3182	1/1	0.28	18.29	0,0,0,0	0
58	MG	CA	3174	1/1	0.32	18.05	0,0,0,0	0
58	MG	CA	3173	1/1	0.25	17.93	0,0,0,0	0
58	MG	CA	3143	1/1	0.29	16.88	0,0,0,0	0
58	MG	AA	1643	1/1	0.27	16.87	0,0,0,0	0
58	MG	AA	1672	1/1	0.24	15.89	3,3,3,3	0
58	MG	DA	3092	1/1	0.23	15.80	34,34,34,34	0
58	MG	CA	3169	1/1	0.24	15.50	7,7,7,7	0
58	MG	DA	3139	1/1	0.26	15.24	0,0,0,0	0
58	MG	DA	3140	1/1	0.27	14.18	0,0,0,0	0
58	MG	AA	1661	1/1	0.19	13.92	15,15,15,15	0
58	MG	CA	3151	1/1	0.32	13.72	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3147	1/1	0.28	13.20	0,0,0,0	0
58	MG	AA	1666	1/1	0.17	12.96	13,13,13,13	0
58	MG	CA	3154	1/1	0.28	12.92	0,0,0,0	0
58	MG	CA	3190	1/1	0.21	12.56	0,0,0,0	0
58	MG	AA	1651	1/1	0.23	12.15	0,0,0,0	0
58	MG	AA	1645	1/1	0.22	11.60	8,8,8,8	0
58	MG	BA	1618	1/1	0.21	11.40	4,4,4,4	0
58	MG	CA	3157	1/1	0.18	11.24	0,0,0,0	0
58	MG	AA	1640	1/1	0.18	11.24	34,34,34,34	0
58	MG	AA	1670	1/1	0.28	11.16	11,11,11,11	0
58	MG	DA	3166	1/1	0.22	11.10	9,9,9,9	0
58	MG	DA	3015	1/1	0.23	11.03	23,23,23,23	0
58	MG	CA	3194	1/1	0.18	11.03	0,0,0,0	0
58	MG	AA	1649	1/1	0.24	10.84	0,0,0,0	0
58	MG	AA	1631	1/1	0.16	10.69	35,35,35,35	0
58	MG	DA	3159	1/1	0.25	10.58	3,3,3,3	0
58	MG	CA	3183	1/1	0.19	10.29	0,0,0,0	0
58	MG	DA	3148	1/1	0.27	10.23	0,0,0,0	0
58	MG	CA	3144	1/1	0.32	10.01	0,0,0,0	0
58	MG	DA	3085	1/1	0.21	9.84	0,0,0,0	0
58	MG	BA	1650	1/1	0.22	9.82	5,5,5,5	0
58	MG	DA	3154	1/1	0.18	9.62	0,0,0,0	0
58	MG	CA	3186	1/1	0.27	9.52	0,0,0,0	0
58	MG	DA	3133	1/1	0.19	9.10	16,16,16,16	0
58	MG	CA	3159	1/1	0.24	9.06	0,0,0,0	0
58	MG	DA	3146	1/1	0.18	8.93	0,0,0,0	0
58	MG	DA	3119	1/1	0.15	8.85	44,44,44,44	0
58	MG	DA	3156	1/1	0.25	8.49	3,3,3,3	0
58	MG	CA	3185	1/1	0.29	8.25	0,0,0,0	0
58	MG	CA	3191	1/1	0.20	8.22	0,0,0,0	0
58	MG	BA	1642	1/1	0.24	8.02	6,6,6,6	0
58	MG	AA	1658	1/1	0.16	7.85	16,16,16,16	0
58	MG	CA	3164	1/1	0.26	7.67	0,0,0,0	0
58	MG	CA	3188	1/1	0.17	7.41	2,2,2,2	0
58	MG	AA	1619	1/1	0.17	7.26	32,32,32,32	0
58	MG	DA	3083	1/1	0.19	7.25	31,31,31,31	0
58	MG	AA	1604	1/1	0.16	7.24	22,22,22,22	0
58	MG	DA	3149	1/1	0.20	7.05	0,0,0,0	0
58	MG	DA	3091	1/1	0.21	7.00	50,50,50,50	0
58	MG	DA	3061	1/1	0.21	6.90	24,24,24,24	0
58	MG	CA	3018	1/1	0.18	6.86	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3031	1/1	0.22	6.60	0,0,0,0	0
58	MG	CA	3184	1/1	0.20	6.56	0,0,0,0	0
58	MG	DA	3025	1/1	0.20	6.52	16,16,16,16	0
58	MG	AA	1646	1/1	0.19	6.12	0,0,0,0	0
58	MG	AA	1657	1/1	0.18	5.88	2,2,2,2	0
58	MG	DA	3157	1/1	0.21	5.84	0,0,0,0	0
58	MG	DA	3143	1/1	0.22	5.73	0,0,0,0	0
58	MG	CA	3095	1/1	0.17	5.40	17,17,17,17	0
58	MG	AA	1608	1/1	0.20	5.28	0,0,0,0	0
58	MG	DA	3152	1/1	0.18	5.23	6,6,6,6	0
58	MG	CA	3116	1/1	0.25	5.02	10,10,10,10	0
58	MG	BA	1615	1/1	0.19	4.92	9,9,9,9	0
58	MG	BA	1656	1/1	0.20	4.75	9,9,9,9	0
58	MG	DA	3147	1/1	0.18	4.55	0,0,0,0	0
58	MG	AA	1644	1/1	0.18	4.54	5,5,5,5	0
58	MG	CA	3066	1/1	0.21	4.43	0,0,0,0	0
58	MG	DA	3037	1/1	0.17	4.39	0,0,0,0	0
58	MG	CA	3153	1/1	0.29	4.34	0,0,0,0	0
58	MG	BA	1637	1/1	0.15	4.17	19,19,19,19	0
58	MG	AA	1667	1/1	0.23	4.03	13,13,13,13	0
58	MG	DA	3165	1/1	0.22	3.81	0,0,0,0	0
58	MG	AA	1653	1/1	0.16	3.79	1,1,1,1	0
58	MG	DA	3007	1/1	0.20	3.40	26,26,26,26	0
58	MG	CA	3155	1/1	0.35	3.19	0,0,0,0	0
58	MG	CA	3165	1/1	0.18	3.19	0,0,0,0	0
58	MG	DA	3142	1/1	0.16	3.14	0,0,0,0	0
58	MG	CA	3163	1/1	0.20	3.10	0,0,0,0	0
58	MG	DA	3150	1/1	0.15	3.08	0,0,0,0	0
58	MG	CA	3166	1/1	0.14	2.88	0,0,0,0	0
58	MG	DA	3115	1/1	0.18	2.88	27,27,27,27	0
58	MG	AA	1622	1/1	0.17	2.83	0,0,0,0	0
58	MG	BA	1608	1/1	0.14	2.81	18,18,18,18	0
58	MG	DA	3116	1/1	0.15	2.78	13,13,13,13	0
58	MG	BA	1649	1/1	0.17	2.62	11,11,11,11	0
58	MG	AA	1655	1/1	0.18	2.37	0,0,0,0	0
58	MG	BA	1648	1/1	0.16	2.02	0,0,0,0	0
58	MG	CA	3110	1/1	0.17	2.00	0,0,0,0	0
58	MG	DA	3106	1/1	0.17	1.98	0,0,0,0	0
58	MG	CA	3177	1/1	0.13	1.89	0,0,0,0	0
58	MG	CA	3134	1/1	0.31	1.77	14,14,14,14	0
58	MG	BA	1640	1/1	0.15	1.71	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3155	1/1	0.16	1.67	1,1,1,1	0
58	MG	DA	3158	1/1	0.15	1.49	0,0,0,0	0
58	MG	AA	1656	1/1	0.14	1.48	14,14,14,14	0
58	MG	DA	3084	1/1	0.13	1.41	32,32,32,32	0
58	MG	DA	3086	1/1	0.15	1.36	0,0,0,0	0
58	MG	DQ	801	1/1	0.24	1.34	0,0,0,0	0
58	MG	CA	3152	1/1	0.19	1.23	0,0,0,0	0
58	MG	AA	1671	1/1	0.14	1.12	6,6,6,6	0
58	MG	DA	3145	1/1	0.12	1.00	0,0,0,0	0
58	MG	AA	1652	1/1	0.11	0.97	13,13,13,13	0
58	MG	AA	1654	1/1	0.18	0.96	5,5,5,5	0
58	MG	DA	3108	1/1	0.15	0.96	0,0,0,0	0
58	MG	BA	1643	1/1	0.15	0.92	3,3,3,3	0
58	MG	DA	3055	1/1	0.14	0.80	28,28,28,28	0
58	MG	CA	3084	1/1	0.11	0.72	22,22,22,22	0
58	MG	DA	3063	1/1	0.15	0.67	0,0,0,0	0
58	MG	DA	3122	1/1	0.14	0.65	0,0,0,0	0
58	MG	AA	1669	1/1	0.12	0.62	10,10,10,10	0
58	MG	DA	3126	1/1	0.14	0.61	0,0,0,0	0
58	MG	BA	1613	1/1	0.13	0.57	0,0,0,0	0
58	MG	BA	1609	1/1	0.11	0.56	26,26,26,26	0
58	MG	CA	3176	1/1	0.12	0.55	10,10,10,10	0
58	MG	DA	3151	1/1	0.17	0.51	11,11,11,11	0
58	MG	CA	3187	1/1	0.16	0.35	0,0,0,0	0
58	MG	DA	3057	1/1	0.15	0.33	14,14,14,14	0
58	MG	DA	3060	1/1	0.13	0.24	5,5,5,5	0
58	MG	BA	1627	1/1	0.14	0.24	35,35,35,35	0
58	MG	BA	1646	1/1	0.14	0.16	10,10,10,10	0
58	MG	AA	1627	1/1	0.14	0.09	19,19,19,19	0
58	MG	CA	3107	1/1	0.17	0.06	0,0,0,0	0
58	MG	DA	3013	1/1	0.14	0.04	0,0,0,0	0
58	MG	CA	3041	1/1	0.17	-0.02	0,0,0,0	0
58	MG	CA	3093	1/1	0.11	-0.11	11,11,11,11	0
58	MG	CA	3050	1/1	0.15	-0.12	0,0,0,0	0
58	MG	DA	3109	1/1	0.12	-0.12	2,2,2,2	0
58	MG	BA	1651	1/1	0.13	-0.20	7,7,7,7	0
58	MG	DA	3164	1/1	0.15	-0.23	0,0,0,0	0
58	MG	CA	3150	1/1	0.11	-0.29	0,0,0,0	0
58	MG	DA	3040	1/1	0.12	-0.36	5,5,5,5	0
58	MG	DA	3074	1/1	0.13	-0.42	0,0,0,0	0
58	MG	DA	3153	1/1	0.12	-0.43	11,11,11,11	0
58	MG	CA	3070	1/1	0.11	-0.52	25,25,25,25	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3120	1/1	0.13	-0.54	2,2,2,2	0
58	MG	DA	3136	1/1	0.12	-0.57	28,28,28,28	0
58	MG	AA	1662	1/1	0.11	-0.59	8,8,8,8	0
58	MG	BA	1631	1/1	0.15	-0.60	35,35,35,35	0
58	MG	CA	3145	1/1	0.13	-0.62	0,0,0,0	0
58	MG	AA	1601	1/1	0.09	-0.64	44,44,44,44	0
58	MG	DA	3030	1/1	0.12	-0.70	0,0,0,0	0
58	MG	AA	1636	1/1	0.08	-0.72	0,0,0,0	0
58	MG	DA	3017	1/1	0.13	-0.74	0,0,0,0	0
58	MG	DA	3088	1/1	0.10	-0.74	12,12,12,12	0
58	MG	DA	3019	1/1	0.11	-0.79	0,0,0,0	0
58	MG	AA	1607	1/1	0.08	-0.82	10,10,10,10	0
58	MG	BA	1641	1/1	0.10	-0.84	20,20,20,20	0
58	MG	BA	1644	1/1	0.09	-0.85	0,0,0,0	0
58	MG	CA	3074	1/1	0.16	-0.90	0,0,0,0	0
58	MG	AA	1632	1/1	0.08	-0.94	15,15,15,15	0
58	MG	DA	3005	1/1	0.10	-0.95	25,25,25,25	0
58	MG	DA	3027	1/1	0.11	-0.95	14,14,14,14	0
58	MG	AA	1648	1/1	0.12	-1.03	4,4,4,4	0
58	MG	DA	3073	1/1	0.12	-1.05	6,6,6,6	0
58	MG	DA	3120	1/1	0.11	-1.05	8,8,8,8	0
58	MG	BA	1611	1/1	0.11	-1.11	13,13,13,13	0
58	MG	DA	3163	1/1	0.09	-1.14	0,0,0,0	0
58	MG	BA	1614	1/1	0.07	-1.17	19,19,19,19	0
58	MG	DA	3059	1/1	0.11	-1.24	6,6,6,6	0
58	MG	DA	3105	1/1	0.12	-1.25	0,0,0,0	0
58	MG	CA	3045	1/1	0.11	-1.25	0,0,0,0	0
58	MG	DA	3077	1/1	0.05	-1.26	12,12,12,12	0
58	MG	AA	1626	1/1	0.10	-1.26	0,0,0,0	0
58	MG	CA	3117	1/1	0.14	-1.26	5,5,5,5	0
58	MG	DA	3101	1/1	0.11	-1.29	0,0,0,0	0
58	MG	BA	1616	1/1	0.10	-1.31	0,0,0,0	0
58	MG	BA	1653	1/1	0.08	-1.35	7,7,7,7	0
58	MG	AA	1616	1/1	0.09	-1.35	11,11,11,11	0
58	MG	DA	3121	1/1	0.07	-1.37	7,7,7,7	0
58	MG	BA	1638	1/1	0.10	-1.37	27,27,27,27	0
58	MG	DA	3008	1/1	0.10	-1.46	0,0,0,0	0
58	MG	DA	3128	1/1	0.10	-1.47	0,0,0,0	0
58	MG	DA	3111	1/1	0.09	-1.49	1,1,1,1	0
58	MG	DA	3036	1/1	0.08	-1.49	21,21,21,21	0
58	MG	DA	3011	1/1	0.08	-1.51	0,0,0,0	0
58	MG	AA	1664	1/1	0.11	-1.51	4,4,4,4	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3038	1/1	0.11	-1.53	0,0,0,0	0
58	MG	DA	3100	1/1	0.06	-1.55	4,4,4,4	0
58	MG	DA	3004	1/1	0.10	-1.56	30,30,30,30	0
58	MG	AA	1623	1/1	0.07	-1.58	24,24,24,24	0
58	MG	AA	1635	1/1	0.08	-1.60	18,18,18,18	0
58	MG	BA	1623	1/1	0.08	-1.61	3,3,3,3	0
58	MG	DA	3075	1/1	0.11	-1.63	8,8,8,8	0
58	MG	CB	202	1/1	0.10	-1.65	0,0,0,0	0
58	MG	DA	3097	1/1	0.06	-1.69	13,13,13,13	0
59	ZN	C4	101	1/1	0.07	-1.71	0,0,0,0	0
58	MG	DA	3054	1/1	0.09	-1.72	0,0,0,0	0
58	MG	BA	1652	1/1	0.09	-1.75	1,1,1,1	0
58	MG	CA	3122	1/1	0.11	-1.77	0,0,0,0	0
58	MG	CA	3048	1/1	0.08	-1.78	13,13,13,13	0
58	MG	AA	1602	1/1	0.10	-1.82	17,17,17,17	0
58	MG	BA	1606	1/1	0.10	-1.83	24,24,24,24	0
58	MG	DA	3078	1/1	0.08	-1.85	15,15,15,15	0
58	MG	DA	3064	1/1	0.09	-1.93	0,0,0,0	0
58	MG	DA	3095	1/1	0.11	-1.93	10,10,10,10	0
58	MG	DA	3062	1/1	0.09	-1.93	0,0,0,0	0
58	MG	AA	1617	1/1	0.05	-2.02	21,21,21,21	0
58	MG	DA	3069	1/1	0.08	-2.04	41,41,41,41	0
58	MG	CA	3075	1/1	0.07	-2.06	0,0,0,0	0
58	MG	AA	1650	1/1	0.11	-2.11	0,0,0,0	0
58	MG	DA	3010	1/1	0.07	-2.16	7,7,7,7	0
58	MG	DA	3003	1/1	0.08	-2.17	8,8,8,8	0
58	MG	AA	1668	1/1	0.08	-2.18	0,0,0,0	0
58	MG	CA	3098	1/1	0.14	-2.19	0,0,0,0	0
58	MG	BA	1601	1/1	0.08	-2.20	2,2,2,2	0
59	ZN	D4	101	1/1	0.05	-2.23	41,41,41,41	0
58	MG	DA	3130	1/1	0.10	-2.24	0,0,0,0	0
58	MG	CA	3092	1/1	0.08	-2.24	16,16,16,16	0
58	MG	BA	1628	1/1	0.10	-2.24	25,25,25,25	0
58	MG	CA	3137	1/1	0.09	-2.29	4,4,4,4	0
58	MG	CA	3058	1/1	0.10	-2.34	10,10,10,10	0
58	MG	BA	1630	1/1	0.07	-2.35	41,41,41,41	0
58	MG	AA	1663	1/1	0.09	-2.36	6,6,6,6	0
58	MG	BA	1603	1/1	0.08	-2.36	13,13,13,13	0
58	MG	CA	3101	1/1	0.11	-2.36	0,0,0,0	0
58	MG	DA	3093	1/1	0.08	-2.38	2,2,2,2	0
58	MG	DA	3112	1/1	0.09	-2.41	5,5,5,5	0
58	MG	CA	3078	1/1	0.08	-2.43	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3113	1/1	0.11	-2.43	0,0,0,0	0
58	MG	CA	3133	1/1	0.05	-2.45	0,0,0,0	0
58	MG	DA	3018	1/1	0.07	-2.46	6,6,6,6	0
58	MG	CA	3033	1/1	0.13	-2.50	0,0,0,0	0
58	MG	DA	3107	1/1	0.08	-2.53	9,9,9,9	0
58	MG	DA	3070	1/1	0.08	-2.56	0,0,0,0	0
58	MG	AA	1660	1/1	0.13	-2.57	15,15,15,15	0
58	MG	DA	3026	1/1	0.09	-2.59	0,0,0,0	0
58	MG	CA	3073	1/1	0.13	-2.63	0,0,0,0	0
58	MG	DA	3028	1/1	0.12	-2.68	0,0,0,0	0
58	MG	DA	3118	1/1	0.09	-2.70	7,7,7,7	0
58	MG	CA	3024	1/1	0.11	-2.70	0,0,0,0	0
58	MG	DA	3132	1/1	0.05	-2.72	6,6,6,6	0
58	MG	AA	1606	1/1	0.06	-2.75	6,6,6,6	0
58	MG	DA	3161	1/1	0.09	-2.77	15,15,15,15	0
58	MG	DL	201	1/1	0.05	-2.79	10,10,10,10	0
58	MG	BA	1605	1/1	0.07	-2.82	21,21,21,21	0
58	MG	BA	1654	1/1	0.09	-2.84	22,22,22,22	0
58	MG	CA	3022	1/1	0.14	-2.87	0,0,0,0	0
58	MG	CA	3114	1/1	0.10	-2.91	0,0,0,0	0
58	MG	CA	3059	1/1	0.07	-2.92	4,4,4,4	0
58	MG	CA	3129	1/1	0.10	-2.93	0,0,0,0	0
58	MG	DA	3134	1/1	0.07	-2.96	0,0,0,0	0
58	MG	DA	3103	1/1	0.08	-2.96	0,0,0,0	0
58	MG	DA	3035	1/1	0.09	-3.05	0,0,0,0	0
58	MG	AA	1603	1/1	0.08	-3.09	28,28,28,28	0
58	MG	CA	3113	1/1	0.11	-3.10	0,0,0,0	0
58	MG	AA	1620	1/1	0.07	-3.15	10,10,10,10	0
58	MG	CA	3052	1/1	0.11	-3.21	0,0,0,0	0
58	MG	BA	1636	1/1	0.09	-3.23	42,42,42,42	0
58	MG	CA	3051	1/1	0.08	-3.23	3,3,3,3	0
58	MG	DA	3071	1/1	0.07	-3.30	0,0,0,0	0
58	MG	AA	1629	1/1	0.07	-3.31	0,0,0,0	0
58	MG	DA	3047	1/1	0.06	-3.39	28,28,28,28	0
58	MG	CA	3056	1/1	0.09	-3.43	10,10,10,10	0
58	MG	AA	1642	1/1	0.06	-3.43	1,1,1,1	0
58	MG	BA	1602	1/1	0.07	-3.46	21,21,21,21	0
58	MG	DA	3033	1/1	0.10	-3.47	0,0,0,0	0
58	MG	DA	3068	1/1	0.06	-3.47	6,6,6,6	0
58	MG	DA	3006	1/1	0.06	-3.48	10,10,10,10	0
58	MG	BA	1604	1/1	0.07	-3.51	13,13,13,13	0
58	MG	AA	1615	1/1	0.09	-3.57	9,9,9,9	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	DA	3001	1/1	0.05	-3.58	0,0,0,0	0
58	MG	DA	3129	1/1	0.08	-3.60	0,0,0,0	0
58	MG	CA	3019	1/1	0.09	-3.63	0,0,0,0	0
58	MG	DA	3123	1/1	0.06	-3.68	6,6,6,6	0
58	MG	DB	203	1/1	0.06	-3.72	16,16,16,16	0
58	MG	AA	1637	1/1	0.09	-3.76	1,1,1,1	0
58	MG	DA	3067	1/1	0.07	-3.79	0,0,0,0	0
58	MG	DA	3053	1/1	0.06	-3.79	0,0,0,0	0
58	MG	DA	3021	1/1	0.08	-3.83	3,3,3,3	0
58	MG	CA	3170	1/1	0.07	-3.87	0,0,0,0	0
58	MG	DA	3046	1/1	0.07	-3.92	1,1,1,1	0
58	MG	BA	1620	1/1	0.06	-3.93	19,19,19,19	0
58	MG	CA	3112	1/1	0.09	-3.94	4,4,4,4	0
58	MG	CA	3047	1/1	0.10	-3.96	0,0,0,0	0
58	MG	BA	1619	1/1	0.07	-3.97	0,0,0,0	0
58	MG	CA	3088	1/1	0.10	-3.98	0,0,0,0	0
58	MG	DA	3114	1/1	0.08	-3.99	14,14,14,14	0
58	MG	DA	3023	1/1	0.06	-4.01	0,0,0,0	0
58	MG	DA	3016	1/1	0.08	-4.03	1,1,1,1	0
58	MG	CA	3008	1/1	0.09	-4.05	0,0,0,0	0
58	MG	DA	3032	1/1	0.08	-4.06	0,0,0,0	0
58	MG	DA	3024	1/1	0.07	-4.08	0,0,0,0	0
58	MG	DA	3090	1/1	0.08	-4.11	15,15,15,15	0
58	MG	DB	202	1/1	0.04	-4.11	9,9,9,9	0
58	MG	AA	1613	1/1	0.06	-4.12	2,2,2,2	0
58	MG	DB	201	1/1	0.05	-4.17	24,24,24,24	0
58	MG	CA	3091	1/1	0.07	-4.17	3,3,3,3	0
58	MG	DA	3094	1/1	0.08	-4.17	43,43,43,43	0
58	MG	DA	3072	1/1	0.07	-4.21	0,0,0,0	0
58	MG	AA	1618	1/1	0.06	-4.22	21,21,21,21	0
58	MG	DA	3079	1/1	0.07	-4.27	27,27,27,27	0
58	MG	DA	3039	1/1	0.08	-4.29	3,3,3,3	0
58	MG	CA	3097	1/1	0.11	-4.32	0,0,0,0	0
58	MG	DA	3089	1/1	0.08	-4.34	24,24,24,24	0
58	MG	DA	3042	1/1	0.06	-4.36	5,5,5,5	0
58	MG	BA	1647	1/1	0.07	-4.40	0,0,0,0	0
58	MG	AA	1641	1/1	0.09	-4.40	0,0,0,0	0
58	MG	AA	1638	1/1	0.06	-4.41	12,12,12,12	0
58	MG	DA	3034	1/1	0.07	-4.45	11,11,11,11	0
58	MG	DA	3045	1/1	0.09	-4.45	0,0,0,0	0
58	MG	AA	1633	1/1	0.04	-4.47	3,3,3,3	0
58	MG	BA	1617	1/1	0.06	-4.49	13,13,13,13	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CB	201	1/1	0.05	-4.57	0,0,0,0	0
58	MG	DA	3044	1/1	0.05	-4.57	11,11,11,11	0
58	MG	BA	1624	1/1	0.07	-4.57	1,1,1,1	0
58	MG	DA	3124	1/1	0.05	-4.58	0,0,0,0	0
58	MG	AA	1630	1/1	0.07	-4.58	16,16,16,16	0
58	MG	BA	1635	1/1	0.08	-4.58	21,21,21,21	0
58	MG	DA	3099	1/1	0.07	-4.60	0,0,0,0	0
58	MG	BA	1645	1/1	0.08	-4.60	8,8,8,8	0
58	MG	CA	3125	1/1	0.08	-4.63	0,0,0,0	0
58	MG	AA	1614	1/1	0.07	-4.69	12,12,12,12	0
58	MG	AA	1612	1/1	0.05	-4.70	0,0,0,0	0
58	MG	DA	3048	1/1	0.06	-4.76	0,0,0,0	0
58	MG	AA	1611	1/1	0.09	-4.79	0,0,0,0	0
58	MG	DA	3009	1/1	0.09	-4.95	4,4,4,4	0
58	MG	CA	3044	1/1	0.06	-5.02	0,0,0,0	0
58	MG	DA	3104	1/1	0.09	-5.06	0,0,0,0	0
58	MG	BA	1607	1/1	0.05	-5.11	1,1,1,1	0
58	MG	BA	1632	1/1	0.04	-5.12	18,18,18,18	0
58	MG	DA	3125	1/1	0.07	-5.13	0,0,0,0	0
58	MG	BA	1626	1/1	0.05	-5.16	14,14,14,14	0
58	MG	DA	3058	1/1	0.07	-5.17	6,6,6,6	0
58	MG	CA	3006	1/1	0.07	-5.20	1,1,1,1	0
58	MG	CA	3065	1/1	0.09	-5.26	0,0,0,0	0
58	MG	CA	3094	1/1	0.06	-5.28	3,3,3,3	0
58	MG	CA	3080	1/1	0.06	-5.28	1,1,1,1	0
58	MG	AA	1634	1/1	0.05	-5.33	2,2,2,2	0
58	MG	DA	3065	1/1	0.08	-5.38	0,0,0,0	0
58	MG	DA	3096	1/1	0.06	-5.45	13,13,13,13	0
58	MG	AA	1639	1/1	0.08	-5.45	22,22,22,22	0
58	MG	DA	3110	1/1	0.05	-5.49	18,18,18,18	0
58	MG	DA	3087	1/1	0.05	-5.65	20,20,20,20	0
58	MG	DA	3020	1/1	0.05	-5.74	0,0,0,0	0
58	MG	CA	3079	1/1	0.05	-5.81	3,3,3,3	0
58	MG	AA	1624	1/1	0.05	-5.82	10,10,10,10	0
58	MG	DA	3076	1/1	0.09	-5.86	5,5,5,5	0
58	MG	CB	203	1/1	0.04	-5.86	5,5,5,5	0
58	MG	AA	1605	1/1	0.07	-5.88	0,0,0,0	0
58	MG	CA	3100	1/1	0.08	-5.93	0,0,0,0	0
58	MG	BA	1625	1/1	0.06	-5.97	0,0,0,0	0
58	MG	BA	1639	1/1	0.07	-6.01	0,0,0,0	0
58	MG	AA	1659	1/1	0.08	-6.05	12,12,12,12	0
58	MG	CA	3090	1/1	0.08	-6.15	1,1,1,1	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	AA	1665	1/1	0.07	-6.17	0,0,0,0	0
58	MG	CA	3049	1/1	0.07	-6.25	0,0,0,0	0
58	MG	DA	3050	1/1	0.06	-6.37	0,0,0,0	0
58	MG	DA	3051	1/1	0.06	-6.42	0,0,0,0	0
58	MG	BA	1622	1/1	0.04	-6.47	4,4,4,4	0
58	MG	AA	1625	1/1	0.07	-6.49	6,6,6,6	0
58	MG	DA	3031	1/1	0.10	-6.67	0,0,0,0	0
58	MG	CA	3057	1/1	0.04	-6.79	0,0,0,0	0
58	MG	BA	1612	1/1	0.05	-7.11	18,18,18,18	0
58	MG	DA	3135	1/1	0.07	-7.34	11,11,11,11	0
58	MG	BA	1634	1/1	0.04	-7.37	10,10,10,10	0
58	MG	AA	1628	1/1	0.04	-7.41	1,1,1,1	0
58	MG	DA	3043	1/1	0.06	-7.46	6,6,6,6	0
58	MG	AA	1609	1/1	0.05	-7.54	0,0,0,0	0
58	MG	DA	3002	1/1	0.05	-7.63	1,1,1,1	0
58	MG	DA	3049	1/1	0.05	-7.88	0,0,0,0	0
58	MG	BA	1633	1/1	0.11	-7.96	11,11,11,11	0
58	MG	DA	3082	1/1	0.05	-8.00	7,7,7,7	0
58	MG	BA	1610	1/1	0.03	-8.94	0,0,0,0	0
58	MG	CA	3115	1/1	0.06	-8.94	0,0,0,0	0
58	MG	DA	3022	1/1	0.07	-9.19	0,0,0,0	0
58	MG	CA	3002	1/1	0.07	-9.32	0,0,0,0	0
58	MG	CA	3046	1/1	0.06	-9.44	0,0,0,0	0
58	MG	BA	1621	1/1	0.05	-9.51	12,12,12,12	0
58	MG	AA	1621	1/1	0.04	-9.57	10,10,10,10	0
58	MG	DA	3052	1/1	0.04	-9.87	0,0,0,0	0
58	MG	BA	1629	1/1	0.05	-10.73	17,17,17,17	0
58	MG	CA	3035	1/1	0.07	-10.81	1,1,1,1	0
58	MG	CA	3007	1/1	0.04	-11.42	0,0,0,0	0
58	MG	CA	3005	1/1	0.04	-11.65	14,14,14,14	0
58	MG	DA	3041	1/1	0.04	-11.85	6,6,6,6	0
58	MG	DA	3080	1/1	0.09	-12.09	1,1,1,1	0
58	MG	AA	1610	1/1	0.05	-12.20	32,32,32,32	0
58	MG	CA	3003	1/1	0.06	-12.55	0,0,0,0	0
58	MG	CA	3119	1/1	0.03	-13.20	8,8,8,8	0
58	MG	DA	3056	1/1	0.05	-14.17	5,5,5,5	0
58	MG	DA	3066	1/1	0.05	-15.62	0,0,0,0	0
58	MG	DA	3029	1/1	0.06	-17.44	0,0,0,0	0
58	MG	CA	3004	1/1	0.06	-18.79	11,11,11,11	0
58	MG	DA	3117	1/1	0.04	-19.37	5,5,5,5	0
58	MG	DA	3144	1/1	0.07	-33.23	0,0,0,0	0
58	MG	CA	3063	1/1	0.12	-	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3013	1/1	0.16	-	0,0,0,0	0
58	MG	CA	3017	1/1	0.15	-	0,0,0,0	0
58	MG	CA	3081	1/1	0.06	-	0,0,0,0	0
58	MG	DA	3014	1/1	0.12	-	12,12,12,12	0
58	MG	CA	3118	1/1	0.07	-	0,0,0,0	0
58	MG	CA	3032	1/1	0.07	-	0,0,0,0	0
58	MG	CA	3105	1/1	0.16	-	0,0,0,0	0
58	MG	CA	3012	1/1	0.17	-	0,0,0,0	0
58	MG	CA	3160	1/1	0.32	-	0,0,0,0	0
58	MG	CA	3037	1/1	0.07	-	11,11,11,11	0
58	MG	CA	3067	1/1	0.12	-	0,0,0,0	0
58	MG	DA	3138	1/1	0.46	-	0,0,0,0	0
58	MG	CA	3148	1/1	0.47	-	0,0,0,0	0
58	MG	CA	3161	1/1	0.21	-	0,0,0,0	0
58	MG	CA	3135	1/1	0.11	-	0,0,0,0	0
58	MG	CA	3099	1/1	0.93	-	53,53,53,53	0
58	MG	CA	3034	1/1	0.20	-	0,0,0,0	0
58	MG	CA	3025	1/1	0.17	-	0,0,0,0	0
58	MG	CA	3072	1/1	0.07	-	0,0,0,0	0
58	MG	CA	3060	1/1	0.05	-	4,4,4,4	0
58	MG	CA	3001	1/1	0.09	-	0,0,0,0	0
58	MG	CA	3104	1/1	0.06	-	0,0,0,0	0
58	MG	CA	3036	1/1	0.16	-	0,0,0,0	0
58	MG	BA	1655	1/1	0.09	-	9,9,9,9	0
58	MG	CA	3062	1/1	0.51	-	46,46,46,46	0
58	MG	CA	3027	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3168	1/1	0.21	-	0,0,0,0	0
58	MG	CA	3010	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3020	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3131	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3053	1/1	0.07	-	0,0,0,0	0
58	MG	DA	3012	1/1	0.10	-	0,0,0,0	0
58	MG	CA	3130	1/1	0.17	-	0,0,0,0	0
58	MG	CA	3076	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3128	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3108	1/1	0.09	-	0,0,0,0	0
58	MG	CA	3068	1/1	0.11	-	0,0,0,0	0
58	MG	CA	3140	1/1	0.50	-	0,0,0,0	0
58	MG	CA	3106	1/1	0.17	-	0,0,0,0	0
58	MG	CA	3026	1/1	0.37	-	30,30,30,30	0
58	MG	CA	3055	1/1	0.09	-	6,6,6,6	0
58	MG	CA	3162	1/1	0.27	-	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3138	1/1	0.42	-	0,0,0,0	0
58	MG	CA	3111	1/1	0.04	-	6,6,6,6	0
58	MG	DA	3162	1/1	0.21	-	4,4,4,4	0
58	MG	CA	3021	1/1	0.09	-	0,0,0,0	0
58	MG	CA	3178	1/1	0.15	-	0,0,0,0	0
58	MG	CA	3030	1/1	0.11	-	0,0,0,0	0
58	MG	CA	3156	1/1	0.28	-	0,0,0,0	0
58	MG	CA	3040	1/1	0.15	-	0,0,0,0	0
58	MG	CA	3015	1/1	0.25	-	36,36,36,36	0
58	MG	CA	3175	1/1	0.19	-	0,0,0,0	0
58	MG	CA	3083	1/1	0.05	-	10,10,10,10	0
58	MG	CA	3136	1/1	0.09	-	0,0,0,0	0
58	MG	CA	3085	1/1	0.20	-	12,12,12,12	0
58	MG	DA	3081	1/1	0.06	-	0,0,0,0	0
58	MG	CA	3038	1/1	0.20	-	0,0,0,0	0
58	MG	CA	3077	1/1	0.07	-	0,0,0,0	0
58	MG	CA	3192	1/1	0.11	-	0,0,0,0	0
58	MG	CA	3023	1/1	0.13	-	0,0,0,0	0
58	MG	CA	3121	1/1	0.18	-	0,0,0,0	0
58	MG	CA	3009	1/1	0.11	-	0,0,0,0	0
58	MG	CA	3043	1/1	0.09	-	0,0,0,0	0
58	MG	CA	3102	1/1	0.15	-	0,0,0,0	0
58	MG	CA	3039	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3123	1/1	0.20	-	0,0,0,0	0
58	MG	CA	3087	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3181	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3011	1/1	0.19	-	0,0,0,0	0
58	MG	CA	3109	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3082	1/1	0.11	-	0,0,0,0	0
58	MG	CA	3061	1/1	0.11	-	9,9,9,9	0
58	MG	DA	3160	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3028	1/1	0.13	-	21,21,21,21	0
58	MG	CA	3016	1/1	0.11	-	0,0,0,0	0
58	MG	CA	3124	1/1	0.09	-	0,0,0,0	0
58	MG	CA	3029	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3126	1/1	0.13	-	0,0,0,0	0
58	MG	DA	3127	1/1	0.04	-	0,0,0,0	0
58	MG	CA	3139	1/1	0.42	-	0,0,0,0	0
58	MG	CA	3089	1/1	0.07	-	19,19,19,19	0
58	MG	CA	3064	1/1	0.19	-	0,0,0,0	0
58	MG	CA	3071	1/1	0.07	-	0,0,0,0	0
58	MG	CA	3172	1/1	0.17	-	0,0,0,0	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
58	MG	CA	3171	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3193	1/1	0.25	-	0,0,0,0	0
58	MG	DA	3102	1/1	0.09	-	12,12,12,12	0
58	MG	CA	3127	1/1	0.12	-	0,0,0,0	0
58	MG	CA	3179	1/1	0.16	-	0,0,0,0	0
58	MG	CA	3189	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3069	1/1	0.14	-	0,0,0,0	0
58	MG	CA	3014	1/1	0.14	-	12,12,12,12	0
58	MG	CA	3086	1/1	0.16	-	0,0,0,0	0
58	MG	CA	3103	1/1	0.09	-	0,0,0,0	0
58	MG	CQ	201	1/1	0.29	-	0,0,0,0	0
58	MG	CA	3054	1/1	0.15	-	0,0,0,0	0
58	MG	CA	3096	1/1	0.07	-	0,0,0,0	0
58	MG	CA	3042	1/1	0.09	-	0,0,0,0	0
58	MG	CA	3146	1/1	0.32	-	0,0,0,0	0
58	MG	CA	3180	1/1	0.18	-	6,6,6,6	0

6.5 Other polymers ⓘ

There are no such residues in this entry.