



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 07:09 PM BST

PDB ID : 4V4Q
Title : Crystal structure of the bacterial ribosome from Escherichia coli at 3.5 Å resolution.
Authors : Schuwirth, B.S.; Borovinskaya, M.A.; Hau, C.W.; Zhang, W.; Vila-Sanjurjo, A.; Holton, J.M.; Cate, J.H.D.
Deposited on : 2005-08-30
Resolution : 3.46 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>

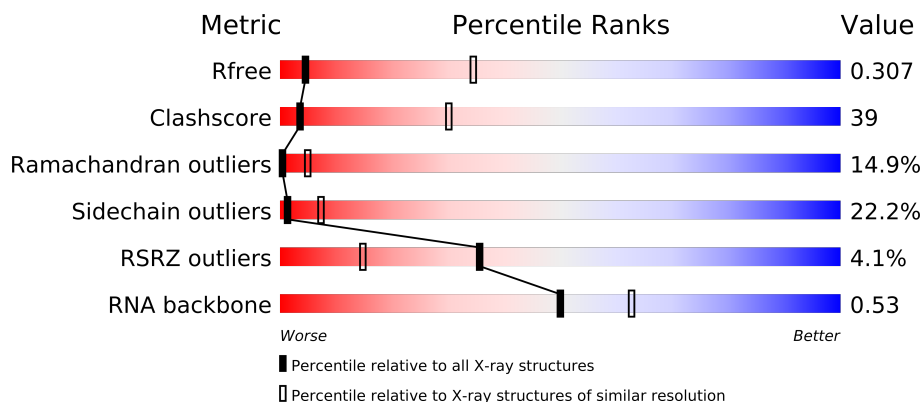
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.46 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	1149 (3.62-3.30)
Clashscore	79885	1012 (3.60-3.32)
Ramachandran outliers	78287	1401 (3.62-3.30)
Sidechain outliers	78261	1401 (3.62-3.30)
RSRZ outliers	66119	1149 (3.62-3.30)
RNA backbone	1838	1004 (4.10-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	1542	
1	CA	1542	
2	AC	232	
2	CC	232	
3	AD	205	
3	CD	205	
4	AE	166	
4	CE	166	
5	AF	135	
5	CF	135	
6	AG	178	
6	CG	178	

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Mol	Chain	Length	Quality of chain
7	AH	129	
7	CH	129	
8	AI	129	
8	CI	129	
9	AJ	103	
9	CJ	103	
10	AK	128	
10	CK	128	
11	AL	123	
11	CL	123	
12	AM	117	
12	CM	117	
13	AN	100	
13	CN	100	
14	AO	89	
14	CO	89	
15	AP	82	
15	CP	82	
16	AQ	83	
16	CQ	83	
17	AR	74	
17	CR	74	
18	AS	91	
18	CS	91	
19	AT	86	
19	CT	86	
20	AB	240	
20	CB	240	
21	AU	71	
21	CU	71	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BV	94	
24	DV	94	
25	BC	273	
25	DC	273	
26	BD	209	
26	DD	209	
27	BE	201	
27	DE	201	

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Mol	Chain	Length	Quality of chain
28	BF	178	
28	DF	178	
29	BG	176	
29	DG	176	
30	BH	149	
30	DH	149	
31	BJ	142	
31	DJ	142	
32	BK	123	
32	DK	123	
33	BL	144	
33	DL	144	
34	BM	136	
34	DM	136	
35	BN	127	
35	DN	127	
36	BO	117	
36	DO	117	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	100	
41	DT	100	
42	BU	103	
42	DU	103	
43	BW	84	
43	DW	84	
44	BX	63	
44	DX	63	
45	BY	58	
45	DY	58	
46	BZ	70	
46	DZ	70	
47	B0	56	
47	D0	56	
48	B1	54	
48	D1	54	

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Mol	Chain	Length	Quality of chain
49	B2	46	
49	D2	46	
50	B3	64	
50	D3	64	
51	B4	38	
51	D4	38	
52	BI	141	
52	DI	141	

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

Mol	Type	Chain	Res	Geometry	Electron density
53	MG	AA	1624	-	X
53	MG	AA	1625	-	X
53	MG	AA	1636	-	X
53	MG	AA	1638	-	X
53	MG	AA	1646	-	X
53	MG	AA	1649	-	X
53	MG	AA	1656	-	X
53	MG	AA	1658	-	X
53	MG	BB	3033	-	X
53	MG	BB	3067	-	X
53	MG	BB	3078	-	X
53	MG	BB	3100	-	X
53	MG	BB	3105	-	X
53	MG	CA	1602	-	X
53	MG	CA	1621	-	X
53	MG	CA	1623	-	X
53	MG	CA	1653	-	X

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 284107 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			
1	CA	1530	Total	C	N	O	P	0	0	0
			32831	14642	6024	10635	1530			

- Molecule 2 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
2	CC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 3 is a protein called 30S ribosomal protein S4.

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

- Molecule 4 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
4	CE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 5 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
5	CF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 6 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	4			
6	CG	152	Total	C	N	O	S	0	0	0
			1196	745	230	217	4			

- Molecule 7 is a protein called 30S ribosomal protein S8.

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

- Molecule 8 is a protein called 30S ribosomal protein S9.

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

- Molecule 9 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
9	CJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 10 is a protein called 30S ribosomal protein S11.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 11 is a protein called 30S ribosomal protein S12.

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

- Molecule 12 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
12	CM	113	Total	C	N	O	S	0	0	0
			876	541	177	155	3			

- Molecule 13 is a protein called 30S ribosomal protein S14.

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

- Molecule 14 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			
14	CO	88	Total	C	N	O	S	0	0	0
			716	440	146	129	1			

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
15	CP	80	Total	C	N	O	S	0	0	0
			638	400	126	111	1			

- Molecule 16 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
16	CQ	81	Total	C	N	O	S	0	0	0
			656	417	122	114	3			

- Molecule 17 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
17	AR	55	Total	C	N	O	0	0	0
			455	288	86	81			
17	CR	55	Total	C	N	O	0	0	0
			455	288	86	81			

- Molecule 18 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
18	CS	80	Total	C	N	O	S	0	0	0
			644	413	121	108	2			

- Molecule 19 is a protein called 30S ribosomal protein S20.

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

- Molecule 20 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
20	CB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- 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
			425	265	86	73	1			
21	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 22 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			
22	DA	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			
23	DB	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			
25	DC	267	Total	C	N	O	S	0	0	0
			2053	1271	416	359	7			

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	BD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

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

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			
28	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 29 is a protein called 50S ribosomal protein L6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			
30	DH	149	Total	C	N	O	S	0	0	0
			1111	699	197	214	1			

- Molecule 31 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			
31	DJ	140	Total	C	N	O	S	0	0	0
			1112	704	210	194	4			

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			
32	DK	121	Total	C	N	O	S	0	0	0
			930	582	179	164	5			

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			
33	DL	144	Total	C	N	O	S	0	0	0
			1053	654	207	190	2			

- Molecule 34 is a protein called 50S ribosomal protein L16.

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

- Molecule 35 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			
35	DN	127	Total	C	N	O	S	0	0	0
			1008	621	204	178	5			

- Molecule 36 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			
36	DO	117	Total	C	N	O	S	0	0	0
			900	557	179	163	1			

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				
38	DQ	117	Total	C	N	O	S	0	0	0
			947	604	192	151				

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			
41	DT	99	Total	C	N	O	S	0	0	0
			777	491	145	139	2			

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0	0
			779	492	146	141				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O			
			779	492	146	141	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BW	84	Total	C	N	O	S		
			634	391	129	113	1	0	0
43	DW	84	Total	C	N	O	S		
			634	391	129	113	1	0	0

- Molecule 44 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BX	63	Total	C	N	O	S		
			509	313	99	95	2	0	0
44	DX	63	Total	C	N	O	S		
			509	313	99	95	2	0	0

- Molecule 45 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BY	58	Total	C	N	O	S		
			449	281	87	79	2	0	0
45	DY	58	Total	C	N	O	S		
			449	281	87	79	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BZ	70	Total	C	N	O	S		
			549	339	104	100	6	0	0
46	DZ	70	Total	C	N	O	S		
			549	339	104	100	6	0	0

- Molecule 47 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
47	B0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0
47	D0	56	Total	C	N	O	S		
			444	269	94	80	1	0	0

- Molecule 48 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
48	B1	54	Total	C	N	O	0	0	0
			441	284	81	76			
48	D1	54	Total	C	N	O	0	0	0
			441	284	81	76			

- Molecule 49 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
49	D2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
50	D3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 51 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
51	D4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 52 is a protein called 50S ribosomal protein L11.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
53	AP	1	Total Mg 1 1	0	0
53	BB	110	Total Mg 110 110	0	0
53	CA	62	Total Mg 62 62	0	0
53	AA	59	Total Mg 59 59	0	0
53	DN	1	Total Mg 1 1	0	0
53	DB	110	Total Mg 110 110	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
54	AA	290	Total O 290 290	0	0
54	AE	3	Total O 3 3	0	0
54	AK	2	Total O 2 2	0	0
54	AN	4	Total O 4 4	0	0
54	AP	1	Total O 1 1	0	0
54	BB	497	Total O 497 497	0	0
54	BC	1	Total O 1 1	0	0
54	BE	5	Total O 5 5	0	0
54	BH	1	Total O 1 1	0	0
54	BL	2	Total O 2 2	0	0
54	BN	1	Total O 1 1	0	0
54	CA	295	Total O 295 295	0	0
54	CE	3	Total O 3 3	0	0
54	CK	1	Total O 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
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54	CN	2	Total 2	O 2	0	0
54	CP	1	Total 1	O 1	0	0
54	CT	2	Total 2	O 2	0	0
54	DB	499	Total 499	O 499	0	0
54	DC	1	Total 1	O 1	0	0
54	DD	1	Total 1	O 1	0	0
54	DE	3	Total 3	O 3	0	0
54	DJ	2	Total 2	O 2	0	0
54	DL	1	Total 1	O 1	0	0
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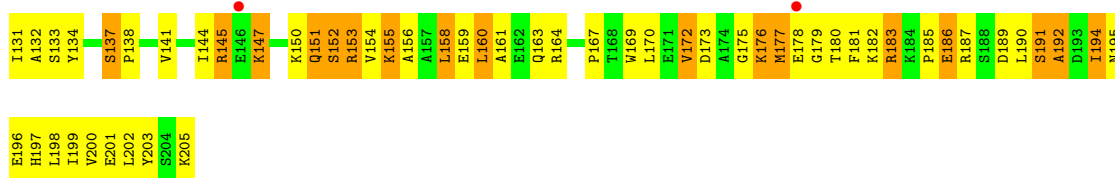
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U835	A914	C980	G1040	A1102		C1244	G1310	U1372		U1506
U836	A915	C981	G1041	C1103	G1178	C1245	G1311	U1373	U1444	A1507
G837	A916	C982	G1042		A1179	C1246	G1312	A1374	U1445	A1508
U838	G917	A983	G1043	G1108	A1180	U1247	G1313	A1375	A1446	C1509
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C839	A919	C985	C1045	A1110	G1182	G1249	G1315	A1377	C1448	G1511
C840	U920	C986	A1046	A1111	U1183	C1250	G1316	C1378	C1449	G1512
C941	U921	C987	G1047	C1112	U1184	A1251	C1317	U1379	U1450	A1513
U842	G922	G988	G1048	C1113	G1190	A1252	A1318	U1380	G1451	G1514
U843	A923	C989	G1049	C1114		G1253	C1319	U1381	C1452	G1515
G844	C924	C990	G1050	U1115	G1193	C1254	C1320	C1382	G1453	G1516
A845	G925	U991	C1051	U1116	U1194	G1255	U1321	C1382	G1454	G1517
G846	G926	C992	U1052	A1117	U1196	A1256	G1322	G1386	G1455	A1518
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	G929	C995	A1055	U1121	G1198	G1259	G1325	C1389	G1458	C1521
C857	C930	A996	U1056	U1122	U1199	G1260	U1326	U1390	G1459	U1522
G858	C931	U997	G1057	U1123	G1200	A1261	C1327	U1391	C1460	G1523
G859		C998	U1058	G1124	A1201	C1262	G1328	G1392	G1461	C1524
A860	C934	C999	G1059	U1125	U1202	C1263	A1329	U1393	C1462	G1525
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C862	C936	C1001	U1061	G1127		A1269	G1331	C1397	U1464	U1527
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G895	U961	G1024	G1084	A1157	C1228	G1294	G1356	C1427	U1490	
C896		U1025	U1085	C1158	A1229	U1295	A1357	A1428	G1491	
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	C967	C1027		G1160	G1231	G1297		A1429	A1493	
A900	A968	C1028	U1090	C1161	U1232	U1298	G1361	A1430	G1494	
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G902	C970	A1030	A1092	A1163	C1234	G1300	A1363	G1432	U1496	
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A906	C972	G1032	G1094		A1236	C1302	G1365	A1434	U1497	
A907	G973	G1033	U1095	U1168	C1237	C1303	C1366	G1435	U1498	
A908	A974	G1034	C1096	A1169	A1238	G1304	C1367	U1436	A1499	
A909	A975	A1035	C1097	A1170	A1239	G1305	C1368	A1437	A1500	
C910	A976	A1036	U1098	A1171	U1240	A1306	C1369	G1438		
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● Molecule 1: 16S ribosomal RNA

Chain CA: 

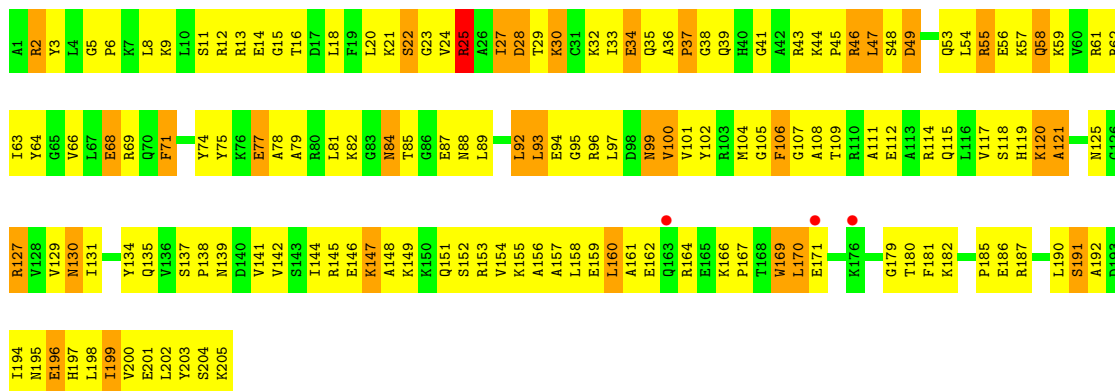
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A65			G69	U70	A71	A72			G75	G76	A77	A78	G79			C83	U84	U85	G86	C87	U88	U89	C90	U91	U92	U93	G94	C95			A98	C99			G105	C106	G107	G108	A109	C110	G111	G112	G113	U114	G115											U118	A119	A120	U121	G122	U123			G128	A129	A130	A131	C132			C135			G138	A139	U140
G141	G142	A143	G144	G145	G146	G147	G148	A149	U150	A151	A152			A155	C156	U157	G158	G159	A160	A161	A162	C163	G164			A167	G168	C169	U170			U173	A174	C175	G176	G177	A178	A179	U180	A181	A182	C183			C186	G187	C188	A189	A190	G191	A192	C193	C194	A195	A196	A197											G202	G203	G204	A205	C206	C207				
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A1311	G1245	G1181	C1114	U1049	C986	A923	U843	G772	A704	G634	G558	G424	G278	G278
G1312	U1246	G1182		G1050	U986	C924	G844	G773	G705	A635	A559	G425	A279	C280
U1313	U1247	U1183	U1118	C1061	G987	G925	A845	A777	G706	U636	A560	U426	G389	G281
G1314	G1184	G988	C1119	U1052	G988	G926	G846	G778	U707	G637	U561	U427	G390	C284
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C1317	A1251	G1187	U1122	U1055	U991	G929		A781	G710	A642	G566	A430	A366	C284
A1318	A1252	A1188	U1123	U1056	U992	C930	C857	A782	U711	G643	G567	A431	U367	C285
A1319	G1253	G993	G1124	G1057	G993	C931	C858	C783	G712	C644	G568	A432	C370	A288
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G1337	C1209	C1209	G1142	U1075	A1012	G951	C882	A807	G733	G664	A596	G454	G391	C314
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A1360	U1298	C1230	G1166	C1100	U1034	C972	A908	G830	G755	U687	C620	U476	A412	C335
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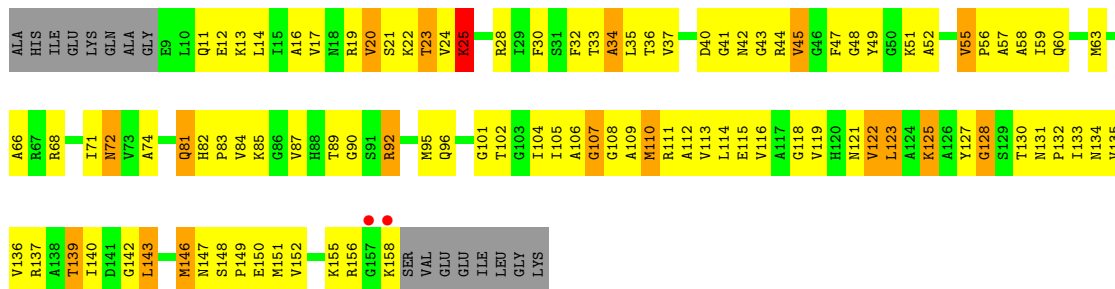
• Molecule 3: 30S ribosomal protein S4

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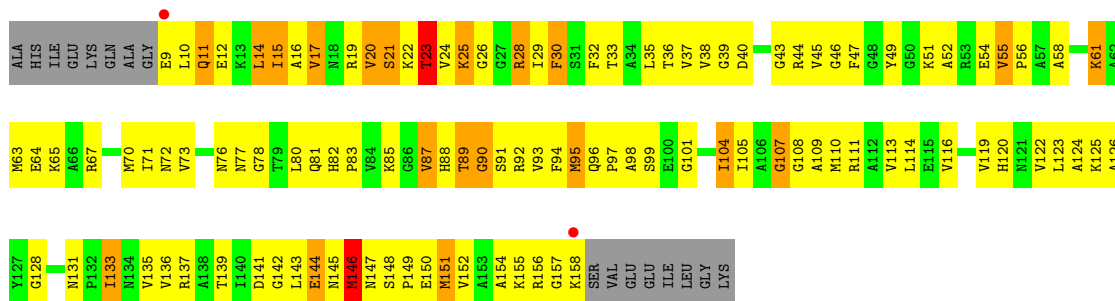
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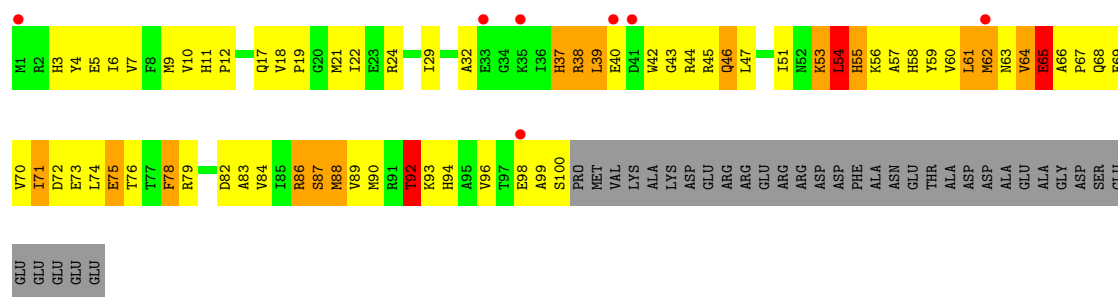
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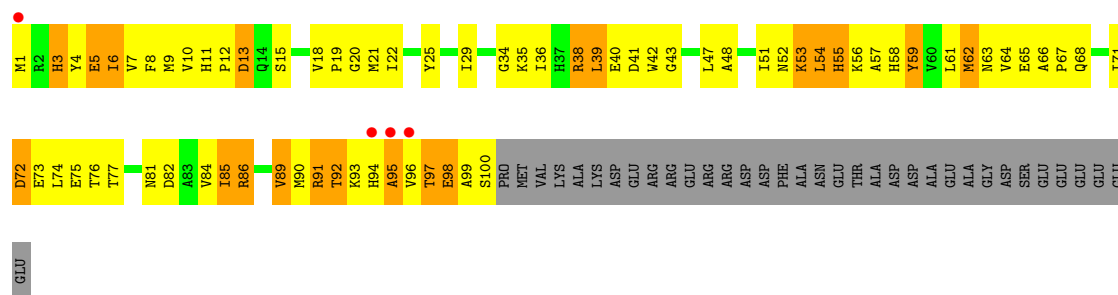
• Molecule 5: 30S ribosomal protein S6

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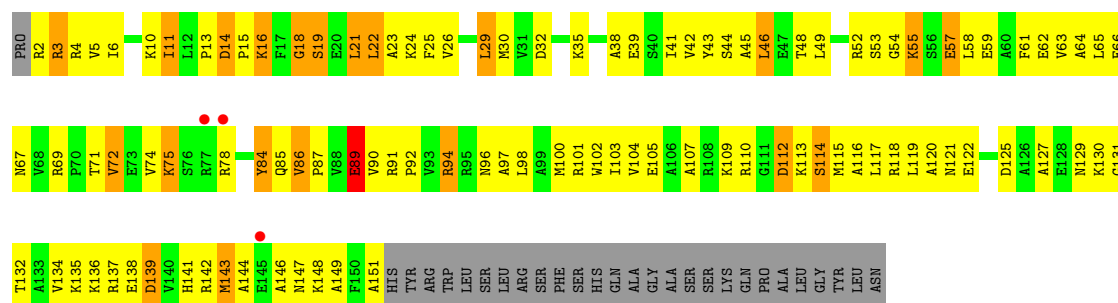
- Molecule 5: 30S ribosomal protein S6

Chain CF:



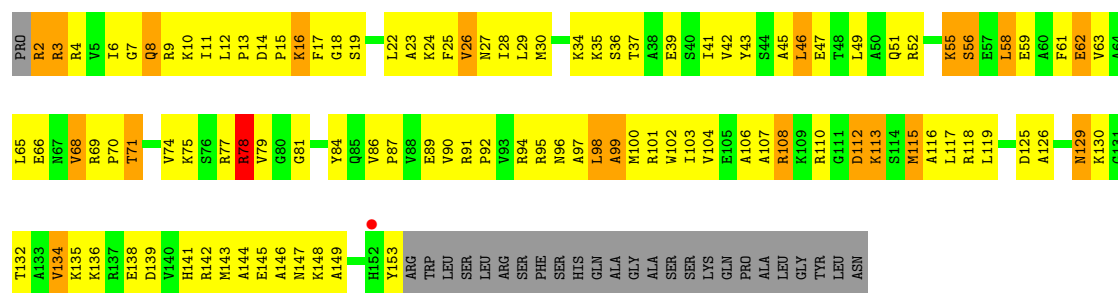
- Molecule 6: 30S ribosomal protein S7

Chain AG:



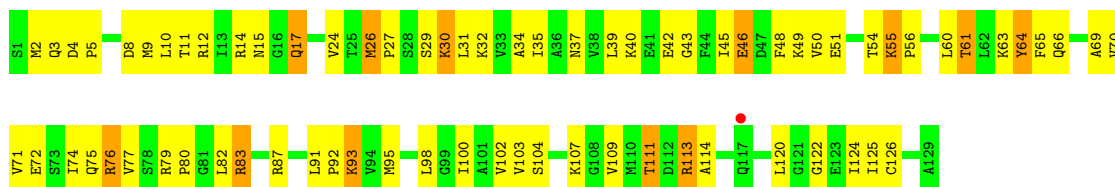
- Molecule 6: 30S ribosomal protein S7

Chain CG:



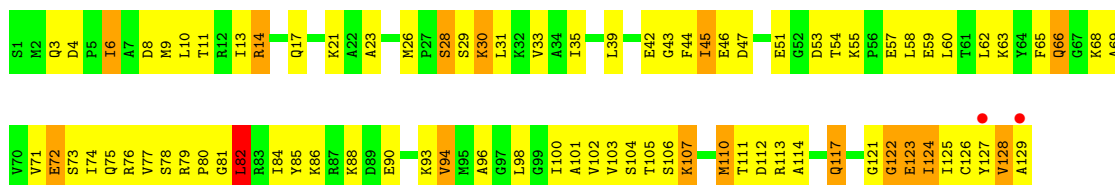
- Molecule 7: 30S ribosomal protein S8

Chain AH:



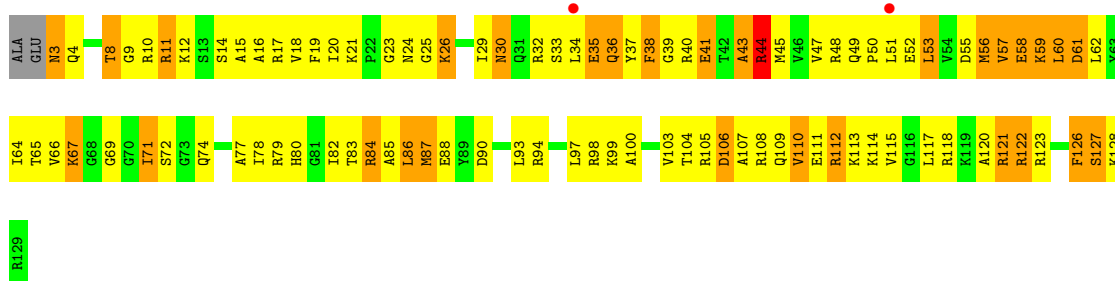
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Chain CH:



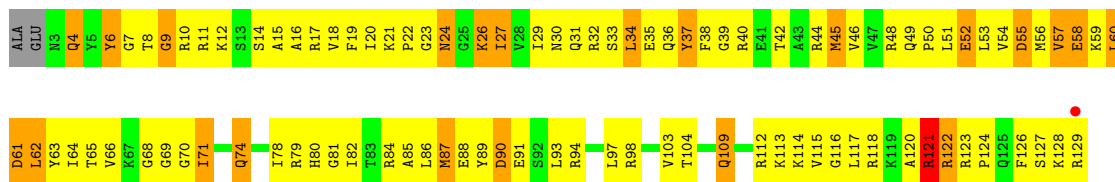
• Molecule 8: 30S ribosomal protein S9

Chain AI:



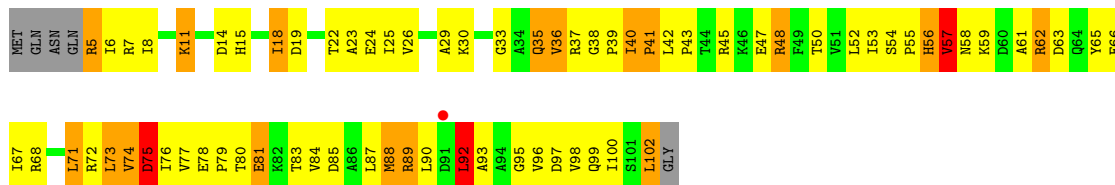
• Molecule 8: 30S ribosomal protein S9

Chain CI:



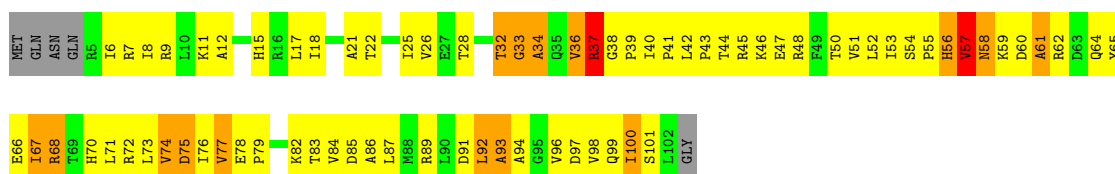
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



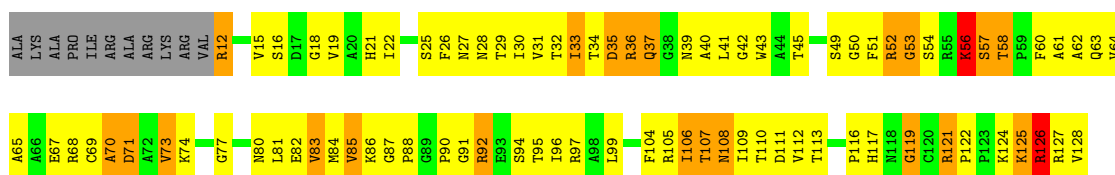
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



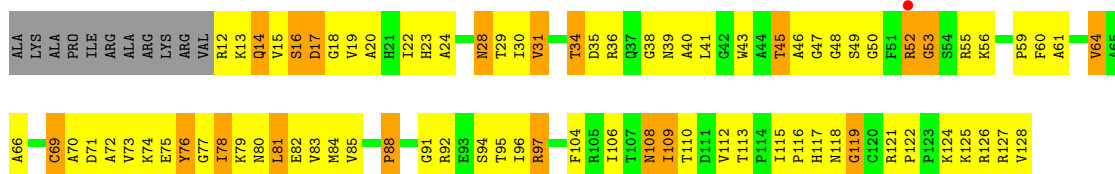
• Molecule 10: 30S ribosomal protein S11

Chain AK:



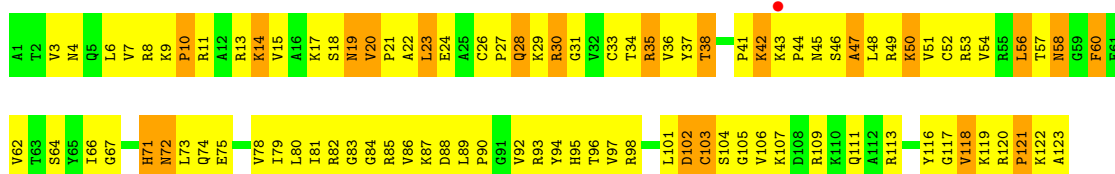
• Molecule 10: 30S ribosomal protein S11

Chain CK:



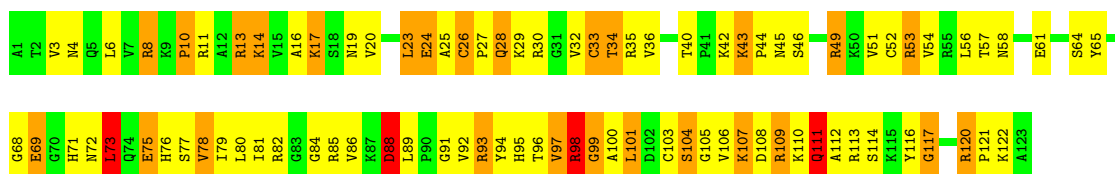
• Molecule 11: 30S ribosomal protein S12

Chain AL:



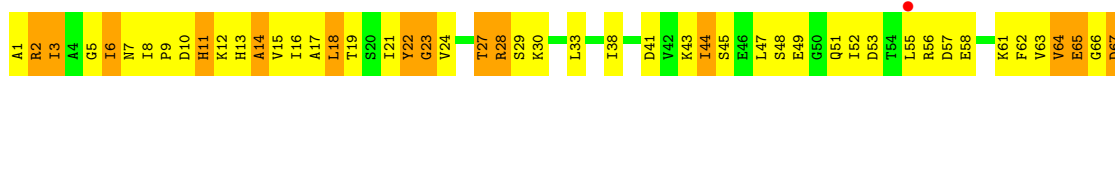
• Molecule 11: 30S ribosomal protein S12

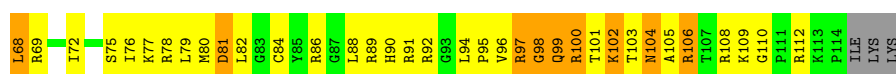
Chain CL:



• Molecule 12: 30S ribosomal protein S13

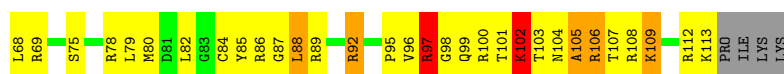
Chain AM:





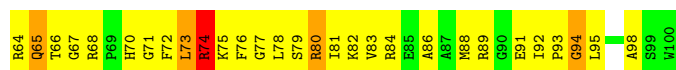
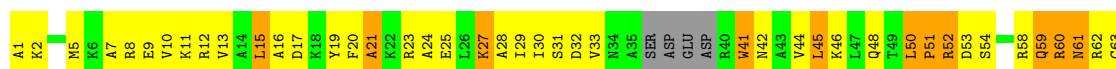
- Molecule 12: 30S ribosomal protein S13

Chain CM:



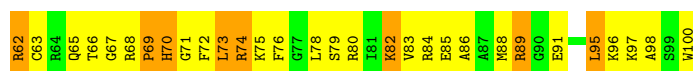
- Molecule 13: 30S ribosomal protein S14

Chain AN:



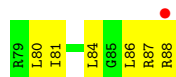
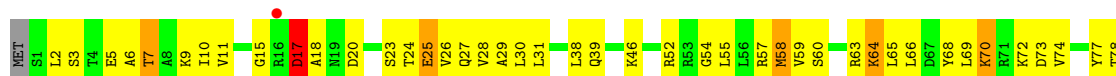
- Molecule 13: 30S ribosomal protein S14

Chain CN:



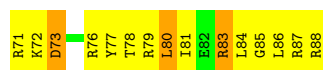
- Molecule 14: 30S ribosomal protein S15

Chain AO:



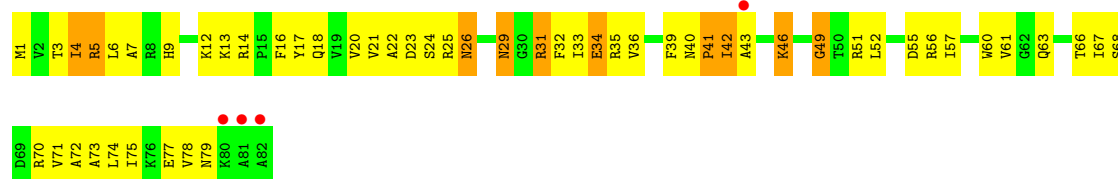
- Molecule 14: 30S ribosomal protein S15

Chain CO:



- Molecule 15: 30S ribosomal protein S16

Chain AP:



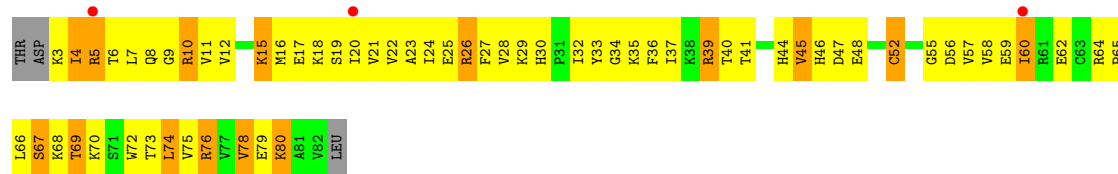
- Molecule 15: 30S ribosomal protein S16

Chain CP:



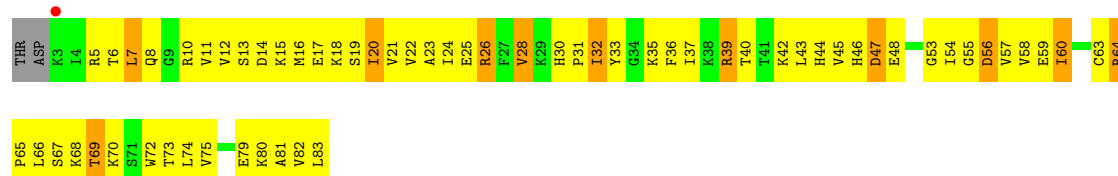
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



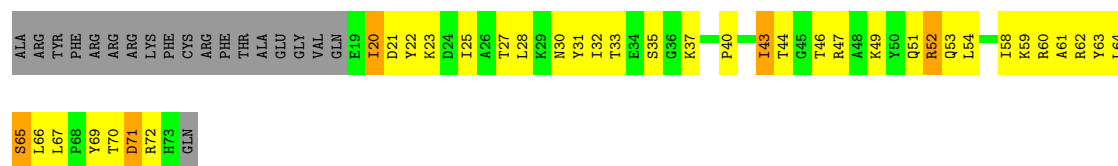
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



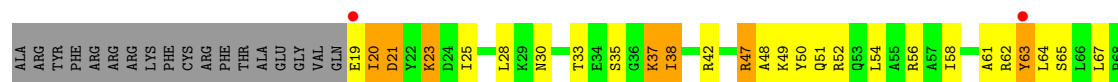
- Molecule 17: 30S ribosomal protein S18

Chain AR:



- Molecule 17: 30S ribosomal protein S18

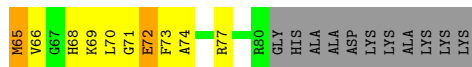
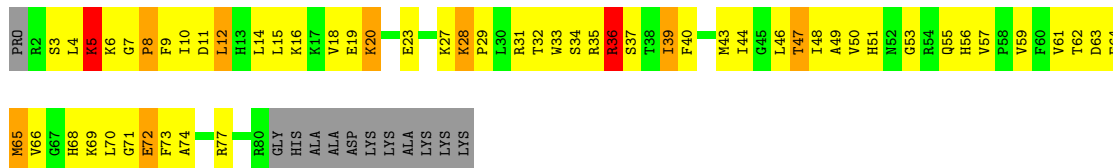
Chain CR:





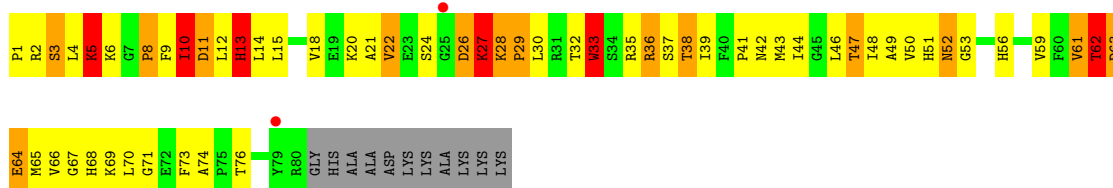
- Molecule 18: 30S ribosomal protein S19

Chain AS:



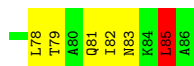
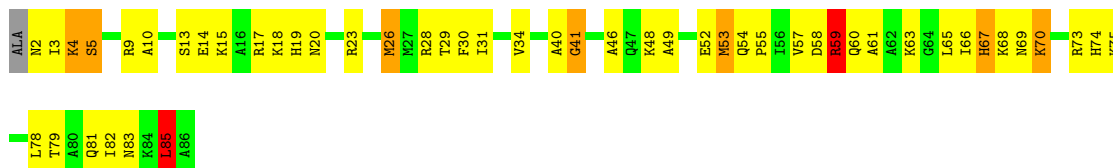
- Molecule 18: 30S ribosomal protein S19

Chain CS:



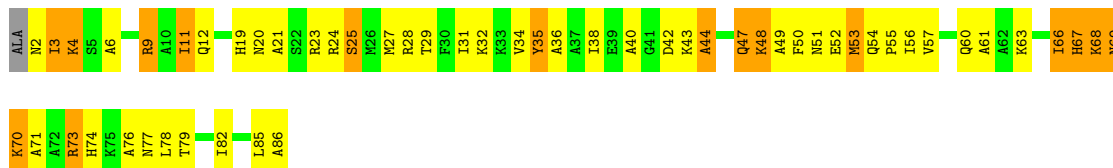
- Molecule 19: 30S ribosomal protein S20

Chain AT:



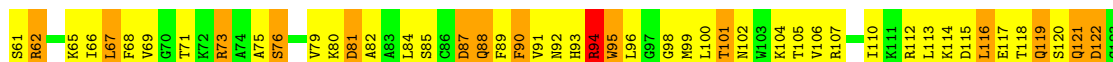
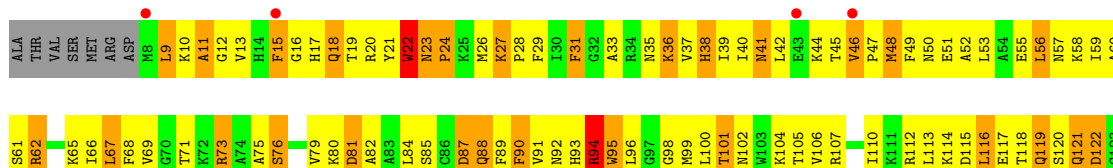
- Molecule 19: 30S ribosomal protein S20

Chain CT:



- Molecule 20: 30S ribosomal protein S2

Chain AB:



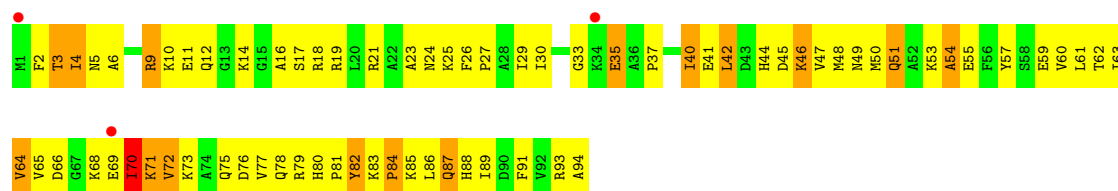
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G1877	U1949	U2024	U2150	U2215	U2276	U2338	U2418	U2493	U2559	G2629	U2691	G2755	A2819
A1878	G1950	G2025	C2151	A2216	U2277	U2339	U2419	U2494	U2560	U2630	U2692	U2756	G2820
G1879	U1951	U2026	U2152	U2217	U2278	U2340	U2420	U2495	U2561	G2631	G2693	U2757	A2821
U1880	A1952	U2027	G2153	U2218	U2279	U2341	U2421	U2496	U2562	U2632	G2694	G2758	G2822
A1881	U1953	U2028	A2154	U2219	U2280	U2342	U2422	U2497	U2563	A2633	U2695	U2759	A2823
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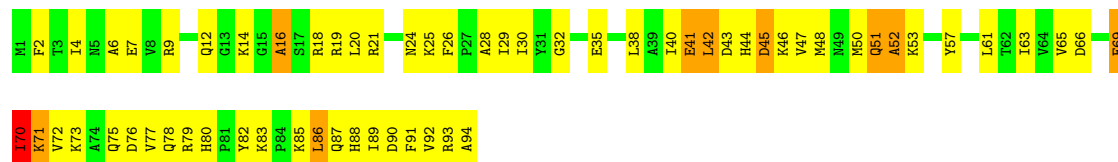
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A1847	U1780	U1713	G1645	G1567	A1503	A1439	U1372	A1301	A1240	U1173	U1109	A1027	C898	
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U1851	U1784	G1715	G1647	A1569	A1505	G1441	G1374	G1303	U1242	A1175	G1112	C1029	G962	
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Chain BV: 



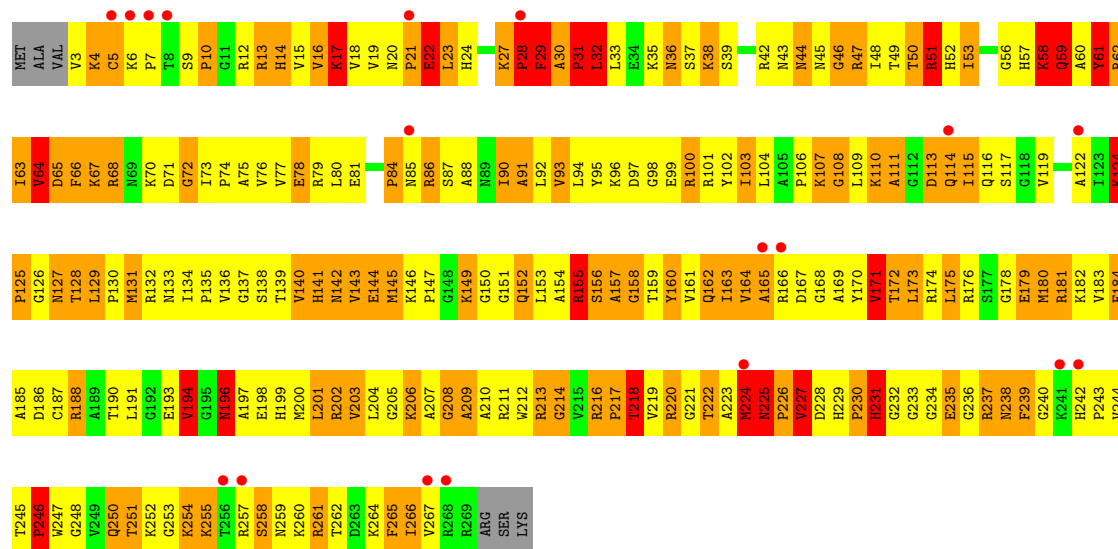
- Molecule 24: 50S ribosomal protein L25

Chain DV: 



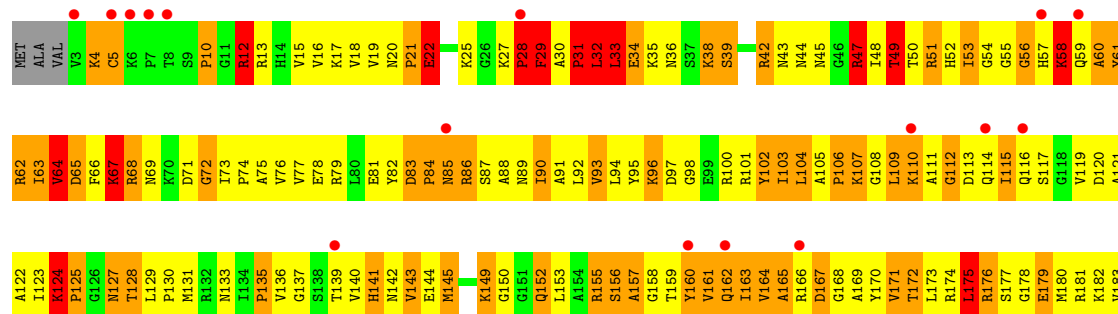
- Molecule 25: 50S ribosomal protein L2

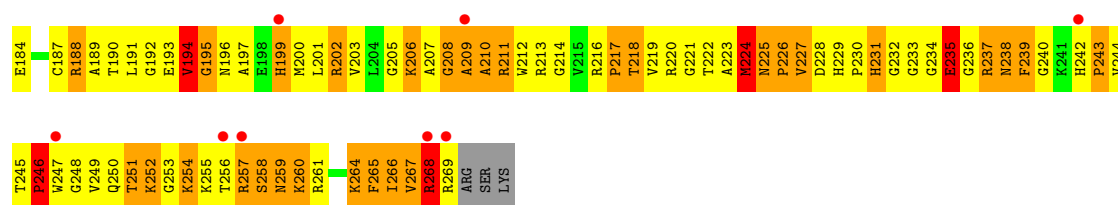
Chain BC: 



- Molecule 25: 50S ribosomal protein L2

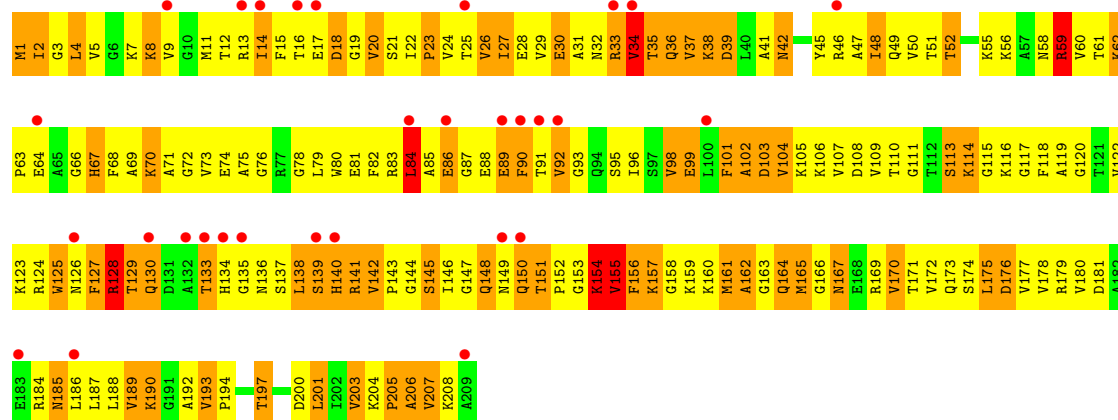
Chain DC: 





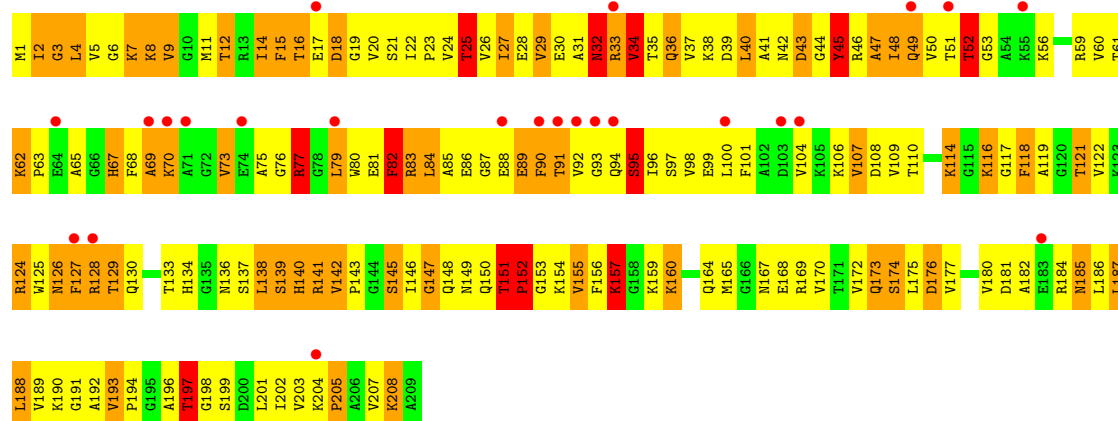
• Molecule 26: 50S ribosomal protein L3

Chain BD:



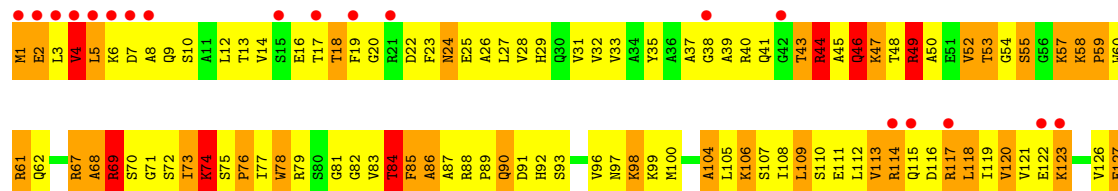
• Molecule 26: 50S ribosomal protein L3

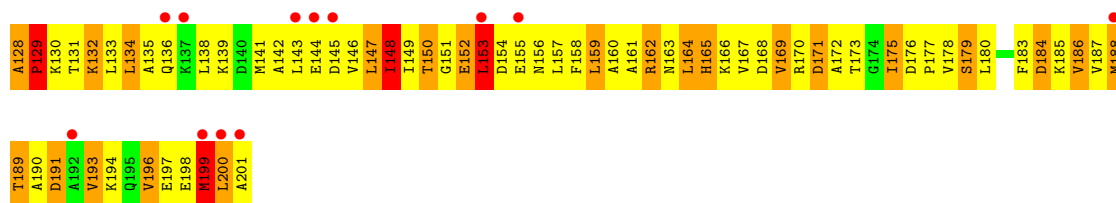
Chain DD:



• Molecule 27: 50S ribosomal protein L4

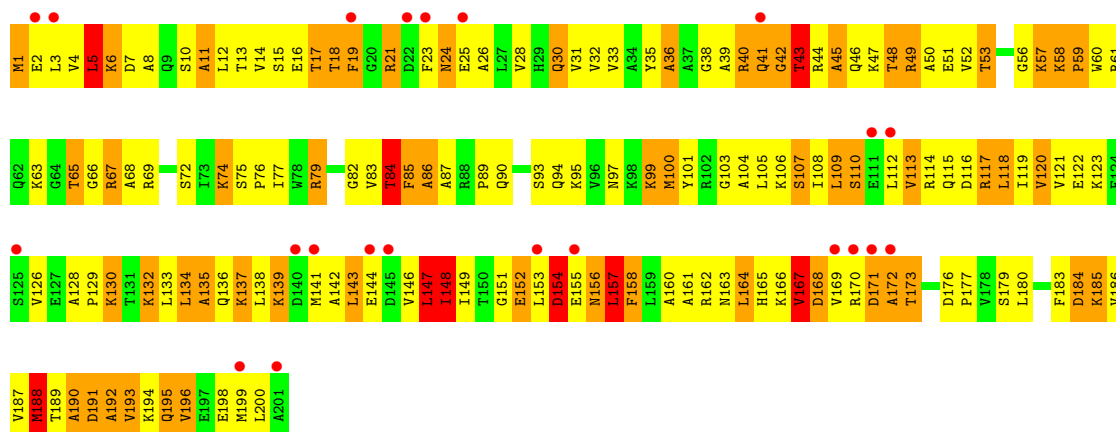
Chain BE:





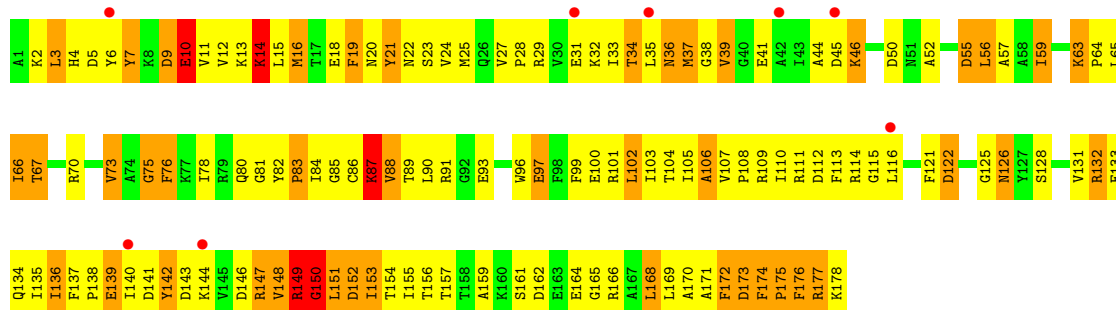
• Molecule 27: 50S ribosomal protein L4

Chain DE:



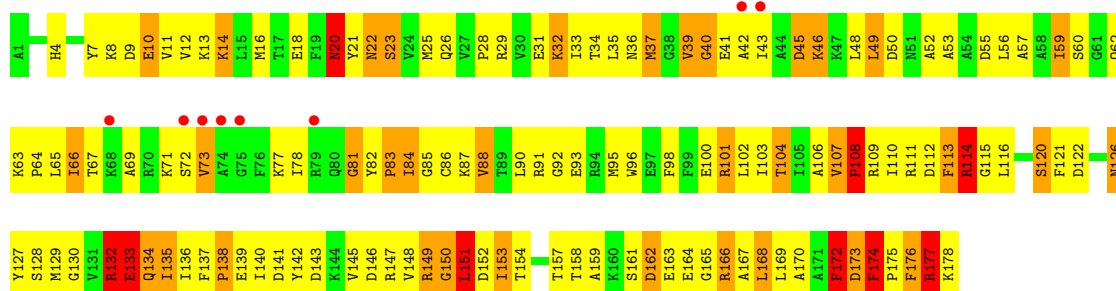
• Molecule 28: 50S ribosomal protein L5

Chain BF:



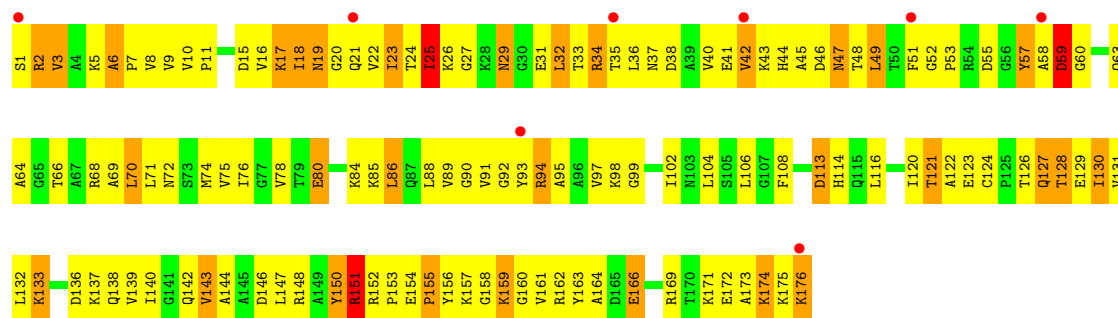
• Molecule 28: 50S ribosomal protein L5

Chain DF:



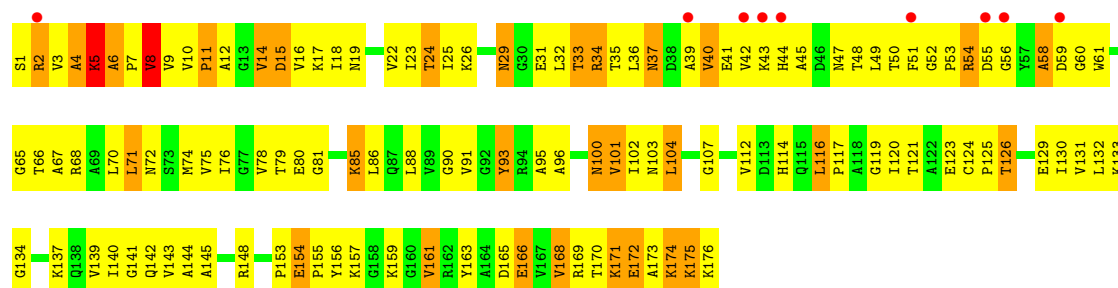
• Molecule 29: 50S ribosomal protein L6

Chain BG:



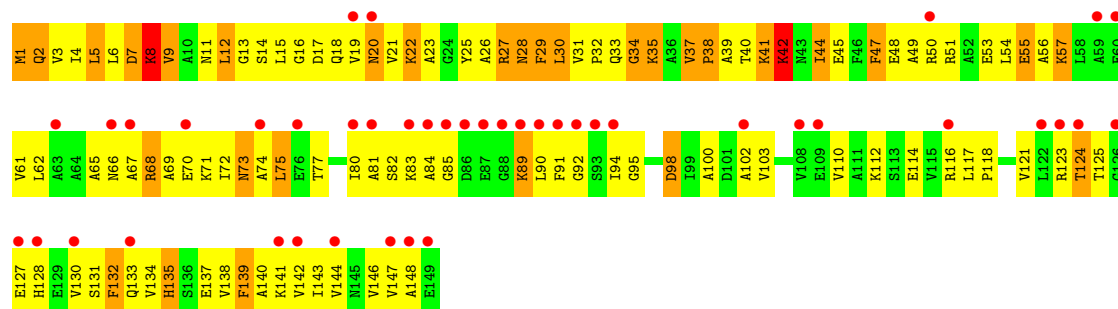
- Molecule 29: 50S ribosomal protein L6

Chain DG:



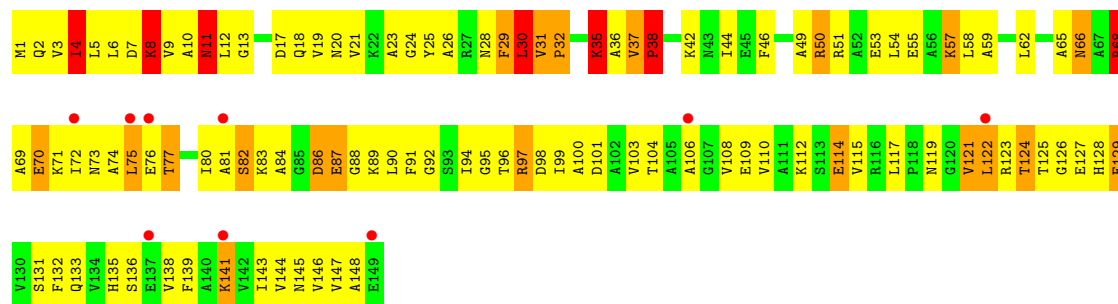
- Molecule 30: 50S ribosomal protein L9

Chain BH:



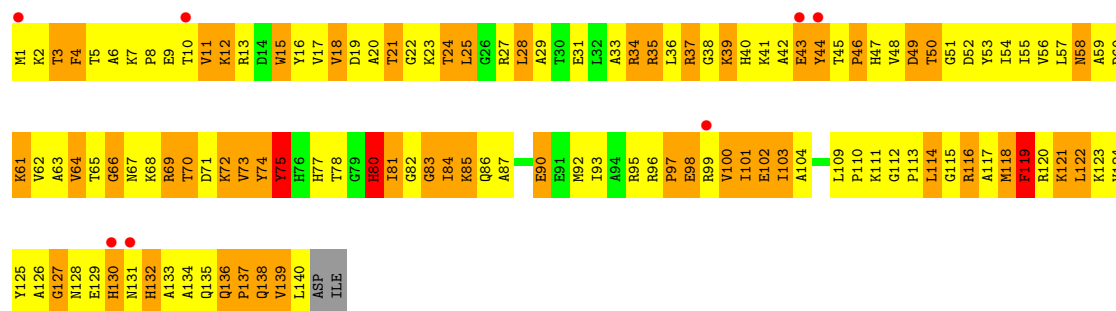
- Molecule 30: 50S ribosomal protein L9

Chain DH:



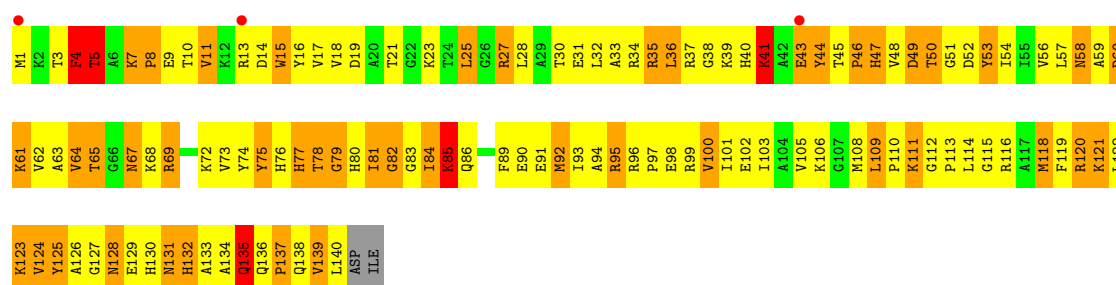
- Molecule 31: 50S ribosomal protein L13

Chain BJ:



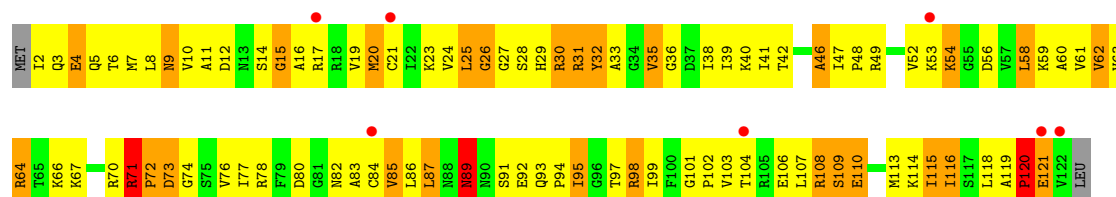
- Molecule 31: 50S ribosomal protein L13

Chain DJ:



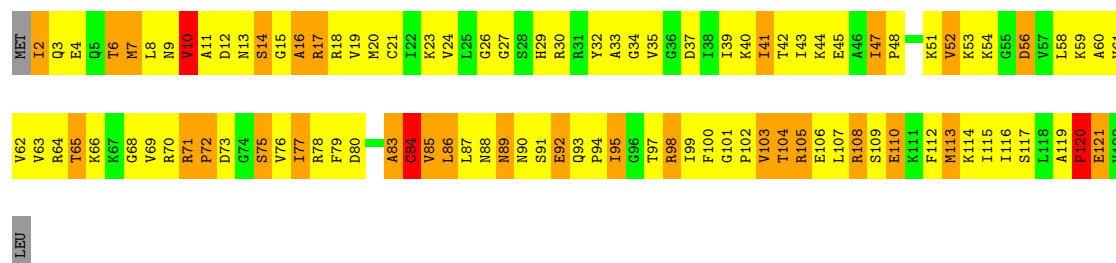
- Molecule 32: 50S ribosomal protein L14

Chain BK:



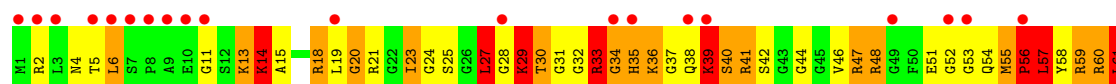
- Molecule 32: 50S ribosomal protein L14

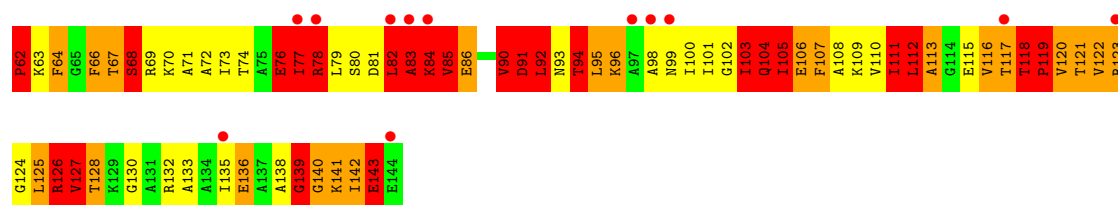
Chain DK:



- Molecule 33: 50S ribosomal protein L15

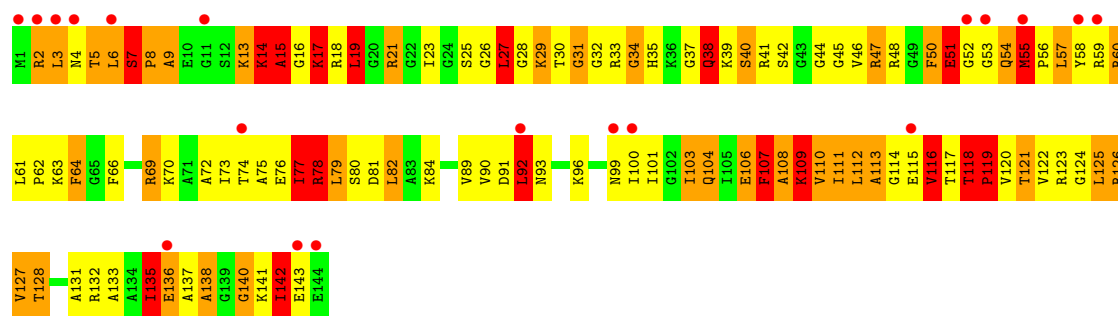
Chain BL:





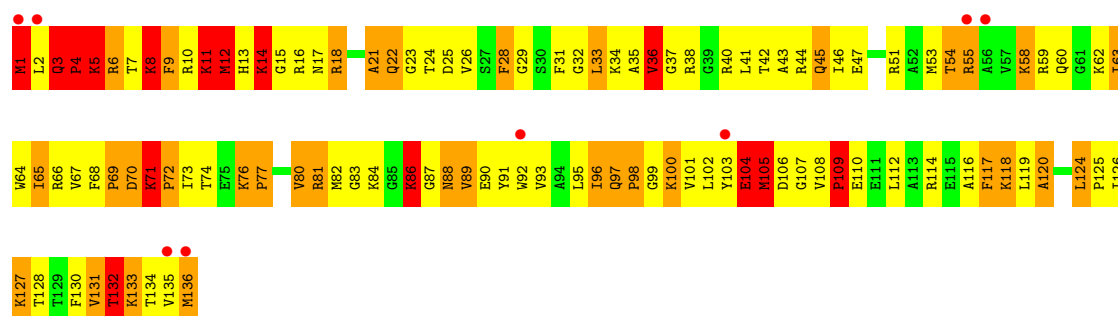
• Molecule 33: 50S ribosomal protein L15

Chain DL:



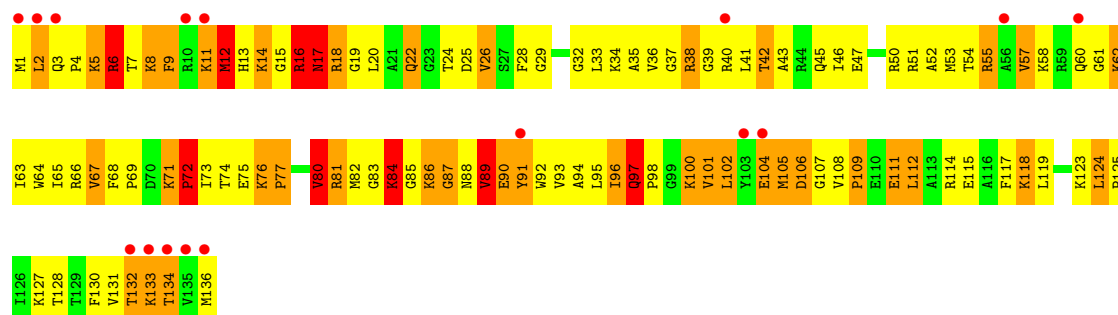
• Molecule 34: 50S ribosomal protein L16

Chain BM:



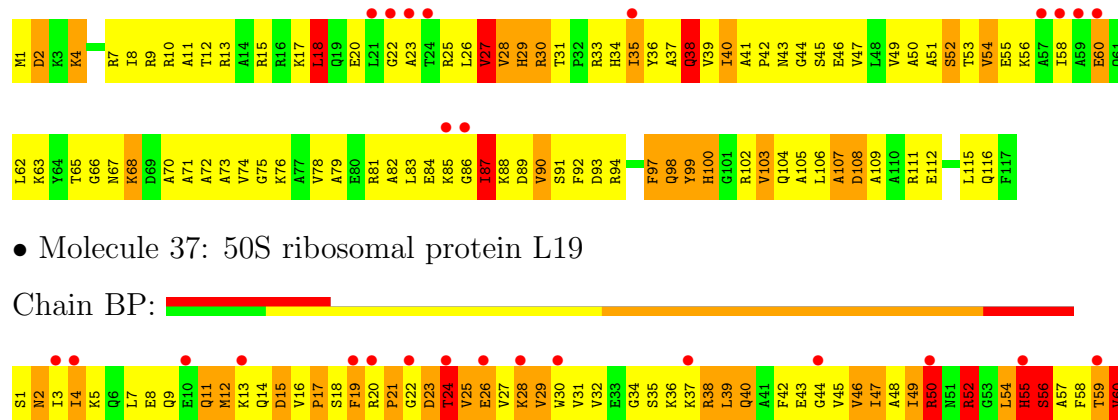
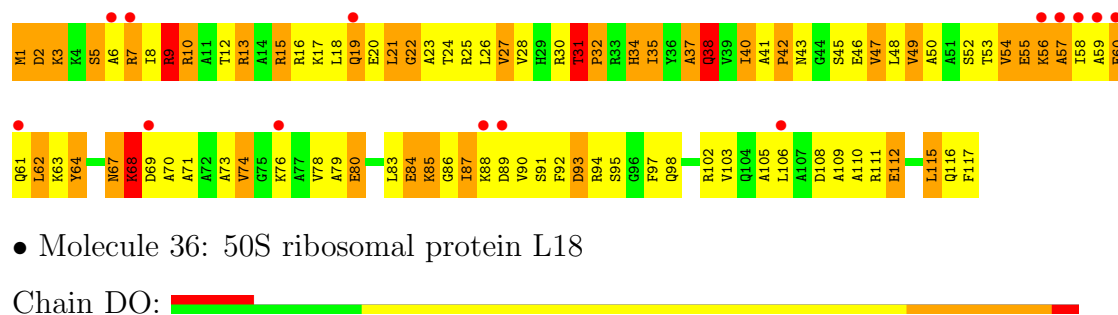
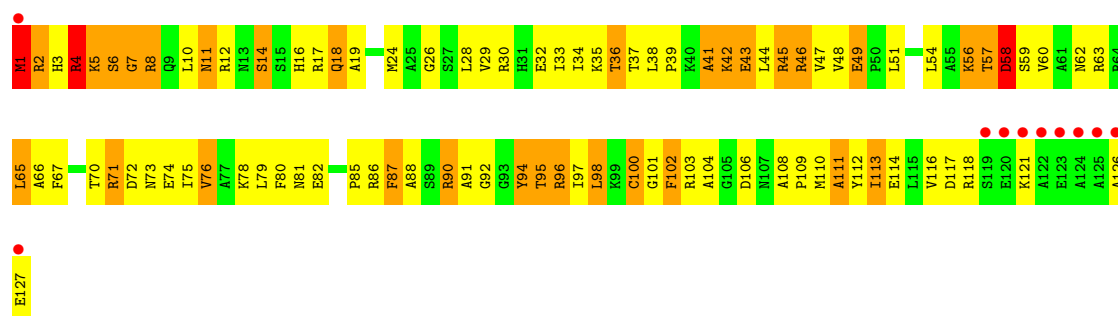
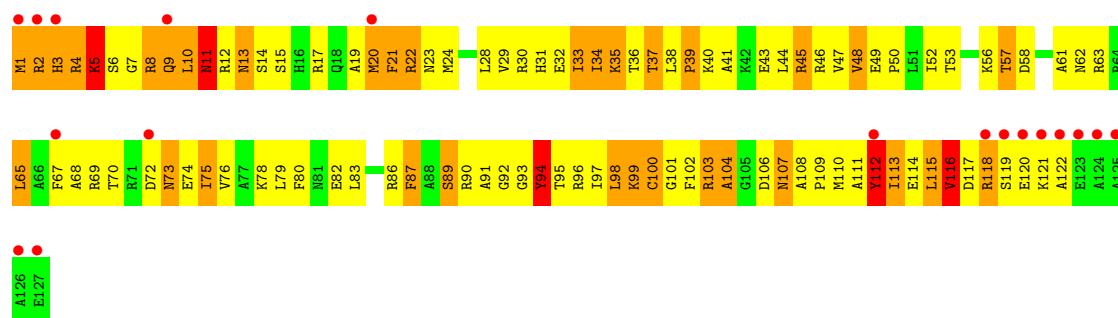
• Molecule 34: 50S ribosomal protein L16

Chain DM:



• Molecule 35: 50S ribosomal protein L17

Chain BN:





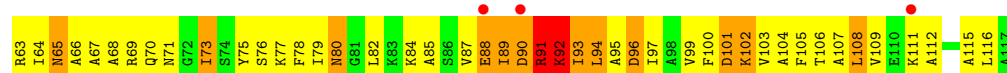
- Molecule 37: 50S ribosomal protein L19

Chain DP:



- Molecule 38: 50S ribosomal protein L20

Chain BQ:



- Molecule 38: 50S ribosomal protein L20

Chain DQ:



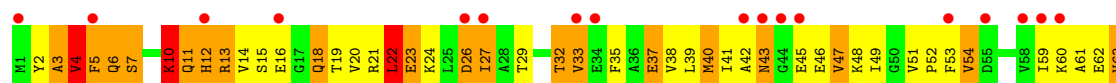
- Molecule 39: 50S ribosomal protein L21

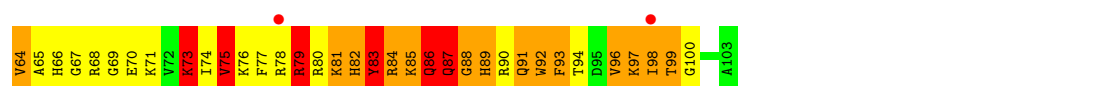
Chain BR:



- Molecule 39: 50S ribosomal protein L21

Chain DR:





- Molecule 40: 50S ribosomal protein L22

Chain BS:



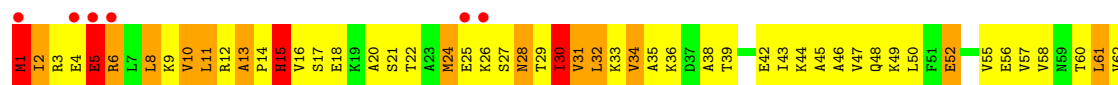
- Molecule 40: 50S ribosomal protein L22

Chain DS:



- Molecule 41: 50S ribosomal protein L23

Chain BT:



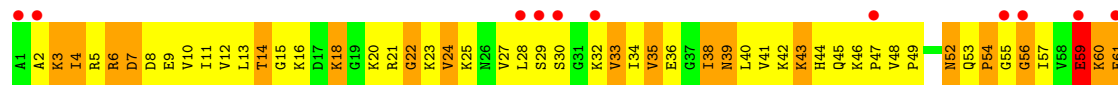
- Molecule 41: 50S ribosomal protein L23

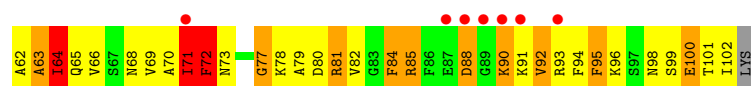
Chain DT:



- Molecule 42: 50S ribosomal protein L24

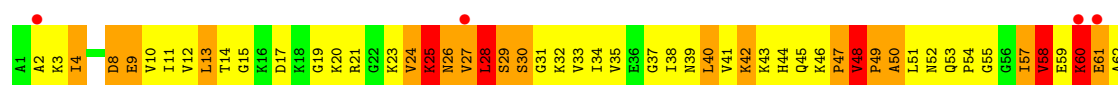
Chain BU:





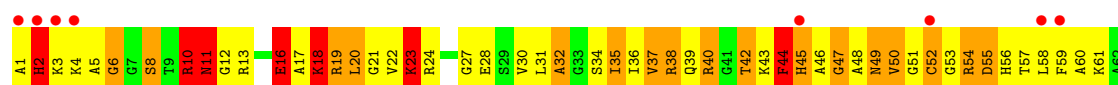
- Molecule 42: 50S ribosomal protein L24

Chain DU:



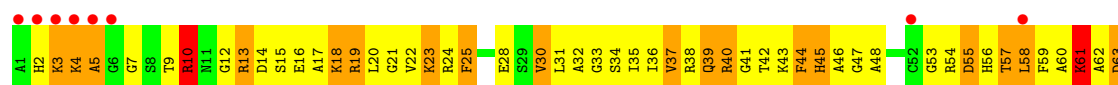
- Molecule 43: 50S ribosomal protein L27

Chain BW:



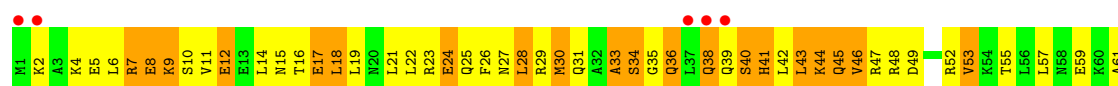
- Molecule 43: 50S ribosomal protein L27

Chain DW:



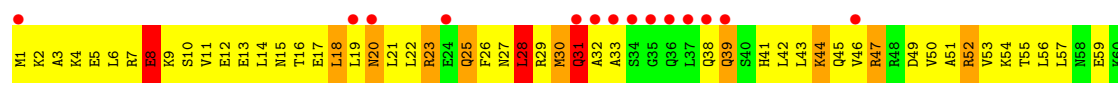
- Molecule 44: 50S ribosomal protein L29

Chain BX:



- Molecule 44: 50S ribosomal protein L29

Chain DX:



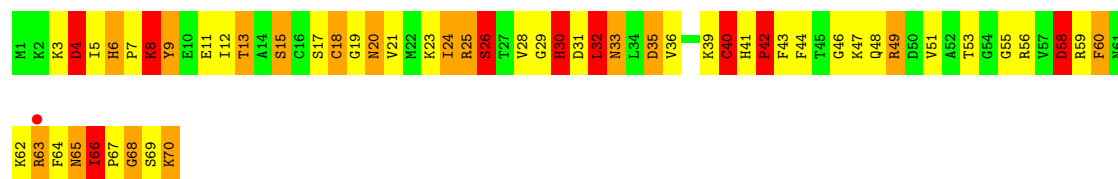
- Molecule 45: 50S ribosomal protein L30

Chain BY: 

- Molecule 45: 50S ribosomal protein L30

Chain DY: 

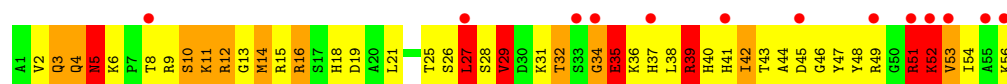
- Molecule 46: 50S ribosomal protein L31

Chain BZ: 

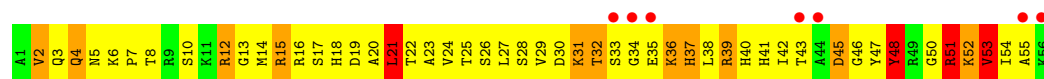
- Molecule 46: 50S ribosomal protein L31

Chain DZ: 

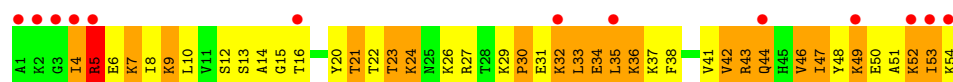
- Molecule 47: 50S ribosomal protein L32

Chain B0: 

- Molecule 47: 50S ribosomal protein L32

Chain D0: 

- Molecule 48: 50S ribosomal protein L33

Chain B1: 

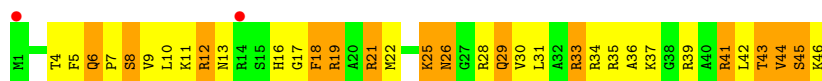
- Molecule 48: 50S ribosomal protein L33

Chain D1: 



- Molecule 49: 50S ribosomal protein L34

Chain B2: 



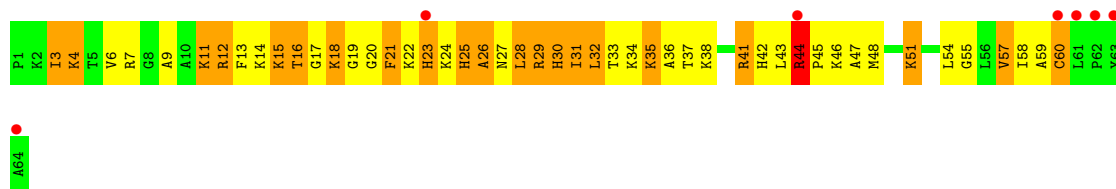
- Molecule 49: 50S ribosomal protein L34

Chain D2: 



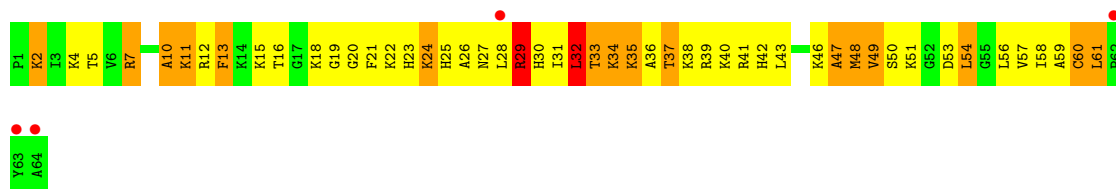
- Molecule 50: 50S ribosomal protein L35

Chain B3: 



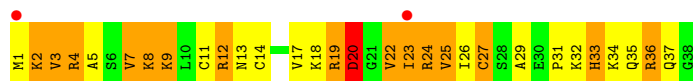
- Molecule 50: 50S ribosomal protein L35

Chain D3: 



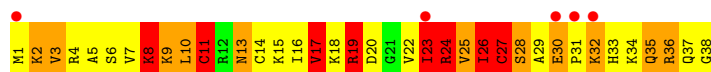
- Molecule 51: 50S ribosomal protein L36

Chain B4: 

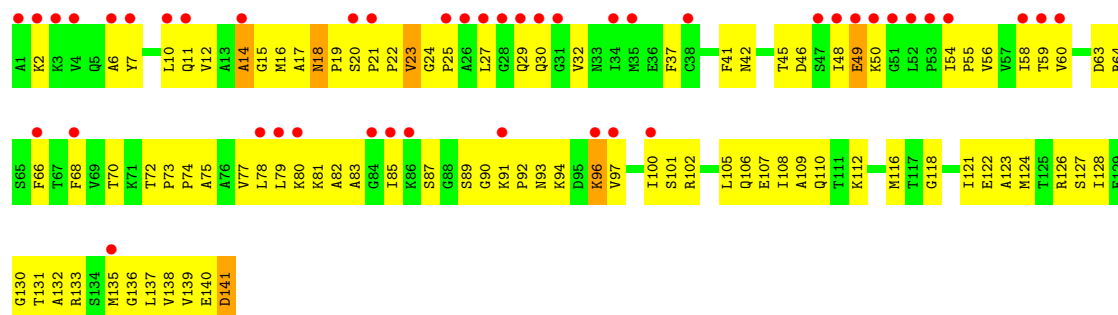


- Molecule 51: 50S ribosomal protein L36

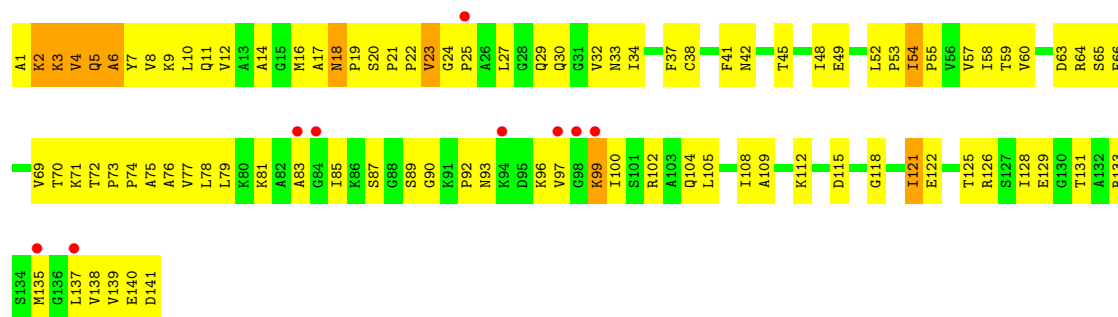
Chain D4: 



• Molecule 52: 50S ribosomal protein L11

Chain BI: 

• Molecule 52: 50S ribosomal protein L11

Chain DI: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.85Å 379.20Å 739.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	70.00 – 3.46 163.96 – 3.46	Depositor EDS
% Data completeness (in resolution range)	91.6 (70.00-3.46) 91.6 (163.96-3.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.49Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.279 , 0.331 0.262 , 0.307	Depositor DCC
R_{free} test set	34250 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.184	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 25.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 720727 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	284107	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.26	1/36762 (0.0%)	0.75	7/57350 (0.0%)
1	CA	0.26	2/36762 (0.0%)	0.75	11/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.47	0/2225
3	AD	0.23	0/1665	0.46	0/2227
3	CD	0.23	0/1665	0.45	0/2227
4	AE	0.23	0/1118	0.45	0/1504
4	CE	0.24	0/1118	0.45	0/1504
5	AF	0.25	0/835	0.47	0/1128
5	CF	0.24	0/835	0.49	0/1128
6	AG	0.23	0/1187	0.45	0/1591
6	CG	0.23	0/1211	0.45	0/1624
7	AH	0.23	0/989	0.45	0/1326
7	CH	0.23	0/989	0.46	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.24	0/1034	0.46	0/1375
9	AJ	0.23	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.47	0/1205
11	AL	0.22	0/969	0.47	0/1300
11	CL	0.22	0/969	0.48	0/1300
12	AM	0.21	0/892	0.48	0/1193
12	CM	0.21	0/884	0.46	0/1181
13	AN	0.24	0/785	0.46	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/724	0.45	0/966
14	CO	0.23	0/724	0.44	0/966
15	AP	0.26	0/659	0.44	0/884
15	CP	0.25	0/648	0.45	0/870
16	AQ	0.23	0/657	0.46	0/881
16	CQ	0.24	0/665	0.47	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.46	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.47	0/888
19	AT	0.23	0/671	0.41	0/888
19	CT	0.24	0/671	0.42	0/888
20	AB	0.25	0/1735	0.47	0/2338
20	CB	0.25	0/1735	0.47	0/2338
21	AU	1.01	4/430 (0.9%)	0.74	2/570 (0.4%)
21	CU	0.98	3/430 (0.7%)	0.82	3/570 (0.5%)
22	BA	0.27	0/2803	0.74	0/4371
22	DA	0.28	0/2803	0.77	0/4371
23	BB	0.33	15/68314 (0.0%)	0.79	63/106569 (0.1%)
23	DB	0.34	18/68314 (0.0%)	0.79	75/106569 (0.1%)
24	BV	0.30	0/766	0.53	0/1025
24	DV	0.25	0/766	0.46	0/1025
25	BC	0.40	0/2092	0.88	7/2813 (0.2%)
25	DC	0.40	0/2092	0.90	8/2813 (0.3%)
26	BD	0.40	0/1586	0.80	2/2134 (0.1%)
26	DD	0.37	0/1586	0.82	4/2134 (0.2%)
27	BE	0.45	1/1571 (0.1%)	0.88	6/2113 (0.3%)
27	DE	0.70	4/1571 (0.3%)	0.83	5/2113 (0.2%)
28	BF	0.33	0/1444	0.87	5/1937 (0.3%)
28	DF	0.41	1/1444 (0.1%)	1.00	10/1937 (0.5%)
29	BG	0.31	0/1343	0.69	0/1816
29	DG	0.30	0/1343	0.67	1/1816 (0.1%)
30	BH	0.28	0/1122	0.60	0/1515
30	DH	0.34	0/1122	0.71	1/1515 (0.1%)
31	BJ	0.41	1/1135 (0.1%)	0.72	3/1529 (0.2%)
31	DJ	0.32	0/1135	0.76	3/1529 (0.2%)
32	BK	0.35	0/939	1.00	2/1258 (0.2%)
32	DK	0.35	0/939	0.99	4/1258 (0.3%)
33	BL	0.69	0/1062	1.60	31/1413 (2.2%)
33	DL	0.74	1/1062 (0.1%)	1.58	25/1413 (1.8%)
34	BM	0.48	0/1093	1.03	8/1460 (0.5%)
34	DM	0.39	0/1093	0.85	5/1460 (0.3%)
35	BN	0.37	0/1021	0.92	7/1364 (0.5%)
35	DN	0.37	0/1021	0.80	3/1364 (0.2%)
36	BO	0.30	0/910	0.67	0/1219
36	DO	0.31	0/910	0.64	0/1219
37	BP	0.55	0/929	1.40	16/1242 (1.3%)
37	DP	0.58	0/929	1.40	16/1242 (1.3%)
38	BQ	0.41	0/960	0.86	3/1278 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.36	0/960	0.75	0/1278
39	BR	1.06	6/829 (0.7%)	1.42	13/1107 (1.2%)
39	DR	0.38	0/829	0.82	3/1107 (0.3%)
40	BS	0.27	0/864	0.68	1/1156 (0.1%)
40	DS	0.26	0/864	0.60	0/1156
41	BT	0.39	0/784	0.78	4/1048 (0.4%)
41	DT	0.45	1/784 (0.1%)	0.80	1/1048 (0.1%)
42	BU	0.33	0/787	0.74	0/1051
42	DU	0.37	0/787	0.94	7/1051 (0.7%)
43	BW	0.36	0/642	0.96	5/848 (0.6%)
43	DW	0.39	0/642	0.80	2/848 (0.2%)
44	BX	0.29	0/510	0.80	1/677 (0.1%)
44	DX	0.29	0/510	0.66	0/677
45	BY	0.31	0/453	0.64	0/605
45	DY	0.31	0/453	0.69	1/605 (0.2%)
46	BZ	0.48	0/559	1.04	5/745 (0.7%)
46	DZ	0.52	0/559	0.91	1/745 (0.1%)
47	B0	0.53	1/450 (0.2%)	1.15	7/599 (1.2%)
47	D0	0.41	0/450	0.97	3/599 (0.5%)
48	B1	0.36	0/448	0.71	0/594
48	D1	0.32	0/448	0.69	0/594
49	B2	0.33	0/380	0.64	0/498
49	D2	0.30	0/380	0.60	0/498
50	B3	0.47	0/513	0.95	1/676 (0.1%)
50	D3	0.39	0/513	0.80	1/676 (0.1%)
51	B4	0.40	0/303	0.73	0/397
51	D4	0.32	0/303	0.77	0/397
52	BI	0.26	0/1046	0.58	0/1410
52	DI	0.60	4/1046 (0.4%)	0.76	4/1410 (0.3%)
All	All	0.33	63/306469 (0.0%)	0.77	396/458101 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	16
1	CA	0	20
21	AU	0	1
22	DA	0	1
23	BB	0	60

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	1	65
25	BC	0	3
25	DC	0	2
31	BJ	0	2
33	BL	0	1
37	BP	0	1
37	DP	0	1
38	BQ	0	1
39	BR	0	1
39	DR	0	1
46	DZ	0	1
47	D0	0	1
All	All	1	178

The worst 5 of 63 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	DE	79	ARG	CD-NE	18.29	1.77	1.46
39	BR	53	PHE	CB-CG	17.86	1.81	1.51
23	DB	1086	A	C5-C6	-17.70	1.25	1.41
23	BB	1086	A	C5-C6	-17.70	1.25	1.41
21	CU	25	ALA	C-N	15.34	1.60	1.33

The worst 5 of 396 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	2791	G	O5'-P-OP1	-28.71	76.25	110.70
23	DB	2791	G	O5'-P-OP2	-27.77	77.38	110.70
23	DB	2791	G	O5'-P-OP1	18.50	132.90	110.70
23	BB	2791	G	O5'-P-OP2	18.20	132.54	110.70
23	DB	448	U	N1-C1'-C2'	17.52	136.78	114.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	DB	2076	U	C3'

5 of 178 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain

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Mol	Chain	Res	Type	Group
1	AA	437	U	Sidechain
1	AA	438	U	Sidechain
1	AA	58	C	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1157	0
1	CA	32831	0	16521	1198	0
2	AC	1624	0	1699	159	0
2	CC	1624	0	1699	148	0
3	AD	1643	0	1710	172	0
3	CD	1643	0	1710	167	0
4	AE	1105	0	1148	109	0
4	CE	1105	0	1148	143	0
5	AF	817	0	808	78	0
5	CF	817	0	808	93	0
6	AG	1174	0	1230	100	0
6	CG	1196	0	1246	98	0
7	AH	979	0	1034	78	0
7	CH	979	0	1034	86	0
8	AI	1022	0	1070	144	0
8	CI	1022	0	1070	127	0
9	AJ	786	0	828	92	0
9	CJ	786	0	828	106	0
10	AK	877	0	887	111	0
10	CK	877	0	887	108	0
11	AL	955	0	1019	103	0
11	CL	955	0	1019	101	0
12	AM	883	0	944	88	0
12	CM	876	0	937	95	0
13	AN	774	0	827	93	0
13	CN	774	0	827	114	0
14	AO	716	0	742	53	0
14	CO	716	0	742	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	AP	649	0	666	77	0
15	CP	638	0	656	71	0
16	AQ	648	0	691	80	0
16	CQ	656	0	702	85	0
17	AR	455	0	478	39	0
17	CR	455	0	478	41	0
18	AS	637	0	665	75	0
18	CS	644	0	675	87	0
19	AT	665	0	714	52	0
19	CT	665	0	714	64	0
20	AB	1704	0	1732	195	0
20	CB	1704	0	1732	152	0
21	AU	425	0	447	104	0
21	CU	425	0	449	84	0
22	BA	2507	0	1270	87	0
22	DA	2507	0	1270	97	0
23	BB	60995	0	30678	2393	0
23	DB	60995	0	30677	2365	0
24	BV	753	0	780	107	0
24	DV	753	0	780	69	0
25	BC	2053	0	2122	436	0
25	DC	2053	0	2122	433	0
26	BD	1565	0	1616	372	0
26	DD	1565	0	1616	316	0
27	BE	1552	0	1619	261	0
27	DE	1552	0	1619	266	0
28	BF	1420	0	1460	169	0
28	DF	1420	0	1460	181	0
29	BG	1323	0	1374	175	0
29	DG	1323	0	1374	162	0
30	BH	1111	0	1148	160	0
30	DH	1111	0	1148	145	0
31	BJ	1112	0	1147	219	0
31	DJ	1112	0	1147	231	0
32	BK	930	0	1000	121	0
32	DK	930	0	1000	126	0
33	BL	1053	0	1129	284	0
33	DL	1053	0	1129	227	0
34	BM	1074	0	1157	237	0
34	DM	1074	0	1157	189	0
35	BN	1008	0	1045	157	0
35	DN	1008	0	1045	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
36	BO	900	0	935	128	0
36	DO	900	0	935	128	0
37	BP	917	0	965	206	0
37	DP	917	0	965	209	0
38	BQ	947	0	1022	178	0
38	DQ	947	0	1022	161	0
39	BR	816	0	838	165	0
39	DR	816	0	839	180	0
40	BS	857	0	922	122	0
40	DS	857	0	922	111	0
41	BT	777	0	840	139	0
41	DT	777	0	840	129	0
42	BU	779	0	834	152	0
42	DU	779	0	834	134	0
43	BW	634	0	656	155	0
43	DW	634	0	656	156	0
44	BX	509	0	543	73	0
44	DX	509	0	543	90	0
45	BY	449	0	491	57	0
45	DY	449	0	491	64	0
46	BZ	549	0	552	114	0
46	DZ	549	0	552	101	0
47	B0	444	0	461	75	0
47	D0	444	0	461	80	0
48	B1	441	0	485	63	0
48	D1	441	0	485	69	0
49	B2	377	0	418	55	0
49	D2	377	0	418	66	0
50	B3	504	0	574	111	0
50	D3	504	0	574	113	0
51	B4	302	0	343	44	0
51	D4	302	0	343	80	0
52	BI	1032	0	1088	129	0
52	DI	1032	0	1088	214	0
53	AA	59	0	0	0	0
53	AP	1	0	0	0	0
53	BB	110	0	0	0	0
53	CA	62	0	0	0	0
53	DB	110	0	0	0	0
53	DN	1	0	0	0	0
54	AA	290	0	0	0	0
54	AE	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	AK	2	0	0	0	0
54	AN	4	0	0	0	0
54	AP	1	0	0	0	0
54	BB	497	0	0	12	0
54	BC	1	0	0	0	0
54	BE	5	0	0	0	0
54	BH	1	0	0	0	0
54	BL	2	0	0	0	0
54	BN	1	0	0	0	0
54	CA	295	0	0	1	0
54	CE	3	0	0	0	0
54	CK	1	0	0	0	0
54	CL	4	0	0	0	0
54	CN	2	0	0	0	0
54	CP	1	0	0	0	0
54	CT	2	0	0	0	0
54	D2	2	0	0	0	0
54	DB	499	0	0	7	0
54	DC	1	0	0	0	0
54	DD	1	0	0	0	0
54	DE	3	0	0	0	0
54	DJ	2	0	0	1	0
54	DL	1	0	0	0	0
54	DN	2	0	0	0	0
54	DQ	1	0	0	0	0
All	All	284107	0	190766	18478	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 39.

The worst 5 of 18478 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
52:DI:3:LYS:CE	52:DI:3:LYS:CD	1.74	1.64
39:BR:53:PHE:CG	39:BR:53:PHE:CB	1.81	1.61
39:BR:54:VAL:CA	39:BR:54:VAL:CB	1.78	1.57
27:DE:79:ARG:CG	27:DE:79:ARG:CD	1.78	1.57
52:DI:3:LYS:CG	52:DI:3:LYS:CD	1.81	1.56

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	AC	204/232 (88%)	135 (66%)	49 (24%)	20 (10%)	1	14
2	CC	204/232 (88%)	139 (68%)	45 (22%)	20 (10%)	1	14
3	AD	203/205 (99%)	131 (64%)	54 (27%)	18 (9%)	1	16
3	CD	203/205 (99%)	137 (68%)	49 (24%)	17 (8%)	1	18
4	AE	148/166 (89%)	107 (72%)	34 (23%)	7 (5%)	4	37
4	CE	148/166 (89%)	108 (73%)	31 (21%)	9 (6%)	2	29
5	AF	98/135 (73%)	69 (70%)	23 (24%)	6 (6%)	2	29
5	CF	98/135 (73%)	65 (66%)	23 (24%)	10 (10%)	1	12
6	AG	148/178 (83%)	103 (70%)	37 (25%)	8 (5%)	3	33
6	CG	150/178 (84%)	101 (67%)	36 (24%)	13 (9%)	1	17
7	AH	127/129 (98%)	105 (83%)	19 (15%)	3 (2%)	9	58
7	CH	127/129 (98%)	90 (71%)	31 (24%)	6 (5%)	4	37
8	AI	125/129 (97%)	87 (70%)	27 (22%)	11 (9%)	1	17
8	CI	125/129 (97%)	82 (66%)	33 (26%)	10 (8%)	1	20
9	AJ	96/103 (93%)	63 (66%)	21 (22%)	12 (12%)	1	8
9	CJ	96/103 (93%)	58 (60%)	21 (22%)	17 (18%)	0	3
10	AK	115/128 (90%)	75 (65%)	27 (24%)	13 (11%)	1	10
10	CK	115/128 (90%)	78 (68%)	27 (24%)	10 (9%)	1	17
11	AL	121/123 (98%)	74 (61%)	30 (25%)	17 (14%)	0	6
11	CL	121/123 (98%)	75 (62%)	28 (23%)	18 (15%)	0	5
12	AM	112/117 (96%)	87 (78%)	14 (12%)	11 (10%)	1	14
12	CM	111/117 (95%)	79 (71%)	17 (15%)	15 (14%)	0	7
13	AN	92/100 (92%)	59 (64%)	24 (26%)	9 (10%)	1	14
13	CN	92/100 (92%)	53 (58%)	24 (26%)	15 (16%)	0	4
14	AO	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	10	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CO	86/89 (97%)	67 (78%)	16 (19%)	3 (4%)	6	49
15	AP	80/82 (98%)	59 (74%)	17 (21%)	4 (5%)	3	35
15	CP	78/82 (95%)	52 (67%)	19 (24%)	7 (9%)	1	16
16	AQ	78/83 (94%)	48 (62%)	26 (33%)	4 (5%)	3	35
16	CQ	79/83 (95%)	61 (77%)	13 (16%)	5 (6%)	2	28
17	AR	53/74 (72%)	27 (51%)	19 (36%)	7 (13%)	0	7
17	CR	53/74 (72%)	39 (74%)	11 (21%)	3 (6%)	3	31
18	AS	77/91 (85%)	57 (74%)	14 (18%)	6 (8%)	1	20
18	CS	78/91 (86%)	48 (62%)	17 (22%)	13 (17%)	0	4
19	AT	83/86 (96%)	69 (83%)	8 (10%)	6 (7%)	2	24
19	CT	83/86 (96%)	61 (74%)	16 (19%)	6 (7%)	2	24
20	AB	216/240 (90%)	145 (67%)	53 (24%)	18 (8%)	1	19
20	CB	216/240 (90%)	150 (69%)	36 (17%)	30 (14%)	0	6
21	AU	49/71 (69%)	22 (45%)	12 (24%)	15 (31%)	0	0
21	CU	49/71 (69%)	28 (57%)	15 (31%)	6 (12%)	1	9
24	BV	92/94 (98%)	62 (67%)	21 (23%)	9 (10%)	1	14
24	DV	92/94 (98%)	59 (64%)	27 (29%)	6 (6%)	2	27
25	BC	265/273 (97%)	103 (39%)	83 (31%)	79 (30%)	0	0
25	DC	265/273 (97%)	97 (37%)	93 (35%)	75 (28%)	0	0
26	BD	207/209 (99%)	90 (44%)	69 (33%)	48 (23%)	0	1
26	DD	207/209 (99%)	96 (46%)	67 (32%)	44 (21%)	0	2
27	BE	199/201 (99%)	98 (49%)	60 (30%)	41 (21%)	0	2
27	DE	199/201 (99%)	87 (44%)	63 (32%)	49 (25%)	0	1
28	BF	176/178 (99%)	95 (54%)	48 (27%)	33 (19%)	0	2
28	DF	176/178 (99%)	91 (52%)	53 (30%)	32 (18%)	0	3
29	BG	174/176 (99%)	118 (68%)	39 (22%)	17 (10%)	1	14
29	DG	174/176 (99%)	117 (67%)	39 (22%)	18 (10%)	1	12
30	BH	147/149 (99%)	87 (59%)	45 (31%)	15 (10%)	1	12
30	DH	147/149 (99%)	84 (57%)	44 (30%)	19 (13%)	0	8
31	BJ	138/142 (97%)	67 (49%)	42 (30%)	29 (21%)	0	2
31	DJ	138/142 (97%)	70 (51%)	36 (26%)	32 (23%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	BK	119/123 (97%)	71 (60%)	32 (27%)	16 (13%)	0	7
32	DK	119/123 (97%)	72 (60%)	25 (21%)	22 (18%)	0	2
33	BL	142/144 (99%)	60 (42%)	40 (28%)	42 (30%)	0	0
33	DL	142/144 (99%)	66 (46%)	37 (26%)	39 (28%)	0	0
34	BM	134/136 (98%)	69 (52%)	37 (28%)	28 (21%)	0	2
34	DM	134/136 (98%)	79 (59%)	31 (23%)	24 (18%)	0	3
35	BN	125/127 (98%)	73 (58%)	35 (28%)	17 (14%)	0	7
35	DN	125/127 (98%)	82 (66%)	32 (26%)	11 (9%)	1	17
36	BO	115/117 (98%)	64 (56%)	26 (23%)	25 (22%)	0	1
36	DO	115/117 (98%)	63 (55%)	33 (29%)	19 (16%)	0	4
37	BP	112/114 (98%)	39 (35%)	36 (32%)	37 (33%)	0	0
37	DP	112/114 (98%)	42 (38%)	38 (34%)	32 (29%)	0	0
38	BQ	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	1	12
38	DQ	115/117 (98%)	79 (69%)	22 (19%)	14 (12%)	1	9
39	BR	101/103 (98%)	44 (44%)	31 (31%)	26 (26%)	0	1
39	DR	101/103 (98%)	42 (42%)	31 (31%)	28 (28%)	0	0
40	BS	108/110 (98%)	63 (58%)	27 (25%)	18 (17%)	0	4
40	DS	108/110 (98%)	67 (62%)	20 (18%)	21 (19%)	0	2
41	BT	97/100 (97%)	42 (43%)	40 (41%)	15 (16%)	0	4
41	DT	97/100 (97%)	42 (43%)	32 (33%)	23 (24%)	0	1
42	BU	100/103 (97%)	33 (33%)	46 (46%)	21 (21%)	0	2
42	DU	100/103 (97%)	46 (46%)	41 (41%)	13 (13%)	0	8
43	BW	82/84 (98%)	29 (35%)	26 (32%)	27 (33%)	0	0
43	DW	82/84 (98%)	31 (38%)	30 (37%)	21 (26%)	0	1
44	BX	61/63 (97%)	28 (46%)	21 (34%)	12 (20%)	0	2
44	DX	61/63 (97%)	38 (62%)	15 (25%)	8 (13%)	0	8
45	BY	56/58 (97%)	29 (52%)	17 (30%)	10 (18%)	0	3
45	DY	56/58 (97%)	35 (62%)	17 (30%)	4 (7%)	2	24
46	BZ	68/70 (97%)	29 (43%)	26 (38%)	13 (19%)	0	2
46	DZ	68/70 (97%)	37 (54%)	22 (32%)	9 (13%)	0	7
47	B0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	D0	54/56 (96%)	30 (56%)	15 (28%)	9 (17%)	0	4
48	B1	52/54 (96%)	19 (36%)	23 (44%)	10 (19%)	0	2
48	D1	52/54 (96%)	21 (40%)	22 (42%)	9 (17%)	0	3
49	B2	44/46 (96%)	23 (52%)	14 (32%)	7 (16%)	0	4
49	D2	44/46 (96%)	24 (54%)	12 (27%)	8 (18%)	0	3
50	B3	62/64 (97%)	30 (48%)	25 (40%)	7 (11%)	1	10
50	D3	62/64 (97%)	35 (56%)	17 (27%)	10 (16%)	0	4
51	B4	36/38 (95%)	18 (50%)	9 (25%)	9 (25%)	0	1
51	D4	36/38 (95%)	13 (36%)	11 (31%)	12 (33%)	0	0
52	BI	139/141 (99%)	124 (89%)	11 (8%)	4 (3%)	7	54
52	DI	139/141 (99%)	123 (88%)	11 (8%)	5 (4%)	5	48
All	All	11263/11902 (95%)	6645 (59%)	2936 (26%)	1682 (15%)	0	5

5 of 1682 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	2	GLN
2	AC	91	ALA
2	AC	153	SER
3	AD	18	LEU
3	AD	31	CYS

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	AC	170/189 (90%)	142 (84%)	28 (16%)	3	19
2	CC	170/189 (90%)	146 (86%)	24 (14%)	5	28
3	AD	172/172 (100%)	140 (81%)	32 (19%)	2	13
3	CD	172/172 (100%)	137 (80%)	35 (20%)	2	10
4	AE	113/125 (90%)	92 (81%)	21 (19%)	2	13
4	CE	113/125 (90%)	92 (81%)	21 (19%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AF	87/116 (75%)	68 (78%)	19 (22%)	1	8
5	CF	87/116 (75%)	74 (85%)	13 (15%)	4	25
6	AG	123/146 (84%)	102 (83%)	21 (17%)	3	17
6	CG	125/146 (86%)	106 (85%)	19 (15%)	4	24
7	AH	104/104 (100%)	87 (84%)	17 (16%)	3	20
7	CH	104/104 (100%)	85 (82%)	19 (18%)	2	13
8	AI	105/106 (99%)	83 (79%)	22 (21%)	1	9
8	CI	105/106 (99%)	89 (85%)	16 (15%)	4	24
9	AJ	86/90 (96%)	66 (77%)	20 (23%)	1	6
9	CJ	86/90 (96%)	78 (91%)	8 (9%)	13	51
10	AK	90/98 (92%)	70 (78%)	20 (22%)	1	7
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	15
11	AL	103/103 (100%)	88 (85%)	15 (15%)	5	26
11	CL	103/103 (100%)	79 (77%)	24 (23%)	1	6
12	AM	92/95 (97%)	70 (76%)	22 (24%)	1	6
12	CM	91/95 (96%)	75 (82%)	16 (18%)	3	15
13	AN	79/83 (95%)	67 (85%)	12 (15%)	4	24
13	CN	79/83 (95%)	68 (86%)	11 (14%)	5	28
14	AO	76/77 (99%)	69 (91%)	7 (9%)	13	52
14	CO	76/77 (99%)	63 (83%)	13 (17%)	3	17
15	AP	65/65 (100%)	56 (86%)	9 (14%)	5	28
15	CP	65/65 (100%)	54 (83%)	11 (17%)	3	18
16	AQ	74/77 (96%)	60 (81%)	14 (19%)	2	12
16	CQ	75/77 (97%)	66 (88%)	9 (12%)	7	36
17	AR	48/64 (75%)	45 (94%)	3 (6%)	25	72
17	CR	48/64 (75%)	41 (85%)	7 (15%)	5	26
18	AS	70/78 (90%)	60 (86%)	10 (14%)	5	27
18	CS	71/78 (91%)	53 (75%)	18 (25%)	1	5
19	AT	65/65 (100%)	56 (86%)	9 (14%)	5	28
19	CT	65/65 (100%)	51 (78%)	14 (22%)	1	8
20	AB	180/198 (91%)	142 (79%)	38 (21%)	1	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CB	180/198 (91%)	153 (85%)	27 (15%)	4	25
21	AU	44/61 (72%)	36 (82%)	8 (18%)	2	14
21	CU	44/61 (72%)	30 (68%)	14 (32%)	0	3
24	BV	78/78 (100%)	66 (85%)	12 (15%)	4	23
24	DV	78/78 (100%)	69 (88%)	9 (12%)	8	38
25	BC	213/218 (98%)	145 (68%)	68 (32%)	0	3
25	DC	213/218 (98%)	150 (70%)	63 (30%)	0	3
26	BD	164/164 (100%)	112 (68%)	52 (32%)	0	3
26	DD	164/164 (100%)	113 (69%)	51 (31%)	0	3
27	BE	165/165 (100%)	115 (70%)	50 (30%)	0	3
27	DE	165/165 (100%)	127 (77%)	38 (23%)	1	7
28	BF	149/149 (100%)	119 (80%)	30 (20%)	2	10
28	DF	149/149 (100%)	122 (82%)	27 (18%)	2	14
29	BG	137/137 (100%)	105 (77%)	32 (23%)	1	6
29	DG	137/137 (100%)	111 (81%)	26 (19%)	2	12
30	BH	114/114 (100%)	85 (75%)	29 (25%)	1	5
30	DH	114/114 (100%)	90 (79%)	24 (21%)	1	9
31	BJ	114/116 (98%)	84 (74%)	30 (26%)	1	4
31	DJ	114/116 (98%)	85 (75%)	29 (25%)	1	5
32	BK	102/104 (98%)	78 (76%)	24 (24%)	1	6
32	DK	102/104 (98%)	81 (79%)	21 (21%)	2	9
33	BL	103/103 (100%)	62 (60%)	41 (40%)	0	1
33	DL	103/103 (100%)	68 (66%)	35 (34%)	0	2
34	BM	109/109 (100%)	77 (71%)	32 (29%)	0	3
34	DM	109/109 (100%)	75 (69%)	34 (31%)	0	3
35	BN	103/103 (100%)	78 (76%)	25 (24%)	1	5
35	DN	103/103 (100%)	76 (74%)	27 (26%)	1	4
36	BO	87/87 (100%)	58 (67%)	29 (33%)	0	2
36	DO	87/87 (100%)	69 (79%)	18 (21%)	2	9
37	BP	99/99 (100%)	77 (78%)	22 (22%)	1	7
37	DP	99/99 (100%)	67 (68%)	32 (32%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	BQ	89/89 (100%)	66 (74%)	23 (26%)	1	4
38	DQ	89/89 (100%)	71 (80%)	18 (20%)	2	10
39	BR	84/84 (100%)	68 (81%)	16 (19%)	2	12
39	DR	84/84 (100%)	58 (69%)	26 (31%)	0	3
40	BS	93/93 (100%)	72 (77%)	21 (23%)	1	7
40	DS	93/93 (100%)	77 (83%)	16 (17%)	3	17
41	BT	83/84 (99%)	60 (72%)	23 (28%)	0	4
41	DT	83/84 (99%)	60 (72%)	23 (28%)	0	4
42	BU	83/84 (99%)	62 (75%)	21 (25%)	1	5
42	DU	83/84 (99%)	60 (72%)	23 (28%)	0	4
43	BW	62/62 (100%)	46 (74%)	16 (26%)	1	4
43	DW	62/62 (100%)	45 (73%)	17 (27%)	0	4
44	BX	55/55 (100%)	40 (73%)	15 (27%)	0	4
44	DX	55/55 (100%)	43 (78%)	12 (22%)	1	8
45	BY	48/48 (100%)	36 (75%)	12 (25%)	1	5
45	DY	48/48 (100%)	33 (69%)	15 (31%)	0	3
46	BZ	62/62 (100%)	43 (69%)	19 (31%)	0	3
46	DZ	62/62 (100%)	46 (74%)	16 (26%)	1	4
47	B0	47/47 (100%)	31 (66%)	16 (34%)	0	2
47	D0	47/47 (100%)	33 (70%)	14 (30%)	0	3
48	B1	48/48 (100%)	33 (69%)	15 (31%)	0	3
48	D1	48/48 (100%)	33 (69%)	15 (31%)	0	3
49	B2	38/38 (100%)	27 (71%)	11 (29%)	0	3
49	D2	38/38 (100%)	27 (71%)	11 (29%)	0	3
50	B3	51/51 (100%)	33 (65%)	18 (35%)	0	2
50	D3	51/51 (100%)	40 (78%)	11 (22%)	1	8
51	B4	34/34 (100%)	21 (62%)	13 (38%)	0	1
51	D4	34/34 (100%)	17 (50%)	17 (50%)	0	0
52	BI	109/109 (100%)	106 (97%)	3 (3%)	56	90
52	DI	109/109 (100%)	104 (95%)	5 (5%)	37	81
All	All	9341/9692 (96%)	7268 (78%)	2073 (22%)	1	7

5 of 2073 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	BW	54	ARG
6	CG	10	LYS
41	DT	82	LYS
45	BY	19	HIS
51	B4	9	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 317 such sidechains are listed below:

Mol	Chain	Res	Type
40	BS	9	HIS
3	CD	53	GLN
39	DR	6	GLN
42	BU	65	GLN
46	BZ	41	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	277 (18%)	25 (1%)
1	CA	1529/1542 (99%)	249 (16%)	26 (1%)
22	BA	116/120 (96%)	23 (19%)	0
22	DA	116/120 (96%)	20 (17%)	1 (0%)
23	BB	2837/2904 (97%)	451 (15%)	18 (0%)
23	DB	2837/2904 (97%)	482 (16%)	22 (0%)
All	All	8964/9132 (98%)	1502 (16%)	92 (1%)

5 of 1502 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	7	A
1	AA	9	G
1	AA	14	U
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A

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Mol	Chain	Res	Type
1	CA	429	U
23	DB	2198	A
23	BB	2756	U
1	CA	279	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 343 ligands modelled in this entry, 343 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
21	AU	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	AU	15:LEU	C	16:ARG	N	0.99

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	1530/1542 (99%)	-0.32	10 (0%) 84 54	16, 66, 135, 180	0
1	CA	1530/1542 (99%)	-0.43	8 (0%) 88 63	11, 49, 119, 180	0
2	AC	206/232 (88%)	0.20	1 (0%) 88 63	8, 56, 116, 163	0
2	CC	206/232 (88%)	0.10	0 100 100	13, 68, 122, 154	0
3	AD	205/205 (100%)	0.40	3 (1%) 70 35	16, 65, 125, 180	0
3	CD	205/205 (100%)	0.26	3 (1%) 70 35	5, 49, 103, 156	0
4	AE	150/166 (90%)	0.16	2 (1%) 74 39	5, 56, 104, 151	0
4	CE	150/166 (90%)	0.27	2 (1%) 74 39	5, 49, 101, 167	0
5	AF	100/135 (74%)	0.75	7 (7%) 16 7	19, 64, 113, 150	0
5	CF	100/135 (74%)	0.84	4 (4%) 36 15	10, 65, 113, 147	0
6	AG	150/178 (84%)	0.17	3 (2%) 62 29	23, 86, 133, 180	0
6	CG	152/178 (85%)	0.04	1 (0%) 84 54	22, 83, 132, 166	0
7	AH	129/129 (100%)	0.43	1 (0%) 83 51	8, 63, 113, 155	0
7	CH	129/129 (100%)	0.32	2 (1%) 68 33	5, 49, 104, 154	0
8	AI	127/129 (98%)	0.18	2 (1%) 68 33	5, 83, 126, 169	0
8	CI	127/129 (98%)	-0.23	1 (0%) 83 51	23, 81, 135, 161	0
9	AJ	98/103 (95%)	0.25	1 (1%) 79 46	14, 76, 141, 160	0
9	CJ	98/103 (95%)	-0.03	0 100 100	27, 78, 122, 143	0
10	AK	117/128 (91%)	0.39	0 100 100	6, 56, 99, 164	0
10	CK	117/128 (91%)	0.29	1 (0%) 81 49	5, 44, 95, 117	0
11	AL	123/123 (100%)	0.30	1 (0%) 83 51	18, 59, 115, 162	0
11	CL	123/123 (100%)	0.13	0 100 100	5, 34, 109, 141	0
12	AM	114/117 (97%)	0.21	1 (0%) 81 49	37, 96, 137, 155	0
12	CM	113/117 (96%)	-0.10	0 100 100	19, 92, 143, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	-0.00	0 100 100	11, 76, 133, 147	0
13	CN	96/100 (96%)	-0.16	1 (1%) 79 46	32, 73, 130, 160	0
14	AO	88/89 (98%)	0.30	2 (2%) 57 26	15, 62, 104, 177	0
14	CO	88/89 (98%)	0.30	2 (2%) 57 26	5, 46, 113, 136	0
15	AP	82/82 (100%)	0.16	4 (4%) 28 11	20, 72, 132, 171	0
15	CP	80/82 (97%)	0.09	1 (1%) 74 39	5, 42, 126, 137	0
16	AQ	80/83 (96%)	0.68	3 (3%) 38 16	34, 77, 119, 158	0
16	CQ	81/83 (97%)	0.43	1 (1%) 75 41	11, 52, 113, 155	0
17	AR	55/74 (74%)	0.45	0 100 100	16, 60, 124, 148	0
17	CR	55/74 (74%)	0.45	2 (3%) 41 17	17, 45, 118, 139	0
18	AS	79/91 (86%)	0.28	0 100 100	44, 110, 140, 169	0
18	CS	80/91 (87%)	0.25	2 (2%) 54 24	47, 99, 151, 161	0
19	AT	85/86 (98%)	0.13	0 100 100	37, 83, 123, 155	0
19	CT	85/86 (98%)	0.13	0 100 100	9, 49, 103, 139	0
20	AB	218/240 (90%)	0.40	6 (2%) 50 22	17, 82, 131, 156	0
20	CB	218/240 (90%)	0.65	11 (5%) 28 11	13, 90, 135, 162	0
21	AU	51/71 (71%)	0.46	2 (3%) 37 16	29, 80, 131, 158	0
21	CU	51/71 (71%)	0.49	1 (1%) 62 29	34, 73, 112, 140	0
22	BA	117/120 (97%)	-0.28	1 (0%) 81 49	36, 62, 94, 157	0
22	DA	117/120 (97%)	-0.31	1 (0%) 81 49	27, 62, 113, 180	0
23	BB	2841/2904 (97%)	-0.16	31 (1%) 77 42	10, 49, 134, 180	0
23	DB	2841/2904 (97%)	-0.24	16 (0%) 86 58	5, 39, 133, 180	0
24	BV	94/94 (100%)	0.39	3 (3%) 45 19	20, 75, 130, 149	0
24	DV	94/94 (100%)	0.55	0 100 100	17, 71, 119, 130	0
25	BC	267/273 (97%)	0.64	18 (6%) 17 8	5, 51, 136, 180	0
25	DC	267/273 (97%)	0.85	24 (8%) 10 6	5, 46, 139, 180	0
26	BD	209/209 (100%)	1.15	30 (14%) 3 3	21, 82, 174, 180	0
26	DD	209/209 (100%)	0.76	24 (11%) 5 4	5, 60, 139, 180	0
27	BE	201/201 (100%)	0.91	31 (15%) 3 2	8, 78, 147, 180	0
27	DE	201/201 (100%)	0.79	22 (10%) 6 4	5, 76, 164, 180	0
28	BF	178/178 (100%)	0.58	8 (4%) 32 13	43, 98, 152, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DF	178/178 (100%)	0.17	8 (4%)	32 13	29, 89, 138, 180	0
29	BG	176/176 (100%)	0.54	8 (4%)	32 13	23, 94, 154, 180	0
29	DG	176/176 (100%)	0.44	9 (5%)	27 11	20, 86, 154, 172	0
30	BH	149/149 (100%)	1.45	43 (28%)	1 1	23, 120, 170, 180	0
30	DH	149/149 (100%)	0.82	9 (6%)	21 9	31, 100, 153, 180	0
31	BJ	140/142 (98%)	0.48	7 (5%)	28 11	14, 79, 160, 180	0
31	DJ	140/142 (98%)	0.48	3 (2%)	60 28	14, 61, 136, 162	0
32	BK	121/123 (98%)	0.95	7 (5%)	22 9	13, 57, 106, 147	0
32	DK	121/123 (98%)	0.21	0	100 100	5, 37, 84, 143	0
33	BL	144/144 (100%)	1.48	32 (22%)	1 2	19, 93, 160, 180	0
33	DL	144/144 (100%)	1.01	19 (13%)	4 3	7, 74, 150, 179	0
34	BM	136/136 (100%)	0.39	8 (5%)	22 9	16, 71, 168, 180	0
34	DM	136/136 (100%)	0.85	16 (11%)	5 4	10, 66, 152, 180	0
35	BN	127/127 (100%)	0.96	18 (14%)	3 3	19, 67, 149, 180	0
35	DN	127/127 (100%)	0.45	10 (7%)	13 7	5, 45, 143, 180	0
36	BO	117/117 (100%)	1.23	14 (11%)	5 4	20, 82, 150, 180	0
36	DO	117/117 (100%)	0.62	11 (9%)	9 5	20, 77, 150, 169	0
37	BP	114/114 (100%)	1.17	21 (18%)	2 2	21, 84, 177, 180	0
37	DP	114/114 (100%)	0.78	8 (7%)	16 7	8, 69, 148, 180	0
38	BQ	117/117 (100%)	0.24	3 (2%)	53 23	8, 63, 125, 174	0
38	DQ	117/117 (100%)	0.48	8 (6%)	17 8	11, 57, 127, 180	0
39	BR	103/103 (100%)	1.01	12 (11%)	5 4	33, 100, 153, 180	0
39	DR	103/103 (100%)	1.18	19 (18%)	2 2	26, 92, 154, 180	0
40	BS	110/110 (100%)	0.54	6 (5%)	24 10	14, 57, 132, 180	0
40	DS	110/110 (100%)	0.43	2 (1%)	65 31	5, 45, 137, 175	0
41	BT	99/100 (99%)	0.78	9 (9%)	9 5	25, 73, 150, 170	0
41	DT	99/100 (99%)	0.95	12 (12%)	5 3	16, 84, 160, 180	0
42	BU	102/103 (99%)	1.04	18 (17%)	2 2	18, 92, 158, 178	0
42	DU	102/103 (99%)	0.26	4 (3%)	37 16	11, 103, 161, 180	0
43	BW	84/84 (100%)	1.07	17 (20%)	2 2	22, 87, 153, 180	0
43	DW	84/84 (100%)	0.86	12 (14%)	3 3	20, 81, 149, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BX	63/63 (100%)	0.98	7 (11%) 6 4	28, 92, 148, 170	0
44	DX	63/63 (100%)	0.92	14 (22%) 1 2	47, 96, 162, 171	0
45	BY	58/58 (100%)	0.88	8 (13%) 4 3	29, 72, 150, 180	0
45	DY	58/58 (100%)	0.56	6 (10%) 7 5	5, 60, 129, 177	0
46	BZ	70/70 (100%)	0.39	1 (1%) 72 37	20, 68, 134, 168	0
46	DZ	70/70 (100%)	0.49	1 (1%) 72 37	16, 59, 132, 180	0
47	B0	56/56 (100%)	1.30	13 (23%) 1 2	23, 89, 163, 180	0
47	D0	56/56 (100%)	0.82	7 (12%) 5 3	12, 61, 148, 180	0
48	B1	54/54 (100%)	1.48	13 (24%) 1 2	18, 89, 142, 179	0
48	D1	54/54 (100%)	1.72	12 (22%) 1 2	22, 77, 153, 173	0
49	B2	46/46 (100%)	0.37	2 (4%) 34 14	11, 47, 152, 180	0
49	D2	46/46 (100%)	0.35	0 100 100	13, 48, 112, 129	0
50	B3	64/64 (100%)	0.73	7 (10%) 6 4	15, 61, 149, 180	0
50	D3	64/64 (100%)	0.64	4 (6%) 19 8	8, 55, 125, 169	0
51	B4	38/38 (100%)	0.67	2 (5%) 25 10	36, 85, 161, 180	0
51	D4	38/38 (100%)	0.86	5 (13%) 4 3	20, 80, 168, 180	0
52	BI	141/141 (100%)	1.60	45 (31%) 1 1	61, 151, 180, 180	0
52	DI	141/141 (100%)	0.71	9 (6%) 19 8	84, 157, 180, 180	0
All	All	20439/21034 (97%)	0.20	830 (4%) 35 15	5, 61, 145, 180	0

The worst 5 of 830 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
36	BO	57	ALA	14.0
36	BO	58	ILE	13.9
23	BB	139	U	10.6
36	BO	59	ALA	10.6
33	BL	98	ALA	9.4

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
53	MG	CA	1653	1/1	0.25	80.00	45,45,45,45	0
53	MG	BB	3100	1/1	0.24	24.68	11,11,11,11	1
53	MG	AA	1636	1/1	0.47	19.90	127,127,127,127	0
53	MG	AA	1649	1/1	0.16	14.50	114,114,114,114	0
53	MG	AA	1625	1/1	0.19	13.00	5,5,5,5	1
53	MG	CA	1621	1/1	0.21	10.19	113,113,113,113	0
53	MG	AA	1638	1/1	0.24	7.53	98,98,98,98	0
53	MG	AA	1656	1/1	0.23	5.95	66,66,66,66	0
53	MG	CA	1623	1/1	0.17	5.10	151,151,151,151	0
53	MG	AA	1646	1/1	0.21	4.62	60,60,60,60	0
53	MG	AA	1658	1/1	0.19	3.91	167,167,167,167	0
53	MG	BB	3078	1/1	0.22	3.09	25,25,25,25	0
53	MG	AA	1624	1/1	0.16	3.01	79,79,79,79	0
53	MG	BB	3105	1/1	0.22	2.27	64,64,64,64	0
53	MG	BB	3033	1/1	0.20	2.13	93,93,93,93	0
53	MG	BB	3067	1/1	0.19	2.05	78,78,78,78	0
53	MG	CA	1602	1/1	0.17	2.04	32,32,32,32	0
53	MG	DB	3065	1/1	0.16	1.71	47,47,47,47	1
53	MG	BB	3093	1/1	0.24	1.62	5,5,5,5	1
53	MG	BB	3039	1/1	0.20	1.43	45,45,45,45	0
53	MG	BB	3028	1/1	0.19	1.37	40,40,40,40	0
53	MG	BB	3031	1/1	0.19	1.19	45,45,45,45	0
53	MG	DB	3094	1/1	0.23	1.08	5,5,5,5	1
53	MG	CA	1649	1/1	0.18	0.96	88,88,88,88	0
53	MG	DB	3058	1/1	0.33	0.78	30,30,30,30	1
53	MG	DB	3110	1/1	0.18	0.72	54,54,54,54	0
53	MG	BB	3097	1/1	0.14	0.46	74,74,74,74	0
53	MG	AA	1612	1/1	0.15	0.38	104,104,104,104	0
53	MG	AA	1619	1/1	0.15	0.30	100,100,100,100	0
53	MG	DB	3052	1/1	0.16	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1609	1/1	0.17	0.22	45,45,45,45	0
53	MG	DB	3029	1/1	0.26	0.16	41,41,41,41	0
53	MG	AA	1629	1/1	0.18	-0.01	138,138,138,138	0
53	MG	CA	1641	1/1	0.14	-0.11	92,92,92,92	0
53	MG	CA	1659	1/1	0.16	-0.18	48,48,48,48	0
53	MG	CA	1660	1/1	0.16	-0.20	65,65,65,65	0
53	MG	CA	1616	1/1	0.12	-0.33	68,68,68,68	0
53	MG	AA	1622	1/1	0.17	-0.38	116,116,116,116	0
53	MG	BB	3088	1/1	0.16	-0.39	34,34,34,34	0
53	MG	DB	3001	1/1	0.16	-0.47	7,7,7,7	0
53	MG	BB	3098	1/1	0.16	-0.48	45,45,45,45	0
53	MG	AA	1615	1/1	0.12	-0.57	43,43,43,43	0
53	MG	CA	1613	1/1	0.13	-0.61	78,78,78,78	0
53	MG	BB	3110	1/1	0.13	-0.68	60,60,60,60	0
53	MG	AA	1655	1/1	0.15	-0.68	75,75,75,75	0
53	MG	DB	3043	1/1	0.14	-0.68	9,9,9,9	0
53	MG	BB	3057	1/1	0.15	-0.74	27,27,27,27	0
53	MG	DB	3057	1/1	0.09	-0.85	28,28,28,28	0
53	MG	BB	3075	1/1	0.18	-0.87	31,31,31,31	0
53	MG	AA	1620	1/1	0.13	-0.89	62,62,62,62	0
53	MG	DN	201	1/1	0.19	-0.94	49,49,49,49	0
53	MG	DB	3077	1/1	0.16	-0.96	57,57,57,57	0
53	MG	AA	1627	1/1	0.14	-0.97	72,72,72,72	0
53	MG	CA	1634	1/1	0.14	-1.01	61,61,61,61	0
53	MG	BB	3005	1/1	0.12	-1.03	5,5,5,5	0
53	MG	CA	1636	1/1	0.11	-1.08	51,51,51,51	0
53	MG	AA	1637	1/1	0.12	-1.08	81,81,81,81	0
53	MG	CA	1662	1/1	0.13	-1.08	26,26,26,26	0
53	MG	AA	1645	1/1	0.12	-1.12	27,27,27,27	0
53	MG	DB	3024	1/1	0.11	-1.16	36,36,36,36	0
53	MG	BB	3036	1/1	0.15	-1.23	37,37,37,37	0
53	MG	AA	1623	1/1	0.16	-1.23	32,32,32,32	1
53	MG	AA	1640	1/1	0.10	-1.24	44,44,44,44	0
53	MG	BB	3054	1/1	0.13	-1.25	72,72,72,72	0
53	MG	DB	3062	1/1	0.13	-1.26	43,43,43,43	0
53	MG	DB	3044	1/1	0.07	-1.27	7,7,7,7	0
53	MG	CA	1615	1/1	0.10	-1.29	101,101,101,101	0
53	MG	DB	3063	1/1	0.08	-1.35	13,13,13,13	0
53	MG	DB	3026	1/1	0.15	-1.36	18,18,18,18	0
53	MG	BB	3021	1/1	0.14	-1.37	55,55,55,55	0
53	MG	DB	3095	1/1	0.15	-1.38	55,55,55,55	0
53	MG	BB	3010	1/1	0.11	-1.39	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3034	1/1	0.12	-1.43	25,25,25,25	0
53	MG	DB	3083	1/1	0.16	-1.47	27,27,27,27	0
53	MG	CA	1624	1/1	0.13	-1.47	48,48,48,48	0
53	MG	DB	3003	1/1	0.07	-1.49	14,14,14,14	0
53	MG	DB	3055	1/1	0.07	-1.50	19,19,19,19	0
53	MG	DB	3010	1/1	0.08	-1.53	12,12,12,12	0
53	MG	CA	1614	1/1	0.09	-1.54	47,47,47,47	0
53	MG	DB	3013	1/1	0.15	-1.57	34,34,34,34	0
53	MG	DB	3059	1/1	0.10	-1.61	127,127,127,127	0
53	MG	DB	3068	1/1	0.11	-1.63	14,14,14,14	0
53	MG	BB	3012	1/1	0.10	-1.64	41,41,41,41	0
53	MG	DB	3023	1/1	0.06	-1.67	34,34,34,34	0
53	MG	BB	3003	1/1	0.06	-1.67	13,13,13,13	0
53	MG	AA	1653	1/1	0.10	-1.70	65,65,65,65	0
53	MG	AA	1604	1/1	0.14	-1.72	45,45,45,45	0
53	MG	DB	3004	1/1	0.12	-1.73	19,19,19,19	0
53	MG	CA	1656	1/1	0.11	-1.75	48,48,48,48	0
53	MG	DB	3070	1/1	0.07	-1.78	46,46,46,46	0
53	MG	BB	3087	1/1	0.13	-1.78	45,45,45,45	0
53	MG	CA	1607	1/1	0.06	-1.79	18,18,18,18	0
53	MG	AA	1634	1/1	0.10	-1.80	85,85,85,85	0
53	MG	CA	1635	1/1	0.11	-1.83	20,20,20,20	0
53	MG	DB	3093	1/1	0.06	-1.86	10,10,10,10	0
53	MG	DB	3030	1/1	0.14	-1.89	23,23,23,23	0
53	MG	BB	3016	1/1	0.15	-1.90	15,15,15,15	0
53	MG	CA	1642	1/1	0.09	-1.90	45,45,45,45	0
53	MG	BB	3051	1/1	0.08	-1.91	71,71,71,71	0
53	MG	BB	3007	1/1	0.15	-1.97	28,28,28,28	0
53	MG	DB	3025	1/1	0.14	-2.00	21,21,21,21	0
53	MG	CA	1655	1/1	0.11	-2.04	48,48,48,48	0
53	MG	BB	3049	1/1	0.10	-2.10	11,11,11,11	0
53	MG	DB	3082	1/1	0.15	-2.14	73,73,73,73	0
53	MG	DB	3034	1/1	0.14	-2.14	66,66,66,66	0
53	MG	CA	1637	1/1	0.10	-2.17	68,68,68,68	0
53	MG	CA	1645	1/1	0.12	-2.18	82,82,82,82	0
53	MG	BB	3032	1/1	0.13	-2.19	9,9,9,9	0
53	MG	AA	1635	1/1	0.07	-2.19	85,85,85,85	0
53	MG	DB	3109	1/1	0.06	-2.23	24,24,24,24	0
53	MG	BB	3104	1/1	0.13	-2.25	18,18,18,18	0
53	MG	AA	1628	1/1	0.11	-2.28	26,26,26,26	0
53	MG	BB	3025	1/1	0.16	-2.40	53,53,53,53	0
53	MG	CA	1612	1/1	0.08	-2.43	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	AA	1617	1/1	0.12	-2.45	78,78,78,78	0
53	MG	BB	3081	1/1	0.15	-2.49	46,46,46,46	0
53	MG	AA	1641	1/1	0.10	-2.51	49,49,49,49	0
53	MG	DB	3086	1/1	0.14	-2.51	69,69,69,69	0
53	MG	AA	1659	1/1	0.12	-2.52	105,105,105,105	0
53	MG	BB	3056	1/1	0.11	-2.53	19,19,19,19	0
53	MG	DB	3053	1/1	0.14	-2.54	27,27,27,27	0
53	MG	DB	3038	1/1	0.09	-2.60	16,16,16,16	0
53	MG	BB	3109	1/1	0.13	-2.65	15,15,15,15	0
53	MG	CA	1630	1/1	0.09	-2.67	5,5,5,5	1
53	MG	AA	1607	1/1	0.10	-2.72	27,27,27,27	0
53	MG	BB	3055	1/1	0.12	-2.72	27,27,27,27	0
53	MG	DB	3073	1/1	0.10	-2.73	16,16,16,16	0
53	MG	BB	3038	1/1	0.04	-2.75	58,58,58,58	0
53	MG	BB	3107	1/1	0.07	-2.75	27,27,27,27	0
53	MG	AA	1639	1/1	0.07	-2.76	47,47,47,47	0
53	MG	AA	1601	1/1	0.06	-2.88	26,26,26,26	0
53	MG	AA	1610	1/1	0.09	-2.88	34,34,34,34	0
53	MG	DB	3060	1/1	0.11	-2.91	77,77,77,77	0
53	MG	DB	3090	1/1	0.12	-2.94	28,28,28,28	0
53	MG	BB	3086	1/1	0.14	-2.95	37,37,37,37	0
53	MG	BB	3029	1/1	0.06	-2.96	13,13,13,13	0
53	MG	CA	1603	1/1	0.12	-2.97	69,69,69,69	0
53	MG	DB	3104	1/1	0.12	-3.01	50,50,50,50	0
53	MG	CA	1629	1/1	0.06	-3.04	45,45,45,45	0
53	MG	AA	1603	1/1	0.11	-3.06	43,43,43,43	0
53	MG	BB	3096	1/1	0.13	-3.06	43,43,43,43	0
53	MG	CA	1622	1/1	0.08	-3.10	67,67,67,67	0
53	MG	BB	3091	1/1	0.06	-3.10	19,19,19,19	0
53	MG	BB	3050	1/1	0.07	-3.13	35,35,35,35	0
53	MG	BB	3071	1/1	0.12	-3.16	24,24,24,24	0
53	MG	DB	3101	1/1	0.11	-3.21	27,27,27,27	0
53	MG	DB	3042	1/1	0.09	-3.23	27,27,27,27	0
53	MG	DB	3072	1/1	0.07	-3.31	30,30,30,30	0
53	MG	DB	3103	1/1	0.13	-3.31	50,50,50,50	0
53	MG	AA	1608	1/1	0.07	-3.31	121,121,121,121	0
53	MG	CA	1657	1/1	0.06	-3.33	37,37,37,37	0
53	MG	DB	3022	1/1	0.07	-3.38	15,15,15,15	0
53	MG	DB	3091	1/1	0.08	-3.43	96,96,96,96	0
53	MG	DB	3036	1/1	0.09	-3.44	16,16,16,16	0
53	MG	BB	3082	1/1	0.14	-3.45	19,19,19,19	0
53	MG	DB	3017	1/1	0.11	-3.46	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1640	1/1	0.07	-3.47	11,11,11,11	0
53	MG	BB	3090	1/1	0.08	-3.53	74,74,74,74	0
53	MG	BB	3058	1/1	0.10	-3.55	28,28,28,28	0
53	MG	AA	1611	1/1	0.07	-3.56	40,40,40,40	0
53	MG	AA	1651	1/1	0.07	-3.57	84,84,84,84	0
53	MG	AA	1616	1/1	0.07	-3.59	46,46,46,46	0
53	MG	BB	3073	1/1	0.09	-3.60	28,28,28,28	0
53	MG	CA	1646	1/1	0.07	-3.65	42,42,42,42	0
53	MG	AA	1652	1/1	0.07	-3.65	25,25,25,25	0
53	MG	CA	1618	1/1	0.10	-3.69	5,5,5,5	0
53	MG	DB	3051	1/1	0.12	-3.71	53,53,53,53	0
53	MG	DB	3014	1/1	0.08	-3.71	5,5,5,5	0
53	MG	DB	3088	1/1	0.13	-3.73	35,35,35,35	0
53	MG	BB	3099	1/1	0.11	-3.73	30,30,30,30	0
53	MG	BB	3102	1/1	0.11	-3.75	19,19,19,19	0
53	MG	AA	1614	1/1	0.11	-3.76	62,62,62,62	0
53	MG	AA	1648	1/1	0.05	-3.76	94,94,94,94	0
53	MG	AA	1632	1/1	0.05	-3.81	53,53,53,53	0
53	MG	AA	1643	1/1	0.09	-3.82	73,73,73,73	0
53	MG	DB	3047	1/1	0.11	-3.83	17,17,17,17	0
53	MG	BB	3018	1/1	0.08	-3.86	27,27,27,27	0
53	MG	CA	1626	1/1	0.08	-3.90	73,73,73,73	0
53	MG	DB	3050	1/1	0.10	-3.92	74,74,74,74	0
53	MG	AA	1609	1/1	0.14	-3.98	8,8,8,8	0
53	MG	BB	3077	1/1	0.09	-4.02	44,44,44,44	0
53	MG	BB	3011	1/1	0.12	-4.03	7,7,7,7	0
53	MG	CA	1639	1/1	0.07	-4.06	117,117,117,117	0
53	MG	DB	3046	1/1	0.07	-4.08	33,33,33,33	0
53	MG	BB	3074	1/1	0.11	-4.11	13,13,13,13	0
53	MG	BB	3080	1/1	0.10	-4.14	31,31,31,31	0
53	MG	BB	3026	1/1	0.10	-4.17	5,5,5,5	0
53	MG	DB	3085	1/1	0.08	-4.21	17,17,17,17	0
53	MG	DB	3035	1/1	0.09	-4.26	30,30,30,30	0
53	MG	CA	1617	1/1	0.10	-4.27	9,9,9,9	0
53	MG	DB	3096	1/1	0.10	-4.31	20,20,20,20	0
53	MG	DB	3108	1/1	0.06	-4.31	5,5,5,5	0
53	MG	AA	1633	1/1	0.06	-4.32	75,75,75,75	0
53	MG	AA	1630	1/1	0.09	-4.36	30,30,30,30	0
53	MG	CA	1648	1/1	0.07	-4.43	56,56,56,56	0
53	MG	BB	3040	1/1	0.10	-4.48	21,21,21,21	0
53	MG	CA	1651	1/1	0.09	-4.49	14,14,14,14	0
53	MG	BB	3046	1/1	0.08	-4.57	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	BB	3092	1/1	0.06	-4.60	11,11,11,11	0
53	MG	BB	3037	1/1	0.07	-4.61	24,24,24,24	0
53	MG	BB	3079	1/1	0.09	-4.62	38,38,38,38	0
53	MG	BB	3063	1/1	0.14	-4.64	27,27,27,27	0
53	MG	CA	1643	1/1	0.09	-4.64	41,41,41,41	0
53	MG	BB	3022	1/1	0.07	-4.71	38,38,38,38	0
53	MG	CA	1620	1/1	0.07	-4.75	35,35,35,35	0
53	MG	DB	3071	1/1	0.07	-4.78	39,39,39,39	0
53	MG	DB	3064	1/1	0.07	-4.80	28,28,28,28	0
53	MG	DB	3007	1/1	0.11	-4.80	12,12,12,12	0
53	MG	DB	3020	1/1	0.11	-4.81	20,20,20,20	0
53	MG	BB	3048	1/1	0.06	-4.81	20,20,20,20	0
53	MG	BB	3019	1/1	0.08	-4.82	27,27,27,27	0
53	MG	CA	1606	1/1	0.08	-4.82	74,74,74,74	0
53	MG	DB	3041	1/1	0.07	-4.88	18,18,18,18	0
53	MG	DB	3107	1/1	0.09	-4.90	19,19,19,19	0
53	MG	DB	3074	1/1	0.08	-4.90	25,25,25,25	0
53	MG	BB	3052	1/1	0.09	-4.93	19,19,19,19	0
53	MG	BB	3066	1/1	0.10	-4.97	59,59,59,59	0
53	MG	CA	1611	1/1	0.10	-4.98	71,71,71,71	0
53	MG	BB	3017	1/1	0.10	-5.00	72,72,72,72	0
53	MG	DB	3098	1/1	0.12	-5.01	18,18,18,18	0
53	MG	DB	3012	1/1	0.11	-5.03	6,6,6,6	0
53	MG	CA	1661	1/1	0.06	-5.04	62,62,62,62	0
53	MG	BB	3084	1/1	0.10	-5.10	5,5,5,5	0
53	MG	BB	3108	1/1	0.08	-5.14	19,19,19,19	0
53	MG	BB	3004	1/1	0.04	-5.15	21,21,21,21	0
53	MG	AA	1621	1/1	0.09	-5.15	23,23,23,23	0
53	MG	DB	3097	1/1	0.10	-5.18	15,15,15,15	0
53	MG	BB	3065	1/1	0.13	-5.18	47,47,47,47	0
53	MG	BB	3083	1/1	0.08	-5.20	20,20,20,20	0
53	MG	CA	1652	1/1	0.08	-5.23	44,44,44,44	0
53	MG	DB	3040	1/1	0.12	-5.23	5,5,5,5	0
53	MG	BB	3061	1/1	0.06	-5.25	42,42,42,42	0
53	MG	CA	1601	1/1	0.04	-5.26	5,5,5,5	0
53	MG	BB	3069	1/1	0.08	-5.28	9,9,9,9	0
53	MG	DB	3087	1/1	0.11	-5.33	6,6,6,6	0
53	MG	DB	3028	1/1	0.10	-5.33	28,28,28,28	0
53	MG	DB	3048	1/1	0.06	-5.37	20,20,20,20	0
53	MG	BB	3013	1/1	0.08	-5.38	31,31,31,31	0
53	MG	DB	3105	1/1	0.11	-5.43	23,23,23,23	0
53	MG	BB	3043	1/1	0.10	-5.45	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	CA	1647	1/1	0.07	-5.45	32,32,32,32	0
53	MG	DB	3031	1/1	0.12	-5.50	18,18,18,18	0
53	MG	DB	3069	1/1	0.09	-5.60	44,44,44,44	0
53	MG	BB	3006	1/1	0.05	-5.64	10,10,10,10	0
53	MG	DB	3054	1/1	0.07	-5.64	15,15,15,15	0
53	MG	BB	3027	1/1	0.10	-5.66	23,23,23,23	0
53	MG	DB	3011	1/1	0.08	-5.67	8,8,8,8	0
53	MG	BB	3094	1/1	0.09	-5.68	35,35,35,35	0
53	MG	CA	1605	1/1	0.07	-5.80	18,18,18,18	0
53	MG	BB	3041	1/1	0.06	-5.86	30,30,30,30	0
53	MG	CA	1608	1/1	0.06	-5.87	110,110,110,110	0
53	MG	DB	3005	1/1	0.07	-5.92	9,9,9,9	0
53	MG	DB	3076	1/1	0.07	-5.94	17,17,17,17	0
53	MG	CA	1650	1/1	0.12	-5.94	82,82,82,82	0
53	MG	CA	1604	1/1	0.08	-5.95	18,18,18,18	0
53	MG	BB	3044	1/1	0.06	-5.97	32,32,32,32	0
53	MG	DB	3067	1/1	0.10	-6.00	17,17,17,17	0
53	MG	BB	3008	1/1	0.06	-6.02	58,58,58,58	0
53	MG	DB	3002	1/1	0.12	-6.03	37,37,37,37	0
53	MG	BB	3053	1/1	0.07	-6.04	6,6,6,6	0
53	MG	DB	3016	1/1	0.10	-6.06	23,23,23,23	0
53	MG	DB	3084	1/1	0.07	-6.07	8,8,8,8	0
53	MG	DB	3081	1/1	0.07	-6.12	25,25,25,25	0
53	MG	DB	3027	1/1	0.07	-6.14	10,10,10,10	0
53	MG	AA	1613	1/1	0.06	-6.16	42,42,42,42	0
53	MG	AA	1642	1/1	0.08	-6.29	70,70,70,70	0
53	MG	DB	3045	1/1	0.07	-6.32	61,61,61,61	0
53	MG	DB	3049	1/1	0.06	-6.38	5,5,5,5	0
53	MG	CA	1625	1/1	0.09	-6.41	26,26,26,26	0
53	MG	DB	3089	1/1	0.05	-6.43	65,65,65,65	0
53	MG	BB	3045	1/1	0.05	-6.52	31,31,31,31	0
53	MG	AA	1606	1/1	0.06	-6.72	59,59,59,59	0
53	MG	CA	1631	1/1	0.08	-6.76	36,36,36,36	0
53	MG	BB	3060	1/1	0.08	-6.86	69,69,69,69	0
53	MG	AA	1644	1/1	0.11	-6.86	96,96,96,96	0
53	MG	BB	3024	1/1	0.10	-6.87	22,22,22,22	0
53	MG	DB	3099	1/1	0.06	-6.89	9,9,9,9	0
53	MG	DB	3033	1/1	0.09	-6.90	11,11,11,11	0
53	MG	BB	3035	1/1	0.08	-7.14	12,12,12,12	0
53	MG	BB	3076	1/1	0.05	-7.17	24,24,24,24	0
53	MG	BB	3095	1/1	0.08	-7.25	34,34,34,34	0
53	MG	DB	3100	1/1	0.09	-7.26	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3080	1/1	0.08	-7.31	12,12,12,12	0
53	MG	CA	1654	1/1	0.06	-7.35	40,40,40,40	0
53	MG	BB	3059	1/1	0.07	-7.38	10,10,10,10	0
53	MG	DB	3021	1/1	0.10	-7.39	16,16,16,16	0
53	MG	CA	1638	1/1	0.04	-7.41	37,37,37,37	0
53	MG	DB	3009	1/1	0.07	-7.49	7,7,7,7	0
53	MG	BB	3047	1/1	0.06	-7.50	114,114,114,114	0
53	MG	DB	3075	1/1	0.04	-7.53	5,5,5,5	0
53	MG	BB	3072	1/1	0.09	-7.59	24,24,24,24	0
53	MG	AA	1647	1/1	0.10	-7.77	23,23,23,23	0
53	MG	CA	1644	1/1	0.06	-7.90	29,29,29,29	0
53	MG	AA	1605	1/1	0.08	-8.03	48,48,48,48	0
53	MG	AA	1650	1/1	0.05	-8.13	72,72,72,72	0
53	MG	CA	1632	1/1	0.11	-8.16	61,61,61,61	0
53	MG	DB	3008	1/1	0.11	-8.39	24,24,24,24	0
53	MG	DB	3018	1/1	0.08	-8.41	29,29,29,29	0
53	MG	BB	3103	1/1	0.07	-8.41	7,7,7,7	0
53	MG	BB	3101	1/1	0.05	-8.44	12,12,12,12	0
53	MG	DB	3106	1/1	0.05	-8.64	21,21,21,21	0
53	MG	BB	3002	1/1	0.10	-8.74	10,10,10,10	0
53	MG	BB	3023	1/1	0.07	-8.84	22,22,22,22	0
53	MG	DB	3015	1/1	0.09	-8.85	49,49,49,49	0
53	MG	DB	3102	1/1	0.09	-9.00	26,26,26,26	0
53	MG	DB	3078	1/1	0.07	-9.05	18,18,18,18	0
53	MG	CA	1658	1/1	0.06	-9.50	38,38,38,38	0
53	MG	BB	3085	1/1	0.06	-9.53	22,22,22,22	0
53	MG	CA	1619	1/1	0.11	-9.89	26,26,26,26	0
53	MG	BB	3001	1/1	0.06	-9.90	10,10,10,10	0
53	MG	AA	1657	1/1	0.06	-9.90	81,81,81,81	0
53	MG	BB	3020	1/1	0.06	-9.94	23,23,23,23	0
53	MG	DB	3019	1/1	0.04	-9.97	5,5,5,5	0
53	MG	DB	3079	1/1	0.09	-10.03	5,5,5,5	0
53	MG	BB	3009	1/1	0.07	-10.04	35,35,35,35	0
53	MG	AA	1626	1/1	0.06	-10.09	35,35,35,35	0
53	MG	BB	3015	1/1	0.07	-10.13	24,24,24,24	0
53	MG	DB	3037	1/1	0.07	-10.78	13,13,13,13	0
53	MG	BB	3030	1/1	0.05	-10.82	53,53,53,53	0
53	MG	AA	1602	1/1	0.08	-10.88	62,62,62,62	0
53	MG	BB	3042	1/1	0.09	-11.00	95,95,95,95	0
53	MG	DB	3092	1/1	0.07	-11.23	23,23,23,23	0
53	MG	AA	1618	1/1	0.05	-11.24	46,46,46,46	0
53	MG	DB	3066	1/1	0.07	-12.40	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
53	MG	DB	3006	1/1	0.07	-12.50	5,5,5,5	0
53	MG	BB	3064	1/1	0.06	-13.01	39,39,39,39	0
53	MG	DB	3032	1/1	0.10	-13.14	46,46,46,46	0
53	MG	DB	3039	1/1	0.07	-13.17	19,19,19,19	0
53	MG	AA	1654	1/1	0.09	-13.89	59,59,59,59	0
53	MG	BB	3089	1/1	0.08	-14.43	45,45,45,45	0
53	MG	DB	3056	1/1	0.07	-14.82	11,11,11,11	0
53	MG	BB	3062	1/1	0.09	-15.04	22,22,22,22	0
53	MG	DB	3061	1/1	0.07	-15.11	78,78,78,78	0
53	MG	CA	1610	1/1	0.03	-15.25	34,34,34,34	0
53	MG	BB	3106	1/1	0.11	-17.60	46,46,46,46	0
53	MG	CA	1633	1/1	0.06	-18.49	47,47,47,47	0
53	MG	BB	3070	1/1	0.08	-19.44	32,32,32,32	0
53	MG	BB	3014	1/1	0.04	-21.81	29,29,29,29	0
53	MG	CA	1628	1/1	0.09	-25.67	55,55,55,55	1
53	MG	BB	3068	1/1	0.09	-38.78	24,24,24,24	0
53	MG	AA	1631	1/1	0.07	-	61,61,61,61	0
53	MG	CA	1627	1/1	0.13	-	29,29,29,29	1
53	MG	AP	101	1/1	0.31	-	53,53,53,53	1

6.5 Other polymers ⓘ

There are no such residues in this entry.