



wwPDB X-ray Structure Validation Summary Report i

Jun 16, 2014 – 06:36 PM BST

PDB ID : 4V55
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with gentamicin and ribosome recycling factor (RRF).
Authors : Borovinskaya, M.A.; Pai, R.D.; Zhang, W.; Schuwirth, B.-S.; Holton, J.M.; Hirokawa, G.; Kaji, H.; Kaji, A.; Cate, J.H.D.
Deposited on : 2007-06-17
Resolution : 4.00 Å(reported)

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

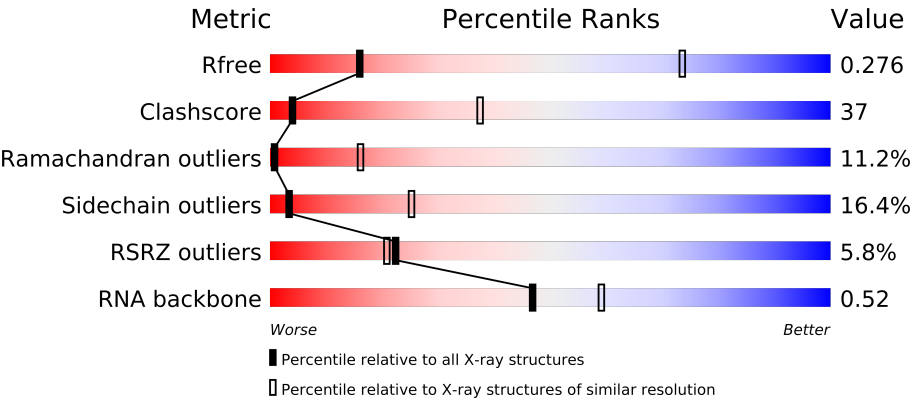
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	66092	1035 (4.52-3.46)
Clashscore	79885	1235 (4.50-3.50)
Ramachandran outliers	78287	1170 (4.50-3.50)
Sidechain outliers	78261	1156 (4.50-3.50)
RSRZ outliers	66119	1035 (4.52-3.46)
RNA backbone	1838	1018 (5.00-2.80)

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	70	
21	CU	70	
22	BA	120	
22	DA	120	
23	BB	2904	
23	DB	2904	
24	BI	141	
24	DI	141	
25	BC	272	
25	DC	272	
26	BD	209	
26	DD	209	
27	BK	123	
27	DK	123	

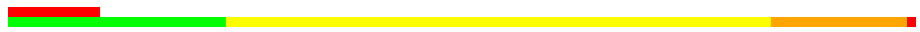
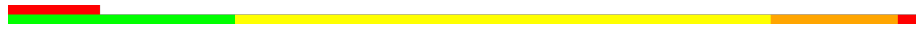


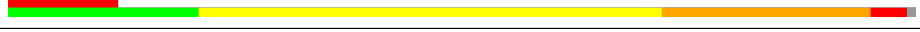
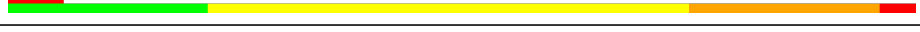
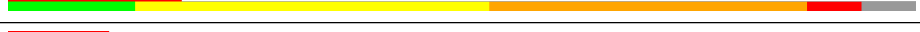


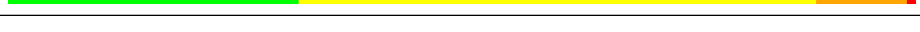
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Mol	Chain	Length	Quality of chain
28	BP	114	
28	DP	114	
29	BE	201	
29	DE	201	
30	BY	58	
30	DY	58	
31	B0	56	
31	D0	56	
32	B4	38	
32	D4	38	
33	B1	54	
33	D1	54	
34	B3	64	
34	D3	64	
35	BV	94	
35	DV	94	
36	B2	46	
36	D2	46	
37	BL	144	
37	DL	144	
38	BM	136	
38	DM	136	
39	BX	63	
39	DX	63	
40	BH	149	
40	DH	149	
41	BJ	142	
41	DJ	142	
42	BN	127	
42	DN	127	
43	BO	117	
43	DO	117	
44	BQ	117	
44	DQ	117	
45	BS	110	
45	DS	110	
46	BU	103	
46	DU	103	
47	BF	178	
47	DF	178	
48	BG	176	
48	DG	176	

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Mol	Chain	Length	Quality of chain
49	BR	103	
49	DR	103	
50	BT	100	
50	DT	100	
51	BZ	78	
51	DZ	78	
52	BW	84	
52	DW	84	
53	B6	185	
53	D6	185	

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

Mol	Type	Chain	Res	Geometry	Electron density
54	MG	AA	1608	-	X
54	MG	AA	1619	-	X
54	MG	AA	1622	-	X
54	MG	AA	1623	-	X
54	MG	AA	1625	-	X
54	MG	AA	1626	-	X
54	MG	AA	1632	-	X
54	MG	AA	1637	-	X
54	MG	AA	1647	-	X
54	MG	AA	1656	-	X
54	MG	AA	1657	-	X
54	MG	AA	1659	-	X
54	MG	BB	3004	-	X
54	MG	BB	3033	-	X
54	MG	BB	3038	-	X
54	MG	BB	3093	-	X
54	MG	CA	1621	-	X
54	MG	CA	1627	-	X
54	MG	CA	1635	-	X
54	MG	CA	1641	-	X
54	MG	CA	1657	-	X
54	MG	CA	1658	-	X
54	MG	DB	3011	-	X
54	MG	DB	3058	-	X
54	MG	DB	3059	-	X
54	MG	DB	3073	-	X
55	LLL	BB	3111	-	X
55	LLL	DB	3112	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 287083 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	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
			1021	634	206	178	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
			714	439	144	130	1			
14	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	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
			657	417	122	115	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 rRNA.

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 rRNA.

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 L11.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
25	DC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	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 L14.

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

- Molecule 28 is a protein called 50S ribosomal protein L19.

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

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

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

- Molecule 30 is a protein called 50S ribosomal protein L30.

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

- Molecule 31 is a protein called 50S ribosomal protein L32.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
33	B1	50	Total	C	N	O	0	0	0
			409	263	75	71			
33	D1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 34 is a protein called 50S ribosomal protein L35.

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

- Molecule 35 is a protein called 50S ribosomal protein L25.

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

- Molecule 36 is a protein called 50S ribosomal protein L34.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

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

- Molecule 39 is a protein called 50S ribosomal protein L29.

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

- Molecule 40 is a protein called 50S ribosomal protein L9.

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

- Molecule 41 is a protein called 50S ribosomal protein L13.

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

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	DN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

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

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

- Molecule 46 is a protein called 50S ribosomal protein L24.

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

- Molecule 47 is a protein called 50S ribosomal protein L5.

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

- Molecule 48 is a protein called 50S ribosomal protein L6.

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

- Molecule 49 is a protein called 50S ribosomal protein L21.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
50	DT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
51	DZ	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 52 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
52	DW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

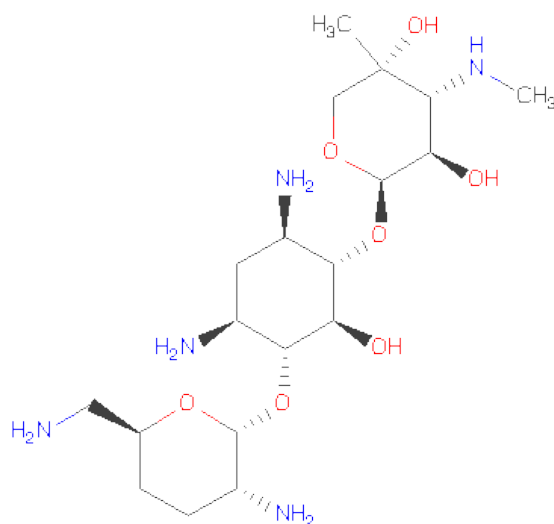
- Molecule 53 is a protein called 50S ribosomal protein RRF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			
53	D6	185	Total	C	N	O	S	0	0	0
			1478	924	270	282	2			

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	DB	111	Total	Mg	0	0
			111	111		
54	BB	110	Total	Mg	0	0
			110	110		
54	AA	60	Total	Mg	0	0
			60	60		
54	CA	61	Total	Mg	0	0
			61	61		
54	CE	1	Total	Mg	0	0
			1	1		

- Molecule 55 is (2R,3R,4R,5R)-2-((1S,2S,3R,4S,6R)-4,6-DIAMINO-3-((2R,3R,6S)-3-AMINO-6-(AMINOMETHYL)-TETRAHYDRO-2H-PYRAN-2-YLOXY)-2-HYDROXYCYCLOHEXYLOXY)-5-METHYL-4-(METHYLAMINO)-TETRAHYDRO-2H-PYRAN-3,5-DIOL (three-letter code: LLL) (formula: C₁₉H₃₉N₅O₇).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	AA	1	Total	C	N	O	0	0
			31	19	5	7		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
55	BB	1	Total	C	N	O	0	0
			31	19	5	7		
55	CA	1	Total	C	N	O	0	0
			31	19	5	7		
55	DB	1	Total	C	N	O	0	0
			31	19	5	7		

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	B4	1	Total	Zn	0	0
			1	1		
56	D4	1	Total	Zn	0	0
			1	1		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	287	Total	O	0	0
			287	287		
57	AE	3	Total	O	0	0
			3	3		
57	AK	1	Total	O	0	0
			1	1		
57	AL	3	Total	O	0	0
			3	3		
57	AN	4	Total	O	0	0
			4	4		
57	AT	2	Total	O	0	0
			2	2		
57	BB	492	Total	O	0	0
			492	492		
57	BC	6	Total	O	0	0
			6	6		
57	BD	1	Total	O	0	0
			1	1		
57	BE	3	Total	O	0	0
			3	3		
57	BL	3	Total	O	0	0
			3	3		
57	BT	1	Total	O	0	0
			1	1		

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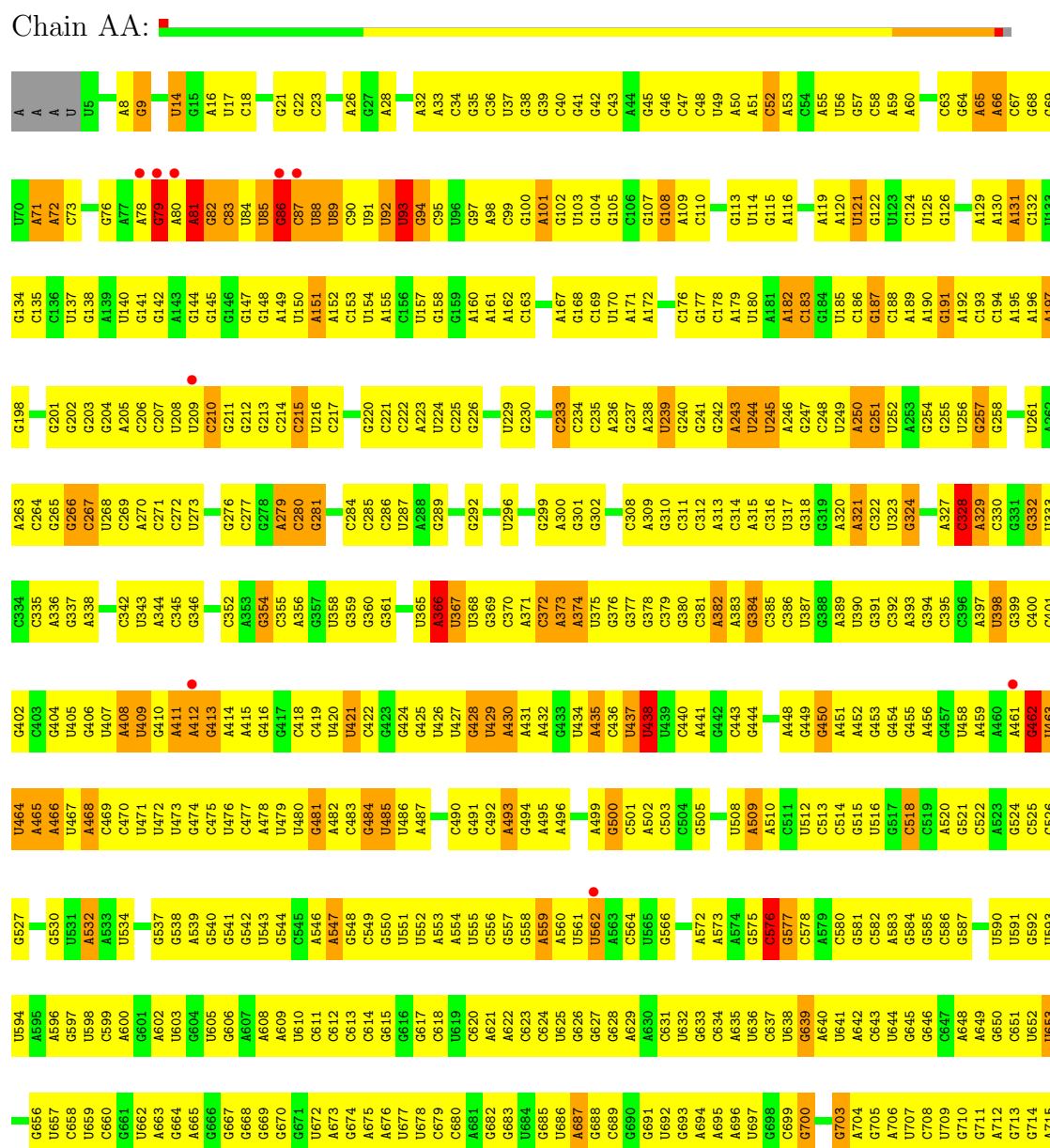
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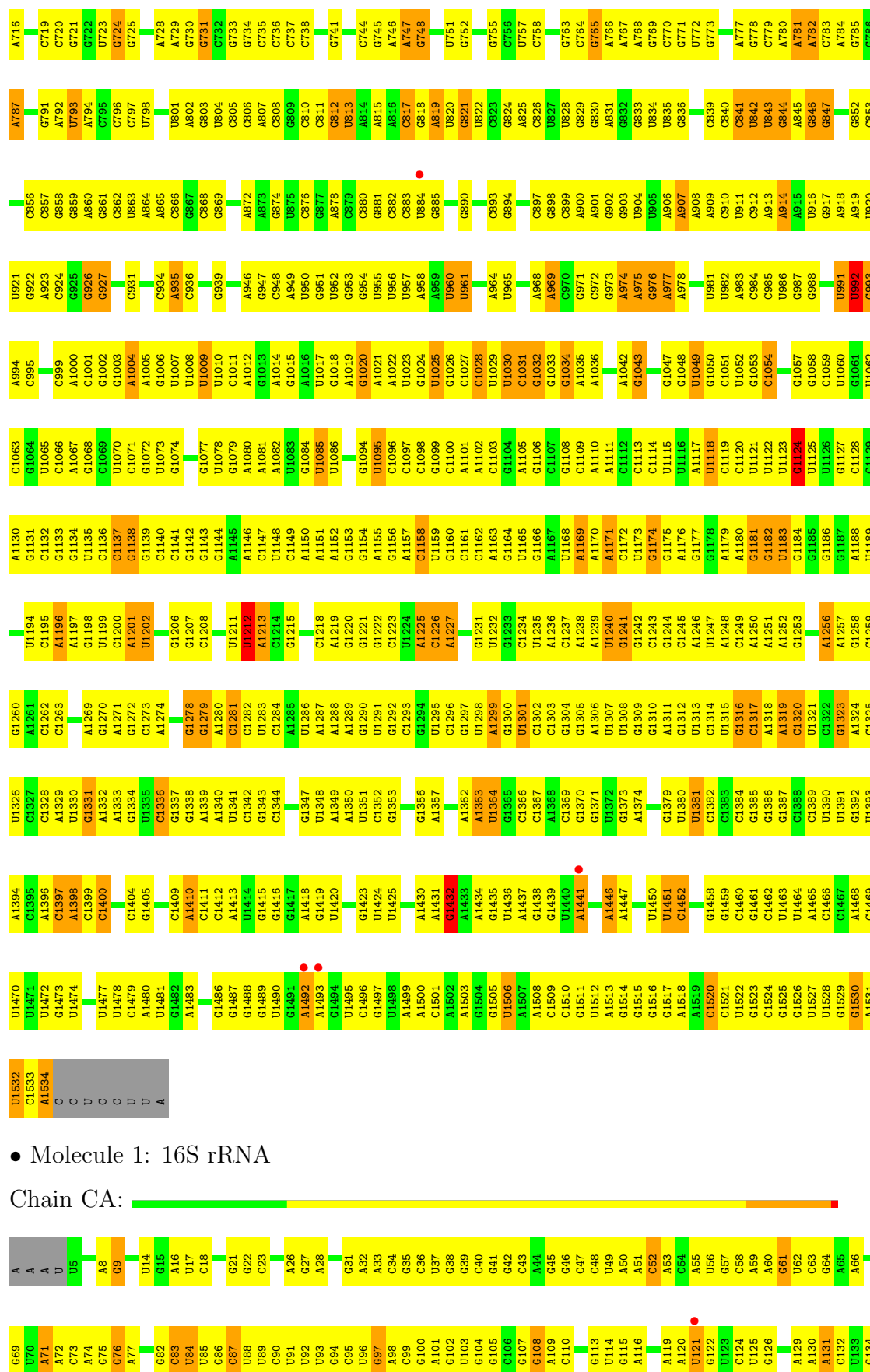
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	CA	296	Total 296	O 296	0	0
57	CE	3	Total 3	O 3	0	0
57	CK	1	Total 1	O 1	0	0
57	CL	3	Total 3	O 3	0	0
57	CN	4	Total 4	O 4	0	0
57	CT	2	Total 2	O 2	0	0
57	DB	500	Total 500	O 500	0	0
57	DC	6	Total 6	O 6	0	0
57	DE	2	Total 2	O 2	0	0
57	DL	2	Total 2	O 2	0	0
57	DR	1	Total 1	O 1	0	0
57	DT	1	Total 1	O 1	0	0

3 Residue-property plots

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

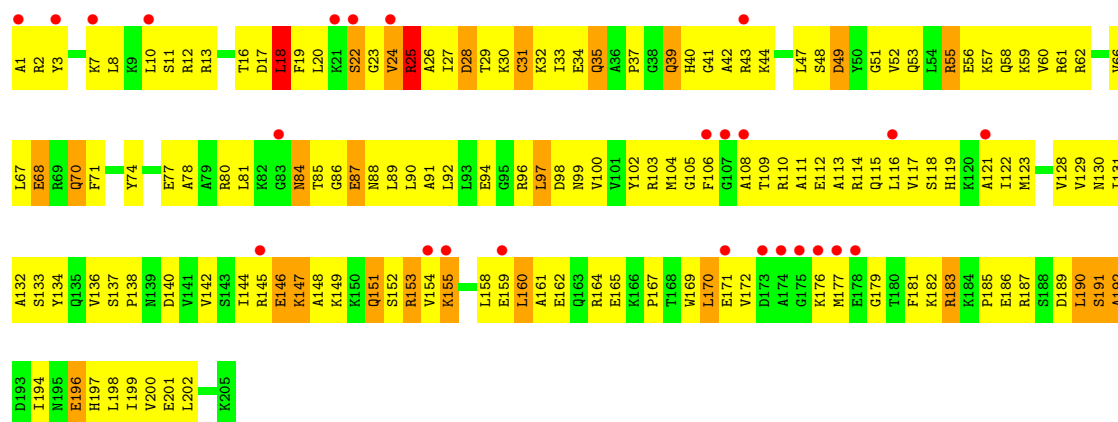
• Molecule 1: 16S rRNA





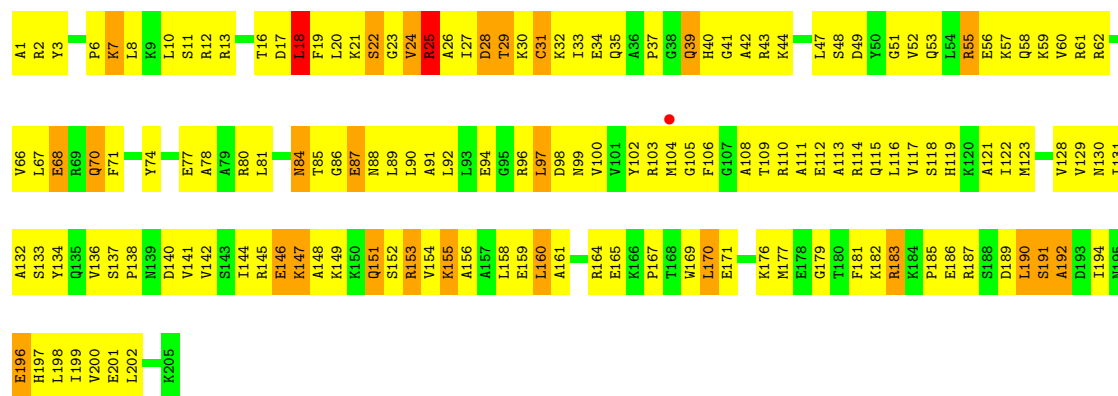
A1179	C1119	G1048	U981	A914	G852	A782	G711	A649	A523	A459	A397	A329	U261	A196	C135
A1180	C1120	U1049	U982	A915	C853	C783	G711	G650	G524	A460	U398	C330	A262	A197	C136
G1181	U1121	C1050	A983	U916	C854	A784	A712	C651	C525	A461	G399	G331	A263	G198	U137
G1182	U1122	C1051	C984	G917	C855	G785	G713	G652	C526	G462	C400	G332	C264	G138	G138
U1183	U1123	C1052	C985	A918	C856	G786	G714	U853	C527	U463	G401	U334	G265	G201	A139
G1184	G1124	U1053	C986	A919	C857	G787	A715	U854	C528	U464	G402	U335	G266	G202	U140
G1185	U1125	C1054	G987	U920	G858	A787	A716	G856	G529	U465	C403	U336	G267	G203	G141
G1186	U1126	G1057	G988	G921	C859	U793	A716	U857	G530	U466	G404	A337	U268	G204	G142
G1187	G1127	G1058	U991	G922	A860	A794	C719	C858	U531	U467	U405	G337	U269	A205	A143
A1188	C1128	C1059	A992	A923	C861	C795	G720	U859	U532	U468	U406	A338	C206	G206	G144
U1189	C129	C1060	G993	G924	C862	C796	G721	C960	A533	A469	U407	A338	C271	C207	G145
A1130	G1130	U1061	A994	G925	U863	C797	G722	G661	U534	C470	A408	C342	C272	U208	G146
C1131	C1131	U1062	C995	G926	A864	C797	U723	U662	G537	U471	U409	U343	C272	U209	G147
C1132	C1132	U1063	A996	G927	A865	U798	G724	A663	G538	U472	G410	A344	U273	G210	G148
G1133	G1133	C1063	A997	G928	C866	A801	G725	A664	G539	U473	A411	A345	G276	G211	G149
G1134	U1134	C1064	U997	C930	G867	A802	A728	A665	G540	G474	A412	G346	G277	G212	U150
U1135	C1135	U1065	C998	C931	C868	G803	A729	G666	G541	G475	G413	A352	G278	G213	A151
G1136	U1136	C1066	C999	C932	C869	U804	A730	G667	G542	U476	A414	A353	A279	C214	A152
C1137	G1137	U1067	A1000	G933	A870	G805	G730	G668	G543	C477	A415	A354	C280	C215	C153
G1138	G1138	C1068	C1001	C934	A871	C806	G731	G669	U544	A478	G416	G354	G281	U216	U154
G1139	G1139	G1069	U1002	A935	C872	C807	C732	G670	G545	U479	G417	C355	G282	C217	A155
C1140	U1140	U1070	G1003	C936	G874	C808	G733	U871	G550	U480	C418	A356	C284	G220	U157
C1141	C1141	C1071	A1004	G937	U875	G809	G734	G672	U551	G481	C419	A357	C285	G221	G158
G1142	G1142	U1072	A1005	G939	C876	C810	G735	A673	U552	G482	U420	U358	C286	C222	G159
G1143	G1143	U1073	G1006	C940	G877	C811	C736	G674	G553	C483	U421	G359	U287	A223	A160
G1144	G1144	U1074	U1007	G941	A878	G812	C737	A675	C549	G484	C422	C360	A288	G224	A161
A1145	A1145	U1075	U1008	G942	C879	U813	C738	A676	G550	U485	G423	G361	G289	C225	C163
U1212	U1212	U1076	U1009	A946	C880	A814	C739	U877	U551	U486	G424	U365	G292	U229	U166
A1213	A1213	U1077	G947	G947	C881	A815	G740	U878	U552	U487	G425	A366	G293	G230	A167
C1214	C1214	U1078	C948	G948	C882	A816	G741	C879	U553	G488	U426	U367	U296	U231	G168
G1215	G1215	U1079	A949	A949	C883	C817	G744	G680	A554	C489	U427	U368	U299	C233	C169
A1150	U1150	U1080	U950	U950	U884	C818	C744	C620	U555	C490	G428	U369	G299	C234	U170
A1151	A1151	A1081	G951	G951	C885	A819	G745	C621	C556	G491	U429	G369	A300	G302	A171
G1152	G1152	U1082	U952	U952	C886	U820	A746	A622	G557	C492	A430	C370	A300	A236	A172
U1085	U1085	G1084	G953	G953	C887	G821	A747	C623	G558	C501	A431	A371	A300	C235	A173
U1086	U1086	U1085	G954	G954	C887	G822	A748	C624	A559	A502	A432	C372	A302	A236	A173
A1019	G1019	U1086	U955	U955	G890	U823	G749	U625	U560	A495	G433	A373	A303	G237	U173
G1020	G1020	U1087	U956	U956	U891	G824	C750	G626	U561	A496	U434	A374	A303	G237	U173
A1021	A1021	U1088	U957	U957	A892	A825	C751	G627	U562	U497	A435	U375	A306	A238	A174
U1022	U1022	C1095	A958	A958	C893	C826	G752	G628	A563	G500	C436	C376	U239	U239	C175
G1023	G1023	C1096	A959	A959	C894	U827	A746	A629	C564	C501	U437	G377	G240	C176	G176
U1024	U1024	C1097	U960	U960	C895	U828	A747	C630	U565	A501	U438	G378	G241	G177	G177
G1025	G1025	U1098	U961	U961	C896	G829	G748	C631	G566	A502	U439	C379	G242	C178	G178
U1026	U1026	C1100	A964	A964	C897	G830	C750	U632	G567	C503	C440	G380	G243	A179	A179
C1027	C1027	A1101	U965	U965	C898	A831	C764	G633	A572	G504	A441	C381	U244	U180	U180
U1028	U1028	U1105	G966	G966	A900	G832	G765	C634	A573	G505	C442	A382	U245	A181	A181
C1029	C1029	C1106	C967	C967	A901	U834	A766	A635	A574	U508	C443	A383	A246	A182	C188
U1030	U1030	U1107	A968	A968	G902	U835	A767	U636	C575	A509	C444	A384	G247	G183	G183
C1031	C1031	C1107	U969	U969	G903	U836	A768	C637	C576	A510	U448	C385	C248	U185	U185
G1032	G1032	U904	C970	C970	U905	G839	G769	U638	G577	A510	U449	C386	U249	C186	C186
U1033	U1033	G971	G971	G971	U906	U701	C770	G639	C578	G511	G450	U387	A250	A250	G187
G1034	G1034	A906	C972	C972	A907	U702	G771	A640	A579	U512	G451	G388	G251	G187	G187
U1035	U1035	U907	G973	G973	C841	G703	U772	U641	C580	C513	A452	A389	U252	C188	C188
A1036	A1036	A908	U942	U942	A909	U704	G773	A642	G581	C514	A453	U390	G253	A189	A189
U975	U975	A909	U943	U943	C910	A705	A777	U644	G582	C514	G454	G391	G322	G190	G190
G976	G976	C911	G844	G844	C912	A706	G778	U645	G583	C515	G455	C392	U323	A191	A191
A977	A977	U911	G845	G845	C912	A707	G779	U646	G584	C516	G456	A393	U324	A192	A192
A978	A978	U912	G846	G846	C913	A708	C780	U647	G585	A520	A457	G394	G257	C193	C193
G1047	G1047	A913	G847	G847	C914	A709	A781	U648	G587	C522	U458	C396	C328	A195	A195





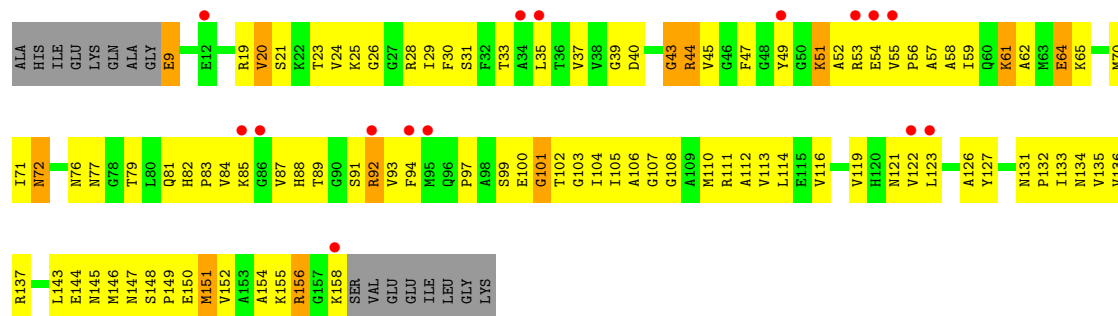
• Molecule 3: 30S ribosomal protein S4

Chain CD:



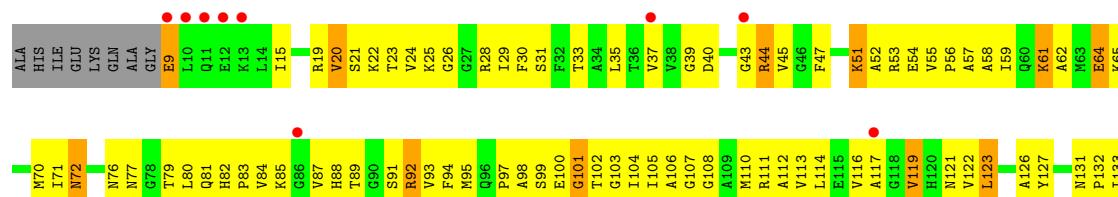
• Molecule 4: 30S ribosomal protein S5

Chain AE:



• Molecule 4: 30S ribosomal protein S5

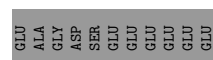
Chain CE:





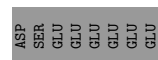
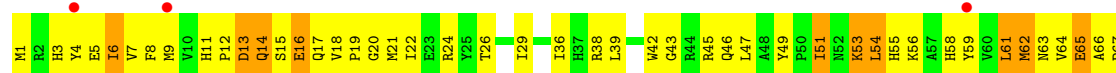
• Molecule 5: 30S ribosomal protein S6

Chain AF:



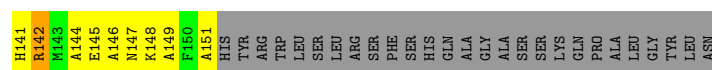
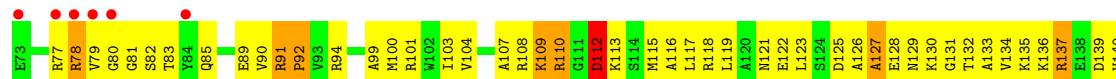
• Molecule 5: 30S ribosomal protein S6

Chain CF:



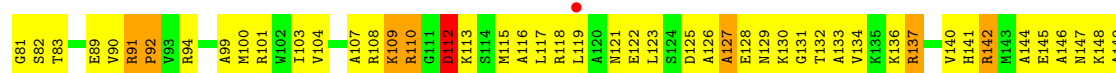
• Molecule 6: 30S ribosomal protein S7

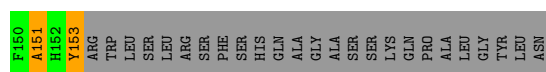
Chain AG:



• Molecule 6: 30S ribosomal protein S7

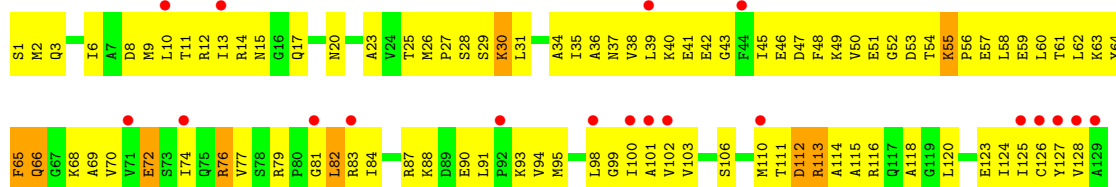
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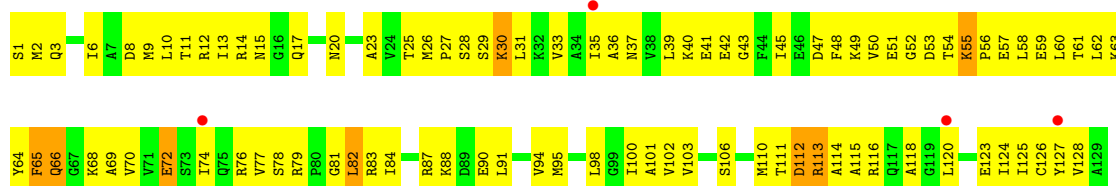
• Molecule 7: 30S ribosomal protein S8

Chain AH:



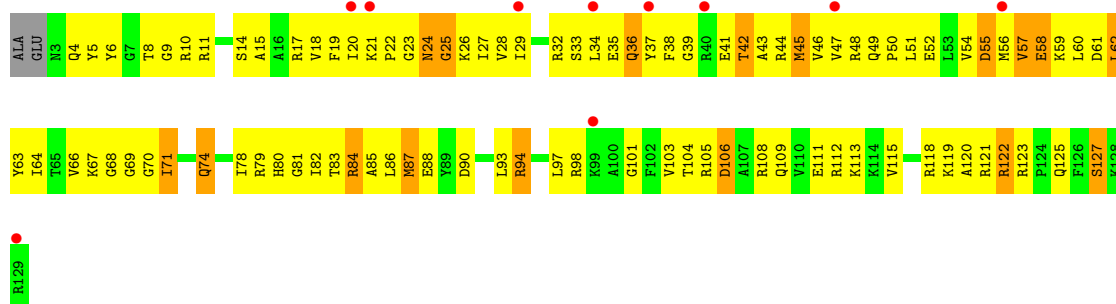
• Molecule 7: 30S ribosomal protein S8

Chain CH:



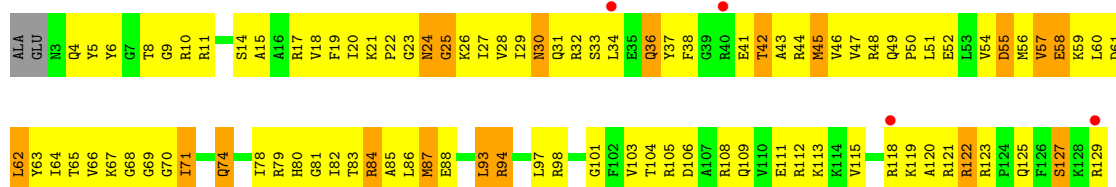
• Molecule 8: 30S ribosomal protein S9

Chain AI:



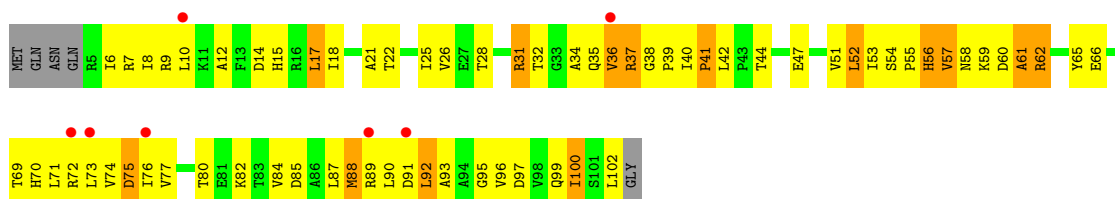
• Molecule 8: 30S ribosomal protein S9

Chain CI:



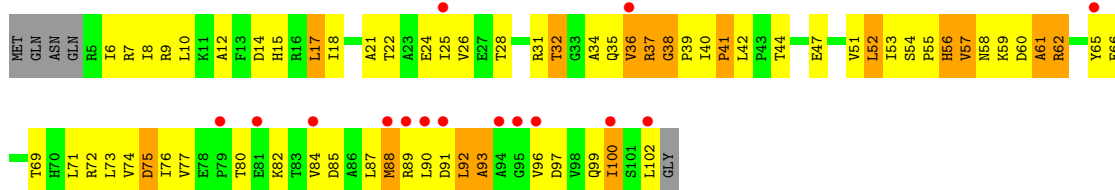
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



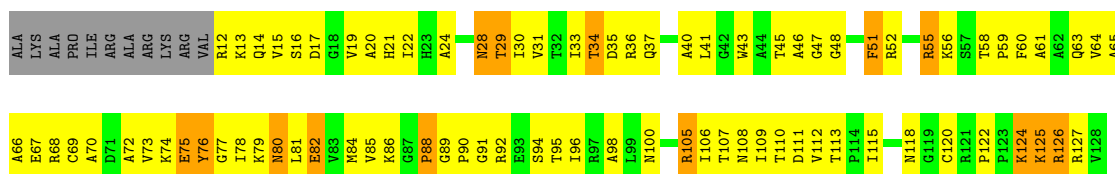
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



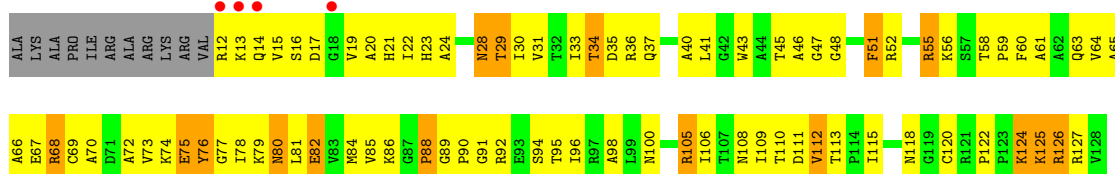
• Molecule 10: 30S ribosomal protein S11

Chain AK:



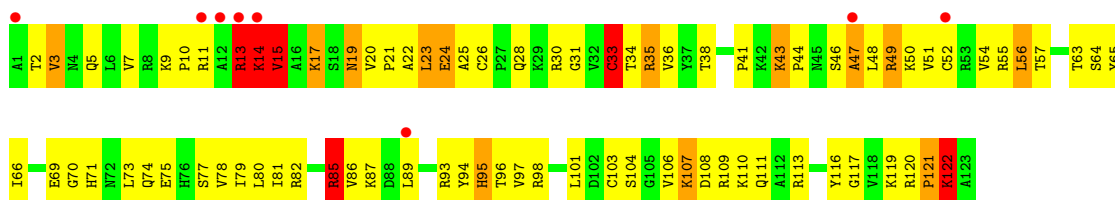
• Molecule 10: 30S ribosomal protein S11

Chain CK:



• Molecule 11: 30S ribosomal protein S12

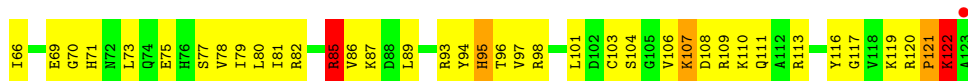
Chain AL:



• Molecule 11: 30S ribosomal protein S12

Chain CL:





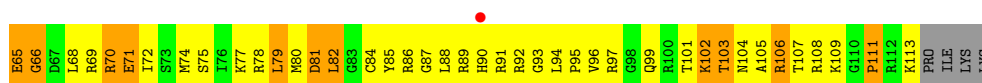
- Molecule 12: 30S ribosomal protein S13

Chain AM:



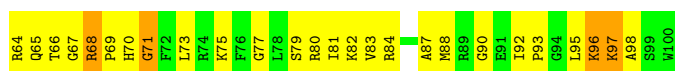
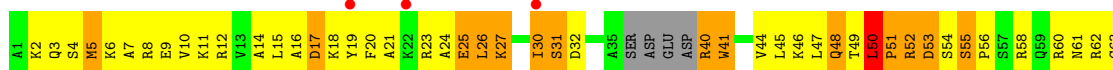
- Molecule 12: 30S ribosomal protein S13

Chain CM:



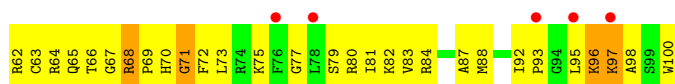
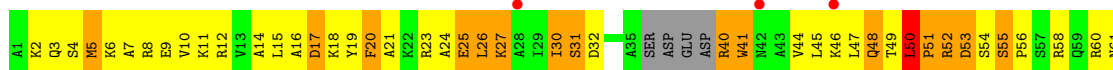
- Molecule 13: 30S ribosomal protein S14

Chain AN:



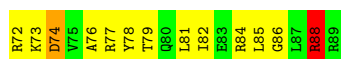
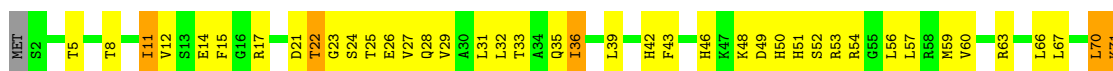
- Molecule 13: 30S ribosomal protein S14

Chain CN:



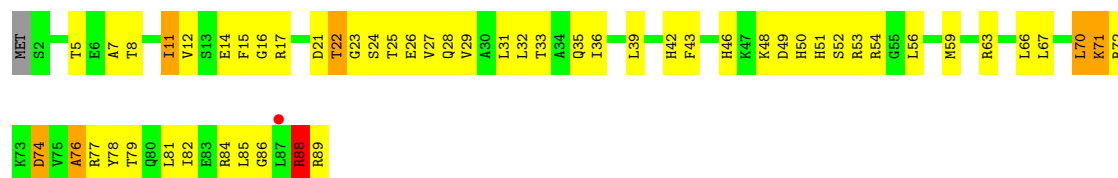
- Molecule 14: 30S ribosomal protein S15

Chain AO:



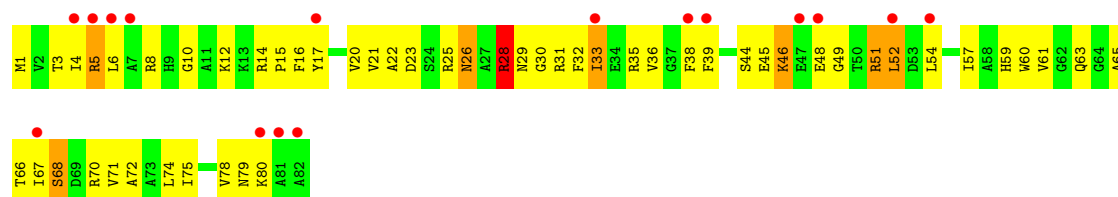
- Molecule 14: 30S ribosomal protein S15

Chain CO:



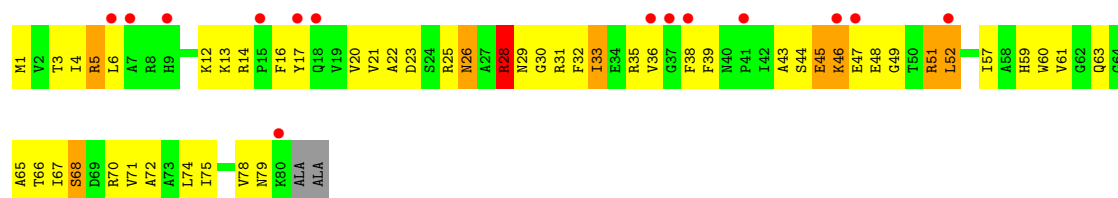
- Molecule 15: 30S ribosomal protein S16

Chain AP:



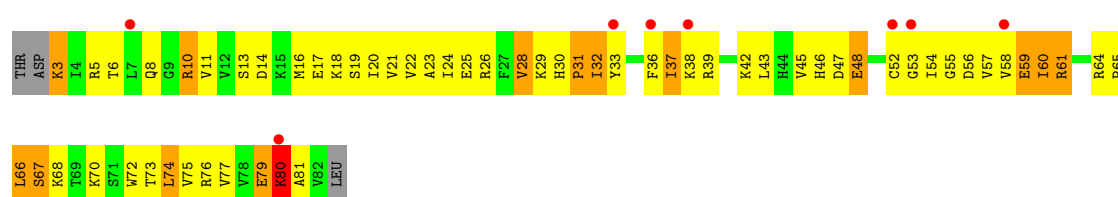
- Molecule 15: 30S ribosomal protein S16

Chain CP:



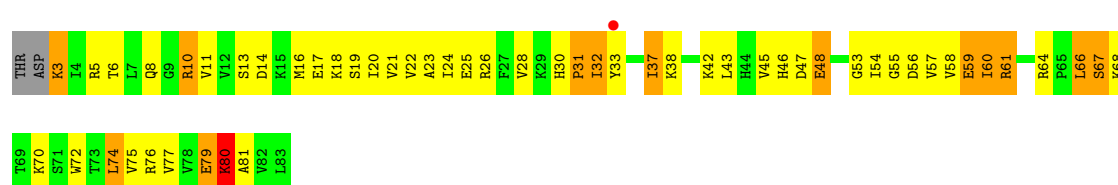
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



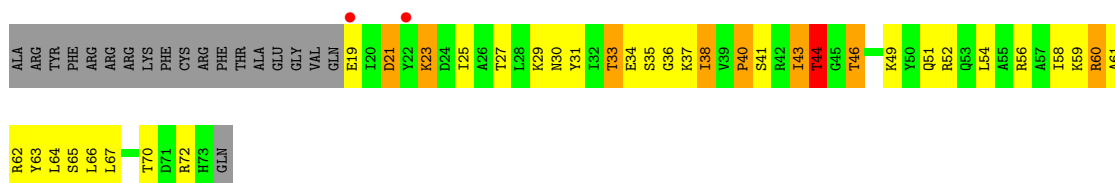
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



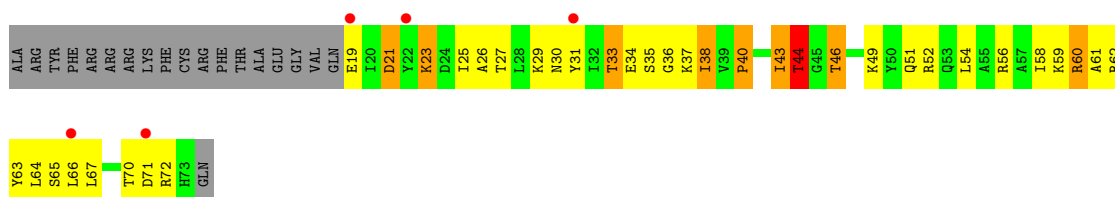
- Molecule 17: 30S ribosomal protein S18

Chain AR:



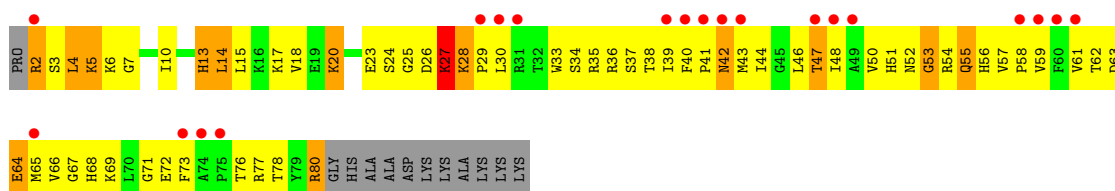
- Molecule 17: 30S ribosomal protein S18

Chain CR:



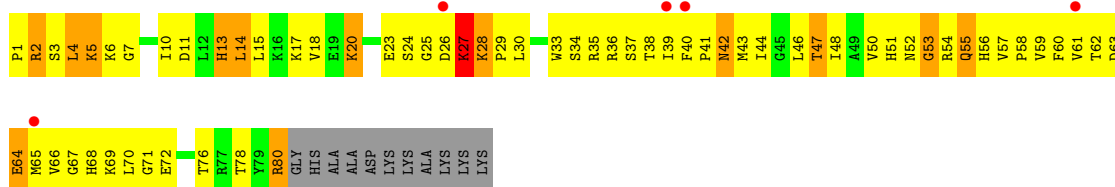
- Molecule 18: 30S ribosomal protein S19

Chain AS:



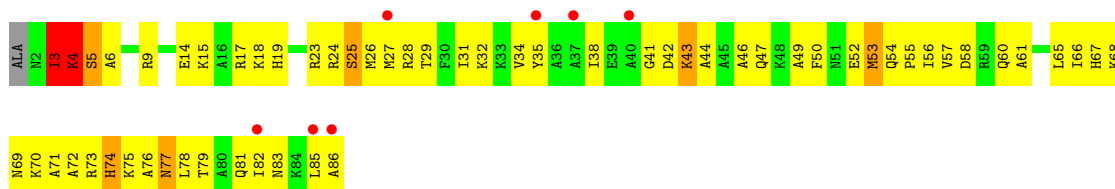
- Molecule 18: 30S ribosomal protein S19

Chain CS:



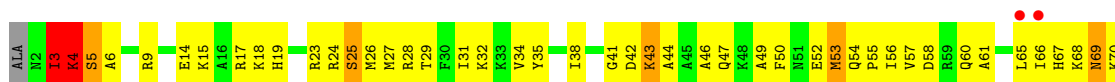
- Molecule 19: 30S ribosomal protein S20

Chain AT:



- Molecule 19: 30S ribosomal protein S20

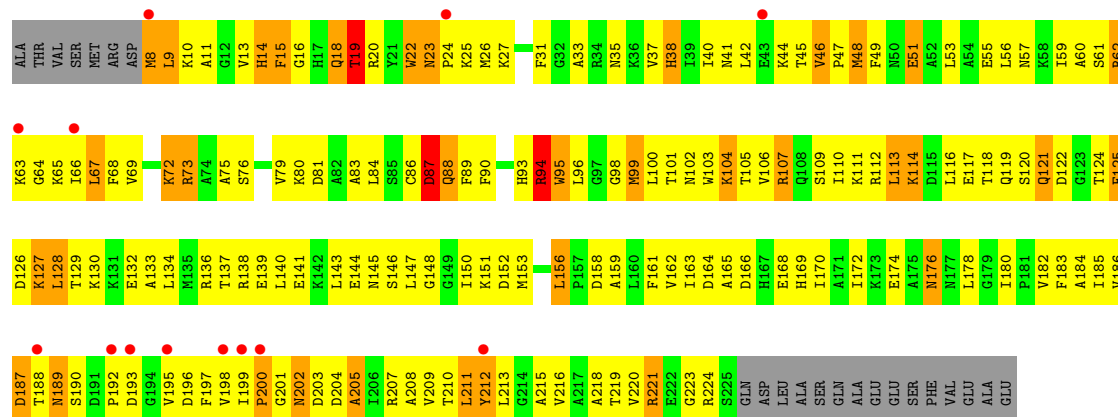
Chain CT:



A71
A72
H74
H75
A76
M77
L78
T79
A80
Q81
I82
N83
K84
L85
A86

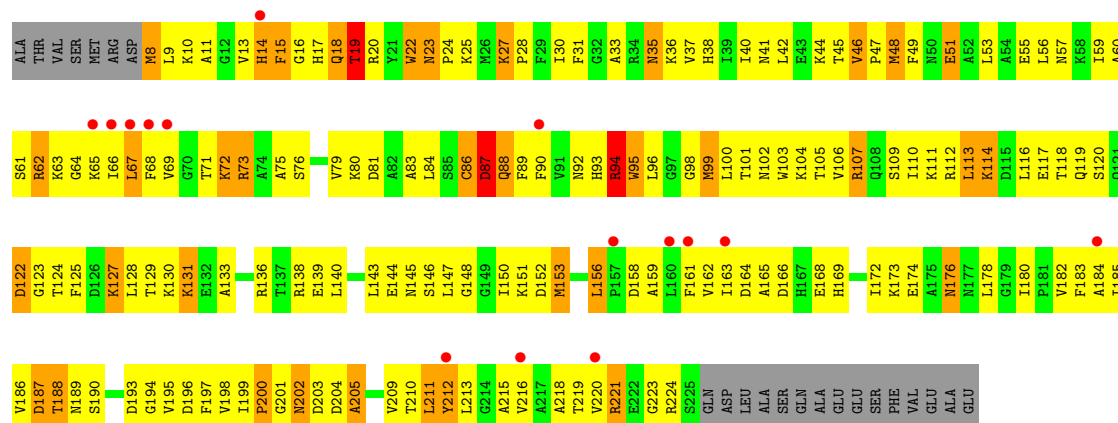
- Molecule 20: 30S ribosomal protein S2

Chain AB:



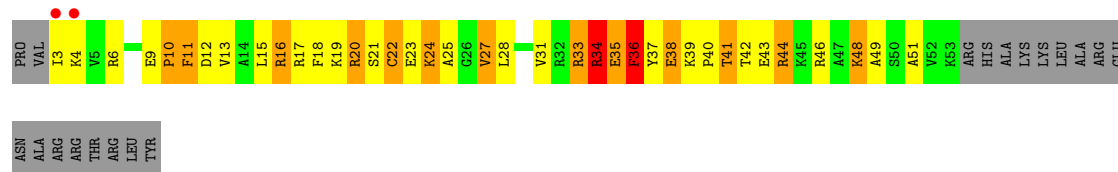
- Molecule 20: 30S ribosomal protein S2

Chain CB:



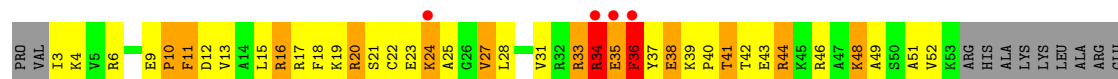
- Molecule 21: 30S ribosomal protein S21

Chain AU:



- Molecule 21: 30S ribosomal protein S21

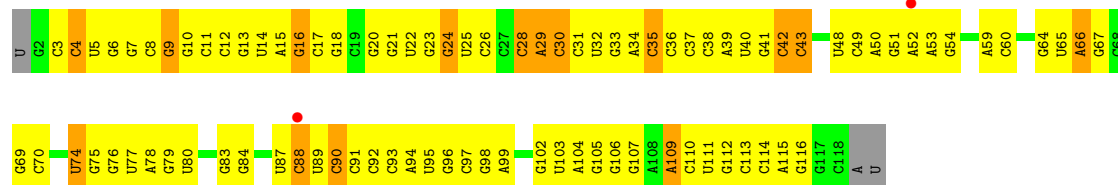
Chain CU:



ASN
ALA
ARG
ARG
THR
ARG
LEU
TYR

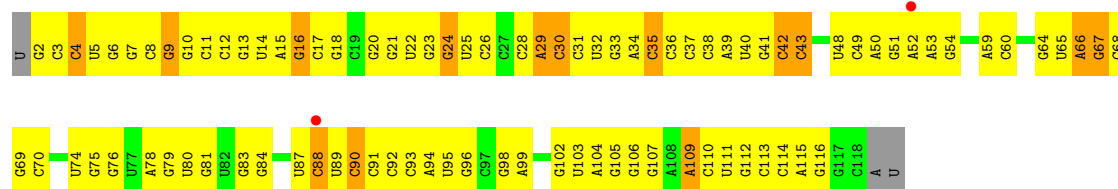
• Molecule 22: 5S rRNA

Chain BA:



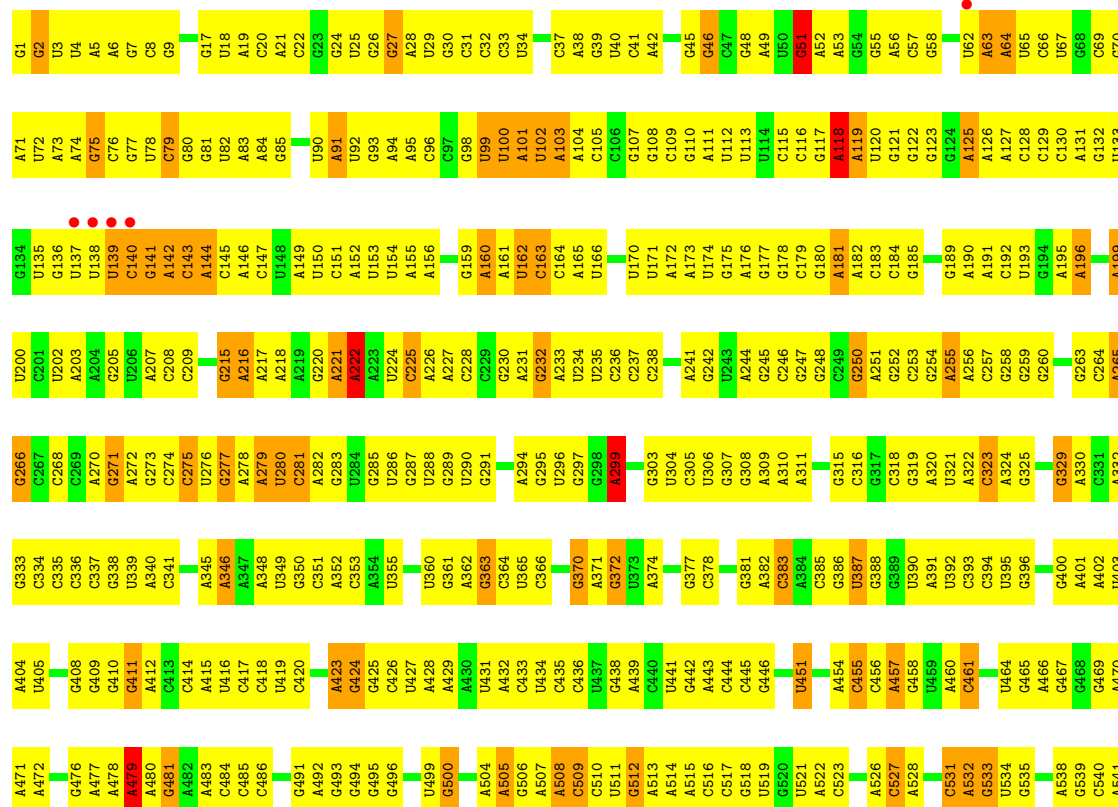
• Molecule 22: 5S rRNA

Chain DA:



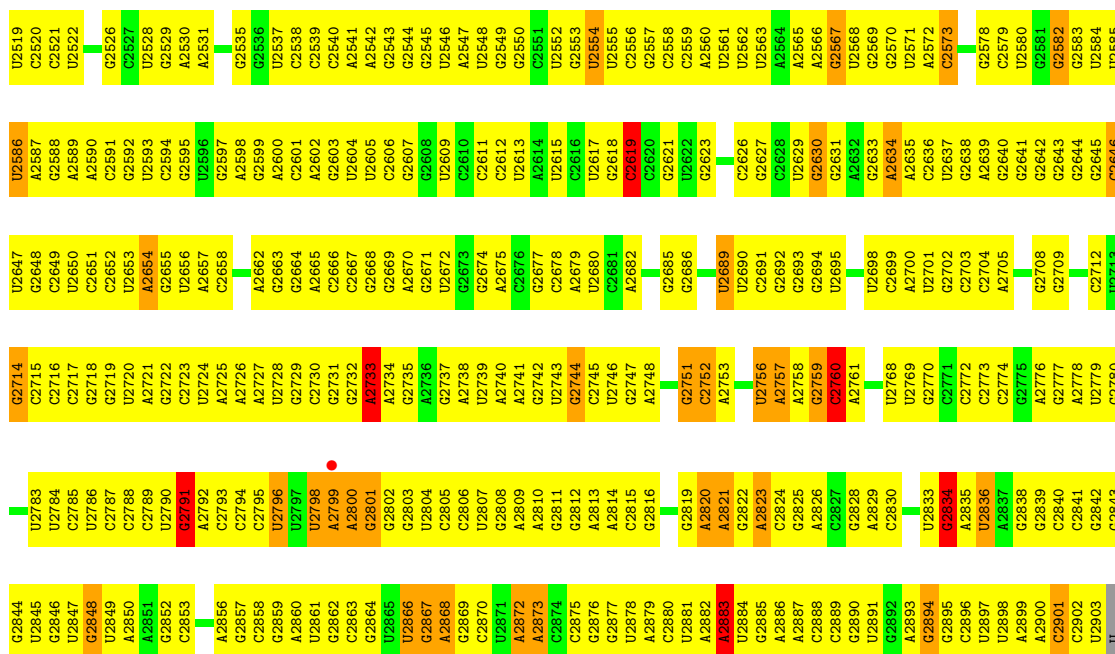
• Molecule 23: 23S rRNA

Chain BB:



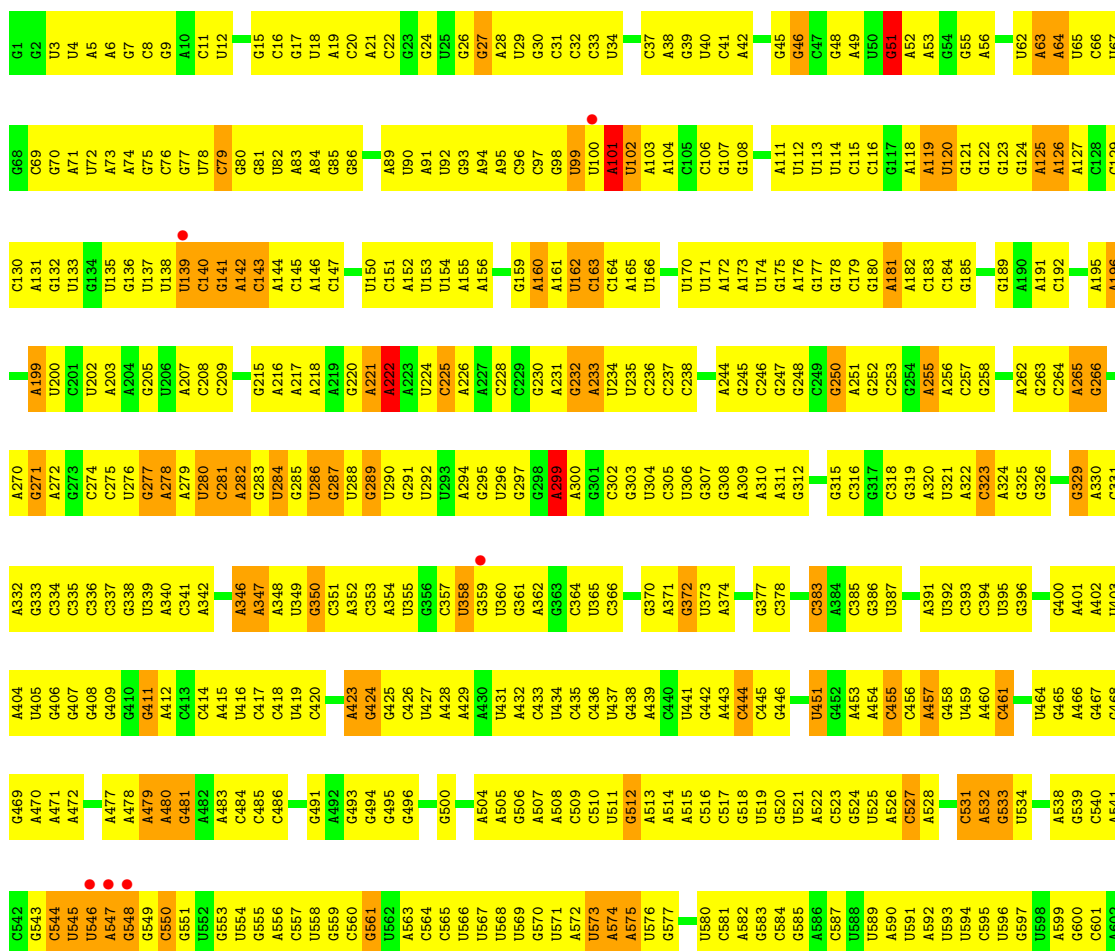
C1463	C1464	G1465	G1466	U1467	U1468	A1469	A1470	G1471	U1472	U1473	U1474	U1475	U1476	U1477	G1478	G1479	C1480	U1481	G1482	G1483	U1484	U1485	U1486	U1487	C1488	C1489	A1490	G1491	G1492	C1493	A1494	A1495	A1496	U1497	G1501	A1502	A1503	A1504	A1505	U1506	C1507	A1508	A1509	G1510	G1511	C1512	U1513	U1514	A1515	G1516	G1517	C1518	G1519	U1520	G1521	A1522	U1523	U1524	
G1401	U1402	A1403	C1404	U1405	U1406	A1407	G1408	U1411	U1412	A1413	U1414	U1415	G1416	C1417	U1418	A1419	A1420	G1421	G1422	G1423	G1424	G1425	G1426	A1427	G1428	G1429	G1430	A1431	G1432	A1433	A1434	G1435	G1436	C1437	U1438	A1439	U1440	G1441	U1442	U1443	U1444	G1445	A1446	C1447	G1448	G1449	C1450	C1451	G1452	A1453	U1454	G1455	U1456	G1457	U1458	U1459	G1460	C1461	U1462
C1335	A1336	G1337	G1338	C1339	U1340	G1341	C1342	C1345	G1346	A1347	C1348	C1349	C1350	C1351	U1352	A1353	A1354	G1355	A1356	C1357	A1358	A1359	A1365	A1366	A1367	G1368	G1369	C1370	C1371	U1372	A1373	G1374	U1375	C1376	G1377	A1378	U1379	C1380	G1381	G1382	A1383	A1384	A1385	C1386	A1387	A1388	G1389	U1390	U1391	A1392	A1393	U1394	A1395	U1396	U1397	C1398	C1399	U1400	
U1267	A1268	A1269	C1270	G1271	A1272	U1273	A1274	A1275	A1276	G1277	C1278	C1279	G1280	U1281	U1282	A1283	A1284	A1285	A1286	G1287	G1288	C1291	G1292	C1293	U1294	C1295	U1296	C1297	U1298	G1299	G1300	A1301	A1302	G1309	G1310	C1314	C1315	U1316	U1317	U1318	U1319	C1320	A1321	A1322	C1323	G1324	U1325	U1326	U1327	A1328	U1329	C1330	G1331	G1332	G1333	G1334			
C1200	U1201	G1202	U1203	A1204	A1205	G1206	G1207	C1208	A1209	G1210	C1211	G1212	A1213	A1214	G1215	G1216	U1217	G1218	U1219	G1220	C1221	U1222	G1223	U1224	G1228	G1229	A1230	U1231	G1236	A1237	U1240	A1241	U1242	C1243	A1244	G1245	A1246	A1247	G1248	U1249	G1250	C1251	G1252	A1253	A1254	U1255	G1256	C1257	U1258	G1259	A1260	C1261	A1262	U1263	G1266				
A1134	C1135	G1136	U1137	G1138	U1139	C1140	U1141	A1142	A1143	U1144	C1145	U1146	A1147	U1148	G1149	C1150	A1151	C1152	G1153	G1157	C1161	G1162	G1163	C1164	A1165	A1166	C1167	G1171	C1172	U1173	U1174	A1175	U1176	G1177	C1178	G1179	U1180	U1181	G1182	U1183	U1184	G1185	G1186	U1187	U1188	A1189	G1190	G1191	U1192	G1193	A1194	G1195	C1196	U1197	U1199				
C994	C995	A996	A1000	A1001	G1002	C1007	C1076	A1077	U1078	C1079	A1080	U1081	U1082	U1083	A1084	U1085	A1086	G1087	A1088	A1089	A1090	G1091	C1092	U1097	A1098	G1099	A1100	U1101	C1102	A1103	C1104	U1105	U1106	G1107	U1108	C1109	G1110	G1111	U1112	U1113	C1114	G1115	U1116	C1117	U1118	U1119	C1121	G1122	G1123	G1124	G1125	U1060	U1061	G1062	G1063	C1064	U1065		
U932	A933	U934	C935	A936	C937	G938	G939	G940	A941	G942	A943	C944	A945	C946	A947	C948	G949	G950	C951	G952	G953	G954	U955	U956	G957	U958	A959	A960	C961	G962	U963	C964	G965	U966	C967	G968	G969	U970	U971	G972	A973	G974	A975	A979	A980	A981	C982	A983	A984	C985	C986	C987	A988	G989	A990	C991	C992	G993	
G862	A863	G864	C865	A866	G869	U870	U871	U872	C873	G874	G875	C876	A877	A878	G	G	G	A820	G822	U823	C824	U825	A826	U827	U828	A829	G830	G831	U832	A833	G834	G835	G836	C837	C838	U839	G840	G841	U842	A845	U846	U847	C848	A849	U850	C851	U852	C853	C854	G855	G856	A927	A928	U929	U931				
C731	C732	G733	A734	C735	C736	C737	G738	A739	C740	U741	A742	U743	U744	G745	U746	C747	G748	A753	U754	U755	A756	C757	G758	G759	G760	A761	C762	A763	G764	C765	U766	U767	G768	G771	C772	U773	G774	G775	G776	G777	G778	U779	G780	A781	A782	A783	U784	C785	C786	C787	C791	A794	C795	G796	G797	G798			
U667	A668	G669	A670	C671	C672	C673	G674	A675	C679	U680	G681	G682	U683	G684	G685	U686	C687	U688	A689	C690	C691	C692	U693	A694	G697	C698	C699	A699	G700	U702	U703	G704	A705	C706	U707	G708	U709	U710	G711	G712	G713	U714	A715	U716	C717	A718	C719	U720	A721	U722	G725	A727	G728	G729	A730				
C544	U545	U546	A547	G548	G549	C550	G553	U554	G555	A556	C557	U558	C560	C561	C562	C563	U562	A563	C564	C565	A627	C566	U567	U568	U569	G570	U571	A572	U573	A574	A575	U576	G577	U580	C581	A582	G583	C584	G585	A586	C587	U588	U589	A590	U591	A592	U593	A594	C595	U596	G597	U598	A599	C601	A602	A603	G604		





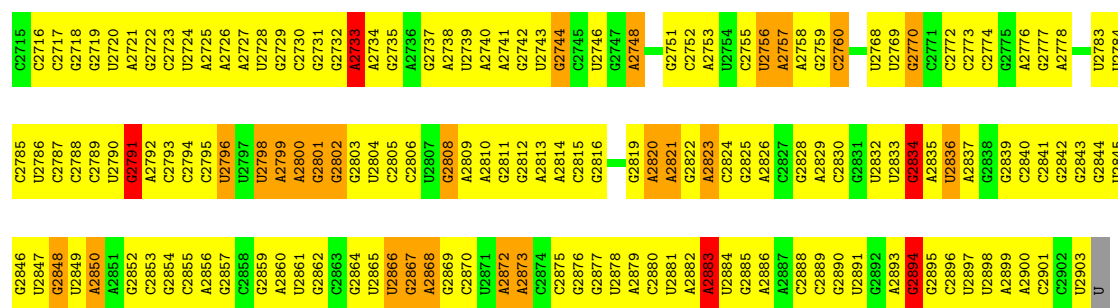
• Molecule 23: 23S rRNA

Chain DB:



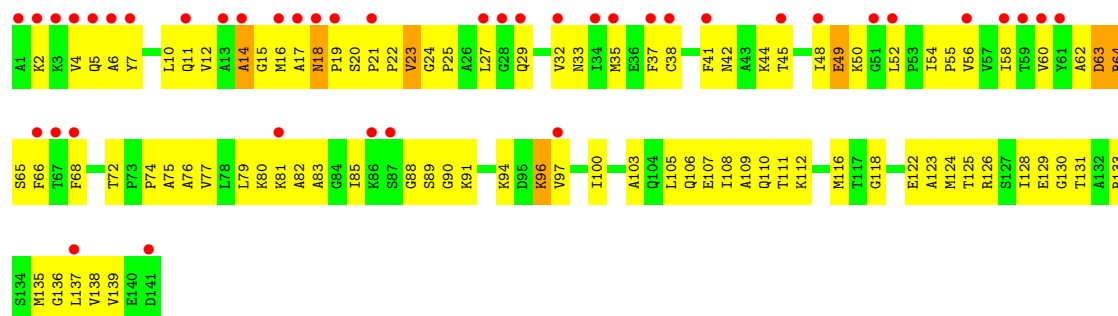






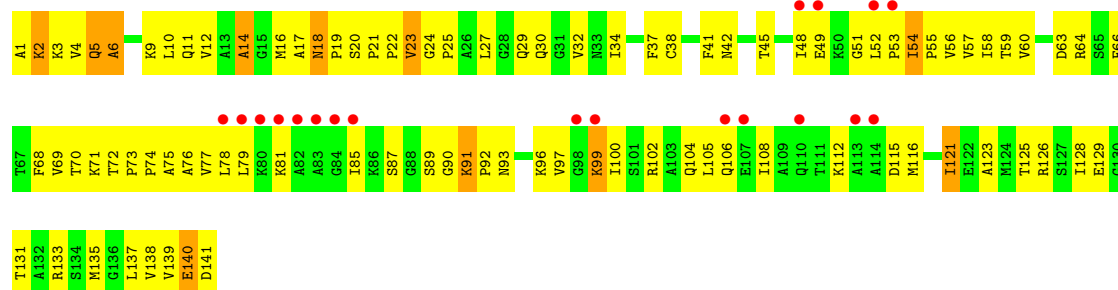
• Molecule 24: 50S ribosomal protein L11

Chain BI:



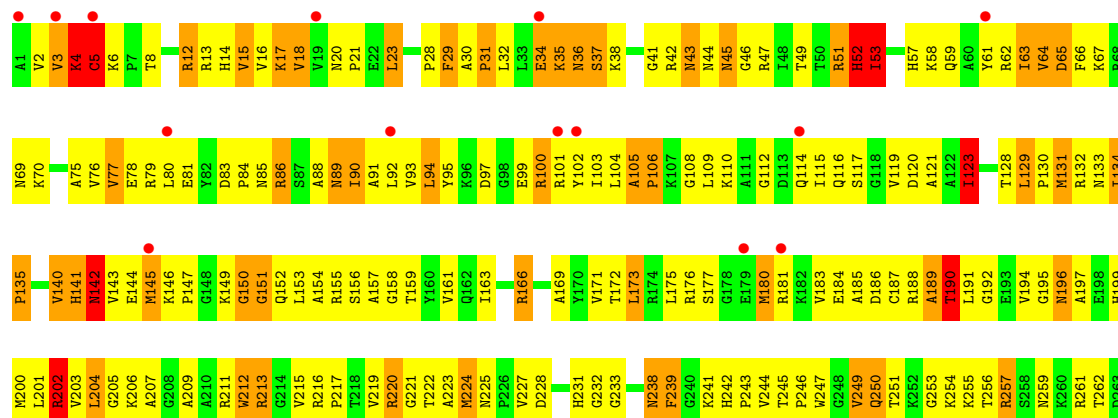
• Molecule 24: 50S ribosomal protein L11

Chain DI:



• Molecule 25: 50S ribosomal protein L2

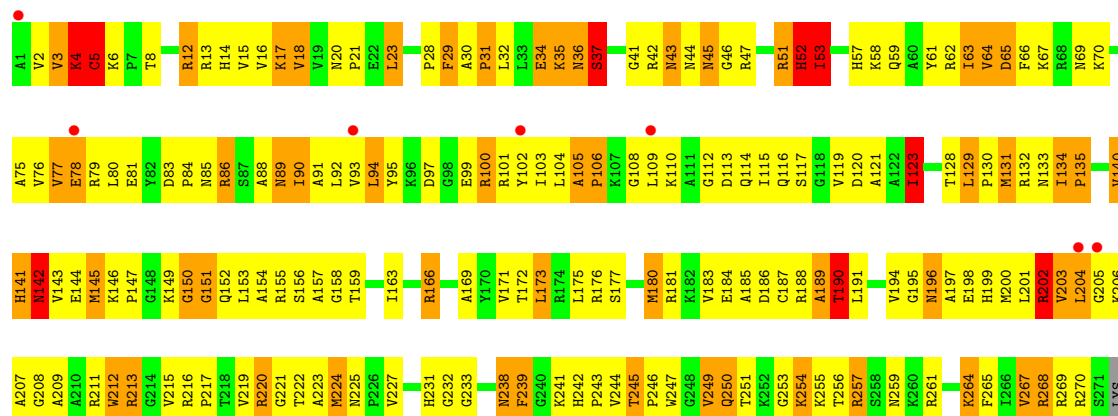
Chain BC:





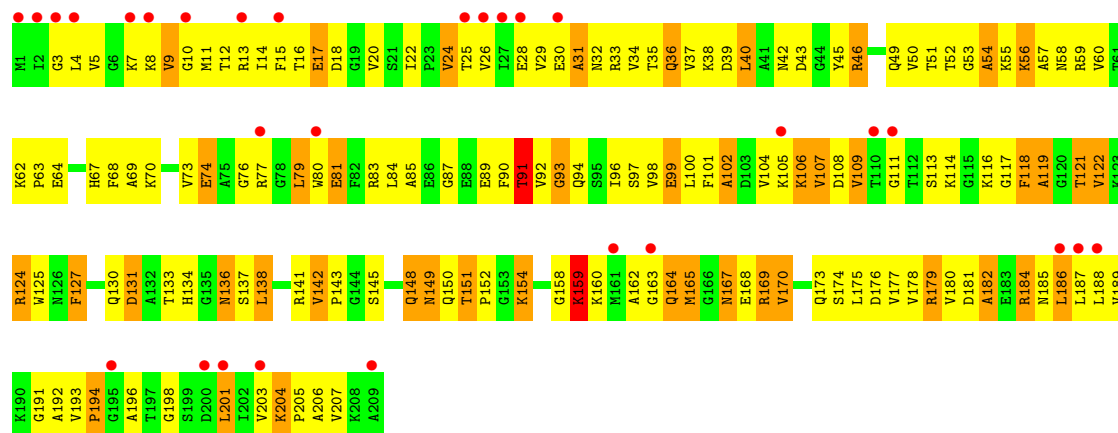
• Molecule 25: 50S ribosomal protein L2

Chain DC:



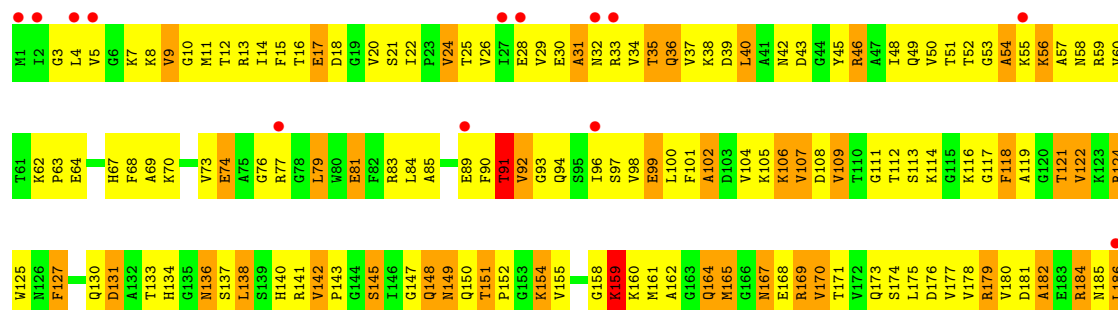
• Molecule 26: 50S ribosomal protein L3

Chain BD:



• Molecule 26: 50S ribosomal protein L3

Chain DD:





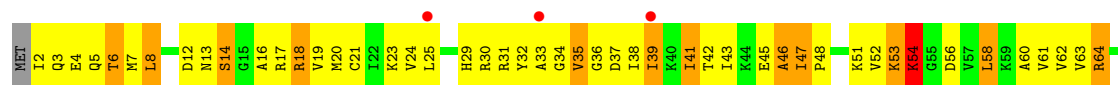
- Molecule 27: 50S ribosomal protein L14

Chain BK:



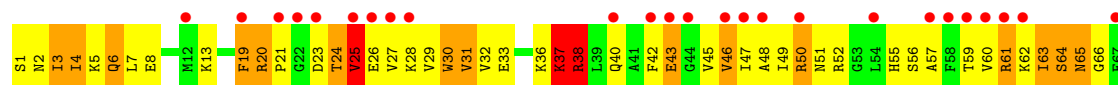
- Molecule 27: 50S ribosomal protein L14

Chain DK:



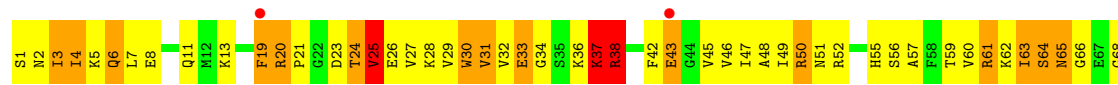
- Molecule 28: 50S ribosomal protein L19

Chain BP:



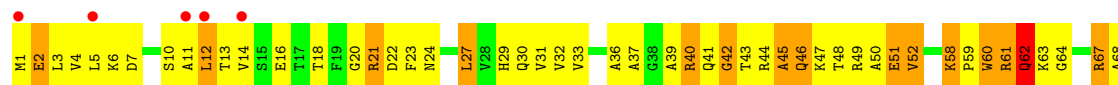
- Molecule 28: 50S ribosomal protein L19

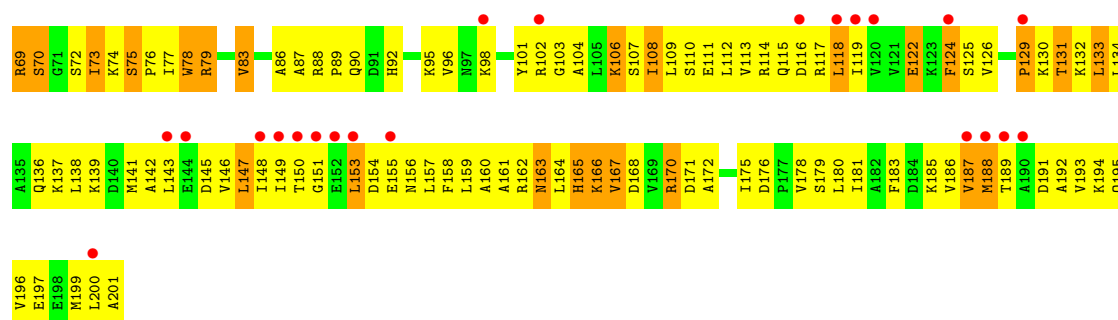
Chain DP:



- Molecule 29: 50S ribosomal protein L4

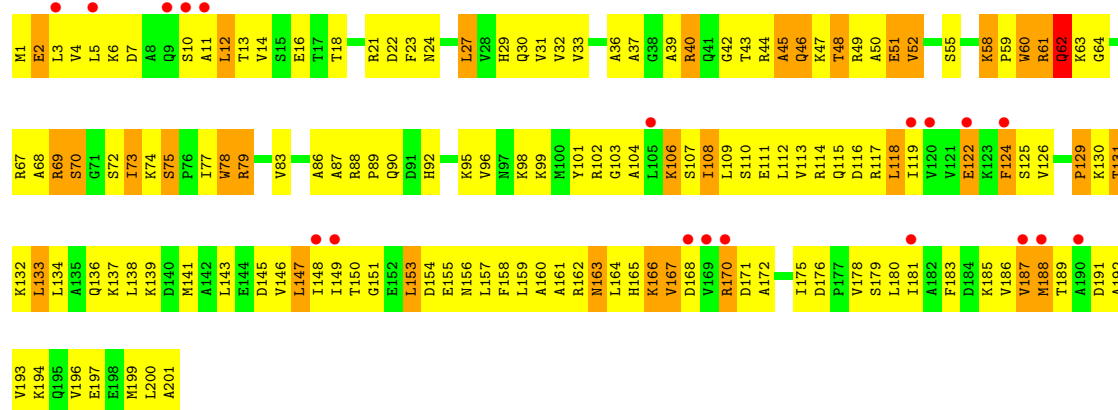
Chain BE:





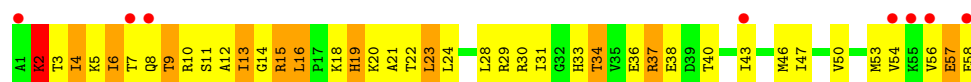
- Molecule 29: 50S ribosomal protein L4

Chain DE:



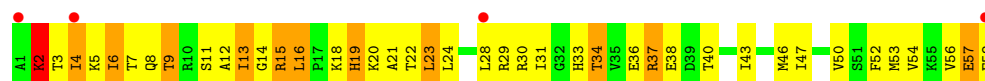
- Molecule 30: 50S ribosomal protein L30

Chain BY:



- Molecule 30: 50S ribosomal protein L30

Chain DY:



- Molecule 31: 50S ribosomal protein L32

Chain B0:



- Molecule 31: 50S ribosomal protein L32

Chain D0:



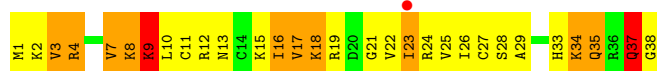
- Molecule 32: 50S ribosomal protein L36

Chain B4:



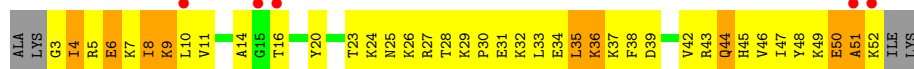
- Molecule 32: 50S ribosomal protein L36

Chain D4:



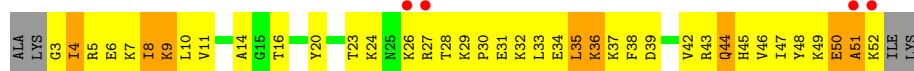
- Molecule 33: 50S ribosomal protein L33

Chain B1:



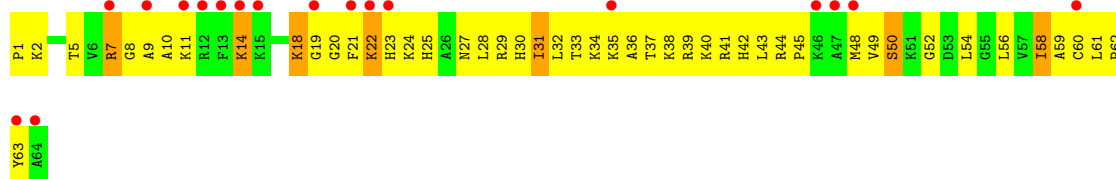
- Molecule 33: 50S ribosomal protein L33

Chain D1:



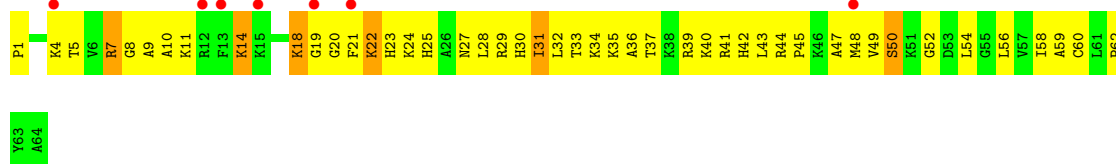
- Molecule 34: 50S ribosomal protein L35

Chain B3:



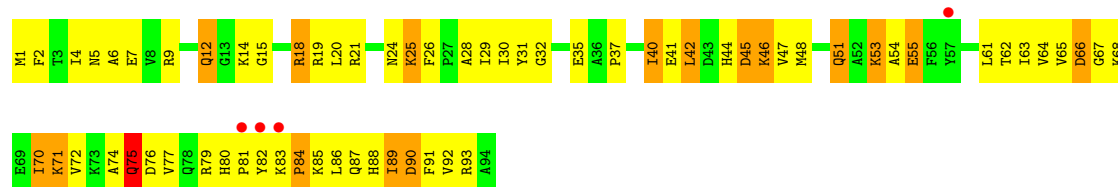
- Molecule 34: 50S ribosomal protein L35

Chain D3:



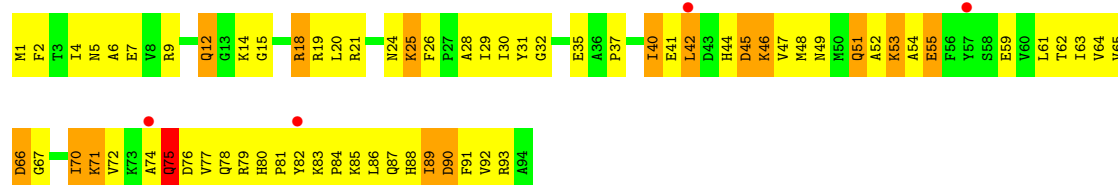
- Molecule 35: 50S ribosomal protein L25

Chain BV:



- Molecule 35: 50S ribosomal protein L25

Chain DV:



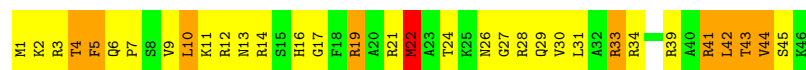
- Molecule 36: 50S ribosomal protein L34

Chain B2:



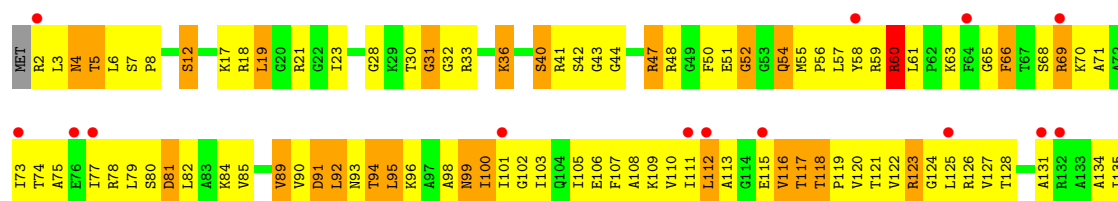
- Molecule 36: 50S ribosomal protein L34

Chain D2:



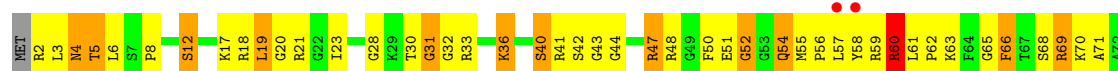
- Molecule 37: 50S ribosomal protein L15

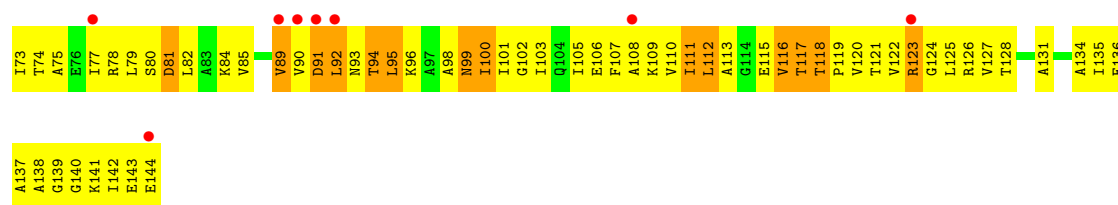
Chain BL:



- Molecule 37: 50S ribosomal protein L15

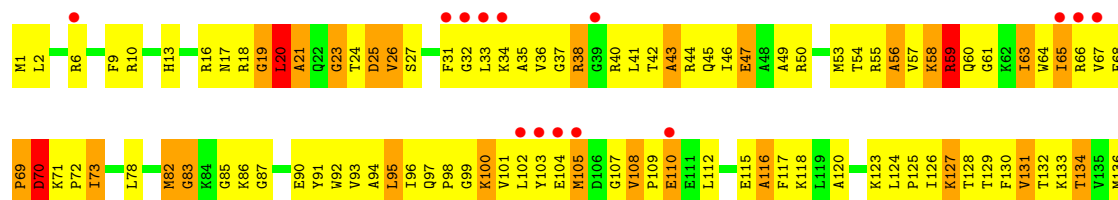
Chain DL:





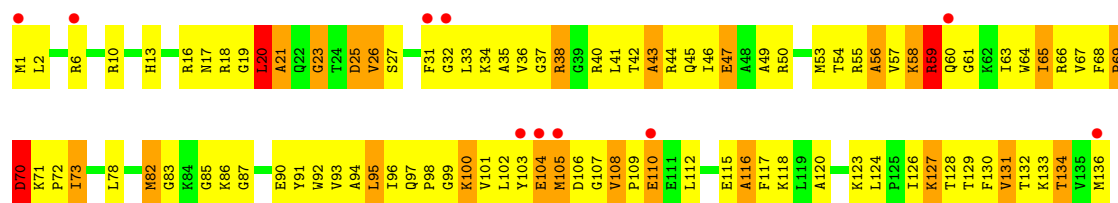
• Molecule 38: 50S ribosomal protein L16

Chain BM:



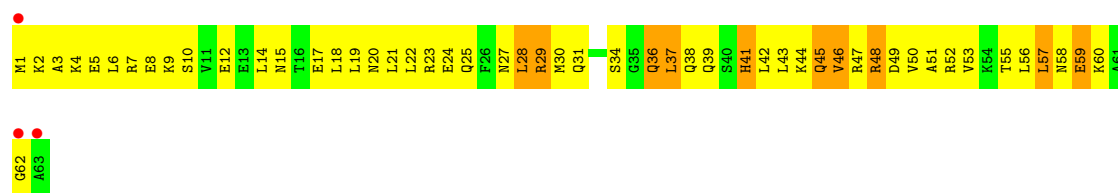
• Molecule 38: 50S ribosomal protein L16

Chain DM:



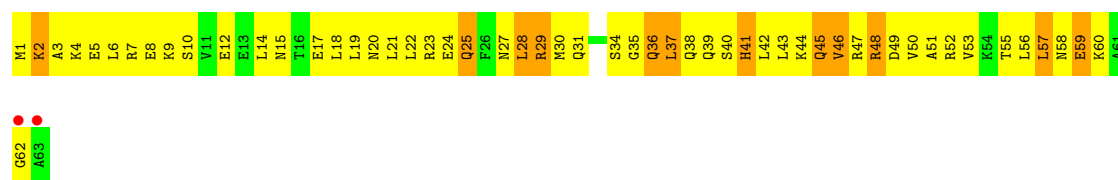
• Molecule 39: 50S ribosomal protein L29

Chain BX:



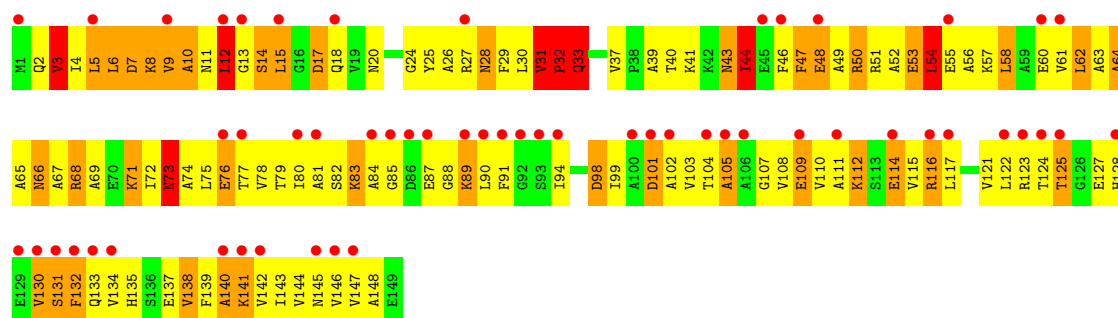
• Molecule 39: 50S ribosomal protein L29

Chain DX:



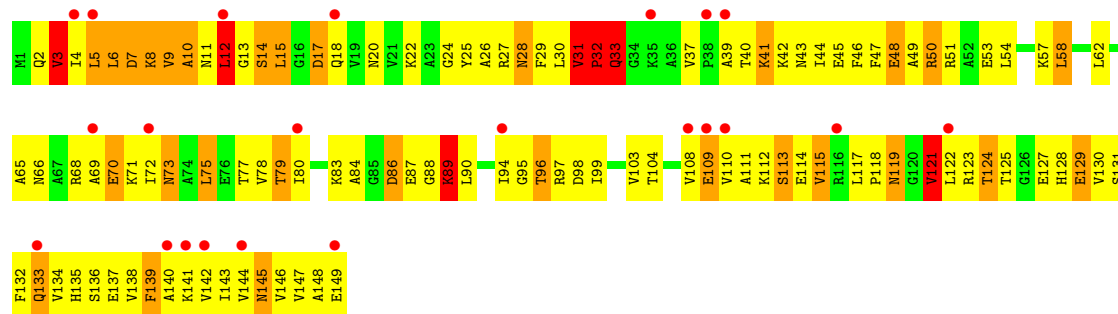
• Molecule 40: 50S ribosomal protein L9

Chain BH:



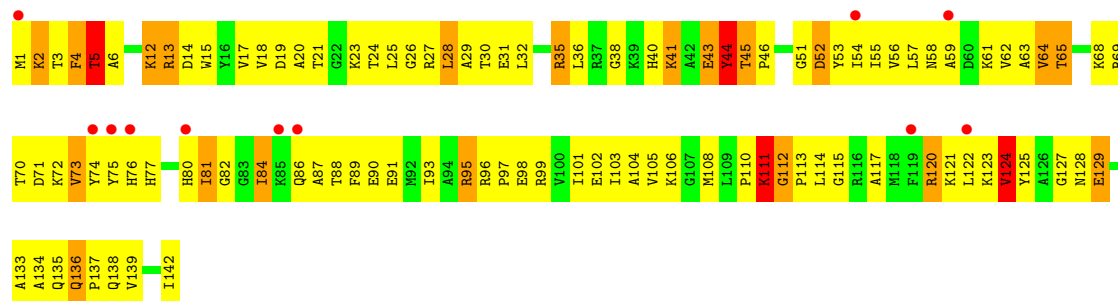
- Molecule 40: 50S ribosomal protein L9

Chain DH:



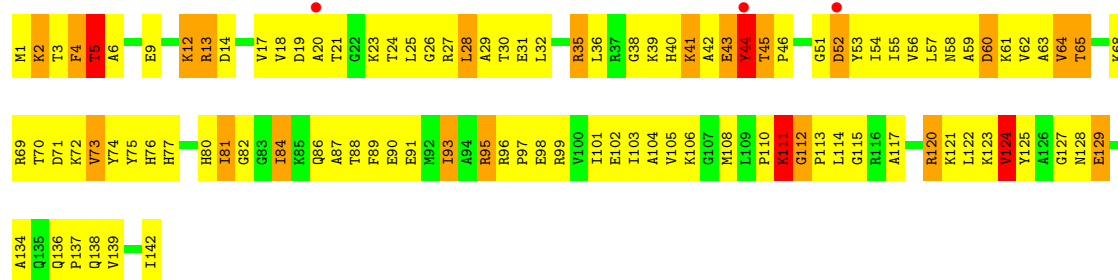
- Molecule 41: 50S ribosomal protein L13

Chain BJ:



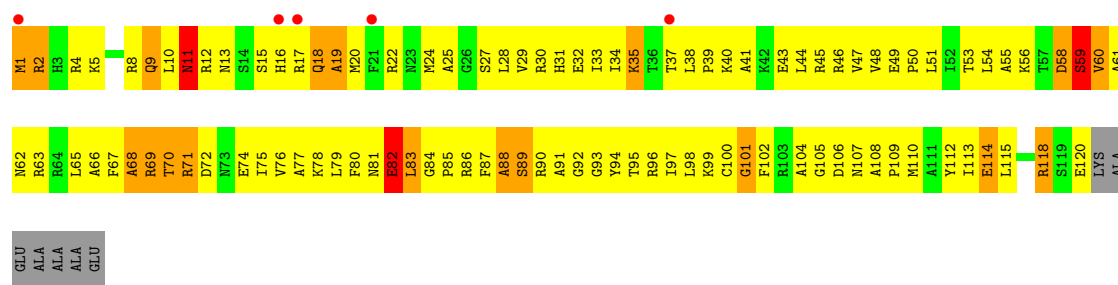
- Molecule 41: 50S ribosomal protein L13

Chain DJ:

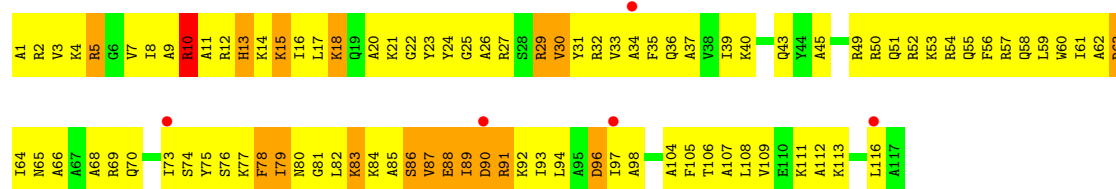


- Molecule 42: 50S ribosomal protein L17

Chain BN:

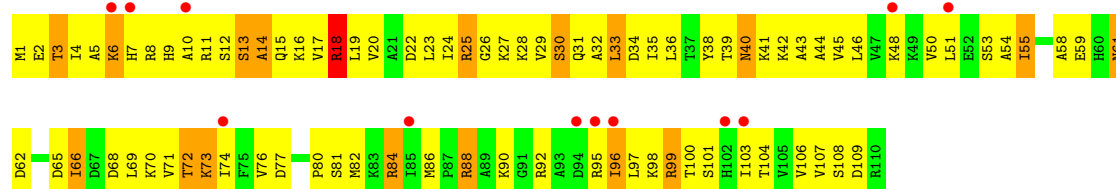


Chain DQ:



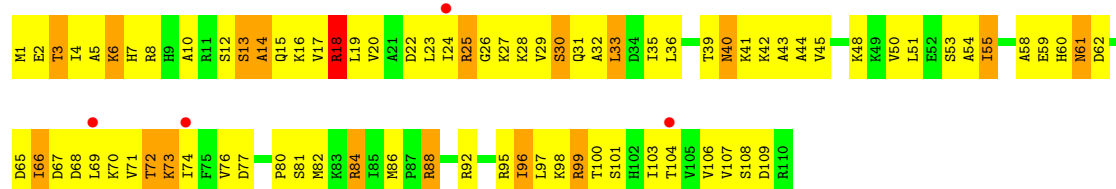
- Molecule 45: 50S ribosomal protein L22

Chain BS:



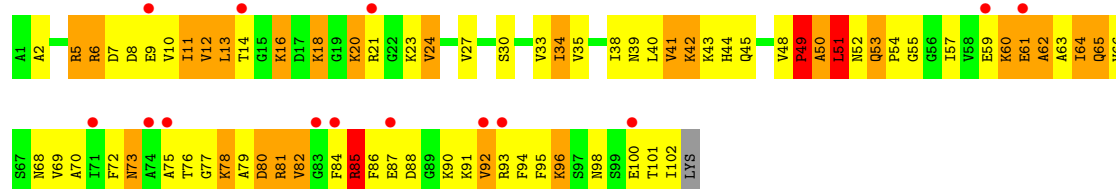
- Molecule 45: 50S ribosomal protein L22

Chain DS:



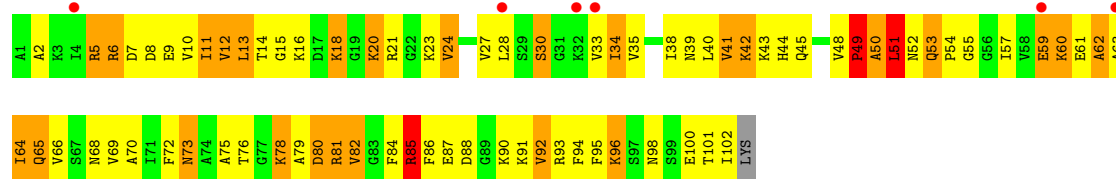
- Molecule 46: 50S ribosomal protein L24

Chain BU:



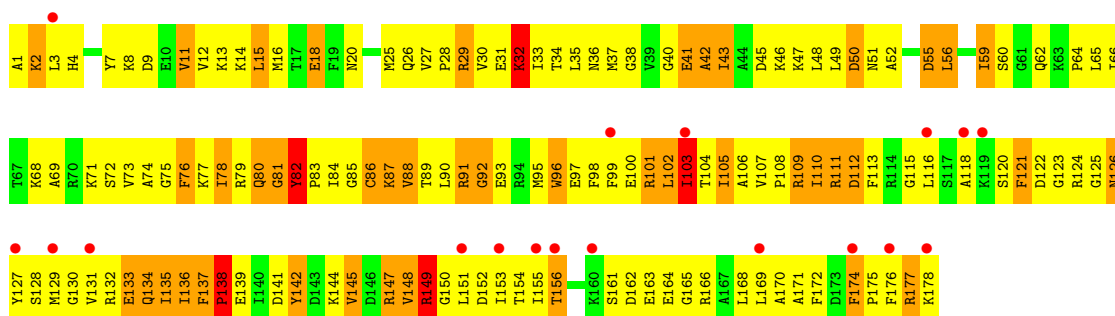
- Molecule 46: 50S ribosomal protein L24

Chain DU:



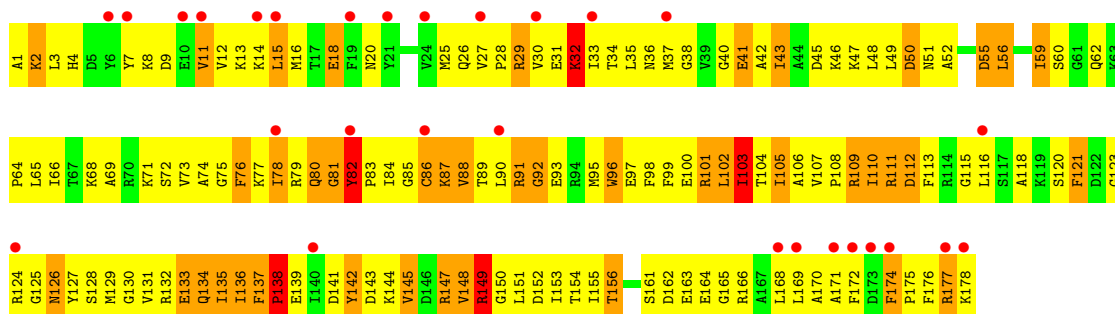
- Molecule 47: 50S ribosomal protein L5

Chain BF:



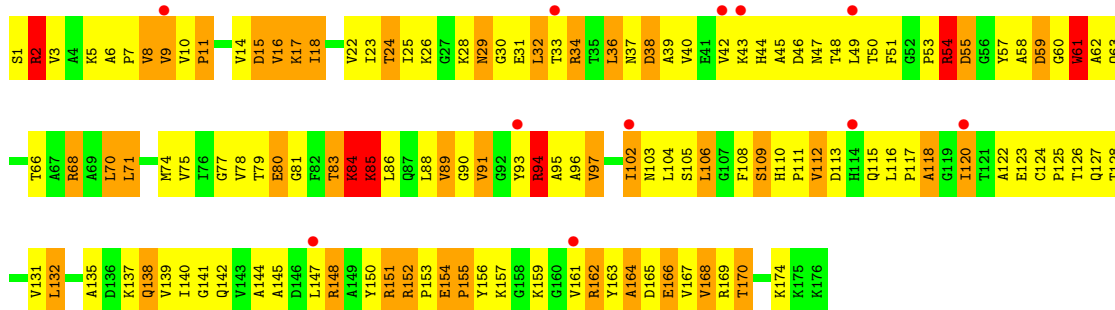
• Molecule 47: 50S ribosomal protein L5

Chain DF:



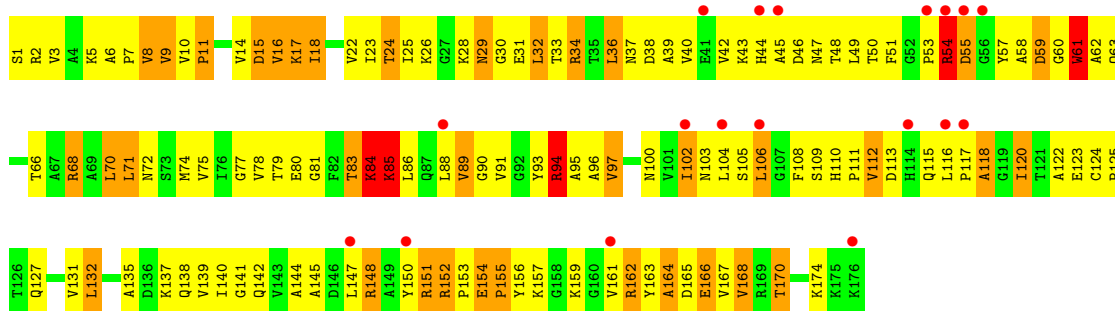
• Molecule 48: 50S ribosomal protein L6

Chain BG:



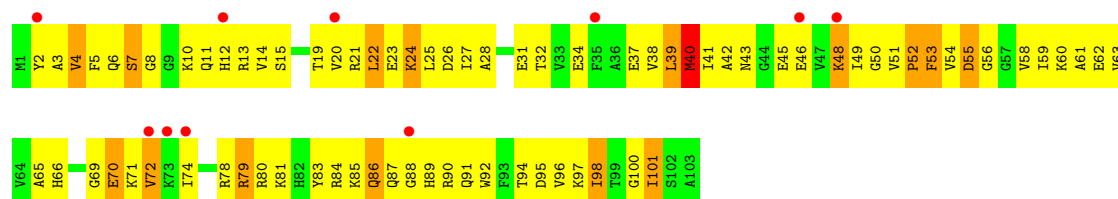
• Molecule 48: 50S ribosomal protein L6

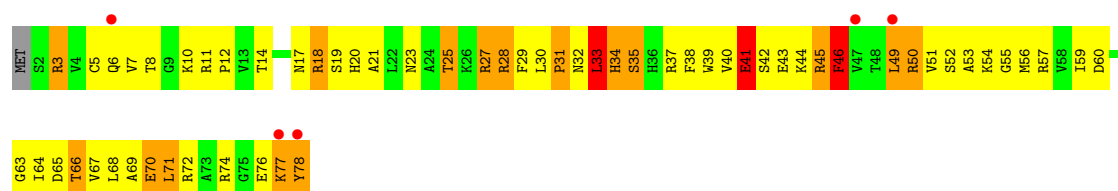
Chain DG:



• Molecule 49: 50S ribosomal protein L21

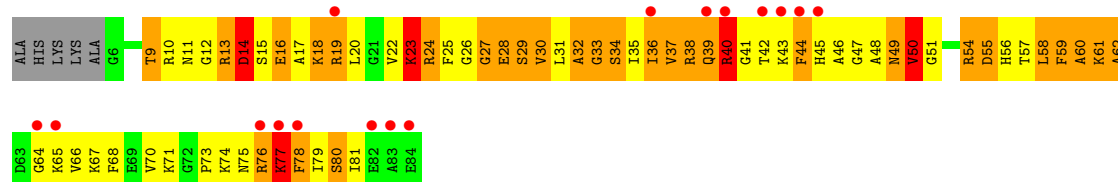
Chain BR: 





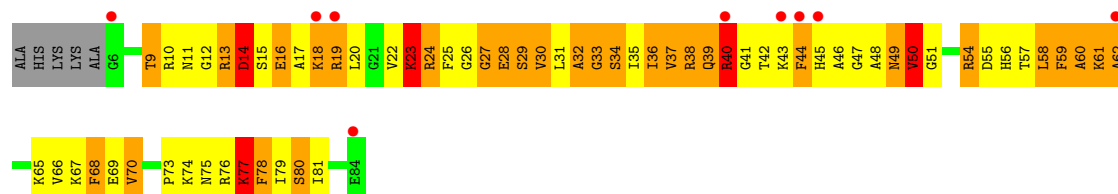
• Molecule 52: 50S ribosomal protein L27

Chain BW:



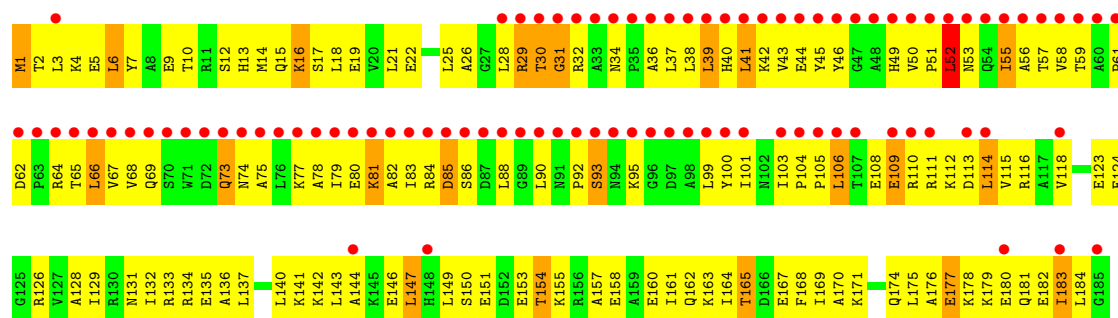
• Molecule 52: 50S ribosomal protein L27

Chain DW:



• Molecule 53: 50S ribosomal protein RRF

Chain B6:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	208.54Å 378.89Å 736.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 4.00 138.07 – 4.15	Depositor EDS
% Data completeness (in resolution range)	87.4 (40.00-4.00) 87.4 (138.07-4.15)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 4.15Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.305 0.242 , 0.276	Depositor DCC
R_{free} test set	18876 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	133.1	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 24.5	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 382905 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	287083	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.29	3/36762 (0.0%)	0.78	21/57350 (0.0%)
1	CA	0.29	4/36762 (0.0%)	0.78	22/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.44	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.44	0/2227
4	AE	0.23	0/1118	0.46	0/1504
4	CE	0.23	0/1118	0.46	0/1504
5	AF	0.24	0/835	0.45	0/1128
5	CF	0.24	0/835	0.45	0/1128
6	AG	0.23	0/1187	0.46	0/1591
6	CG	0.23	0/1211	0.46	0/1624
7	AH	0.23	0/989	0.44	0/1326
7	CH	0.23	0/989	0.44	0/1326
8	AI	0.24	0/1034	0.46	0/1375
8	CI	0.24	0/1033	0.46	0/1375
9	AJ	0.22	0/796	0.48	0/1077
9	CJ	0.22	0/796	0.48	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.50	0/1300
11	CL	0.22	0/969	0.50	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.46	0/1181
13	AN	0.24	0/785	0.45	0/1043
13	CN	0.24	0/785	0.45	0/1043
14	AO	0.23	0/722	0.47	0/964
14	CO	0.23	0/722	0.47	0/964
15	AP	0.25	0/659	0.46	0/884
15	CP	0.25	0/648	0.47	0/870
16	AQ	0.24	0/657	0.47	0/881
16	CQ	0.24	0/666	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	0.46	0/621
18	AS	0.25	0/652	0.47	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.23	0/671	0.39	0/888
19	CT	0.23	0/671	0.39	0/888
20	AB	0.25	0/1735	0.45	0/2338
20	CB	0.25	0/1735	0.45	0/2338
21	AU	0.26	0/430	0.48	0/570
21	CU	0.26	0/430	0.48	0/570
22	BA	0.28	0/2803	0.76	1/4371 (0.0%)
22	DA	0.28	0/2803	0.76	0/4371
23	BB	0.28	6/68314 (0.0%)	0.78	48/106569 (0.0%)
23	DB	0.30	6/68314 (0.0%)	0.79	48/106569 (0.0%)
24	BI	0.24	0/1046	0.47	0/1410
24	DI	0.25	0/1046	0.48	0/1410
25	BC	0.22	0/2121	0.48	0/2852
25	DC	0.22	0/2121	0.48	0/2852
26	BD	0.24	0/1586	0.49	0/2134
26	DD	0.24	0/1586	0.49	0/2134
27	BK	0.24	0/939	0.55	0/1258
27	DK	0.24	0/939	0.55	0/1258
28	BP	0.24	0/929	0.51	0/1242
28	DP	0.24	0/929	0.51	0/1242
29	BE	0.24	0/1571	0.51	0/2113
29	DE	0.24	0/1571	0.51	0/2113
30	BY	0.23	0/453	0.49	0/605
30	DY	0.23	0/453	0.49	0/605
31	B0	0.22	0/450	0.55	0/599
31	D0	0.23	0/450	0.55	0/599
32	B4	0.23	0/303	0.47	0/397
32	D4	0.23	0/303	0.47	0/397
33	B1	0.27	0/416	0.49	0/554
33	D1	0.27	0/416	0.49	0/554
34	B3	0.24	0/513	0.48	0/676
34	D3	0.24	0/513	0.48	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.25	0/380	0.48	0/498
36	D2	0.25	0/380	0.48	0/498
37	BL	0.23	0/1054	0.48	0/1403
37	DL	0.23	0/1054	0.48	0/1403
38	BM	0.25	0/1093	0.48	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.48	0/1460
39	BX	0.24	0/510	0.53	0/677
39	DX	0.24	0/510	0.53	0/677
40	BH	0.25	0/1122	0.48	0/1515
40	DH	0.25	0/1122	0.48	0/1515
41	BJ	0.24	0/1152	0.48	0/1551
41	DJ	0.23	0/1152	0.48	0/1551
42	BN	0.24	0/973	0.51	0/1301
42	DN	0.24	0/973	0.51	0/1301
43	BO	0.23	0/902	0.49	0/1209
43	DO	0.23	0/902	0.49	0/1209
44	BQ	0.25	0/960	0.49	0/1278
44	DQ	0.26	0/960	0.49	0/1278
45	BS	0.22	0/864	0.52	0/1156
45	DS	0.22	0/864	0.52	0/1156
46	BU	0.25	0/787	0.47	0/1051
46	DU	0.25	0/787	0.47	0/1051
47	BF	0.26	0/1444	0.52	0/1937
47	DF	0.26	0/1444	0.52	0/1937
48	BG	0.23	0/1343	0.47	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.50	0/1107
49	DR	0.25	0/829	0.50	0/1107
50	BT	0.23	0/744	0.55	0/994
50	DT	0.22	0/744	0.55	0/994
51	BZ	0.25	0/635	0.51	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.51	0/797
52	DW	0.28	0/603	0.51	0/797
53	B6	0.23	0/1497	0.52	1/2017 (0.0%)
53	D6	0.30	0/1497	0.58	1/2017 (0.0%)
All	All	0.28	19/309353 (0.0%)	0.71	142/462003 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	16
1	CA	0	17
23	BB	0	35

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Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	0	47
All	All	0	115

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.56	1.26	1.41
23	DB	1086	A	C5-C6	-16.53	1.26	1.41
23	DB	1088	A	C6-N1	-10.57	1.28	1.35
23	BB	1088	A	C6-N1	-10.52	1.28	1.35
1	CA	1213	A	P-OP1	-9.61	1.32	1.49

The worst 5 of 142 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CA	1213	A	O5'-P-OP1	-31.90	72.42	110.70
1	AA	1213	A	O5'-P-OP2	-30.12	74.56	110.70
23	DB	2204	G	O5'-P-OP1	-29.74	75.02	110.70
23	BB	2204	G	O5'-P-OP2	-28.90	76.02	110.70
23	BB	2791	G	O5'-P-OP1	-28.07	77.02	110.70

There are no chirality outliers.

5 of 115 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	187	G	Sidechain
1	AA	281	G	Sidechain
1	AA	324	G	Sidechain
1	AA	437	U	Sidechain
1	AA	86	G	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32831	0	16521	1290	0
1	CA	32831	0	16521	1350	0
2	AC	1624	0	1699	140	0
2	CC	1624	0	1699	146	0
3	AD	1643	0	1710	174	0
3	CD	1643	0	1710	170	0
4	AE	1105	0	1148	95	0
4	CE	1105	0	1148	96	0
5	AF	817	0	808	96	0
5	CF	817	0	808	94	0
6	AG	1174	0	1230	112	0
6	CG	1196	0	1246	106	0
7	AH	979	0	1034	95	0
7	CH	979	0	1034	96	0
8	AI	1022	0	1070	149	0
8	CI	1021	0	1070	149	0
9	AJ	786	0	828	77	0
9	CJ	786	0	828	80	0
10	AK	877	0	887	111	0
10	CK	877	0	887	114	0
11	AL	955	0	1019	92	0
11	CL	955	0	1019	91	0
12	AM	883	0	944	119	0
12	CM	876	0	937	120	0
13	AN	774	0	827	121	0
13	CN	774	0	827	131	0
14	AO	714	0	734	60	0
14	CO	714	0	734	54	0
15	AP	649	0	666	56	0
15	CP	638	0	656	57	0
16	AQ	648	0	691	71	0
16	CQ	657	0	702	67	0
17	AR	455	0	478	51	0
17	CR	455	0	478	56	0
18	AS	637	0	665	85	0
18	CS	644	0	675	87	0
19	AT	665	0	714	68	0
19	CT	665	0	714	70	0
20	AB	1704	0	1732	220	0
20	CB	1704	0	1732	211	0
21	AU	425	0	449	79	0
21	CU	425	0	449	89	0
22	BA	2507	0	1270	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	108	0
23	BB	60995	0	30678	2536	0
23	DB	60995	0	30678	2543	0
24	BI	1032	0	1088	119	0
24	DI	1032	0	1088	181	0
25	BC	2082	0	2157	239	0
25	DC	2082	0	2157	241	0
26	BD	1565	0	1616	206	0
26	DD	1565	0	1616	216	0
27	BK	930	0	1000	122	0
27	DK	930	0	1000	122	0
28	BP	917	0	965	102	0
28	DP	917	0	965	108	0
29	BE	1552	0	1619	194	0
29	DE	1552	0	1619	181	0
30	BY	449	0	491	49	0
30	DY	449	0	491	55	0
31	B0	444	0	461	49	0
31	D0	444	0	461	47	0
32	B4	302	0	340	38	0
32	D4	302	0	340	44	0
33	B1	409	0	440	58	0
33	D1	409	0	440	54	0
34	B3	504	0	574	51	0
34	D3	504	0	574	48	0
35	BV	753	0	780	97	0
35	DV	753	0	780	102	0
36	B2	377	0	418	38	0
36	D2	377	0	418	38	0
37	BL	1045	0	1117	148	0
37	DL	1045	0	1117	153	0
38	BM	1074	0	1157	129	0
38	DM	1074	0	1157	121	0
39	BX	509	0	543	55	0
39	DX	509	0	543	60	0
40	BH	1111	0	1148	186	0
40	DH	1111	0	1148	158	0
41	BJ	1129	0	1162	136	0
41	DJ	1129	0	1162	137	0
42	BN	960	0	1000	130	0
42	DN	960	0	1000	129	0
43	BO	892	0	923	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	96	0
44	BQ	947	0	1022	171	0
44	DQ	947	0	1022	178	0
45	BS	857	0	922	101	0
45	DS	857	0	922	101	0
46	BU	779	0	834	114	0
46	DU	779	0	834	109	0
47	BF	1420	0	1460	223	0
47	DF	1420	0	1460	216	0
48	BG	1323	0	1374	218	0
48	DG	1323	0	1374	195	0
49	BR	816	0	839	113	0
49	DR	816	0	839	128	0
50	BT	738	0	807	125	0
50	DT	738	0	807	121	0
51	BZ	625	0	652	82	0
51	DZ	625	0	652	82	0
52	BW	596	0	610	120	0
52	DW	596	0	610	126	0
53	B6	1478	0	1526	192	0
53	D6	1478	0	1526	150	0
54	AA	60	0	0	0	0
54	BB	110	0	0	0	0
54	CA	61	0	0	0	0
54	CE	1	0	0	0	0
54	DB	111	0	0	0	0
55	AA	31	0	39	0	0
55	BB	31	0	39	2	0
55	CA	31	0	39	3	0
55	DB	31	0	39	0	0
56	B4	1	0	0	0	0
56	D4	1	0	0	0	0
57	AA	287	0	0	1	0
57	AE	3	0	0	0	0
57	AK	1	0	0	0	0
57	AL	3	0	0	0	0
57	AN	4	0	0	0	0
57	AT	2	0	0	0	0
57	BB	492	0	0	8	0
57	BC	6	0	0	0	0
57	BD	1	0	0	0	0
57	BE	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	BL	3	0	0	0	0
57	BT	1	0	0	0	0
57	CA	296	0	0	2	0
57	CE	3	0	0	0	0
57	CK	1	0	0	0	0
57	CL	3	0	0	0	0
57	CN	4	0	0	0	0
57	CT	2	0	0	0	0
57	DB	500	0	0	7	0
57	DC	6	0	0	0	0
57	DE	2	0	0	0	0
57	DL	2	0	0	0	0
57	DR	1	0	0	0	0
57	DT	1	0	0	0	0
All	All	287083	0	193870	17818	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 37.

The worst 5 of 17818 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:DB:1099:G:H8	24:DI:3:LYS:N	1.36	1.20
40:BH:31:VAL:HB	40:BH:32:PRO:HD2	1.23	1.17
21:CU:36:PHE:HB3	21:CU:40:PRO:HD3	1.28	1.14
21:AU:36:PHE:HB3	21:AU:40:PRO:HD3	1.29	1.11
25:DC:144:GLU:HA	25:DC:151:GLY:HA2	1.33	1.11

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%)	151 (74%)	38 (19%)	15 (7%)	2	31
2	CC	204/232 (88%)	152 (74%)	37 (18%)	15 (7%)	2	31
3	AD	203/205 (99%)	151 (74%)	39 (19%)	13 (6%)	2	36
3	CD	203/205 (99%)	148 (73%)	42 (21%)	13 (6%)	2	36
4	AE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	4	49
4	CE	148/166 (89%)	117 (79%)	25 (17%)	6 (4%)	4	49
5	AF	98/135 (73%)	64 (65%)	25 (26%)	9 (9%)	1	24
5	CF	98/135 (73%)	65 (66%)	24 (24%)	9 (9%)	1	24
6	AG	148/178 (83%)	106 (72%)	33 (22%)	9 (6%)	2	37
6	CG	150/178 (84%)	112 (75%)	29 (19%)	9 (6%)	2	38
7	AH	127/129 (98%)	98 (77%)	23 (18%)	6 (5%)	4	45
7	CH	127/129 (98%)	96 (76%)	25 (20%)	6 (5%)	4	45
8	AI	125/129 (97%)	99 (79%)	17 (14%)	9 (7%)	2	32
8	CI	125/129 (97%)	98 (78%)	18 (14%)	9 (7%)	2	32
9	AJ	96/103 (93%)	70 (73%)	13 (14%)	13 (14%)	0	11
9	CJ	96/103 (93%)	71 (74%)	12 (12%)	13 (14%)	0	11
10	AK	115/128 (90%)	87 (76%)	22 (19%)	6 (5%)	3	42
10	CK	115/128 (90%)	87 (76%)	22 (19%)	6 (5%)	3	42
11	AL	121/123 (98%)	73 (60%)	33 (27%)	15 (12%)	1	13
11	CL	121/123 (98%)	75 (62%)	31 (26%)	15 (12%)	1	13
12	AM	112/117 (96%)	79 (70%)	24 (21%)	9 (8%)	1	28
12	CM	111/117 (95%)	76 (68%)	25 (22%)	10 (9%)	1	24
13	AN	92/100 (92%)	59 (64%)	26 (28%)	7 (8%)	2	29
13	CN	92/100 (92%)	60 (65%)	24 (26%)	8 (9%)	1	25
14	AO	86/89 (97%)	59 (69%)	22 (26%)	5 (6%)	3	39
14	CO	86/89 (97%)	60 (70%)	22 (26%)	4 (5%)	4	45
15	AP	80/82 (98%)	59 (74%)	16 (20%)	5 (6%)	2	37
15	CP	78/82 (95%)	56 (72%)	16 (20%)	6 (8%)	1	29
16	AQ	78/83 (94%)	58 (74%)	15 (19%)	5 (6%)	2	36
16	CQ	79/83 (95%)	59 (75%)	15 (19%)	5 (6%)	2	37
17	AR	53/74 (72%)	41 (77%)	9 (17%)	3 (6%)	3	39
17	CR	53/74 (72%)	41 (77%)	9 (17%)	3 (6%)	3	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	AS	77/91 (85%)	60 (78%)	12 (16%)	5 (6%)	2	36
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	29
19	AT	83/86 (96%)	63 (76%)	15 (18%)	5 (6%)	2	38
19	CT	83/86 (96%)	62 (75%)	16 (19%)	5 (6%)	2	38
20	AB	216/240 (90%)	142 (66%)	57 (26%)	17 (8%)	1	28
20	CB	216/240 (90%)	134 (62%)	65 (30%)	17 (8%)	1	28
21	AU	49/70 (70%)	28 (57%)	11 (22%)	10 (20%)	0	4
21	CU	49/70 (70%)	28 (57%)	12 (24%)	9 (18%)	0	5
24	BI	139/141 (99%)	120 (86%)	14 (10%)	5 (4%)	5	54
24	DI	139/141 (99%)	114 (82%)	20 (14%)	5 (4%)	5	54
25	BC	269/272 (99%)	155 (58%)	66 (24%)	48 (18%)	0	5
25	DC	269/272 (99%)	155 (58%)	65 (24%)	49 (18%)	0	5
26	BD	207/209 (99%)	122 (59%)	54 (26%)	31 (15%)	0	8
26	DD	207/209 (99%)	124 (60%)	51 (25%)	32 (16%)	0	8
27	BK	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	10
27	DK	119/123 (97%)	78 (66%)	24 (20%)	17 (14%)	0	10
28	BP	112/114 (98%)	61 (54%)	32 (29%)	19 (17%)	0	6
28	DP	112/114 (98%)	61 (54%)	34 (30%)	17 (15%)	0	8
29	BE	199/201 (99%)	125 (63%)	50 (25%)	24 (12%)	1	14
29	DE	199/201 (99%)	125 (63%)	51 (26%)	23 (12%)	1	15
30	BY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	25
30	DY	56/58 (97%)	39 (70%)	12 (21%)	5 (9%)	1	25
31	B0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	12
31	D0	54/56 (96%)	39 (72%)	8 (15%)	7 (13%)	0	12
32	B4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	1
32	D4	36/38 (95%)	16 (44%)	10 (28%)	10 (28%)	0	1
33	B1	48/54 (89%)	37 (77%)	7 (15%)	4 (8%)	1	27
33	D1	48/54 (89%)	36 (75%)	8 (17%)	4 (8%)	1	27
34	B3	62/64 (97%)	35 (56%)	21 (34%)	6 (10%)	1	21
34	D3	62/64 (97%)	34 (55%)	22 (36%)	6 (10%)	1	21
35	BV	92/94 (98%)	64 (70%)	22 (24%)	6 (6%)	2	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	DV	92/94 (98%)	62 (67%)	24 (26%)	6 (6%)	2	36
36	B2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	1	24
36	D2	44/46 (96%)	30 (68%)	10 (23%)	4 (9%)	1	24
37	BL	141/144 (98%)	89 (63%)	31 (22%)	21 (15%)	0	8
37	DL	141/144 (98%)	89 (63%)	32 (23%)	20 (14%)	0	10
38	BM	134/136 (98%)	84 (63%)	29 (22%)	21 (16%)	0	7
38	DM	134/136 (98%)	83 (62%)	31 (23%)	20 (15%)	0	8
39	BX	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	12
39	DX	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	12
40	BH	147/149 (99%)	76 (52%)	46 (31%)	25 (17%)	0	6
40	DH	147/149 (99%)	91 (62%)	33 (22%)	23 (16%)	0	7
41	BJ	140/142 (99%)	85 (61%)	37 (26%)	18 (13%)	0	12
41	DJ	140/142 (99%)	85 (61%)	36 (26%)	19 (14%)	0	11
42	BN	118/127 (93%)	76 (64%)	29 (25%)	13 (11%)	1	16
42	DN	118/127 (93%)	77 (65%)	28 (24%)	13 (11%)	1	16
43	BO	114/117 (97%)	74 (65%)	29 (25%)	11 (10%)	1	21
43	DO	114/117 (97%)	75 (66%)	27 (24%)	12 (10%)	1	18
44	BQ	115/117 (98%)	75 (65%)	31 (27%)	9 (8%)	1	28
44	DQ	115/117 (98%)	75 (65%)	29 (25%)	11 (10%)	1	21
45	BS	108/110 (98%)	68 (63%)	29 (27%)	11 (10%)	1	19
45	DS	108/110 (98%)	66 (61%)	31 (29%)	11 (10%)	1	19
46	BU	100/103 (97%)	58 (58%)	23 (23%)	19 (19%)	0	4
46	DU	100/103 (97%)	59 (59%)	22 (22%)	19 (19%)	0	4
47	BF	176/178 (99%)	103 (58%)	44 (25%)	29 (16%)	0	7
47	DF	176/178 (99%)	105 (60%)	42 (24%)	29 (16%)	0	7
48	BG	174/176 (99%)	99 (57%)	42 (24%)	33 (19%)	0	4
48	DG	174/176 (99%)	101 (58%)	41 (24%)	32 (18%)	0	5
49	BR	101/103 (98%)	72 (71%)	20 (20%)	9 (9%)	1	25
49	DR	101/103 (98%)	74 (73%)	18 (18%)	9 (9%)	1	25
50	BT	91/100 (91%)	48 (53%)	23 (25%)	20 (22%)	0	2
50	DT	91/100 (91%)	46 (50%)	27 (30%)	18 (20%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BZ	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	7
51	DZ	75/78 (96%)	50 (67%)	13 (17%)	12 (16%)	0	7
52	BW	77/84 (92%)	28 (36%)	23 (30%)	26 (34%)	0	0
52	DW	77/84 (92%)	28 (36%)	24 (31%)	25 (32%)	0	0
53	B6	183/185 (99%)	162 (88%)	16 (9%)	5 (3%)	8	61
53	D6	183/185 (99%)	152 (83%)	24 (13%)	7 (4%)	5	52
All	All	11607/12284 (94%)	7731 (67%)	2581 (22%)	1295 (11%)	1	16

5 of 1295 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	54	ILE
2	AC	205	GLU
3	AD	24	VAL
3	AD	25	ARG

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%)	144 (85%)	26 (15%)	4	29
2	CC	170/189 (90%)	143 (84%)	27 (16%)	4	27
3	AD	172/172 (100%)	146 (85%)	26 (15%)	4	30
3	CD	172/172 (100%)	147 (86%)	25 (14%)	5	31
4	AE	113/125 (90%)	95 (84%)	18 (16%)	4	27
4	CE	113/125 (90%)	96 (85%)	17 (15%)	4	30
5	AF	87/116 (75%)	76 (87%)	11 (13%)	7	39
5	CF	87/116 (75%)	76 (87%)	11 (13%)	7	39
6	AG	123/146 (84%)	105 (85%)	18 (15%)	5	31
6	CG	125/146 (86%)	106 (85%)	19 (15%)	4	29
7	AH	104/104 (100%)	96 (92%)	8 (8%)	18	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	CH	104/104 (100%)	97 (93%)	7 (7%)	23	71
8	AI	105/106 (99%)	91 (87%)	14 (13%)	6	37
8	CI	105/106 (99%)	89 (85%)	16 (15%)	4	29
9	AJ	86/90 (96%)	76 (88%)	10 (12%)	8	43
9	CJ	86/90 (96%)	76 (88%)	10 (12%)	8	43
10	AK	90/98 (92%)	77 (86%)	13 (14%)	5	32
10	CK	90/98 (92%)	75 (83%)	15 (17%)	3	24
11	AL	103/103 (100%)	86 (84%)	17 (16%)	3	25
11	CL	103/103 (100%)	85 (82%)	18 (18%)	3	21
12	AM	92/95 (97%)	77 (84%)	15 (16%)	3	26
12	CM	91/95 (96%)	76 (84%)	15 (16%)	3	25
13	AN	79/83 (95%)	62 (78%)	17 (22%)	1	11
13	CN	79/83 (95%)	62 (78%)	17 (22%)	1	11
14	AO	76/77 (99%)	69 (91%)	7 (9%)	13	56
14	CO	76/77 (99%)	69 (91%)	7 (9%)	13	56
15	AP	65/65 (100%)	59 (91%)	6 (9%)	13	56
15	CP	65/65 (100%)	59 (91%)	6 (9%)	13	56
16	AQ	74/77 (96%)	61 (82%)	13 (18%)	3	20
16	CQ	75/77 (97%)	63 (84%)	12 (16%)	3	27
17	AR	48/64 (75%)	40 (83%)	8 (17%)	3	24
17	CR	48/64 (75%)	39 (81%)	9 (19%)	2	17
18	AS	70/78 (90%)	56 (80%)	14 (20%)	2	14
18	CS	71/78 (91%)	57 (80%)	14 (20%)	2	15
19	AT	65/65 (100%)	55 (85%)	10 (15%)	4	28
19	CT	65/65 (100%)	55 (85%)	10 (15%)	4	28
20	AB	180/198 (91%)	148 (82%)	32 (18%)	2	20
20	CB	180/198 (91%)	150 (83%)	30 (17%)	3	24
21	AU	44/60 (73%)	32 (73%)	12 (27%)	0	6
21	CU	44/60 (73%)	32 (73%)	12 (27%)	0	6
24	BI	109/109 (100%)	107 (98%)	2 (2%)	71	93
24	DI	109/109 (100%)	103 (94%)	6 (6%)	30	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	BC	216/217 (100%)	179 (83%)	37 (17%)	3	22
25	DC	216/217 (100%)	176 (82%)	40 (18%)	2	18
26	BD	164/164 (100%)	135 (82%)	29 (18%)	3	20
26	DD	164/164 (100%)	134 (82%)	30 (18%)	2	18
27	BK	102/104 (98%)	80 (78%)	22 (22%)	1	11
27	DK	102/104 (98%)	81 (79%)	21 (21%)	2	13
28	BP	99/99 (100%)	80 (81%)	19 (19%)	2	16
28	DP	99/99 (100%)	80 (81%)	19 (19%)	2	16
29	BE	165/165 (100%)	143 (87%)	22 (13%)	6	37
29	DE	165/165 (100%)	142 (86%)	23 (14%)	5	34
30	BY	48/48 (100%)	38 (79%)	10 (21%)	2	13
30	DY	48/48 (100%)	38 (79%)	10 (21%)	2	13
31	B0	47/47 (100%)	38 (81%)	9 (19%)	2	16
31	D0	47/47 (100%)	38 (81%)	9 (19%)	2	16
32	B4	34/34 (100%)	28 (82%)	6 (18%)	3	20
32	D4	34/34 (100%)	29 (85%)	5 (15%)	4	31
33	B1	45/48 (94%)	40 (89%)	5 (11%)	9	46
33	D1	45/48 (94%)	41 (91%)	4 (9%)	14	58
34	B3	51/51 (100%)	45 (88%)	6 (12%)	8	42
34	D3	51/51 (100%)	46 (90%)	5 (10%)	12	52
35	BV	78/78 (100%)	64 (82%)	14 (18%)	2	19
35	DV	78/78 (100%)	64 (82%)	14 (18%)	2	19
36	B2	38/38 (100%)	28 (74%)	10 (26%)	1	7
36	D2	38/38 (100%)	28 (74%)	10 (26%)	1	7
37	BL	102/103 (99%)	91 (89%)	11 (11%)	9	48
37	DL	102/103 (99%)	91 (89%)	11 (11%)	9	48
38	BM	109/109 (100%)	87 (80%)	22 (20%)	2	14
38	DM	109/109 (100%)	87 (80%)	22 (20%)	2	14
39	BX	55/55 (100%)	46 (84%)	9 (16%)	3	25
39	DX	55/55 (100%)	46 (84%)	9 (16%)	3	25
40	BH	114/114 (100%)	79 (69%)	35 (31%)	0	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	DH	114/114 (100%)	89 (78%)	25 (22%)	1	11
41	BJ	116/116 (100%)	100 (86%)	16 (14%)	5	34
41	DJ	116/116 (100%)	100 (86%)	16 (14%)	5	34
42	BN	100/103 (97%)	84 (84%)	16 (16%)	3	27
42	DN	100/103 (97%)	84 (84%)	16 (16%)	3	27
43	BO	86/87 (99%)	71 (83%)	15 (17%)	3	21
43	DO	86/87 (99%)	72 (84%)	14 (16%)	3	26
44	BQ	89/89 (100%)	79 (89%)	10 (11%)	9	45
44	DQ	89/89 (100%)	79 (89%)	10 (11%)	9	45
45	BS	93/93 (100%)	77 (83%)	16 (17%)	3	22
45	DS	93/93 (100%)	77 (83%)	16 (17%)	3	22
46	BU	83/84 (99%)	65 (78%)	18 (22%)	1	11
46	DU	83/84 (99%)	65 (78%)	18 (22%)	1	11
47	BF	149/149 (100%)	117 (78%)	32 (22%)	1	11
47	DF	149/149 (100%)	117 (78%)	32 (22%)	1	11
48	BG	137/137 (100%)	110 (80%)	27 (20%)	2	15
48	DG	137/137 (100%)	112 (82%)	25 (18%)	2	18
49	BR	84/84 (100%)	71 (84%)	13 (16%)	4	28
49	DR	84/84 (100%)	70 (83%)	14 (17%)	3	24
50	BT	80/84 (95%)	64 (80%)	16 (20%)	2	14
50	DT	80/84 (95%)	64 (80%)	16 (20%)	2	14
51	BZ	67/68 (98%)	53 (79%)	14 (21%)	1	12
51	DZ	67/68 (98%)	56 (84%)	11 (16%)	3	25
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	5
52	DW	59/62 (95%)	42 (71%)	17 (29%)	0	5
53	B6	157/157 (100%)	137 (87%)	20 (13%)	6	39
53	D6	157/157 (100%)	134 (85%)	23 (15%)	5	31
All	All	9647/10014 (96%)	8066 (84%)	1581 (16%)	3	25

5 of 1581 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	BR	39	LEU

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Mol	Chain	Res	Type
6	CG	110	ARG
47	DF	103	ILE
50	BT	68	LYS
2	CC	61	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 320 such sidechains are listed below:

Mol	Chain	Res	Type
48	BG	37	ASN
7	CH	3	GLN
46	DU	65	GLN
49	BR	86	GLN
2	CC	2	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	244 (15%)	21 (1%)
1	CA	1529/1542 (99%)	235 (15%)	19 (1%)
22	BA	116/120 (96%)	17 (14%)	0
22	DA	116/120 (96%)	16 (13%)	0
23	BB	2837/2904 (97%)	457 (16%)	17 (0%)
23	DB	2837/2904 (97%)	435 (15%)	22 (0%)
All	All	8964/9132 (98%)	1404 (15%)	79 (0%)

5 of 1404 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2425	A
1	CA	372	C
23	DB	2336	A

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Mol	Chain	Res	Type
23	BB	2756	U
1	CA	243	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 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	LLL	AA	1661	-	33,33,33	2.39	13 (39%)	49,49,49	1.39	6 (12%)
55	LLL	BB	3111	-	33,33,33	2.36	13 (39%)	49,49,49	1.37	5 (10%)
55	LLL	CA	1662	-	33,33,33	2.38	13 (39%)	49,49,49	1.40	6 (12%)
55	LLL	DB	3112	-	33,33,33	2.39	13 (39%)	49,49,49	1.39	5 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	LLL	AA	1661	-	-	0/12/65/65	0/3/3/3
55	LLL	BB	3111	-	-	0/12/65/65	0/3/3/3
55	LLL	CA	1662	-	-	0/12/65/65	0/3/3/3
55	LLL	DB	3112	-	-	0/12/65/65	0/3/3/3

The worst 5 of 52 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	CA	1662	LLL	O53-C53	5.73	1.52	1.43
55	AA	1661	LLL	O53-C53	5.71	1.52	1.43
55	DB	3112	LLL	O53-C53	5.70	1.52	1.43
55	BB	3111	LLL	O53-C53	5.66	1.52	1.43
55	DB	3112	LLL	C43-C33	4.98	1.63	1.54

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BB	3111	LLL	C93-N33-C33	4.68	117.55	113.75
55	DB	3112	LLL	C93-N33-C33	4.60	117.48	113.75
55	CA	1662	LLL	C53-O53-C13	4.49	117.62	111.22
55	DB	3112	LLL	C53-O53-C13	4.47	117.59	111.22
55	AA	1661	LLL	C53-O53-C13	4.37	117.45	111.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.48	13 (0%) 83 70	13, 75, 157, 180	0
1	CA	1530/1542 (99%)	-0.56	5 (0%) 91 86	8, 52, 139, 180	0
2	AC	206/232 (88%)	0.40	8 (3%) 37 31	5, 72, 147, 180	0
2	CC	206/232 (88%)	0.46	6 (2%) 49 39	6, 72, 131, 180	0
3	AD	205/205 (100%)	0.79	25 (12%) 5 7	20, 95, 159, 180	0
3	CD	205/205 (100%)	0.35	1 (0%) 88 78	5, 56, 145, 180	0
4	AE	150/166 (90%)	0.76	15 (10%) 8 10	7, 69, 146, 180	0
4	CE	150/166 (90%)	0.70	10 (6%) 17 18	5, 49, 112, 180	0
5	AF	100/135 (74%)	0.89	15 (15%) 3 5	5, 69, 150, 177	0
5	CF	100/135 (74%)	0.54	5 (5%) 28 24	5, 72, 143, 166	0
6	AG	150/178 (84%)	0.58	12 (8%) 12 14	20, 97, 159, 175	0
6	CG	152/178 (85%)	0.47	4 (2%) 53 42	29, 85, 147, 180	0
7	AH	129/129 (100%)	0.88	19 (14%) 3 5	26, 80, 143, 177	0
7	CH	129/129 (100%)	0.44	4 (3%) 47 37	6, 49, 117, 174	0
8	AI	127/129 (98%)	0.64	10 (7%) 13 14	18, 89, 171, 180	0
8	CI	127/129 (98%)	0.42	4 (3%) 47 37	22, 92, 160, 180	0
9	AJ	98/103 (95%)	0.77	7 (7%) 16 16	16, 92, 169, 180	0
9	CJ	98/103 (95%)	0.99	15 (15%) 3 5	26, 87, 153, 180	0
10	AK	117/128 (91%)	0.22	0 100 100	7, 59, 119, 180	0
10	CK	117/128 (91%)	0.33	4 (3%) 43 35	5, 52, 120, 180	0
11	AL	123/123 (100%)	0.65	8 (6%) 18 19	14, 78, 152, 180	0
11	CL	123/123 (100%)	0.38	1 (0%) 83 70	5, 46, 127, 170	0
12	AM	114/117 (97%)	0.37	5 (4%) 33 28	40, 114, 180, 180	0
12	CM	113/117 (96%)	0.32	2 (1%) 65 52	27, 100, 173, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.62	3 (3%) 47 37	8, 86, 158, 180	0
13	CN	96/100 (96%)	0.76	8 (8%) 11 13	14, 87, 147, 178	0
14	AO	88/89 (98%)	0.13	0 100 100	5, 76, 128, 180	0
14	CO	88/89 (98%)	0.35	1 (1%) 77 63	10, 63, 132, 159	0
15	AP	82/82 (100%)	1.32	16 (19%) 2 3	24, 94, 154, 180	0
15	CP	80/82 (97%)	1.10	14 (17%) 2 4	5, 46, 128, 180	0
16	AQ	80/83 (96%)	0.69	8 (10%) 8 10	36, 96, 168, 180	0
16	CQ	81/83 (97%)	0.58	1 (1%) 75 61	5, 52, 135, 180	0
17	AR	55/74 (74%)	0.47	2 (3%) 41 33	14, 70, 148, 180	0
17	CR	55/74 (74%)	0.90	5 (9%) 9 12	12, 64, 136, 180	0
18	AS	79/91 (86%)	1.14	20 (25%) 1 3	44, 120, 176, 180	0
18	CS	80/91 (87%)	0.51	5 (6%) 19 19	34, 107, 180, 180	0
19	AT	85/86 (98%)	0.53	7 (8%) 12 13	34, 101, 168, 180	0
19	CT	85/86 (98%)	0.16	2 (2%) 56 43	5, 62, 140, 180	0
20	AB	218/240 (90%)	0.48	13 (5%) 21 20	18, 97, 160, 180	0
20	CB	218/240 (90%)	0.54	15 (6%) 17 17	16, 93, 160, 180	0
21	AU	51/70 (72%)	0.63	2 (3%) 37 31	27, 89, 171, 180	0
21	CU	51/70 (72%)	0.44	4 (7%) 13 14	23, 81, 137, 180	0
22	BA	117/120 (97%)	-0.56	2 (1%) 67 53	49, 85, 136, 180	0
22	DA	117/120 (97%)	-0.48	2 (1%) 67 53	36, 88, 148, 180	0
23	BB	2841/2904 (97%)	-0.26	25 (0%) 81 68	6, 60, 150, 180	0
23	DB	2841/2904 (97%)	-0.33	14 (0%) 88 78	5, 46, 154, 180	0
24	BI	141/141 (100%)	1.50	42 (29%) 1 2	72, 166, 180, 180	0
24	DI	141/141 (100%)	1.01	19 (13%) 4 6	63, 162, 180, 180	0
25	BC	271/272 (99%)	0.67	14 (5%) 26 23	5, 47, 107, 156	0
25	DC	271/272 (99%)	0.57	7 (2%) 53 42	5, 38, 99, 145	0
26	BD	209/209 (100%)	0.94	29 (13%) 4 5	8, 72, 145, 180	0
26	DD	209/209 (100%)	0.73	17 (8%) 12 14	5, 51, 131, 180	0
27	BK	121/123 (98%)	1.17	17 (14%) 3 5	16, 62, 142, 180	0
27	DK	121/123 (98%)	0.88	4 (3%) 44 36	5, 42, 103, 180	0
28	BP	114/114 (100%)	1.83	48 (42%) 1 2	28, 86, 155, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.43	3 (2%) 53 42	5, 52, 119, 161	0
29	BE	201/201 (100%)	0.96	27 (13%) 4 6	5, 76, 143, 180	0
29	DE	201/201 (100%)	0.64	19 (9%) 8 11	5, 66, 138, 180	0
30	BY	58/58 (100%)	0.93	8 (13%) 4 5	22, 84, 137, 180	0
30	DY	58/58 (100%)	0.51	4 (6%) 17 17	10, 66, 149, 158	0
31	B0	56/56 (100%)	0.70	4 (7%) 16 16	5, 81, 149, 180	0
31	D0	56/56 (100%)	0.21	1 (1%) 65 52	9, 54, 119, 180	0
32	B4	38/38 (100%)	0.47	2 (5%) 25 23	5, 71, 153, 168	0
32	D4	38/38 (100%)	0.49	1 (2%) 53 42	17, 62, 132, 171	0
33	B1	50/54 (92%)	0.78	5 (10%) 8 10	32, 87, 132, 174	0
33	D1	50/54 (92%)	0.45	4 (8%) 12 14	24, 73, 125, 155	0
34	B3	64/64 (100%)	1.36	18 (28%) 1 2	19, 64, 105, 133	0
34	D3	64/64 (100%)	0.68	7 (10%) 6 9	6, 49, 107, 180	0
35	BV	94/94 (100%)	0.39	4 (4%) 34 28	37, 92, 143, 180	0
35	DV	94/94 (100%)	0.53	4 (4%) 34 28	27, 94, 160, 180	0
36	B2	46/46 (100%)	0.55	1 (2%) 59 46	5, 50, 123, 143	0
36	D2	46/46 (100%)	0.48	0 100 100	7, 43, 103, 180	0
37	BL	143/144 (99%)	0.85	16 (11%) 6 8	7, 72, 131, 180	0
37	DL	143/144 (99%)	0.65	10 (6%) 16 16	5, 61, 128, 162	0
38	BM	136/136 (100%)	0.77	14 (10%) 7 10	16, 68, 144, 165	0
38	DM	136/136 (100%)	0.66	10 (7%) 14 15	5, 63, 134, 171	0
39	BX	63/63 (100%)	0.72	3 (4%) 29 25	24, 92, 169, 180	0
39	DX	63/63 (100%)	0.39	2 (3%) 45 36	38, 94, 166, 180	0
40	BH	149/149 (100%)	1.77	56 (37%) 1 2	13, 125, 180, 180	0
40	DH	149/149 (100%)	0.97	22 (14%) 3 5	5, 109, 171, 180	0
41	BJ	142/142 (100%)	0.66	11 (7%) 13 14	13, 77, 132, 166	0
41	DJ	142/142 (100%)	0.48	3 (2%) 60 47	5, 65, 128, 180	0
42	BN	120/127 (94%)	0.67	5 (4%) 35 29	5, 68, 136, 180	0
42	DN	120/127 (94%)	0.15	0 100 100	5, 44, 116, 141	0
43	BO	116/117 (99%)	1.18	26 (22%) 1 3	29, 94, 144, 180	0
43	DO	116/117 (99%)	0.29	3 (2%) 53 42	5, 93, 156, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.18	1 (0%) 81 68	5, 72, 134, 171	0
44	DQ	117/117 (100%)	0.50	5 (4%) 34 28	5, 50, 131, 156	0
45	BS	110/110 (100%)	0.97	12 (10%) 6 9	5, 67, 129, 180	0
45	DS	110/110 (100%)	0.79	4 (3%) 41 33	5, 50, 120, 157	0
46	BU	102/103 (99%)	1.22	14 (13%) 4 5	13, 88, 148, 177	0
46	DU	102/103 (99%)	0.62	6 (5%) 22 20	26, 93, 154, 180	0
47	BF	178/178 (100%)	0.79	18 (10%) 7 10	39, 115, 174, 180	0
47	DF	178/178 (100%)	1.09	28 (15%) 3 5	22, 106, 175, 180	0
48	BG	176/176 (100%)	0.70	11 (6%) 19 19	8, 102, 172, 180	0
48	DG	176/176 (100%)	0.61	18 (10%) 7 10	32, 104, 164, 180	0
49	BR	103/103 (100%)	0.86	10 (9%) 8 11	18, 99, 151, 173	0
49	DR	103/103 (100%)	0.85	10 (9%) 8 11	5, 85, 144, 180	0
50	BT	93/100 (93%)	1.05	13 (13%) 3 5	13, 83, 160, 180	0
50	DT	93/100 (93%)	1.00	10 (10%) 6 9	15, 79, 167, 180	0
51	BZ	77/78 (98%)	0.98	9 (11%) 5 8	12, 57, 112, 152	0
51	DZ	77/78 (98%)	0.63	5 (6%) 18 19	5, 56, 101, 131	0
52	BW	79/84 (94%)	1.09	16 (20%) 1 3	19, 88, 139, 180	0
52	DW	79/84 (94%)	0.69	9 (11%) 6 8	5, 79, 143, 180	0
53	B6	185/185 (100%)	2.99	91 (49%) 1 2	23, 123, 180, 180	0
53	D6	185/185 (100%)	1.54	59 (31%) 1 2	5, 104, 180, 180	0
All	All	20787/21416 (97%)	0.26	1206 (5%) 22 21	5, 69, 159, 180	0

The worst 5 of 1206 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	B6	88	LEU	14.0
53	B6	96	GLY	13.5
53	B6	98	ALA	12.4
53	B6	95	LYS	11.0
53	B6	97	ASP	10.5

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
54	MG	CA	1621	1/1	0.46	113.11	110,110,110,110	0
54	MG	AA	1659	1/1	0.54	49.17	180,180,180,180	0
54	MG	CA	1635	1/1	0.12	43.00	98,98,98,98	0
54	MG	DB	3058	1/1	0.83	36.95	162,162,162,162	0
54	MG	AA	1637	1/1	2.26	35.55	151,151,151,151	0
54	MG	AA	1656	1/1	0.75	30.69	161,161,161,161	0
54	MG	AA	1647	1/1	0.88	28.43	180,180,180,180	0
54	MG	AA	1625	1/1	0.74	20.65	84,84,84,84	1
54	MG	AA	1623	1/1	0.60	17.86	73,73,73,73	1
54	MG	CA	1641	1/1	0.22	14.34	42,42,42,42	0
54	MG	AA	1626	1/1	0.15	13.67	49,49,49,49	1
54	MG	CA	1658	1/1	0.33	8.96	53,53,53,53	0
54	MG	AA	1619	1/1	0.16	8.74	180,180,180,180	0
54	MG	AA	1657	1/1	0.36	8.35	124,124,124,124	0
54	MG	CA	1627	1/1	0.27	7.99	69,69,69,69	1
54	MG	BB	3033	1/1	0.66	7.73	141,141,141,141	0
54	MG	DB	3011	1/1	0.29	7.20	33,33,33,33	0
55	LLL	DB	3112	31/31	0.35	6.43	121,121,121,121	0
55	LLL	BB	3111	31/31	0.32	6.37	107,107,107,107	0
54	MG	AA	1632	1/1	0.24	6.10	62,62,62,62	0
54	MG	CA	1657	1/1	0.21	5.19	89,89,89,89	0
54	MG	BB	3004	1/1	0.20	5.14	73,73,73,73	0
54	MG	BB	3093	1/1	0.40	4.72	131,131,131,131	0
54	MG	AA	1608	1/1	0.25	4.42	147,147,147,147	0
54	MG	AA	1622	1/1	0.40	3.76	163,163,163,163	0
54	MG	DB	3073	1/1	0.22	3.75	67,67,67,67	0
54	MG	DB	3059	1/1	0.25	2.50	166,166,166,166	0
54	MG	BB	3038	1/1	0.26	2.19	152,152,152,152	0
54	MG	DB	3101	1/1	0.27	2.00	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1604	1/1	0.31	1.99	16,16,16,16	0
54	MG	CA	1652	1/1	0.18	1.84	65,65,65,65	0
54	MG	CA	1630	1/1	0.31	1.78	52,52,52,52	0
54	MG	BB	3022	1/1	0.32	1.66	37,37,37,37	0
54	MG	AA	1612	1/1	0.17	1.63	88,88,88,88	0
54	MG	BB	3017	1/1	0.18	1.59	73,73,73,73	0
54	MG	BB	3087	1/1	0.22	1.55	114,114,114,114	0
54	MG	BB	3108	1/1	0.25	1.52	44,44,44,44	0
54	MG	DB	3089	1/1	0.20	1.43	61,61,61,61	0
55	LLL	CA	1662	31/31	0.22	1.36	14,14,14,14	0
54	MG	BB	3013	1/1	0.16	1.29	92,92,92,92	0
54	MG	DB	3050	1/1	0.19	1.29	123,123,123,123	0
54	MG	DB	3028	1/1	0.20	1.29	58,58,58,58	0
54	MG	DB	3106	1/1	0.19	1.18	64,64,64,64	0
54	MG	BB	3080	1/1	0.19	1.13	77,77,77,77	0
54	MG	AA	1639	1/1	0.42	1.07	134,134,134,134	0
54	MG	AA	1644	1/1	0.13	0.86	98,98,98,98	0
54	MG	DB	3035	1/1	0.20	0.85	75,75,75,75	0
54	MG	DB	3020	1/1	0.20	0.83	13,13,13,13	0
54	MG	DB	3037	1/1	0.16	0.75	54,54,54,54	0
54	MG	BB	3073	1/1	0.22	0.72	38,38,38,38	0
54	MG	DB	3099	1/1	0.20	0.65	5,5,5,5	0
54	MG	BB	3010	1/1	0.14	0.60	40,40,40,40	0
54	MG	CA	1620	1/1	0.16	0.53	37,37,37,37	0
54	MG	CA	1638	1/1	0.12	0.43	98,98,98,98	0
54	MG	DB	3052	1/1	0.18	0.42	113,113,113,113	0
54	MG	AA	1650	1/1	0.12	0.38	122,122,122,122	0
54	MG	BB	3018	1/1	0.16	0.38	50,50,50,50	0
54	MG	BB	3028	1/1	0.14	0.37	61,61,61,61	0
54	MG	BB	3011	1/1	0.25	0.37	29,29,29,29	0
55	LLL	AA	1661	31/31	0.25	0.37	21,21,21,21	0
54	MG	DB	3097	1/1	0.17	0.36	64,64,64,64	0
54	MG	DB	3086	1/1	0.19	0.35	52,52,52,52	0
54	MG	DB	3090	1/1	0.28	0.30	64,64,64,64	0
54	MG	BB	3104	1/1	0.17	0.21	28,28,28,28	0
54	MG	DB	3051	1/1	0.20	0.16	32,32,32,32	0
54	MG	BB	3034	1/1	0.31	0.16	59,59,59,59	0
54	MG	DB	3005	1/1	0.23	0.14	45,45,45,45	0
54	MG	CA	1651	1/1	0.11	0.14	38,38,38,38	0
54	MG	AA	1615	1/1	0.28	0.07	106,106,106,106	0
54	MG	CA	1614	1/1	0.21	0.05	90,90,90,90	0
54	MG	AA	1653	1/1	0.15	0.05	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3008	1/1	0.23	-0.01	75,75,75,75	0
54	MG	BB	3026	1/1	0.21	-0.03	43,43,43,43	0
54	MG	AA	1646	1/1	0.17	-0.03	104,104,104,104	0
54	MG	AA	1602	1/1	0.20	-0.06	147,147,147,147	0
54	MG	CA	1622	1/1	0.11	-0.11	18,18,18,18	0
54	MG	BB	3098	1/1	0.19	-0.11	16,16,16,16	0
54	MG	BB	3036	1/1	0.14	-0.14	62,62,62,62	0
54	MG	BB	3057	1/1	0.21	-0.17	65,65,65,65	0
54	MG	DB	3006	1/1	0.18	-0.19	15,15,15,15	0
54	MG	DB	3110	1/1	0.18	-0.20	38,38,38,38	0
54	MG	CA	1648	1/1	0.22	-0.25	14,14,14,14	0
54	MG	AA	1624	1/1	0.12	-0.30	77,77,77,77	0
54	MG	BB	3009	1/1	0.13	-0.35	96,96,96,96	0
54	MG	DB	3027	1/1	0.17	-0.44	28,28,28,28	0
54	MG	BB	3083	1/1	0.21	-0.46	28,28,28,28	0
54	MG	BB	3072	1/1	0.15	-0.46	79,79,79,79	0
54	MG	BB	3023	1/1	0.22	-0.47	11,11,11,11	0
54	MG	DB	3069	1/1	0.21	-0.50	14,14,14,14	0
54	MG	DB	3003	1/1	0.16	-0.51	33,33,33,33	0
54	MG	BB	3079	1/1	0.20	-0.53	63,63,63,63	0
54	MG	DB	3100	1/1	0.22	-0.55	46,46,46,46	0
54	MG	BB	3021	1/1	0.13	-0.57	51,51,51,51	0
54	MG	BB	3063	1/1	0.14	-0.58	28,28,28,28	0
54	MG	CA	1642	1/1	0.11	-0.58	108,108,108,108	0
54	MG	AA	1617	1/1	0.16	-0.59	100,100,100,100	0
54	MG	AA	1635	1/1	0.09	-0.59	103,103,103,103	0
54	MG	CA	1605	1/1	0.14	-0.59	18,18,18,18	0
54	MG	BB	3070	1/1	0.21	-0.60	59,59,59,59	0
54	MG	BB	3005	1/1	0.22	-0.62	20,20,20,20	0
54	MG	DB	3014	1/1	0.13	-0.64	43,43,43,43	0
54	MG	CA	1613	1/1	0.12	-0.65	40,40,40,40	0
54	MG	BB	3042	1/1	0.13	-0.65	135,135,135,135	0
54	MG	CA	1608	1/1	0.10	-0.66	139,139,139,139	0
54	MG	AA	1640	1/1	0.10	-0.67	56,56,56,56	0
54	MG	DB	3098	1/1	0.19	-0.69	28,28,28,28	0
54	MG	BB	3047	1/1	0.10	-0.70	116,116,116,116	0
54	MG	CA	1616	1/1	0.11	-0.71	88,88,88,88	0
54	MG	CA	1660	1/1	0.09	-0.71	63,63,63,63	0
54	MG	DB	3111	1/1	0.17	-0.73	32,32,32,32	0
54	MG	DB	3088	1/1	0.16	-0.73	46,46,46,46	0
54	MG	AA	1613	1/1	0.08	-0.74	71,71,71,71	0
54	MG	BB	3055	1/1	0.18	-0.77	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1618	1/1	0.13	-0.77	30,30,30,30	0
54	MG	CE	201	1/1	0.16	-0.77	113,113,113,113	0
54	MG	CA	1601	1/1	0.17	-0.77	5,5,5,5	0
54	MG	AA	1631	1/1	0.12	-0.78	88,88,88,88	0
54	MG	CA	1633	1/1	0.14	-0.81	50,50,50,50	0
54	MG	BB	3051	1/1	0.16	-0.81	65,65,65,65	0
54	MG	AA	1627	1/1	0.17	-0.82	68,68,68,68	0
54	MG	BB	3084	1/1	0.19	-0.83	77,77,77,77	0
54	MG	CA	1649	1/1	0.15	-0.84	127,127,127,127	0
54	MG	BB	3053	1/1	0.06	-0.84	79,79,79,79	0
54	MG	BB	3078	1/1	0.18	-0.87	101,101,101,101	0
54	MG	BB	3099	1/1	0.22	-0.88	56,56,56,56	0
54	MG	CA	1645	1/1	0.10	-0.91	66,66,66,66	0
54	MG	AA	1611	1/1	0.10	-0.92	77,77,77,77	0
54	MG	AA	1618	1/1	0.12	-0.94	93,93,93,93	0
54	MG	DB	3096	1/1	0.17	-0.95	20,20,20,20	0
54	MG	BB	3016	1/1	0.20	-0.98	91,91,91,91	0
54	MG	AA	1636	1/1	0.07	-1.00	93,93,93,93	0
54	MG	DB	3026	1/1	0.18	-1.02	54,54,54,54	0
54	MG	DB	3083	1/1	0.17	-1.05	83,83,83,83	0
54	MG	AA	1628	1/1	0.13	-1.06	59,59,59,59	0
54	MG	BB	3054	1/1	0.14	-1.07	46,46,46,46	0
54	MG	CA	1646	1/1	0.08	-1.08	99,99,99,99	0
54	MG	DB	3104	1/1	0.17	-1.13	71,71,71,71	0
54	MG	DB	3009	1/1	0.17	-1.14	18,18,18,18	0
54	MG	AA	1658	1/1	0.07	-1.14	85,85,85,85	0
54	MG	DB	3025	1/1	0.16	-1.15	42,42,42,42	0
54	MG	DB	3092	1/1	0.12	-1.17	56,56,56,56	0
54	MG	CA	1607	1/1	0.07	-1.18	83,83,83,83	0
54	MG	DB	3029	1/1	0.11	-1.19	59,59,59,59	0
54	MG	CA	1636	1/1	0.06	-1.20	92,92,92,92	0
54	MG	DB	3057	1/1	0.09	-1.21	77,77,77,77	0
54	MG	DB	3093	1/1	0.16	-1.22	10,10,10,10	0
54	MG	BB	3092	1/1	0.07	-1.24	45,45,45,45	0
54	MG	BB	3041	1/1	0.15	-1.25	8,8,8,8	0
54	MG	BB	3075	1/1	0.16	-1.29	29,29,29,29	0
54	MG	BB	3040	1/1	0.10	-1.32	27,27,27,27	0
54	MG	DB	3030	1/1	0.17	-1.33	10,10,10,10	0
54	MG	AA	1651	1/1	0.09	-1.35	112,112,112,112	0
54	MG	DB	3094	1/1	0.10	-1.36	55,55,55,55	0
54	MG	BB	3096	1/1	0.16	-1.37	67,67,67,67	0
54	MG	CA	1615	1/1	0.09	-1.37	180,180,180,180	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1606	1/1	0.10	-1.40	47,47,47,47	0
54	MG	DB	3024	1/1	0.14	-1.40	45,45,45,45	0
54	MG	BB	3032	1/1	0.17	-1.44	49,49,49,49	0
54	MG	AA	1652	1/1	0.09	-1.45	90,90,90,90	0
54	MG	AA	1607	1/1	0.06	-1.48	42,42,42,42	0
54	MG	DB	3087	1/1	0.14	-1.50	75,75,75,75	0
54	MG	AA	1642	1/1	0.10	-1.50	41,41,41,41	0
54	MG	CA	1661	1/1	0.10	-1.52	48,48,48,48	0
54	MG	DB	3060	1/1	0.10	-1.52	104,104,104,104	0
56	ZN	D4	101	1/1	0.05	-1.59	45,45,45,45	0
54	MG	BB	3100	1/1	0.13	-1.62	151,151,151,151	0
54	MG	AA	1660	1/1	0.09	-1.63	37,37,37,37	0
54	MG	AA	1609	1/1	0.11	-1.69	5,5,5,5	0
54	MG	BB	3089	1/1	0.17	-1.69	25,25,25,25	0
56	ZN	B4	101	1/1	0.08	-1.73	64,64,64,64	0
54	MG	CA	1650	1/1	0.08	-1.73	33,33,33,33	0
54	MG	AA	1601	1/1	0.12	-1.74	41,41,41,41	0
54	MG	DB	3067	1/1	0.13	-1.75	16,16,16,16	0
54	MG	BB	3090	1/1	0.10	-1.78	91,91,91,91	0
54	MG	DB	3070	1/1	0.12	-1.78	38,38,38,38	0
54	MG	BB	3095	1/1	0.10	-1.78	81,81,81,81	0
54	MG	DB	3013	1/1	0.13	-1.78	41,41,41,41	0
54	MG	AA	1610	1/1	0.05	-1.79	62,62,62,62	0
54	MG	CA	1612	1/1	0.08	-1.80	72,72,72,72	0
54	MG	AA	1630	1/1	0.11	-1.81	88,88,88,88	0
54	MG	BB	3086	1/1	0.15	-1.82	18,18,18,18	0
54	MG	CA	1606	1/1	0.13	-1.88	138,138,138,138	0
54	MG	AA	1645	1/1	0.08	-1.88	95,95,95,95	0
54	MG	DB	3068	1/1	0.17	-1.88	22,22,22,22	0
54	MG	CA	1624	1/1	0.10	-1.94	56,56,56,56	0
54	MG	DB	3082	1/1	0.08	-1.95	57,57,57,57	0
54	MG	AA	1620	1/1	0.07	-2.00	113,113,113,113	0
54	MG	BB	3019	1/1	0.08	-2.02	40,40,40,40	0
54	MG	DB	3055	1/1	0.12	-2.06	41,41,41,41	0
54	MG	BB	3071	1/1	0.09	-2.07	89,89,89,89	0
54	MG	DB	3007	1/1	0.13	-2.08	13,13,13,13	0
54	MG	AA	1634	1/1	0.07	-2.08	67,67,67,67	0
54	MG	BB	3014	1/1	0.12	-2.08	58,58,58,58	0
54	MG	BB	3043	1/1	0.08	-2.08	122,122,122,122	0
54	MG	AA	1614	1/1	0.08	-2.09	113,113,113,113	0
54	MG	BB	3097	1/1	0.08	-2.10	88,88,88,88	0
54	MG	DB	3033	1/1	0.12	-2.10	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3048	1/1	0.10	-2.10	7,7,7,7	0
54	MG	CA	1625	1/1	0.14	-2.11	6,6,6,6	0
54	MG	BB	3082	1/1	0.16	-2.11	5,5,5,5	0
54	MG	CA	1659	1/1	0.08	-2.13	90,90,90,90	0
54	MG	DB	3047	1/1	0.14	-2.16	19,19,19,19	0
54	MG	CA	1617	1/1	0.07	-2.16	5,5,5,5	0
54	MG	DB	3023	1/1	0.11	-2.19	17,17,17,17	0
54	MG	DB	3062	1/1	0.04	-2.20	67,67,67,67	0
54	MG	BB	3077	1/1	0.08	-2.20	83,83,83,83	0
54	MG	DB	3084	1/1	0.13	-2.22	16,16,16,16	0
54	MG	BB	3020	1/1	0.11	-2.23	36,36,36,36	0
54	MG	AA	1629	1/1	0.07	-2.23	26,26,26,26	0
54	MG	BB	3029	1/1	0.12	-2.26	17,17,17,17	0
54	MG	DB	3004	1/1	0.13	-2.27	69,69,69,69	0
54	MG	BB	3037	1/1	0.11	-2.27	44,44,44,44	0
54	MG	BB	3066	1/1	0.14	-2.30	25,25,25,25	0
54	MG	AA	1648	1/1	0.07	-2.30	40,40,40,40	0
54	MG	CA	1637	1/1	0.07	-2.30	92,92,92,92	0
54	MG	CA	1639	1/1	0.08	-2.33	7,7,7,7	0
54	MG	BB	3061	1/1	0.08	-2.35	56,56,56,56	0
54	MG	DB	3081	1/1	0.13	-2.37	19,19,19,19	0
54	MG	DB	3095	1/1	0.12	-2.38	88,88,88,88	0
54	MG	DB	3046	1/1	0.07	-2.39	11,11,11,11	0
54	MG	BB	3074	1/1	0.13	-2.44	13,13,13,13	0
54	MG	BB	3044	1/1	0.07	-2.44	52,52,52,52	0
54	MG	AA	1605	1/1	0.09	-2.48	47,47,47,47	0
54	MG	DB	3085	1/1	0.12	-2.59	49,49,49,49	0
54	MG	BB	3085	1/1	0.11	-2.64	43,43,43,43	0
54	MG	BB	3046	1/1	0.07	-2.66	64,64,64,64	0
54	MG	DB	3015	1/1	0.09	-2.66	24,24,24,24	0
54	MG	BB	3025	1/1	0.07	-2.67	42,42,42,42	0
54	MG	BB	3109	1/1	0.07	-2.68	59,59,59,59	0
54	MG	BB	3107	1/1	0.07	-2.69	30,30,30,30	0
54	MG	BB	3110	1/1	0.09	-2.69	40,40,40,40	0
54	MG	CA	1654	1/1	0.09	-2.72	59,59,59,59	0
54	MG	BB	3031	1/1	0.12	-2.75	63,63,63,63	0
54	MG	DB	3078	1/1	0.08	-2.76	32,32,32,32	0
54	MG	BB	3007	1/1	0.07	-2.77	53,53,53,53	0
54	MG	DB	3042	1/1	0.07	-2.83	23,23,23,23	0
54	MG	AA	1604	1/1	0.07	-2.83	19,19,19,19	0
54	MG	CA	1611	1/1	0.06	-2.85	57,57,57,57	0
54	MG	DB	3039	1/1	0.07	-2.86	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1602	1/1	0.11	-2.87	11,11,11,11	0
54	MG	BB	3024	1/1	0.06	-2.88	44,44,44,44	0
54	MG	DB	3103	1/1	0.11	-2.89	42,42,42,42	0
54	MG	DB	3075	1/1	0.12	-2.91	35,35,35,35	0
54	MG	DB	3018	1/1	0.09	-2.92	22,22,22,22	0
54	MG	DB	3072	1/1	0.09	-2.92	54,54,54,54	0
54	MG	BB	3012	1/1	0.10	-2.94	53,53,53,53	0
54	MG	DB	3091	1/1	0.14	-2.95	5,5,5,5	0
54	MG	DB	3045	1/1	0.06	-2.96	68,68,68,68	0
54	MG	BB	3045	1/1	0.07	-2.97	38,38,38,38	0
54	MG	CA	1647	1/1	0.07	-3.01	65,65,65,65	0
54	MG	DB	3008	1/1	0.12	-3.01	17,17,17,17	0
54	MG	DB	3022	1/1	0.09	-3.02	71,71,71,71	0
54	MG	AA	1638	1/1	0.06	-3.06	20,20,20,20	0
54	MG	DB	3038	1/1	0.13	-3.08	37,37,37,37	0
54	MG	AA	1621	1/1	0.14	-3.13	26,26,26,26	0
54	MG	DB	3034	1/1	0.19	-3.14	69,69,69,69	0
54	MG	BB	3076	1/1	0.06	-3.16	20,20,20,20	0
54	MG	DB	3074	1/1	0.10	-3.21	17,17,17,17	0
54	MG	BB	3081	1/1	0.17	-3.22	16,16,16,16	0
54	MG	DB	3036	1/1	0.09	-3.23	20,20,20,20	0
54	MG	CA	1603	1/1	0.08	-3.23	29,29,29,29	0
54	MG	BB	3062	1/1	0.05	-3.26	27,27,27,27	0
54	MG	CA	1644	1/1	0.07	-3.26	68,68,68,68	0
54	MG	CA	1632	1/1	0.08	-3.30	18,18,18,18	0
54	MG	AA	1654	1/1	0.07	-3.34	82,82,82,82	0
54	MG	DB	3071	1/1	0.05	-3.35	37,37,37,37	0
54	MG	BB	3002	1/1	0.09	-3.37	30,30,30,30	0
54	MG	AA	1603	1/1	0.12	-3.39	14,14,14,14	0
54	MG	CA	1653	1/1	0.05	-3.39	51,51,51,51	0
54	MG	BB	3069	1/1	0.14	-3.45	10,10,10,10	0
54	MG	DB	3031	1/1	0.08	-3.52	24,24,24,24	0
54	MG	DB	3010	1/1	0.09	-3.52	16,16,16,16	0
54	MG	BB	3001	1/1	0.07	-3.59	29,29,29,29	0
54	MG	BB	3039	1/1	0.08	-3.60	5,5,5,5	0
54	MG	DB	3053	1/1	0.09	-3.61	80,80,80,80	0
54	MG	BB	3088	1/1	0.09	-3.63	36,36,36,36	0
54	MG	BB	3049	1/1	0.16	-3.67	35,35,35,35	0
54	MG	DB	3076	1/1	0.13	-3.76	104,104,104,104	0
54	MG	DB	3105	1/1	0.10	-3.77	30,30,30,30	0
54	MG	DB	3016	1/1	0.06	-3.79	25,25,25,25	0
54	MG	DB	3064	1/1	0.09	-3.80	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1655	1/1	0.07	-3.81	54,54,54,54	0
54	MG	DB	3043	1/1	0.09	-3.82	32,32,32,32	0
54	MG	BB	3003	1/1	0.11	-3.87	51,51,51,51	0
54	MG	AA	1616	1/1	0.04	-3.88	42,42,42,42	0
54	MG	DB	3044	1/1	0.07	-4.04	21,21,21,21	0
54	MG	BB	3059	1/1	0.09	-4.06	60,60,60,60	0
54	MG	CA	1609	1/1	0.04	-4.12	84,84,84,84	0
54	MG	BB	3052	1/1	0.08	-4.18	36,36,36,36	0
54	MG	DB	3001	1/1	0.10	-4.18	6,6,6,6	0
54	MG	DB	3032	1/1	0.08	-4.29	51,51,51,51	0
54	MG	BB	3058	1/1	0.10	-4.32	11,11,11,11	0
54	MG	CA	1656	1/1	0.06	-4.34	11,11,11,11	0
54	MG	DB	3077	1/1	0.07	-4.45	15,15,15,15	0
54	MG	BB	3035	1/1	0.13	-4.46	82,82,82,82	0
54	MG	DB	3021	1/1	0.09	-4.46	51,51,51,51	0
54	MG	AA	1641	1/1	0.04	-4.46	69,69,69,69	0
54	MG	DB	3108	1/1	0.09	-4.49	5,5,5,5	0
54	MG	DB	3012	1/1	0.08	-4.50	12,12,12,12	0
54	MG	DB	3109	1/1	0.08	-4.50	83,83,83,83	0
54	MG	BB	3060	1/1	0.10	-4.51	22,22,22,22	0
54	MG	BB	3065	1/1	0.06	-4.63	5,5,5,5	0
54	MG	DB	3049	1/1	0.07	-4.66	9,9,9,9	0
54	MG	BB	3105	1/1	0.06	-4.73	60,60,60,60	0
54	MG	BB	3103	1/1	0.09	-4.75	20,20,20,20	0
54	MG	DB	3080	1/1	0.08	-4.82	5,5,5,5	0
54	MG	BB	3056	1/1	0.07	-4.88	31,31,31,31	0
54	MG	CA	1643	1/1	0.07	-4.90	32,32,32,32	0
54	MG	BB	3027	1/1	0.13	-4.94	42,42,42,42	0
54	MG	DB	3002	1/1	0.10	-4.96	6,6,6,6	0
54	MG	BB	3094	1/1	0.13	-4.97	47,47,47,47	0
54	MG	AA	1633	1/1	0.03	-5.01	48,48,48,48	0
54	MG	CA	1640	1/1	0.08	-5.08	5,5,5,5	0
54	MG	CA	1655	1/1	0.07	-5.16	25,25,25,25	0
54	MG	DB	3063	1/1	0.09	-5.23	19,19,19,19	0
54	MG	BB	3015	1/1	0.09	-5.26	42,42,42,42	0
54	MG	BB	3106	1/1	0.10	-5.36	39,39,39,39	0
54	MG	BB	3050	1/1	0.11	-5.42	33,33,33,33	0
54	MG	BB	3101	1/1	0.06	-5.42	5,5,5,5	0
54	MG	CA	1634	1/1	0.10	-5.43	23,23,23,23	0
54	MG	AA	1649	1/1	0.05	-5.49	82,82,82,82	0
54	MG	DB	3056	1/1	0.11	-5.57	12,12,12,12	0
54	MG	CA	1619	1/1	0.17	-5.66	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	BB	3067	1/1	0.13	-5.99	24,24,24,24	0
54	MG	DB	3040	1/1	0.09	-6.02	18,18,18,18	0
54	MG	DB	3017	1/1	0.09	-6.05	5,5,5,5	0
54	MG	CA	1610	1/1	0.07	-6.17	75,75,75,75	0
54	MG	DB	3065	1/1	0.07	-6.41	45,45,45,45	0
54	MG	BB	3091	1/1	0.10	-6.46	37,37,37,37	0
54	MG	BB	3006	1/1	0.08	-6.76	20,20,20,20	0
54	MG	DB	3107	1/1	0.07	-7.01	11,11,11,11	0
54	MG	DB	3048	1/1	0.06	-7.58	34,34,34,34	0
54	MG	DB	3079	1/1	0.10	-7.61	34,34,34,34	0
54	MG	AA	1643	1/1	0.03	-8.02	29,29,29,29	0
54	MG	DB	3041	1/1	0.08	-8.64	34,34,34,34	0
54	MG	BB	3030	1/1	0.05	-9.46	70,70,70,70	0
54	MG	CA	1628	1/1	0.07	-9.73	44,44,44,44	0
54	MG	DB	3054	1/1	0.06	-9.76	29,29,29,29	0
54	MG	DB	3061	1/1	0.09	-10.71	69,69,69,69	0
54	MG	CA	1631	1/1	0.10	-11.13	40,40,40,40	0
54	MG	BB	3064	1/1	0.09	-12.73	37,37,37,37	0
54	MG	BB	3068	1/1	0.05	-13.14	61,61,61,61	0
54	MG	CA	1623	1/1	0.09	-14.14	173,173,173,173	0
54	MG	DB	3019	1/1	0.06	-14.37	5,5,5,5	0
54	MG	DB	3102	1/1	0.08	-26.41	22,22,22,22	0
54	MG	BB	3102	1/1	0.04	-29.15	31,31,31,31	0
54	MG	CA	1629	1/1	0.11	-	65,65,65,65	1
54	MG	CA	1626	1/1	0.30	-	41,41,41,41	1
54	MG	DB	3066	1/1	0.28	-	158,158,158,158	0

6.5 Other polymers ⓘ

There are no such residues in this entry.