



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 06:35 PM BST

PDB ID : 4V54
Title : Crystal structure of the bacterial ribosome from Escherichia coli in complex with 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 : 2007-06-16
Resolution : 3.30 Å(reported)

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

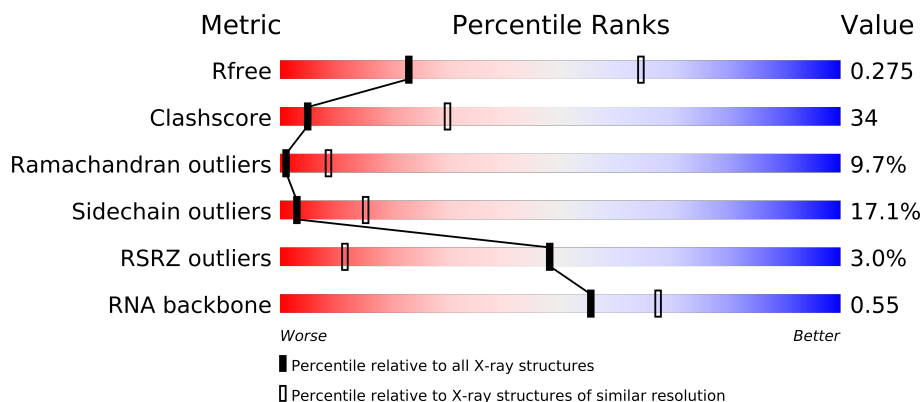
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.30 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	1341 (3.40-3.20)
Clashscore	79885	1696 (3.40-3.20)
Ramachandran outliers	78287	1664 (3.40-3.20)
Sidechain outliers	78261	1662 (3.40-3.20)
RSRZ outliers	66119	1342 (3.40-3.20)
RNA backbone	1838	1042 (3.90-2.70)

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	2017	-	X
54	MG	AA	2023	-	X
54	MG	AA	2025	-	X
54	MG	AA	2026	-	X
54	MG	AA	2027	-	X
54	MG	AA	2032	-	X
54	MG	AA	2039	-	X
54	MG	AA	2047	-	X
54	MG	AA	2056	-	X
54	MG	AA	2057	-	X
54	MG	AA	2059	-	X
54	MG	BB	3008	-	X
54	MG	BB	3033	-	X
54	MG	BB	3087	-	X
54	MG	BB	3093	-	X
54	MG	BB	3100	-	X
54	MG	CA	1615	-	X
54	MG	CA	1621	-	X
54	MG	CA	1623	-	X
54	MG	CA	1626	-	X
54	MG	CA	1627	-	X
54	MG	CA	1641	-	X
54	MG	DB	3013	-	X
54	MG	DB	3030	-	X
54	MG	DB	3052	-	X
54	MG	DB	3058	-	X
54	MG	DB	3066	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	DB	3095	-	X
54	MG	DB	3110	-	X

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 286960 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
			1022	634	206	179	3			

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AO	88	Total	C	N	O	S	0	0	0
			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 ribosome recycling factor.

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

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

- Molecule 56 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AA	289	Total	O	0	0
			289	289		
56	AE	4	Total	O	0	0
			4	4		
56	AK	1	Total	O	0	0
			1	1		
56	AL	1	Total	O	0	0
			1	1		
56	AN	3	Total	O	0	0
			3	3		
56	AP	1	Total	O	0	0
			1	1		

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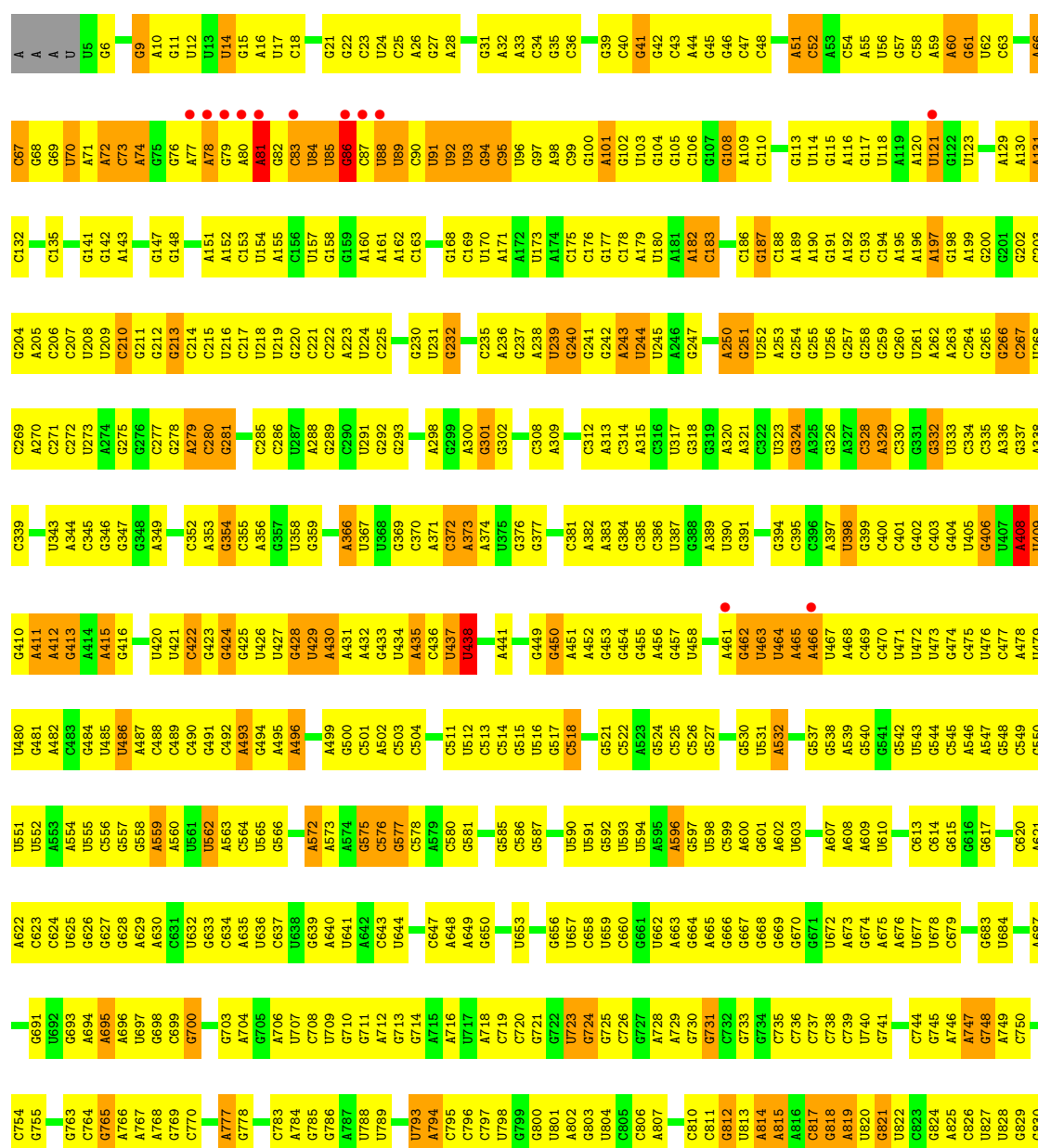
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
56	AT	1	Total 1	O 1	0	0
56	BB	495	Total 495	O 495	0	0
56	BC	4	Total 4	O 4	0	0
56	BD	1	Total 1	O 1	0	0
56	BE	3	Total 3	O 3	0	0
56	B2	1	Total 1	O 1	0	0
56	BL	1	Total 1	O 1	0	0
56	BT	1	Total 1	O 1	0	0
56	CE	2	Total 2	O 2	0	0
56	CK	1	Total 1	O 1	0	0
56	CL	1	Total 1	O 1	0	0
56	CN	4	Total 4	O 4	0	0
56	CT	1	Total 1	O 1	0	0
56	CA	300	Total 300	O 300	0	0
56	DB	505	Total 505	O 505	0	0
56	DC	4	Total 4	O 4	0	0
56	DD	1	Total 1	O 1	0	0
56	DE	2	Total 2	O 2	0	0

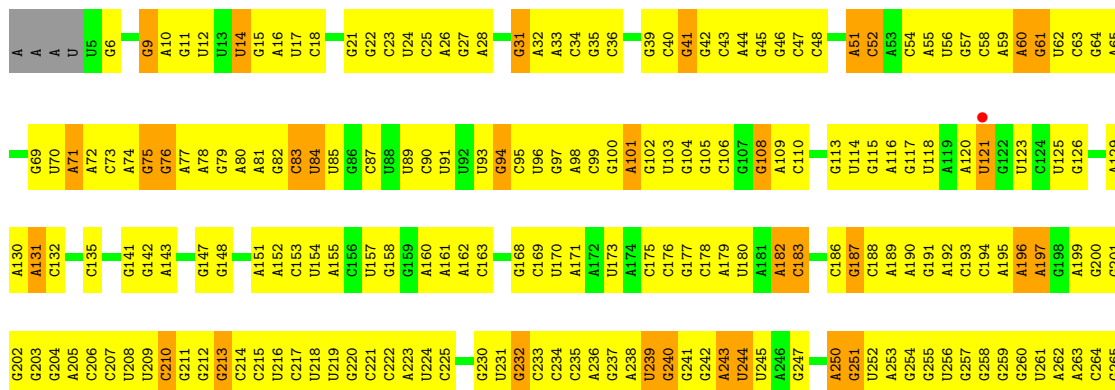
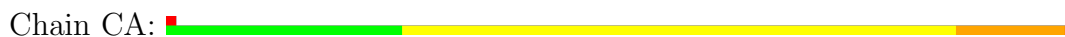
3 Residue-property plots

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

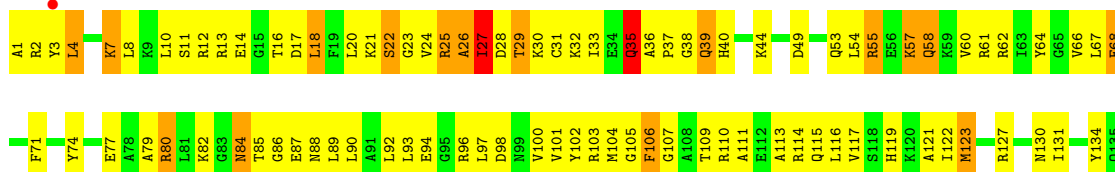
• Molecule 1: 16S rRNA

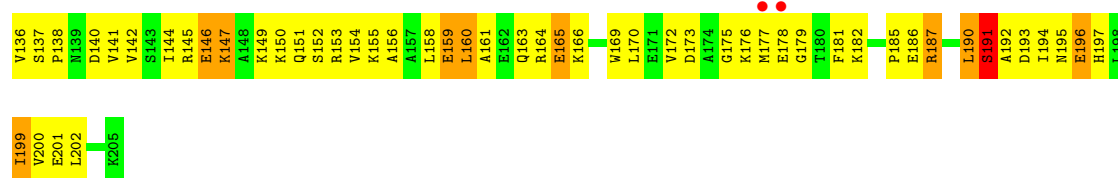
Chain AA: 





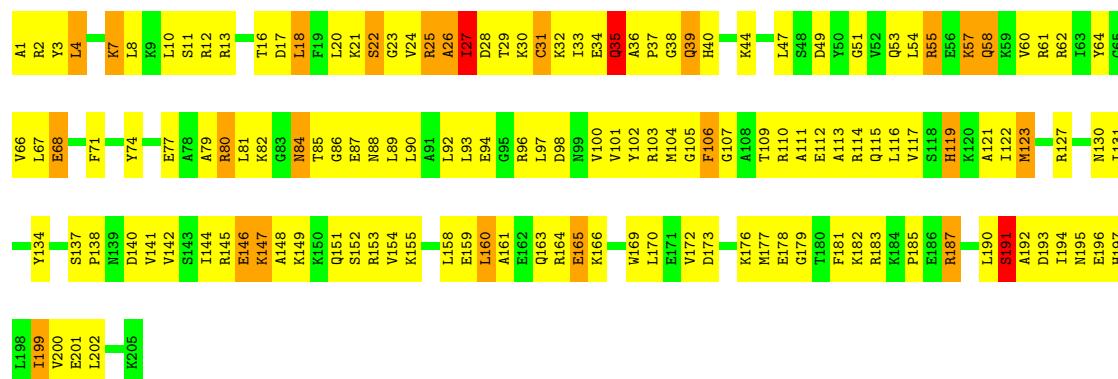
G1304	G1242	A1176	G1100	A1036	G976	A909	G830	A749	G683	G617	C548	U476	G406	A336	C266
G1305	C1243	G1177	A1101	C1037	A977	A910	A831	C760	U684	C620	C549	C477	U407	G337	C267
A1306	G1244	A1178	C1102	G1038	A978	C910	G832	C754	A887	C620	G550	A478	A408	A338	U268
U1307	C1245	A1179	C1103	U1040	C979	U911	G833	G765	U685	A621	U551	U479	U409	C339	C269
U1308	U1246	G1180	U1115	G1041	C980	C912	U835	G763	G691	A622	U553	G481	A410	C344	A270
G1309	U1247	G1181	U1116	U1042	U982	A914	G836	C764	U686	A623	A554	A482	A412	A344	C271
G1310	U1248	G1182	U1117	G1043	A983	A915	G837	C765	A694	C624	U555	G483	G413	C345	C272
A1311	G1249	U1183	U1118	A1044	C984	A916	G838	G766	A695	U625	C556	G484	A414	G346	U273
A1312	A1250	G1184	C1119	A1045	A985	U916	G839	G767	A696	G626	G557	U485	A415	G275	U274
A1313	A1251	U1185	U1120	C1046	C986	A917	C839	A766	U697	G627	G558	U486	A416	G276	G275
C1314	G1252	A1188	U1121	U1047	U986	A918	C840	A767	U698	G628	G559	A487	C277	C277	C277
U1315	G1253	U1189	U1122	G1048	C987	A919	C841	A768	G698	A629	A560	C488	U420	C352	G278
G1316	U1254	G1190	U1123	U1049	C988	U920	U842	C769	C699	A630	A561	C489	U421	A353	A279
C1317	G1255	A1191	G1124	U1050	U989	U921	U843	C770	G700	G631	U562	C490	U422	C354	C280
A1318	A1256	C1192	C1125	G1051	C990	G922	A844	A777	G703	U632	U563	C491	A423	G355	C281
A1319	A1257	G1193	U1130	C1051	U991	A923	G845	G778	A704	U633	U564	G492	G424	A356	C285
C1320	U1194	U1195	A1131	G1052	U992	C924	G846	C783	G705	C634	U565	C493	G425	G357	C286
U1321	G1258	C1136	G1130	U1053	C993	G925	G847	A784	U706	U635	U566	A495	U426	U358	U287
C1322	A1196	C1137	C1132	C1054	A994	G926	U848	C785	U707	U636	G566	A496	U427	C359	C288
A1323	A1197	C1138	G1133	G1057	C995	G927	G849	A785	C708	U637	A572	A497	U428	A363	A289
A1324	C1262	U1135	U1134	G1058	A996	G928	G852	C786	U709	U638	A573	C500	U429	A364	C290
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C1327	U1265	U1202	G1138	U1061	C999	C931	C855	U789	A712	A642	C576	C503	G433	U367	G293
A1328	A1261	C1203	C1139	U1062	A1000	C934	C856	U790	G713	C643	C577	C504	U434	A370	A303
A1329	A1262	G1206	G1139	U1063	C1001	A935	C857	U793	G714	U644	C578	C511	A435	C370	C298
U1330	C1270	G1207	C1140	G1064	G1002	U935	G858	A794	U723	U657	A579	C512	A451	A371	G299
G1331	A1271	A1270	C1141	U1065	G1003	G939	G859	C795	G724	U658	G592	C522	A452	A382	A313
A1332	G1272	G1208	G1142	U1066	A1004	C940	A860	C796	G725	U659	U593	C523	G453	A383	C314
C1333	C1273	U1211	G1143	C1066	A1005	G941	G861	C797	G726	C660	U594	A523	G454	A384	A315
G1334	A1274	U1212	C1144	U1067	A1006	G942	G862	U798	G727	G661	A595	C524	G455	C385	C316
A1275	A1275	A1213	A1145	G1068	U1007	U952	U863	U799	A718	A649	A596	C525	A456	C386	U317
G1336	G1276	C1214	A1146	U1069	U1008	A946	A864	U802	C720	G650	G585	C526	G457	U387	G318
C1337	C1277	G1215	C1147	U1070	G947	C948	A865	A803	G721	U653	C586	C527	U458	G388	C319
G1338	G1278	A1216	U1148	C1071	U1009	U949	C866	U804	U723	G656	G587	C518	G459	A389	A320
A1339	A1279	C1217	C1149	U1072	C1011	A950	G867	C805	G724	U657	U591	G530	A461	U390	A321
A1340	C1280	C1218	A1150	U1073	A1012	U951	G868	C806	G725	C658	G592	C524	A462	A397	C322
U1341	C1281	A1219	A1151	G1074	G1013	C951	G869	A807	G726	U659	U593	C525	U463	U398	C328
C1342	C1282	G1220	A1152	U1075	A1014	U952	G870	C807	G727	C660	U594	C526	U464	A399	A329
G1343	U1283	G1221	G1153	U1076	G1015	U953	U875	C810	A728	G661	A596	C527	U465	C400	C330
C1344	C1284	G1222	A1157	U1077	A1016	U954	C876	C811	A729	U662	A597	C528	A466	G402	G332
G1347	U1286	C1223	U1158	U1078	G1017	U955	G877	C812	A730	A663	G597	C529	A467	C403	U333
U1348	A1287	U1224	G1159	A1080	G1018	U957	A878	G813	G731	G664	U598	C530	U468	G404	C334
A1288	A1288	C1225	U1159	A1081	A1019	U958	C882	U814	C732	A665	C599	G531	A469	U405	C335
A1289	A1289	A1226	G1160	U1082	G1020	A959	C883	A815	G733	G666	A600	G532	A470	C406	G336
G1290	C1290	C1227	C1161	U1084	A1021	U960	U884	A816	G734	G667	G601	A533	U471	C407	C337
U1291	U1291	C1228	C1162	U1085	A1022	U961	U885	C817	G735	G668	A602	A534	U472	C408	C338
G1292	C1292	A1229	A1163	U1086	U1023	C962	G886	C818	C736	G669	U603	G537	U473	C409	C339
C1293	C1293	G1231	G1164	G1089	G1024	G963	G887	A819	C737	G670	A607	G538	U474	C410	C340
U1294	G1294	U1232	U1165	U1090	U1025	A964	U892	U820	C738	G671	A608	G539	U475	C411	C341
U1295	U1295	G1233	G1166	U1091	G1026	U965	C893	G821	C739	U672	A609	A540	U476	C412	C342
C1296	C1296	A1292	U1168	A1092	C1028	C967	G894	U822	U740	A673	U610	G541	U477	C413	C343
G1297	G1297	U1234	U1169	U1093	U1029	A968	U901	C823	G741	C674	G611	G542	U478	C414	C344
U1298	U1298	A1236	A1169	G1094	U1030	A969	G902	G824	C744	A675	C612	G543	U479	C415	C345
A1299	A1299	C1237	A1170	U1095	U1031	C972	G903	A825	G745	A676	C613	G544	U480	C416	C346
A1300	G1300	A1238	C1172	C1096	G1032	G973	U904	C826	G746	U677	C614	G545	U481	C417	C347
A1301	U1301	C1239	U1173	C1097	G1033	A974	U905	U827	A747	G678	C615	G546	U482	C418	C348
U1302	C1302	U1240	G1174	C1098	G1034	A975	U906	U828	A748	C679	C616	A547	U483	C419	C349
C1303	C1303	G1241	G1175	G1099	A1035	A976	A906	C829	G749	U679	G616	A548	U484	C420	C350





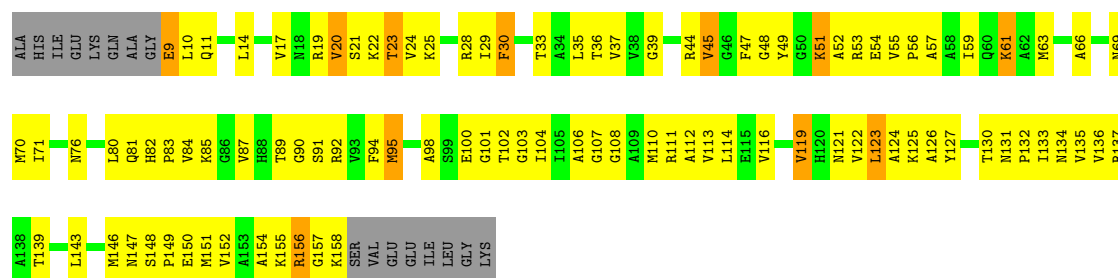
• Molecule 3: 30S ribosomal protein S4

Chain CD:



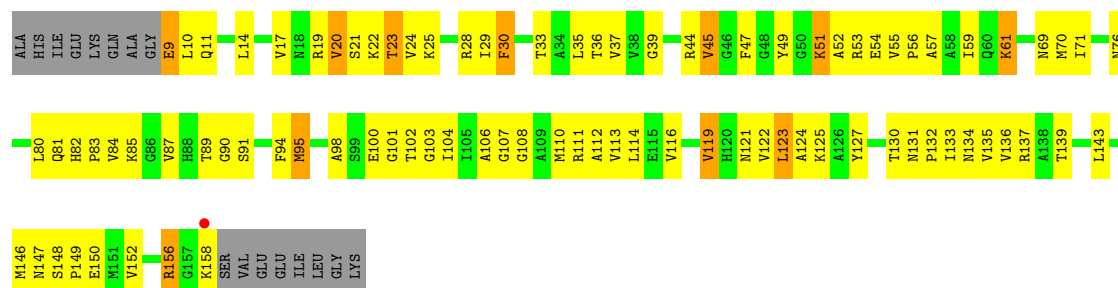
• Molecule 4: 30S ribosomal protein S5

Chain AE:



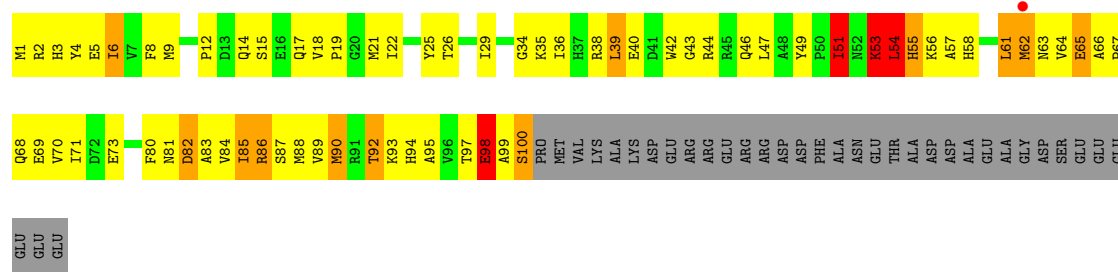
• Molecule 4: 30S ribosomal protein S5

Chain CE:



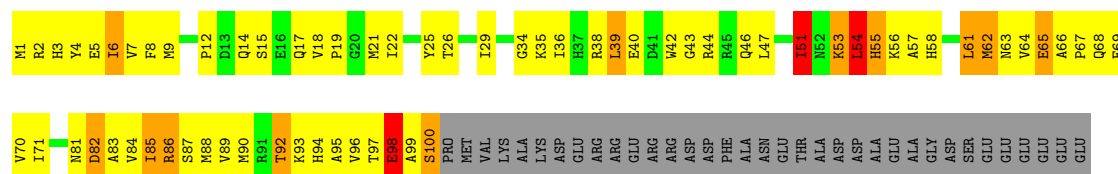
• Molecule 5: 30S ribosomal protein S6

Chain AF:



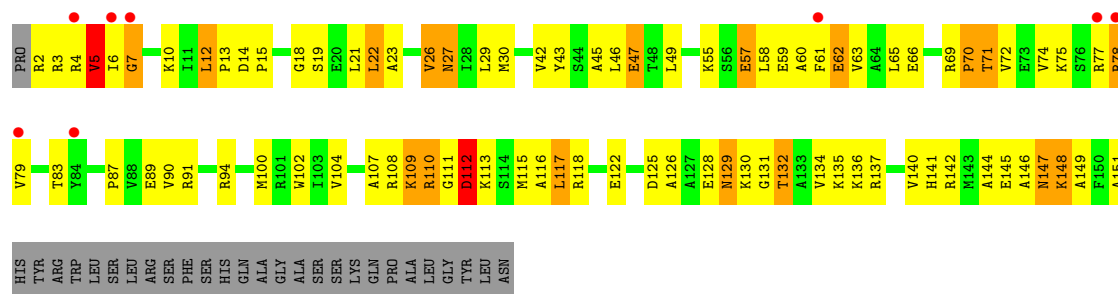
- Molecule 5: 30S ribosomal protein S6

Chain CF:



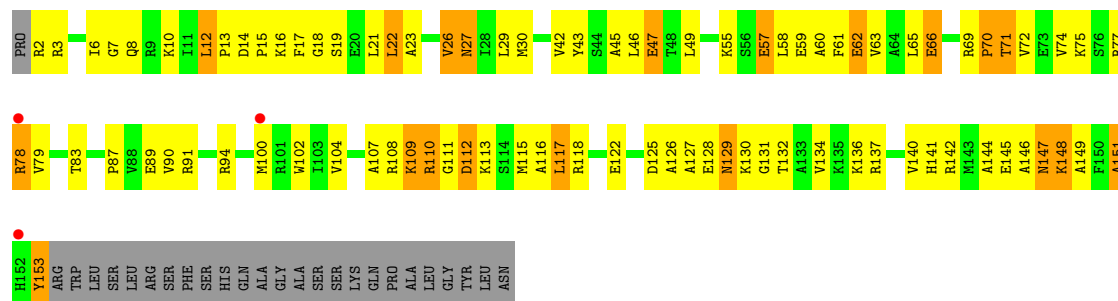
- Molecule 6: 30S ribosomal protein S7

Chain AG:



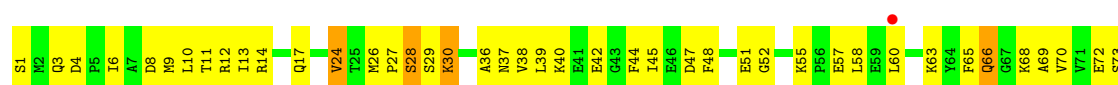
- Molecule 6: 30S ribosomal protein S7

Chain CG:



- Molecule 7: 30S ribosomal protein S8

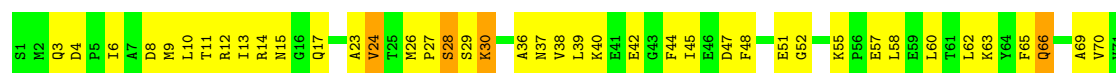
Chain AH:





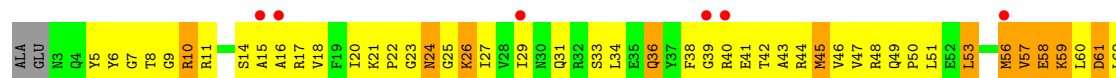
- Molecule 7: 30S ribosomal protein S8

Chain CH:



- Molecule 8: 30S ribosomal protein S9

Chain AI:



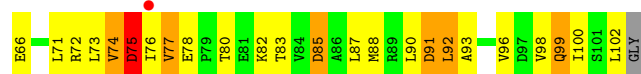
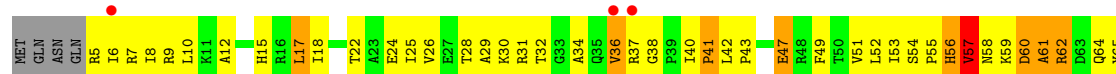
- Molecule 8: 30S ribosomal protein S9

Chain CI:



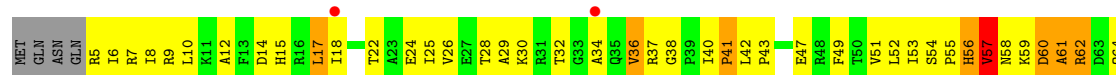
- Molecule 9: 30S ribosomal protein S10

Chain AJ:

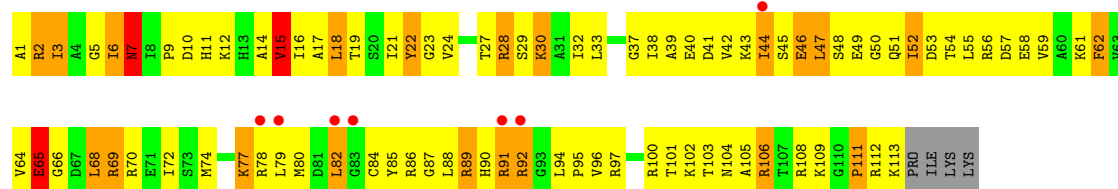


- Molecule 9: 30S ribosomal protein S10

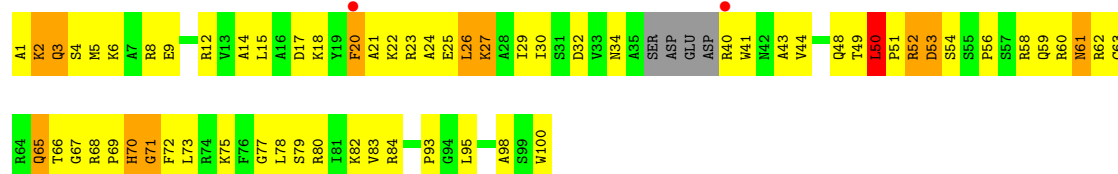
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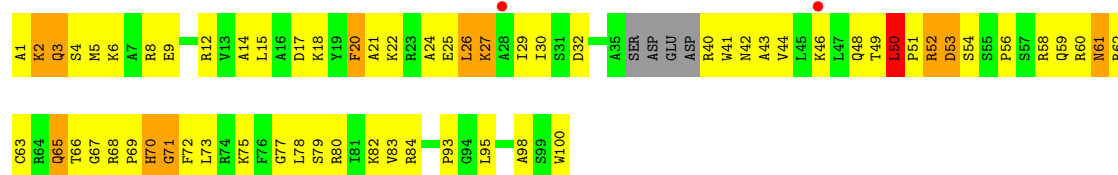
- Molecule 12: 30S ribosomal protein S13

Chain CM: 

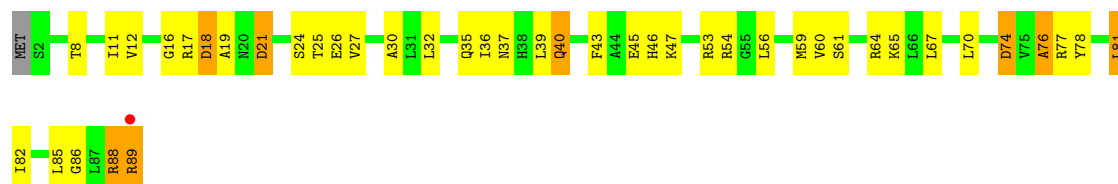
- Molecule 13: 30S ribosomal protein S14

Chain AN: 

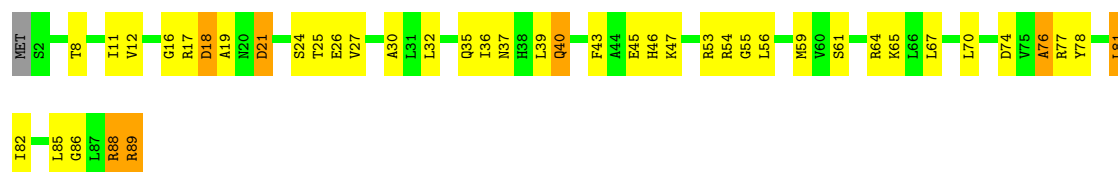
- Molecule 13: 30S ribosomal protein S14

Chain CN: 

- Molecule 14: 30S ribosomal protein S15

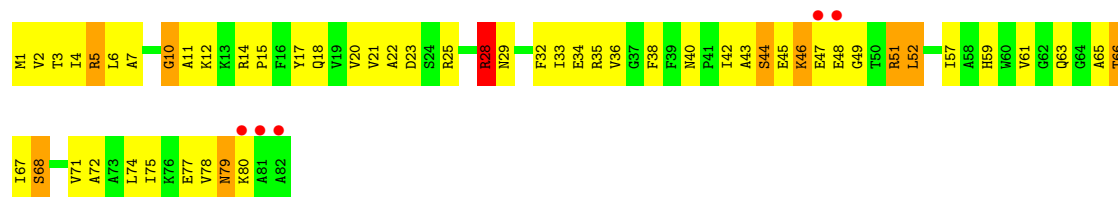
Chain AO: 

- Molecule 14: 30S ribosomal protein S15

Chain CO: 

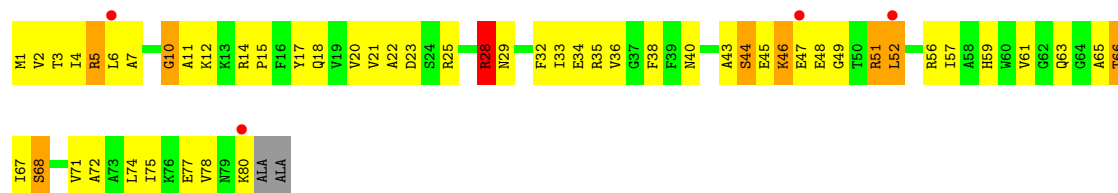
- Molecule 15: 30S ribosomal protein S16

Chain AP: 



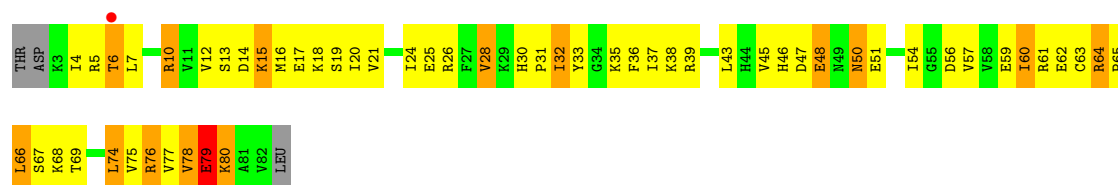
• Molecule 15: 30S ribosomal protein S16

Chain CP:



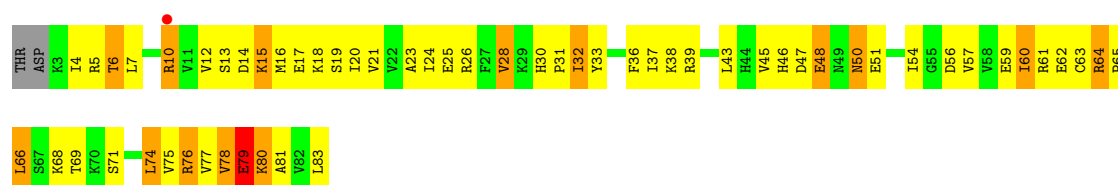
• Molecule 16: 30S ribosomal protein S17

Chain AQ:



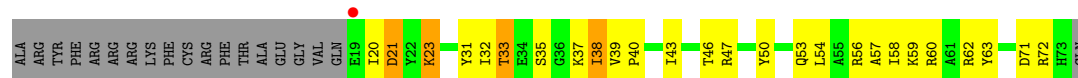
• Molecule 16: 30S ribosomal protein S17

Chain CQ:



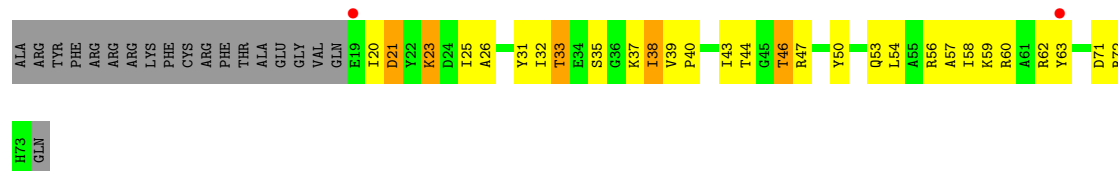
• Molecule 17: 30S ribosomal protein S18

Chain AR:

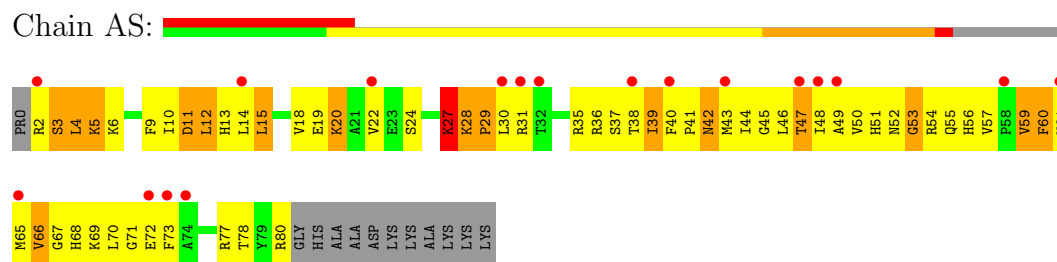


• Molecule 17: 30S ribosomal protein S18

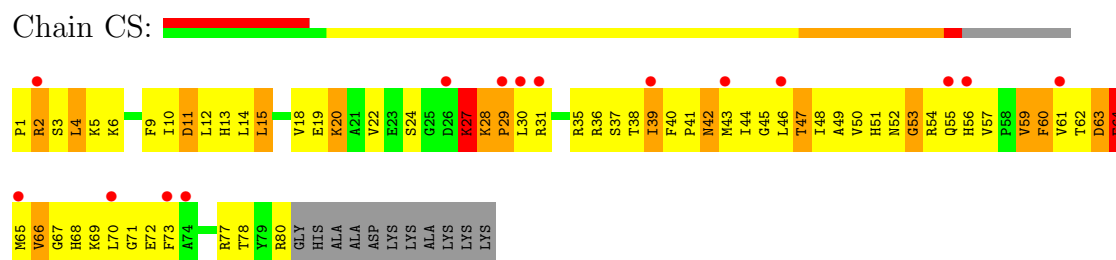
Chain CR:



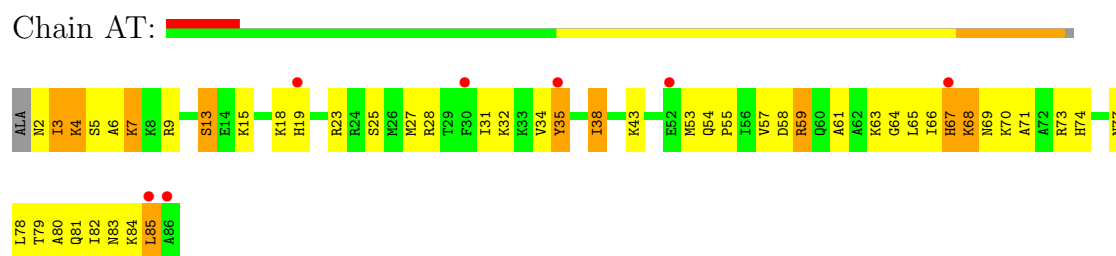
- Molecule 18: 30S ribosomal protein S19



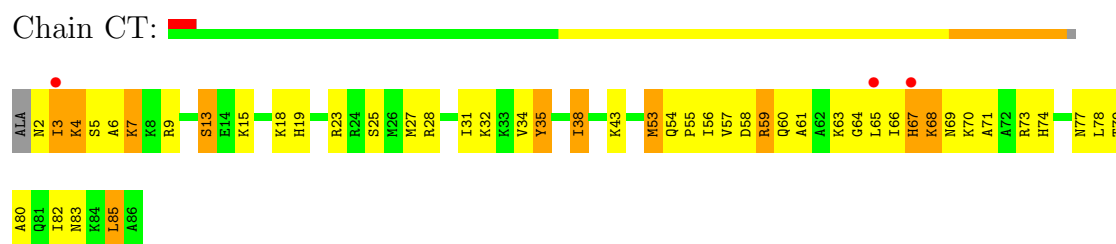
- Molecule 18: 30S ribosomal protein S19



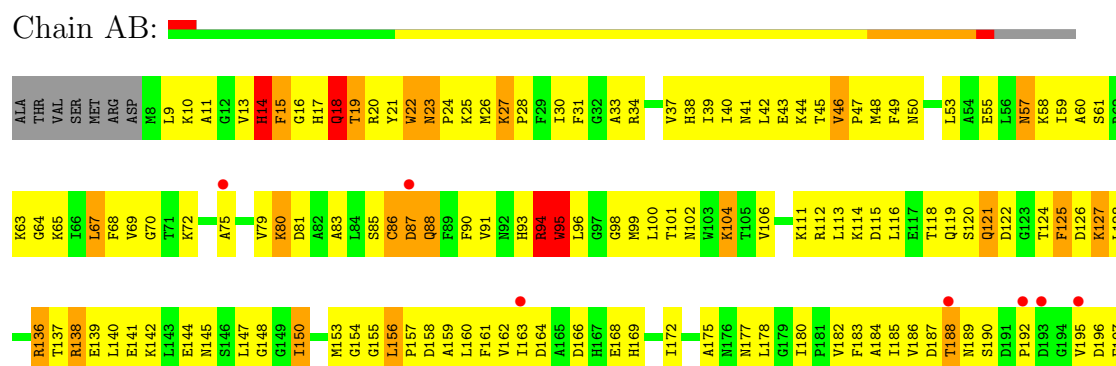
- Molecule 19: 30S ribosomal protein S20



- Molecule 19: 30S ribosomal protein S20



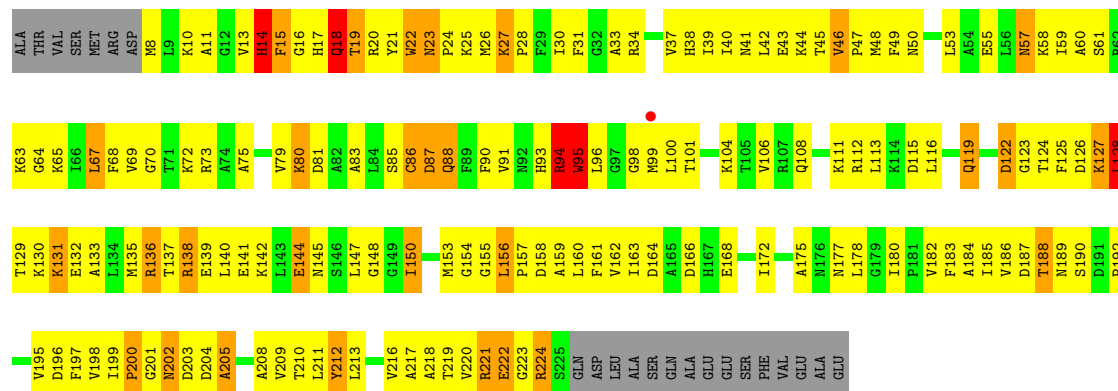
- Molecule 20: 30S ribosomal protein S2





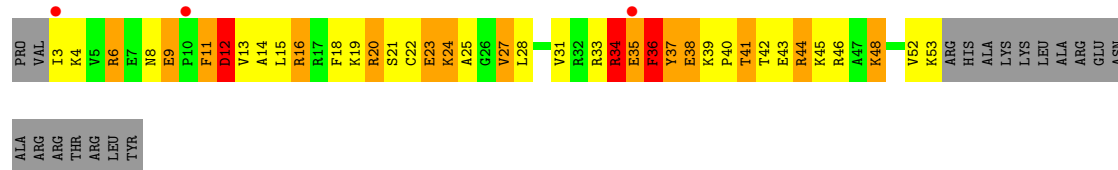
- Molecule 20: 30S ribosomal protein S2

Chain CB:



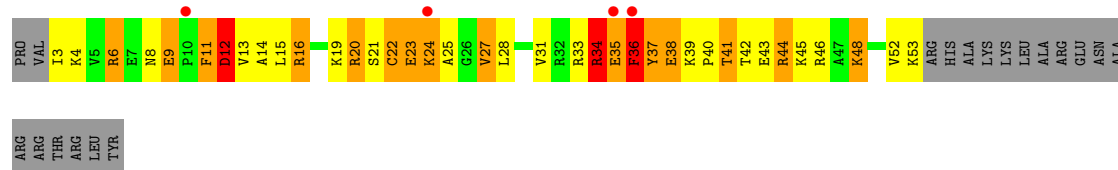
- Molecule 21: 30S ribosomal protein S21

Chain AU:



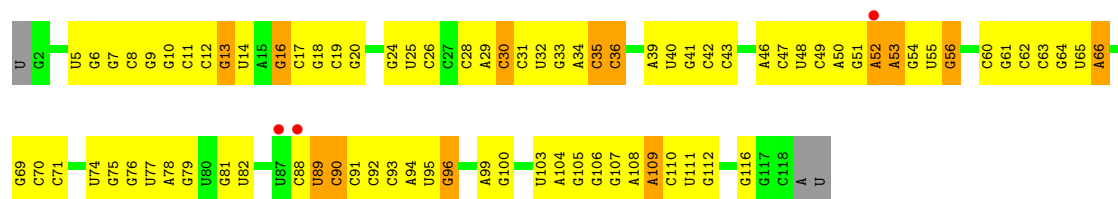
- Molecule 21: 30S ribosomal protein S21

Chain CU:



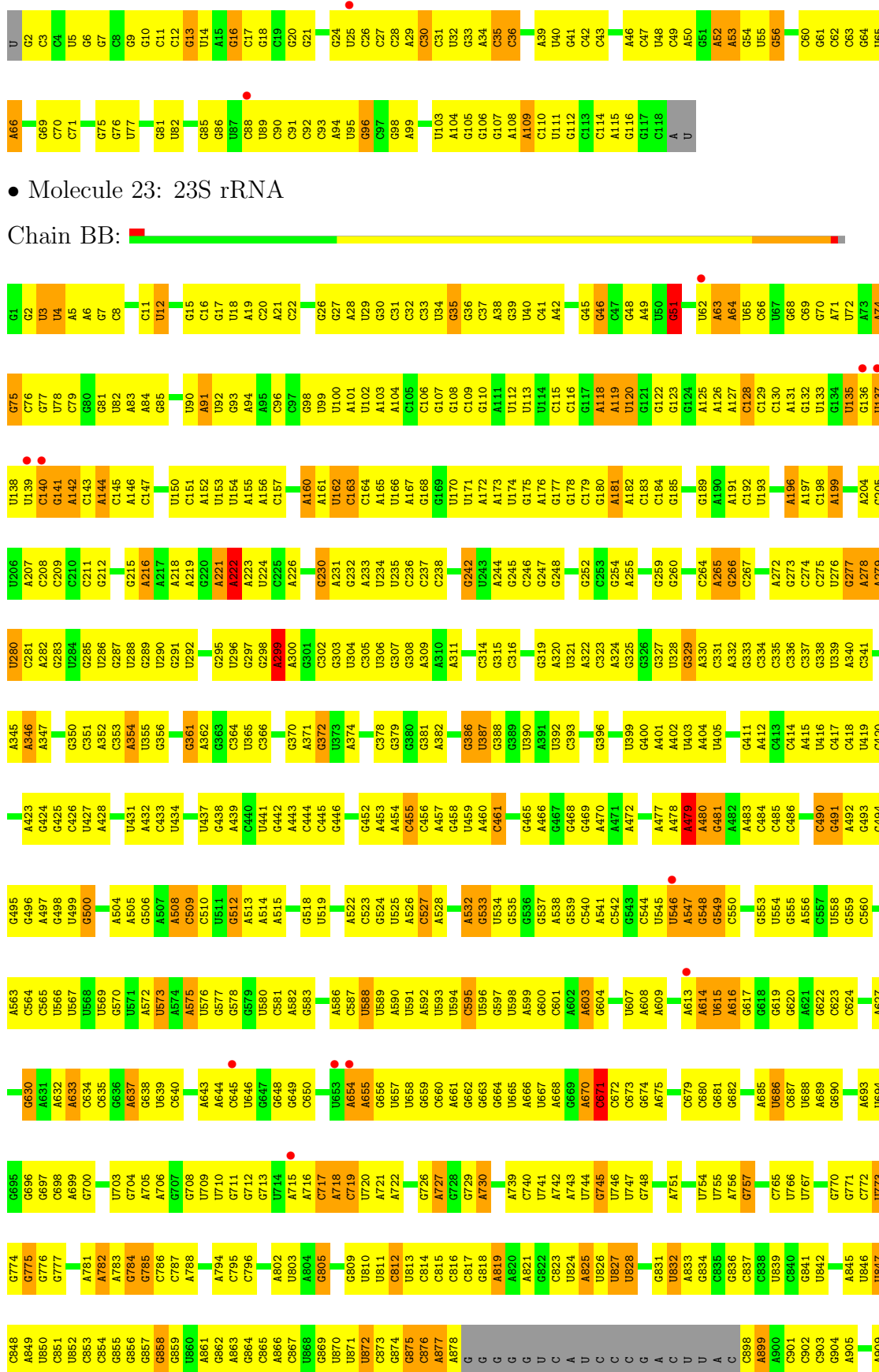
- Molecule 22: 5S rRNA

Chain BA:



- Molecule 22: 5S rRNA

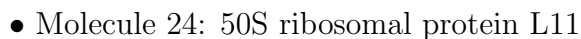
Chain DA:



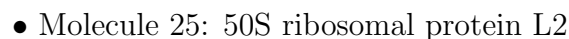


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C1053	A984	C853	A782	U703	C635	G570	A504	A432	A352	U288	G215	A146	G2
A1054	C985	C854	G783	A705	G636	U571	A505	A433	C353	U289	A216	A147	U3
G1055	C986	G855	G784	A705	A637	A572	A506	C433	A354	U290	A217	U148	U4
G1056	C987	G856	G785	G708	G638	U573	G507	U434	G355	G291	A218	U149	A5
A1057	C988	G857	C786	G709	U639	A574	A508	U437	G356	U292	A219	U150	A6
U1058	G989	G858	C787	U710	C640	A575	A509	U438	G357	G293	G220	A151	G7
U1059	A990	G859	A786	U711	A643	G577	C509	A439	U358	G295	A221	A152	C11
U1060	A925	A861	G794	G711	A643	U577	C510	A439	G359	U296	A222	U153	U12
C992	C926	G862	G795	G712	A644	U580	U511	A440	U360	G297	A223	U154	C16
G993	A927	G863	C796	G713	C645	C581	A513	U441	G361	G298	A224	U155	C17
C994	A928	A863	G797	U714	U646	A582	A514	A442	A362	A299	U224	A156	C18
C995	U929	G864	G797	A715	G647	A583	A515	A443	G363	A300	G230	C157	G16
G930	G930	C865	A716	A716	G648	C584	A515	C444	C364	G301	G231	A160	U18
U931	U931	A866	C717	C717	G649	C585	A515	C445	U365	G302	A231	A161	U19
U932	U932	C867	A718	A718	C650	C586	U519	G446	C366	G303	A232	U162	C20
A933	A933	U868	C719	C719	A654	A586	A522	G452	G370	U304	A233	U163	A21
U934	U934	G869	U720	U720	A655	C587	C523	A453	A371	U306	A234	C164	G26
C935	C935	U870	A721	A721	G656	U588	C524	A454	G372	G307	U235	A165	G27
A936	A936	U871	A722	A722	G657	U589	G525	A455	U373	G308	C236	U166	A28
C937	C937	G873	G725	G725	U657	U591	A526	C456	G374	C237	C237	A167	U29
G938	G938	C874	G726	G726	U658	A592	C527	A457	A375	A310	C238	G168	G30
A941	A941	U813	A727	A727	C660	U593	A528	G458	G375	A311	G242	G169	C31
G942	G942	C814	G728	G728	A661	U594	A528	U459	G381	U170	U243	U171	C32
A943	A943	C815	G729	G729	G662	C595	C531	A460	A382	C314	A244	U172	C33
C944	C944	C816	A730	A730	G663	U596	A532	C461	G386	G315	C245	A173	U34
U945	U945	C817	G738	G738	G664	U597	G533	C462	U387	C316	G246	A174	G35
C946	C946	U818	U665	U665	U665	U598	U534	G463	G318	G317	G247	G175	G36
A947	A947	A819	A666	A666	U666	A599	G536	U464	A391	G319	G248	A176	C37
C948	C948	A820	U667	U667	U667	G600	G537	G465	A392	A320	C249	G177	A38
G949	G949	A821	U668	U668	A668	C601	G602	A466	U393	U321	G250	G178	G39
C950	C950	G822	G669	G669	G669	A602	A603	G467	G393	A322	G252	G179	U40
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G956	G956	U824	C672	C672	C672	G605	C542	A470	G400	A324	A255	A182	A42
C957	C957	A825	C673	C673	C673	U606	C544	A471	A401	G325	A256	C183	G45
U958	U958	U826	C674	C674	G674	U607	G543	A472	A402	G327	G259	G184	G46
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C961	C961	U828	C679	C679	C679	A609	U545	A477	A404	G329	G261	G189	A48
G962	G962	A832	C680	C680	C680	A613	U546	A479	U405	A330	C264	A190	A49
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C964	C964	C834	G682	G682	G682	U615	G549	C481	C332	A127	C129	C192	G51
G965	G965	C835	U755	U755	U755	A616	G553	A482	C333	C128	C129	U193	U62
C966	C966	G836	A756	A756	A756	G617	U554	A483	C334	C129	C129	C193	U63
U967	U967	C837	C765	C765	U686	U618	U555	C484	C335	C130	C130	A196	A63
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G969	G969	A839	U767	U767	U688	G620	A556	C486	C337	G133	U133	C198	U65
U970	U970	C840	U767	U767	A689	A621	C557	C487	C338	U676	U676	A199	C66
C971	C971	G841	G690	G690	G690	G622	U558	C488	U339	G277	G277	U200	U67
A972	A972	U842	A693	A693	A693	C623	G559	U491	C341	A278	A278	U201	G68
G973	G973	A845	U694	U694	U694	C624	C560	A492	A342	U280	U280	A204	G69
C974	C974	U846	G695	G695	G695	A627	A563	G493	A423	C281	C281	G205	A71
A975	A975	U847	G696	G696	G696	A630	C564	G494	A424	A282	A282	C208	A74
G978	G978	C848	G697	G697	G697	G630	C565	C495	G425	G347	G347	C209	G75
A981	A981	U849	C698	C698	C698	A631	U566	A497	C426	U284	U284	C210	G76
C982	C982	U850	A699	A699	A699	A633	U568	G498	U427	G285	G285	C211	G77
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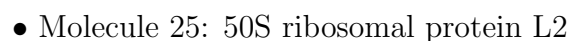
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A	A2051	U1971	G1905	G1895	A1755	G1685	A1598	C1534	C1463	A1396	A1327	U1263	G1192	G1120
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G	A2060	G1980	G1910	U1831	C1760	A1690	C1607	G1539	A1471	U1405	G1333	U1268	G1197	
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G	C2063	G1985	A1913	U1833	G1762	U1692	A1609	G1540	A1473	G1407	G1335	G1270	U1199	G1131
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G	C2065		U1915	G1842	U1765	C1694	G1611	U1551	U1482	A1413	A1337	A1272	U1202	A1133
C	C2066	U1991	U1916	C1843	C1771	A1700	A1545	A1547	U1475	U1408	G1341	A1275	U1203	C1135
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C	G2102	G2029	U1955	U1883	A1805	G1733	U1662	A1583	G1514	C1447	U1378	G1310	G1245	U1173
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G	A2108	C1961	C1961	A1889	G1740	U1692	C1675	U1589	U1523	A1453	A1385	G1318	G1252	U1181
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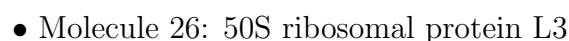
Age Group	Percentage
18-24	10%
25-34	25%
35-44	35%
45-54	15%
55-64	5%
65-74	5%
75-84	5%
85+	5%



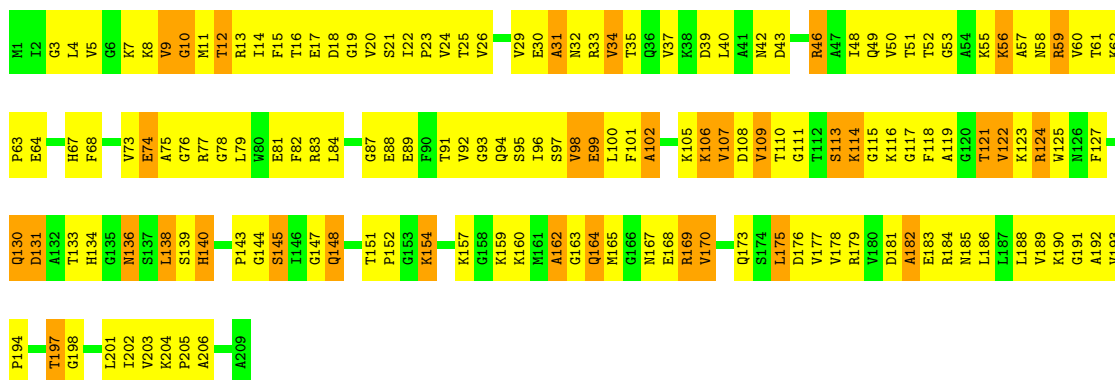
Age Group	Percentage
18-24	15%
25-34	25%
35-44	20%
45-54	15%
55-64	10%
65-74	5%
75-84	5%
85+	5%



Age Group	Percentage
18-24	15%
25-34	25%
35-44	20%
45-54	15%
55-64	10%
65-74	5%
75-84	2%
85+	1%

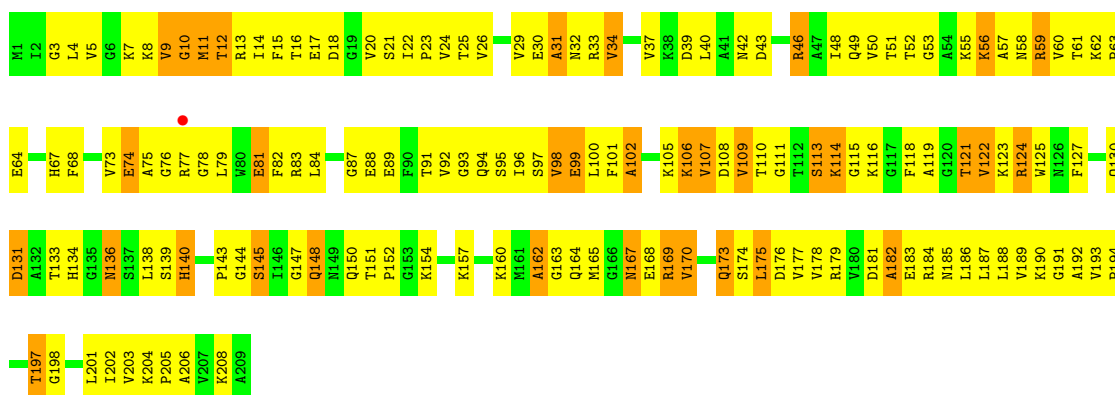


Frequency	Percentage
Daily	60%
Weekly	30%
Monthly	10%



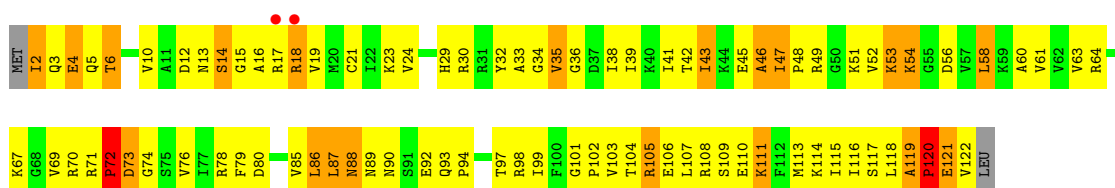
• Molecule 26: 50S ribosomal protein L3

Chain DD:



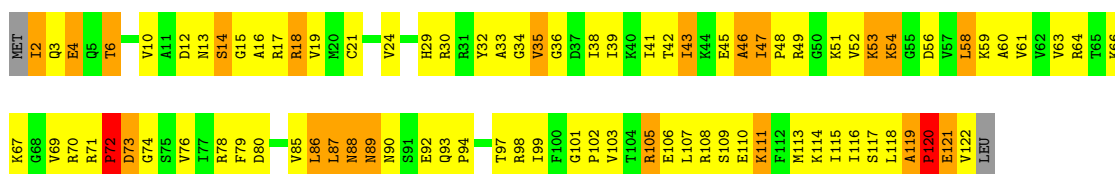
• Molecule 27: 50S ribosomal protein L14

Chain BK:



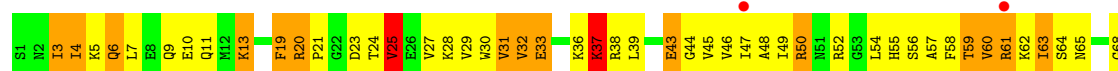
• Molecule 27: 50S ribosomal protein L14

Chain DK:



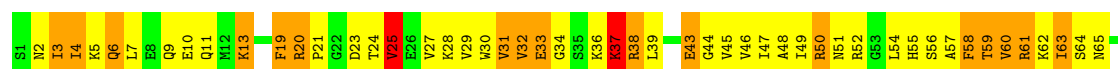
• Molecule 28: 50S ribosomal protein L19

Chain BP:



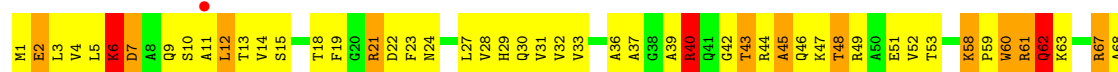
• Molecule 28: 50S ribosomal protein L19

Chain DP:



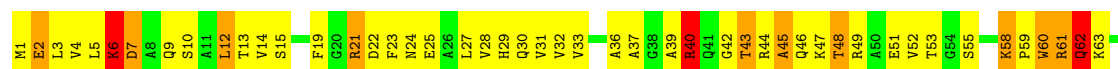
• Molecule 29: 50S ribosomal protein L4

Chain BE:



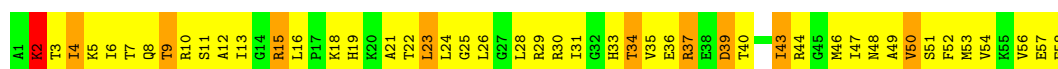
• Molecule 29: 50S ribosomal protein L4

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:



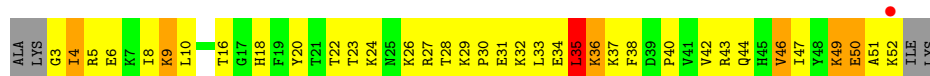
- Molecule 33: 50S ribosomal protein L33

Chain B1:



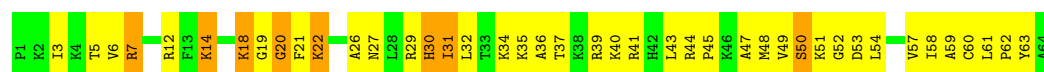
- Molecule 33: 50S ribosomal protein L33

Chain D1:



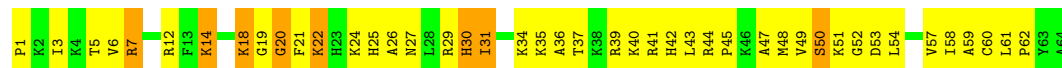
- Molecule 34: 50S ribosomal protein L35

Chain B3:



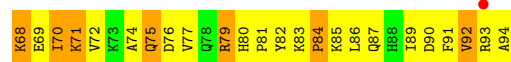
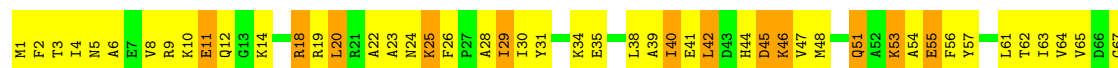
- Molecule 34: 50S ribosomal protein L35

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:



I135
E136
A137
A138
G139
G140
K141
I142
E143
E144

- Molecule 37: 50S ribosomal protein L15

Chain DL:

MET R2 L3 M4 T5 L6 S7 P8 A9 S12 K13 K14 A15 G16 K17 R18 R19 G20 R21 G22 I23 G28 K29 T30 G31 G32 R33 K36 S40 R41 S42 R48 E51 G52 G53 Q54 M55 P56 L57 Y58 R59 R60 L61 P62 K63 F64 G65 F66 T67 S68 R69 K70 I73

T74 A75 E76 I77 R78 L79 S80 D81 L82 K83 K84 V85 E86 W89 V90 D91 L92 N93 T94 R95 K96 A97 I100 I101 G102 I103 G104 I105 K109 V110 I111 L112 A113 G114 E115 V116 T117 T118 P119 V120 T121 V122 R123 G124 L125 R126 V127 T128 K129 G130 A131 R132 A133 A134 I135 E136 A137

A138 G139 K140 K141 I142 E143 E144

- Molecule 38: 50S ribosomal protein L16

Chain BM:

M1 L2 Q3 P4 K5 R6 R10 K11 M12 R16 R17 R18 G19 L20 A21 D25 V26 S27 F28 G29 S30 F31 G32 L33 K34 A35 V36 G37 R38 G39 R40 L41 T42 M105 A43 R44 Q45 I46 E47 R50 R51 A52 M53 T54 R55 A56 V57 K58 R59 Q60 G61 R62 I63 W64 R65 I66 T67 V67

F68 P69 D70 K71 P72 T73 T74 E75 E76 P77 L78 A79 V80 R81 M82 G83 G87 N88 V89 E90 Y91 W92 V93 A94 L95 I96 I97 P98 G99 K100 K101 V101 L102 Y103 E104 M105 D106 G107 V108 P109 E110 E111 E112 L113 A114 E115 A116 F117 K118 L119 A120 A121 A122 K123 L124 P125 I126 K127 T128 T129

F130 V131 T132 K133 T134 V135 M136

- Molecule 38: 50S ribosomal protein L16

Chain DM:

M1 L2 Q3 P4 K5 R6 R10 K11 M12 R16 R17 R18 G19 L20 A21 D25 V26 S27 F28 G29 S30 F31 G32 L33 K34 A35 V36 G37 R38 G39 R40 L41 T42 M105 A43 R44 Q45 I46 E47 A52 M53 T54 R55 A56 V57 K58 R59 Q60 G61 R62 I63 W64 R65 I66 T67 V67 P69

D70 K71 P72 T73 T74 E75 E76 P77 L78 A79 V80 R81 M82 G83 K86 G87 N88 V89 E90 Y91 W92 V93 A94 L95 I96 I97 P98 G99 K100 K101 V101 L102 Y103 E104 M105 D106 G107 V108 P109 E110 E111 E112 L113 A114 E115 A116 F117 K118 L119 A120 A121 A122 K123 L124 P125 I126 K127 T128 T129 F130

V131 T132 K133 T134 V135 M136

- Molecule 39: 50S ribosomal protein L29

Chain BX:

M1 K2 A3 K4 E5 L6 R7 E8 K9 E12 E13 E14 M15 T16 E17 L18 L19 N20 N21 L22 L23 R24 E25 Q26 F26 N27 L28 R29 M30 Q31 Q32 A33 S34 G35 Q36 L37 S40 H41 L42 L43 K44 Q45 V46 R47 R48 D49 V50 A51 A52 V53 R54 T55 L56 L57 N58 E59 A60 A61 G62

L63

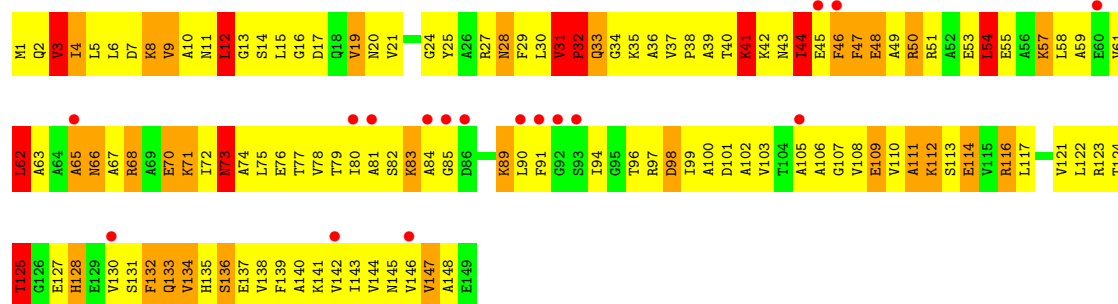
- Molecule 39: 50S ribosomal protein L29

Chain DX: 



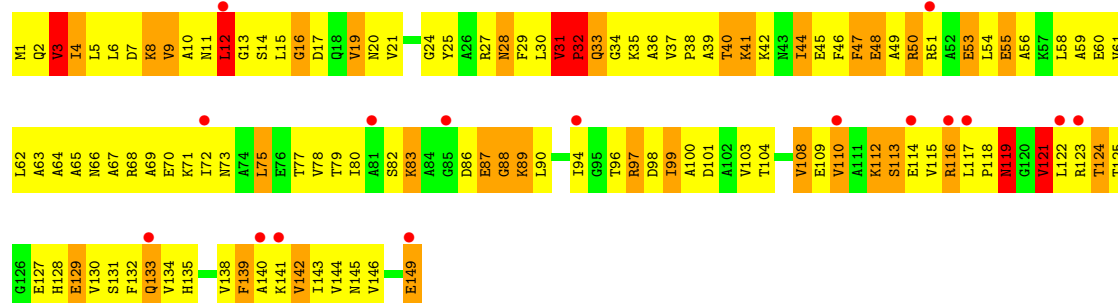
- Molecule 40: 50S ribosomal protein L9

Chain BH: 



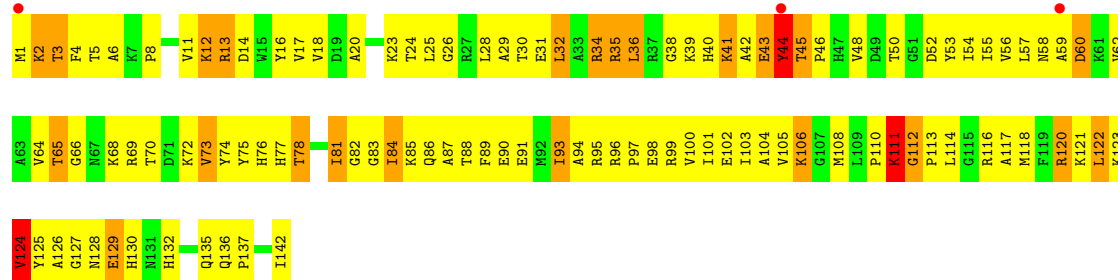
- Molecule 40: 50S ribosomal protein L9

Chain DH: 



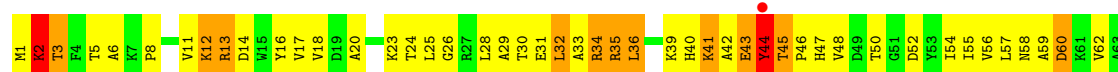
- Molecule 41: 50S ribosomal protein L13

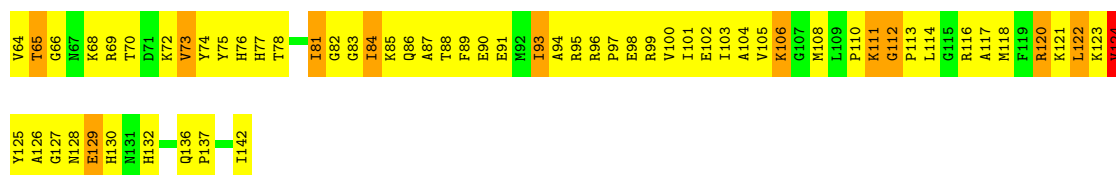
Chain BJ: 



- Molecule 41: 50S ribosomal protein L13

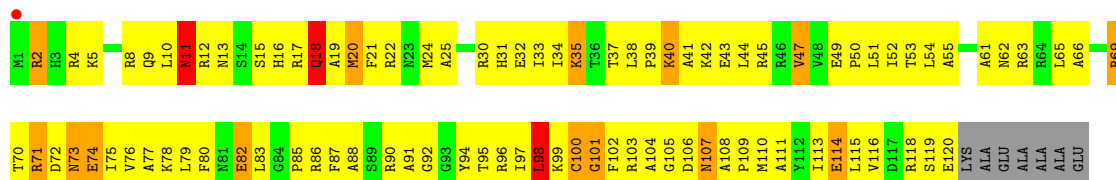
Chain DJ: 





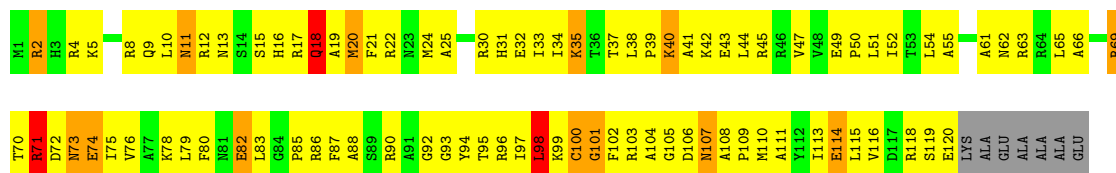
• Molecule 42: 50S ribosomal protein L17

Chain BN:



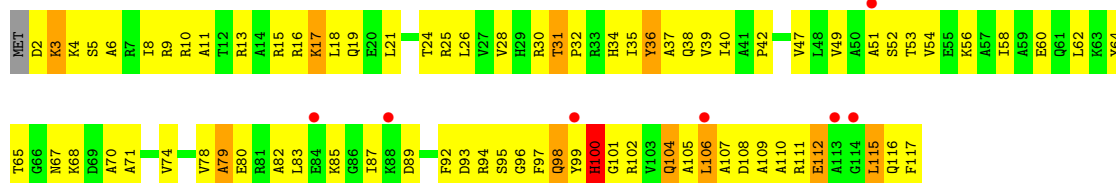
• Molecule 42: 50S ribosomal protein L17

Chain DN:



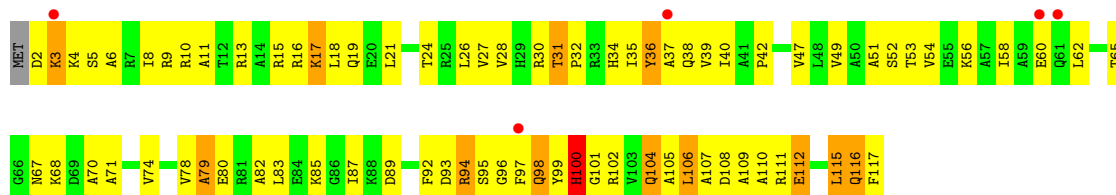
• Molecule 43: 50S ribosomal protein L18

Chain BO:



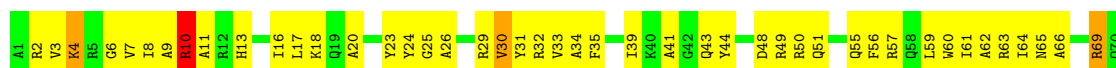
• Molecule 43: 50S ribosomal protein L18

Chain DO:



• Molecule 44: 50S ribosomal protein L20

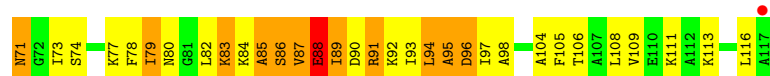
Chain BQ:





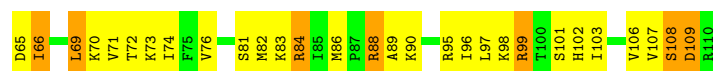
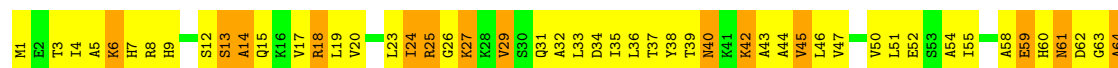
• Molecule 44: 50S ribosomal protein L20

Chain DQ:



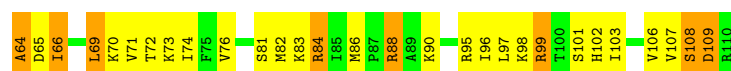
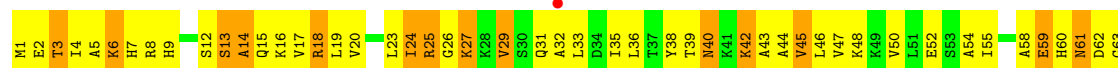
• Molecule 45: 50S ribosomal protein L22

Chain BS:



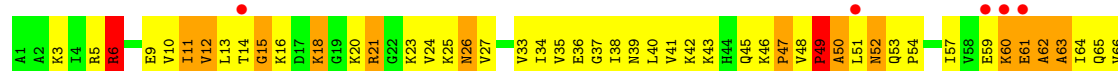
• Molecule 45: 50S ribosomal protein L22

Chain DS:



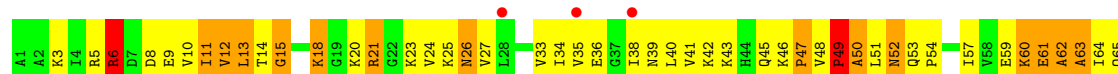
• Molecule 46: 50S ribosomal protein L24

Chain BU:

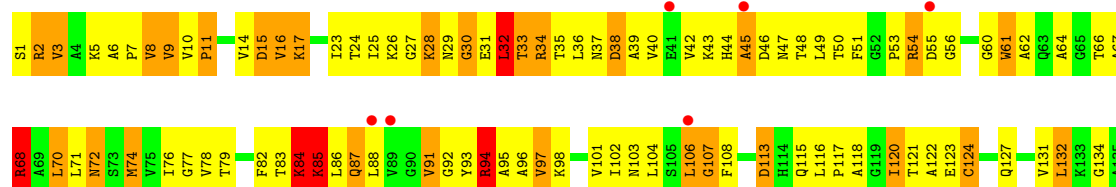


• Molecule 46: 50S ribosomal protein L24

Chain DU:



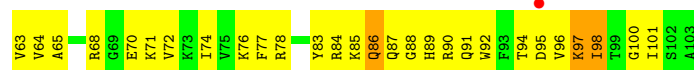
- Chain BF: 





• Molecule 49: 50S ribosomal protein L21

Chain BR:



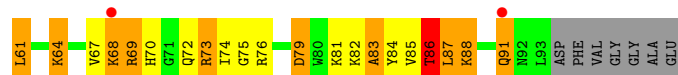
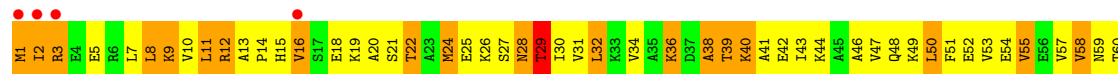
• Molecule 49: 50S ribosomal protein L21

Chain DR:



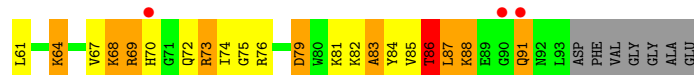
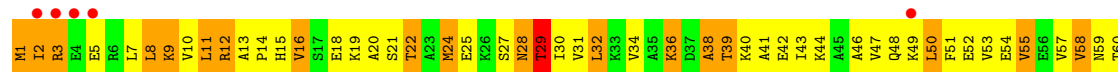
• Molecule 50: 50S ribosomal protein L23

Chain BT:



• Molecule 50: 50S ribosomal protein L23

Chain DT:



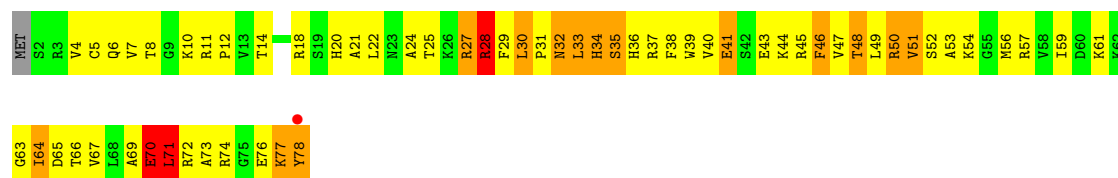
• Molecule 51: 50S ribosomal protein L28

Chain BZ:



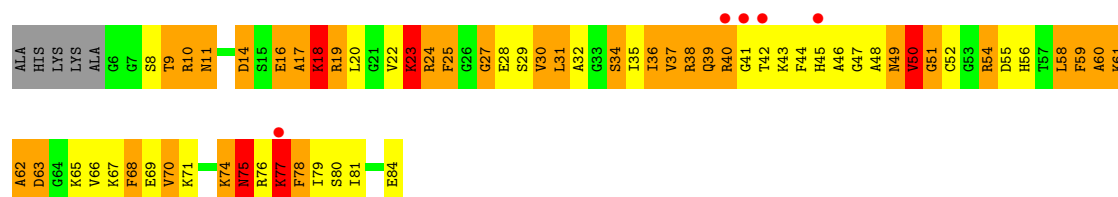
- Molecule 51: 50S ribosomal protein L28

Chain DZ:



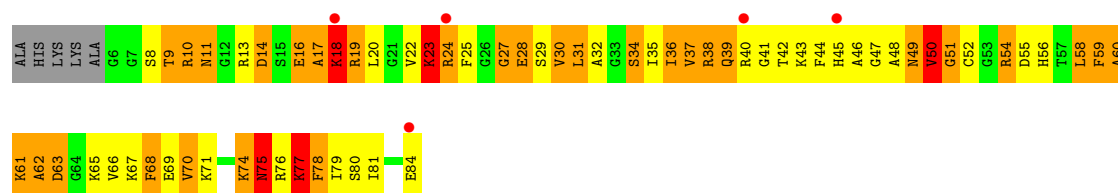
- Molecule 52: 50S ribosomal protein L27

Chain BW:



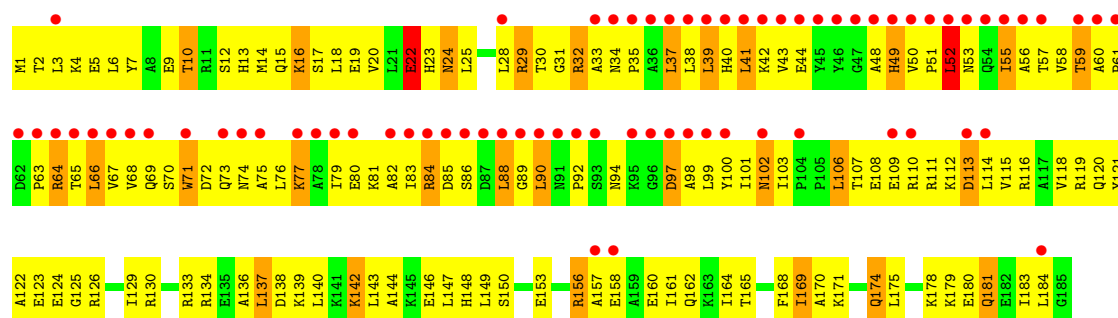
- Molecule 52: 50S ribosomal protein L27

Chain DW:



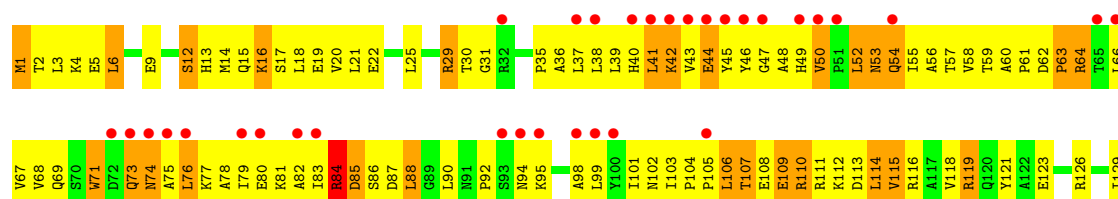
- Molecule 53: ribosome recycling factor

Chain B6:



- Molecule 53: ribosome recycling factor

Chain D6:



R130	R131	I132	R133	R134	E135	A136	L137	D138	K139	L140	K141	K142	L143	E146	L147	H148	L149	S150	E151	D152	E153	T154	K155	R156	E160	I161	F168	K171	Q174	L175	K178	K179	E180	I183	L184	G185
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	207.90Å 378.20Å 736.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.30 82.86 – 3.32	Depositor EDS
% Data completeness (in resolution range)	85.8 (40.00-3.30) 87.1 (82.86-3.32)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.33Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.275 , 0.304 0.250 , 0.275	Depositor DCC
R_{free} test set	35399 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 20.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 738833 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	286960	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	AA	0.26	0/36762	0.75	11/57350 (0.0%)
1	CA	0.26	0/36762	0.75	18/57350 (0.0%)
2	AC	0.23	0/1651	0.44	0/2225
2	CC	0.23	0/1651	0.45	0/2225
3	AD	0.23	0/1665	0.44	0/2227
3	CD	0.23	0/1665	0.43	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	0.45	0/1591
6	CG	0.23	0/1211	0.45	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	0/1034	0.46	0/1375
9	AJ	0.22	0/796	0.49	0/1077
9	CJ	0.22	0/796	0.49	0/1077
10	AK	0.24	0/893	0.46	0/1205
10	CK	0.24	0/893	0.46	0/1205
11	AL	0.22	0/969	0.48	0/1300
11	CL	0.22	0/969	0.49	0/1300
12	AM	0.21	0/892	0.46	0/1193
12	CM	0.21	0/884	0.45	0/1181
13	AN	0.24	0/785	0.44	0/1043
13	CN	0.24	0/785	0.44	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	0.45	0/884
15	CP	0.25	0/648	0.45	0/870
16	AQ	0.23	0/657	0.47	0/881
16	CQ	0.24	0/666	0.48	0/892

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.23	0/462	0.45	0/621
17	CR	0.23	0/462	0.45	0/621
18	AS	0.25	0/652	0.46	0/877
18	CS	0.25	0/660	0.48	0/888
19	AT	0.23	0/671	0.40	0/888
19	CT	0.23	0/671	0.40	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	0.25	0/2803	0.74	1/4371 (0.0%)
22	DA	0.25	0/2803	0.74	1/4371 (0.0%)
23	BB	0.28	6/68314 (0.0%)	0.77	55/106569 (0.1%)
23	DB	0.28	8/68314 (0.0%)	0.78	51/106569 (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	0.25	0/929	0.50	0/1242
28	DP	0.24	0/929	0.50	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	0.50	0/605
30	DY	0.23	0/453	0.50	0/605
31	B0	0.22	0/450	0.56	0/599
31	D0	0.22	0/450	0.56	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	0.47	0/676
34	D3	0.24	0/513	0.47	0/676
35	BV	0.25	0/766	0.43	0/1025
35	DV	0.25	0/766	0.43	0/1025
36	B2	0.26	0/380	0.48	0/498
36	D2	0.26	0/380	0.48	0/498
37	BL	0.23	0/1054	0.49	0/1403
37	DL	0.23	0/1054	0.49	0/1403
38	BM	0.25	0/1093	0.49	0/1460

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DM	0.25	0/1093	0.49	0/1460
39	BX	0.24	0/510	0.52	0/677
39	DX	0.24	0/510	0.52	0/677
40	BH	0.25	0/1122	0.48	0/1515
40	DH	0.25	0/1122	0.49	0/1515
41	BJ	0.23	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	0.25	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	0.48	0/1816
48	DG	0.23	0/1343	0.47	0/1816
49	BR	0.25	0/829	0.49	0/1107
49	DR	0.25	0/829	0.49	0/1107
50	BT	0.23	0/744	0.55	0/994
50	DT	0.23	0/744	0.55	0/994
51	BZ	0.25	0/635	0.52	0/848
51	DZ	0.25	0/635	0.52	0/848
52	BW	0.28	0/603	0.52	0/797
52	DW	0.28	0/603	0.52	0/797
53	B6	0.24	0/1497	0.48	0/2017
53	D6	0.23	0/1497	0.48	0/2017
All	All	0.26	14/309354 (0.0%)	0.70	137/462003 (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	14
1	CA	0	13
23	BB	0	29

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
23	DB	0	29
All	All	0	85

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	BB	1086	A	C5-C6	-16.41	1.26	1.41
23	DB	1086	A	C5-C6	-16.29	1.26	1.41
23	DB	1088	A	C6-N1	-10.64	1.28	1.35
23	BB	1088	A	C6-N1	-10.54	1.28	1.35
23	DB	1060	U	C2-N3	7.91	1.43	1.37

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	DB	2204	G	O5'-P-OP1	-29.30	75.55	110.70
23	BB	2204	G	O5'-P-OP2	-27.99	77.11	110.70
23	BB	2791	G	O5'-P-OP1	-27.68	77.49	110.70
23	DB	2791	G	O5'-P-OP2	-27.63	77.54	110.70
23	DB	2791	G	O5'-P-OP1	18.08	132.40	110.70

There are no chirality outliers.

5 of 85 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	81	A	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	1174	0
1	CA	32831	0	16521	1151	0
2	AC	1624	0	1699	141	0
2	CC	1624	0	1699	138	0
3	AD	1643	0	1710	151	0
3	CD	1643	0	1710	155	0
4	AE	1105	0	1148	107	0
4	CE	1105	0	1148	102	0
5	AF	817	0	808	85	0
5	CF	817	0	808	82	0
6	AG	1174	0	1230	102	0
6	CG	1196	0	1246	91	0
7	AH	979	0	1034	62	0
7	CH	979	0	1034	62	0
8	AI	1022	0	1070	123	0
8	CI	1022	0	1070	126	0
9	AJ	786	0	828	76	0
9	CJ	786	0	828	76	0
10	AK	877	0	887	84	0
10	CK	877	0	887	73	0
11	AL	955	0	1019	85	0
11	CL	955	0	1019	92	0
12	AM	883	0	944	104	0
12	CM	876	0	937	109	0
13	AN	774	0	827	96	0
13	CN	774	0	827	95	0
14	AO	714	0	734	46	0
14	CO	714	0	734	51	0
15	AP	649	0	666	60	0
15	CP	638	0	656	60	0
16	AQ	648	0	691	64	0
16	CQ	657	0	702	65	0
17	AR	455	0	478	36	0
17	CR	455	0	478	37	0
18	AS	637	0	665	89	0
18	CS	644	0	675	91	0
19	AT	665	0	714	45	0
19	CT	665	0	714	44	0
20	AB	1704	0	1732	195	0
20	CB	1704	0	1732	198	0
21	AU	425	0	449	69	0
21	CU	425	0	449	68	0
22	BA	2507	0	1270	89	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	DA	2507	0	1270	83	0
23	BB	60995	0	30679	2163	0
23	DB	60995	0	30677	2184	0
24	BI	1032	0	1088	112	0
24	DI	1032	0	1088	183	0
25	BC	2082	0	2157	232	0
25	DC	2082	0	2157	232	0
26	BD	1565	0	1616	186	0
26	DD	1565	0	1616	184	0
27	BK	930	0	1000	110	0
27	DK	930	0	1000	113	0
28	BP	917	0	965	136	0
28	DP	917	0	965	145	0
29	BE	1552	0	1619	188	0
29	DE	1552	0	1619	191	0
30	BY	449	0	491	52	0
30	DY	449	0	491	52	0
31	B0	444	0	461	39	0
31	D0	444	0	461	31	0
32	B4	302	0	340	50	0
32	D4	302	0	340	53	0
33	B1	409	0	440	51	0
33	D1	409	0	440	43	0
34	B3	504	0	574	54	0
34	D3	504	0	574	57	0
35	BV	753	0	780	86	0
35	DV	753	0	780	84	0
36	B2	377	0	418	34	0
36	D2	377	0	418	32	0
37	BL	1045	0	1117	138	0
37	DL	1045	0	1117	144	0
38	BM	1074	0	1157	120	0
38	DM	1074	0	1157	118	0
39	BX	509	0	543	56	0
39	DX	509	0	543	58	0
40	BH	1111	0	1148	220	0
40	DH	1111	0	1148	161	0
41	BJ	1129	0	1162	156	0
41	DJ	1129	0	1162	161	0
42	BN	960	0	1000	111	0
42	DN	960	0	1000	108	0
43	BO	892	0	923	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	DO	892	0	923	81	0
44	BQ	947	0	1022	125	0
44	DQ	947	0	1022	136	0
45	BS	857	0	922	94	0
45	DS	857	0	922	93	0
46	BU	779	0	834	111	0
46	DU	779	0	834	111	0
47	BF	1420	0	1460	242	0
47	DF	1420	0	1460	233	0
48	BG	1323	0	1374	158	0
48	DG	1323	0	1374	159	0
49	BR	816	0	839	85	0
49	DR	816	0	839	96	0
50	BT	738	0	807	120	0
50	DT	738	0	807	115	0
51	BZ	625	0	652	63	0
51	DZ	625	0	652	61	0
52	BW	596	0	610	138	0
52	DW	596	0	610	152	0
53	B6	1478	0	1526	204	0
53	D6	1478	0	1526	177	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	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	AA	289	0	0	1	0
56	AE	4	0	0	0	0
56	AK	1	0	0	0	0
56	AL	1	0	0	0	0
56	AN	3	0	0	0	0
56	AP	1	0	0	0	0
56	AT	1	0	0	0	0
56	B2	1	0	0	0	0
56	BB	495	0	0	5	0
56	BC	4	0	0	0	0
56	BD	1	0	0	0	0
56	BE	3	0	0	0	0
56	BL	1	0	0	0	0
56	BT	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	CA	300	0	0	0	0
56	CE	2	0	0	0	0
56	CK	1	0	0	0	0
56	CL	1	0	0	0	0
56	CN	4	0	0	0	0
56	CT	1	0	0	0	0
56	DB	505	0	0	7	0
56	DC	4	0	0	1	0
56	DD	1	0	0	0	0
56	DE	2	0	0	0	0
All	All	286960	0	193714	16198	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 34.

The worst 5 of 16198 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	1.39	1.17
13:CN:63:CYS:HB3	13:CN:67:GLY:H	1.09	1.16
13:AN:63:CYS:HB3	13:AN:67:GLY:H	1.05	1.15
10:AK:124:LYS:HA	21:AU:34:ARG:HB3	1.27	1.14
29:DE:21:ARG:HD2	29:DE:107:SER:HB3	1.30	1.13

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%)	152 (74%)	36 (18%)	16 (8%)	1	14
2	CC	204/232 (88%)	151 (74%)	37 (18%)	16 (8%)	1	14
3	AD	203/205 (99%)	151 (74%)	39 (19%)	13 (6%)	2	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CD	203/205 (99%)	150 (74%)	41 (20%)	12 (6%)	2	23
4	AE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	11	58
4	CE	148/166 (89%)	125 (84%)	20 (14%)	3 (2%)	11	58
5	AF	98/135 (73%)	71 (72%)	18 (18%)	9 (9%)	1	9
5	CF	98/135 (73%)	69 (70%)	21 (21%)	8 (8%)	1	13
6	AG	148/178 (83%)	114 (77%)	28 (19%)	6 (4%)	4	35
6	CG	150/178 (84%)	118 (79%)	25 (17%)	7 (5%)	4	30
7	AH	127/129 (98%)	106 (84%)	17 (13%)	4 (3%)	7	45
7	CH	127/129 (98%)	105 (83%)	18 (14%)	4 (3%)	7	45
8	AI	125/129 (97%)	92 (74%)	28 (22%)	5 (4%)	5	36
8	CI	125/129 (97%)	93 (74%)	28 (22%)	4 (3%)	6	43
9	AJ	96/103 (93%)	73 (76%)	13 (14%)	10 (10%)	1	7
9	CJ	96/103 (93%)	74 (77%)	12 (12%)	10 (10%)	1	7
10	AK	115/128 (90%)	85 (74%)	25 (22%)	5 (4%)	4	34
10	CK	115/128 (90%)	84 (73%)	25 (22%)	6 (5%)	3	27
11	AL	121/123 (98%)	84 (69%)	28 (23%)	9 (7%)	2	15
11	CL	121/123 (98%)	86 (71%)	25 (21%)	10 (8%)	1	12
12	AM	112/117 (96%)	85 (76%)	16 (14%)	11 (10%)	1	8
12	CM	111/117 (95%)	83 (75%)	17 (15%)	11 (10%)	1	8
13	AN	92/100 (92%)	65 (71%)	19 (21%)	8 (9%)	1	11
13	CN	92/100 (92%)	66 (72%)	18 (20%)	8 (9%)	1	11
14	AO	86/89 (97%)	68 (79%)	15 (17%)	3 (4%)	6	41
14	CO	86/89 (97%)	70 (81%)	14 (16%)	2 (2%)	10	54
15	AP	80/82 (98%)	62 (78%)	10 (12%)	8 (10%)	1	8
15	CP	78/82 (95%)	61 (78%)	11 (14%)	6 (8%)	1	14
16	AQ	78/83 (94%)	59 (76%)	15 (19%)	4 (5%)	3	28
16	CQ	79/83 (95%)	60 (76%)	15 (19%)	4 (5%)	3	28
17	AR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
17	CR	53/74 (72%)	48 (91%)	5 (9%)	0	100	100
18	AS	77/91 (85%)	59 (77%)	12 (16%)	6 (8%)	1	14
18	CS	78/91 (86%)	61 (78%)	11 (14%)	6 (8%)	1	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	AT	83/86 (96%)	64 (77%)	15 (18%)	4 (5%)	4	30
19	CT	83/86 (96%)	65 (78%)	14 (17%)	4 (5%)	4	30
20	AB	216/240 (90%)	153 (71%)	48 (22%)	15 (7%)	2	17
20	CB	216/240 (90%)	150 (69%)	49 (23%)	17 (8%)	1	13
21	AU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
21	CU	49/70 (70%)	31 (63%)	10 (20%)	8 (16%)	0	1
24	BI	139/141 (99%)	119 (86%)	15 (11%)	5 (4%)	5	40
24	DI	139/141 (99%)	114 (82%)	21 (15%)	4 (3%)	7	47
25	BC	269/272 (99%)	176 (65%)	61 (23%)	32 (12%)	1	4
25	DC	269/272 (99%)	177 (66%)	59 (22%)	33 (12%)	1	4
26	BD	207/209 (99%)	123 (59%)	56 (27%)	28 (14%)	0	3
26	DD	207/209 (99%)	122 (59%)	55 (27%)	30 (14%)	0	2
27	BK	119/123 (97%)	80 (67%)	25 (21%)	14 (12%)	1	4
27	DK	119/123 (97%)	81 (68%)	24 (20%)	14 (12%)	1	4
28	BP	112/114 (98%)	68 (61%)	29 (26%)	15 (13%)	0	3
28	DP	112/114 (98%)	69 (62%)	28 (25%)	15 (13%)	0	3
29	BE	199/201 (99%)	126 (63%)	54 (27%)	19 (10%)	1	9
29	DE	199/201 (99%)	127 (64%)	52 (26%)	20 (10%)	1	8
30	BY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	1	6
30	DY	56/58 (97%)	39 (70%)	11 (20%)	6 (11%)	1	6
31	B0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
31	D0	54/56 (96%)	40 (74%)	5 (9%)	9 (17%)	0	1
32	B4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
32	D4	36/38 (95%)	22 (61%)	5 (14%)	9 (25%)	0	0
33	B1	48/54 (89%)	37 (77%)	6 (12%)	5 (10%)	1	7
33	D1	48/54 (89%)	36 (75%)	7 (15%)	5 (10%)	1	7
34	B3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	1	8
34	D3	62/64 (97%)	42 (68%)	14 (23%)	6 (10%)	1	8
35	BV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	6	43
35	DV	92/94 (98%)	71 (77%)	18 (20%)	3 (3%)	6	43
36	B2	44/46 (96%)	36 (82%)	7 (16%)	1 (2%)	10	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	D2	44/46 (96%)	35 (80%)	7 (16%)	2 (4%)	4	32
37	BL	141/144 (98%)	92 (65%)	31 (22%)	18 (13%)	0	3
37	DL	141/144 (98%)	94 (67%)	28 (20%)	19 (14%)	0	3
38	BM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	2
38	DM	134/136 (98%)	90 (67%)	24 (18%)	20 (15%)	0	2
39	BX	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	2	19
39	DX	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	2	19
40	BH	147/149 (99%)	74 (50%)	50 (34%)	23 (16%)	0	1
40	DH	147/149 (99%)	92 (63%)	38 (26%)	17 (12%)	1	5
41	BJ	140/142 (99%)	96 (69%)	31 (22%)	13 (9%)	1	9
41	DJ	140/142 (99%)	95 (68%)	32 (23%)	13 (9%)	1	9
42	BN	118/127 (93%)	84 (71%)	25 (21%)	9 (8%)	2	15
42	DN	118/127 (93%)	82 (70%)	25 (21%)	11 (9%)	1	9
43	BO	114/117 (97%)	87 (76%)	21 (18%)	6 (5%)	3	26
43	DO	114/117 (97%)	86 (75%)	21 (18%)	7 (6%)	2	22
44	BQ	115/117 (98%)	81 (70%)	21 (18%)	13 (11%)	1	5
44	DQ	115/117 (98%)	81 (70%)	22 (19%)	12 (10%)	1	7
45	BS	108/110 (98%)	72 (67%)	21 (19%)	15 (14%)	0	2
45	DS	108/110 (98%)	73 (68%)	20 (18%)	15 (14%)	0	2
46	BU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	2
46	DU	100/103 (97%)	58 (58%)	27 (27%)	15 (15%)	0	2
47	BF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	1
47	DF	176/178 (99%)	106 (60%)	36 (20%)	34 (19%)	0	1
48	BG	174/176 (99%)	108 (62%)	41 (24%)	25 (14%)	0	2
48	DG	174/176 (99%)	109 (63%)	39 (22%)	26 (15%)	0	2
49	BR	101/103 (98%)	74 (73%)	16 (16%)	11 (11%)	1	6
49	DR	101/103 (98%)	73 (72%)	17 (17%)	11 (11%)	1	6
50	BT	91/100 (91%)	52 (57%)	23 (25%)	16 (18%)	0	1
50	DT	91/100 (91%)	52 (57%)	24 (26%)	15 (16%)	0	1
51	BZ	75/78 (96%)	50 (67%)	16 (21%)	9 (12%)	1	4
51	DZ	75/78 (96%)	50 (67%)	17 (23%)	8 (11%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
52	BW	77/84 (92%)	32 (42%)	20 (26%)	25 (32%)	0	0
52	DW	77/84 (92%)	33 (43%)	18 (23%)	26 (34%)	0	0
53	B6	183/185 (99%)	140 (76%)	36 (20%)	7 (4%)	5	37
53	D6	183/185 (99%)	146 (80%)	28 (15%)	9 (5%)	3	29
All	All	11607/12284 (94%)	8146 (70%)	2335 (20%)	1126 (10%)	1	8

5 of 1126 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	14	VAL
2	AC	25	THR
2	AC	54	ILE
2	AC	100	ILE
2	AC	104	GLU

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%)	145 (85%)	25 (15%)	4	22
2	CC	170/189 (90%)	145 (85%)	25 (15%)	4	22
3	AD	172/172 (100%)	138 (80%)	34 (20%)	2	9
3	CD	172/172 (100%)	138 (80%)	34 (20%)	2	9
4	AE	113/125 (90%)	99 (88%)	14 (12%)	7	31
4	CE	113/125 (90%)	99 (88%)	14 (12%)	7	31
5	AF	87/116 (75%)	70 (80%)	17 (20%)	2	9
5	CF	87/116 (75%)	70 (80%)	17 (20%)	2	9
6	AG	123/146 (84%)	101 (82%)	22 (18%)	2	13
6	CG	125/146 (86%)	103 (82%)	22 (18%)	3	13
7	AH	104/104 (100%)	95 (91%)	9 (9%)	15	53
7	CH	104/104 (100%)	96 (92%)	8 (8%)	18	60
8	AI	105/106 (99%)	86 (82%)	19 (18%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CI	105/106 (99%)	86 (82%)	19 (18%)	2	12
9	AJ	86/90 (96%)	75 (87%)	11 (13%)	6	29
9	CJ	86/90 (96%)	76 (88%)	10 (12%)	8	35
10	AK	90/98 (92%)	74 (82%)	16 (18%)	2	13
10	CK	90/98 (92%)	74 (82%)	16 (18%)	2	13
11	AL	103/103 (100%)	87 (84%)	16 (16%)	4	19
11	CL	103/103 (100%)	87 (84%)	16 (16%)	4	19
12	AM	92/95 (97%)	71 (77%)	21 (23%)	1	5
12	CM	91/95 (96%)	69 (76%)	22 (24%)	1	4
13	AN	79/83 (95%)	71 (90%)	8 (10%)	11	42
13	CN	79/83 (95%)	71 (90%)	8 (10%)	11	42
14	AO	76/77 (99%)	70 (92%)	6 (8%)	18	59
14	CO	76/77 (99%)	70 (92%)	6 (8%)	18	59
15	AP	65/65 (100%)	57 (88%)	8 (12%)	7	32
15	CP	65/65 (100%)	56 (86%)	9 (14%)	5	25
16	AQ	74/77 (96%)	59 (80%)	15 (20%)	2	8
16	CQ	75/77 (97%)	60 (80%)	15 (20%)	2	9
17	AR	48/64 (75%)	43 (90%)	5 (10%)	10	41
17	CR	48/64 (75%)	43 (90%)	5 (10%)	10	41
18	AS	70/78 (90%)	53 (76%)	17 (24%)	1	3
18	CS	71/78 (91%)	55 (78%)	16 (22%)	1	6
19	AT	65/65 (100%)	54 (83%)	11 (17%)	3	15
19	CT	65/65 (100%)	54 (83%)	11 (17%)	3	15
20	AB	180/198 (91%)	145 (81%)	35 (19%)	2	10
20	CB	180/198 (91%)	144 (80%)	36 (20%)	2	9
21	AU	44/60 (73%)	28 (64%)	16 (36%)	0	1
21	CU	44/60 (73%)	27 (61%)	17 (39%)	0	0
24	BI	109/109 (100%)	107 (98%)	2 (2%)	71	93
24	DI	109/109 (100%)	103 (94%)	6 (6%)	30	75
25	BC	216/217 (100%)	186 (86%)	30 (14%)	5	25
25	DC	216/217 (100%)	187 (87%)	29 (13%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	BD	164/164 (100%)	146 (89%)	18 (11%)	9	38
26	DD	164/164 (100%)	148 (90%)	16 (10%)	12	45
27	BK	102/104 (98%)	84 (82%)	18 (18%)	3	13
27	DK	102/104 (98%)	84 (82%)	18 (18%)	3	13
28	BP	99/99 (100%)	78 (79%)	21 (21%)	1	7
28	DP	99/99 (100%)	78 (79%)	21 (21%)	1	7
29	BE	165/165 (100%)	136 (82%)	29 (18%)	3	13
29	DE	165/165 (100%)	137 (83%)	28 (17%)	3	15
30	BY	48/48 (100%)	41 (85%)	7 (15%)	5	23
30	DY	48/48 (100%)	41 (85%)	7 (15%)	5	23
31	B0	47/47 (100%)	37 (79%)	10 (21%)	1	7
31	D0	47/47 (100%)	37 (79%)	10 (21%)	1	7
32	B4	34/34 (100%)	26 (76%)	8 (24%)	1	4
32	D4	34/34 (100%)	26 (76%)	8 (24%)	1	4
33	B1	45/48 (94%)	39 (87%)	6 (13%)	6	27
33	D1	45/48 (94%)	39 (87%)	6 (13%)	6	27
34	B3	51/51 (100%)	47 (92%)	4 (8%)	18	60
34	D3	51/51 (100%)	47 (92%)	4 (8%)	18	60
35	BV	78/78 (100%)	59 (76%)	19 (24%)	1	3
35	DV	78/78 (100%)	59 (76%)	19 (24%)	1	3
36	B2	38/38 (100%)	32 (84%)	6 (16%)	4	18
36	D2	38/38 (100%)	32 (84%)	6 (16%)	4	18
37	BL	102/103 (99%)	92 (90%)	10 (10%)	12	45
37	DL	102/103 (99%)	92 (90%)	10 (10%)	12	45
38	BM	109/109 (100%)	90 (83%)	19 (17%)	3	14
38	DM	109/109 (100%)	90 (83%)	19 (17%)	3	14
39	BX	55/55 (100%)	43 (78%)	12 (22%)	1	7
39	DX	55/55 (100%)	43 (78%)	12 (22%)	1	7
40	BH	114/114 (100%)	79 (69%)	35 (31%)	0	1
40	DH	114/114 (100%)	82 (72%)	32 (28%)	0	2
41	BJ	116/116 (100%)	96 (83%)	20 (17%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	DJ	116/116 (100%)	98 (84%)	18 (16%)	4	19
42	BN	100/103 (97%)	84 (84%)	16 (16%)	3	18
42	DN	100/103 (97%)	84 (84%)	16 (16%)	3	18
43	BO	86/87 (99%)	74 (86%)	12 (14%)	5	25
43	DO	86/87 (99%)	72 (84%)	14 (16%)	3	17
44	BQ	89/89 (100%)	78 (88%)	11 (12%)	7	31
44	DQ	89/89 (100%)	78 (88%)	11 (12%)	7	31
45	BS	93/93 (100%)	82 (88%)	11 (12%)	8	34
45	DS	93/93 (100%)	82 (88%)	11 (12%)	8	34
46	BU	83/84 (99%)	71 (86%)	12 (14%)	5	23
46	DU	83/84 (99%)	70 (84%)	13 (16%)	4	19
47	BF	149/149 (100%)	114 (76%)	35 (24%)	1	4
47	DF	149/149 (100%)	115 (77%)	34 (23%)	1	5
48	BG	137/137 (100%)	106 (77%)	31 (23%)	1	5
48	DG	137/137 (100%)	105 (77%)	32 (23%)	1	4
49	BR	84/84 (100%)	71 (84%)	13 (16%)	4	19
49	DR	84/84 (100%)	71 (84%)	13 (16%)	4	19
50	BT	80/84 (95%)	59 (74%)	21 (26%)	1	2
50	DT	80/84 (95%)	59 (74%)	21 (26%)	1	2
51	BZ	67/68 (98%)	52 (78%)	15 (22%)	1	6
51	DZ	67/68 (98%)	52 (78%)	15 (22%)	1	6
52	BW	59/62 (95%)	42 (71%)	17 (29%)	0	2
52	DW	59/62 (95%)	43 (73%)	16 (27%)	1	2
53	B6	157/157 (100%)	126 (80%)	31 (20%)	2	9
53	D6	157/157 (100%)	121 (77%)	36 (23%)	1	5
All	All	9647/10014 (96%)	7996 (83%)	1651 (17%)	3	15

5 of 1651 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
50	BT	12	ARG
6	CG	75	LYS
48	DG	37	ASN

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Mol	Chain	Res	Type
51	BZ	41	GLU
2	CC	120	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 342 such sidechains are listed below:

Mol	Chain	Res	Type
49	BR	43	ASN
5	CF	46	GLN
47	DF	51	ASN
50	BT	92	ASN
53	B6	102	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1529/1542 (99%)	248 (16%)	28 (1%)
1	CA	1529/1542 (99%)	239 (15%)	25 (1%)
22	BA	116/120 (96%)	18 (15%)	0
22	DA	116/120 (96%)	19 (16%)	0
23	BB	2837/2904 (97%)	448 (15%)	20 (0%)
23	DB	2837/2904 (97%)	432 (15%)	19 (0%)
All	All	8964/9132 (98%)	1404 (15%)	92 (1%)

5 of 1404 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	14	U
1	AA	15	G
1	AA	31	G
1	AA	32	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
23	BB	2213	U
1	CA	243	A
23	DB	2213	U
23	BB	2282	G
23	BB	2873	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 345 ligands modelled in this entry, 345 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1530/1542 (99%)	-0.20	18 (1%) 75 29	20, 68, 149, 180	0
1	CA	1530/1542 (99%)	-0.28	9 (0%) 86 46	10, 51, 126, 180	0
2	AC	206/232 (88%)	0.26	2 (0%) 79 33	24, 58, 114, 180	0
2	CC	206/232 (88%)	0.19	1 (0%) 88 51	28, 67, 117, 175	0
3	AD	205/205 (100%)	0.28	3 (1%) 70 24	22, 77, 137, 154	0
3	CD	205/205 (100%)	0.07	0 100 100	15, 53, 129, 160	0
4	AE	150/166 (90%)	0.23	0 100 100	16, 62, 116, 154	0
4	CE	150/166 (90%)	0.21	1 (0%) 84 42	20, 50, 105, 159	0
5	AF	100/135 (74%)	0.31	1 (1%) 79 33	33, 73, 126, 163	0
5	CF	100/135 (74%)	0.12	0 100 100	20, 63, 115, 146	0
6	AG	150/178 (84%)	0.35	8 (5%) 25 6	40, 87, 140, 168	0
6	CG	152/178 (85%)	0.44	3 (1%) 62 19	21, 80, 132, 169	0
7	AH	129/129 (100%)	0.51	3 (2%) 57 15	34, 71, 116, 137	0
7	CH	129/129 (100%)	0.18	0 100 100	18, 50, 96, 131	0
8	AI	127/129 (98%)	0.59	8 (6%) 19 5	23, 81, 151, 180	0
8	CI	127/129 (98%)	0.37	2 (1%) 68 22	26, 82, 135, 180	0
9	AJ	98/103 (95%)	0.65	4 (4%) 35 8	21, 74, 134, 180	0
9	CJ	98/103 (95%)	0.76	8 (8%) 12 3	34, 83, 136, 163	0
10	AK	117/128 (91%)	0.20	2 (1%) 67 21	19, 57, 100, 155	0
10	CK	117/128 (91%)	0.11	0 100 100	18, 48, 100, 142	0
11	AL	123/123 (100%)	0.52	3 (2%) 56 15	29, 68, 124, 169	0
11	CL	123/123 (100%)	0.21	1 (0%) 83 39	10, 44, 107, 159	0
12	AM	114/117 (97%)	0.62	4 (3%) 42 10	48, 105, 157, 171	0
12	CM	113/117 (96%)	0.51	7 (6%) 20 5	44, 98, 149, 166	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AN	96/100 (96%)	0.52	2 (2%)	60	17	31, 77, 136, 171	0
13	CN	96/100 (96%)	0.50	2 (2%)	60	17	31, 78, 137, 161	0
14	AO	88/89 (98%)	0.16	1 (1%)	77	30	33, 67, 119, 173	0
14	CO	88/89 (98%)	0.02	0	100	100	18, 53, 105, 133	0
15	AP	82/82 (100%)	0.72	5 (6%)	21	5	38, 78, 140, 157	0
15	CP	80/82 (97%)	0.76	4 (5%)	28	6	16, 44, 124, 180	0
16	AQ	80/83 (96%)	0.52	1 (1%)	74	27	47, 86, 139, 155	0
16	CQ	81/83 (97%)	0.35	1 (1%)	75	29	25, 56, 117, 151	0
17	AR	55/74 (74%)	0.48	1 (1%)	65	20	27, 66, 125, 149	0
17	CR	55/74 (74%)	0.33	2 (3%)	41	9	24, 51, 105, 154	0
18	AS	79/91 (86%)	1.25	19 (24%)	1	1	61, 116, 158, 179	0
18	CS	80/91 (87%)	1.11	15 (18%)	2	1	54, 107, 165, 177	0
19	AT	85/86 (98%)	0.89	7 (8%)	12	3	52, 92, 133, 180	0
19	CT	85/86 (98%)	0.48	3 (3%)	42	10	24, 52, 103, 156	0
20	AB	218/240 (90%)	0.43	7 (3%)	45	11	29, 88, 139, 180	0
20	CB	218/240 (90%)	0.36	1 (0%)	88	51	40, 92, 143, 161	0
21	AU	51/70 (72%)	0.67	3 (5%)	22	5	36, 90, 150, 153	0
21	CU	51/70 (72%)	0.61	4 (7%)	13	4	26, 74, 136, 174	0
22	BA	117/120 (97%)	-0.33	3 (2%)	53	13	46, 80, 115, 168	0
22	DA	117/120 (97%)	-0.16	2 (1%)	67	21	35, 69, 110, 178	0
23	BB	2841/2904 (97%)	-0.14	45 (1%)	68	22	16, 56, 145, 180	0
23	DB	2841/2904 (97%)	-0.16	31 (1%)	77	30	7, 45, 142, 180	0
24	BI	141/141 (100%)	1.68	43 (30%)	1	1	62, 152, 180, 180	0
24	DI	141/141 (100%)	1.93	52 (36%)	1	0	85, 155, 180, 180	0
25	BC	271/272 (99%)	0.23	1 (0%)	90	57	9, 45, 87, 170	0
25	DC	271/272 (99%)	0.20	1 (0%)	90	57	5, 37, 75, 125	0
26	BD	209/209 (100%)	0.29	0	100	100	22, 66, 124, 167	0
26	DD	209/209 (100%)	0.27	1 (0%)	88	51	10, 44, 112, 139	0
27	BK	121/123 (98%)	0.53	2 (1%)	67	21	16, 67, 120, 154	0
27	DK	121/123 (98%)	0.18	0	100	100	8, 39, 93, 152	0
28	BP	114/114 (100%)	0.70	5 (4%)	33	7	27, 77, 122, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DP	114/114 (100%)	0.25	0 100 100	5, 42, 104, 160	0
29	BE	201/201 (100%)	0.34	3 (1%) 70 24	16, 67, 132, 148	0
29	DE	201/201 (100%)	0.32	4 (1%) 62 19	5, 65, 124, 156	0
30	BY	58/58 (100%)	0.46	0 100 100	42, 73, 129, 143	0
30	DY	58/58 (100%)	0.34	0 100 100	9, 58, 127, 150	0
31	B0	56/56 (100%)	0.34	2 (3%) 41 9	33, 71, 126, 141	0
31	D0	56/56 (100%)	0.23	1 (1%) 65 20	11, 45, 122, 170	0
32	B4	38/38 (100%)	0.60	0 100 100	23, 75, 134, 149	0
32	D4	38/38 (100%)	0.48	0 100 100	29, 54, 106, 125	0
33	B1	50/54 (92%)	0.56	3 (6%) 21 5	43, 79, 117, 132	0
33	D1	50/54 (92%)	0.42	1 (2%) 62 19	34, 66, 111, 135	0
34	B3	64/64 (100%)	0.45	0 100 100	31, 51, 91, 115	0
34	D3	64/64 (100%)	0.29	0 100 100	20, 40, 75, 110	0
35	BV	94/94 (100%)	0.41	1 (1%) 77 30	32, 90, 135, 169	0
35	DV	94/94 (100%)	0.35	0 100 100	28, 74, 131, 167	0
36	B2	46/46 (100%)	0.29	0 100 100	13, 40, 87, 121	0
36	D2	46/46 (100%)	0.16	0 100 100	11, 32, 67, 131	0
37	BL	143/144 (99%)	0.31	1 (0%) 84 42	13, 64, 117, 161	0
37	DL	143/144 (99%)	0.22	0 100 100	13, 54, 108, 133	0
38	BM	136/136 (100%)	0.53	4 (2%) 49 12	24, 68, 124, 174	0
38	DM	136/136 (100%)	0.26	0 100 100	13, 46, 109, 131	0
39	BX	63/63 (100%)	0.42	4 (6%) 19 5	20, 86, 141, 171	0
39	DX	63/63 (100%)	0.25	2 (3%) 45 11	38, 84, 134, 172	0
40	BH	149/149 (100%)	0.96	17 (11%) 6 2	37, 121, 160, 180	0
40	DH	149/149 (100%)	0.84	16 (10%) 6 2	20, 108, 147, 180	0
41	BJ	142/142 (100%)	0.44	3 (2%) 60 17	25, 73, 126, 137	0
41	DJ	142/142 (100%)	0.42	1 (0%) 84 42	19, 55, 104, 167	0
42	BN	120/127 (94%)	0.23	1 (0%) 83 39	20, 65, 117, 173	0
42	DN	120/127 (94%)	0.23	0 100 100	8, 40, 80, 125	0
43	BO	116/117 (99%)	0.82	7 (6%) 21 5	27, 82, 128, 179	0
43	DO	116/117 (99%)	0.46	5 (4%) 34 8	19, 68, 119, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BQ	117/117 (100%)	0.28	0 100 100	5, 64, 111, 163	0
44	DQ	117/117 (100%)	0.18	1 (0%) 81 37	14, 48, 96, 180	0
45	BS	110/110 (100%)	0.34	0 100 100	15, 58, 112, 161	0
45	DS	110/110 (100%)	0.29	1 (0%) 81 37	8, 42, 101, 132	0
46	BU	102/103 (99%)	0.57	6 (5%) 22 5	26, 75, 130, 171	0
46	DU	102/103 (99%)	0.58	3 (2%) 49 12	27, 83, 143, 180	0
47	BF	178/178 (100%)	0.72	15 (8%) 11 3	42, 113, 160, 180	0
47	DF	178/178 (100%)	0.57	8 (4%) 32 7	38, 97, 155, 180	0
48	BG	176/176 (100%)	0.61	10 (5%) 23 5	51, 103, 141, 162	0
48	DG	176/176 (100%)	0.51	8 (4%) 32 7	34, 91, 142, 169	0
49	BR	103/103 (100%)	0.87	9 (8%) 10 3	27, 86, 128, 157	0
49	DR	103/103 (100%)	0.37	1 (0%) 79 33	18, 76, 122, 148	0
50	BT	93/100 (93%)	0.79	6 (6%) 18 5	31, 70, 134, 164	0
50	DT	93/100 (93%)	0.81	8 (8%) 11 3	21, 66, 136, 173	0
51	BZ	77/78 (98%)	0.38	0 100 100	22, 50, 93, 129	0
51	DZ	77/78 (98%)	0.26	1 (1%) 74 27	17, 46, 95, 130	0
52	BW	79/84 (94%)	0.60	5 (6%) 19 5	29, 81, 126, 153	0
52	DW	79/84 (94%)	0.69	5 (6%) 19 5	20, 59, 119, 135	0
53	B6	185/185 (100%)	1.56	73 (39%) 1 0	33, 116, 167, 180	0
53	D6	185/185 (100%)	0.92	33 (17%) 2 1	19, 88, 157, 180	0
All	All	20787/21416 (97%)	0.19	621 (2%) 48 11	5, 63, 142, 180	0

The worst 5 of 621 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
15	AP	81	ALA	7.8
24	DI	99	LYS	7.7
24	DI	81	LYS	7.2
23	DB	1175	A	7.1
53	D6	42	LYS	6.7

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	DB	3058	1/1	2.05	117.19	145,145,145,145	0
54	MG	AA	2059	1/1	2.10	106.08	127,127,127,127	0
54	MG	CA	1626	1/1	0.31	53.00	42,42,42,42	1
54	MG	BB	3100	1/1	0.69	34.61	75,75,75,75	1
54	MG	AA	2025	1/1	0.72	34.16	54,54,54,54	1
54	MG	AA	2057	1/1	0.56	27.54	93,93,93,93	0
54	MG	DB	3066	1/1	0.28	24.80	63,63,63,63	1
54	MG	CA	1641	1/1	0.22	23.52	61,61,61,61	0
54	MG	AA	2017	1/1	0.28	16.68	75,75,75,75	0
54	MG	CA	1623	1/1	0.22	15.18	101,101,101,101	0
54	MG	AA	2047	1/1	0.48	11.39	126,126,126,126	0
54	MG	DB	3052	1/1	0.34	11.26	114,114,114,114	0
54	MG	BB	3093	1/1	0.65	11.00	38,38,38,38	1
54	MG	CA	1621	1/1	0.38	10.97	110,110,110,110	0
54	MG	AA	2032	1/1	0.40	10.53	64,64,64,64	0
54	MG	DB	3030	1/1	0.34	9.98	47,47,47,47	0
54	MG	AA	2023	1/1	0.28	8.27	32,32,32,32	1
54	MG	CA	1627	1/1	0.39	8.02	5,5,5,5	1
54	MG	AA	2056	1/1	0.32	7.40	46,46,46,46	0
54	MG	AA	2039	1/1	0.41	7.31	108,108,108,108	0
54	MG	CA	1615	1/1	0.18	6.72	121,121,121,121	0
54	MG	DB	3095	1/1	0.34	5.95	19,19,19,19	1
54	MG	AA	2026	1/1	0.16	4.00	5,5,5,5	1
54	MG	DB	3110	1/1	0.25	3.60	40,40,40,40	0
54	MG	BB	3087	1/1	0.24	3.50	100,100,100,100	0
54	MG	BB	3033	1/1	0.18	3.36	94,94,94,94	0
54	MG	DB	3013	1/1	0.23	2.72	47,47,47,47	0
54	MG	BB	3008	1/1	0.25	2.38	93,93,93,93	0
54	MG	AA	2027	1/1	0.21	2.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1658	1/1	0.19	1.70	33,33,33,33	0
54	MG	DB	3089	1/1	0.21	1.69	50,50,50,50	0
54	MG	DB	3077	1/1	0.18	1.48	51,51,51,51	0
54	MG	BB	3081	1/1	0.22	1.42	35,35,35,35	0
54	MG	BB	3040	1/1	0.20	1.24	60,60,60,60	0
54	MG	AA	2022	1/1	0.33	0.43	77,77,77,77	0
54	MG	DB	3011	1/1	0.18	0.38	16,16,16,16	0
54	MG	DB	3020	1/1	0.20	0.28	14,14,14,14	0
54	MG	BB	3057	1/1	0.27	0.28	37,37,37,37	0
54	MG	CA	1650	1/1	0.16	0.22	41,41,41,41	0
54	MG	DB	3037	1/1	0.17	0.21	45,45,45,45	0
54	MG	BB	3086	1/1	0.20	0.16	45,45,45,45	0
54	MG	CA	1602	1/1	0.20	0.12	34,34,34,34	0
54	MG	DB	3086	1/1	0.18	0.06	26,26,26,26	0
54	MG	DB	3022	1/1	0.17	0.02	32,32,32,32	0
54	MG	DB	3099	1/1	0.19	-0.06	15,15,15,15	0
54	MG	AA	2053	1/1	0.16	-0.14	46,46,46,46	0
54	MG	BB	3105	1/1	0.17	-0.22	65,65,65,65	0
54	MG	DB	3096	1/1	0.17	-0.24	30,30,30,30	0
54	MG	BB	3028	1/1	0.16	-0.28	46,46,46,46	0
54	MG	DB	3084	1/1	0.20	-0.30	34,34,34,34	0
54	MG	AA	2008	1/1	0.15	-0.40	94,94,94,94	0
54	MG	BB	3090	1/1	0.20	-0.48	78,78,78,78	0
54	MG	BB	3010	1/1	0.15	-0.49	70,70,70,70	0
54	MG	DB	3051	1/1	0.16	-0.57	25,25,25,25	0
54	MG	AA	2019	1/1	0.12	-0.62	120,120,120,120	0
54	MG	BB	3039	1/1	0.17	-0.66	43,43,43,43	0
54	MG	AA	2004	1/1	0.18	-0.68	36,36,36,36	0
54	MG	BB	3044	1/1	0.13	-0.69	70,70,70,70	0
54	MG	DB	3059	1/1	0.14	-0.70	65,65,65,65	1
54	MG	CE	201	1/1	0.20	-0.77	102,102,102,102	0
54	MG	DB	3111	1/1	0.19	-0.93	51,51,51,51	0
54	MG	BB	3043	1/1	0.16	-0.94	53,53,53,53	0
54	MG	DB	3062	1/1	0.09	-1.06	41,41,41,41	0
54	MG	CA	1659	1/1	0.10	-1.08	64,64,64,64	0
54	MG	BB	3016	1/1	0.16	-1.10	34,34,34,34	0
54	MG	DB	3034	1/1	0.19	-1.14	82,82,82,82	0
54	MG	CA	1614	1/1	0.13	-1.19	58,58,58,58	0
54	MG	CA	1654	1/1	0.14	-1.23	52,52,52,52	0
54	MG	DB	3057	1/1	0.09	-1.24	40,40,40,40	0
54	MG	BB	3099	1/1	0.12	-1.26	51,51,51,51	0
54	MG	DB	3063	1/1	0.16	-1.28	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3017	1/1	0.14	-1.33	59,59,59,59	0
54	MG	BB	3042	1/1	0.12	-1.33	123,123,123,123	0
54	MG	CA	1632	1/1	0.17	-1.33	41,41,41,41	0
54	MG	BB	3055	1/1	0.18	-1.34	41,41,41,41	0
54	MG	DB	3027	1/1	0.17	-1.43	27,27,27,27	0
54	MG	BB	3062	1/1	0.16	-1.43	41,41,41,41	0
54	MG	BB	3110	1/1	0.14	-1.46	56,56,56,56	0
54	MG	AA	2051	1/1	0.12	-1.49	80,80,80,80	0
54	MG	DB	3097	1/1	0.14	-1.50	32,32,32,32	0
54	MG	DB	3003	1/1	0.15	-1.56	29,29,29,29	0
54	MG	CA	1616	1/1	0.09	-1.58	42,42,42,42	0
54	MG	DB	3071	1/1	0.13	-1.61	57,57,57,57	0
54	MG	DB	3047	1/1	0.16	-1.62	13,13,13,13	0
54	MG	AA	2015	1/1	0.10	-1.64	86,86,86,86	0
55	ZN	B4	101	1/1	0.09	-1.69	55,55,55,55	0
54	MG	DB	3060	1/1	0.10	-1.76	89,89,89,89	0
54	MG	DB	3094	1/1	0.08	-1.76	39,39,39,39	0
54	MG	AA	2006	1/1	0.06	-1.79	71,71,71,71	0
54	MG	BB	3085	1/1	0.15	-1.80	56,56,56,56	0
54	MG	AA	2002	1/1	0.14	-1.83	85,85,85,85	0
54	MG	DB	3078	1/1	0.11	-1.85	45,45,45,45	0
54	MG	AA	2036	1/1	0.09	-1.87	65,65,65,65	0
54	MG	CA	1636	1/1	0.12	-1.89	63,63,63,63	0
54	MG	DB	3100	1/1	0.10	-1.91	17,17,17,17	0
54	MG	BB	3082	1/1	0.15	-1.91	38,38,38,38	0
54	MG	CA	1639	1/1	0.12	-1.94	24,24,24,24	0
54	MG	BB	3021	1/1	0.12	-1.94	43,43,43,43	0
54	MG	BB	3054	1/1	0.09	-1.95	57,57,57,57	0
54	MG	BB	3009	1/1	0.15	-1.96	87,87,87,87	0
54	MG	AA	2013	1/1	0.10	-1.98	85,85,85,85	0
54	MG	CA	1624	1/1	0.08	-2.06	22,22,22,22	0
54	MG	BB	3025	1/1	0.12	-2.12	49,49,49,49	0
55	ZN	D4	101	1/1	0.07	-2.13	55,55,55,55	0
54	MG	DB	3006	1/1	0.14	-2.15	26,26,26,26	0
54	MG	BB	3047	1/1	0.11	-2.17	70,70,70,70	0
54	MG	CA	1638	1/1	0.12	-2.18	90,90,90,90	0
54	MG	BB	3046	1/1	0.16	-2.19	69,69,69,69	0
54	MG	DB	3068	1/1	0.15	-2.21	8,8,8,8	0
54	MG	BB	3037	1/1	0.10	-2.24	23,23,23,23	0
54	MG	CA	1642	1/1	0.05	-2.24	63,63,63,63	0
54	MG	CA	1617	1/1	0.11	-2.25	21,21,21,21	0
54	MG	CA	1633	1/1	0.12	-2.26	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DB	3045	1/1	0.09	-2.29	61,61,61,61	0
54	MG	BB	3107	1/1	0.07	-2.30	31,31,31,31	0
54	MG	DB	3048	1/1	0.11	-2.31	41,41,41,41	0
54	MG	AA	2011	1/1	0.09	-2.32	45,45,45,45	0
54	MG	DB	3026	1/1	0.19	-2.35	41,41,41,41	0
54	MG	DB	3012	1/1	0.17	-2.38	23,23,23,23	0
54	MG	CA	1609	1/1	0.10	-2.41	56,56,56,56	0
54	MG	BB	3029	1/1	0.11	-2.41	28,28,28,28	0
54	MG	AA	2020	1/1	0.08	-2.44	84,84,84,84	0
54	MG	BB	3034	1/1	0.13	-2.46	35,35,35,35	0
54	MG	BB	3096	1/1	0.08	-2.54	37,37,37,37	0
54	MG	AA	2003	1/1	0.12	-2.56	31,31,31,31	0
54	MG	BB	3075	1/1	0.14	-2.58	37,37,37,37	0
54	MG	DB	3029	1/1	0.15	-2.64	67,67,67,67	0
54	MG	CA	1612	1/1	0.07	-2.72	46,46,46,46	0
54	MG	DB	3064	1/1	0.14	-2.73	37,37,37,37	0
54	MG	BB	3097	1/1	0.12	-2.80	101,101,101,101	0
54	MG	AA	2009	1/1	0.12	-2.81	21,21,21,21	0
54	MG	BB	3003	1/1	0.10	-2.82	47,47,47,47	0
54	MG	AA	2018	1/1	0.08	-2.85	78,78,78,78	0
54	MG	BB	3032	1/1	0.12	-2.85	34,34,34,34	0
54	MG	CA	1613	1/1	0.07	-2.86	39,39,39,39	0
54	MG	BB	3058	1/1	0.14	-2.88	33,33,33,33	0
54	MG	AA	2010	1/1	0.07	-2.89	36,36,36,36	0
54	MG	DB	3008	1/1	0.14	-2.92	33,33,33,33	0
54	MG	CA	1647	1/1	0.07	-2.96	102,102,102,102	0
54	MG	DB	3069	1/1	0.14	-2.99	21,21,21,21	0
54	MG	CA	1656	1/1	0.09	-2.99	22,22,22,22	0
54	MG	AA	2055	1/1	0.10	-2.99	54,54,54,54	0
54	MG	BB	3074	1/1	0.14	-3.02	21,21,21,21	0
54	MG	AA	2042	1/1	0.12	-3.02	32,32,32,32	0
54	MG	DB	3049	1/1	0.12	-3.04	26,26,26,26	0
54	MG	BB	3006	1/1	0.08	-3.05	28,28,28,28	0
54	MG	AA	2035	1/1	0.09	-3.08	102,102,102,102	0
54	MG	CA	1643	1/1	0.07	-3.09	20,20,20,20	0
54	MG	CA	1625	1/1	0.09	-3.10	19,19,19,19	0
54	MG	AA	2024	1/1	0.10	-3.12	61,61,61,61	0
54	MG	BB	3091	1/1	0.10	-3.12	31,31,31,31	0
54	MG	DB	3018	1/1	0.12	-3.16	23,23,23,23	0
54	MG	BB	3049	1/1	0.14	-3.16	26,26,26,26	0
54	MG	AA	2030	1/1	0.10	-3.17	102,102,102,102	0
54	MG	AA	2049	1/1	0.09	-3.18	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3002	1/1	0.11	-3.19	12,12,12,12	0
54	MG	BB	3092	1/1	0.05	-3.21	51,51,51,51	0
54	MG	CA	1644	1/1	0.11	-3.21	52,52,52,52	0
54	MG	BB	3007	1/1	0.10	-3.23	74,74,74,74	0
54	MG	DB	3023	1/1	0.09	-3.24	33,33,33,33	0
54	MG	BB	3098	1/1	0.13	-3.24	30,30,30,30	0
54	MG	AA	2040	1/1	0.11	-3.27	56,56,56,56	0
54	MG	CA	1653	1/1	0.05	-3.28	55,55,55,55	0
54	MG	BB	3031	1/1	0.11	-3.33	46,46,46,46	0
54	MG	AA	2045	1/1	0.07	-3.33	63,63,63,63	0
54	MG	BB	3104	1/1	0.14	-3.33	20,20,20,20	0
54	MG	BB	3014	1/1	0.13	-3.33	58,58,58,58	0
54	MG	BB	3059	1/1	0.12	-3.34	32,32,32,32	0
54	MG	AA	2038	1/1	0.10	-3.34	63,63,63,63	0
54	MG	BB	3088	1/1	0.09	-3.34	75,75,75,75	0
54	MG	BB	3063	1/1	0.14	-3.36	52,52,52,52	0
54	MG	AA	2048	1/1	0.10	-3.37	27,27,27,27	0
54	MG	CA	1637	1/1	0.09	-3.38	53,53,53,53	0
54	MG	BB	3109	1/1	0.10	-3.38	42,42,42,42	0
54	MG	BB	3073	1/1	0.16	-3.41	70,70,70,70	0
54	MG	BB	3027	1/1	0.12	-3.42	34,34,34,34	0
54	MG	CA	1640	1/1	0.11	-3.43	43,43,43,43	0
54	MG	DB	3007	1/1	0.09	-3.47	30,30,30,30	0
54	MG	CA	1649	1/1	0.07	-3.47	80,80,80,80	0
54	MG	DB	3050	1/1	0.05	-3.47	70,70,70,70	0
54	MG	CA	1620	1/1	0.07	-3.48	58,58,58,58	0
54	MG	CA	1605	1/1	0.13	-3.48	38,38,38,38	0
54	MG	DB	3081	1/1	0.11	-3.50	17,17,17,17	0
54	MG	BB	3020	1/1	0.14	-3.54	20,20,20,20	0
54	MG	BB	3053	1/1	0.07	-3.58	61,61,61,61	0
54	MG	AA	2043	1/1	0.10	-3.61	42,42,42,42	0
54	MG	DB	3035	1/1	0.10	-3.62	57,57,57,57	0
54	MG	CA	1646	1/1	0.10	-3.66	46,46,46,46	0
54	MG	DB	3090	1/1	0.07	-3.68	49,49,49,49	0
54	MG	DB	3102	1/1	0.11	-3.70	15,15,15,15	0
54	MG	DB	3009	1/1	0.15	-3.70	17,17,17,17	0
54	MG	BB	3038	1/1	0.09	-3.73	98,98,98,98	0
54	MG	DB	3088	1/1	0.12	-3.74	28,28,28,28	0
54	MG	BB	3019	1/1	0.08	-3.74	37,37,37,37	0
54	MG	BB	3036	1/1	0.08	-3.77	39,39,39,39	0
54	MG	BB	3024	1/1	0.10	-3.80	47,47,47,47	0
54	MG	BB	3012	1/1	0.10	-3.80	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BB	3060	1/1	0.11	-3.83	47,47,47,47	0
54	MG	CA	1601	1/1	0.10	-3.84	9,9,9,9	0
54	MG	DB	3072	1/1	0.10	-3.88	23,23,23,23	0
54	MG	DB	3053	1/1	0.09	-3.91	28,28,28,28	0
54	MG	AA	2034	1/1	0.10	-3.91	40,40,40,40	0
54	MG	BB	3001	1/1	0.08	-3.93	35,35,35,35	0
54	MG	AA	2044	1/1	0.08	-3.95	47,47,47,47	0
54	MG	BB	3018	1/1	0.14	-3.96	45,45,45,45	0
54	MG	DB	3032	1/1	0.12	-3.97	33,33,33,33	0
54	MG	DB	3024	1/1	0.12	-3.98	30,30,30,30	0
54	MG	DB	3054	1/1	0.07	-3.99	25,25,25,25	0
54	MG	CA	1608	1/1	0.11	-4.00	106,106,106,106	0
54	MG	DB	3065	1/1	0.07	-4.02	12,12,12,12	0
54	MG	DB	3091	1/1	0.11	-4.05	29,29,29,29	0
54	MG	DB	3085	1/1	0.11	-4.13	5,5,5,5	0
54	MG	CA	1634	1/1	0.11	-4.14	32,32,32,32	0
54	MG	AA	2028	1/1	0.08	-4.14	66,66,66,66	0
54	MG	DB	3042	1/1	0.10	-4.22	45,45,45,45	0
54	MG	DB	3055	1/1	0.12	-4.23	17,17,17,17	0
54	MG	DB	3073	1/1	0.11	-4.27	29,29,29,29	0
54	MG	DB	3056	1/1	0.10	-4.30	11,11,11,11	0
54	MG	DB	3017	1/1	0.12	-4.30	18,18,18,18	0
54	MG	AA	2033	1/1	0.07	-4.31	40,40,40,40	0
54	MG	BB	3067	1/1	0.09	-4.32	45,45,45,45	0
54	MG	DB	3038	1/1	0.15	-4.44	26,26,26,26	0
54	MG	DB	3025	1/1	0.12	-4.46	28,28,28,28	0
54	MG	BB	3013	1/1	0.08	-4.47	36,36,36,36	0
54	MG	DB	3036	1/1	0.12	-4.51	25,25,25,25	0
54	MG	BB	3045	1/1	0.05	-4.52	41,41,41,41	0
54	MG	BB	3069	1/1	0.08	-4.52	17,17,17,17	0
54	MG	DB	3021	1/1	0.12	-4.61	21,21,21,21	0
54	MG	BB	3094	1/1	0.09	-4.62	21,21,21,21	0
54	MG	CA	1622	1/1	0.08	-4.65	46,46,46,46	0
54	MG	DB	3041	1/1	0.12	-4.70	36,36,36,36	0
54	MG	BB	3051	1/1	0.10	-4.70	35,35,35,35	0
54	MG	DB	3015	1/1	0.10	-4.72	60,60,60,60	0
54	MG	DB	3083	1/1	0.13	-4.73	72,72,72,72	0
54	MG	AA	2007	1/1	0.07	-4.73	42,42,42,42	0
54	MG	BB	3011	1/1	0.10	-4.76	30,30,30,30	0
54	MG	AA	2001	1/1	0.07	-4.81	29,29,29,29	0
54	MG	CA	1657	1/1	0.11	-4.82	62,62,62,62	0
54	MG	BB	3041	1/1	0.08	-4.88	22,22,22,22	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	0.08	-4.96	30,30,30,30	0
54	MG	BB	3083	1/1	0.10	-4.97	30,30,30,30	0
54	MG	BB	3026	1/1	0.08	-4.98	28,28,28,28	0
54	MG	DB	3109	1/1	0.09	-4.99	35,35,35,35	0
54	MG	BB	3106	1/1	0.09	-5.00	36,36,36,36	0
54	MG	BB	3070	1/1	0.09	-5.06	35,35,35,35	0
54	MG	DB	3010	1/1	0.09	-5.09	19,19,19,19	0
54	MG	CA	1629	1/1	0.08	-5.11	20,20,20,20	1
54	MG	CA	1648	1/1	0.15	-5.14	47,47,47,47	0
54	MG	BB	3035	1/1	0.10	-5.17	41,41,41,41	0
54	MG	CA	1618	1/1	0.07	-5.27	18,18,18,18	0
54	MG	DB	3087	1/1	0.11	-5.30	54,54,54,54	0
54	MG	DB	3076	1/1	0.06	-5.30	17,17,17,17	0
54	MG	DB	3074	1/1	0.09	-5.42	30,30,30,30	0
54	MG	BB	3061	1/1	0.07	-5.43	38,38,38,38	0
54	MG	BB	3005	1/1	0.10	-5.43	24,24,24,24	0
54	MG	DB	3039	1/1	0.08	-5.44	34,34,34,34	0
54	MG	DB	3014	1/1	0.06	-5.45	21,21,21,21	0
54	MG	BB	3108	1/1	0.10	-5.46	37,37,37,37	0
54	MG	CA	1604	1/1	0.09	-5.63	36,36,36,36	0
54	MG	DB	3004	1/1	0.14	-5.63	17,17,17,17	0
54	MG	DB	3070	1/1	0.12	-5.67	26,26,26,26	0
54	MG	DB	3101	1/1	0.15	-5.74	5,5,5,5	0
54	MG	AA	2016	1/1	0.09	-5.80	50,50,50,50	0
54	MG	CA	1645	1/1	0.10	-5.81	45,45,45,45	0
54	MG	BB	3030	1/1	0.07	-5.88	40,40,40,40	0
54	MG	DB	3092	1/1	0.11	-5.91	65,65,65,65	0
54	MG	BB	3071	1/1	0.07	-5.94	25,25,25,25	0
54	MG	DB	3108	1/1	0.10	-5.97	11,11,11,11	0
54	MG	CA	1660	1/1	0.07	-6.00	96,96,96,96	0
54	MG	BB	3023	1/1	0.07	-6.05	23,23,23,23	0
54	MG	CA	1619	1/1	0.11	-6.05	51,51,51,51	0
54	MG	DB	3082	1/1	0.11	-6.10	21,21,21,21	0
54	MG	CA	1655	1/1	0.08	-6.14	28,28,28,28	0
54	MG	BB	3015	1/1	0.09	-6.22	40,40,40,40	0
54	MG	CA	1606	1/1	0.09	-6.24	59,59,59,59	0
54	MG	BB	3103	1/1	0.09	-6.30	20,20,20,20	0
54	MG	DB	3019	1/1	0.07	-6.33	21,21,21,21	0
54	MG	DB	3046	1/1	0.05	-6.42	22,22,22,22	0
54	MG	BB	3052	1/1	0.08	-6.43	25,25,25,25	0
54	MG	BB	3072	1/1	0.09	-6.45	44,44,44,44	0
54	MG	BB	3084	1/1	0.14	-6.47	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	CA	1611	1/1	0.10	-6.56	81,81,81,81	0
54	MG	CA	1635	1/1	0.07	-6.76	55,55,55,55	0
54	MG	DB	3028	1/1	0.12	-6.81	29,29,29,29	0
54	MG	AA	2029	1/1	0.07	-6.89	40,40,40,40	0
54	MG	AA	2041	1/1	0.04	-6.93	40,40,40,40	0
54	MG	BB	3101	1/1	0.09	-7.02	22,22,22,22	0
54	MG	BB	3089	1/1	0.08	-7.05	38,38,38,38	0
54	MG	BB	3077	1/1	0.07	-7.13	36,36,36,36	0
54	MG	DB	3103	1/1	0.09	-7.26	26,26,26,26	0
54	MG	DB	3043	1/1	0.09	-7.35	8,8,8,8	0
54	MG	CA	1631	1/1	0.09	-7.41	38,38,38,38	0
54	MG	DB	3044	1/1	0.07	-7.46	12,12,12,12	0
54	MG	DB	3080	1/1	0.14	-7.47	29,29,29,29	0
54	MG	BB	3066	1/1	0.06	-7.64	21,21,21,21	0
54	MG	BB	3022	1/1	0.05	-7.71	44,44,44,44	0
54	MG	AA	2012	1/1	0.06	-7.71	63,63,63,63	0
54	MG	BB	3076	1/1	0.06	-7.75	43,43,43,43	0
54	MG	AA	2060	1/1	0.05	-7.94	75,75,75,75	0
54	MG	BB	3078	1/1	0.10	-7.96	47,47,47,47	0
54	MG	DB	3079	1/1	0.07	-7.96	34,34,34,34	0
54	MG	CA	1630	1/1	0.11	-7.99	39,39,39,39	0
54	MG	BB	3080	1/1	0.11	-8.27	57,57,57,57	0
54	MG	DB	3001	1/1	0.10	-8.27	9,9,9,9	0
54	MG	DB	3067	1/1	0.08	-8.35	18,18,18,18	0
54	MG	AA	2046	1/1	0.10	-8.37	46,46,46,46	0
54	MG	DB	3002	1/1	0.06	-8.61	11,11,11,11	0
54	MG	CA	1610	1/1	0.07	-8.73	56,56,56,56	0
54	MG	BB	3064	1/1	0.10	-8.85	31,31,31,31	0
54	MG	DB	3005	1/1	0.06	-8.86	56,56,56,56	0
54	MG	AA	2052	1/1	0.07	-9.28	50,50,50,50	0
54	MG	DB	3093	1/1	0.11	-9.38	6,6,6,6	0
54	MG	DB	3016	1/1	0.09	-9.55	28,28,28,28	0
54	MG	DB	3105	1/1	0.07	-9.61	32,32,32,32	0
54	MG	CA	1607	1/1	0.06	-9.81	37,37,37,37	0
54	MG	BB	3056	1/1	0.07	-10.13	31,31,31,31	0
54	MG	BB	3102	1/1	0.08	-10.63	38,38,38,38	0
54	MG	DB	3061	1/1	0.04	-10.80	51,51,51,51	0
54	MG	AA	2014	1/1	0.10	-10.87	101,101,101,101	0
54	MG	DB	3075	1/1	0.05	-10.89	33,33,33,33	0
54	MG	AA	2058	1/1	0.06	-10.90	88,88,88,88	0
54	MG	CA	1628	1/1	0.12	-11.00	38,38,38,38	0
54	MG	BB	3095	1/1	0.08	-11.14	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	DB	3107	1/1	0.07	-11.14	34,34,34,34	0
54	MG	AA	2031	1/1	0.08	-11.28	51,51,51,51	0
54	MG	DB	3040	1/1	0.09	-11.55	9,9,9,9	0
54	MG	CA	1661	1/1	0.06	-11.71	49,49,49,49	0
54	MG	BB	3065	1/1	0.07	-11.71	40,40,40,40	0
54	MG	DB	3098	1/1	0.11	-12.61	29,29,29,29	0
54	MG	BB	3004	1/1	0.09	-13.01	52,52,52,52	0
54	MG	CA	1603	1/1	0.11	-13.19	29,29,29,29	0
54	MG	BB	3050	1/1	0.10	-13.22	28,28,28,28	0
54	MG	AA	2054	1/1	0.04	-14.70	49,49,49,49	0
54	MG	BB	3079	1/1	0.11	-15.77	63,63,63,63	0
54	MG	DB	3031	1/1	0.09	-17.84	17,17,17,17	0
54	MG	DB	3104	1/1	0.09	-17.99	28,28,28,28	0
54	MG	AA	2021	1/1	0.07	-18.12	52,52,52,52	0
54	MG	CA	1651	1/1	0.05	-21.08	50,50,50,50	0
54	MG	DB	3106	1/1	0.10	-22.42	9,9,9,9	0
54	MG	CA	1652	1/1	0.10	-24.33	54,54,54,54	0
54	MG	BB	3068	1/1	0.11	-29.90	43,43,43,43	0
54	MG	DB	3033	1/1	0.11	-35.10	20,20,20,20	0
54	MG	AA	2005	1/1	0.07	-42.18	36,36,36,36	0
54	MG	AA	2050	1/1	0.14	-	101,101,101,101	0
54	MG	AA	2037	1/1	1.47	-	139,139,139,139	0

6.5 Other polymers ⓘ

There are no such residues in this entry.