



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:51 PM BST

PDB ID : 4V6E
Title : Crystal structure of the E. coli 70S ribosome in an intermediate state of ratcheting
Authors : Zhang, W.; Dunkle, J.A.; Cate, J.H.D.
Deposited on : 2009-06-28
Resolution : 3.71 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>

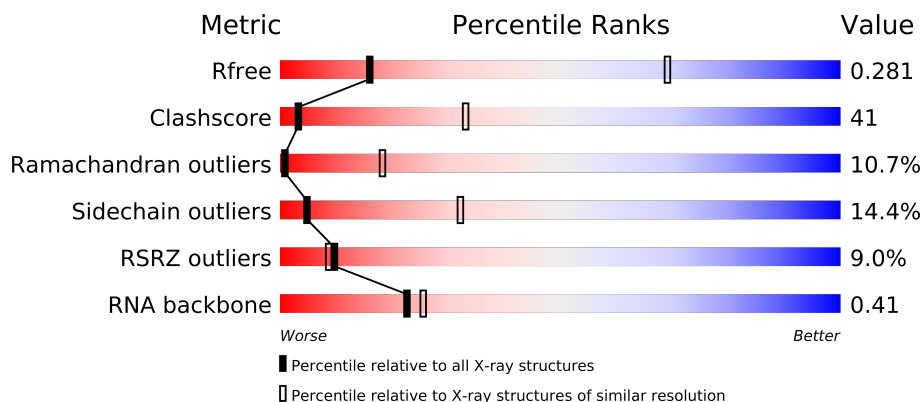
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.71 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	1103 (4.04-3.40)
Clashscore	79885	1026 (3.98-3.46)
Ramachandran outliers	78287	1082 (4.00-3.44)
Sidechain outliers	78261	1075 (4.00-3.44)
RSRZ outliers	66119	1104 (4.04-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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

Mol	Chain	Length	Quality of chain
1	AB	241	
1	CB	241	
2	AC	233	
2	CC	233	
3	AD	206	
3	CD	206	
4	AE	167	
4	CE	167	
5	AF	135	
5	CF	135	
6	AG	179	
6	CG	179	

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Mol	Chain	Length	Quality of chain
7	AH	130	
7	CH	130	
8	AI	130	
8	CI	130	
9	AJ	103	
9	CJ	103	
10	AK	129	
10	CK	129	
11	AL	124	
11	CL	124	
12	AM	118	
12	CM	118	
13	AN	101	
13	CN	101	
14	AO	89	
14	CO	89	
15	AP	82	
15	CP	82	
16	AQ	84	
16	CQ	84	
17	AR	75	
17	CR	75	
18	AS	92	
18	CS	92	
19	AT	87	
19	CT	87	
20	AU	71	
20	CU	71	
21	AA	1533	
22	AV	17	
22	AX	17	
22	CV	17	
22	CX	17	
23	AW	6	
23	CW	6	
24	BA	2903	
24	DA	2903	
25	BB	118	
26	BC	273	
26	DC	273	
27	BD	209	
27	DD	209	

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Mol	Chain	Length	Quality of chain
28	BE	201	
28	DE	201	
29	BF	179	
29	DF	179	
30	BG	177	
30	DG	177	
31	BH	149	
31	DH	149	
32	BI	142	
32	DI	142	
33	BJ	142	
33	DJ	142	
34	BK	123	
34	DK	123	
35	BL	144	
35	DL	144	
36	BM	136	
36	DM	136	
37	BN	127	
37	DN	127	
38	BO	117	
38	DO	117	
39	BP	115	
39	DP	115	
40	BQ	118	
40	DQ	118	
41	BR	103	
41	DR	103	
42	BS	110	
42	DS	110	
43	BT	100	
43	DT	100	
44	BU	104	
44	DU	104	
45	BV	94	
45	DV	94	
46	BW	85	
46	DW	85	
47	BX	78	
47	DX	78	
48	BY	63	
48	DY	63	

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Mol	Chain	Length	Quality of chain
49	BZ	59	
49	DZ	59	
50	B0	57	
50	D0	57	
51	B1	55	
51	D1	55	
52	B2	46	
52	D2	46	
53	B3	65	
53	D3	65	
54	B4	38	
54	D4	38	
55	CA	1530	
56	DB	117	

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

Mol	Type	Chain	Res	Geometry	Electron density
57	MG	AA	1602	-	X
57	MG	AA	1605	-	X
57	MG	AA	1607	-	X
57	MG	AA	1610	-	X
57	MG	AA	1619	-	X
57	MG	AA	1621	-	X
57	MG	AA	1624	-	X
57	MG	AA	1625	-	X
57	MG	AA	1626	-	X
57	MG	AA	1627	-	X
57	MG	AA	1628	-	X
57	MG	AA	1629	-	X
57	MG	AA	1636	-	X
57	MG	AA	1637	-	X
57	MG	AA	1641	-	X
57	MG	AA	1642	-	X
57	MG	BA	3002	-	X
57	MG	BA	3007	-	X
57	MG	BA	3011	-	X
57	MG	BA	3014	-	X
57	MG	BA	3015	-	X
57	MG	BA	3016	-	X
57	MG	BA	3020	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BA	3021	-	X
57	MG	BA	3022	-	X
57	MG	BA	3026	-	X
57	MG	BA	3028	-	X
57	MG	BA	3030	-	X
57	MG	BA	3031	-	X
57	MG	BA	3035	-	X
57	MG	BA	3037	-	X
57	MG	BA	3041	-	X
57	MG	BA	3045	-	X
57	MG	BA	3056	-	X
57	MG	BA	3057	-	X
57	MG	BA	3058	-	X
57	MG	BA	3060	-	X
57	MG	BA	3061	-	X
57	MG	BA	3062	-	X
57	MG	BA	3071	-	X
57	MG	BA	3072	-	X
57	MG	BA	3084	-	X
57	MG	BA	3085	-	X
57	MG	BA	3088	-	X
57	MG	BA	3093	-	X
57	MG	BA	3096	-	X
57	MG	BA	3098	-	X
57	MG	BA	3112	-	X
57	MG	BA	3115	-	X
57	MG	BA	3119	-	X
57	MG	BA	3124	-	X
57	MG	BA	3125	-	X
57	MG	BA	3126	-	X
57	MG	BA	3131	-	X
57	MG	BA	3133	-	X
57	MG	BA	3135	-	X
57	MG	BA	3136	-	X
57	MG	BB	201	-	X
57	MG	CA	1610	-	X
57	MG	CA	1611	-	X
57	MG	CA	1614	-	X
57	MG	CA	1615	-	X
57	MG	CA	1619	-	X
57	MG	CA	1620	-	X
57	MG	CA	1623	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
57	MG	CA	1625	-	X
57	MG	CA	1626	-	X
57	MG	CA	1627	-	X
57	MG	CA	1628	-	X
57	MG	CA	1636	-	X
57	MG	CA	1637	-	X
57	MG	CA	1640	-	X
57	MG	D4	101	-	X
57	MG	DA	3001	-	X
57	MG	DA	3002	-	X
57	MG	DA	3004	-	X
57	MG	DA	3005	-	X
57	MG	DA	3007	-	X
57	MG	DA	3011	-	X
57	MG	DA	3015	-	X
57	MG	DA	3016	-	X
57	MG	DA	3020	-	X
57	MG	DA	3021	-	X
57	MG	DA	3022	-	X
57	MG	DA	3026	-	X
57	MG	DA	3028	-	X
57	MG	DA	3036	-	X
57	MG	DA	3038	-	X
57	MG	DA	3041	-	X
57	MG	DA	3045	-	X
57	MG	DA	3046	-	X
57	MG	DA	3051	-	X
57	MG	DA	3053	-	X
57	MG	DA	3054	-	X
57	MG	DA	3058	-	X
57	MG	DA	3059	-	X
57	MG	DA	3060	-	X
57	MG	DA	3062	-	X
57	MG	DA	3063	-	X
57	MG	DA	3064	-	X
57	MG	DA	3071	-	X
57	MG	DA	3072	-	X
57	MG	DA	3074	-	X
57	MG	DA	3075	-	X
57	MG	DA	3076	-	X
57	MG	DA	3078	-	X
57	MG	DA	3082	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
57	MG	DA	3086	-	X
57	MG	DA	3088	-	X
57	MG	DA	3091	-	X
57	MG	DA	3092	-	X
57	MG	DA	3094	-	X
57	MG	DA	3097	-	X
57	MG	DA	3104	-	X
57	MG	DA	3106	-	X
57	MG	DA	3108	-	X
57	MG	DA	3109	-	X
57	MG	DA	3114	-	X
57	MG	DA	3117	-	X
57	MG	DA	3121	-	X
57	MG	DA	3122	-	X
57	MG	DA	3124	-	X
57	MG	DA	3125	-	X
57	MG	DA	3127	-	X
57	MG	DA	3128	-	X
57	MG	DA	3129	-	X
57	MG	DA	3131	-	X
57	MG	DJ	201	-	X

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 286150 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 protein called 30S ribosomal protein S2.

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

- 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	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
6	CG	150	Total	C	N	O	S	0	0	0
			1174	730	226	214	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	95	Total	C	N	O	S	0	0	0
			769	480	159	127	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	80	Total	C	N	O	S	0	0	0
			648	411	121	113	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	79	Total	C	N	O	S	0	0	0
			637	408	120	107	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 S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
20	CU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 22 is a RNA chain called P-site tRNA ASL fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	AX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CV	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
22	CX	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 23 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			
23	CW	6	Total	C	N	O	P	0	0	0
			120	54	12	48	6			

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
24	DA	2841	Total	C	N	O	P	0	0	0
			60995	27210	11229	19715	2841			

- Molecule 25 is a RNA chain called 5S rRNA.

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

- Molecule 26 is a protein called 50S ribosomal protein L2.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L3.

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

- Molecule 28 is a protein called 50S ribosomal protein L4.

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

- Molecule 29 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
29	DF	178	Total	C	N	O	S	0	0	0
			1420	905	251	258	6			

- Molecule 30 is a protein called 50S ribosomal protein L6.

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

- Molecule 31 is a protein called 50S ribosomal protein L9.

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

- Molecule 32 is a protein called 50S ribosomal protein L11.

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
34	DK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 35 is a protein called 50S ribosomal protein L15.

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

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called 50S ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

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

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

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

- Molecule 49 is a protein called 50S ribosomal protein L30.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L33.

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

- Molecule 52 is a protein called 50S ribosomal protein L34.

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

- Molecule 53 is a protein called 50S ribosomal protein L35.

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

- Molecule 54 is a protein called 50S ribosomal protein L36.

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

- Molecule 55 is a RNA chain called 16S rRNA.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	DB	117	Total	C	N	O	P	0	0	0
			2507	1116	459	815	117			

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	BB	4	Total	Mg	0	0
			4	4		
57	BA	136	Total	Mg	0	0
			136	136		
57	CA	42	Total	Mg	0	0
			42	42		
57	DJ	1	Total	Mg	0	0
			1	1		
57	BD	1	Total	Mg	0	0
			1	1		
57	AA	43	Total	Mg	0	0
			43	43		
57	D4	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DA	132	Total 132	Mg 132	0	0
57	DC	2	Total 2	Mg 2	0	0
57	DB	1	Total 1	Mg 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AE	1	Total 1	O 1	0	0
59	AL	3	Total 3	O 3	0	0
59	AN	6	Total 6	O 6	0	0
59	AT	1	Total 1	O 1	0	0
59	AU	1	Total 1	O 1	0	0
59	AA	196	Total 196	O 196	0	0
59	BA	615	Total 615	O 615	0	0
59	BB	20	Total 20	O 20	0	0
59	BC	8	Total 8	O 8	0	0
59	BD	3	Total 3	O 3	0	0
59	BE	1	Total 1	O 1	0	0
59	BL	3	Total 3	O 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BN	3	Total 3	O 3	0	0
59	BT	1	Total 1	O 1	0	0
59	B2	1	Total 1	O 1	0	0
59	B3	3	Total 3	O 3	0	0
59	B4	2	Total 2	O 2	0	0
59	CE	4	Total 4	O 4	0	0
59	CI	1	Total 1	O 1	0	0
59	CL	1	Total 1	O 1	0	0
59	CN	2	Total 2	O 2	0	0
59	CT	2	Total 2	O 2	0	0
59	CU	2	Total 2	O 2	0	0
59	CA	195	Total 195	O 195	0	0
59	DA	600	Total 600	O 600	0	0
59	DB	4	Total 4	O 4	0	0
59	DC	12	Total 12	O 12	0	0
59	DD	2	Total 2	O 2	0	0
59	DE	3	Total 3	O 3	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	6	Total 6	O 6	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0

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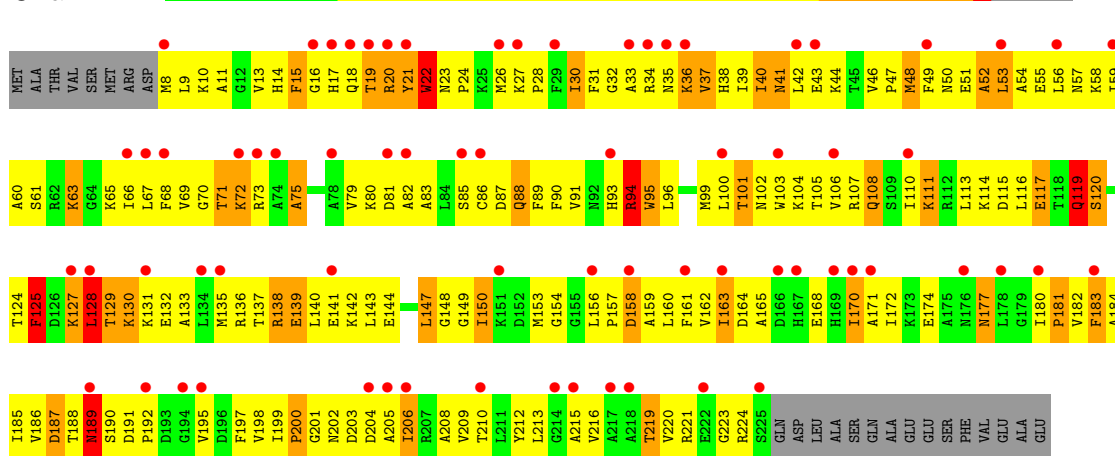
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DU	1	Total 1	O 1	0	0
59	DV	1	Total 1	O 1	0	0
59	D2	1	Total 1	O 1	0	0
59	D3	1	Total 1	O 1	0	0
59	D4	5	Total 5	O 5	0	0

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.

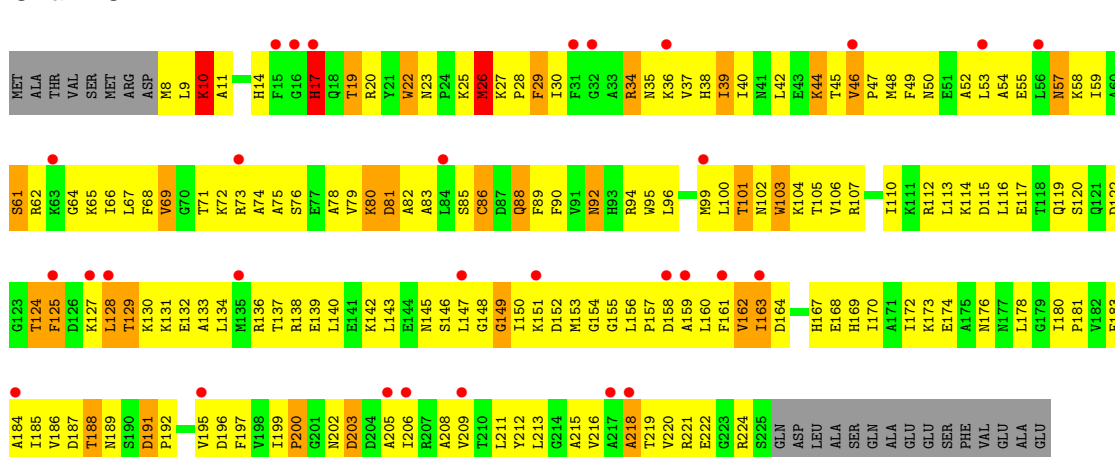
- Molecule 1: 30S ribosomal protein S2

Chain AB:



- Molecule 1: 30S ribosomal protein S2

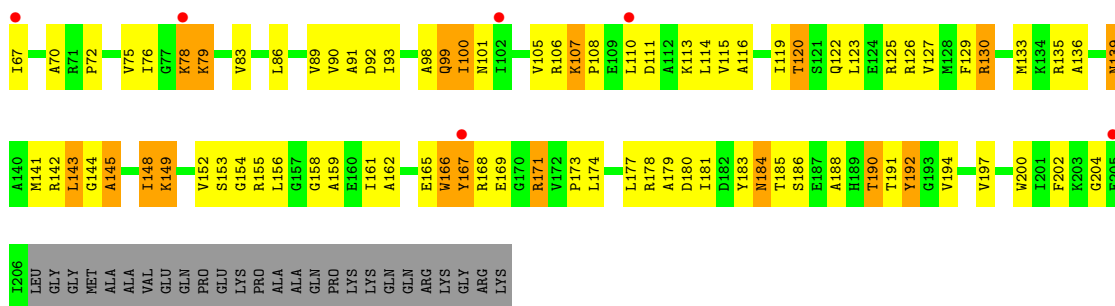
Chain CB:



- Molecule 2: 30S ribosomal protein S3

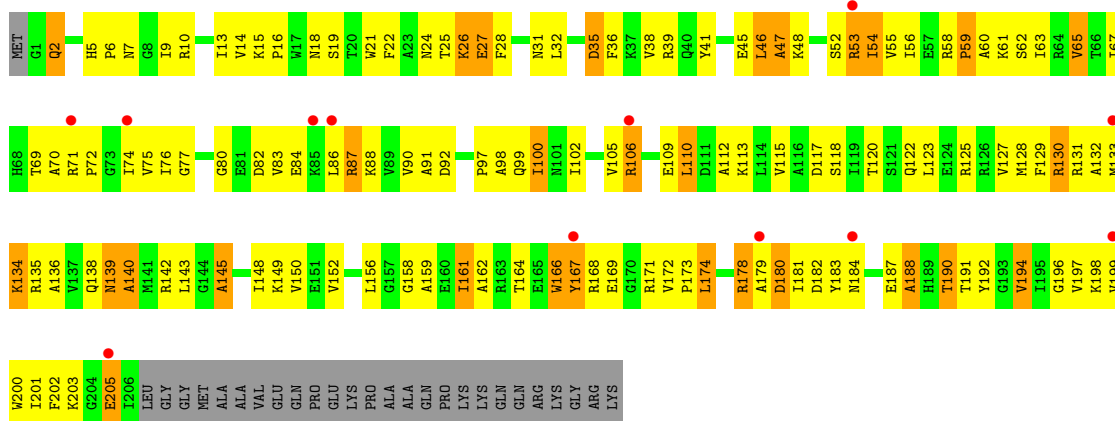
Chain AC:





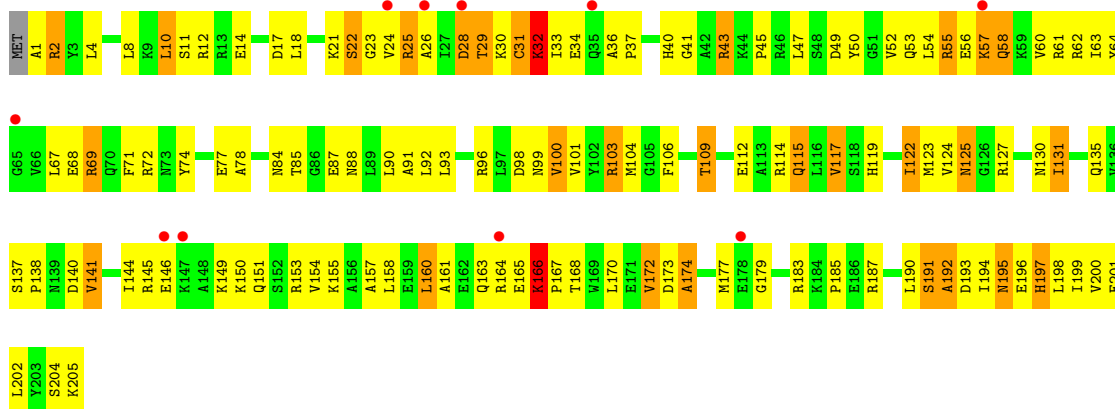
• Molecule 2: 30S ribosomal protein S3

Chain CC:



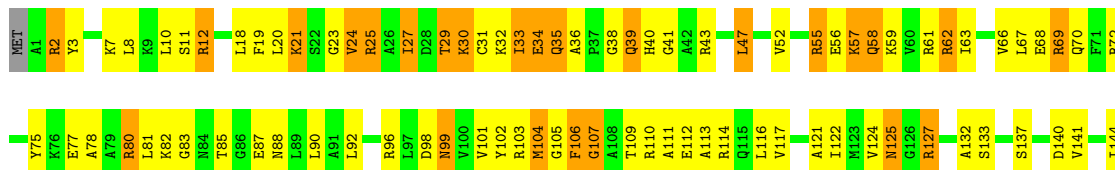
• Molecule 3: 30S ribosomal protein S4

Chain AD:



• Molecule 3: 30S ribosomal protein S4

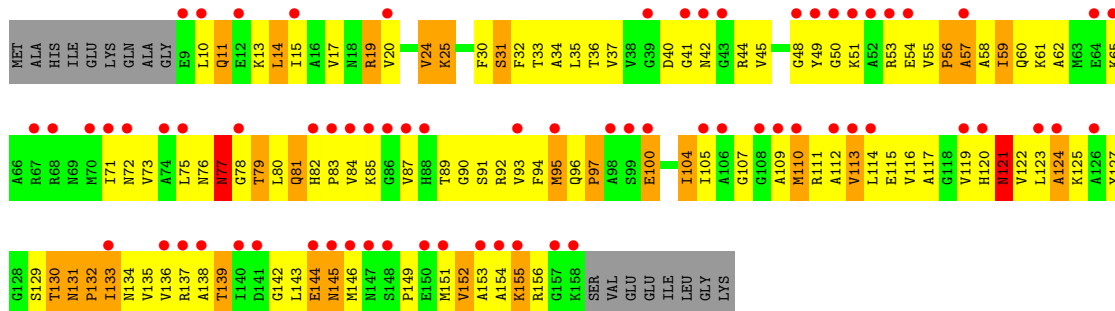
Chain CD:





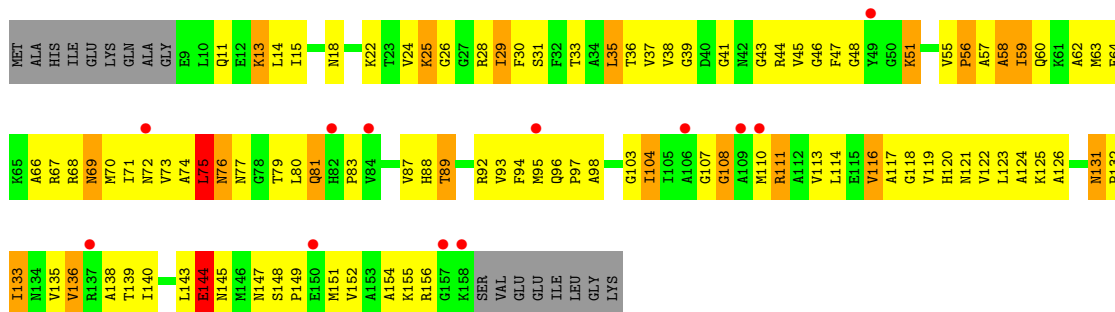
• Molecule 4: 30S ribosomal protein S5

Chain AE:



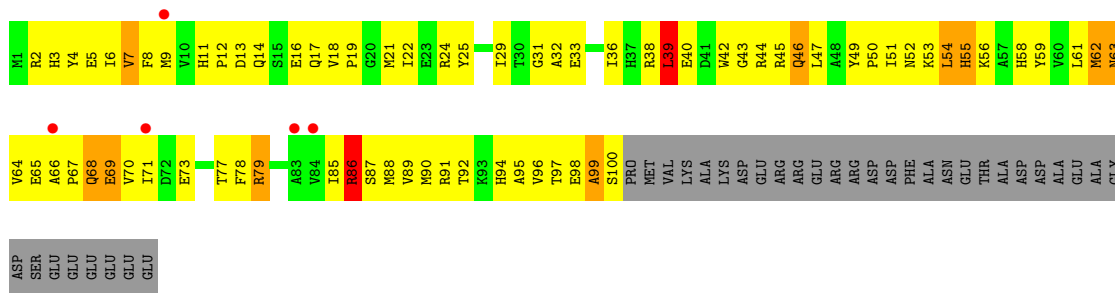
• Molecule 4: 30S ribosomal protein S5

Chain CE:



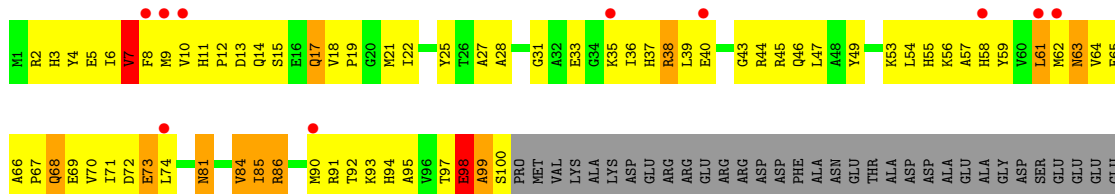
• Molecule 5: 30S ribosomal protein S6

Chain AF:



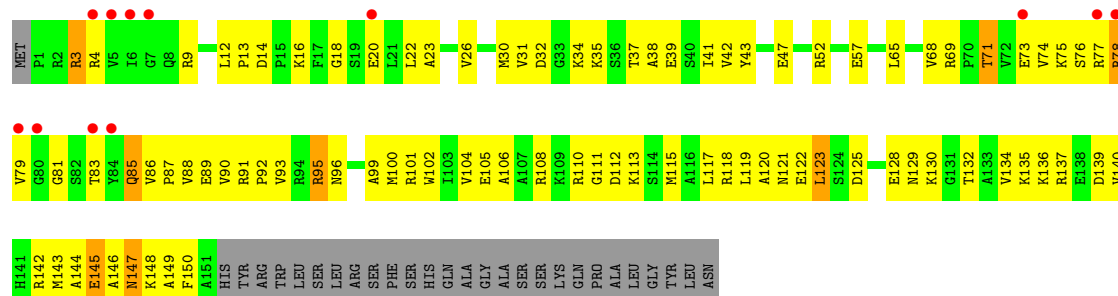
• Molecule 5: 30S ribosomal protein S6

Chain CF:

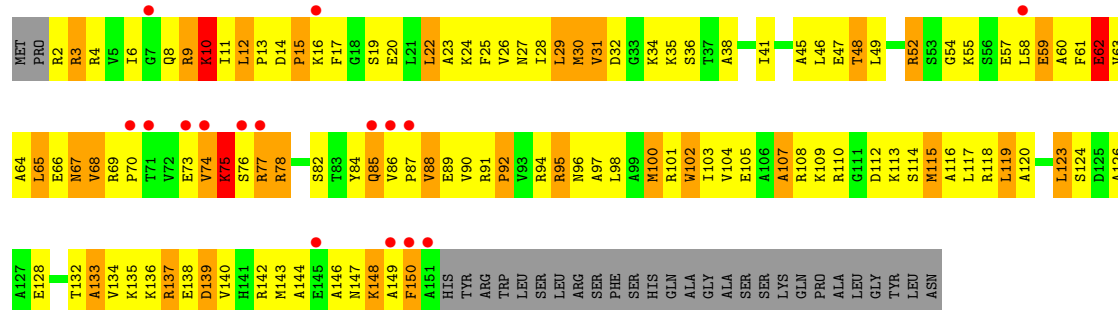


GLU
GLU

- Molecule 6: 30S ribosomal protein S7

Chain AG: 

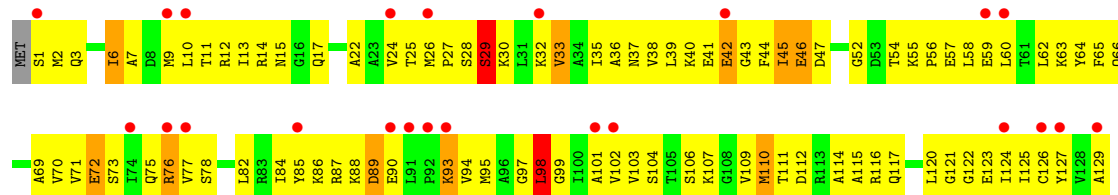
- Molecule 6: 30S ribosomal protein S7

Chain CG: 

- Molecule 7: 30S ribosomal protein S8

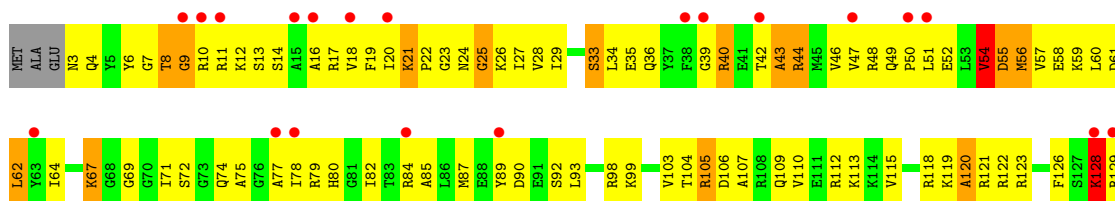
Chain AH: 

- Molecule 7: 30S ribosomal protein S8

Chain CH: 

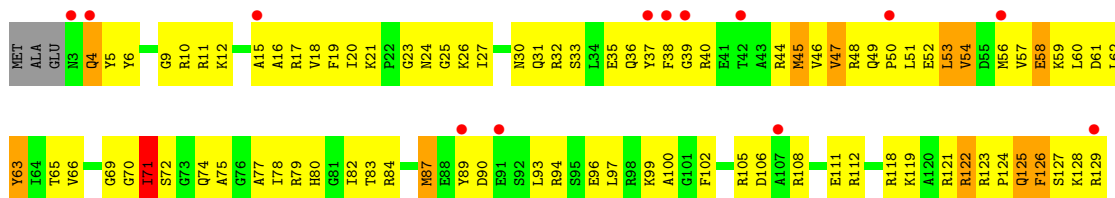
- Molecule 8: 30S ribosomal protein S9

Chain AI: 



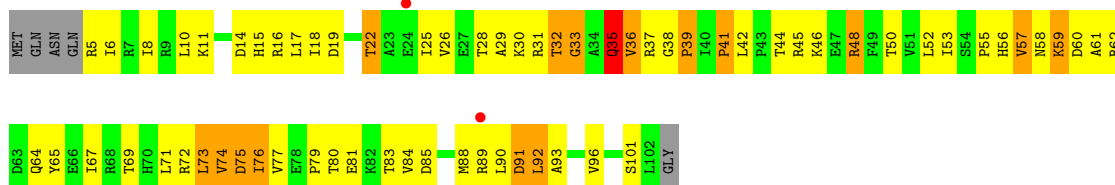
• Molecule 8: 30S ribosomal protein S9

Chain CI:



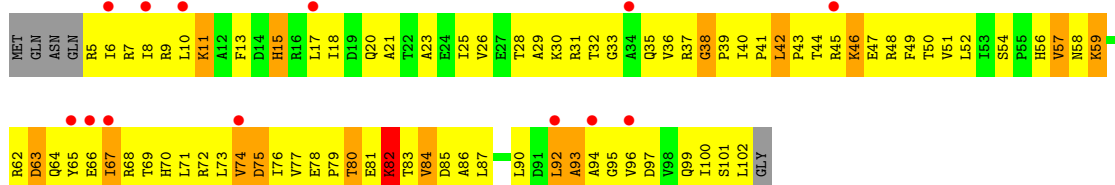
• Molecule 9: 30S ribosomal protein S10

Chain AJ:



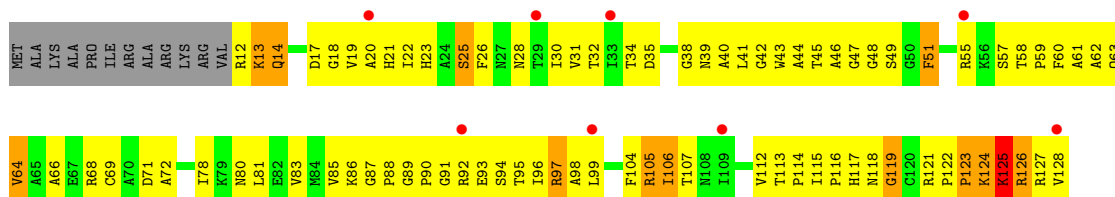
• Molecule 9: 30S ribosomal protein S10

Chain CJ:



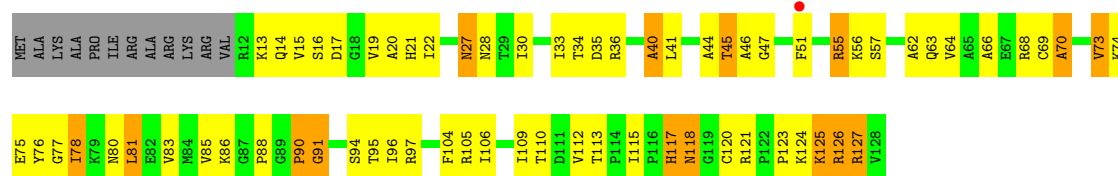
• Molecule 10: 30S ribosomal protein S11

Chain AK:



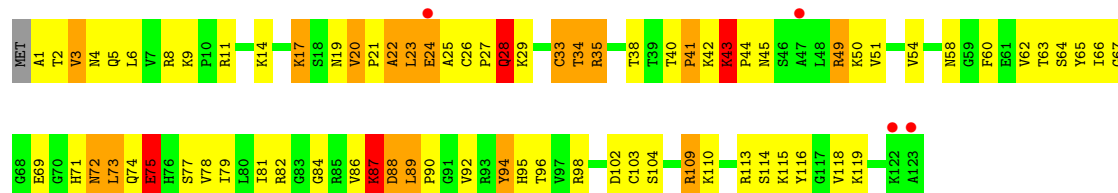
• Molecule 10: 30S ribosomal protein S11

Chain CK:



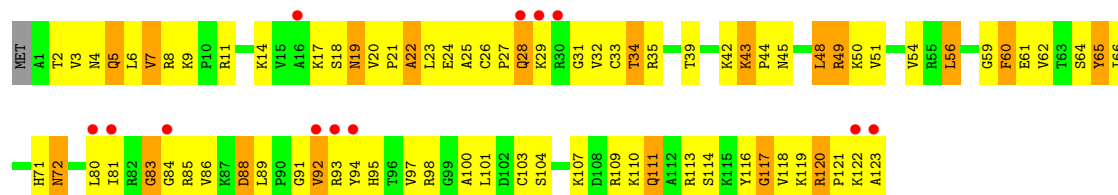
• Molecule 11: 30S ribosomal protein S12

Chain AL:



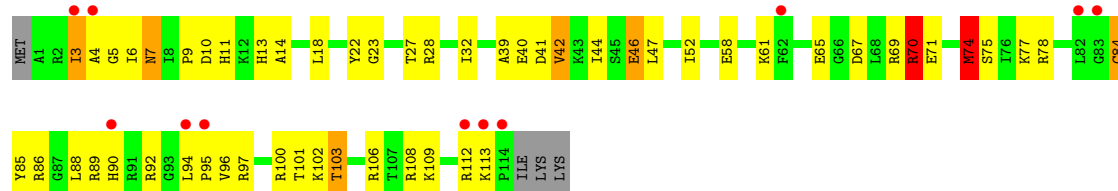
• Molecule 11: 30S ribosomal protein S12

Chain CL:



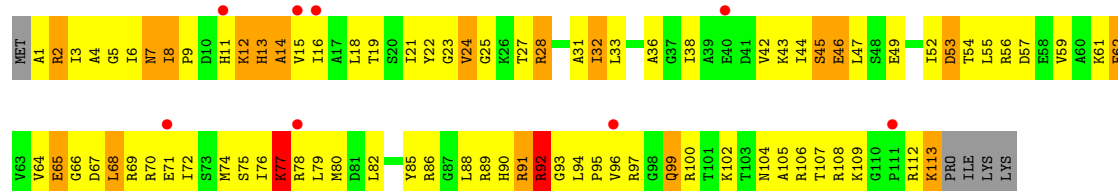
• Molecule 12: 30S ribosomal protein S13

Chain AM:



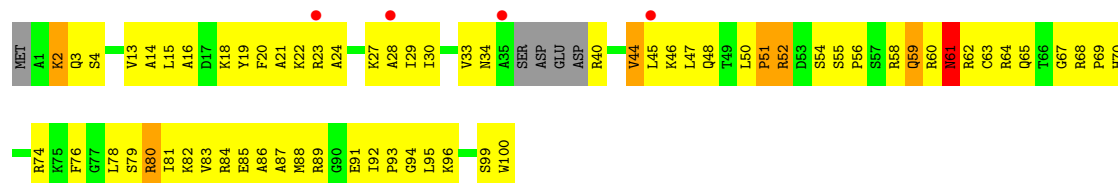
• Molecule 12: 30S ribosomal protein S13

Chain CM:



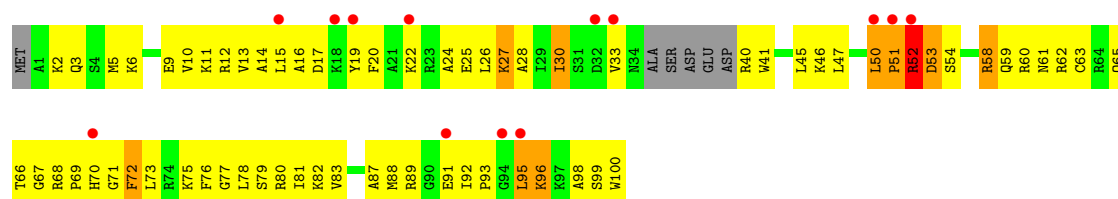
• Molecule 13: 30S ribosomal protein S14

Chain AN:



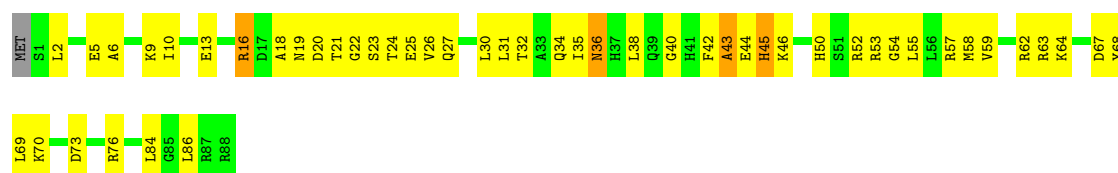
• Molecule 13: 30S ribosomal protein S14

Chain CN:



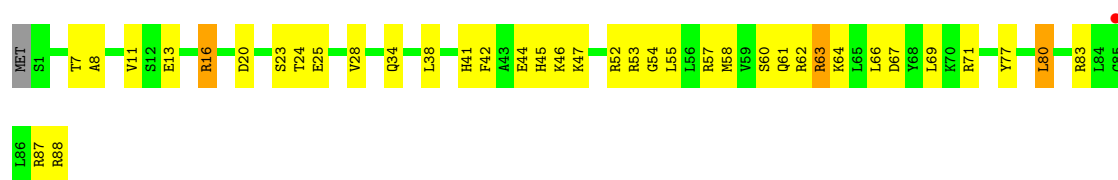
• Molecule 14: 30S ribosomal protein S15

Chain AO:



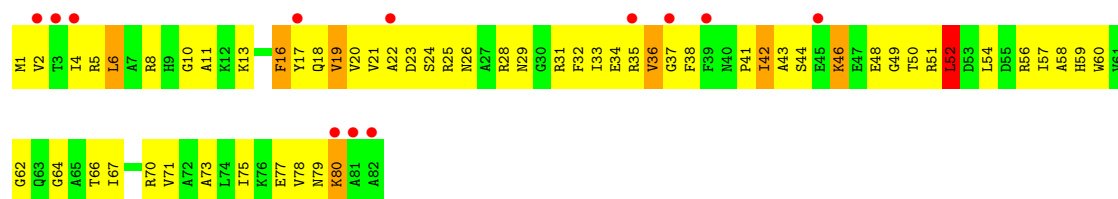
• Molecule 14: 30S ribosomal protein S15

Chain CO:



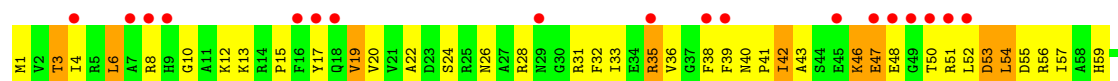
• Molecule 15: 30S ribosomal protein S16

Chain AP:



• Molecule 15: 30S ribosomal protein S16

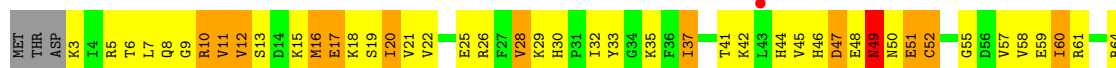
Chain CP:





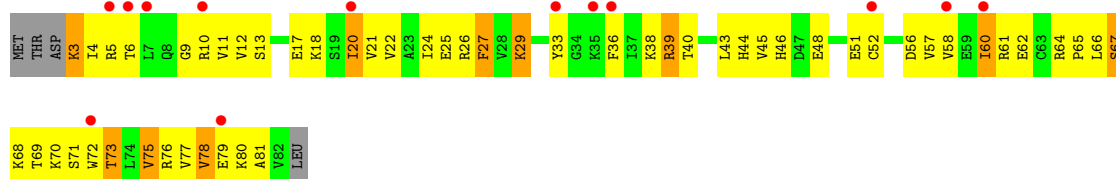
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



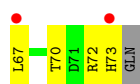
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



- Molecule 17: 30S ribosomal protein S18

Chain AR:



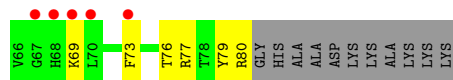
- Molecule 17: 30S ribosomal protein S18

Chain CR:

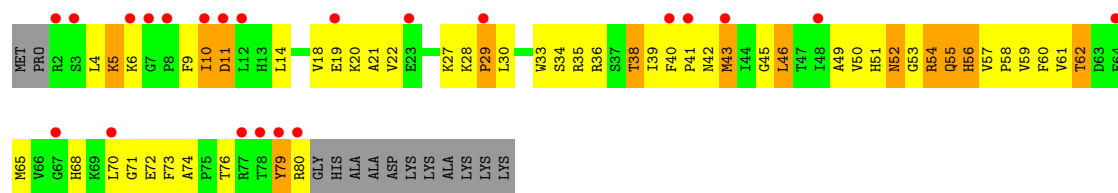


- Molecule 18: 30S ribosomal protein S19

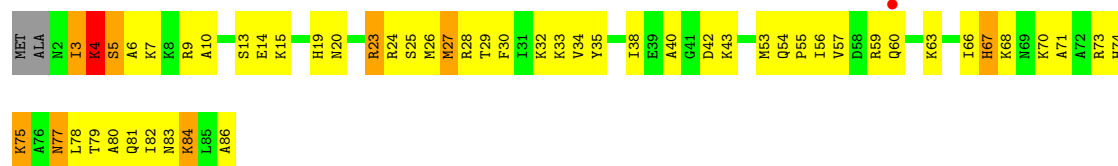
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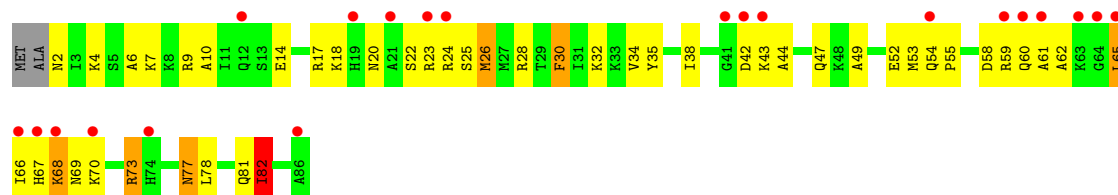
- Molecule 18: 30S ribosomal protein S19

Chain CS: 

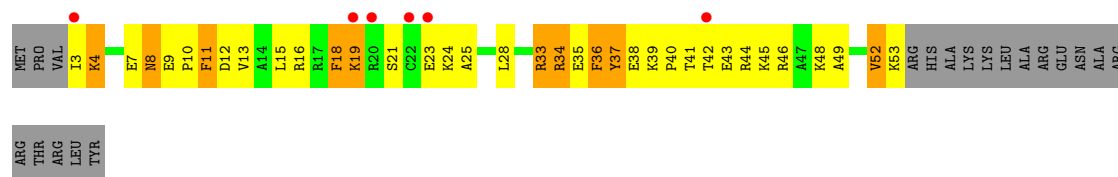
- Molecule 19: 30S ribosomal protein S20

Chain AT: 

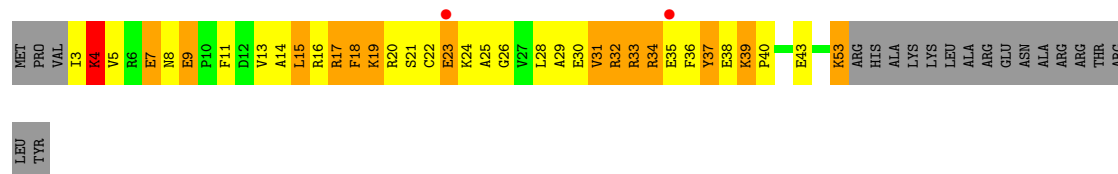
- Molecule 19: 30S ribosomal protein S20

Chain CT: 

- Molecule 20: 30S ribosomal protein S21

Chain AU: 

- Molecule 20: 30S ribosomal protein S21

Chain CU: 

- Molecule 21: 16S rRNA

Chain AA: 

A2	A3	U4	U5	G6	G6	A7	A8	G9	A10	G11	U12	U13	U14	G15	A16	U17	C18	A19	A18	U20	G21	G22	C23	U24	C25	A26	U29	U30	G31	A32	A33	C34	G35	U37	G38	G39	C40	G41	G42	C43	A44	G45	G46	C47	C48	U49	A50	A51	G52	A53	C54	G57	C58	A59	A60	G61	U62	C63	
G64	A65	A66	C67	G68	G69	U70	A71	A72	C73	A74	G75	G76	U77	A78	U79	A80	A81	G82	C83	U84	U85	C87	U88	U89	C90	A91	U92	U93	G94	C95	A96	A97	A98	C99	G100	A101	U102	U103	G104	G105	C106	A109	C110	G111	G112	G113	U114	G115	A116	U117	U118	A119	A120	U121	U122	C124			
U125	G126	G127	G128	G129	A130	A131	C132	U133	G134	C135	G138	A139	U140	U141	G142	A143	G144	G145	U146	U147	G148	A151	U154	A155	C156	U157	U158	G159	A160	A161	A162	C163	G164	G165	U166	A167	G168	C169	U170	A171	A172	U173	A174	C175	G176	U177	C178	A179	U180	A181	A182	C183	G184	U185	G187	U188	U189		
C188	A189	A190	G191	A192	C193	C194	A195	A196	A197	G198	A199	G200	G201	G202	G203	G204	A205	C206	C207	U208	U209	G211	G212	G213	C214	A215	U216	U217	A218	U219	G220	A223	U224	C225	G226	G227	A228	U229	G230	C231	U232	C233	C234	C235	A236	G237	U240	A243	U244	C245	A246	C247	U248	A250					
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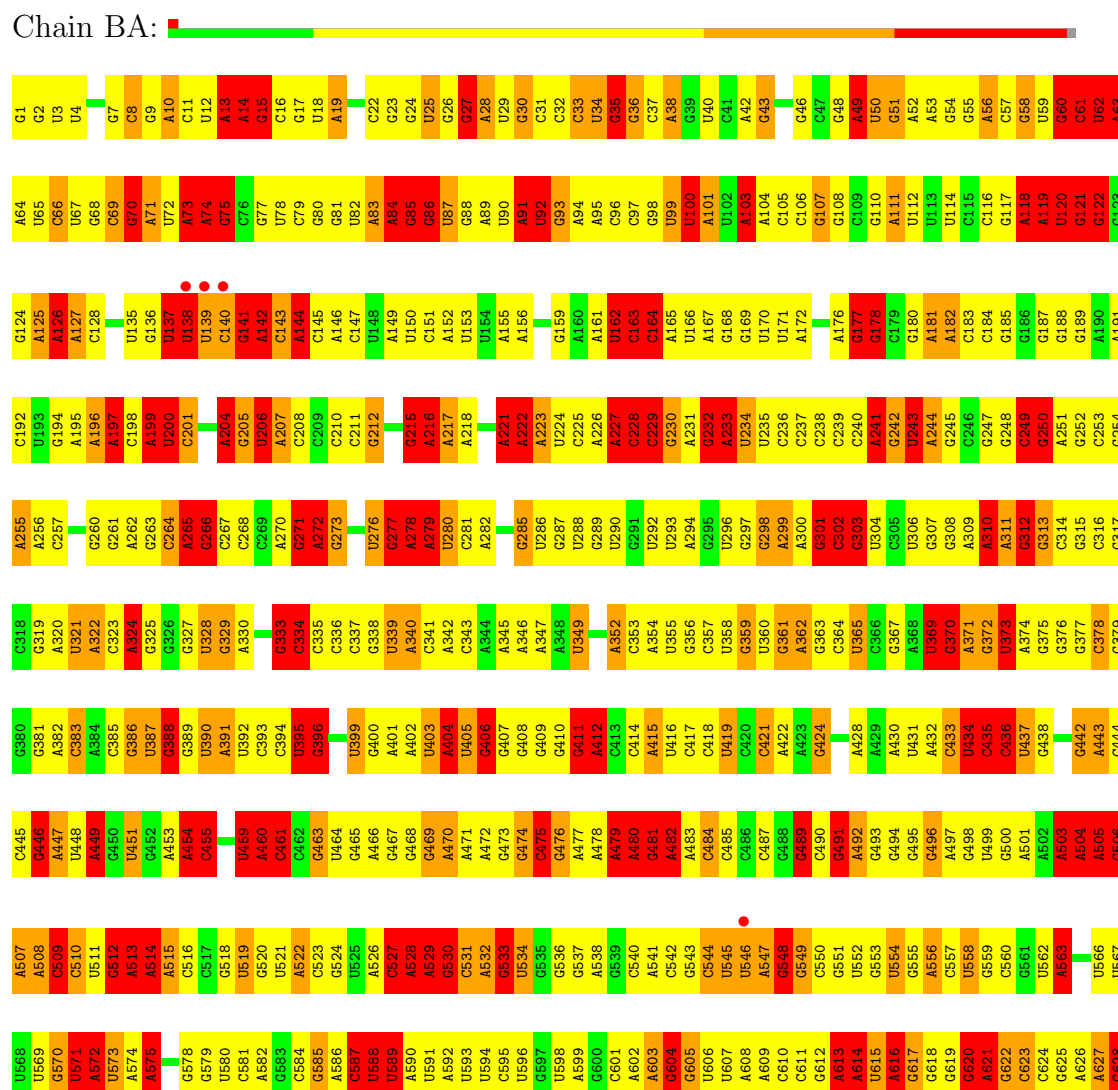
- Molecule 23: messenger RNA



- Molecule 23: messenger RNA



- Molecule 24: 23S rRNA

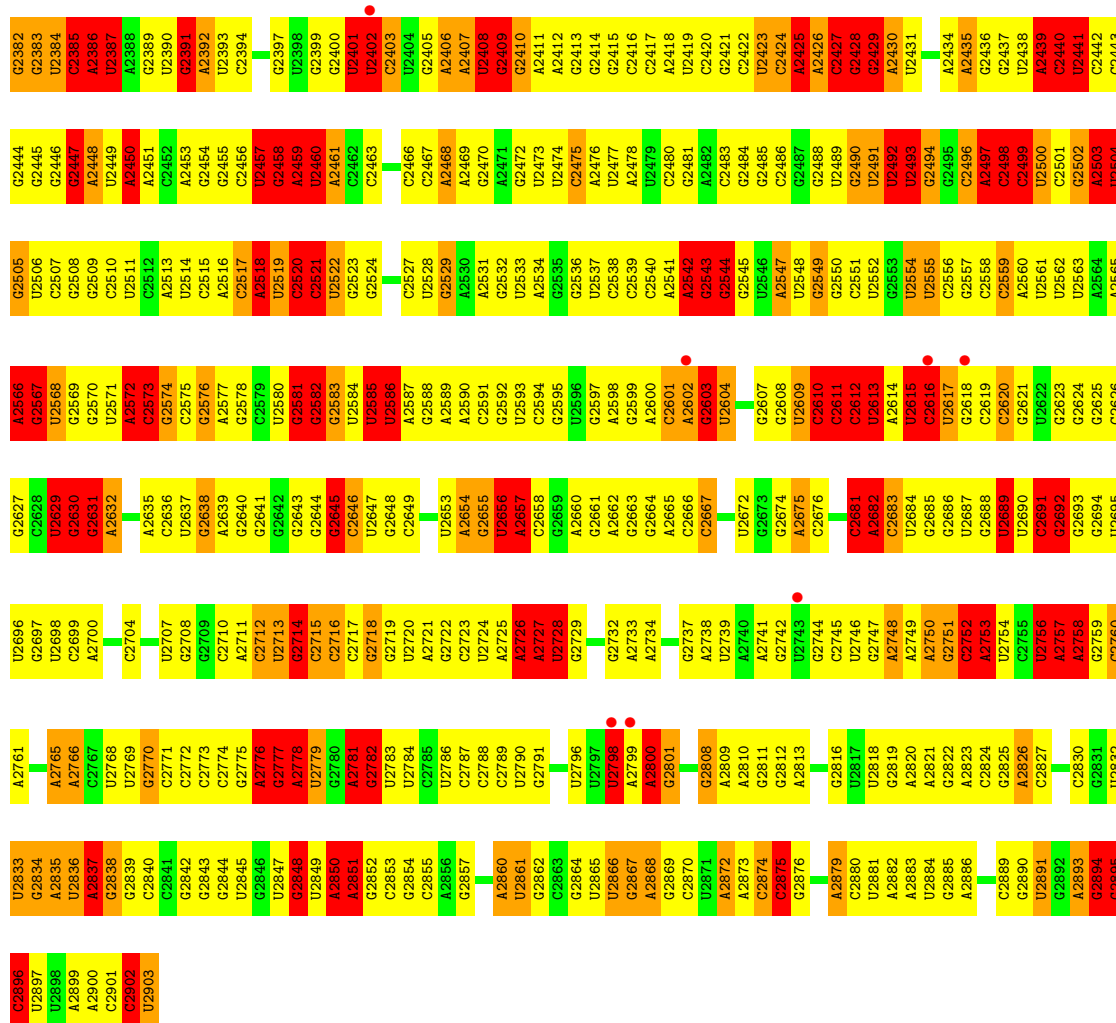


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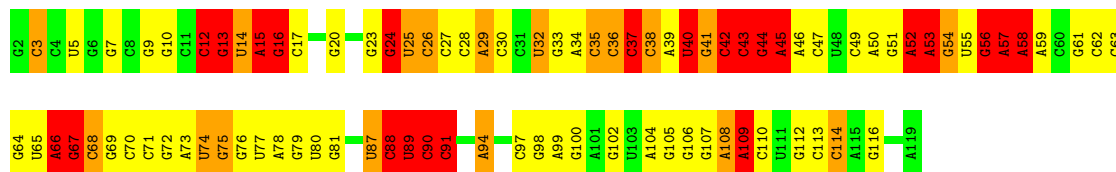
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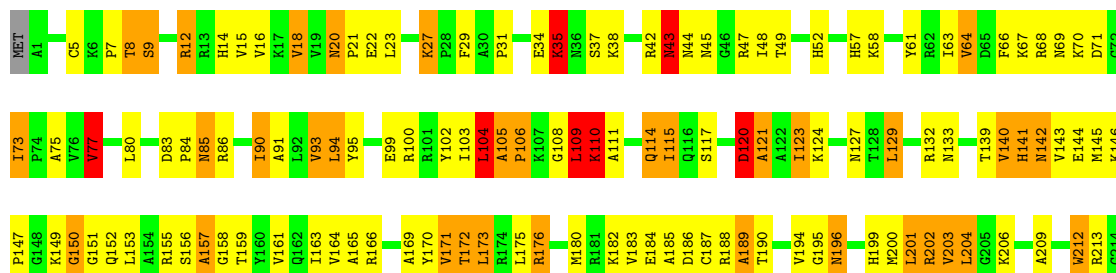
• Molecule 25: 5S rRNA

Chain BB:



• Molecule 26: 50S ribosomal protein L2

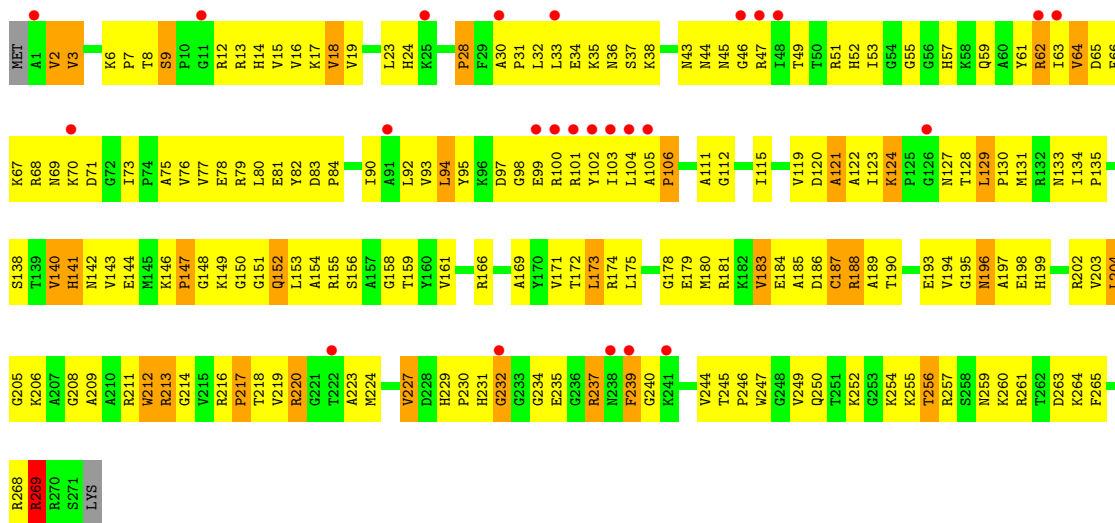
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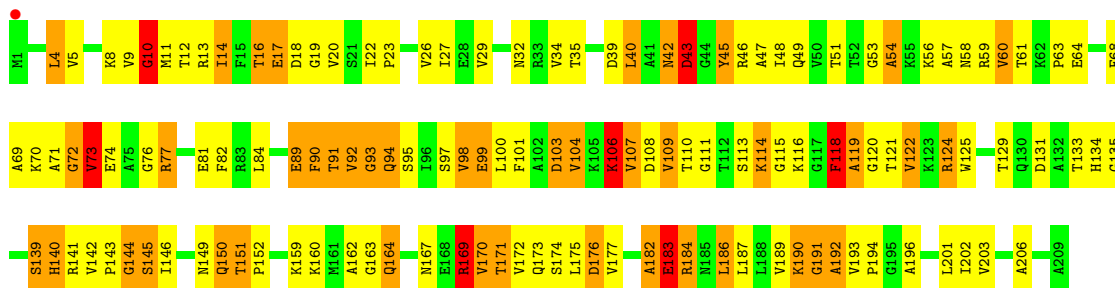
• Molecule 26: 50S ribosomal protein L2

Chain DC:



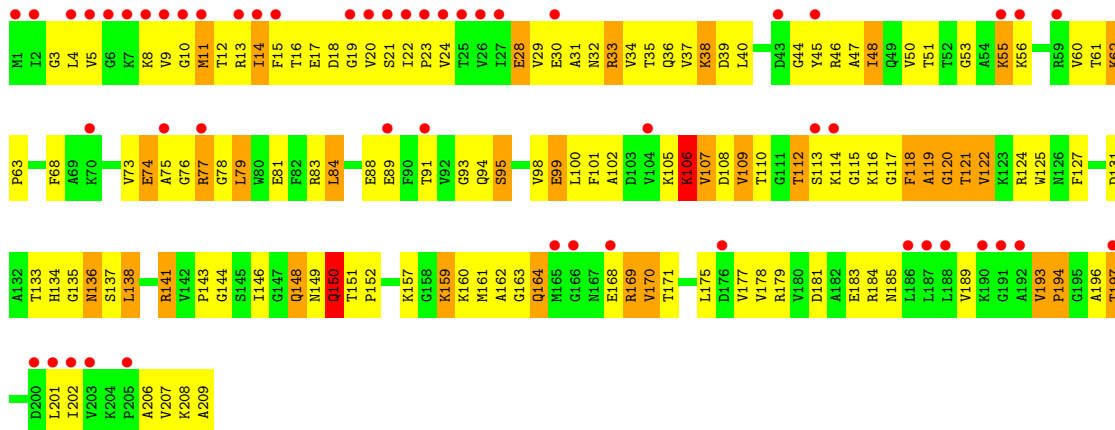
• Molecule 27: 50S ribosomal protein L3

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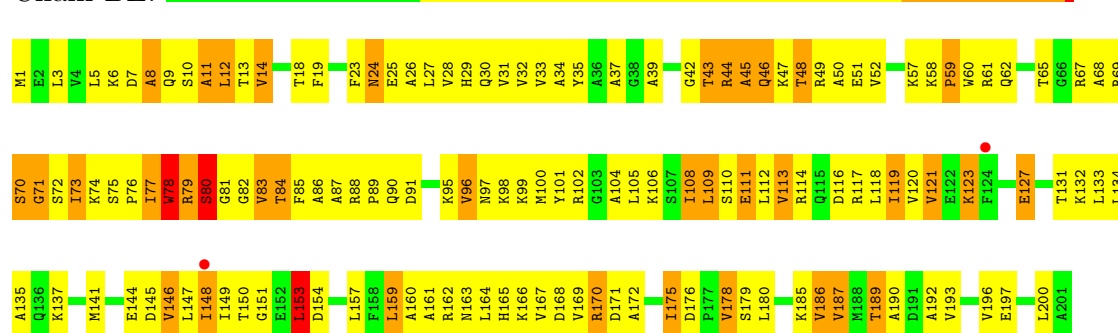
• Molecule 27: 50S ribosomal protein L3

Chain DD:



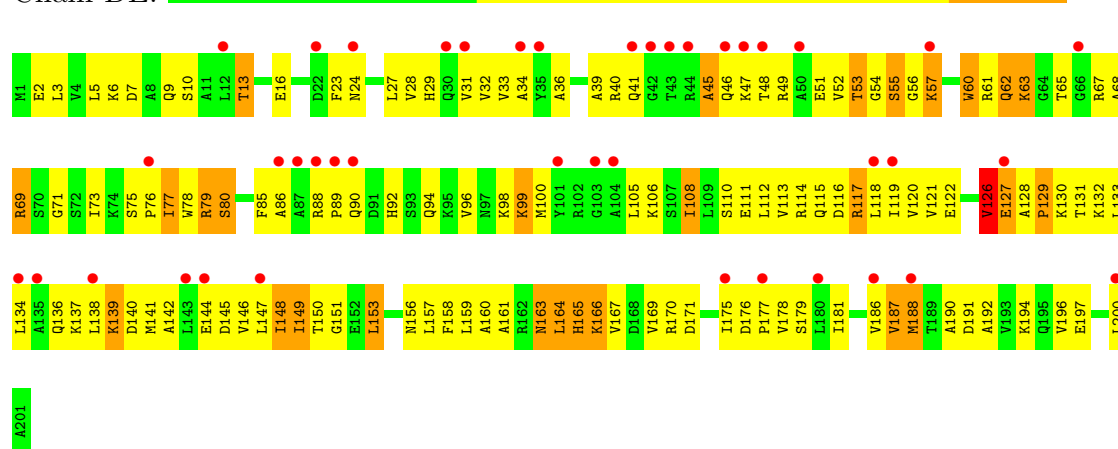
- Molecule 28: 50S ribosomal protein L4

Chain BE:



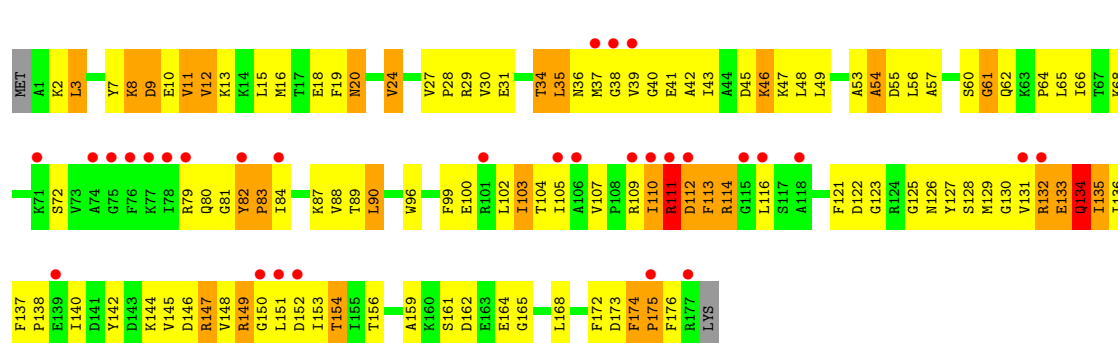
- Molecule 28: 50S ribosomal protein L4

Chain DE:



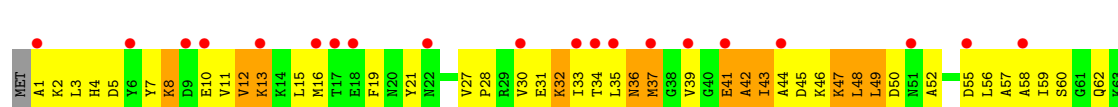
- Molecule 29: 50S ribosomal protein L5

Chain BF:

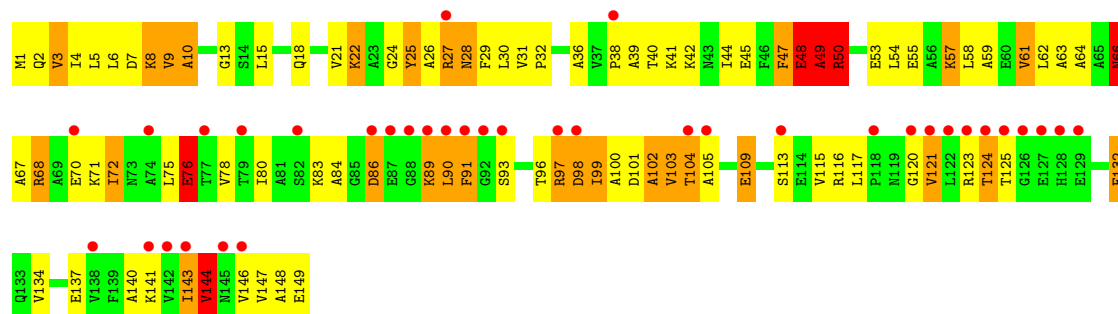


- Molecule 29: 50S ribosomal protein L5

Chain DF:







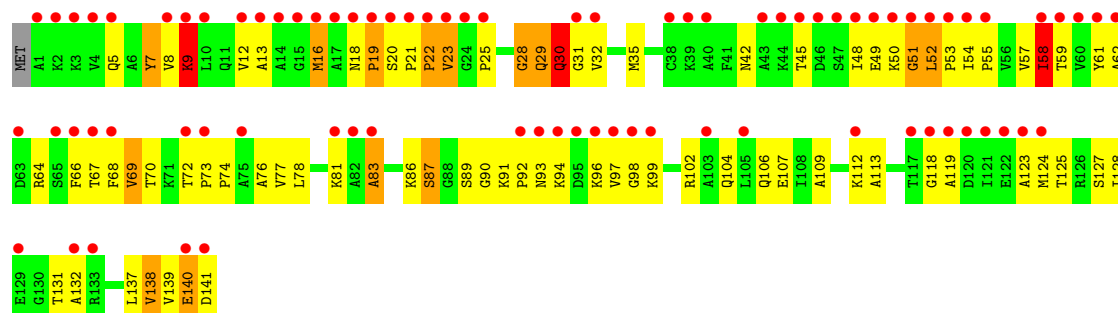
• Molecule 32: 50S ribosomal protein L11

Chain BI:



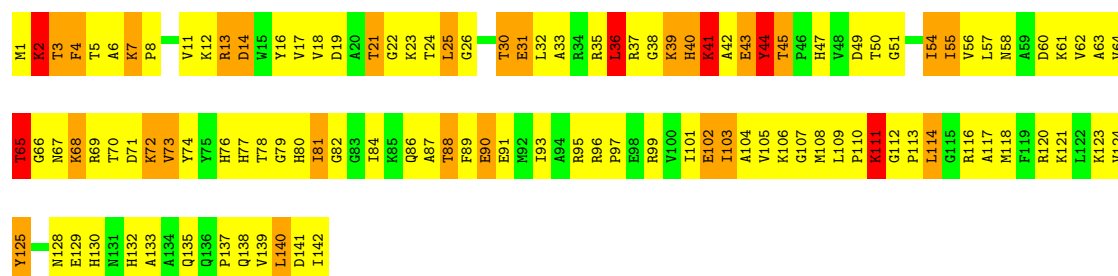
• Molecule 32: 50S ribosomal protein L11

Chain DI:



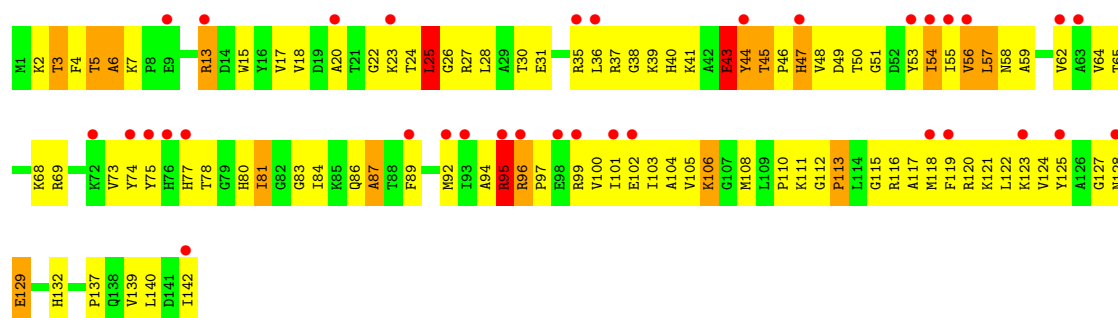
• Molecule 33: 50S ribosomal protein L13

Chain BJ:



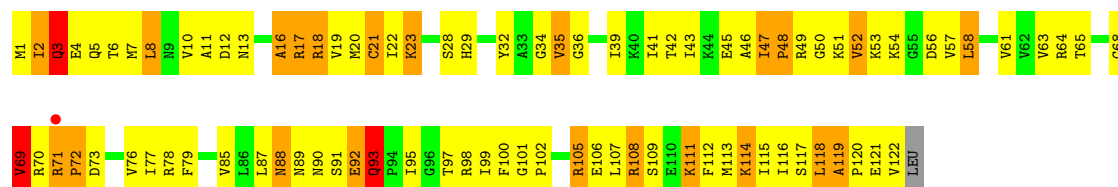
• Molecule 33: 50S ribosomal protein L13

Chain DJ:



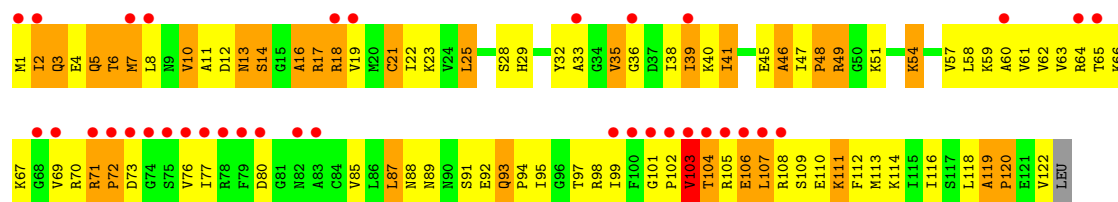
- Molecule 34: 50S ribosomal protein L14

Chain BK:



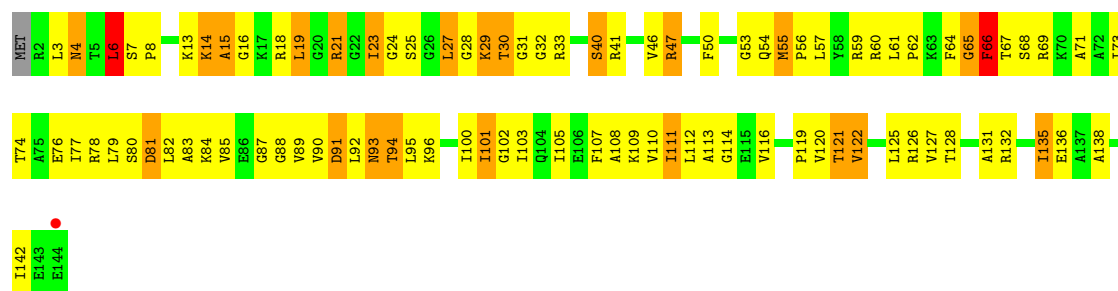
- Molecule 34: 50S ribosomal protein L14

Chain DK:



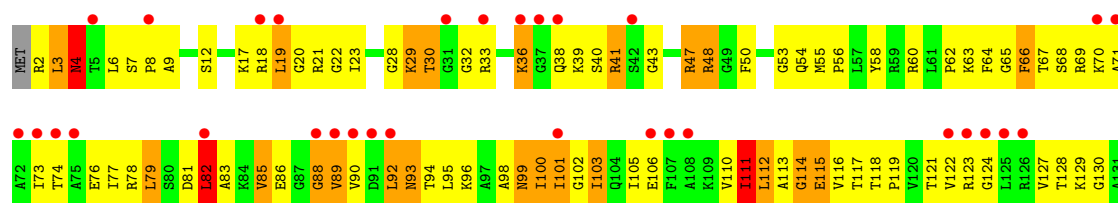
- Molecule 35: 50S ribosomal protein L15

Chain BL:



- Molecule 35: 50S ribosomal protein L15

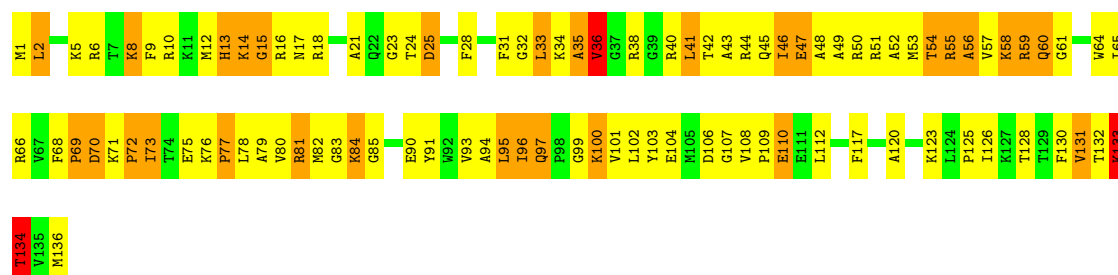
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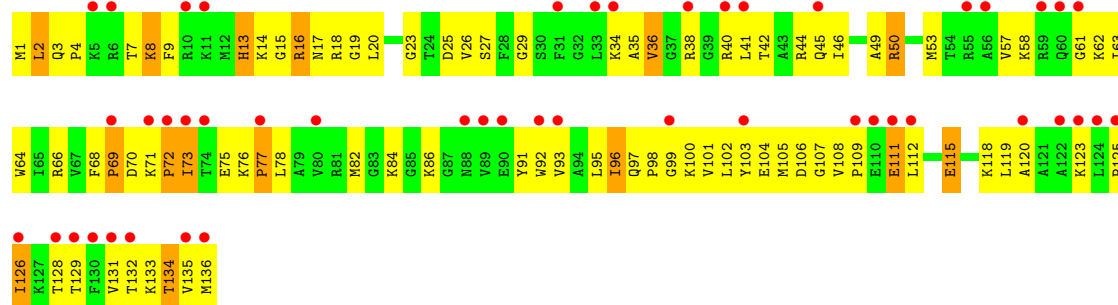
- Molecule 36: 50S ribosomal protein L16

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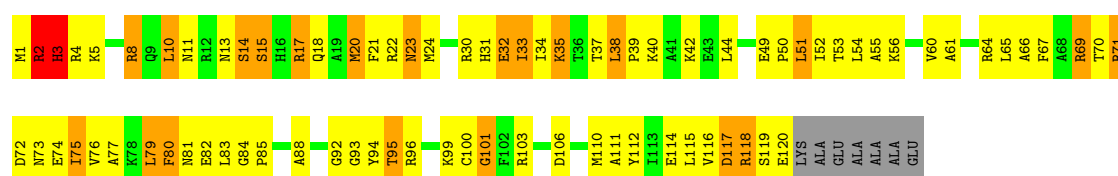
- Molecule 36: 50S ribosomal protein L16

Chain DM:



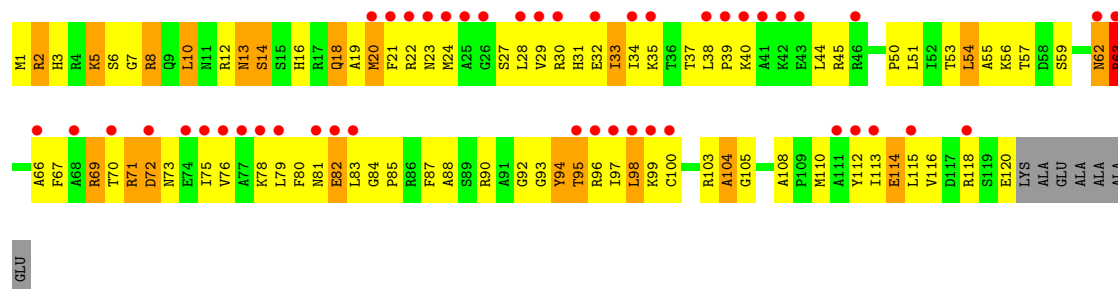
- Molecule 37: 50S ribosomal protein L17

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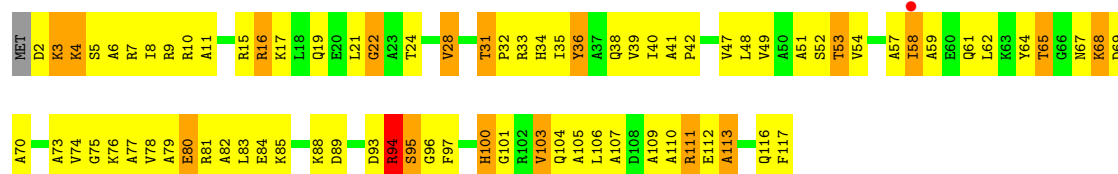
- Molecule 37: 50S ribosomal protein L17

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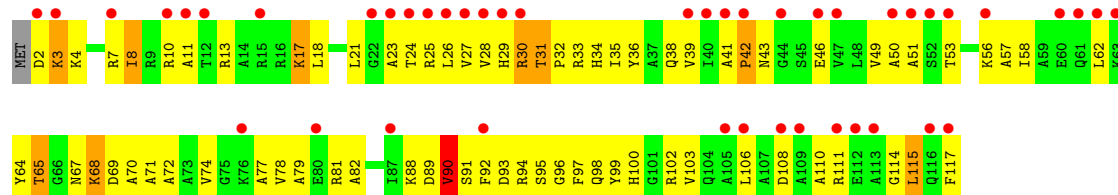
- Molecule 38: 50S ribosomal protein L18

Chain BO:



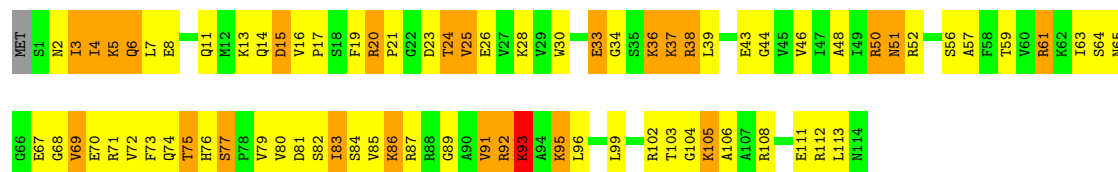
- Molecule 38: 50S ribosomal protein L18

Chain DO:



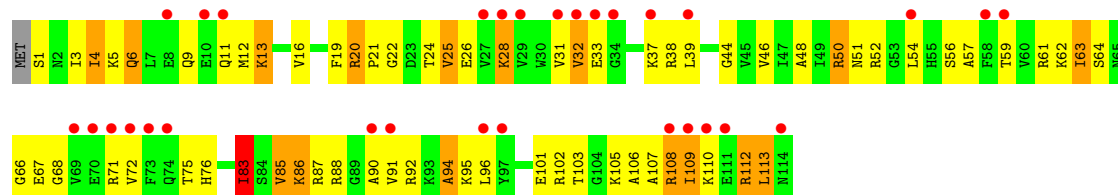
- Molecule 39: 50S ribosomal protein L19

Chain BP:



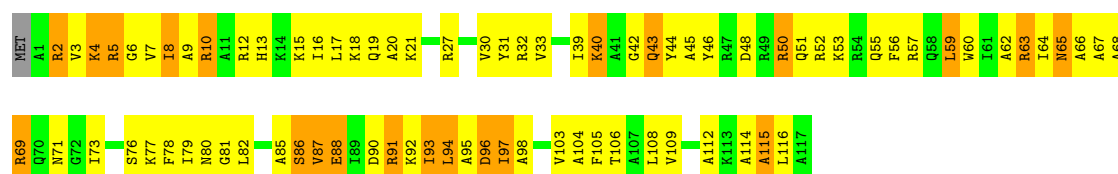
- Molecule 39: 50S ribosomal protein L19

Chain DP:



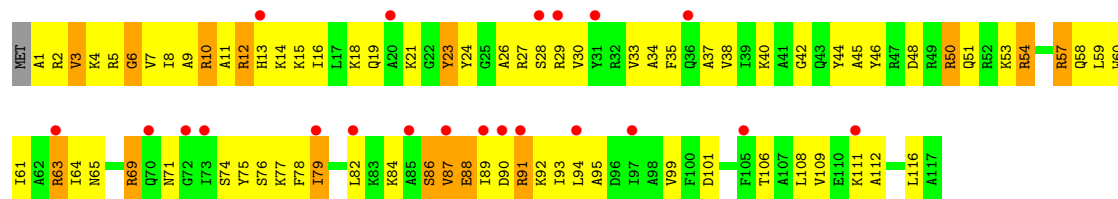
- Molecule 40: 50S ribosomal protein L20

Chain BQ:



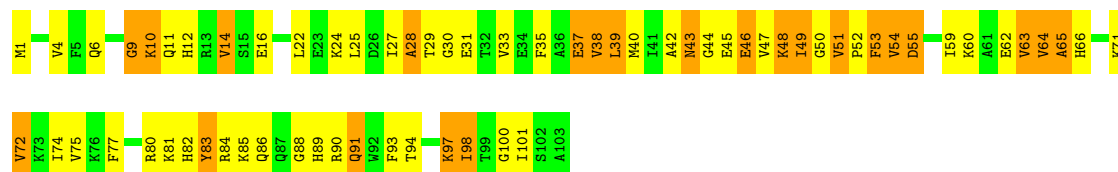
- Molecule 40: 50S ribosomal protein L20

Chain DQ:



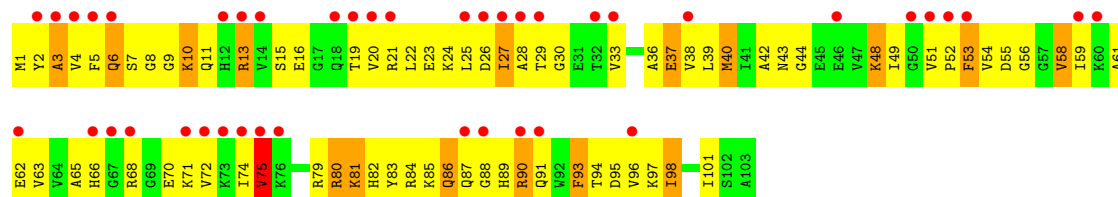
• Molecule 41: 50S ribosomal protein L21

Chain BR:



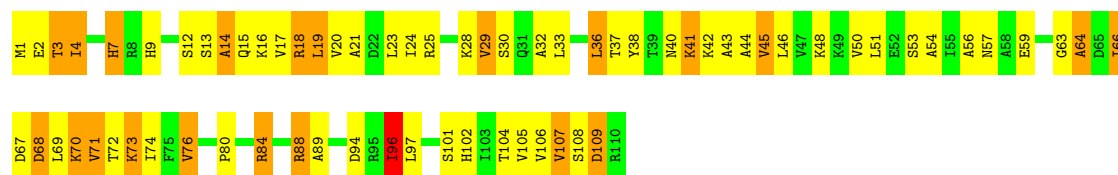
• Molecule 41: 50S ribosomal protein L21

Chain DR:



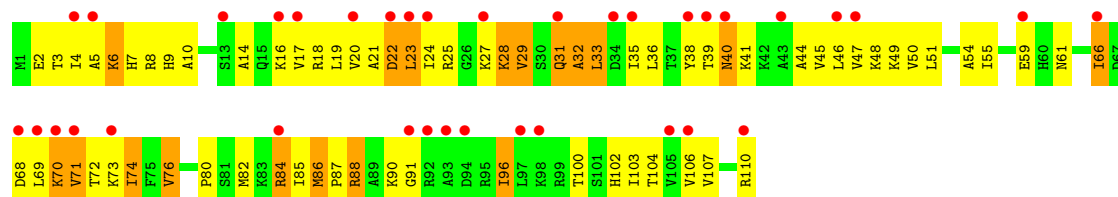
• Molecule 42: 50S ribosomal protein L22

Chain BS:



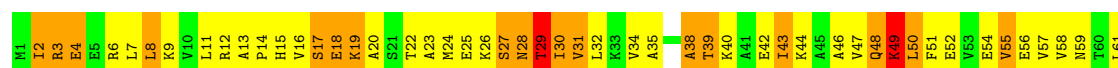
• Molecule 42: 50S ribosomal protein L22

Chain DS:



• Molecule 43: 50S ribosomal protein L23

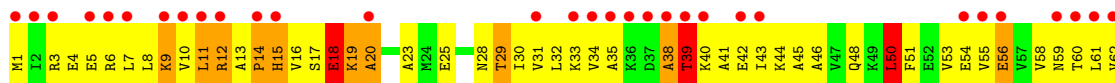
Chain BT:





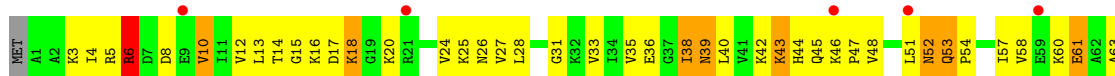
- Molecule 43: 50S ribosomal protein L23

Chain DT:



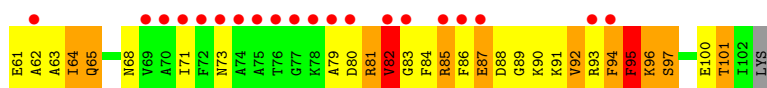
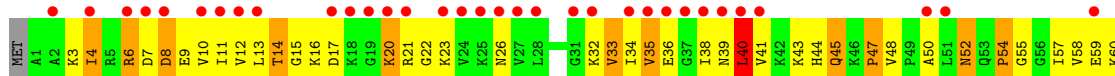
- Molecule 44: 50S ribosomal protein L24

Chain BU:



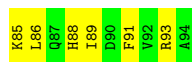
- Molecule 44: 50S ribosomal protein L24

Chain DU:



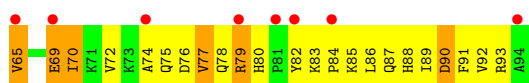
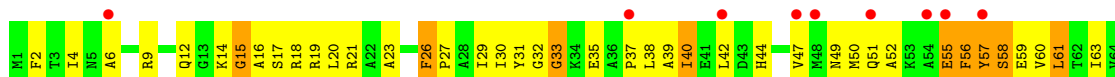
- Molecule 45: 50S ribosomal protein L25

Chain BV:



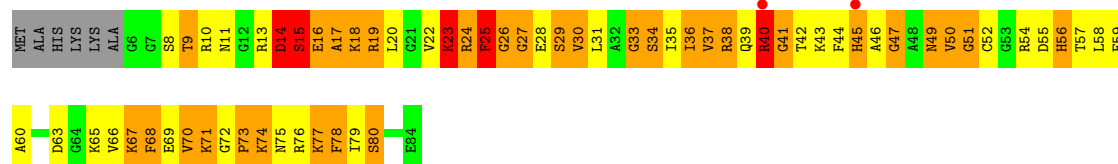
- Molecule 45: 50S ribosomal protein L25

Chain DV:



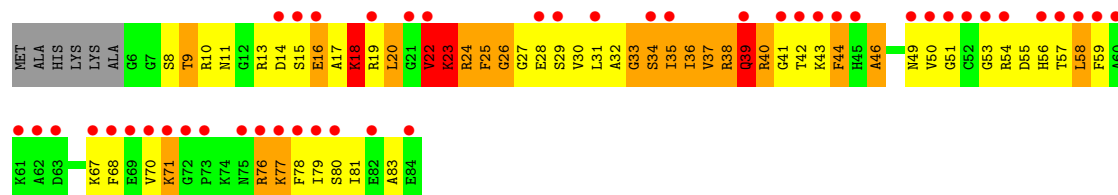
- Molecule 46: 50S ribosomal protein L27

Chain BW:



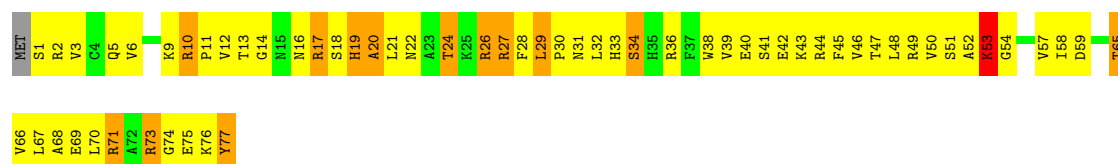
- Molecule 46: 50S ribosomal protein L27

Chain DW:



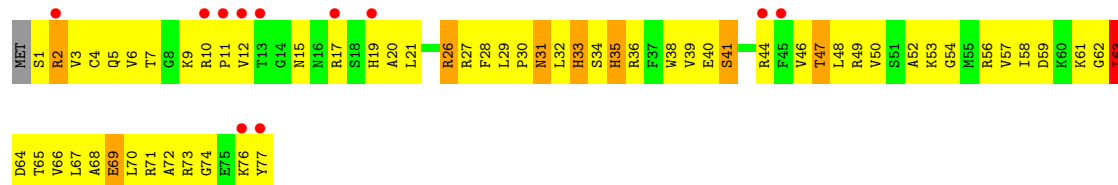
- Molecule 47: 50S ribosomal protein L28

Chain BX:



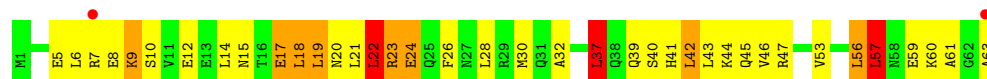
- Molecule 47: 50S ribosomal protein L28

Chain DX:



- Molecule 48: 50S ribosomal protein L29

Chain BY:



- Molecule 48: 50S ribosomal protein L29

Chain DY:



- Molecule 49: 50S ribosomal protein L30

Chain BZ:



- Molecule 49: 50S ribosomal protein L30

Chain DZ:



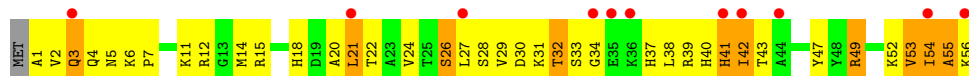
- Molecule 50: 50S ribosomal protein L32

Chain B0:



- Molecule 50: 50S ribosomal protein L32

Chain D0:



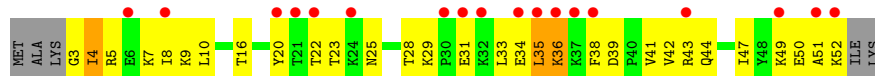
- Molecule 51: 50S ribosomal protein L33

Chain B1:



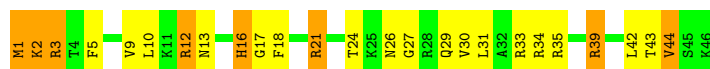
- Molecule 51: 50S ribosomal protein L33

Chain D1:



- Molecule 52: 50S ribosomal protein L34

Chain B2:



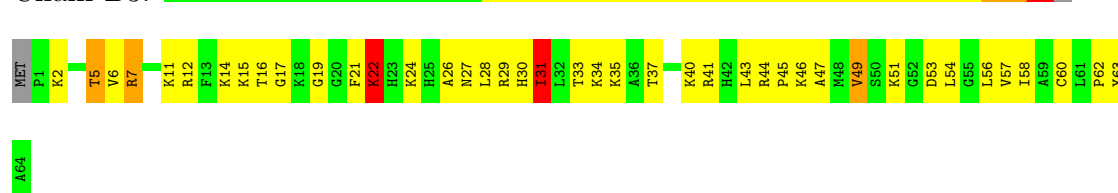
- Molecule 52: 50S ribosomal protein L34

Chain D2:



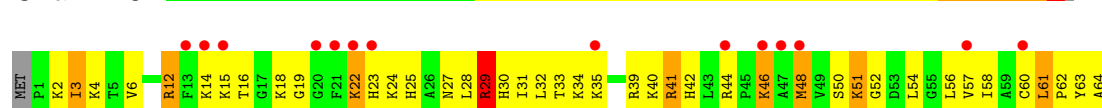
- Molecule 53: 50S ribosomal protein L35

Chain B3:



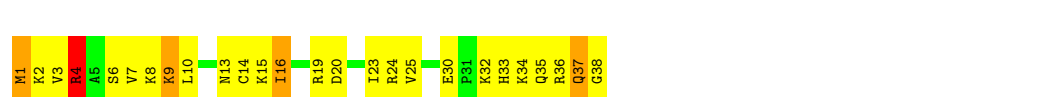
- Molecule 53: 50S ribosomal protein L35

Chain D3:



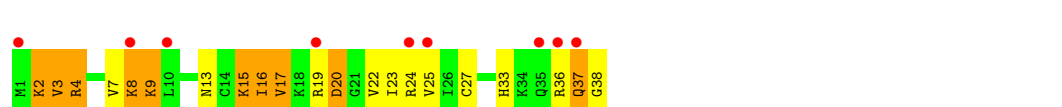
- Molecule 54: 50S ribosomal protein L36

Chain B4:



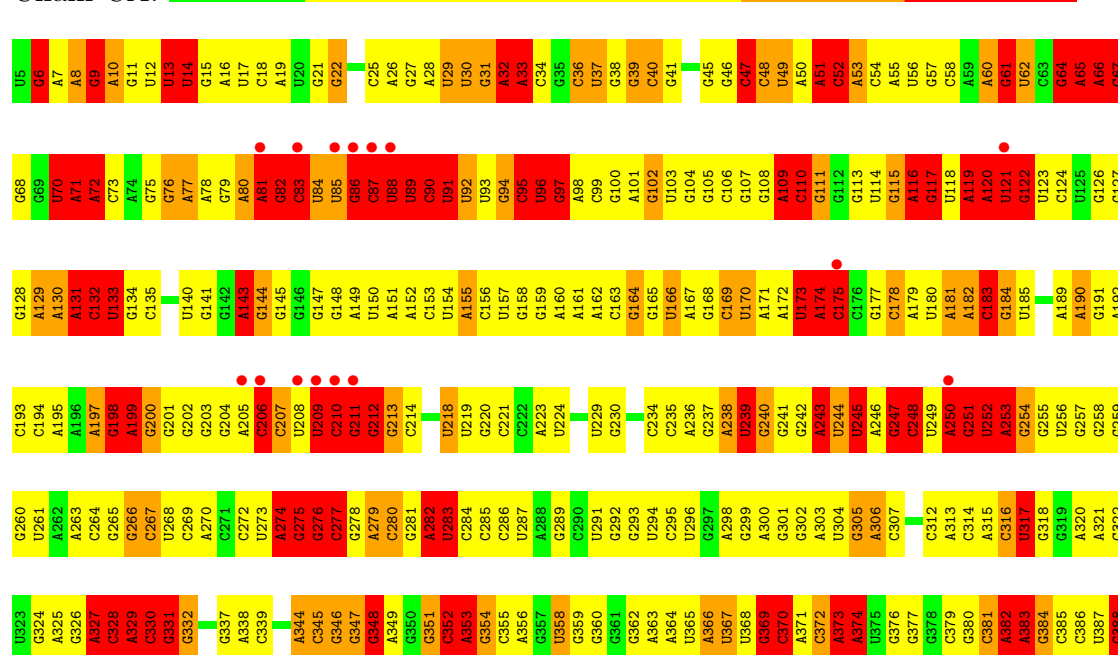
- Molecule 54: 50S ribosomal protein L36

Chain D4:

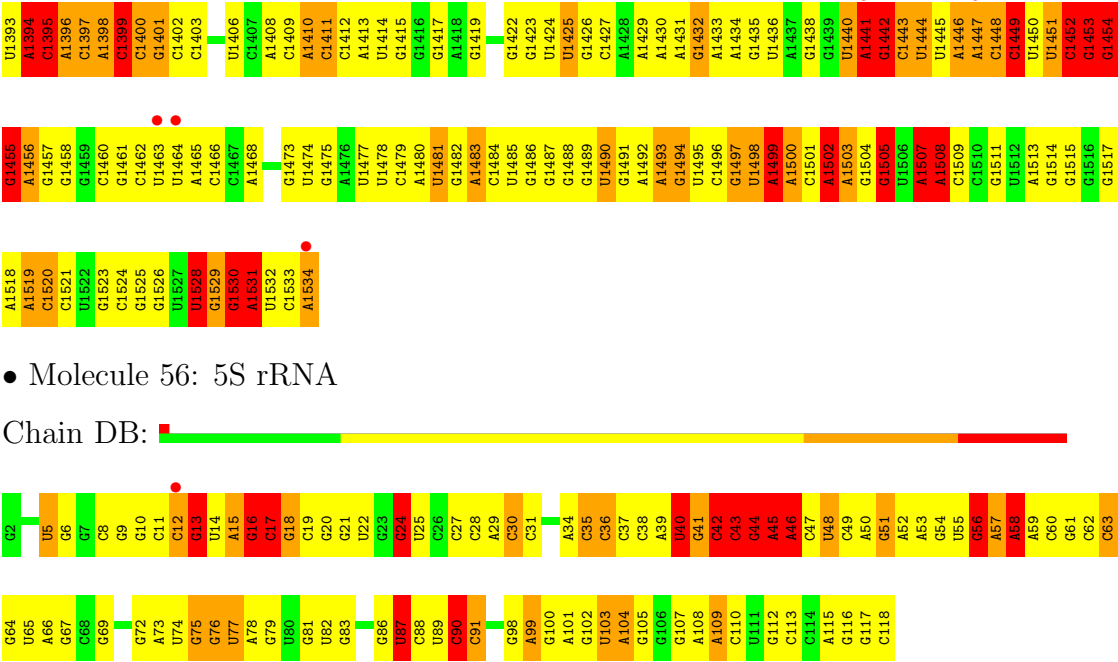


- Molecule 55: 16S rRNA

Chain CA:



U1330	A1269	C1209	G1083	A1021	A959	U891	G830	A768	A704	A642	C576	C514	G454	A389
G1331	G1270	C1210	G1084	A1022	U960	A892	A831	G769	G705	G643	G577	G517	G455	U390
A1332	G1271	U1211	U1085	U1023	U961	C993	G832	C770	A706	U644	C578	C518	A456	C392
A1333	G1272	U1212	U1086	G1024	C962		G833	G771	U707	G645	A579	C520	G457	C393
G1334	A1151	A1213	G1087	G1025	U965	C899	U834	G774	C708	G647	C580	A520	U458	A394
U1335	A1152	G1214	G1088	U1026	G966	A900	U835	G775	U709	G646	C581	A521	A459	G395
C1336	G1276	G1215	G1089		C967	A901	G836	G776	G710	A648	C582	G521	A460	C396
G1337	C1277	A1216	U1090	U1029	C968	A906	G837	G777	G711	A649	A583	C522	A461	A397
G1338	G1278	C1217	U1091	U1030	C969	A907	G838	G778	G714	G650	G584	C525	A462	U397
A1339	G1279	U1218	G1092	G1031	A969	A908	C841	G779	A715	C651	C585	C526	U463	U398
A1340	A1280	A1219	A1093	G1032	C970	A909	U842	C780	A716	U653	C587	G527	U464	
U1341	G1281	G1220	U1094	G1033	G971	C910	U843	A781	U717	G654	C588	C528	A465	C401
C1282	U1342	G1221	U1095	G1034	C972	U911	G844	A782	A718	A655	U589	C529	U466	C403
U1283	G1343	G1222	C1096	A1035	G973	C912	A845	G783	C719	G656	U590	G530	U467	G404
C1284	C1344	C1223	G1097	A1036	A974	A908	A846	C784	C720	U657	C591	U531	A468	U405
U1345	U1346	U1224	C1098	C1037	A975	A913	G847	A784	G721	C658	C592	A532	C469	G406
A1346	A1285	A1225	G1099	G1038	G976	A914	G847	G785	G722	U659	C593	A533	C470	U407
G1347	U1286	C1226	C1100	G1039	A977	A915	C948	G786	G723	C660	U594	U534	U471	G408
U1348	A1287	A1227	U1041	U1040	A978	U916	G849	A787	U723	G661	A595	A535	U473	U409
A1349	A1288	C1228	G1101	G1041	C979	G917	U850		G724	U662	A596	A536	G474	G410
A1350	U1289	U1229	A1102	G1042	C980	A918	C851	A790	G725	G663	C597	G537	C475	A411
U1351	G1290	C1230	C1103	A1043	U981	A919	C852	G791	C726	A663	C597	G538	U476	A412
C1352	U1291	U1231	G1106	G1044	U982	U920	C853	A792	G727	G664	C599	A539	C477	G413
G1353	A1347	U1232	C1107	C1045	A983	U921	U854	A793	A728	A665	A600	G540	U478	A414
	U1348	C1233	G1108	A1046	C984	G922	U855	A794	A729	G666	A601	C541	U479	A415
A1349	A1290	C1234	C1109	G1047	C985	A923	C856	C795	G730		A602	G542	U480	G416
A1350	G1291	U1235	U1048	G1048	U986	C924	C857	C796	G731	G669		G543	G481	G417
U1351	U1292	U1236	G1113	U1049	C987	G925	C858	C797	C732	G670	A607	U543	G482	C418
C1352	U1293	A1237	C1114	G1050	U988	G926	C859	U798	G733	G671	A608	C544	C483	C419
G1353	A1348	U1238	U1115	C1051	U989	G927	A860	G799	G734	U672	A609	A546	G484	U420
A1361	U1299	A1239	U1116	U1052	C990	G928	G861	G800	C735	A673	U610	A547	U485	U421
A1362	U1300	U1240	U1117	G1053	U991	G929	C862	U801	C736	G674	U611	A548	U486	C422
C1363	U1301	G1241	U1118	C1054	U992	C930	U863	A802	C737	A675	C612	C549	U487	G423
U1364	C1302	U1242	C1119	A1055	G993	C931	A864	G803		A676	C613	G550	C488	G424
G1365	G1304	C1243	C1120	U1056	A994	C932	A865	U804	G741	U677	C614	U551	C489	G425
C1366	U1244	G1245	G1057	C995	C996	G933	C866	C805	G742		C615	U552	C490	G426
A1367	G1245	U1246	U1058	A996	U997	C934	C867	C806	A743		C616	A553	C491	U427
A1368	U1307	A1247	C1059	U998	C998	A935	C868	A807	C744		C617	A554	C492	G428
C1369	U1308	U1248	U1060	U999	C999	C936	C869	C808		G680	C618	U555	A493	U429
G1370	G1309	C1249	U1126	U1061	C999	A937	U870	G809	A747	G682	C619	U556	C501	U438
U1371	A1310	U1250	G1127	U1062	A1000	A938	U871	C810	G748	G683	U619	C556	G494	A430
G1372	G1311	C1251	C1128	C1063	C1001	G939	A872	C811	A749	U684	C620	C557	A495	A431
U1373	U1312	A1251	C1129	G1064	G1002	C940	A873	G812	C750	U685		G558	A496	A432
A1374	G1313	C1252	A1130	U1065	G1003	C941	G874	U813	U751	U686	C624	A559	C497	G433
C1375	C1314	G1253	G1131	C1066	A1004	G942	U875	A814	G752	G688	U625	A560	A498	
U1376	U1315	U1254	C1132	A1067	A1005	U943	C876	A815	A753	C689	U626	U561	A499	C436
A1377	G1316	G1255	G1133	G1068	G1006	G944	C877	A816	C754	G690		U562	G500	U437
C1378	C1317	A1256	U1134	C1069	U1007	G945	A878	C817	G755	G691	A629	A563	C501	U438
G1379	A1318	A1257	U1135	U1070	U1008	A946	C879	G818	C756	U692	A630	C564	A502	U439
U1380	C1319	G1258	C1136	C1071	U1009	G947	C880	A819	U757	G693	C631	U565	C503	C440
U1381	A1320	C1259	U1137	G1072	U1010	C948	G881	U820	G758	A694	U632	G566	C504	A441
C1382	U1321	G1260	G1138	U1073	C1011		C882	G821	A759	A695	G633	G567	G505	G444
C1383	C1322	A1261	C1139	A1012	U1012	U952	C883	U822	G760	A696	C634	C569	G506	G445
A1384	G1323	C1262	C1140	G1013	U1013	U953	U884	C823	G761	U697	A635	G570	C507	G446
G1385	A1324	C1263	C1141	A1014	G1014	G954	G885	G824	U762	G698	U636	U571	U508	A448
C1386	U1325	U1264	G1142	U1015	G1015	U955	G886	A825	G763	C699	C637	A572	A509	A451
U1387	U1326	C1265	G1143	G1078	G1079	U956	G887	C826	C764	G700	U638	A573	A510	C451
C1388	G1327	U1266	C1144	U1077	G1077	U957	U888	U827	G765	U701	U640	A574	C511	U512
	U1328	C1267	A1145	A1081	U1081	U958	G889	U828	A766	A702		A575	C512	G453
A1329	G1329	G1268	C1208	A1082	G1020	A958	C890	G829	A767	G703	U641	G575	C513	



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.95Å 433.08Å 624.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.44 – 3.71 73.44 – 3.71	Depositor EDS
% Data completeness (in resolution range)	75.7 (73.44-3.71) 75.7 (73.44-3.71)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.227 , 0.268 0.242 , 0.281	Depositor DCC
R_{free} test set	9161 reflections (2.06%)	DCC
Wilson B-factor (Å ²)	109.1	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 80.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 452802 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	286150	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.08% 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	AB	0.25	0/1735	0.47	0/2338
1	CB	0.25	0/1735	0.46	0/2338
2	AC	0.27	0/1651	0.48	0/2225
2	CC	0.26	0/1651	0.47	0/2225
3	AD	0.27	0/1665	0.48	0/2227
3	CD	0.30	0/1665	0.50	0/2227
4	AE	0.30	0/1118	0.54	0/1504
4	CE	0.29	0/1118	0.53	0/1504
5	AF	0.26	0/835	0.46	0/1128
5	CF	0.26	0/835	0.46	0/1128
6	AG	0.25	0/1195	0.43	0/1602
6	CG	0.27	0/1187	0.50	0/1591
7	AH	0.27	0/989	0.50	0/1326
7	CH	0.25	0/989	0.47	0/1326
8	AI	0.24	0/1034	0.45	0/1375
8	CI	0.25	0/1034	0.47	0/1375
9	AJ	0.25	0/796	0.48	0/1077
9	CJ	0.24	0/796	0.47	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.26	0/893	0.50	0/1205
11	AL	0.33	0/969	0.62	0/1300
11	CL	0.31	0/969	0.53	0/1300
12	AM	0.36	0/892	0.64	3/1193 (0.3%)
12	CM	0.38	0/884	0.53	0/1181
13	AN	0.26	0/785	0.48	0/1043
13	CN	0.25	0/780	0.43	0/1036
14	AO	0.26	0/722	0.48	0/964
14	CO	0.24	0/722	0.46	0/964
15	AP	0.27	0/659	0.46	0/884
15	CP	0.27	0/648	0.47	0/870
16	AQ	0.33	0/657	0.55	0/881
16	CQ	0.26	0/657	0.46	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AR	0.25	0/462	0.48	0/621
17	CR	0.27	0/462	0.49	0/621
18	AS	0.24	0/652	0.43	0/877
18	CS	0.23	0/652	0.46	0/877
19	AT	0.29	0/671	0.51	0/888
19	CT	0.24	0/671	0.44	0/888
20	AU	0.27	0/430	0.46	0/570
20	CU	0.29	0/430	0.54	0/570
21	AA	0.55	1/36834 (0.0%)	1.44	678/57462 (1.2%)
22	AV	0.59	0/408	1.14	1/634 (0.2%)
22	AX	0.52	0/408	1.04	0/634
22	CV	0.56	0/408	1.14	0/634
22	CX	0.41	0/408	0.82	0/634
23	AW	0.88	0/131	1.88	5/200 (2.5%)
23	CW	0.73	0/131	1.93	7/200 (3.5%)
24	BA	0.76	12/68626 (0.0%)	1.69	1758/107056 (1.6%)
24	DA	0.53	1/68314 (0.0%)	1.46	1365/106569 (1.3%)
25	BB	0.66	0/2828	1.67	74/4410 (1.7%)
26	BC	0.45	0/2121	0.72	1/2852 (0.0%)
26	DC	0.33	0/2121	0.54	0/2852
27	BD	0.50	0/1586	0.75	1/2134 (0.0%)
27	DD	0.31	0/1586	0.55	0/2134
28	BE	0.44	0/1571	0.67	0/2113
28	DE	0.25	0/1571	0.47	0/2113
29	BF	0.41	0/1434	0.68	3/1926 (0.2%)
29	DF	0.35	0/1444	0.73	5/1937 (0.3%)
30	BG	0.43	0/1343	0.65	0/1816
30	DG	0.23	0/1343	0.46	0/1816
31	BH	0.70	6/1122 (0.5%)	0.83	6/1515 (0.4%)
31	DH	0.53	3/1122 (0.3%)	0.67	3/1515 (0.2%)
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.23	0/1046	0.44	0/1410
33	BJ	0.55	0/1152	0.75	0/1551
33	DJ	0.28	0/1152	0.55	0/1551
34	BK	0.55	0/947	0.83	0/1268
34	DK	0.31	0/947	0.54	0/1268
35	BL	0.42	0/1054	0.77	1/1403 (0.1%)
35	DL	0.27	0/1054	0.51	0/1403
36	BM	0.51	0/1093	0.77	1/1460 (0.1%)
36	DM	0.31	0/1093	0.48	0/1460
37	BN	0.55	0/973	0.79	0/1301
37	DN	0.27	0/973	0.49	0/1301
38	BO	0.42	0/902	0.63	0/1209

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DO	0.24	0/902	0.44	0/1209
39	BP	0.51	0/929	0.77	0/1242
39	DP	0.28	0/929	0.49	0/1242
40	BQ	0.60	0/960	0.71	0/1278
40	DQ	0.28	0/960	0.46	0/1278
41	BR	0.56	0/829	0.85	1/1107 (0.1%)
41	DR	0.28	0/829	0.50	0/1107
42	BS	0.50	0/864	0.75	0/1156
42	DS	0.29	0/864	0.54	0/1156
43	BT	0.48	0/744	0.70	0/994
43	DT	0.25	0/744	0.49	0/994
44	BU	0.41	0/787	0.70	0/1051
44	DU	0.25	0/787	0.47	0/1051
45	BV	0.48	0/766	0.66	0/1025
45	DV	0.38	0/766	0.54	0/1025
46	BW	0.51	0/603	0.76	0/797
46	DW	0.26	0/603	0.47	0/797
47	BX	0.42	0/635	0.67	0/848
47	DX	0.30	0/635	0.55	0/848
48	BY	0.40	0/510	0.66	0/677
48	DY	0.23	0/510	0.44	0/677
49	BZ	0.52	0/453	0.77	0/605
49	DZ	0.28	0/453	0.51	0/605
50	B0	0.45	0/450	0.79	0/599
50	D0	0.28	0/450	0.51	0/599
51	B1	0.40	0/416	0.63	0/554
51	D1	0.28	0/416	0.46	0/554
52	B2	0.47	0/380	0.73	0/498
52	D2	0.28	0/380	0.55	0/498
53	B3	0.51	0/513	0.76	0/676
53	D3	0.26	0/513	0.51	0/676
54	B4	0.47	0/303	0.76	0/397
54	D4	0.30	0/303	0.49	0/397
55	CA	0.53	0/36762	1.45	712/57350 (1.2%)
56	DB	0.52	0/2803	1.35	52/4371 (1.2%)
All	All	0.55	23/308631 (0.0%)	1.35	4677/461501 (1.0%)

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
12	AM	0	1
27	BD	0	1
31	BH	0	2
31	DH	0	3
37	BN	0	1
All	All	0	8

The worst 5 of 23 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-13.92	1.29	1.37
31	BH	48	GLU	C-O	9.51	1.41	1.23
24	BA	2451	A	C8-N7	9.03	1.37	1.31
31	DH	49	ALA	CA-CB	-7.88	1.35	1.52
31	BH	48	GLU	CA-CB	6.93	1.69	1.53

The worst 5 of 4677 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BA	2447	G	C6-N1-C2	-22.51	111.59	125.10
24	BA	2451	A	C5-N7-C8	-17.23	95.28	103.90
24	BA	2347	C	N1-C1'-C2'	-16.79	92.17	114.00
24	BA	790	U	P-O3'-C3'	-16.12	100.36	119.70
25	BB	88	C	O4'-C1'-N1	-15.24	96.01	108.20

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	AM	70	ARG	Peptide
27	BD	10	GLY	Peptide
31	BH	48	GLU	Mainchain
31	BH	49	ALA	Mainchain
37	BN	101	GLY	Peptide

5.2 Close contacts

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

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AB	1704	0	1732	253	0
1	CB	1704	0	1732	203	0
2	AC	1624	0	1699	133	0
2	CC	1624	0	1699	149	0
3	AD	1643	0	1710	139	0
3	CD	1643	0	1710	139	0
4	AE	1105	0	1148	196	0
4	CE	1105	0	1148	127	0
5	AF	817	0	808	91	0
5	CF	817	0	808	76	0
6	AG	1181	0	1240	100	0
6	CG	1174	0	1230	154	0
7	AH	979	0	1034	107	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	122	0
8	CI	1022	0	1070	108	0
9	AJ	786	0	828	69	0
9	CJ	786	0	828	114	0
10	AK	877	0	887	103	0
10	CK	877	0	887	82	0
11	AL	955	0	1019	97	0
11	CL	955	0	1019	101	0
12	AM	883	0	944	69	0
12	CM	876	0	937	123	0
13	AN	774	0	827	72	0
13	CN	769	0	822	83	0
14	AO	714	0	737	50	0
14	CO	714	0	737	40	0
15	AP	649	0	666	63	0
15	CP	638	0	656	56	0
16	AQ	648	0	691	70	0
16	CQ	648	0	691	59	0
17	AR	455	0	478	36	0
17	CR	455	0	478	41	0
18	AS	637	0	665	42	0
18	CS	637	0	665	79	0
19	AT	665	0	714	56	0
19	CT	665	0	714	58	0
20	AU	425	0	449	65	0
20	CU	425	0	449	70	0
21	AA	32895	0	16553	1800	0
22	AV	365	0	185	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	AX	365	0	185	20	0
22	CV	365	0	185	26	0
22	CX	365	0	185	11	0
23	AW	120	0	61	8	0
23	CW	120	0	61	4	0
24	BA	61274	0	30819	3133	0
24	DA	60995	0	30679	3843	0
25	BB	2529	0	1281	109	0
26	BC	2082	0	2157	226	0
26	DC	2082	0	2157	230	0
27	BD	1565	0	1616	200	0
27	DD	1565	0	1616	162	0
28	BE	1552	0	1619	158	0
28	DE	1552	0	1619	170	0
29	BF	1410	0	1447	144	0
29	DF	1420	0	1460	183	0
30	BG	1323	0	1374	149	0
30	DG	1323	0	1374	116	0
31	BH	1111	0	1148	108	0
31	DH	1111	0	1148	100	0
32	BI	1032	0	1088	116	0
32	DI	1032	0	1088	69	0
33	BJ	1129	0	1162	160	0
33	DJ	1129	0	1162	122	0
34	BK	938	0	1012	102	0
34	DK	938	0	1012	114	0
35	BL	1045	0	1117	133	0
35	DL	1045	0	1117	130	0
36	BM	1074	0	1157	129	0
36	DM	1074	0	1157	96	0
37	BN	960	0	1000	102	0
37	DN	960	0	1000	107	0
38	BO	892	0	923	82	0
38	DO	892	0	923	90	0
39	BP	917	0	965	120	0
39	DP	917	0	965	87	0
40	BQ	947	0	1022	147	0
40	DQ	947	0	1022	120	0
41	BR	816	0	839	102	0
41	DR	816	0	839	90	0
42	BS	857	0	922	89	0
42	DS	857	0	922	83	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BT	738	0	807	103	0
43	DT	738	0	807	96	0
44	BU	779	0	834	65	0
44	DU	779	0	834	93	0
45	BV	753	0	780	54	0
45	DV	753	0	780	98	0
46	BW	596	0	610	179	0
46	DW	596	0	610	105	0
47	BX	625	0	655	68	0
47	DX	625	0	655	76	0
48	BY	509	0	543	45	0
48	DY	509	0	543	55	0
49	BZ	449	0	491	41	0
49	DZ	449	0	491	40	0
50	B0	444	0	461	36	0
50	D0	444	0	461	63	0
51	B1	409	0	440	43	0
51	D1	409	0	440	33	0
52	B2	377	0	418	28	0
52	D2	377	0	418	42	0
53	B3	504	0	574	41	0
53	D3	504	0	574	54	0
54	B4	302	0	340	40	0
54	D4	302	0	340	27	0
55	CA	32831	0	16521	2003	0
56	DB	2507	0	1270	160	0
57	AA	43	0	0	0	0
57	BA	136	0	0	0	0
57	BB	4	0	0	0	0
57	BD	1	0	0	0	0
57	CA	42	0	0	0	0
57	D4	1	0	0	0	0
57	DA	132	0	0	0	0
57	DB	1	0	0	0	0
57	DC	2	0	0	0	0
57	DJ	1	0	0	0	0
58	B4	1	0	0	0	0
58	D4	1	0	0	0	0
59	AA	196	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	0	0
59	AN	6	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	AT	1	0	0	0	0
59	AU	1	0	0	0	0
59	B2	1	0	0	0	0
59	B3	3	0	0	0	0
59	B4	2	0	0	0	0
59	BA	615	0	0	21	0
59	BB	20	0	0	1	0
59	BC	8	0	0	1	0
59	BD	3	0	0	4	0
59	BE	1	0	0	0	0
59	BL	3	0	0	0	0
59	BN	3	0	0	0	0
59	BT	1	0	0	1	0
59	CA	195	0	0	6	0
59	CE	4	0	0	0	0
59	CI	1	0	0	0	0
59	CL	1	0	0	0	0
59	CN	2	0	0	0	0
59	CT	2	0	0	0	0
59	CU	2	0	0	0	0
59	D2	1	0	0	0	0
59	D3	1	0	0	0	0
59	D4	5	0	0	0	0
59	DA	600	0	0	17	0
59	DB	4	0	0	0	0
59	DC	12	0	0	0	0
59	DD	2	0	0	0	0
59	DE	3	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	6	0	0	0	0
59	DN	2	0	0	1	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	286150	0	191700	19249	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 41.

The worst 5 of 19249 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:AM:67:ASP:O	12:AM:70:ARG:HD2	1.23	1.31

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
55:CA:1213:A:O2'	55:CA:1214:C:H5'	1.29	1.25
24:DA:604:G:O2'	24:DA:605:G:H5'	1.40	1.19
40:BQ:63:ARG:NH1	40:BQ:96:ASP:HA	1.56	1.18
24:DA:297:G:H5''	44:DU:84:PHE:HB2	1.26	1.18

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	
1	AB	216/241 (90%)	119 (55%)	69 (32%)	28 (13%)	0	13
1	CB	216/241 (90%)	144 (67%)	50 (23%)	22 (10%)	1	20
2	AC	204/233 (88%)	140 (69%)	48 (24%)	16 (8%)	1	30
2	CC	204/233 (88%)	136 (67%)	52 (26%)	16 (8%)	1	30
3	AD	203/206 (98%)	143 (70%)	43 (21%)	17 (8%)	1	27
3	CD	203/206 (98%)	136 (67%)	46 (23%)	21 (10%)	1	20
4	AE	148/167 (89%)	105 (71%)	27 (18%)	16 (11%)	1	18
4	CE	148/167 (89%)	100 (68%)	34 (23%)	14 (10%)	1	23
5	AF	98/135 (73%)	68 (69%)	22 (22%)	8 (8%)	1	28
5	CF	98/135 (73%)	65 (66%)	27 (28%)	6 (6%)	2	39
6	AG	149/179 (83%)	103 (69%)	36 (24%)	10 (7%)	2	36
6	CG	148/179 (83%)	84 (57%)	44 (30%)	20 (14%)	0	12
7	AH	127/130 (98%)	90 (71%)	27 (21%)	10 (8%)	1	30
7	CH	127/130 (98%)	88 (69%)	30 (24%)	9 (7%)	2	34
8	AI	125/130 (96%)	81 (65%)	32 (26%)	12 (10%)	1	23
8	CI	125/130 (96%)	88 (70%)	33 (26%)	4 (3%)	6	58
9	AJ	96/103 (93%)	69 (72%)	16 (17%)	11 (12%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	CJ	96/103 (93%)	62 (65%)	22 (23%)	12 (12%)	1	14
10	AK	115/129 (89%)	84 (73%)	22 (19%)	9 (8%)	1	30
10	CK	115/129 (89%)	86 (75%)	19 (16%)	10 (9%)	1	26
11	AL	121/124 (98%)	82 (68%)	27 (22%)	12 (10%)	1	21
11	CL	121/124 (98%)	86 (71%)	26 (22%)	9 (7%)	2	32
12	AM	112/118 (95%)	89 (80%)	16 (14%)	7 (6%)	2	38
12	CM	111/118 (94%)	71 (64%)	28 (25%)	12 (11%)	1	18
13	AN	92/101 (91%)	63 (68%)	18 (20%)	11 (12%)	1	15
13	CN	91/101 (90%)	62 (68%)	24 (26%)	5 (6%)	3	42
14	AO	86/89 (97%)	64 (74%)	20 (23%)	2 (2%)	10	66
14	CO	86/89 (97%)	67 (78%)	19 (22%)	0	100	100
15	AP	80/82 (98%)	52 (65%)	22 (28%)	6 (8%)	2	32
15	CP	78/82 (95%)	52 (67%)	20 (26%)	6 (8%)	1	30
16	AQ	78/84 (93%)	47 (60%)	20 (26%)	11 (14%)	0	11
16	CQ	78/84 (93%)	57 (73%)	16 (20%)	5 (6%)	2	38
17	AR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	3	41
17	CR	53/75 (71%)	39 (74%)	11 (21%)	3 (6%)	3	41
18	AS	77/92 (84%)	61 (79%)	13 (17%)	3 (4%)	5	52
18	CS	77/92 (84%)	55 (71%)	20 (26%)	2 (3%)	8	63
19	AT	83/87 (95%)	63 (76%)	14 (17%)	6 (7%)	2	34
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	5	55
20	AU	49/71 (69%)	26 (53%)	16 (33%)	7 (14%)	0	11
20	CU	49/71 (69%)	23 (47%)	17 (35%)	9 (18%)	0	5
26	BC	269/273 (98%)	192 (71%)	48 (18%)	29 (11%)	1	18
26	DC	269/273 (98%)	169 (63%)	73 (27%)	27 (10%)	1	21
27	BD	207/209 (99%)	141 (68%)	35 (17%)	31 (15%)	0	9
27	DD	207/209 (99%)	129 (62%)	48 (23%)	30 (14%)	0	10
28	BE	199/201 (99%)	138 (69%)	41 (21%)	20 (10%)	1	21
28	DE	199/201 (99%)	129 (65%)	49 (25%)	21 (11%)	1	18
29	BF	175/179 (98%)	133 (76%)	26 (15%)	16 (9%)	1	25
29	DF	176/179 (98%)	94 (53%)	43 (24%)	39 (22%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	BG	174/177 (98%)	114 (66%)	34 (20%)	26 (15%)	0	9
30	DG	174/177 (98%)	109 (63%)	36 (21%)	29 (17%)	0	7
31	BH	147/149 (99%)	63 (43%)	53 (36%)	31 (21%)	0	3
31	DH	147/149 (99%)	78 (53%)	48 (33%)	21 (14%)	0	11
32	BI	139/142 (98%)	84 (60%)	42 (30%)	13 (9%)	1	24
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	12
33	BJ	140/142 (99%)	100 (71%)	22 (16%)	18 (13%)	0	13
33	DJ	140/142 (99%)	95 (68%)	31 (22%)	14 (10%)	1	21
34	BK	120/123 (98%)	86 (72%)	17 (14%)	17 (14%)	0	11
34	DK	120/123 (98%)	79 (66%)	22 (18%)	19 (16%)	0	8
35	BL	141/144 (98%)	106 (75%)	23 (16%)	12 (8%)	1	27
35	DL	141/144 (98%)	80 (57%)	42 (30%)	19 (14%)	0	12
36	BM	134/136 (98%)	95 (71%)	16 (12%)	23 (17%)	0	7
36	DM	134/136 (98%)	89 (66%)	32 (24%)	13 (10%)	1	22
37	BN	118/127 (93%)	85 (72%)	23 (20%)	10 (8%)	1	27
37	DN	118/127 (93%)	73 (62%)	32 (27%)	13 (11%)	1	17
38	BO	114/117 (97%)	84 (74%)	20 (18%)	10 (9%)	1	26
38	DO	114/117 (97%)	80 (70%)	28 (25%)	6 (5%)	3	43
39	BP	112/115 (97%)	74 (66%)	23 (20%)	15 (13%)	0	12
39	DP	112/115 (97%)	67 (60%)	30 (27%)	15 (13%)	0	12
40	BQ	115/118 (98%)	85 (74%)	23 (20%)	7 (6%)	2	39
40	DQ	115/118 (98%)	85 (74%)	22 (19%)	8 (7%)	2	34
41	BR	101/103 (98%)	75 (74%)	14 (14%)	12 (12%)	1	15
41	DR	101/103 (98%)	71 (70%)	20 (20%)	10 (10%)	1	21
42	BS	108/110 (98%)	81 (75%)	20 (18%)	7 (6%)	2	37
42	DS	108/110 (98%)	80 (74%)	18 (17%)	10 (9%)	1	25
43	BT	91/100 (91%)	55 (60%)	20 (22%)	16 (18%)	0	6
43	DT	91/100 (91%)	47 (52%)	30 (33%)	14 (15%)	0	9
44	BU	100/104 (96%)	68 (68%)	16 (16%)	16 (16%)	0	8
44	DU	100/104 (96%)	49 (49%)	29 (29%)	22 (22%)	0	2
45	BV	92/94 (98%)	76 (83%)	15 (16%)	1 (1%)	21	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	DV	92/94 (98%)	59 (64%)	25 (27%)	8 (9%)	1	26
46	BW	77/85 (91%)	32 (42%)	18 (23%)	27 (35%)	0	0
46	DW	77/85 (91%)	34 (44%)	25 (32%)	18 (23%)	0	2
47	BX	75/78 (96%)	58 (77%)	12 (16%)	5 (7%)	2	36
47	DX	75/78 (96%)	49 (65%)	19 (25%)	7 (9%)	1	25
48	BY	61/63 (97%)	39 (64%)	15 (25%)	7 (12%)	1	16
48	DY	61/63 (97%)	45 (74%)	11 (18%)	5 (8%)	1	28
49	BZ	56/59 (95%)	43 (77%)	10 (18%)	3 (5%)	3	43
49	DZ	56/59 (95%)	35 (62%)	14 (25%)	7 (12%)	1	14
50	B0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	13
50	D0	54/57 (95%)	39 (72%)	8 (15%)	7 (13%)	0	13
51	B1	48/55 (87%)	32 (67%)	9 (19%)	7 (15%)	0	10
51	D1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	28
52	B2	44/46 (96%)	36 (82%)	6 (14%)	2 (4%)	4	48
52	D2	44/46 (96%)	30 (68%)	9 (20%)	5 (11%)	1	17
53	B3	62/65 (95%)	50 (81%)	10 (16%)	2 (3%)	6	58
53	D3	62/65 (95%)	42 (68%)	15 (24%)	5 (8%)	1	29
54	B4	36/38 (95%)	27 (75%)	6 (17%)	3 (8%)	1	28
54	D4	36/38 (95%)	22 (61%)	8 (22%)	6 (17%)	0	7
All	All	11238/11970 (94%)	7515 (67%)	2516 (22%)	1207 (11%)	1	18

5 of 1207 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	37	VAL
1	AB	71	THR
1	AB	125	PHE

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	
1	AB	180/199 (90%)	147 (82%)	33 (18%)	2	18
1	CB	180/199 (90%)	158 (88%)	22 (12%)	7	41
2	AC	170/190 (90%)	148 (87%)	22 (13%)	6	38
2	CC	170/190 (90%)	146 (86%)	24 (14%)	5	34
3	AD	172/173 (99%)	147 (86%)	25 (14%)	5	32
3	CD	172/173 (99%)	152 (88%)	20 (12%)	8	44
4	AE	113/126 (90%)	93 (82%)	20 (18%)	3	20
4	CE	113/126 (90%)	100 (88%)	13 (12%)	8	44
5	AF	87/116 (75%)	75 (86%)	12 (14%)	5	35
5	CF	87/116 (75%)	74 (85%)	13 (15%)	4	31
6	AG	124/147 (84%)	117 (94%)	7 (6%)	30	78
6	CG	123/147 (84%)	95 (77%)	28 (23%)	1	10
7	AH	104/105 (99%)	92 (88%)	12 (12%)	8	44
7	CH	104/105 (99%)	91 (88%)	13 (12%)	7	40
8	AI	105/107 (98%)	90 (86%)	15 (14%)	5	33
8	CI	105/107 (98%)	91 (87%)	14 (13%)	6	37
9	AJ	86/90 (96%)	74 (86%)	12 (14%)	5	34
9	CJ	86/90 (96%)	77 (90%)	9 (10%)	10	49
10	AK	90/99 (91%)	80 (89%)	10 (11%)	9	47
10	CK	90/99 (91%)	80 (89%)	10 (11%)	9	47
11	AL	103/104 (99%)	85 (82%)	18 (18%)	3	21
11	CL	103/104 (99%)	88 (85%)	15 (15%)	5	31
12	AM	92/96 (96%)	87 (95%)	5 (5%)	31	79
12	CM	91/96 (95%)	74 (81%)	17 (19%)	2	17
13	AN	79/84 (94%)	73 (92%)	6 (8%)	19	67
13	CN	79/84 (94%)	68 (86%)	11 (14%)	5	35
14	AO	76/77 (99%)	72 (95%)	4 (5%)	32	80
14	CO	76/77 (99%)	72 (95%)	4 (5%)	32	80
15	AP	65/65 (100%)	60 (92%)	5 (8%)	18	66
15	CP	65/65 (100%)	59 (91%)	6 (9%)	13	57
16	AQ	74/78 (95%)	60 (81%)	14 (19%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	6	36
17	AR	48/65 (74%)	46 (96%)	2 (4%)	40	84
17	CR	48/65 (74%)	46 (96%)	2 (4%)	40	84
18	AS	70/79 (89%)	63 (90%)	7 (10%)	11	53
18	CS	70/79 (89%)	59 (84%)	11 (16%)	4	28
19	AT	65/66 (98%)	55 (85%)	10 (15%)	4	29
19	CT	65/66 (98%)	56 (86%)	9 (14%)	5	35
20	AU	44/61 (72%)	37 (84%)	7 (16%)	4	27
20	CU	44/61 (72%)	35 (80%)	9 (20%)	2	13
26	BC	216/218 (99%)	173 (80%)	43 (20%)	2	14
26	DC	216/218 (99%)	191 (88%)	25 (12%)	8	44
27	BD	164/164 (100%)	136 (83%)	28 (17%)	3	23
27	DD	164/164 (100%)	144 (88%)	20 (12%)	7	41
28	BE	165/165 (100%)	130 (79%)	35 (21%)	1	12
28	DE	165/165 (100%)	152 (92%)	13 (8%)	18	65
29	BF	148/150 (99%)	130 (88%)	18 (12%)	7	41
29	DF	149/150 (99%)	124 (83%)	25 (17%)	3	24
30	BG	137/138 (99%)	107 (78%)	30 (22%)	1	11
30	DG	137/138 (99%)	120 (88%)	17 (12%)	7	41
31	BH	114/114 (100%)	97 (85%)	17 (15%)	4	31
31	DH	114/114 (100%)	95 (83%)	19 (17%)	3	24
32	BI	109/110 (99%)	94 (86%)	15 (14%)	5	35
32	DI	109/110 (99%)	102 (94%)	7 (6%)	25	74
33	BJ	116/116 (100%)	90 (78%)	26 (22%)	1	10
33	DJ	116/116 (100%)	106 (91%)	10 (9%)	15	62
34	BK	103/104 (99%)	84 (82%)	19 (18%)	2	18
34	DK	103/104 (99%)	85 (82%)	18 (18%)	3	21
35	BL	102/103 (99%)	81 (79%)	21 (21%)	2	13
35	DL	102/103 (99%)	90 (88%)	12 (12%)	8	43
36	BM	109/109 (100%)	90 (83%)	19 (17%)	3	21
36	DM	109/109 (100%)	100 (92%)	9 (8%)	16	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BN	100/103 (97%)	81 (81%)	19 (19%)	2	16
37	DN	100/103 (97%)	85 (85%)	15 (15%)	4	30
38	BO	86/87 (99%)	69 (80%)	17 (20%)	2	15
38	DO	86/87 (99%)	78 (91%)	8 (9%)	13	57
39	BP	99/100 (99%)	79 (80%)	20 (20%)	2	14
39	DP	99/100 (99%)	91 (92%)	8 (8%)	17	64
40	BQ	89/90 (99%)	73 (82%)	16 (18%)	2	19
40	DQ	89/90 (99%)	79 (89%)	10 (11%)	9	46
41	BR	84/84 (100%)	69 (82%)	15 (18%)	2	20
41	DR	84/84 (100%)	70 (83%)	14 (17%)	3	24
42	BS	93/93 (100%)	73 (78%)	20 (22%)	1	11
42	DS	93/93 (100%)	79 (85%)	14 (15%)	4	30
43	BT	80/84 (95%)	61 (76%)	19 (24%)	1	8
43	DT	80/84 (95%)	74 (92%)	6 (8%)	19	68
44	BU	83/85 (98%)	69 (83%)	14 (17%)	3	24
44	DU	83/85 (98%)	72 (87%)	11 (13%)	6	37
45	BV	78/78 (100%)	64 (82%)	14 (18%)	2	20
45	DV	78/78 (100%)	68 (87%)	10 (13%)	6	39
46	BW	59/63 (94%)	43 (73%)	16 (27%)	1	6
46	DW	59/63 (94%)	44 (75%)	15 (25%)	1	8
47	BX	67/68 (98%)	53 (79%)	14 (21%)	1	12
47	DX	67/68 (98%)	58 (87%)	9 (13%)	6	36
48	BY	55/55 (100%)	44 (80%)	11 (20%)	2	14
48	DY	55/55 (100%)	52 (94%)	3 (6%)	30	79
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	5
49	DZ	48/49 (98%)	41 (85%)	7 (15%)	5	31
50	B0	47/48 (98%)	42 (89%)	5 (11%)	10	49
50	D0	47/48 (98%)	42 (89%)	5 (11%)	10	49
51	B1	45/49 (92%)	37 (82%)	8 (18%)	2	20
51	D1	45/49 (92%)	41 (91%)	4 (9%)	14	60
52	B2	38/38 (100%)	32 (84%)	6 (16%)	4	28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
52	D2	38/38 (100%)	34 (90%)	4 (10%)	10 49
53	B3	51/52 (98%)	44 (86%)	7 (14%)	5 35
53	D3	51/52 (98%)	42 (82%)	9 (18%)	3 21
54	B4	34/34 (100%)	30 (88%)	4 (12%)	8 43
54	D4	34/34 (100%)	29 (85%)	5 (15%)	4 31
All	All	9331/9756 (96%)	7983 (86%)	1348 (14%)	5 32

5 of 1348 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BS	41	LYS
54	B4	9	LYS
41	DR	95	ASP
43	BT	8	LEU
46	BW	71	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 323 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	51	GLN
4	CE	77	ASN
45	DV	51	GLN
47	BX	5	GLN
1	CB	167	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	465 (30%)	230 (15%)
22	AV	17/17 (100%)	2 (11%)	1 (5%)
22	AX	17/17 (100%)	2 (11%)	1 (5%)
22	CV	17/17 (100%)	3 (17%)	1 (5%)
22	CX	16/17 (94%)	2 (12%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	1 (20%)	1 (20%)
24	BA	2850/2903 (98%)	925 (32%)	497 (17%)
24	DA	2838/2903 (97%)	1020 (35%)	505 (17%)
25	BB	117/118 (99%)	32 (27%)	22 (18%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	CA	1529/1530 (99%)	516 (33%)	245 (16%)
56	DB	116/117 (99%)	29 (25%)	13 (11%)
All	All	9059/9184 (98%)	3000 (33%)	1517 (16%)

5 of 3000 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	AA	5	U
21	AA	6	G
21	AA	7	A
21	AA	9	G
21	AA	13	U

5 of 1517 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2638	G
55	CA	497	G
24	DA	2283	C
24	BA	2778	A
55	CA	82	G

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 365 ligands modelled in this entry, 365 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	AB	218/241 (90%)	1.61	70 (32%) 1 2	170, 274, 284, 290	0
1	CB	218/241 (90%)	0.87	30 (13%) 4 4	159, 222, 233, 241	0
2	AC	206/233 (88%)	0.53	6 (2%) 49 31	133, 162, 187, 202	0
2	CC	206/233 (88%)	0.68	12 (5%) 22 15	140, 172, 212, 228	0
3	AD	205/206 (99%)	0.38	10 (4%) 28 18	122, 157, 195, 218	0
3	CD	205/206 (99%)	-0.01	0 100 100	112, 131, 152, 165	0
4	AE	150/167 (89%)	2.45	70 (46%) 1 1	108, 211, 223, 227	0
4	CE	150/167 (89%)	0.64	12 (8%) 12 10	100, 156, 171, 176	0
5	AF	100/135 (74%)	0.46	5 (5%) 28 18	197, 229, 250, 260	0
5	CF	100/135 (74%)	0.86	10 (10%) 8 8	164, 186, 203, 209	0
6	AG	151/179 (84%)	0.41	12 (7%) 13 10	158, 192, 220, 237	0
6	CG	150/179 (83%)	0.53	16 (10%) 6 7	142, 194, 228, 244	0
7	AH	129/130 (99%)	0.43	3 (2%) 57 36	127, 155, 181, 193	0
7	CH	129/130 (99%)	0.93	23 (17%) 2 3	152, 177, 195, 203	0
8	AI	127/130 (97%)	0.95	20 (15%) 3 4	142, 193, 220, 233	0
8	CI	127/130 (97%)	0.66	13 (10%) 7 8	155, 195, 223, 232	0
9	AJ	98/103 (95%)	0.45	2 (2%) 62 39	135, 181, 216, 239	0
9	CJ	98/103 (95%)	0.84	13 (13%) 4 4	155, 196, 230, 240	0
10	AK	117/129 (90%)	0.79	8 (6%) 17 12	132, 195, 243, 254	0
10	CK	117/129 (90%)	0.40	1 (0%) 81 61	125, 155, 181, 196	0
11	AL	123/124 (99%)	0.38	4 (3%) 44 28	89, 106, 131, 150	0
11	CL	123/124 (99%)	0.81	12 (9%) 8 8	117, 139, 155, 161	0
12	AM	114/118 (96%)	0.78	11 (9%) 8 8	157, 219, 252, 264	0
12	CM	113/118 (95%)	0.79	8 (7%) 16 11	195, 269, 309, 322	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AN	96/101 (95%)	0.52	4 (4%) 35 22	142, 165, 217, 227	0
13	CN	95/101 (94%)	1.04	13 (13%) 4 4	155, 207, 265, 284	0
14	AO	88/89 (98%)	0.07	0 100 100	138, 168, 199, 219	0
14	CO	88/89 (98%)	0.16	1 (1%) 77 54	142, 174, 193, 201	0
15	AP	82/82 (100%)	0.93	12 (14%) 3 4	117, 144, 178, 192	0
15	CP	80/82 (97%)	1.44	19 (23%) 1 2	151, 180, 203, 207	0
16	AQ	80/84 (95%)	0.76	2 (2%) 54 34	90, 113, 135, 144	0
16	CQ	80/84 (95%)	1.02	13 (16%) 2 3	99, 123, 145, 163	0
17	AR	55/75 (73%)	0.85	7 (12%) 4 5	175, 198, 219, 234	0
17	CR	55/75 (73%)	0.48	2 (3%) 41 26	148, 165, 180, 187	0
18	AS	79/92 (85%)	1.42	26 (32%) 1 2	171, 203, 244, 257	0
18	CS	79/92 (85%)	1.33	22 (27%) 1 2	223, 265, 319, 334	0
19	AT	85/87 (97%)	0.31	1 (1%) 75 52	114, 141, 164, 180	0
19	CT	85/87 (97%)	1.11	21 (24%) 1 2	194, 242, 275, 283	0
20	AU	51/71 (71%)	0.96	6 (11%) 5 6	133, 168, 248, 252	0
20	CU	51/71 (71%)	0.43	2 (3%) 37 24	126, 150, 183, 193	0
21	AA	1533/1533 (100%)	-0.48	13 (0%) 83 63	76, 150, 233, 282	0
22	AV	17/17 (100%)	0.41	1 (5%) 22 15	142, 154, 182, 203	0
22	AX	17/17 (100%)	-0.19	1 (5%) 22 15	139, 144, 186, 195	0
22	CV	17/17 (100%)	0.01	1 (5%) 22 15	158, 162, 193, 208	0
22	CX	17/17 (100%)	2.27	9 (52%) 0 1	187, 193, 221, 222	0
23	AW	6/6 (100%)	0.27	0 100 100	136, 138, 143, 152	0
23	CW	6/6 (100%)	0.65	0 100 100	160, 160, 168, 179	0
24	BA	2854/2903 (98%)	-0.40	36 (1%) 74 50	52, 81, 194, 355	0
24	DA	2841/2903 (97%)	0.24	112 (3%) 37 24	132, 200, 303, 402	0
25	BB	118/118 (100%)	-0.60	0 100 100	66, 101, 133, 171	0
26	BC	271/273 (99%)	0.18	3 (1%) 77 54	60, 99, 129, 161	0
26	DC	271/273 (99%)	0.71	25 (9%) 9 8	133, 157, 179, 190	0
27	BD	209/209 (100%)	0.07	1 (0%) 88 73	55, 75, 114, 129	0
27	DD	209/209 (100%)	1.30	52 (24%) 1 2	147, 200, 232, 242	0
28	BE	201/201 (100%)	0.10	2 (0%) 79 57	56, 96, 129, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DE	201/201 (100%)	1.15	41 (20%) 1 2	154, 282, 335, 351	0
29	BF	177/179 (98%)	0.96	30 (16%) 2 3	120, 166, 201, 215	0
29	DF	178/179 (99%)	1.71	54 (30%) 1 2	307, 314, 321, 323	0
30	BG	176/177 (99%)	0.29	2 (1%) 77 54	83, 108, 134, 152	0
30	DG	176/177 (99%)	1.51	50 (28%) 1 2	186, 221, 245, 259	0
31	BH	149/149 (100%)	1.75	54 (36%) 1 1	110, 239, 259, 264	0
31	DH	149/149 (100%)	1.38	37 (24%) 1 2	186, 240, 256, 260	0
32	BI	141/142 (99%)	1.96	53 (37%) 1 1	243, 307, 359, 366	0
32	DI	141/142 (99%)	2.47	80 (56%) 0 1	367, 394, 412, 419	0
33	BJ	142/142 (100%)	-0.02	0 100 100	59, 76, 102, 132	0
33	DJ	142/142 (100%)	1.21	34 (23%) 1 2	161, 201, 223, 233	0
34	BK	122/123 (99%)	0.16	1 (0%) 83 63	55, 73, 113, 169	0
34	DK	122/123 (99%)	1.32	36 (29%) 1 2	151, 171, 189, 198	0
35	BL	143/144 (99%)	-0.00	1 (0%) 84 66	55, 93, 124, 136	0
35	DL	143/144 (99%)	1.20	34 (23%) 1 2	166, 240, 288, 297	0
36	BM	136/136 (100%)	0.18	0 100 100	58, 81, 111, 138	0
36	DM	136/136 (100%)	1.67	47 (34%) 1 1	144, 181, 210, 232	0
37	BN	120/127 (94%)	0.23	0 100 100	61, 76, 96, 141	0
37	DN	120/127 (94%)	1.94	46 (38%) 1 1	183, 222, 252, 266	0
38	BO	116/117 (99%)	0.13	1 (0%) 81 61	96, 105, 123, 147	0
38	DO	116/117 (99%)	1.92	45 (38%) 1 1	286, 293, 297, 303	0
39	BP	114/115 (99%)	0.22	0 100 100	64, 81, 119, 134	0
39	DP	114/115 (99%)	1.40	30 (26%) 1 2	179, 203, 220, 230	0
40	BQ	117/118 (99%)	-0.15	0 100 100	56, 77, 99, 120	0
40	DQ	117/118 (99%)	1.16	21 (17%) 2 3	184, 211, 240, 247	0
41	BR	103/103 (100%)	0.07	0 100 100	55, 87, 114, 131	0
41	DR	103/103 (100%)	1.89	42 (40%) 1 1	173, 249, 271, 277	0
42	BS	110/110 (100%)	-0.04	0 100 100	55, 70, 105, 159	0
42	DS	110/110 (100%)	1.59	36 (32%) 1 2	159, 223, 269, 278	0
43	BT	93/100 (93%)	0.37	1 (1%) 77 54	65, 105, 142, 151	0
43	DT	93/100 (93%)	2.14	46 (49%) 1 1	206, 253, 285, 294	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BU	102/104 (98%)	0.55	5 (4%) 28 18	89, 114, 136, 158	0
44	DU	102/104 (98%)	2.57	53 (51%) 0 1	272, 312, 355, 358	0
45	BV	94/94 (100%)	0.10	0 100 100	71, 90, 116, 126	0
45	DV	94/94 (100%)	1.13	17 (18%) 2 3	228, 241, 252, 254	0
46	BW	79/85 (92%)	0.16	2 (2%) 54 34	68, 86, 136, 156	0
46	DW	79/85 (92%)	2.49	46 (58%) 0 1	156, 216, 233, 252	0
47	BX	77/78 (98%)	0.11	0 100 100	65, 101, 124, 137	0
47	DX	77/78 (98%)	0.93	11 (14%) 3 4	157, 185, 209, 224	0
48	BY	63/63 (100%)	0.23	2 (3%) 45 28	101, 123, 149, 159	0
48	DY	63/63 (100%)	1.25	14 (22%) 1 2	264, 288, 316, 329	0
49	BZ	58/59 (98%)	0.35	1 (1%) 67 44	64, 74, 111, 141	0
49	DZ	58/59 (98%)	1.15	10 (17%) 2 3	188, 215, 238, 248	0
50	B0	56/57 (98%)	-0.22	0 100 100	54, 77, 113, 132	0
50	D0	56/57 (98%)	1.28	11 (19%) 2 2	157, 230, 260, 265	0
51	B1	50/55 (90%)	0.66	3 (6%) 21 15	76, 100, 118, 132	0
51	D1	50/55 (90%)	1.65	18 (36%) 1 1	174, 207, 228, 238	0
52	B2	46/46 (100%)	0.04	0 100 100	62, 75, 103, 137	0
52	D2	46/46 (100%)	0.77	3 (6%) 18 13	155, 182, 198, 202	0
53	B3	64/65 (98%)	-0.00	0 100 100	58, 73, 96, 120	0
53	D3	64/65 (98%)	1.38	14 (21%) 1 2	180, 194, 211, 215	0
54	B4	38/38 (100%)	0.32	0 100 100	69, 84, 110, 120	0
54	D4	38/38 (100%)	1.37	9 (23%) 1 2	171, 187, 198, 203	0
55	CA	1530/1530 (100%)	-0.14	31 (2%) 62 39	109, 171, 272, 362	0
56	DB	117/117 (100%)	-0.00	1 (0%) 81 61	219, 294, 300, 302	0
All	All	20511/21154 (96%)	0.40	1851 (9%) 10 9	52, 166, 293, 419	0

The worst 5 of 1851 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
55	CA	209	U	14.0
24	BA	2179	C	13.3
24	BA	2180	U	13.0
24	DA	2799	A	12.9
1	AB	194	GLY	12.8

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
57	MG	DA	3020	1/1	1.88	423.75	229,229,229,229	0
57	MG	CA	1619	1/1	0.95	201.75	135,135,135,135	0
57	MG	DA	3058	1/1	0.96	106.12	162,162,162,162	0
57	MG	DA	3074	1/1	1.52	62.26	187,187,187,187	0
57	MG	BA	3015	1/1	0.55	48.17	55,55,55,55	0
57	MG	BA	3119	1/1	0.37	47.68	68,68,68,68	0
57	MG	CA	1627	1/1	0.38	47.40	136,136,136,136	0
57	MG	DA	3063	1/1	1.63	47.07	157,157,157,157	0
57	MG	DA	3064	1/1	0.49	46.77	157,157,157,157	0
57	MG	DA	3011	1/1	1.17	40.31	184,184,184,184	0
57	MG	DA	3109	1/1	0.74	39.45	145,145,145,145	0
57	MG	DA	3060	1/1	0.90	39.26	132,132,132,132	0
57	MG	DA	3002	1/1	1.22	38.48	212,212,212,212	0
57	MG	BA	3062	1/1	0.74	37.61	55,55,55,55	0
57	MG	BB	201	1/1	0.43	37.32	118,118,118,118	0
57	MG	AA	1627	1/1	1.51	36.43	142,142,142,142	0
57	MG	DA	3005	1/1	1.03	31.83	197,197,197,197	0
57	MG	BA	3026	1/1	0.41	29.22	59,59,59,59	0
57	MG	BA	3096	1/1	0.20	28.99	61,61,61,61	0
57	MG	DA	3078	1/1	0.61	28.04	144,144,144,144	0
57	MG	AA	1619	1/1	0.47	27.61	162,162,162,162	0
57	MG	BA	3061	1/1	0.37	27.06	56,56,56,56	0
57	MG	BA	3136	1/1	0.41	24.61	64,64,64,64	0
57	MG	DA	3038	1/1	0.38	23.52	197,197,197,197	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1628	1/1	1.03	22.03	99,99,99,99	0
57	MG	DA	3076	1/1	0.99	19.70	145,145,145,145	0
57	MG	BA	3002	1/1	0.36	18.75	61,61,61,61	0
57	MG	AA	1602	1/1	0.39	18.53	97,97,97,97	0
57	MG	BA	3131	1/1	0.51	17.67	68,68,68,68	0
57	MG	AA	1636	1/1	0.30	17.55	154,154,154,154	0
57	MG	BA	3071	1/1	0.35	16.73	55,55,55,55	0
57	MG	CA	1625	1/1	0.48	16.23	127,127,127,127	0
57	MG	BA	3085	1/1	0.39	16.10	59,59,59,59	0
57	MG	BA	3058	1/1	0.49	15.71	63,63,63,63	0
57	MG	AA	1641	1/1	0.41	15.63	108,108,108,108	0
57	MG	DA	3108	1/1	0.61	15.14	172,172,172,172	0
57	MG	BA	3037	1/1	0.24	14.92	58,58,58,58	0
57	MG	DA	3086	1/1	0.30	14.23	196,196,196,196	0
57	MG	DA	3062	1/1	0.99	14.22	160,160,160,160	0
57	MG	CA	1620	1/1	0.49	13.82	150,150,150,150	0
57	MG	DA	3091	1/1	0.83	13.66	174,174,174,174	0
57	MG	CA	1640	1/1	0.59	13.65	118,118,118,118	0
57	MG	BA	3124	1/1	0.92	13.34	59,59,59,59	0
57	MG	BA	3016	1/1	0.29	13.26	56,56,56,56	0
57	MG	BA	3098	1/1	0.36	12.94	72,72,72,72	0
57	MG	DA	3127	1/1	0.60	11.90	138,138,138,138	0
57	MG	BA	3133	1/1	0.60	11.79	73,73,73,73	0
57	MG	BA	3045	1/1	0.32	11.68	80,80,80,80	0
57	MG	AA	1625	1/1	0.36	11.66	114,114,114,114	0
57	MG	DA	3022	1/1	0.90	10.88	152,152,152,152	0
57	MG	AA	1607	1/1	0.48	10.64	113,113,113,113	0
57	MG	DA	3016	1/1	1.10	9.87	175,175,175,175	0
57	MG	CA	1614	1/1	0.53	9.57	146,146,146,146	0
57	MG	DA	3075	1/1	0.78	9.49	155,155,155,155	0
57	MG	DA	3004	1/1	0.22	9.47	206,206,206,206	0
57	MG	BA	3060	1/1	0.32	9.43	56,56,56,56	0
57	MG	DJ	201	1/1	0.65	9.27	183,183,183,183	0
57	MG	DA	3121	1/1	0.43	9.21	206,206,206,206	0
57	MG	DA	3094	1/1	0.58	9.17	173,173,173,173	0
57	MG	BA	3057	1/1	0.31	9.12	61,61,61,61	0
57	MG	DA	3131	1/1	0.55	9.07	181,181,181,181	0
57	MG	DA	3088	1/1	0.29	9.02	180,180,180,180	0
57	MG	BA	3072	1/1	0.33	8.72	55,55,55,55	0
57	MG	BA	3011	1/1	0.29	8.63	62,62,62,62	0
57	MG	BA	3135	1/1	0.33	8.54	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	1621	1/1	0.25	8.32	80,80,80,80	0
57	MG	AA	1626	1/1	0.30	8.30	136,136,136,136	0
57	MG	CA	1636	1/1	1.57	8.22	120,120,120,120	0
57	MG	CA	1626	1/1	0.33	7.65	139,139,139,139	0
57	MG	BA	3030	1/1	0.40	7.64	58,58,58,58	0
57	MG	DA	3082	1/1	0.42	7.56	220,220,220,220	0
57	MG	DA	3071	1/1	0.33	7.23	184,184,184,184	0
57	MG	DA	3129	1/1	1.47	7.12	132,132,132,132	0
57	MG	BA	3021	1/1	0.25	6.97	59,59,59,59	0
57	MG	DA	3072	1/1	0.41	6.78	182,182,182,182	0
57	MG	DA	3045	1/1	0.26	6.49	188,188,188,188	0
57	MG	CA	1623	1/1	0.27	6.25	123,123,123,123	0
57	MG	CA	1610	1/1	0.23	6.22	181,181,181,181	0
57	MG	DA	3122	1/1	0.32	6.21	146,146,146,146	0
57	MG	BA	3028	1/1	0.31	6.18	57,57,57,57	0
57	MG	DA	3036	1/1	0.43	6.04	212,212,212,212	0
57	MG	BA	3035	1/1	0.27	5.90	72,72,72,72	0
57	MG	BA	3115	1/1	0.48	5.86	65,65,65,65	0
57	MG	BA	3020	1/1	0.36	5.76	63,63,63,63	0
57	MG	BA	3056	1/1	0.31	5.65	64,64,64,64	0
57	MG	BA	3014	1/1	0.28	5.57	55,55,55,55	0
57	MG	CA	1615	1/1	0.19	5.55	156,156,156,156	0
57	MG	BA	3093	1/1	0.27	5.44	104,104,104,104	0
57	MG	DA	3124	1/1	0.37	5.36	168,168,168,168	0
57	MG	BA	3022	1/1	0.23	5.35	55,55,55,55	0
57	MG	DA	3059	1/1	0.29	5.31	136,136,136,136	0
57	MG	D4	101	1/1	1.37	5.29	183,183,183,183	0
57	MG	DA	3106	1/1	0.41	4.93	228,228,228,228	0
57	MG	DA	3007	1/1	0.34	4.83	250,250,250,250	0
57	MG	DA	3046	1/1	0.26	4.73	172,172,172,172	0
57	MG	DA	3021	1/1	0.38	4.73	151,151,151,151	0
57	MG	DA	3041	1/1	0.36	4.60	176,176,176,176	0
57	MG	BA	3031	1/1	0.23	4.57	59,59,59,59	0
57	MG	CA	1611	1/1	0.27	4.54	132,132,132,132	0
57	MG	DA	3053	1/1	0.17	4.51	144,144,144,144	0
57	MG	DA	3015	1/1	1.18	4.44	164,164,164,164	0
57	MG	DA	3097	1/1	0.36	4.31	156,156,156,156	0
57	MG	AA	1629	1/1	0.24	4.26	161,161,161,161	0
57	MG	BA	3112	1/1	0.22	4.22	64,64,64,64	0
57	MG	DA	3092	1/1	0.28	4.08	198,198,198,198	0
57	MG	AA	1642	1/1	0.25	3.98	90,90,90,90	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3117	1/1	0.46	3.44	170,170,170,170	0
57	MG	DA	3026	1/1	0.95	3.41	160,160,160,160	0
57	MG	BA	3126	1/1	0.25	3.41	70,70,70,70	0
57	MG	DA	3054	1/1	0.33	3.41	155,155,155,155	0
57	MG	DA	3114	1/1	0.27	3.40	135,135,135,135	0
57	MG	BA	3088	1/1	0.13	3.38	77,77,77,77	0
57	MG	CA	1637	1/1	0.28	3.35	112,112,112,112	0
57	MG	BA	3007	1/1	0.16	3.28	111,111,111,111	0
57	MG	DA	3104	1/1	0.26	3.03	142,142,142,142	0
57	MG	DA	3128	1/1	0.72	2.64	132,132,132,132	0
57	MG	DA	3125	1/1	0.29	2.62	187,187,187,187	0
57	MG	BA	3041	1/1	0.20	2.61	60,60,60,60	0
57	MG	DA	3051	1/1	0.25	2.55	160,160,160,160	0
57	MG	BA	3084	1/1	0.19	2.54	61,61,61,61	0
57	MG	AA	1610	1/1	0.13	2.53	155,155,155,155	0
57	MG	AA	1637	1/1	0.57	2.46	118,118,118,118	0
57	MG	AA	1605	1/1	0.21	2.18	124,124,124,124	0
57	MG	DA	3001	1/1	0.28	2.11	206,206,206,206	0
57	MG	BA	3125	1/1	0.24	2.10	58,58,58,58	0
57	MG	AA	1628	1/1	0.27	2.07	134,134,134,134	0
57	MG	AA	1624	1/1	0.17	2.03	131,131,131,131	0
57	MG	BA	3109	1/1	0.20	1.99	60,60,60,60	0
57	MG	CA	1630	1/1	0.22	1.97	99,99,99,99	0
57	MG	DA	3028	1/1	0.56	1.94	165,165,165,165	0
57	MG	BA	3048	1/1	0.20	1.94	91,91,91,91	0
57	MG	DA	3084	1/1	0.30	1.94	214,214,214,214	0
57	MG	DA	3098	1/1	0.28	1.90	170,170,170,170	0
57	MG	CA	1607	1/1	0.23	1.90	134,134,134,134	0
57	MG	DA	3069	1/1	0.49	1.80	139,139,139,139	0
57	MG	BA	3095	1/1	0.16	1.72	92,92,92,92	0
57	MG	BD	301	1/1	0.20	1.67	55,55,55,55	0
57	MG	BA	3108	1/1	0.20	1.57	58,58,58,58	0
57	MG	AA	1630	1/1	0.25	1.55	99,99,99,99	0
57	MG	DA	3089	1/1	0.38	1.55	179,179,179,179	0
57	MG	BA	3067	1/1	0.18	1.42	57,57,57,57	0
57	MG	AA	1635	1/1	0.18	1.39	148,148,148,148	0
57	MG	DA	3065	1/1	0.32	1.31	152,152,152,152	0
57	MG	DA	3118	1/1	0.24	1.31	181,181,181,181	0
57	MG	AA	1611	1/1	0.21	1.30	126,126,126,126	0
57	MG	DA	3096	1/1	0.39	1.29	190,190,190,190	0
57	MG	DA	3029	1/1	0.40	1.22	179,179,179,179	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	BA	3043	1/1	0.19	1.18	68,68,68,68	0
57	MG	DA	3047	1/1	0.24	1.18	208,208,208,208	0
57	MG	DA	3100	1/1	0.32	1.16	150,150,150,150	0
57	MG	BA	3122	1/1	0.22	1.15	57,57,57,57	0
57	MG	DA	3018	1/1	0.37	1.13	248,248,248,248	0
57	MG	DA	3123	1/1	0.23	1.08	225,225,225,225	0
57	MG	AA	1633	1/1	0.15	1.04	128,128,128,128	0
57	MG	DA	3044	1/1	0.25	0.93	210,210,210,210	0
57	MG	CA	1618	1/1	0.28	0.91	148,148,148,148	0
57	MG	DA	3068	1/1	0.25	0.89	143,143,143,143	0
57	MG	BA	3116	1/1	0.17	0.87	55,55,55,55	0
57	MG	CA	1608	1/1	0.20	0.86	121,121,121,121	0
57	MG	CA	1624	1/1	0.27	0.83	99,99,99,99	0
57	MG	BA	3074	1/1	0.17	0.82	54,54,54,54	0
57	MG	BA	3102	1/1	0.19	0.80	57,57,57,57	0
57	MG	DA	3111	1/1	0.35	0.77	160,160,160,160	0
57	MG	BA	3005	1/1	0.14	0.76	91,91,91,91	0
57	MG	BA	3004	1/1	0.20	0.74	86,86,86,86	0
57	MG	AA	1620	1/1	0.16	0.74	186,186,186,186	0
57	MG	AA	1608	1/1	0.20	0.71	105,105,105,105	0
57	MG	AA	1614	1/1	0.19	0.67	150,150,150,150	0
57	MG	BA	3080	1/1	0.17	0.63	93,93,93,93	0
57	MG	AA	1617	1/1	0.28	0.63	150,150,150,150	0
57	MG	CA	1616	1/1	0.35	0.61	199,199,199,199	0
57	MG	DA	3013	1/1	0.29	0.60	165,165,165,165	0
57	MG	CA	1641	1/1	0.18	0.58	151,151,151,151	0
57	MG	BA	3075	1/1	0.28	0.48	58,58,58,58	0
57	MG	DA	3057	1/1	0.33	0.47	133,133,133,133	0
57	MG	DA	3132	1/1	0.25	0.43	198,198,198,198	0
57	MG	BB	202	1/1	0.14	0.42	127,127,127,127	0
57	MG	CA	1603	1/1	0.14	0.40	141,141,141,141	0
57	MG	BA	3132	1/1	0.27	0.39	61,61,61,61	0
57	MG	DA	3113	1/1	0.18	0.36	182,182,182,182	0
57	MG	CA	1631	1/1	0.21	0.34	130,130,130,130	0
57	MG	AA	1638	1/1	0.19	0.30	107,107,107,107	0
57	MG	BA	3068	1/1	0.17	0.30	65,65,65,65	0
57	MG	AA	1616	1/1	0.26	0.26	161,161,161,161	0
57	MG	BA	3089	1/1	0.18	0.25	66,66,66,66	0
57	MG	DA	3037	1/1	0.22	0.19	204,204,204,204	0
57	MG	BA	3051	1/1	0.13	0.07	57,57,57,57	0
57	MG	DA	3042	1/1	0.24	0.07	179,179,179,179	0
57	MG	BA	3047	1/1	0.19	-0.01	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	CA	1617	1/1	0.24	-0.04	183,183,183,183	0
57	MG	DA	3120	1/1	0.23	-0.08	159,159,159,159	0
57	MG	AA	1631	1/1	0.18	-0.16	114,114,114,114	0
57	MG	BA	3130	1/1	0.16	-0.19	68,68,68,68	0
57	MG	DA	3040	1/1	0.26	-0.22	171,171,171,171	0
57	MG	CA	1633	1/1	0.13	-0.22	123,123,123,123	0
57	MG	DA	3023	1/1	0.24	-0.29	148,148,148,148	0
57	MG	DA	3030	1/1	0.30	-0.30	164,164,164,164	0
57	MG	DA	3009	1/1	0.22	-0.32	199,199,199,199	0
57	MG	BA	3070	1/1	0.17	-0.35	158,158,158,158	0
57	MG	BA	3019	1/1	0.12	-0.37	86,86,86,86	0
57	MG	DA	3017	1/1	0.21	-0.37	187,187,187,187	0
57	MG	BA	3046	1/1	0.18	-0.37	77,77,77,77	0
57	MG	DA	3019	1/1	0.15	-0.41	245,245,245,245	0
57	MG	DA	3039	1/1	0.23	-0.41	186,186,186,186	0
57	MG	DA	3081	1/1	0.21	-0.46	182,182,182,182	0
57	MG	BA	3107	1/1	0.18	-0.48	67,67,67,67	0
57	MG	DA	3073	1/1	0.17	-0.52	312,312,312,312	0
57	MG	BA	3050	1/1	0.15	-0.52	56,56,56,56	0
57	MG	DA	3006	1/1	0.15	-0.52	296,296,296,296	0
57	MG	BA	3013	1/1	0.18	-0.52	55,55,55,55	0
57	MG	BA	3128	1/1	0.13	-0.53	64,64,64,64	0
57	MG	DA	3126	1/1	0.18	-0.60	199,199,199,199	0
57	MG	DA	3056	1/1	0.20	-0.61	141,141,141,141	0
57	MG	BA	3076	1/1	0.16	-0.61	62,62,62,62	0
57	MG	DA	3014	1/1	0.28	-0.64	162,162,162,162	0
57	MG	DB	201	1/1	0.16	-0.64	224,224,224,224	0
57	MG	CA	1632	1/1	0.15	-0.71	210,210,210,210	0
57	MG	BA	3104	1/1	0.17	-0.72	55,55,55,55	0
57	MG	DA	3102	1/1	0.20	-0.76	141,141,141,141	0
57	MG	AA	1601	1/1	0.10	-0.76	133,133,133,133	0
57	MG	BA	3105	1/1	0.17	-0.77	55,55,55,55	0
57	MG	BA	3100	1/1	0.14	-0.79	74,74,74,74	0
57	MG	BA	3120	1/1	0.17	-0.79	59,59,59,59	0
57	MG	DC	302	1/1	0.18	-0.82	140,140,140,140	0
57	MG	CA	1602	1/1	0.17	-0.84	177,177,177,177	0
57	MG	DA	3087	1/1	0.17	-0.90	208,208,208,208	0
57	MG	BA	3024	1/1	0.15	-0.91	60,60,60,60	0
57	MG	AA	1609	1/1	0.16	-0.91	118,118,118,118	0
57	MG	DA	3095	1/1	0.19	-0.93	152,152,152,152	0
57	MG	DA	3116	1/1	0.13	-0.93	133,133,133,133	0
57	MG	BA	3106	1/1	0.14	-0.94	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	DA	3099	1/1	0.17	-0.97	211,211,211,211	0
57	MG	DA	3110	1/1	0.15	-0.99	219,219,219,219	0
57	MG	DA	3034	1/1	0.17	-1.01	158,158,158,158	0
57	MG	AA	1606	1/1	0.14	-1.08	119,119,119,119	0
57	MG	BA	3121	1/1	0.11	-1.10	64,64,64,64	0
57	MG	DA	3024	1/1	0.19	-1.11	162,162,162,162	0
57	MG	CA	1606	1/1	0.15	-1.14	124,124,124,124	0
57	MG	DA	3119	1/1	0.12	-1.15	147,147,147,147	0
57	MG	BA	3114	1/1	0.11	-1.19	88,88,88,88	0
57	MG	DA	3130	1/1	0.20	-1.21	170,170,170,170	0
57	MG	AA	1618	1/1	0.17	-1.22	131,131,131,131	0
57	MG	AA	1603	1/1	0.10	-1.24	93,93,93,93	0
57	MG	BA	3034	1/1	0.16	-1.25	57,57,57,57	0
57	MG	DA	3031	1/1	0.17	-1.28	159,159,159,159	0
57	MG	BA	3038	1/1	0.14	-1.29	59,59,59,59	0
57	MG	DA	3049	1/1	0.09	-1.30	249,249,249,249	0
57	MG	DA	3035	1/1	0.10	-1.31	155,155,155,155	0
57	MG	DA	3079	1/1	0.21	-1.31	148,148,148,148	0
57	MG	DA	3115	1/1	0.15	-1.33	154,154,154,154	0
57	MG	DA	3012	1/1	0.29	-1.34	168,168,168,168	0
57	MG	BB	203	1/1	0.10	-1.36	69,69,69,69	0
57	MG	CA	1609	1/1	0.16	-1.36	131,131,131,131	0
57	MG	AA	1615	1/1	0.14	-1.37	153,153,153,153	0
57	MG	DA	3027	1/1	0.16	-1.46	171,171,171,171	0
57	MG	DA	3101	1/1	0.18	-1.52	155,155,155,155	0
57	MG	DA	3083	1/1	0.08	-1.54	303,303,303,303	0
57	MG	DA	3033	1/1	0.14	-1.56	162,162,162,162	0
57	MG	DA	3105	1/1	0.13	-1.56	159,159,159,159	0
58	ZN	D4	102	1/1	0.09	-1.57	99,99,99,99	0
57	MG	BA	3091	1/1	0.13	-1.59	88,88,88,88	0
57	MG	AA	1639	1/1	0.08	-1.61	143,143,143,143	0
57	MG	AA	1623	1/1	0.06	-1.61	129,129,129,129	0
57	MG	DA	3080	1/1	0.09	-1.63	134,134,134,134	0
57	MG	AA	1613	1/1	0.12	-1.63	95,95,95,95	0
57	MG	AA	1634	1/1	0.11	-1.69	121,121,121,121	0
57	MG	CA	1622	1/1	0.09	-1.70	216,216,216,216	0
57	MG	BA	3101	1/1	0.14	-1.72	54,54,54,54	0
57	MG	DA	3093	1/1	0.16	-1.72	208,208,208,208	0
57	MG	CA	1601	1/1	0.11	-1.74	224,224,224,224	0
57	MG	BA	3066	1/1	0.11	-1.75	61,61,61,61	0
57	MG	BA	3033	1/1	0.17	-1.79	56,56,56,56	0
57	MG	DA	3085	1/1	0.21	-1.79	167,167,167,167	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
57	MG	CA	1621	1/1	0.14	-1.80	115,115,115,115	0
57	MG	BA	3111	1/1	0.10	-1.80	55,55,55,55	0
57	MG	CA	1638	1/1	0.10	-1.81	226,226,226,226	0
57	MG	CA	1612	1/1	0.18	-1.81	124,124,124,124	0
57	MG	BA	3052	1/1	0.11	-1.82	54,54,54,54	0
57	MG	DA	3050	1/1	0.20	-1.82	180,180,180,180	0
57	MG	DA	3061	1/1	0.13	-1.84	134,134,134,134	0
57	MG	DA	3025	1/1	0.10	-1.89	135,135,135,135	0
57	MG	BA	3017	1/1	0.12	-1.93	56,56,56,56	0
57	MG	BA	3010	1/1	0.13	-1.94	64,64,64,64	0
57	MG	BA	3077	1/1	0.14	-1.94	63,63,63,63	0
57	MG	BA	3006	1/1	0.07	-1.94	101,101,101,101	0
57	MG	AA	1604	1/1	0.08	-1.95	157,157,157,157	0
57	MG	BA	3127	1/1	0.10	-2.02	57,57,57,57	0
57	MG	CA	1642	1/1	0.10	-2.03	170,170,170,170	0
57	MG	BA	3092	1/1	0.08	-2.03	127,127,127,127	0
57	MG	BA	3134	1/1	0.14	-2.03	55,55,55,55	0
57	MG	BA	3023	1/1	0.16	-2.09	59,59,59,59	0
58	ZN	B4	101	1/1	0.08	-2.14	99,99,99,99	0
57	MG	BA	3103	1/1	0.07	-2.18	81,81,81,81	0
57	MG	CA	1613	1/1	0.11	-2.19	121,121,121,121	0
57	MG	CA	1629	1/1	0.19	-2.21	157,157,157,157	0
57	MG	CA	1634	1/1	0.11	-2.28	153,153,153,153	0
57	MG	DA	3107	1/1	0.15	-2.33	137,137,137,137	0
57	MG	DA	3112	1/1	0.12	-2.40	143,143,143,143	0
57	MG	BA	3008	1/1	0.12	-2.42	59,59,59,59	0
57	MG	BA	3012	1/1	0.12	-2.43	54,54,54,54	0
57	MG	BA	3055	1/1	0.10	-2.52	62,62,62,62	0
57	MG	AA	1622	1/1	0.10	-2.52	113,113,113,113	0
57	MG	CA	1604	1/1	0.04	-2.60	117,117,117,117	0
57	MG	BA	3094	1/1	0.11	-2.61	92,92,92,92	0
57	MG	DA	3066	1/1	0.13	-2.64	150,150,150,150	0
57	MG	DA	3055	1/1	0.13	-2.68	136,136,136,136	0
57	MG	DA	3103	1/1	0.15	-2.74	150,150,150,150	0
57	MG	BA	3123	1/1	0.13	-2.78	79,79,79,79	0
57	MG	BA	3063	1/1	0.11	-2.86	54,54,54,54	0
57	MG	BA	3032	1/1	0.13	-2.90	57,57,57,57	0
57	MG	DA	3043	1/1	0.12	-2.92	208,208,208,208	0
57	MG	BA	3078	1/1	0.08	-2.92	100,100,100,100	0
57	MG	DA	3052	1/1	0.10	-2.92	144,144,144,144	0
57	MG	BA	3018	1/1	0.07	-2.94	80,80,80,80	0
57	MG	BA	3079	1/1	0.07	-3.01	110,110,110,110	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	DA	3090	1/1	0.08	-3.01	200,200,200,200	0
57	MG	AA	1643	1/1	0.09	-3.03	101,101,101,101	0
57	MG	BA	3069	1/1	0.11	-3.04	65,65,65,65	0
57	MG	BA	3025	1/1	0.10	-3.08	59,59,59,59	0
57	MG	BB	204	1/1	0.08	-3.22	74,74,74,74	0
57	MG	DA	3008	1/1	0.12	-3.28	198,198,198,198	0
57	MG	DA	3067	1/1	0.14	-3.33	147,147,147,147	0
57	MG	DA	3048	1/1	0.14	-3.38	203,203,203,203	0
57	MG	BA	3113	1/1	0.12	-3.42	54,54,54,54	0
57	MG	BA	3040	1/1	0.17	-3.46	58,58,58,58	0
57	MG	BA	3039	1/1	0.13	-3.49	57,57,57,57	0
57	MG	BA	3059	1/1	0.09	-3.51	69,69,69,69	0
57	MG	BA	3042	1/1	0.10	-3.55	68,68,68,68	0
57	MG	AA	1640	1/1	0.06	-3.60	160,160,160,160	0
57	MG	CA	1639	1/1	0.08	-3.70	266,266,266,266	0
57	MG	BA	3087	1/1	0.12	-3.72	61,61,61,61	0
57	MG	BA	3099	1/1	0.10	-3.85	58,58,58,58	0
57	MG	DA	3032	1/1	0.13	-3.90	161,161,161,161	0
57	MG	AA	1612	1/1	0.09	-3.90	106,106,106,106	0
57	MG	BA	3003	1/1	0.07	-3.94	90,90,90,90	0
57	MG	BA	3027	1/1	0.07	-3.95	59,59,59,59	0
57	MG	CA	1635	1/1	0.09	-3.99	142,142,142,142	0
57	MG	BA	3117	1/1	0.13	-4.01	67,67,67,67	0
57	MG	BA	3009	1/1	0.10	-4.12	61,61,61,61	0
57	MG	DA	3070	1/1	0.08	-4.18	147,147,147,147	0
57	MG	BA	3053	1/1	0.08	-4.67	57,57,57,57	0
57	MG	BA	3097	1/1	0.08	-4.75	65,65,65,65	0
57	MG	BA	3064	1/1	0.06	-4.84	55,55,55,55	0
57	MG	BA	3086	1/1	0.13	-4.98	60,60,60,60	0
57	MG	BA	3073	1/1	0.09	-5.27	61,61,61,61	0
57	MG	DC	301	1/1	0.15	-5.99	135,135,135,135	0
57	MG	BA	3054	1/1	0.07	-6.04	62,62,62,62	0
57	MG	BA	3036	1/1	0.09	-6.14	65,65,65,65	0
57	MG	DA	3077	1/1	0.12	-6.40	162,162,162,162	0
57	MG	BA	3090	1/1	0.10	-6.57	63,63,63,63	0
57	MG	BA	3065	1/1	0.04	-6.65	55,55,55,55	0
57	MG	BA	3001	1/1	0.05	-6.79	61,61,61,61	0
57	MG	BA	3081	1/1	0.10	-7.12	56,56,56,56	0
57	MG	BA	3082	1/1	0.10	-7.49	55,55,55,55	0
57	MG	BA	3118	1/1	0.08	-7.61	60,60,60,60	0
57	MG	BA	3129	1/1	0.09	-8.02	55,55,55,55	0
57	MG	BA	3083	1/1	0.07	-9.08	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BA	3049	1/1	0.07	-9.93	61,61,61,61	0
57	MG	BA	3110	1/1	0.09	-10.54	61,61,61,61	0
57	MG	BA	3044	1/1	0.08	-11.06	88,88,88,88	0
57	MG	BA	3029	1/1	0.06	-11.96	54,54,54,54	0
57	MG	CA	1605	1/1	0.12	-12.16	115,115,115,115	0
57	MG	AA	1632	1/1	0.10	-13.86	117,117,117,117	0
57	MG	DA	3010	1/1	0.26	-	210,210,210,210	0
57	MG	DA	3003	1/1	1.26	-	229,229,229,229	0

6.5 Other polymers ⓘ

There are no such residues in this entry.