



# wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:23 PM BST

PDB ID : 4V6D  
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 : 2009-06-27  
Resolution : 3.81 Å(reported)

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

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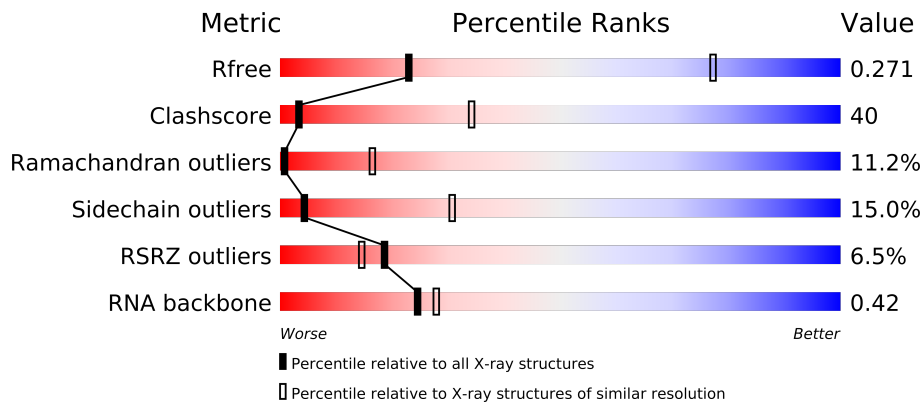
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.81 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	1165 (4.24-3.40)
Clashscore	79885	1105 (4.14-3.50)
Ramachandran outliers	78287	1055 (4.14-3.50)
Sidechain outliers	78261	1047 (4.14-3.50)
RSRZ outliers	66119	1166 (4.24-3.40)
RNA backbone	1838	1010 (4.84-2.80)

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  $\geq 3$ , 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	CV	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	
28	BE	201	
28	DE	201	

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Mol	Chain	Length	Quality of chain
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	
49	BZ	59	
49	DZ	59	

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Mol	Chain	Length	Quality of chain
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	1607	-	X
57	MG	AA	1610	-	X
57	MG	AA	1614	-	X
57	MG	AA	1619	-	X
57	MG	AA	1621	-	X
57	MG	AA	1623	-	X
57	MG	AA	1624	-	X
57	MG	AA	1626	-	X
57	MG	AA	1627	-	X
57	MG	AA	1628	-	X
57	MG	AA	1629	-	X
57	MG	AA	1631	-	X
57	MG	AA	1636	-	X
57	MG	AA	1641	-	X
57	MG	AA	1642	-	X
57	MG	BA	3002	-	X
57	MG	BA	3004	-	X
57	MG	BA	3005	-	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	3026	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
57	MG	BA	3028	-	X
57	MG	BA	3030	-	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	3065	-	X
57	MG	BA	3068	-	X
57	MG	BA	3071	-	X
57	MG	BA	3072	-	X
57	MG	BA	3077	-	X
57	MG	BA	3084	-	X
57	MG	BA	3085	-	X
57	MG	BA	3092	-	X
57	MG	BA	3093	-	X
57	MG	BA	3095	-	X
57	MG	BA	3098	-	X
57	MG	BA	3099	-	X
57	MG	BA	3102	-	X
57	MG	BA	3104	-	X
57	MG	BA	3105	-	X
57	MG	BA	3109	-	X
57	MG	BA	3112	-	X
57	MG	BA	3115	-	X
57	MG	BA	3118	-	X
57	MG	BA	3119	-	X
57	MG	BA	3123	-	X
57	MG	BA	3124	-	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	1602	-	X
57	MG	CA	1603	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
57	MG	CA	1605	-	X
57	MG	CA	1608	-	X
57	MG	CA	1612	-	X
57	MG	CA	1614	-	X
57	MG	CA	1615	-	X
57	MG	CA	1619	-	X
57	MG	CA	1620	-	X
57	MG	CA	1624	-	X
57	MG	CA	1625	-	X
57	MG	CA	1627	-	X
57	MG	CA	1628	-	X
57	MG	CA	1629	-	X
57	MG	CA	1636	-	X
57	MG	CA	1637	-	X
57	MG	CA	1639	-	X
57	MG	CA	1640	-	X
57	MG	DA	3001	-	X
57	MG	DA	3002	-	X
57	MG	DA	3008	-	X
57	MG	DA	3012	-	X
57	MG	DA	3015	-	X
57	MG	DA	3016	-	X
57	MG	DA	3017	-	X
57	MG	DA	3021	-	X
57	MG	DA	3023	-	X
57	MG	DA	3028	-	X
57	MG	DA	3029	-	X
57	MG	DA	3030	-	X
57	MG	DA	3031	-	X
57	MG	DA	3032	-	X
57	MG	DA	3038	-	X
57	MG	DA	3040	-	X
57	MG	DA	3041	-	X
57	MG	DA	3054	-	X
57	MG	DA	3060	-	X
57	MG	DA	3061	-	X
57	MG	DA	3062	-	X
57	MG	DA	3064	-	X
57	MG	DA	3065	-	X
57	MG	DA	3066	-	X
57	MG	DA	3071	-	X
57	MG	DA	3073	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
57	MG	DA	3076	-	X
57	MG	DA	3077	-	X
57	MG	DA	3078	-	X
57	MG	DA	3080	-	X
57	MG	DA	3088	-	X
57	MG	DA	3089	-	X
57	MG	DA	3090	-	X
57	MG	DA	3093	-	X
57	MG	DA	3096	-	X
57	MG	DA	3099	-	X
57	MG	DA	3100	-	X
57	MG	DA	3101	-	X
57	MG	DA	3107	-	X
57	MG	DA	3109	-	X
57	MG	DA	3110	-	X
57	MG	DA	3112	-	X
57	MG	DA	3118	-	X
57	MG	DA	3120	-	X
57	MG	DA	3121	-	X
57	MG	DA	3126	-	X
57	MG	DA	3128	-	X
57	MG	DA	3130	-	X
57	MG	DA	3131	-	X
57	MG	DA	3133	-	X
57	MG	DA	3134	-	X
57	MG	DC	301	-	X
57	MG	DJ	201	-	X

## 2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 285420 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
			360	161	64	118	17			
22	CV	17	Total	C	N	O	P	0	0	0
			360	161	64	118	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
			125	56	18	45	6			
23	CW	6	Total	C	N	O	P	0	0	0
			125	56	18	45	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			
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			

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	DA	134	Total	Mg	0	0
			134	134		
57	DC	1	Total	Mg	0	0
			1	1		
57	DB	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AE	1	Total O 1 1	0	0
59	AL	3	Total O 3 3	0	0
59	AN	5	Total O 5 5	0	0
59	AT	3	Total O 3 3	0	0
59	AU	1	Total O 1 1	0	0
59	AA	195	Total O 195 195	0	0
59	BA	615	Total O 615 615	0	0
59	BB	19	Total O 19 19	0	0
59	BC	7	Total O 7 7	0	0
59	BD	2	Total O 2 2	0	0
59	BE	1	Total O 1 1	0	0
59	BL	4	Total O 4 4	0	0
59	BN	2	Total O 2 2	0	0
59	BQ	1	Total O 1 1	0	0
59	BT	1	Total O 1 1	0	0
59	BV	1	Total O 1 1	0	0
59	B2	2	Total O 2 2	0	0
59	B3	3	Total O 3 3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	B4	2	Total 2	O 2	0	0
59	CE	3	Total 3	O 3	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	196	Total 196	O 196	0	0
59	DC	14	Total 14	O 14	0	0
59	DD	4	Total 4	O 4	0	0
59	DE	2	Total 2	O 2	0	0
59	DJ	3	Total 3	O 3	0	0
59	DL	5	Total 5	O 5	0	0
59	DN	2	Total 2	O 2	0	0
59	DT	2	Total 2	O 2	0	0
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
59	DA	598	Total 598	O 598	0	0

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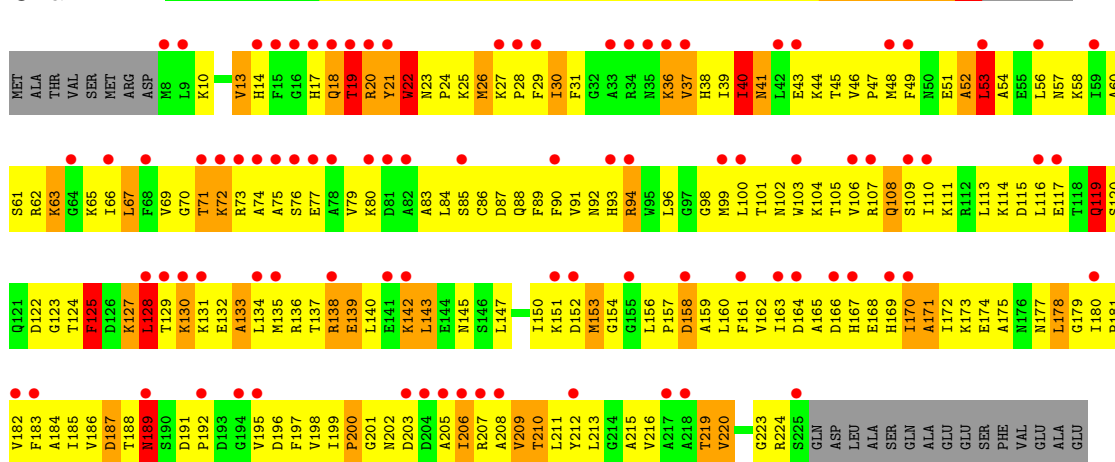
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DB	4	Total	O	0	0
			4	4		

### 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.

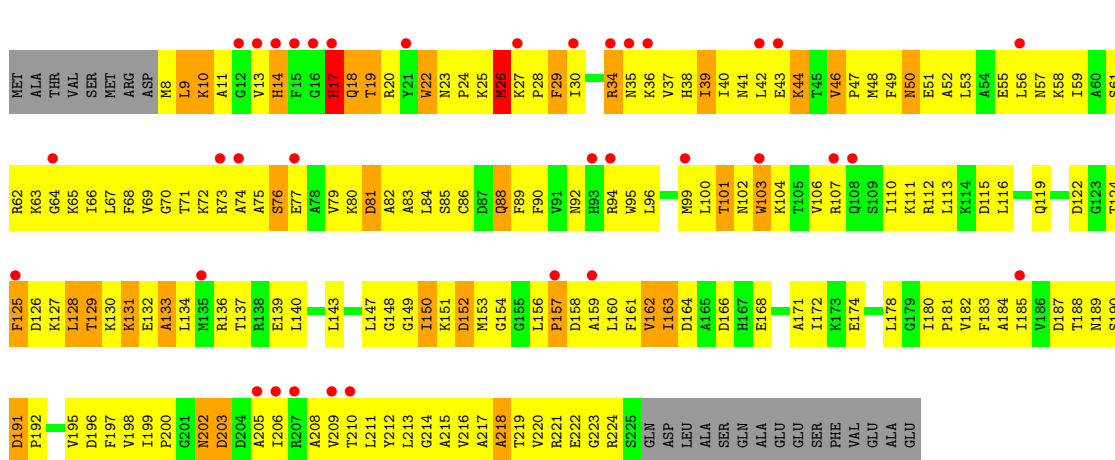
#### • Molecule 1: 30S ribosomal protein S2

Chain AB:



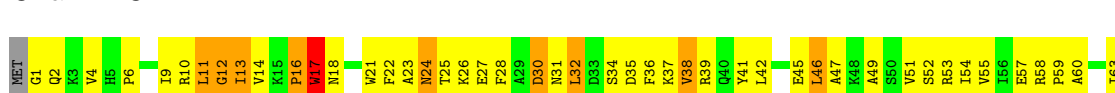
#### • Molecule 1: 30S ribosomal protein S2

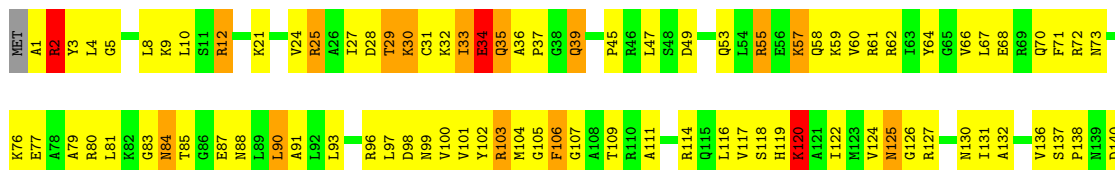
Chain CB:



#### • Molecule 2: 30S ribosomal protein S3

Chain AC:



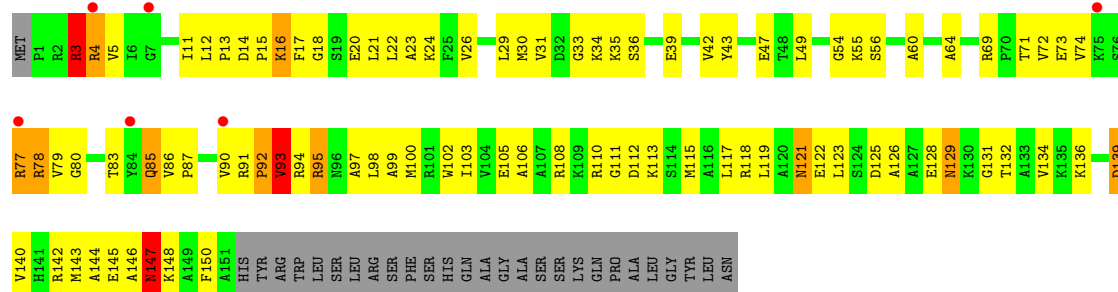




GLU  
GLU  
GLU  
GLU

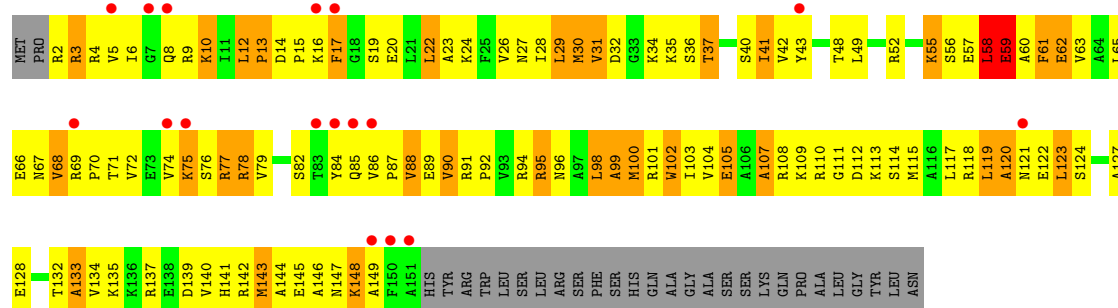
• Molecule 6: 30S ribosomal protein S7

Chain AG:



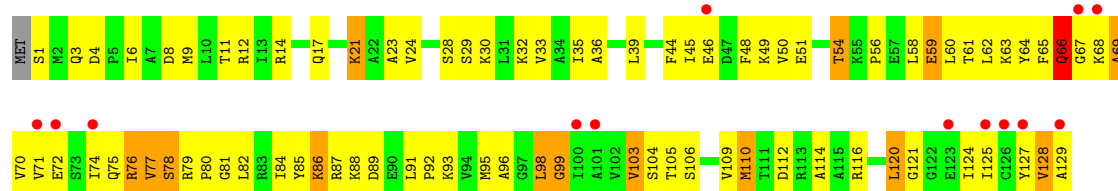
• Molecule 6: 30S ribosomal protein S7

Chain CG:



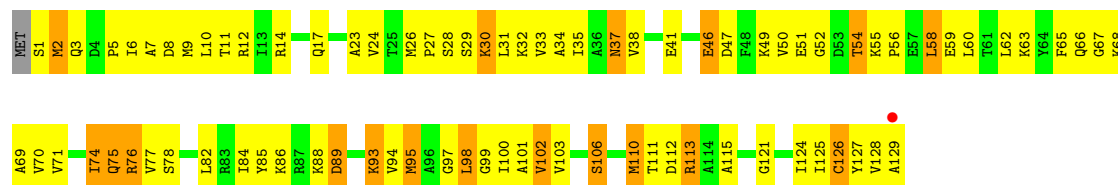
• Molecule 7: 30S ribosomal protein S8

Chain AH:



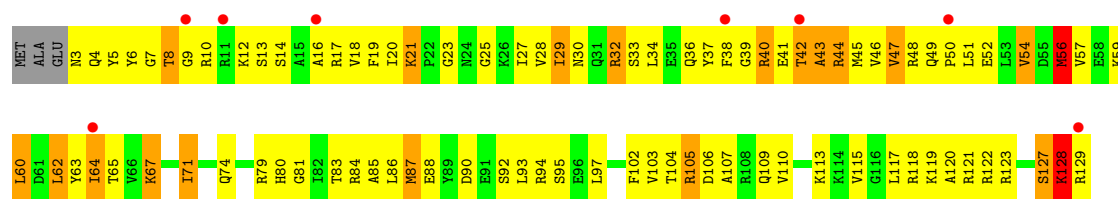
• Molecule 7: 30S ribosomal protein S8

Chain CH:



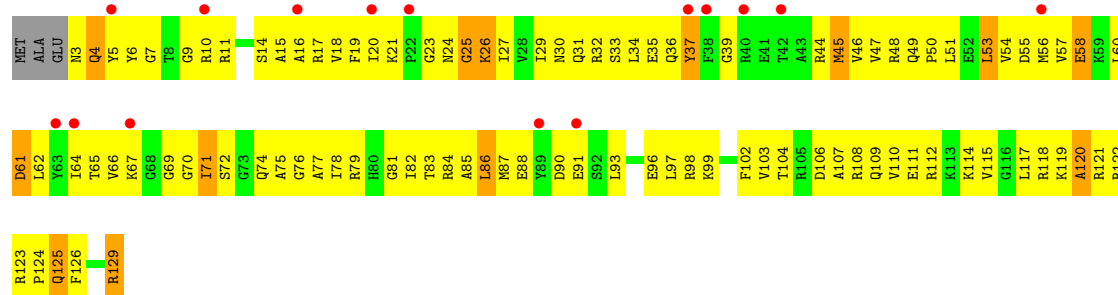
• Molecule 8: 30S ribosomal protein S9

Chain AI:



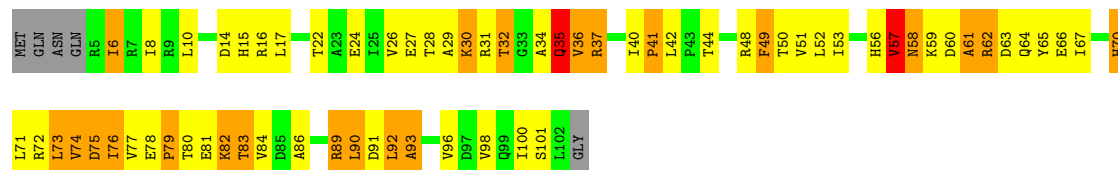
• Molecule 8: 30S ribosomal protein S9

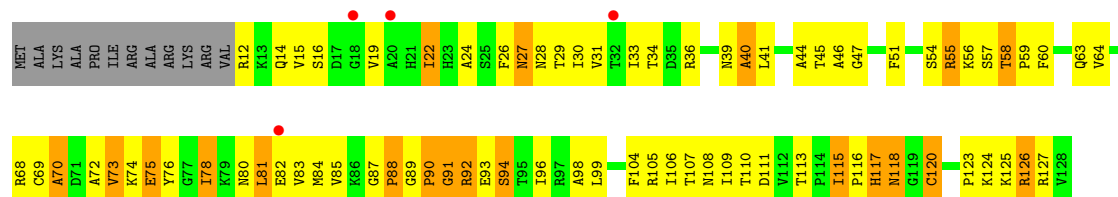
Chain CI:



• Molecule 9: 30S ribosomal protein S10

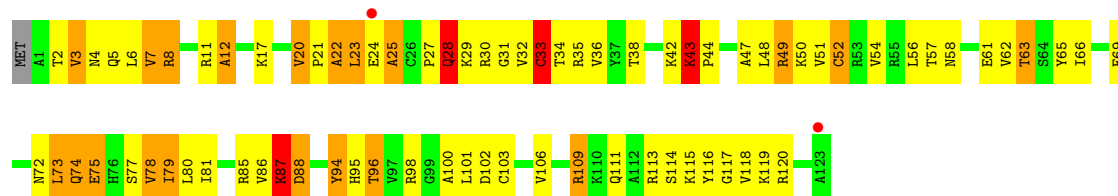
Chain AJ:





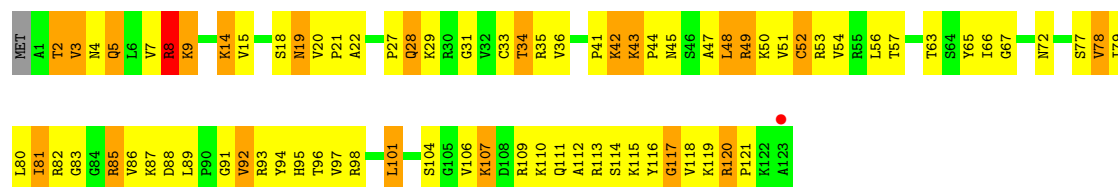
- Molecule 11: 30S ribosomal protein S12

Chain AL:



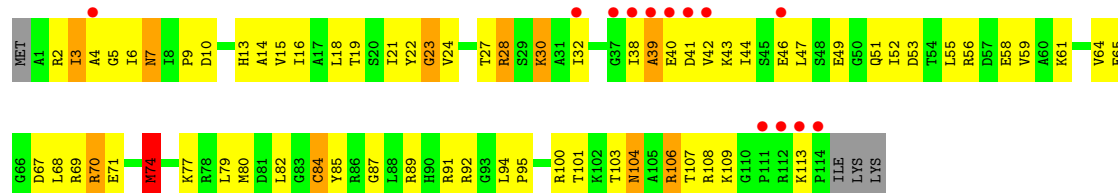
- Molecule 11: 30S ribosomal protein S12

Chain CL:



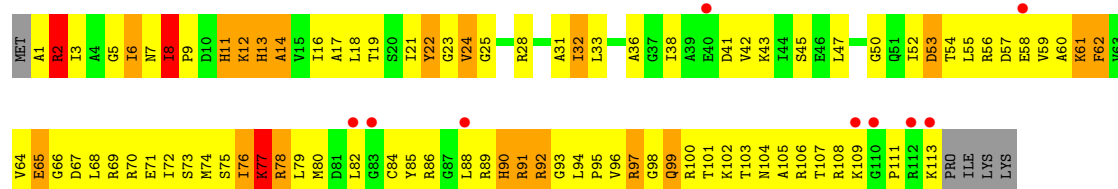
- Molecule 12: 30S ribosomal protein S13

Chain AM:



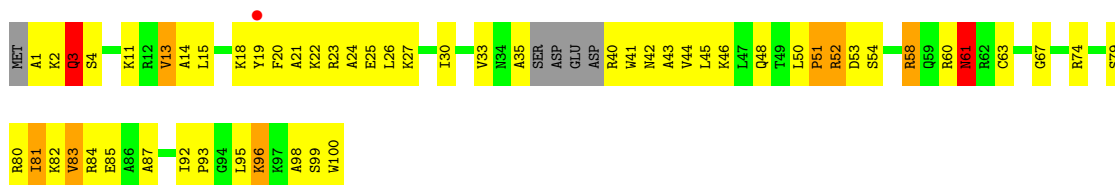
- Molecule 12: 30S ribosomal protein S13

Chain CM:



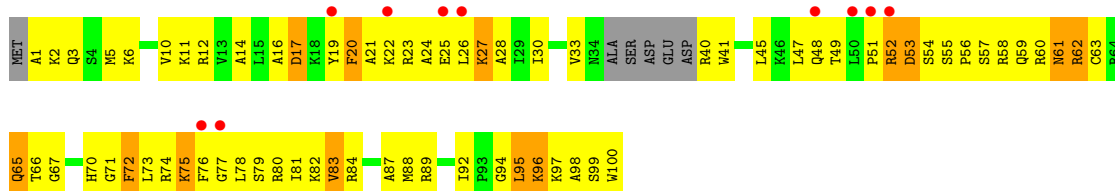
- Molecule 13: 30S ribosomal protein S14

Chain AN:



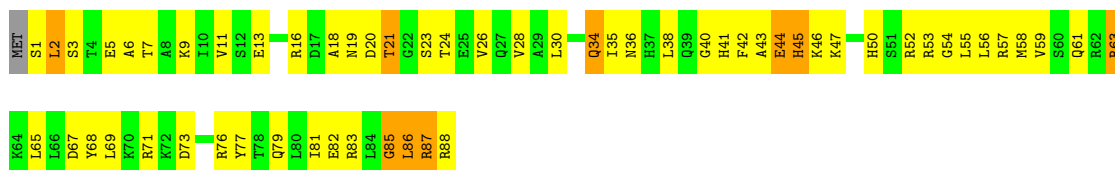
• Molecule 13: 30S ribosomal protein S14

Chain CN:



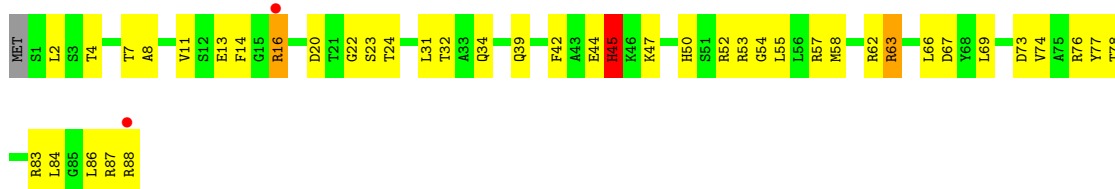
• Molecule 14: 30S ribosomal protein S15

Chain AO:



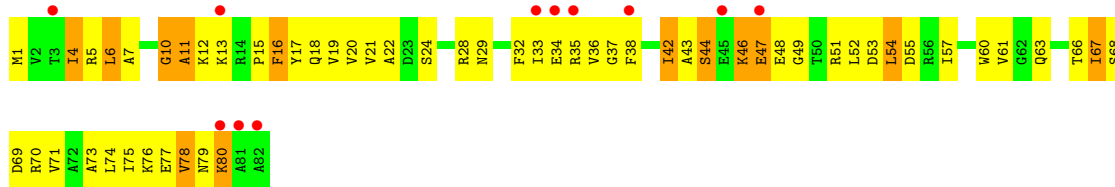
• Molecule 14: 30S ribosomal protein S15

Chain CO:



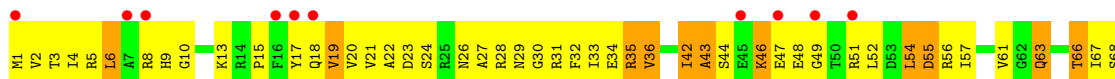
• Molecule 15: 30S ribosomal protein S16

Chain AP:



• Molecule 15: 30S ribosomal protein S16

Chain CP:





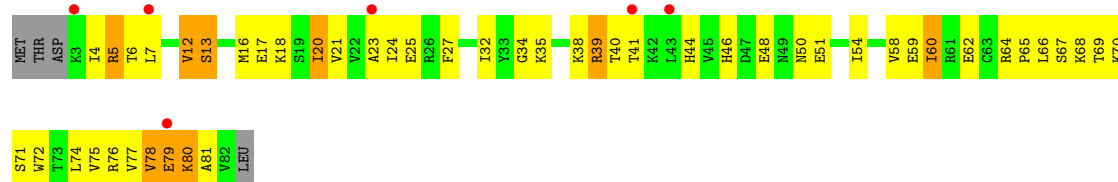
- Molecule 16: 30S ribosomal protein S17

Chain AQ:



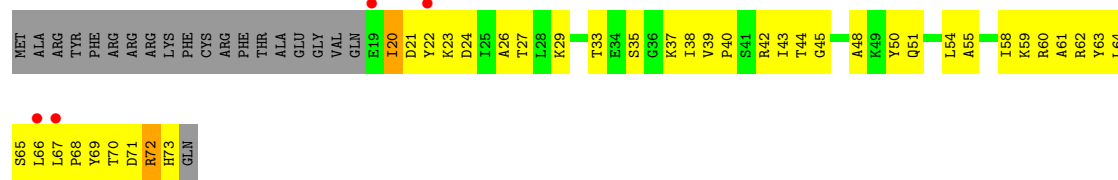
- Molecule 16: 30S ribosomal protein S17

Chain CQ:



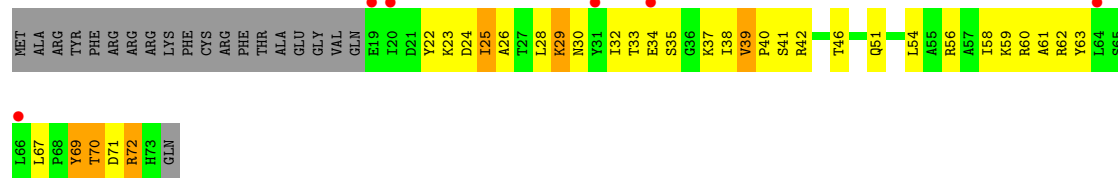
- Molecule 17: 30S ribosomal protein S18

Chain AR:



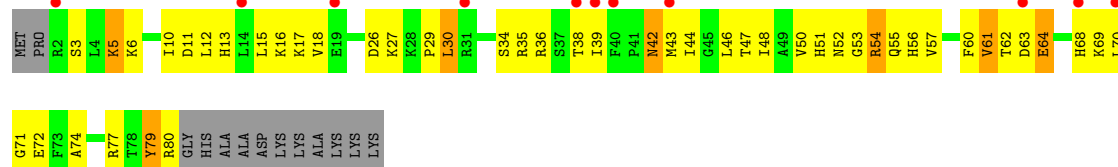
- Molecule 17: 30S ribosomal protein S18

Chain CR:



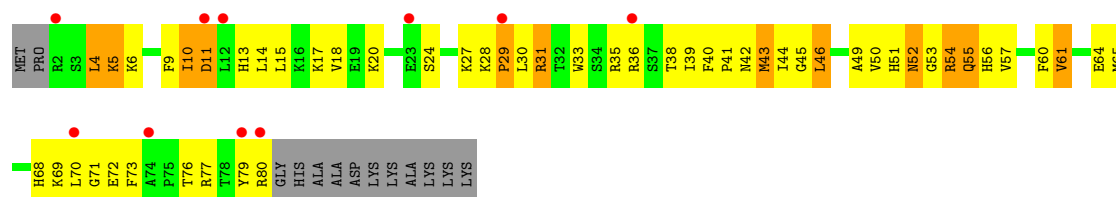
- Molecule 18: 30S ribosomal protein S19

Chain AS:



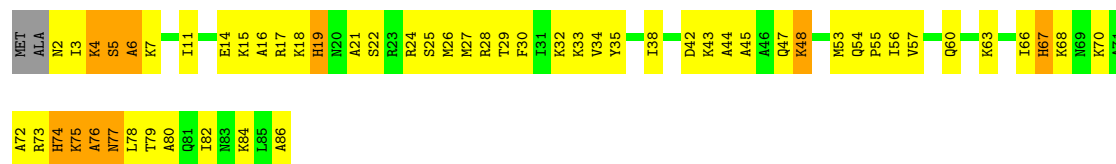
- Molecule 18: 30S ribosomal protein S19

Chain CS:



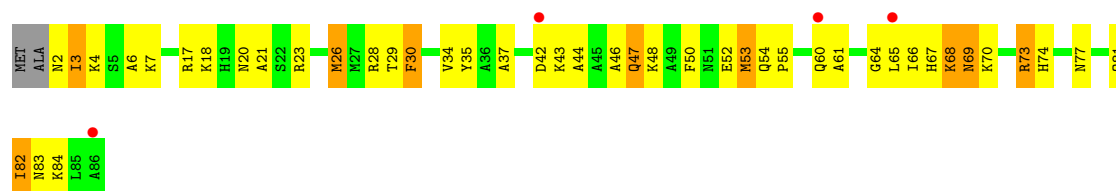
- Molecule 19: 30S ribosomal protein S20

Chain AT:



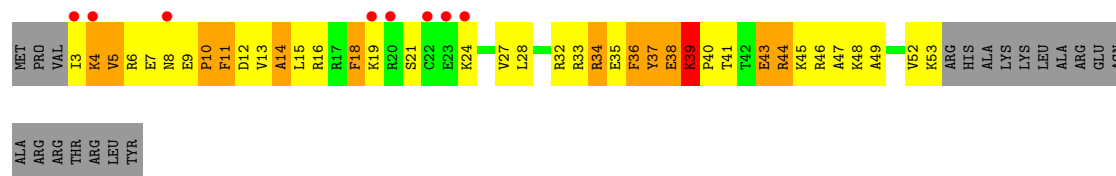
- Molecule 19: 30S ribosomal protein S20

Chain CT:



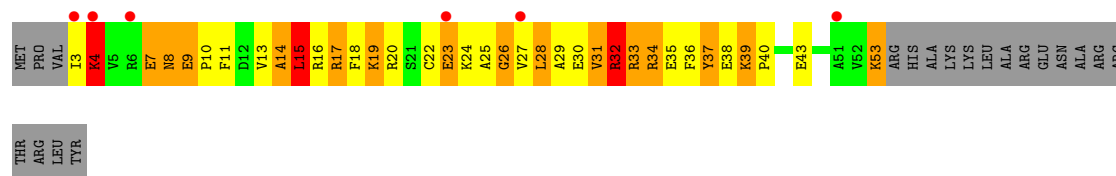
- Molecule 20: 30S ribosomal protein S21

Chain AU:



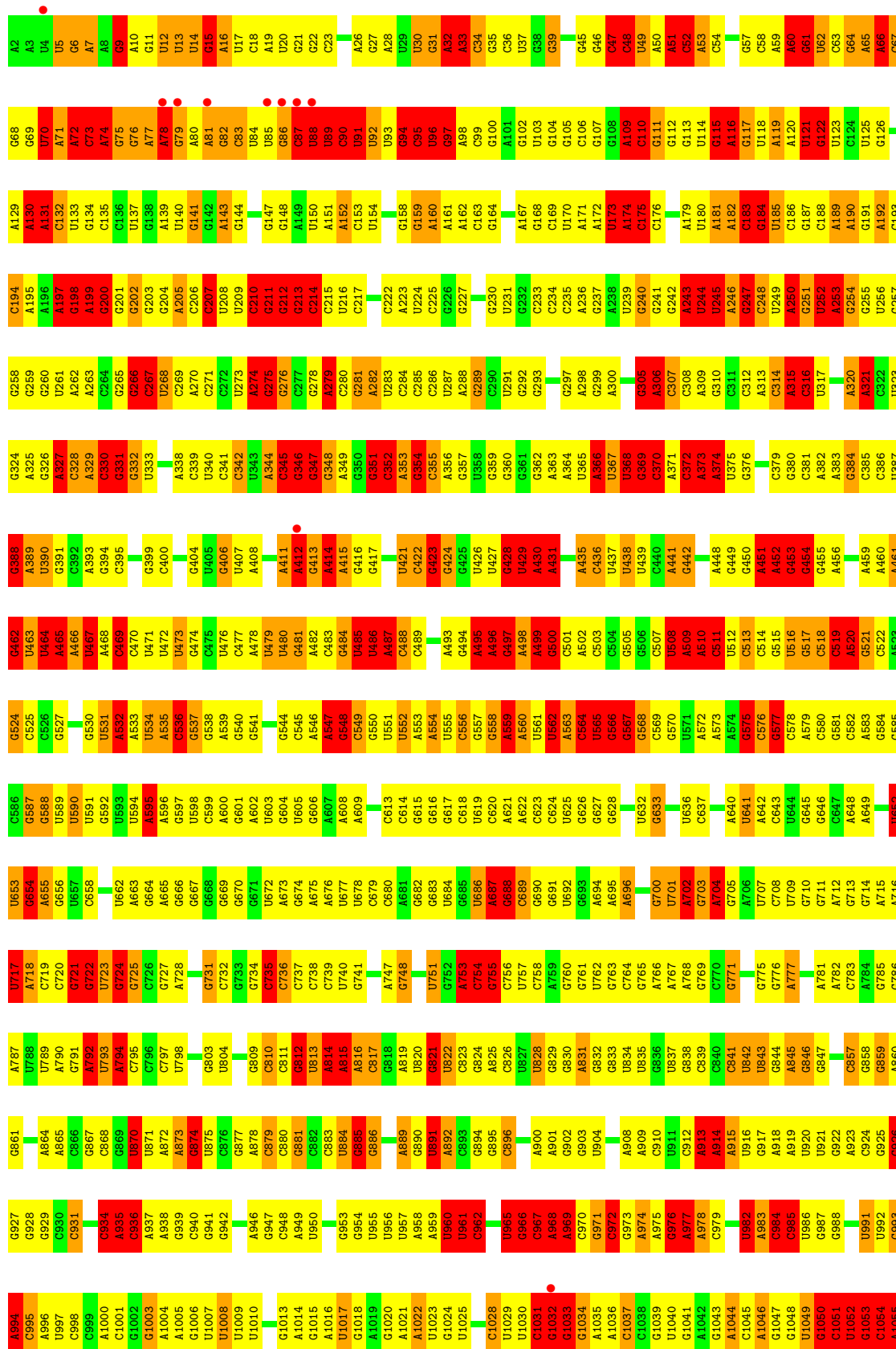
- Molecule 20: 30S ribosomal protein S21

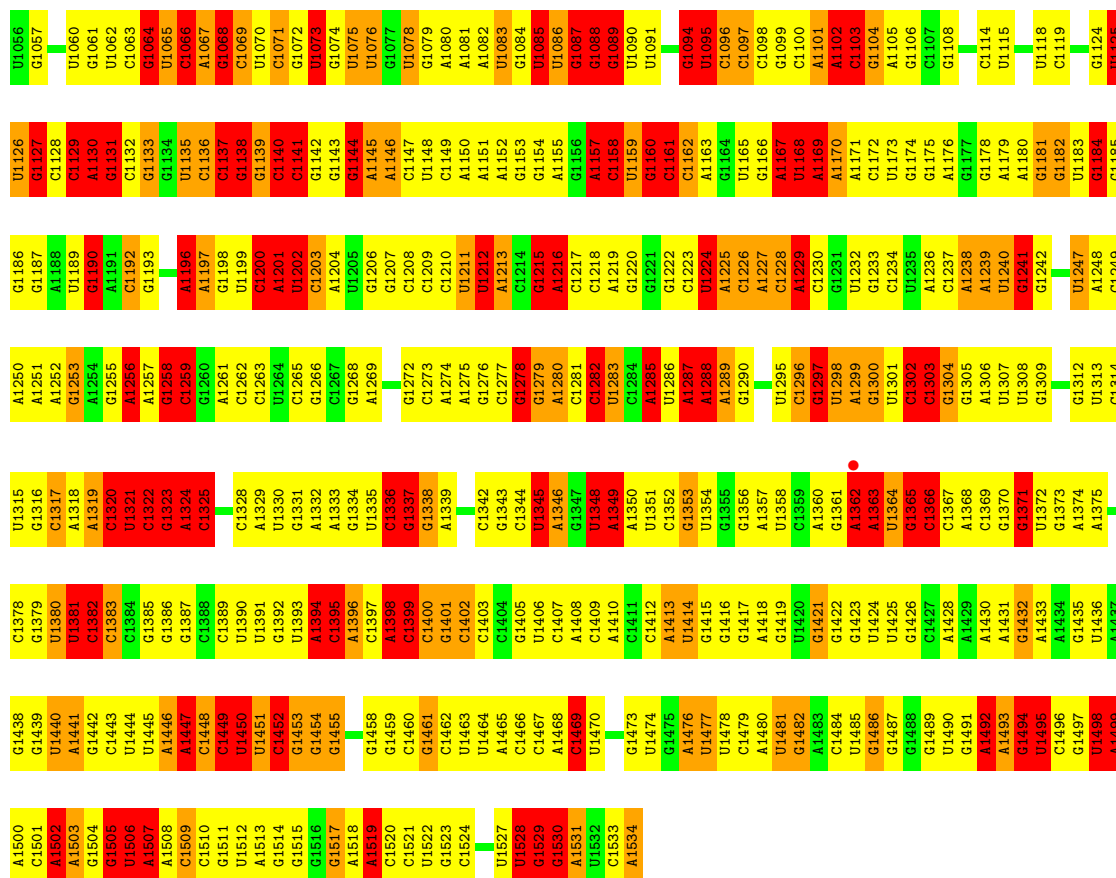
Chain CU:



- Molecule 21: 16S rRNA

Chain AA:





- Molecule 22: P-site tRNA ASL fragment

Chain AV:



- Molecule 22: P-site tRNA ASL fragment

Chain CV:



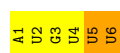
- Molecule 23: messenger RNA

Chain AW:



- Molecule 23: messenger RNA

Chain CW:



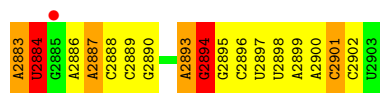
● Molecule 24: 23S rRNA

Chain BA: 

A900	U939	G778	A718	U653	G585	C523	C462	U395	U328	C264	U200	U135	U62	G1
C901	C940	U779	C719	A654	A586	C523	G463	C396	C329	A265	C201	U135	A63	G2
G904	G841	U780	U720	A655	C587	A526	U464	U397	A330	C266	C201	U136	A64	U3
U942	U943	A781	A721	C656	U589	C527	C465	C398	C331	C267	A203	U137		U4
U906	G844	A782	A722	U657	U588	A528	A466	U399	A332	C268	A204	U138	G68	A5
G907	A845	A783	C723	U658	A590	A529	C467	G400	G333	C269	G205	U139	C69	A6
		G784	U724	G659	U591	C530	C468	A401	G334	A270	U206	C140	G70	G7
		G785	G725	G785	A592	C531	G469	A402	C335	G271	A207	G141	A71	C8
		C786	G726		U593	A532	C470	U403	C336	A272	C208	A142	U73	G9
A910	U947	A787	A727		U594	G533	A471	A404	C337	G273	C209	C143	A73	A10
A911	C948	A788	G728	A666	C595	U534	A472	G405	G338	U276	C210	A144	A74	C11
U913	U950	A789	G729	A668		G535	G473	U406	U339	G277	C211	A145	G75	U12
C951	C851	U790	A730	G669	G600	G536	G474	G407	A340			A146	G76	A13
G915	U852	C791	C731	A670	C601	G537	C475	G408	A341	G277	G215	A147	G77	A14
A917	C853	A792	C732	C671	A602	A538	G476	G409	A342	A278	A216	U148		G15
A918	G854	A793	G733	C672	A603	G539	A477	G410	A343	U280	A217	U149	U82	C16
G955	A917	A794	A734	C673	G604	C540	A478	G411	A344	C281	A218	U150	A83	G17
U919	G956	C795	A735	G674	G605	A541	A479	G412	A345	A282		C151	A84	U18
A920	G857	C796	C736	A675		C542	A480	C413	A346	G283	A221	C151	G85	A19
			C737	A676	A608	C543	G481	C414	A347	U284	A222		G86	C20
C921	G858	G799	C738	A677	C609	C544	A482	C415	U348	G285	A223	A155	G87	A21
G922	G859	A800	A739	C678	C610	U545	A483	U416	A349	U286	U224	C157	G88	C22
G923	U960	G801	C740	C679	C611	U546	C484	C417		G287	C225	U158	G89	G23
G924	A861	A802	U741	C680	G612	A547	C485	C418	A352	U288	A226	G159	U90	G24
A925	G862	U803	A742	G681	A613	G548	C486	U419	C353	G289	A227	A160	A91	U25
G926	A863	U804	A743	G682	A614	C549	C487	C420		U290	A228	A161	U92	U26
A927	G864	G805	U744	U683	U615	C550	G488	C421	C357		C229	U162	G93	G27
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G874	G874	U813	A752	C692	G625	C559	A497	C433	C366	G302	C238	U171	U102	G36
C975	C875	C814	A753	C692	A626	C559	G497	U434	C367	G303	C239	U172	A103	C37
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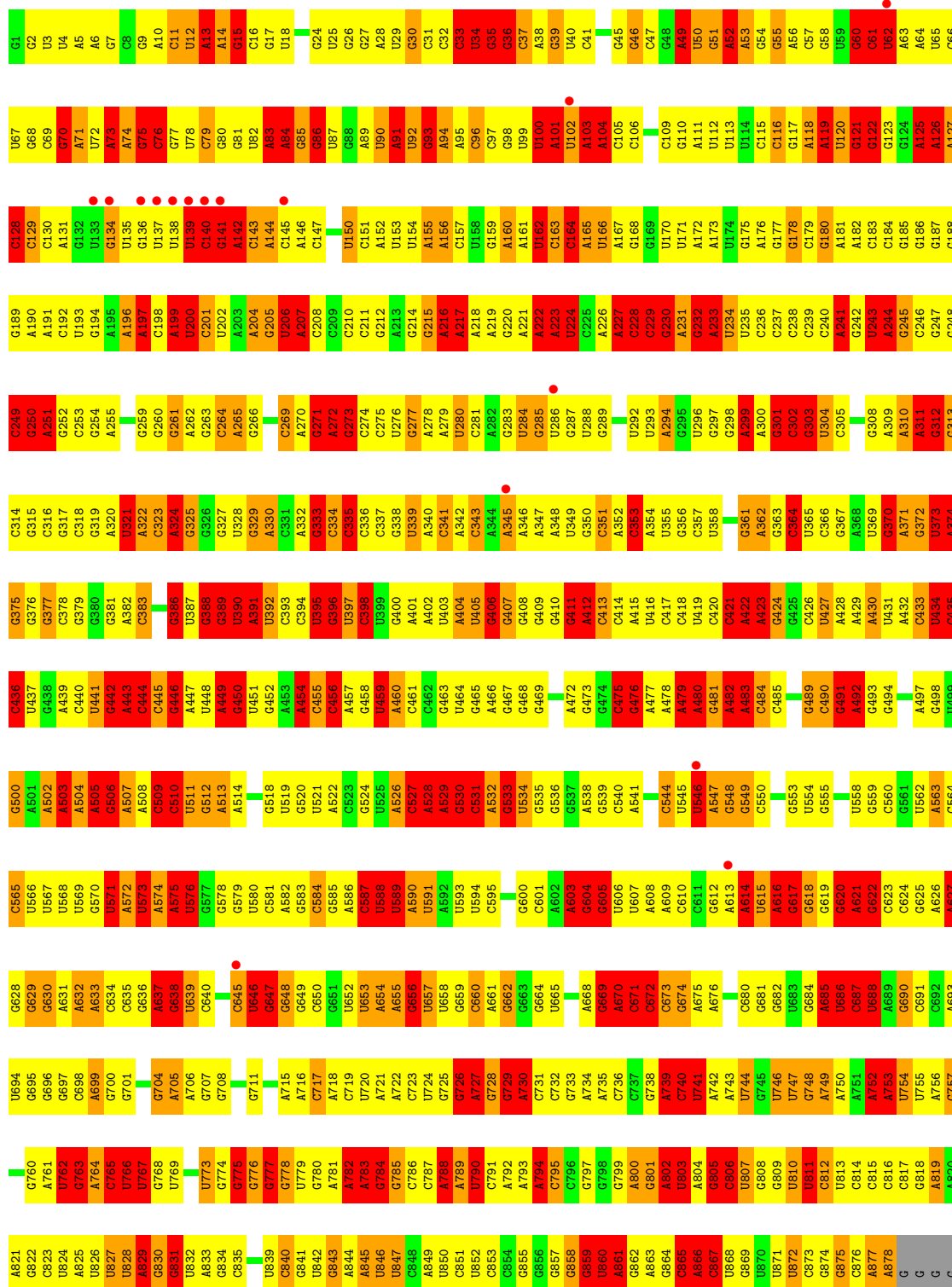
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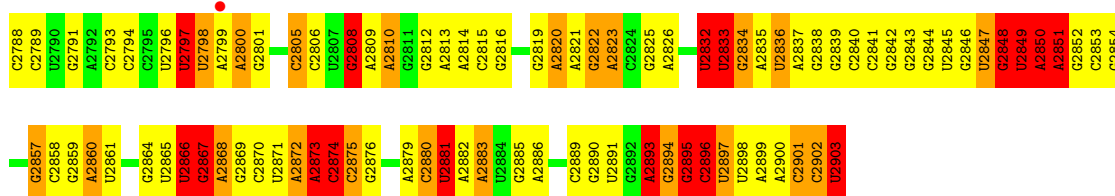
• Molecule 24: 23S rRNA

Chain DA:



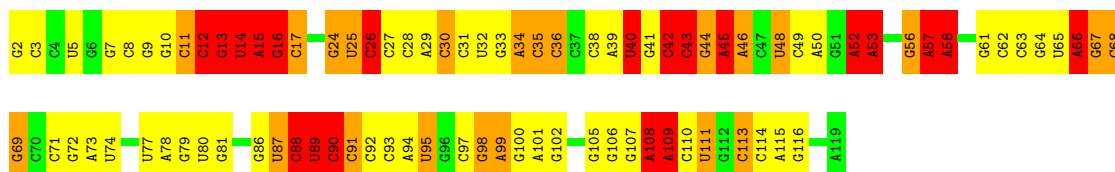


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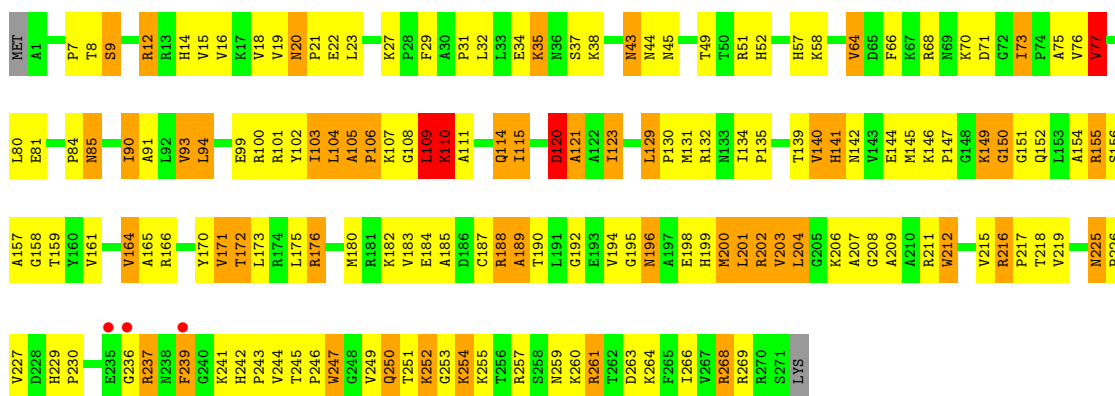
- Molecule 25: 5S rRNA

Chain BB:



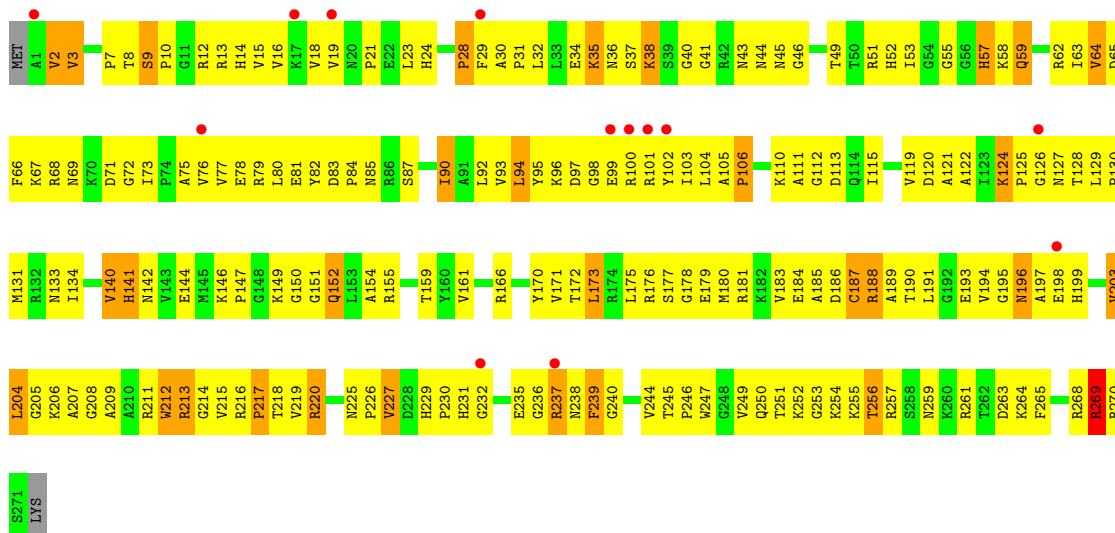
- Molecule 26: 50S ribosomal protein L2

Chain BC:



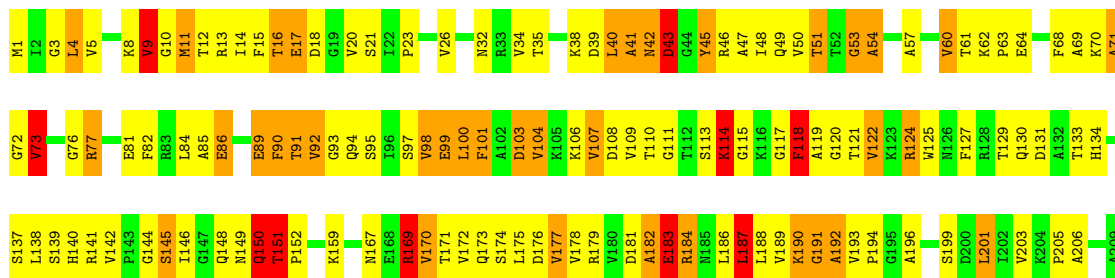
- Molecule 26: 50S ribosomal protein L2

Chain DC:



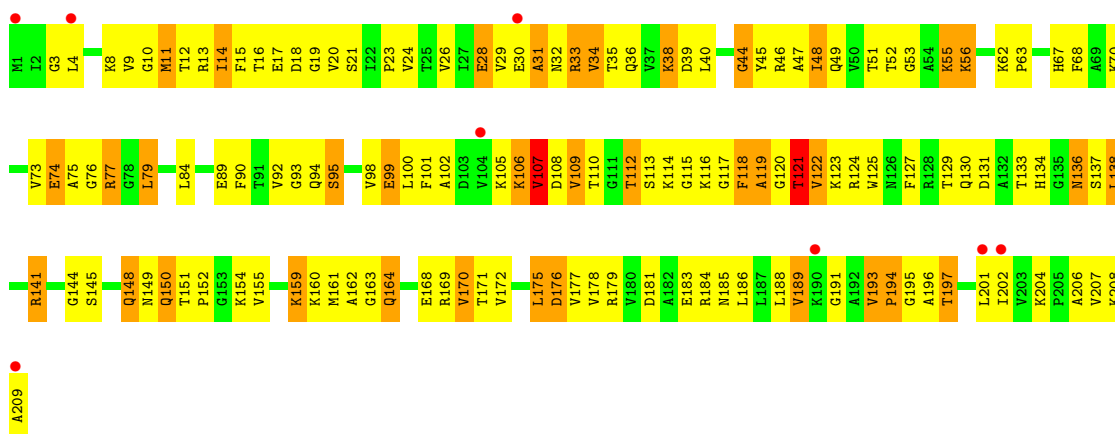
- Molecule 27: 50S ribosomal protein L3

Chain BD:



- Molecule 27: 50S ribosomal protein L3

Chain DD:



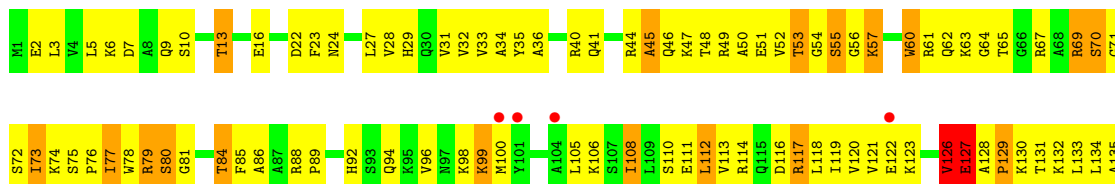
- Molecule 28: 50S ribosomal protein L4

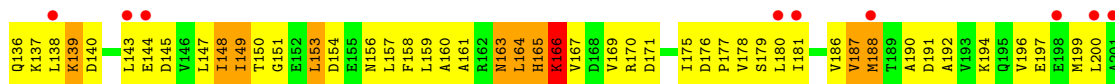
Chain BE:



- Molecule 28: 50S ribosomal protein L4

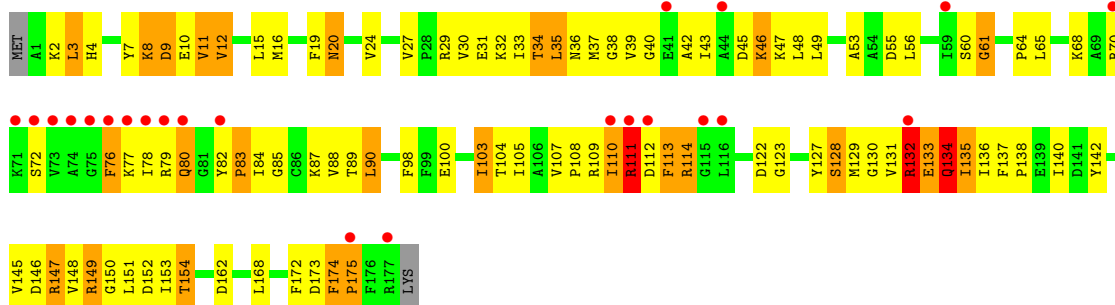
Chain DE:





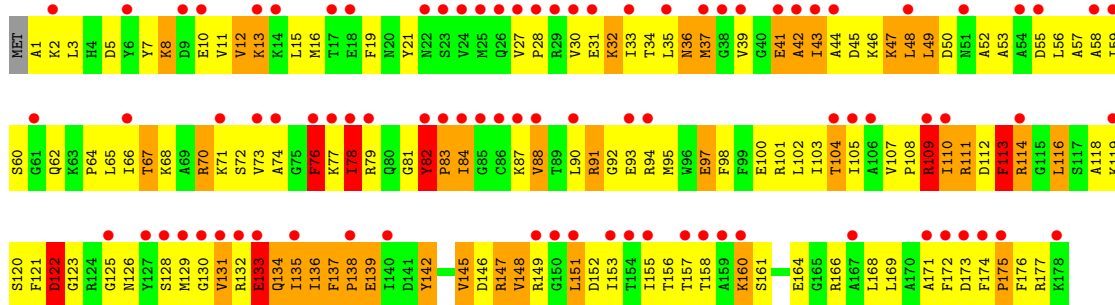
• Molecule 29: 50S ribosomal protein L5

Chain BF:



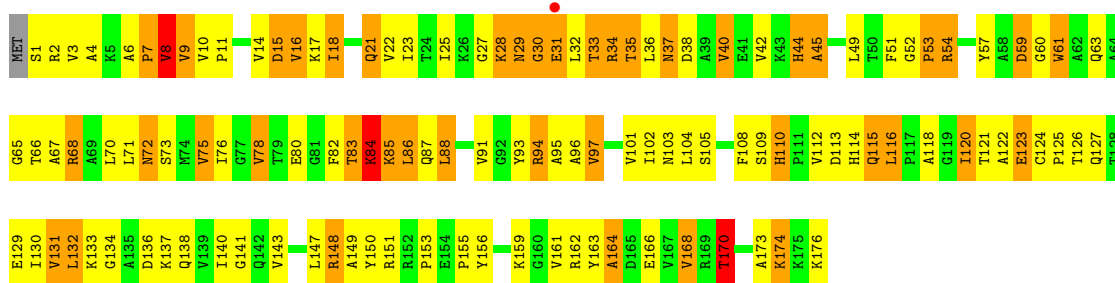
• Molecule 29: 50S ribosomal protein L5

Chain DF:



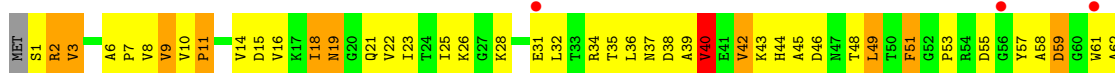
• Molecule 30: 50S ribosomal protein L6

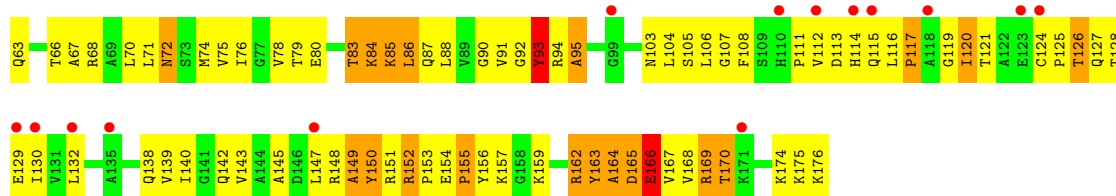
Chain BG:



• Molecule 30: 50S ribosomal protein L6

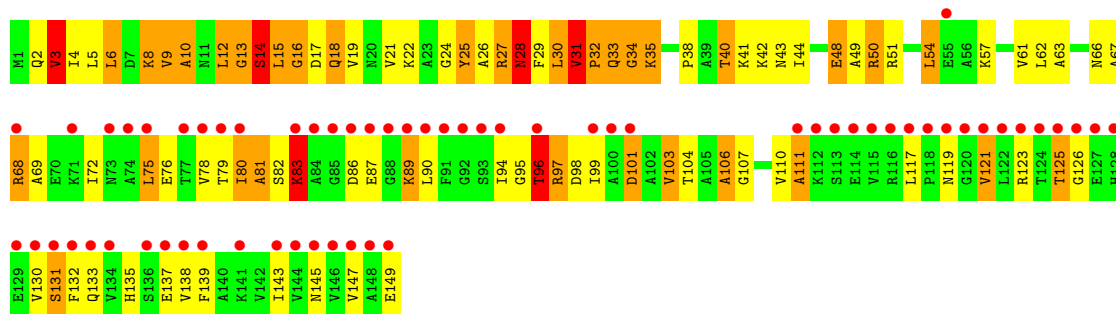
Chain DG:





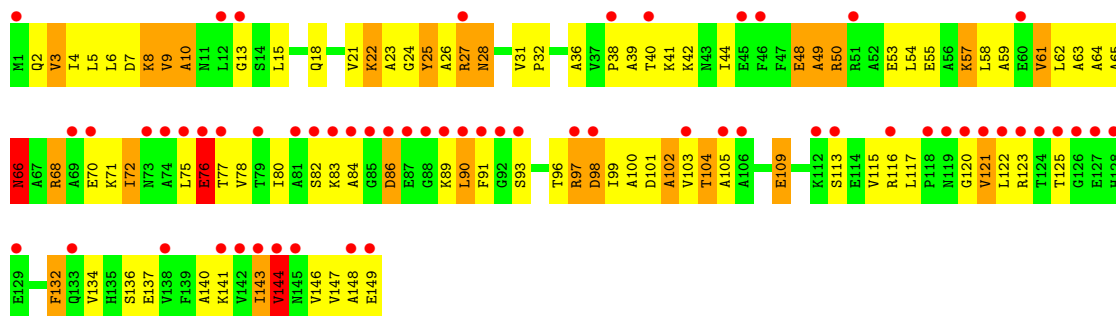
• Molecule 31: 50S ribosomal protein L9

Chain BH:



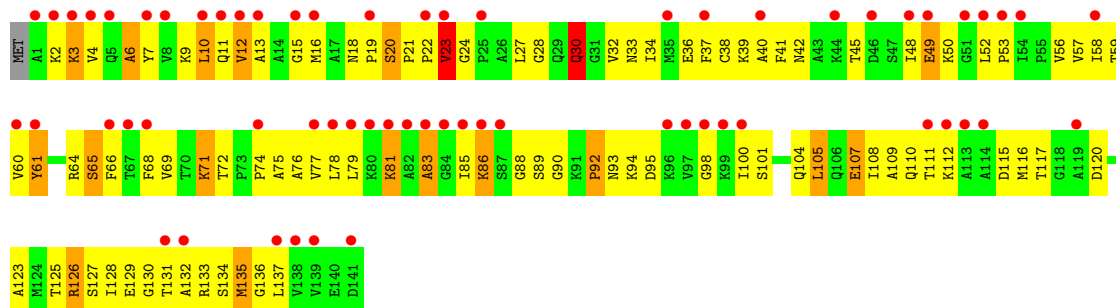
• Molecule 31: 50S ribosomal protein L9

Chain DH:



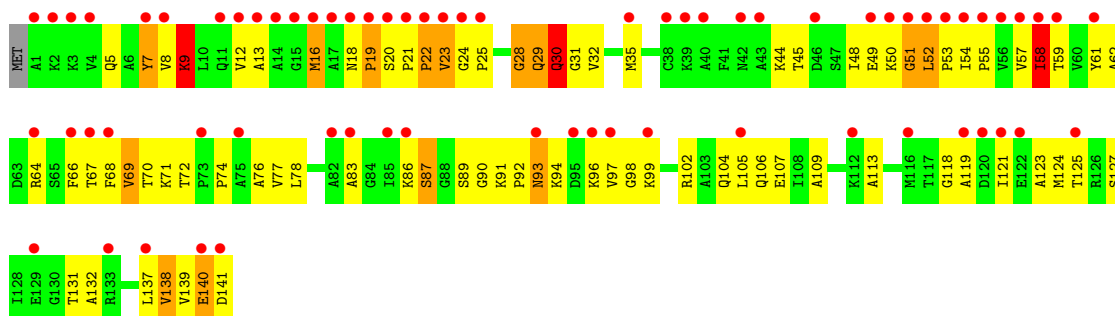
• Molecule 32: 50S ribosomal protein L11

Chain BI:



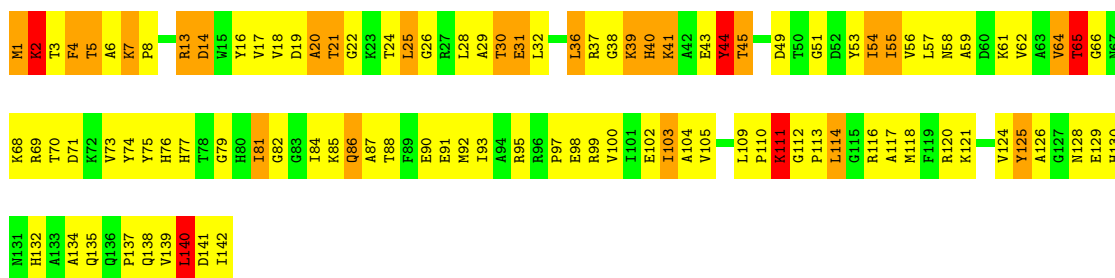
• Molecule 32: 50S ribosomal protein L11

Chain DI:



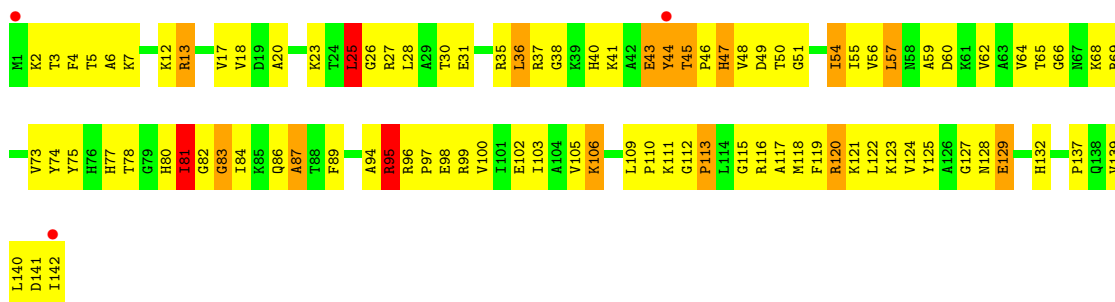
- Molecule 33: 50S ribosomal protein L13

Chain BJ:



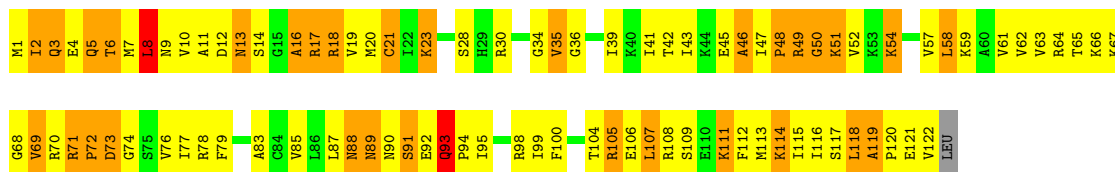
- Molecule 33: 50S ribosomal protein L13

Chain DJ:



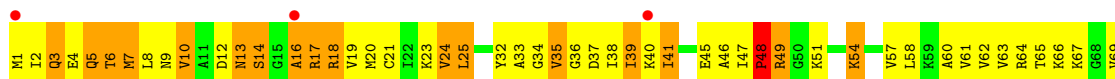
- Molecule 34: 50S ribosomal protein L14

Chain BK:



- Molecule 34: 50S ribosomal protein L14

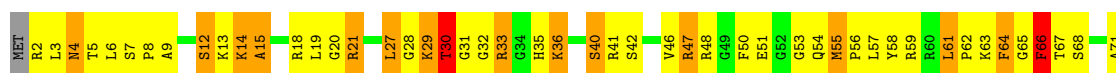
Chain DK:





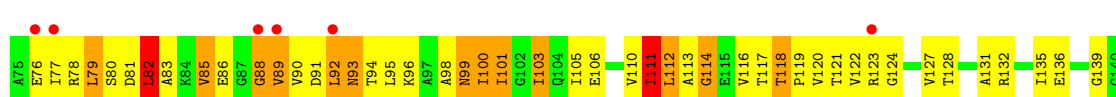
- Molecule 35: 50S ribosomal protein L15

Chain BL:



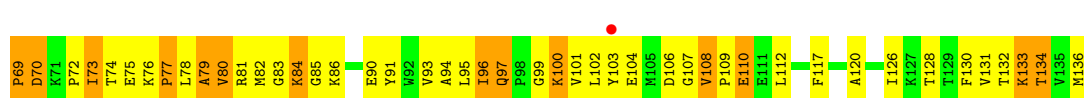
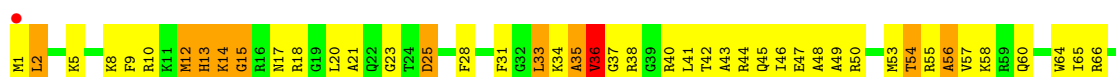
- Molecule 35: 50S ribosomal protein L15

Chain DL:



- Molecule 36: 50S ribosomal protein L16

Chain BM:



- Molecule 36: 50S ribosomal protein L16

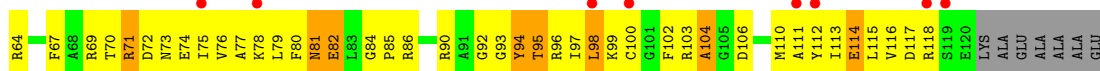
Chain DM:



- Molecule 37: 50S ribosomal protein L17



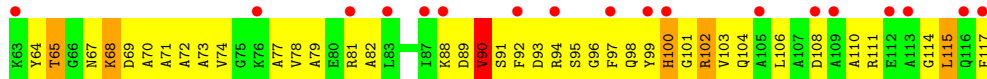
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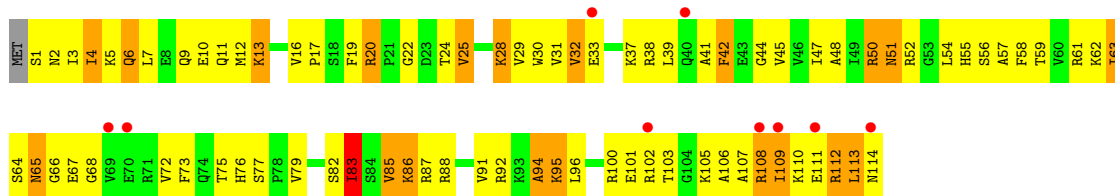
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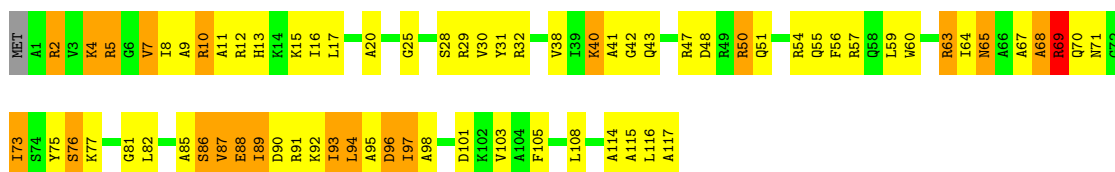


- 
- | Response | Percentage |
|----------|------------|
| Yes      | 100%       |
| No       | 0%         |



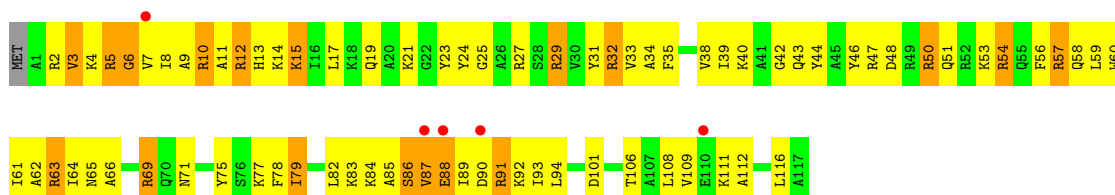
• Molecule 40: 50S ribosomal protein L20

Chain BQ:



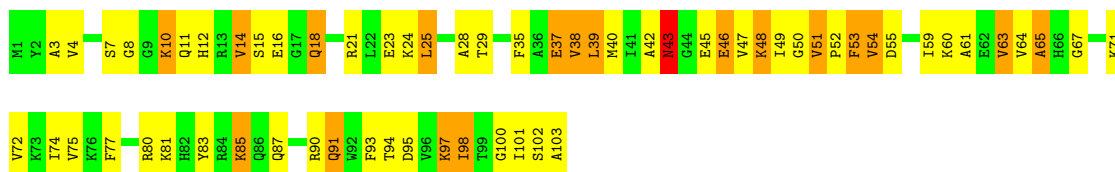
• Molecule 40: 50S ribosomal protein L20

Chain DQ:



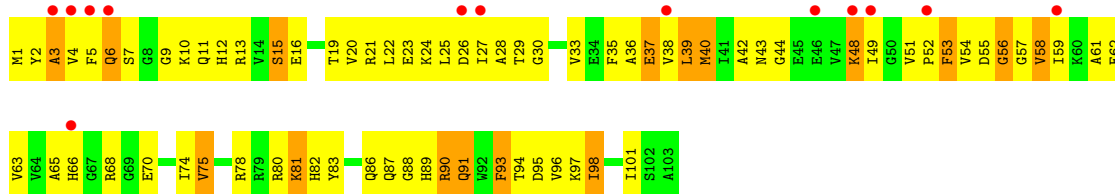
• Molecule 41: 50S ribosomal protein L21

Chain BR:



• Molecule 41: 50S ribosomal protein L21

Chain DR:



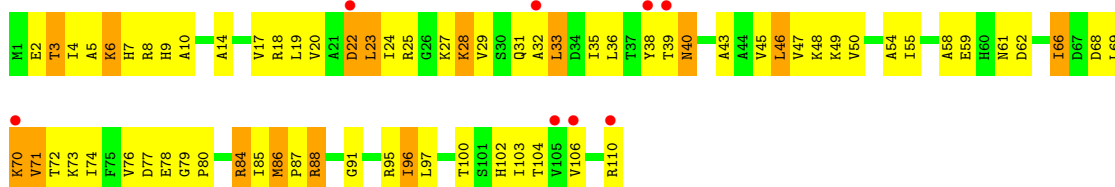
• Molecule 42: 50S ribosomal protein L22

Chain BS:

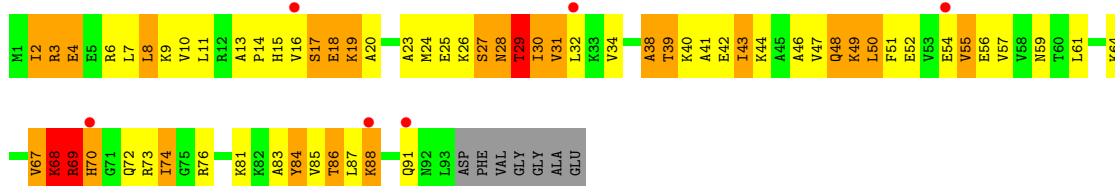




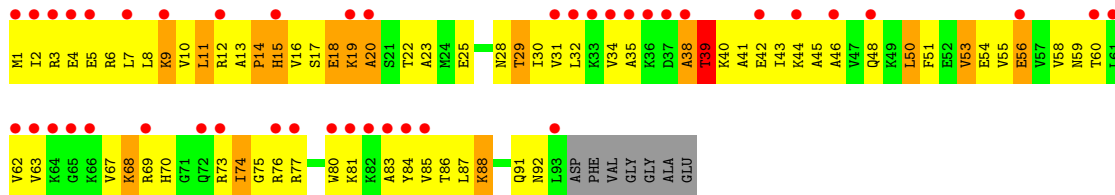
• Molecule 42: 50S ribosomal protein L22



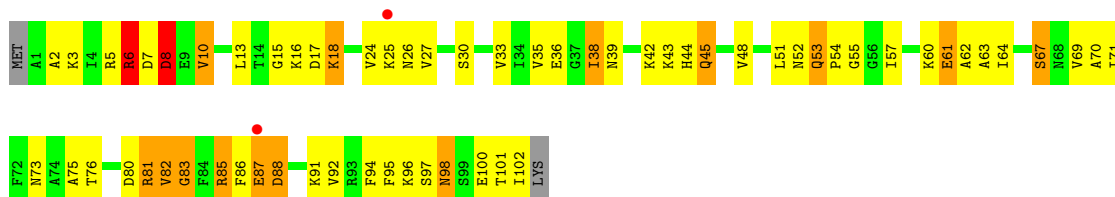
• Molecule 43: 50S ribosomal protein L23



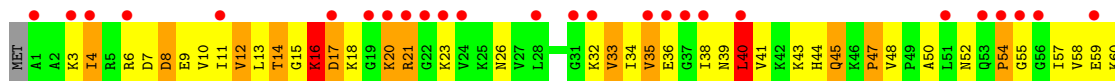
• Molecule 43: 50S ribosomal protein L23

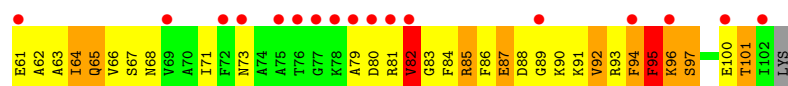


• Molecule 44: 50S ribosomal protein L24



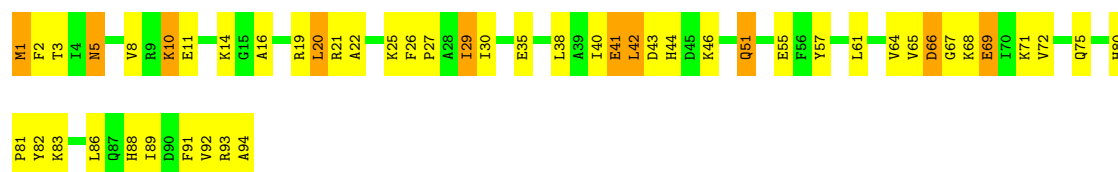
• Molecule 44: 50S ribosomal protein L24





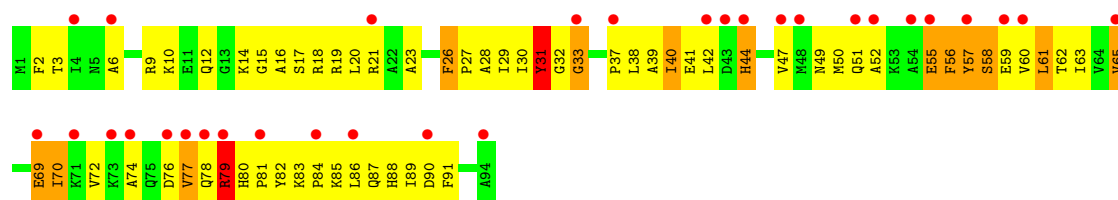
- Molecule 45: 50S ribosomal protein L25

Chain BV:



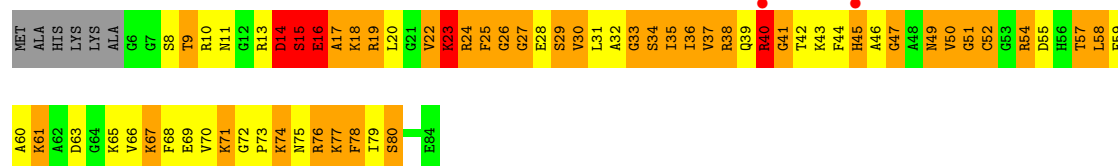
- Molecule 45: 50S ribosomal protein L25

Chain DV:



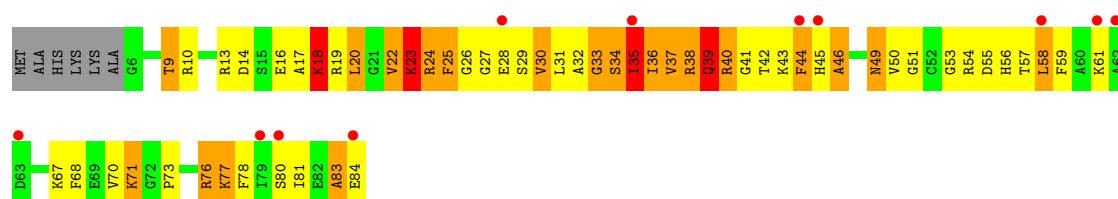
- Molecule 46: 50S ribosomal protein L27

Chain BW:



- Molecule 46: 50S ribosomal protein L27

Chain DW:



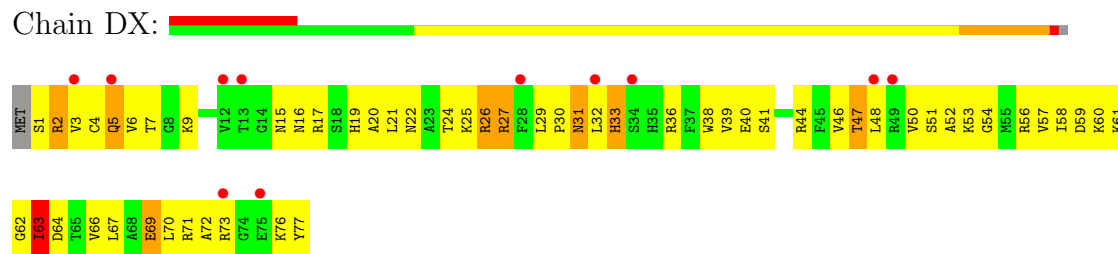
- Molecule 47: 50S ribosomal protein L28

Chain BX:



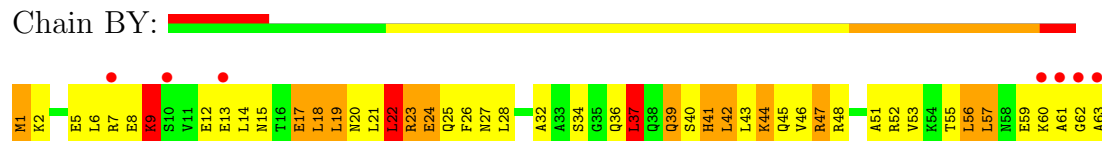
- Molecule 47: 50S ribosomal protein L28

Chain DX:



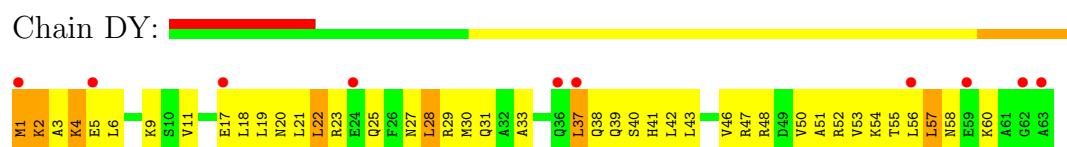
- Molecule 48: 50S ribosomal protein L29

Chain BY:



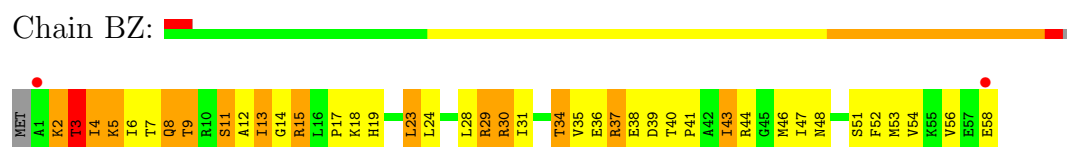
- Molecule 48: 50S ribosomal protein L29

Chain DY:



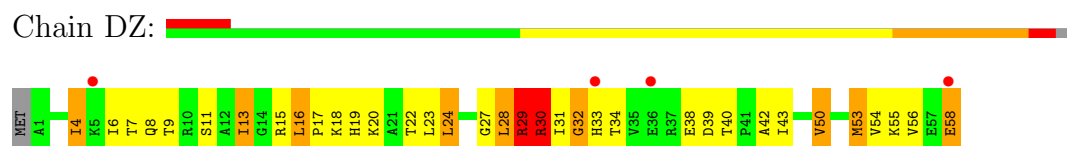
- Molecule 49: 50S ribosomal protein L30

Chain BZ:



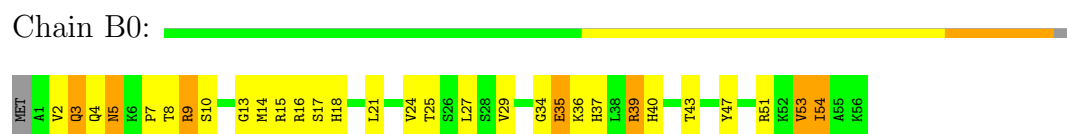
- Molecule 49: 50S ribosomal protein L30

Chain DZ:



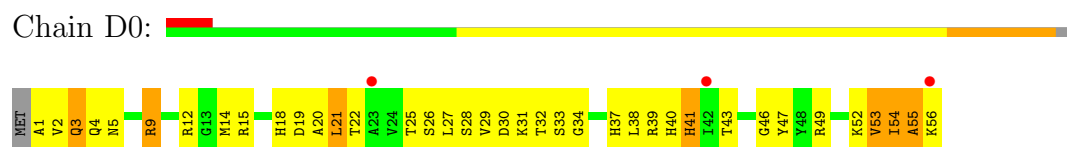
- Molecule 50: 50S ribosomal protein L32

Chain B0:



- Molecule 50: 50S ribosomal protein L32

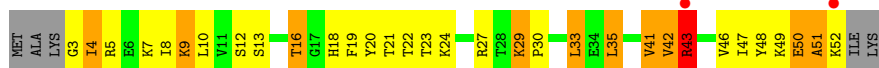
Chain D0:



- Molecule 51: 50S ribosomal protein L33

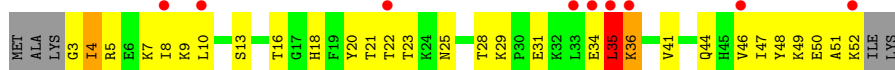
Chain B1:





- Molecule 51: 50S ribosomal protein L33

Chain D1:



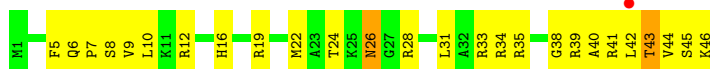
- Molecule 52: 50S ribosomal protein L34

Chain B2:



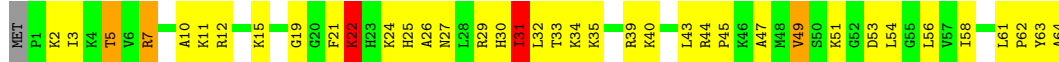
- Molecule 52: 50S ribosomal protein L34

Chain D2:



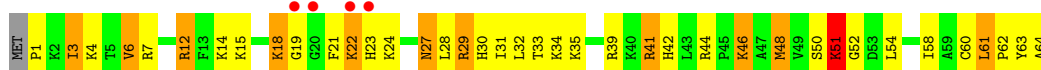
- Molecule 53: 50S ribosomal protein L35

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:

G971	A909	G844	C779	A718	A649	G581	C519	A456	A393	C328	A262	G200	C132	A71	U5
C972	A913	A845	A780	C719	G650	C582	A520	G457	G394	A329	A263	G201	U133	A72	G6
G973	A914	G846	A781	C720	C651	A583	G521	U458	C395	C330	G264	G202	C134	C73	A7
A974	A915	G847	A782	G721	G652	G584	C522	A459	C396	G331	G265	G203	C135	A74	A8
A975	A916	C848	C783	G722	U653	G585	U561	A460	A397	G332	G266	G204	U140	G75	G9
G976	A917	G849	A784	G723	G654	C586	U562	A461	U398	U333	C267	A205	G140	G76	A10
A977	A918	U850	G785	G724	A655	U589	C525	G462	G399	U334	C268	C206	G141	A77	G11
A978	A919	G851	G786	G725	G656	U590	C526	U463	C400	C339	A270	C207	G142	A78	U12
C979	A920	G852	A787	G726	U657	G591	C527	U464	C401	U340	U273	U208	A143	A79	U13
C980	U921	C853	A790	G727	C658	G592	C528	A465	C402	C341	U274	U209	G144	A80	U14
U981	U922	U854	G791	A728	U659	G593	U534	A466	G403		G275	G211	G147	A81	G15
U982	G922	U855	G792	G729	C660	U594	U535	U467	G404	A344	G276	G212	G148	G82	A16
A983	A923	C856	A793	G730	U661	A595	U536	U468	U405	C345	C277	G213	G149	C33	U17
C984	C924	C857	U793	G731	U662	A596	A537	C470	G406	G346	G278	G214	A150	U85	A19
C985	G925	G858	A794	C732	A663	A597	U538	U471	U407	G347	G279	C215	U151	G86	U20
G988	G926	G859	C795	G733	G664	G598	U539	U472	U408	G348	C280	C216	A152	C87	G21
U989	G927	A860	A665	G734	A665	C599	A535	U473	U409	A349	G281	C217	C153	U88	
G990	G928	G861	A666	G735	G666	C600	G537	G474	C410	G350	A282	U218	G154	U89	
C991	G929	C862	G667	G736	G667	G601	G538	C475	A411	G351	U283	U219	A155	C90	
U992	C930	U863	U801	C737	G668	A602	U539	U476	G412	C352	U284	G220		A26	
C993	C931	A864	A802	C738		A603	A540	C477	A413	A353	C285	U92	G158	U29	
A994	C932	A865	G803	G741	G674	G604	U541	A478	A414	G354	C286	U93	G159	U30	
C995	C933	C866	U804	A675	A675	G605	U542	U479	A415	C355	U287	U94	A160	G31	
A996	A935	U870	C805	A743	A676	G606	U543	U480	C416	A356	A288	U96	A161	A32	
U997	C936	U871	A807	C744	U677	A607	U544	G481	C419	G357	G289	U97	A162	A33	
C998	A937	G874	C808	G745	G682	A608	C545	A482	U420	U358	G292	G227	C163	G34	
G999	A938	U875	G809	A746	U682	A609	A546	G483	U421	G359	C288	U228	G164	G35	
A1000	C939	C876	C811	G747	G683	U610	A547	G484	C422	G360	U294	U229	G165	C96	
C1001	C940	C877	G812	G748	U684		G548	U485	G423	G361	U294	G230	U166	C99	
G1002	G941	C877	G813	A749	G685	G617	C549	U486	G424	G362	C295	U231	A167	U37	
G1003	G942	A878	U813	C750	U686	C618	G550	A487	G425	A363	U296	G232	G168	G38	
A1004	U943	C879	A814	U751	U687	U619	U551	C488	U426	A364	G297	C233	C169	C40	
A1005	G944	C880	A815	G752	G688	C620	U552	C489	U427	U365	A298	C234	G170	G41	
G945	G945	C881	A816	C753	C689		A553		G428	U366	G299	C235	A171	G42	
A946	A946	C882	C817	C754	G690	C623	U554	U429	U430	A300	A236	A236	A172	G107	
G947	C947	C883	G818	G755	G691	G494	U555	G494	A431	U368	G301	G237	U173	G108	
C948	C948	U884	A819	C756	U692	A495	U556	A495	A432	G369	G302		A174	A109	
A949	U950	G886	G821	U757	G693	A496		G497	G433	C370	G305	U239	C175	C110	
G951	G951		U822	A759	A695	G628	A559	G498	G434	A371	G306	G240	C176	G111	
U952	U952	A889	C823	G760	A696	A629	U561	A498	U434	C372	A306	G241	G177	G112	
G953	G953	C890	G824	G761	U697	A630	U562	A499	U435	A373	C307	G242	G178	G113	
G954	G954	U891	A825	U762		G631	U563	G500	C436	A374	C308	U243	A179	U114	
U955	U955	A892	C826	G763	G700	G632	A564	C501	U437	U375	A309	U244	U180	G115	
A1019	U956		U827	C764	U701	G633	C564	A502	U438	G376		U245	A181	C52	
G1015	U957	G895	G828	G765	A702	C634	U565	C503		G377	C312	A246	A182	A53	
A1016	G958	C896	G829	A766	G703	A635	U566	C504			A313	G247	C183	G57	
G1017	G959	C897	G830	A767	A704	U636	G567	G505			C314	C248	G184	C58	
G1018	U955	C898	A831	A768	G705	G637	U568				A315	U249	U185	A59	
A1019	U956	C899		G769	A706	U638	C569	U508	G444	G380	C316	G250	G190	A60	
G1020	U957	A900	U835	C770	U709	G639	U570	A509	G445	A382	U317	G251	A191	G61	
A1021	C958	A901	G836	G771	U710	A640	U571	A510	G446	A383	G318	U252	G192	G62	
A1022	A959	C897	U837	U772	G710	U641	A572	C385	A448	C385		A253	A192	C63	
U1023	U960	C898	G838	U773	G711	A642	A573	C386	G449	C386		G254	C193	G64	
G1024	U961	C899	C839	G774	A712	U643	A574	U387	C450	U387	A321	G257	C194	A65	
U1025	C962	A900	U840	G775	G713	U644	C575	C514	A451	G388	U323	G257	C195	A66	
G1026	A964	G902	U841	G776	G714	G645	C576	C515	A452	A389	G324	G258	A196	C67	
U1029	U965	U985	C941	A777	U715	G646	U577	U516	A453	U390	A325	G259	A197	G68	
U1030	C967	A963	U842	G778	U717	C647	C578	G517	G454	G391	G326	G260	A198	G69	
C1031	G1032	G1033	U843			A648		C518	G455	C392	A327	U261	A199	A131	



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	210.72Å 435.07Å 628.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	75.71 – 3.81 75.71 – 3.81	Depositor EDS
% Data completeness (in resolution range)	78.6 (75.71-3.81) 78.7 (75.71-3.81)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.59 (at 3.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.207 , 0.253 0.228 , 0.271	Depositor DCC
$R_{free}$ test set	8842 reflections (2.06%)	DCC
Wilson B-factor (Å <sup>2</sup> )	99.2	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	1 of 438428 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	285420	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	125.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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	0.27	0/1735	0.48	0/2338
1	CB	0.28	0/1735	0.52	0/2338
2	AC	0.28	0/1651	0.50	0/2225
2	CC	0.29	0/1651	0.48	0/2225
3	AD	0.29	0/1665	0.48	0/2227
3	CD	0.36	0/1665	0.53	0/2227
4	AE	0.35	0/1118	0.64	1/1504 (0.1%)
4	CE	0.34	0/1118	0.55	0/1504
5	AF	0.27	0/835	0.49	0/1128
5	CF	0.26	0/835	0.48	0/1128
6	AG	0.26	0/1195	0.45	0/1602
6	CG	0.30	0/1187	0.51	0/1591
7	AH	0.31	0/989	0.49	0/1326
7	CH	0.30	0/989	0.50	0/1326
8	AI	0.26	0/1034	0.46	0/1375
8	CI	0.26	0/1034	0.46	0/1375
9	AJ	0.26	0/796	0.49	0/1077
9	CJ	0.26	0/796	0.50	0/1077
10	AK	0.26	0/893	0.48	0/1205
10	CK	0.30	0/893	0.52	0/1205
11	AL	0.34	0/969	0.60	0/1300
11	CL	0.30	0/969	0.56	0/1300
12	AM	0.27	0/892	0.54	1/1193 (0.1%)
12	CM	0.36	0/884	1.04	4/1181 (0.3%)
13	AN	0.25	0/785	0.45	0/1043
13	CN	0.26	0/780	0.45	0/1036
14	AO	0.25	0/722	0.45	0/964
14	CO	0.26	0/722	0.47	0/964
15	AP	0.30	0/659	0.50	0/884
15	CP	0.30	0/648	0.49	0/870
16	AQ	0.32	0/657	0.57	0/881
16	CQ	0.31	0/657	0.49	0/881

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	AR	0.25	0/462	0.46	0/621
17	CR	0.31	0/462	0.49	0/621
18	AS	0.25	0/652	0.44	0/877
18	CS	0.25	0/652	0.46	0/877
19	AT	0.30	0/671	0.51	0/888
19	CT	0.27	0/671	0.46	0/888
20	AU	0.28	0/430	0.53	0/570
20	CU	0.33	0/430	0.57	0/570
21	AA	0.57	0/36834	1.45	646/57462 (1.1%)
22	AV	0.56	0/401	1.20	2/622 (0.3%)
22	CV	0.55	0/401	1.18	1/622 (0.2%)
23	AW	0.76	0/138	1.54	3/212 (1.4%)
23	CW	0.79	0/138	1.93	4/212 (1.9%)
24	BA	0.77	12/68626 (0.0%)	1.70	1788/107056 (1.7%)
24	DA	0.57	3/68314 (0.0%)	1.49	1376/106569 (1.3%)
25	BB	0.71	0/2828	1.59	62/4410 (1.4%)
26	BC	0.47	0/2121	0.73	1/2852 (0.0%)
26	DC	0.35	0/2121	0.58	0/2852
27	BD	0.52	0/1586	0.81	1/2134 (0.0%)
27	DD	0.32	0/1586	0.60	0/2134
28	BE	0.45	0/1571	0.67	0/2113
28	DE	0.33	0/1571	0.53	0/2113
29	BF	0.44	1/1434 (0.1%)	0.62	1/1926 (0.1%)
29	DF	0.45	3/1444 (0.2%)	0.79	5/1937 (0.3%)
30	BG	0.38	0/1343	0.64	0/1816
30	DG	0.28	0/1343	0.50	0/1816
31	BH	0.48	1/1122 (0.1%)	0.62	1/1515 (0.1%)
31	DH	0.39	0/1122	0.54	0/1515
32	BI	0.24	0/1046	0.50	0/1410
32	DI	0.24	0/1046	0.44	0/1410
33	BJ	0.56	0/1152	0.77	1/1551 (0.1%)
33	DJ	0.37	0/1152	0.62	0/1551
34	BK	0.53	0/947	0.82	1/1268 (0.1%)
34	DK	0.35	0/947	0.61	0/1268
35	BL	0.47	0/1054	0.76	1/1403 (0.1%)
35	DL	0.34	0/1054	0.58	0/1403
36	BM	0.50	0/1093	0.70	0/1460
36	DM	0.45	0/1093	0.63	0/1460
37	BN	0.48	0/973	0.73	1/1301 (0.1%)
37	DN	0.32	0/973	0.56	0/1301
38	BO	0.41	0/902	0.61	0/1209
38	DO	0.44	0/902	0.71	2/1209 (0.2%)
39	BP	0.48	0/929	0.74	0/1242

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
39	DP	0.33	0/929	0.52	0/1242
40	BQ	0.58	0/960	0.74	0/1278
40	DQ	0.36	0/960	0.54	0/1278
41	BR	0.57	0/829	0.77	0/1107
41	DR	0.38	0/829	0.58	0/1107
42	BS	0.54	0/864	0.78	0/1156
42	DS	0.30	0/864	0.56	0/1156
43	BT	0.44	0/744	0.67	0/994
43	DT	0.27	0/744	0.51	0/994
44	BU	0.42	0/787	0.71	1/1051 (0.1%)
44	DU	0.35	0/787	0.56	1/1051 (0.1%)
45	BV	0.47	0/766	0.68	0/1025
45	DV	0.68	3/766 (0.4%)	0.81	3/1025 (0.3%)
46	BW	0.54	0/603	0.84	0/797
46	DW	0.34	0/603	0.55	0/797
47	BX	0.41	0/635	0.68	1/848 (0.1%)
47	DX	0.32	0/635	0.55	0/848
48	BY	0.42	0/510	0.67	0/677
48	DY	0.28	0/510	0.49	0/677
49	BZ	0.47	0/453	0.73	0/605
49	DZ	0.32	0/453	0.58	0/605
50	B0	0.40	0/450	0.70	0/599
50	D0	0.31	0/450	0.55	0/599
51	B1	0.40	0/416	0.59	0/554
51	D1	0.31	0/416	0.49	0/554
52	B2	0.48	0/380	0.80	0/498
52	D2	0.31	0/380	0.53	0/498
53	B3	0.46	0/513	0.67	0/676
53	D3	0.36	0/513	0.57	0/676
54	B4	0.50	0/303	0.80	0/397
54	D4	0.41	0/303	0.60	0/397
55	CA	0.55	1/36762 (0.0%)	1.45	694/57350 (1.2%)
56	DB	0.68	4/2803 (0.1%)	1.79	112/4371 (2.6%)
All	All	0.57	28/307815 (0.0%)	1.37	4715/460233 (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
27	BD	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	DF	0	1
36	DM	0	1
All	All	0	4

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BA	1142	A	N9-C4	-11.34	1.31	1.37
45	DV	31	TYR	CE1-CZ	10.97	1.52	1.38
24	DA	1060	U	C2-N3	7.54	1.43	1.37
24	BA	1142	A	C8-N7	7.36	1.36	1.31
24	BA	2857	G	N3-C4	7.16	1.40	1.35

The worst 5 of 4715 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	CM	2	ARG	NE-CZ-NH1	-22.49	109.06	120.30
24	BA	2447	G	C6-N1-C2	-18.42	114.05	125.10
12	CM	2	ARG	NE-CZ-NH2	17.95	129.28	120.30
24	BA	1330	C	N1-C1'-C2'	-17.28	91.53	114.00
56	DB	104	A	C8-N9-C4	-16.28	99.29	105.80

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
27	BD	10	GLY	Peptide
27	BD	9	VAL	Peptide
29	DF	78	ILE	Peptide
36	DM	135	VAL	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	269	0
1	CB	1704	0	1732	208	0
2	AC	1624	0	1699	139	0
2	CC	1624	0	1699	159	0
3	AD	1643	0	1710	172	0
3	CD	1643	0	1710	143	0
4	AE	1105	0	1148	242	0
4	CE	1105	0	1148	122	0
5	AF	817	0	808	78	0
5	CF	817	0	808	79	0
6	AG	1181	0	1240	98	0
6	CG	1174	0	1230	151	0
7	AH	979	0	1034	118	0
7	CH	979	0	1034	95	0
8	AI	1022	0	1070	116	0
8	CI	1022	0	1070	141	0
9	AJ	786	0	828	77	0
9	CJ	786	0	828	124	0
10	AK	877	0	887	85	0
10	CK	877	0	887	99	0
11	AL	955	0	1019	96	0
11	CL	955	0	1019	102	0
12	AM	883	0	944	71	0
12	CM	876	0	937	137	0
13	AN	774	0	827	80	0
13	CN	769	0	822	89	0
14	AO	714	0	737	54	0
14	CO	714	0	737	40	0
15	AP	649	0	666	55	0
15	CP	638	0	656	65	0
16	AQ	648	0	691	82	0
16	CQ	648	0	691	47	0
17	AR	455	0	478	42	0
17	CR	455	0	478	40	0
18	AS	637	0	665	51	0
18	CS	637	0	665	78	0
19	AT	665	0	714	59	0
19	CT	665	0	714	47	0
20	AU	425	0	449	68	0
20	CU	425	0	449	76	0
21	AA	32895	0	16553	1701	0
22	AV	360	0	185	10	0
22	CV	360	0	185	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	AW	125	0	63	4	0
23	CW	125	0	63	6	0
24	BA	61274	0	30819	3143	0
24	DA	60995	0	30677	3530	0
25	BB	2529	0	1281	108	0
26	BC	2082	0	2157	200	0
26	DC	2082	0	2157	211	0
27	BD	1565	0	1616	189	0
27	DD	1565	0	1616	165	0
28	BE	1552	0	1619	150	0
28	DE	1552	0	1619	167	0
29	BF	1410	0	1447	123	0
29	DF	1420	0	1460	197	0
30	BG	1323	0	1374	163	0
30	DG	1323	0	1374	147	0
31	BH	1111	0	1148	109	0
31	DH	1111	0	1148	106	0
32	BI	1032	0	1088	110	0
32	DI	1032	0	1088	67	0
33	BJ	1129	0	1162	158	0
33	DJ	1129	0	1162	118	0
34	BK	938	0	1012	113	0
34	DK	938	0	1012	112	0
35	BL	1045	0	1117	123	0
35	DL	1045	0	1117	142	0
36	BM	1074	0	1157	111	0
36	DM	1074	0	1157	109	0
37	BN	960	0	1000	99	0
37	DN	960	0	1000	115	0
38	BO	892	0	923	67	0
38	DO	892	0	923	155	0
39	BP	917	0	965	134	0
39	DP	917	0	965	106	0
40	BQ	947	0	1022	130	0
40	DQ	947	0	1022	129	0
41	BR	816	0	839	88	0
41	DR	816	0	839	97	0
42	BS	857	0	922	69	0
42	DS	857	0	922	69	0
43	BT	738	0	807	108	0
43	DT	738	0	807	93	0
44	BU	779	0	834	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DU	779	0	834	107	0
45	BV	753	0	780	53	0
45	DV	753	0	780	118	0
46	BW	596	0	610	179	0
46	DW	596	0	610	120	0
47	BX	625	0	655	69	0
47	DX	625	0	655	73	0
48	BY	509	0	543	67	0
48	DY	509	0	543	62	0
49	BZ	449	0	491	46	0
49	DZ	449	0	491	38	0
50	B0	444	0	461	32	0
50	D0	444	0	461	52	0
51	B1	409	0	440	37	0
51	D1	409	0	440	33	0
52	B2	377	0	418	32	0
52	D2	377	0	418	33	0
53	B3	504	0	574	46	0
53	D3	504	0	574	50	0
54	B4	302	0	340	32	0
54	D4	302	0	340	24	0
55	CA	32831	0	16521	1808	0
56	DB	2507	0	1270	203	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	DA	134	0	0	0	0
57	DB	1	0	0	0	0
57	DC	1	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	195	0	0	7	0
59	AE	1	0	0	0	0
59	AL	3	0	0	1	0
59	AN	5	0	0	0	0
59	AT	3	0	0	0	0
59	AU	1	0	0	0	0
59	B2	2	0	0	0	0
59	B3	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	B4	2	0	0	0	0
59	BA	615	0	0	31	0
59	BB	19	0	0	0	0
59	BC	7	0	0	1	0
59	BD	2	0	0	3	0
59	BE	1	0	0	1	0
59	BL	4	0	0	1	0
59	BN	2	0	0	0	0
59	BQ	1	0	0	0	0
59	BT	1	0	0	1	0
59	BV	1	0	0	1	0
59	CA	196	0	0	4	0
59	CE	3	0	0	1	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	598	0	0	14	0
59	DB	4	0	0	0	0
59	DC	14	0	0	2	0
59	DD	4	0	0	0	0
59	DE	2	0	0	0	0
59	DJ	3	0	0	0	0
59	DL	5	0	0	0	0
59	DN	2	0	0	0	0
59	DT	2	0	0	0	0
59	DU	1	0	0	0	0
59	DV	1	0	0	0	0
All	All	285420	0	191332	18973	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 40.

The worst 5 of 18973 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:DA:1439:A:C2	24:DA:1552:A:C6	2.21	1.28
24:DA:1439:A:N1	24:DA:1552:A:C5	2.03	1.26
24:DA:1439:A:C2	24:DA:1552:A:C5	2.25	1.25

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
38:DO:100:HIS:CE1	56:DB:48:U:O2'	1.89	1.25
38:DO:30:ARG:HB2	38:DO:30:ARG:NH1	1.53	1.21

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%)	128 (59%)	60 (28%)	28 (13%)	0	13
1	CB	216/241 (90%)	145 (67%)	49 (23%)	22 (10%)	1	20
2	AC	204/233 (88%)	139 (68%)	51 (25%)	14 (7%)	2	34
2	CC	204/233 (88%)	146 (72%)	41 (20%)	17 (8%)	1	27
3	AD	203/206 (98%)	126 (62%)	52 (26%)	25 (12%)	1	14
3	CD	203/206 (98%)	141 (70%)	40 (20%)	22 (11%)	1	17
4	AE	148/167 (89%)	100 (68%)	31 (21%)	17 (12%)	1	16
4	CE	148/167 (89%)	98 (66%)	37 (25%)	13 (9%)	1	25
5	AF	98/135 (73%)	62 (63%)	25 (26%)	11 (11%)	1	16
5	CF	98/135 (73%)	65 (66%)	21 (21%)	12 (12%)	1	14
6	AG	149/179 (83%)	109 (73%)	29 (20%)	11 (7%)	2	32
6	CG	148/179 (83%)	80 (54%)	44 (30%)	24 (16%)	0	7
7	AH	127/130 (98%)	97 (76%)	22 (17%)	8 (6%)	2	38
7	CH	127/130 (98%)	96 (76%)	24 (19%)	7 (6%)	3	42
8	AI	125/130 (96%)	80 (64%)	34 (27%)	11 (9%)	1	25
8	CI	125/130 (96%)	86 (69%)	33 (26%)	6 (5%)	4	45
9	AJ	96/103 (93%)	69 (72%)	12 (12%)	15 (16%)	0	8
9	CJ	96/103 (93%)	61 (64%)	20 (21%)	15 (16%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	AK	115/129 (89%)	86 (75%)	22 (19%)	7 (6%)	2	38
10	CK	115/129 (89%)	74 (64%)	31 (27%)	10 (9%)	1	26
11	AL	121/124 (98%)	80 (66%)	24 (20%)	17 (14%)	0	11
11	CL	121/124 (98%)	86 (71%)	25 (21%)	10 (8%)	1	27
12	AM	112/118 (95%)	87 (78%)	16 (14%)	9 (8%)	1	29
12	CM	111/118 (94%)	65 (59%)	30 (27%)	16 (14%)	0	10
13	AN	92/101 (91%)	58 (63%)	25 (27%)	9 (10%)	1	21
13	CN	91/101 (90%)	59 (65%)	24 (26%)	8 (9%)	1	25
14	AO	86/89 (97%)	64 (74%)	17 (20%)	5 (6%)	3	39
14	CO	86/89 (97%)	72 (84%)	13 (15%)	1 (1%)	19	77
15	AP	80/82 (98%)	54 (68%)	15 (19%)	11 (14%)	0	11
15	CP	78/82 (95%)	56 (72%)	14 (18%)	8 (10%)	1	19
16	AQ	78/84 (93%)	48 (62%)	21 (27%)	9 (12%)	1	16
16	CQ	78/84 (93%)	59 (76%)	13 (17%)	6 (8%)	1	30
17	AR	53/75 (71%)	40 (76%)	11 (21%)	2 (4%)	5	53
17	CR	53/75 (71%)	44 (83%)	6 (11%)	3 (6%)	3	40
18	AS	77/92 (84%)	67 (87%)	6 (8%)	4 (5%)	3	42
18	CS	77/92 (84%)	54 (70%)	19 (25%)	4 (5%)	3	42
19	AT	83/87 (95%)	55 (66%)	21 (25%)	7 (8%)	1	27
19	CT	83/87 (95%)	59 (71%)	21 (25%)	3 (4%)	5	54
20	AU	49/71 (69%)	22 (45%)	18 (37%)	9 (18%)	0	5
20	CU	49/71 (69%)	20 (41%)	17 (35%)	12 (24%)	0	2
26	BC	269/273 (98%)	184 (68%)	59 (22%)	26 (10%)	1	22
26	DC	269/273 (98%)	181 (67%)	60 (22%)	28 (10%)	1	19
27	BD	207/209 (99%)	141 (68%)	32 (16%)	34 (16%)	0	7
27	DD	207/209 (99%)	132 (64%)	45 (22%)	30 (14%)	0	10
28	BE	199/201 (99%)	151 (76%)	24 (12%)	24 (12%)	1	14
28	DE	199/201 (99%)	130 (65%)	43 (22%)	26 (13%)	0	13
29	BF	175/179 (98%)	133 (76%)	25 (14%)	17 (10%)	1	22
29	DF	176/179 (98%)	97 (55%)	45 (26%)	34 (19%)	0	4
30	BG	174/177 (98%)	112 (64%)	35 (20%)	27 (16%)	0	8

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	DG	174/177 (98%)	105 (60%)	41 (24%)	28 (16%)	0	7
31	BH	147/149 (99%)	62 (42%)	54 (37%)	31 (21%)	0	3
31	DH	147/149 (99%)	76 (52%)	50 (34%)	21 (14%)	0	10
32	BI	139/142 (98%)	84 (60%)	44 (32%)	11 (8%)	1	29
32	DI	139/142 (98%)	81 (58%)	39 (28%)	19 (14%)	0	11
33	BJ	140/142 (99%)	106 (76%)	20 (14%)	14 (10%)	1	20
33	DJ	140/142 (99%)	95 (68%)	33 (24%)	12 (9%)	1	26
34	BK	120/123 (98%)	84 (70%)	18 (15%)	18 (15%)	0	9
34	DK	120/123 (98%)	80 (67%)	21 (18%)	19 (16%)	0	7
35	BL	141/144 (98%)	101 (72%)	28 (20%)	12 (8%)	1	27
35	DL	141/144 (98%)	83 (59%)	37 (26%)	21 (15%)	0	9
36	BM	134/136 (98%)	94 (70%)	25 (19%)	15 (11%)	1	16
36	DM	134/136 (98%)	92 (69%)	25 (19%)	17 (13%)	0	13
37	BN	118/127 (93%)	87 (74%)	21 (18%)	10 (8%)	1	27
37	DN	118/127 (93%)	71 (60%)	35 (30%)	12 (10%)	1	20
38	BO	114/117 (97%)	79 (69%)	26 (23%)	9 (8%)	1	29
38	DO	114/117 (97%)	76 (67%)	29 (25%)	9 (8%)	1	29
39	BP	112/115 (97%)	71 (63%)	22 (20%)	19 (17%)	0	6
39	DP	112/115 (97%)	67 (60%)	28 (25%)	17 (15%)	0	8
40	BQ	115/118 (98%)	88 (76%)	18 (16%)	9 (8%)	1	29
40	DQ	115/118 (98%)	79 (69%)	26 (23%)	10 (9%)	1	26
41	BR	101/103 (98%)	79 (78%)	14 (14%)	8 (8%)	1	29
41	DR	101/103 (98%)	72 (71%)	19 (19%)	10 (10%)	1	21
42	BS	108/110 (98%)	76 (70%)	27 (25%)	5 (5%)	4	46
42	DS	108/110 (98%)	81 (75%)	18 (17%)	9 (8%)	1	27
43	BT	91/100 (91%)	53 (58%)	23 (25%)	15 (16%)	0	7
43	DT	91/100 (91%)	48 (53%)	28 (31%)	15 (16%)	0	7
44	BU	100/104 (96%)	71 (71%)	13 (13%)	16 (16%)	0	7
44	DU	100/104 (96%)	51 (51%)	28 (28%)	21 (21%)	0	3
45	BV	92/94 (98%)	75 (82%)	15 (16%)	2 (2%)	10	66
45	DV	92/94 (98%)	59 (64%)	26 (28%)	7 (8%)	2	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	BW	77/85 (91%)	29 (38%)	22 (29%)	26 (34%)	0	0
46	DW	77/85 (91%)	32 (42%)	27 (35%)	18 (23%)	0	2
47	BX	75/78 (96%)	59 (79%)	13 (17%)	3 (4%)	5	51
47	DX	75/78 (96%)	48 (64%)	21 (28%)	6 (8%)	1	29
48	BY	61/63 (97%)	36 (59%)	17 (28%)	8 (13%)	0	13
48	DY	61/63 (97%)	44 (72%)	12 (20%)	5 (8%)	1	28
49	BZ	56/59 (95%)	39 (70%)	13 (23%)	4 (7%)	2	33
49	DZ	56/59 (95%)	31 (55%)	18 (32%)	7 (12%)	1	14
50	B0	54/57 (95%)	39 (72%)	9 (17%)	6 (11%)	1	17
50	D0	54/57 (95%)	40 (74%)	8 (15%)	6 (11%)	1	17
51	B1	48/55 (87%)	37 (77%)	7 (15%)	4 (8%)	1	27
51	D1	48/55 (87%)	35 (73%)	9 (19%)	4 (8%)	1	27
52	B2	44/46 (96%)	35 (80%)	8 (18%)	1 (2%)	10	65
52	D2	44/46 (96%)	32 (73%)	7 (16%)	5 (11%)	1	16
53	B3	62/65 (95%)	49 (79%)	11 (18%)	2 (3%)	6	57
53	D3	62/65 (95%)	39 (63%)	17 (27%)	6 (10%)	1	22
54	B4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	27
54	D4	36/38 (95%)	22 (61%)	9 (25%)	5 (14%)	0	11
All	All	11238/11970 (94%)	7499 (67%)	2485 (22%)	1254 (11%)	1	16

5 of 1254 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AB	20	ARG
1	AB	22	TRP
1	AB	40	ILE
1	AB	71	THR
1	AB	72	LYS

### 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%)	157 (87%)	23 (13%)	6	39
2	AC	170/190 (90%)	148 (87%)	22 (13%)	6	38
2	CC	170/190 (90%)	153 (90%)	17 (10%)	11	53
3	AD	172/173 (99%)	144 (84%)	28 (16%)	3	26
3	CD	172/173 (99%)	146 (85%)	26 (15%)	4	30
4	AE	113/126 (90%)	90 (80%)	23 (20%)	2	14
4	CE	113/126 (90%)	97 (86%)	16 (14%)	5	34
5	AF	87/116 (75%)	77 (88%)	10 (12%)	8	44
5	CF	87/116 (75%)	78 (90%)	9 (10%)	10	51
6	AG	124/147 (84%)	116 (94%)	8 (6%)	24	73
6	CG	123/147 (84%)	97 (79%)	26 (21%)	1	12
7	AH	104/105 (99%)	92 (88%)	12 (12%)	8	44
7	CH	104/105 (99%)	87 (84%)	17 (16%)	3	26
8	AI	105/107 (98%)	88 (84%)	17 (16%)	3	26
8	CI	105/107 (98%)	91 (87%)	14 (13%)	6	37
9	AJ	86/90 (96%)	72 (84%)	14 (16%)	3	26
9	CJ	86/90 (96%)	74 (86%)	12 (14%)	5	34
10	AK	90/99 (91%)	81 (90%)	9 (10%)	11	53
10	CK	90/99 (91%)	73 (81%)	17 (19%)	2	17
11	AL	103/104 (99%)	85 (82%)	18 (18%)	3	21
11	CL	103/104 (99%)	85 (82%)	18 (18%)	3	21
12	AM	92/96 (96%)	87 (95%)	5 (5%)	31	79
12	CM	91/96 (95%)	75 (82%)	16 (18%)	3	21
13	AN	79/84 (94%)	74 (94%)	5 (6%)	25	74
13	CN	79/84 (94%)	67 (85%)	12 (15%)	4	30
14	AO	76/77 (99%)	69 (91%)	7 (9%)	13	57
14	CO	76/77 (99%)	71 (93%)	5 (7%)	24	73
15	AP	65/65 (100%)	59 (91%)	6 (9%)	13	57
15	CP	65/65 (100%)	59 (91%)	6 (9%)	13	57
16	AQ	74/78 (95%)	57 (77%)	17 (23%)	1	10
16	CQ	74/78 (95%)	64 (86%)	10 (14%)	6	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	AR	48/65 (74%)	47 (98%)	1 (2%)	66	92
17	CR	48/65 (74%)	45 (94%)	3 (6%)	25	74
18	AS	70/79 (89%)	62 (89%)	8 (11%)	8	44
18	CS	70/79 (89%)	59 (84%)	11 (16%)	4	28
19	AT	65/66 (98%)	56 (86%)	9 (14%)	5	35
19	CT	65/66 (98%)	58 (89%)	7 (11%)	9	49
20	AU	44/61 (72%)	36 (82%)	8 (18%)	2	19
20	CU	44/61 (72%)	33 (75%)	11 (25%)	1	8
26	BC	216/218 (99%)	177 (82%)	39 (18%)	2	19
26	DC	216/218 (99%)	191 (88%)	25 (12%)	8	44
27	BD	164/164 (100%)	133 (81%)	31 (19%)	2	17
27	DD	164/164 (100%)	144 (88%)	20 (12%)	7	42
28	BE	165/165 (100%)	128 (78%)	37 (22%)	1	11
28	DE	165/165 (100%)	150 (91%)	15 (9%)	14	58
29	BF	148/150 (99%)	129 (87%)	19 (13%)	6	39
29	DF	149/150 (99%)	121 (81%)	28 (19%)	2	17
30	BG	137/138 (99%)	108 (79%)	29 (21%)	1	12
30	DG	137/138 (99%)	120 (88%)	17 (12%)	7	41
31	BH	114/114 (100%)	98 (86%)	16 (14%)	5	34
31	DH	114/114 (100%)	97 (85%)	17 (15%)	4	31
32	BI	109/110 (99%)	92 (84%)	17 (16%)	4	28
32	DI	109/110 (99%)	102 (94%)	7 (6%)	25	74
33	BJ	116/116 (100%)	91 (78%)	25 (22%)	1	11
33	DJ	116/116 (100%)	105 (90%)	11 (10%)	12	55
34	BK	103/104 (99%)	82 (80%)	21 (20%)	2	14
34	DK	103/104 (99%)	85 (82%)	18 (18%)	3	21
35	BL	102/103 (99%)	77 (76%)	25 (24%)	1	8
35	DL	102/103 (99%)	87 (85%)	15 (15%)	4	31
36	BM	109/109 (100%)	89 (82%)	20 (18%)	2	18
36	DM	109/109 (100%)	96 (88%)	13 (12%)	8	43
37	BN	100/103 (97%)	78 (78%)	22 (22%)	1	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DN	100/103 (97%)	87 (87%)	13 (13%)	6	38
38	BO	86/87 (99%)	69 (80%)	17 (20%)	2	15
38	DO	86/87 (99%)	76 (88%)	10 (12%)	8	44
39	BP	99/100 (99%)	77 (78%)	22 (22%)	1	11
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%)	78 (88%)	11 (12%)	7	41
41	BR	84/84 (100%)	68 (81%)	16 (19%)	2	17
41	DR	84/84 (100%)	72 (86%)	12 (14%)	5	33
42	BS	93/93 (100%)	76 (82%)	17 (18%)	2	18
42	DS	93/93 (100%)	80 (86%)	13 (14%)	5	34
43	BT	80/84 (95%)	63 (79%)	17 (21%)	1	12
43	DT	80/84 (95%)	75 (94%)	5 (6%)	25	74
44	BU	83/85 (98%)	73 (88%)	10 (12%)	7	42
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%)	65 (83%)	13 (17%)	3	24
46	BW	59/63 (94%)	39 (66%)	20 (34%)	0	3
46	DW	59/63 (94%)	43 (73%)	16 (27%)	1	6
47	BX	67/68 (98%)	56 (84%)	11 (16%)	3	25
47	DX	67/68 (98%)	58 (87%)	9 (13%)	6	37
48	BY	55/55 (100%)	41 (74%)	14 (26%)	1	8
48	DY	55/55 (100%)	51 (93%)	4 (7%)	20	68
49	BZ	48/49 (98%)	34 (71%)	14 (29%)	0	5
49	DZ	48/49 (98%)	39 (81%)	9 (19%)	2	17
50	B0	47/48 (98%)	43 (92%)	4 (8%)	15	62
50	D0	47/48 (98%)	41 (87%)	6 (13%)	6	39
51	B1	45/49 (92%)	35 (78%)	10 (22%)	1	11
51	D1	45/49 (92%)	41 (91%)	4 (9%)	14	59
52	B2	38/38 (100%)	32 (84%)	6 (16%)	4	28
52	D2	38/38 (100%)	34 (90%)	4 (10%)	10	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	B3	51/52 (98%)	45 (88%)	6 (12%)	8	43
53	D3	51/52 (98%)	42 (82%)	9 (18%)	3	21
54	B4	34/34 (100%)	29 (85%)	5 (15%)	4	31
54	D4	34/34 (100%)	29 (85%)	5 (15%)	4	31
All	All	9331/9756 (96%)	7927 (85%)	1404 (15%)	4	31

5 of 1404 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
42	BS	29	VAL
1	CB	19	THR
42	DS	22	ASP
43	BT	17	SER
47	BX	24	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 327 such sidechains are listed below:

Mol	Chain	Res	Type
45	BV	51	GLN
3	CD	125	ASN
44	DU	53	GLN
46	BW	49	ASN
1	CB	14	HIS

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	AA	1532/1533 (99%)	474 (30%)	255 (16%)
22	AV	16/17 (94%)	0	0
22	CV	16/17 (94%)	1 (6%)	0
23	AW	5/6 (83%)	3 (60%)	1 (20%)
23	CW	5/6 (83%)	2 (40%)	1 (20%)
24	BA	2850/2903 (98%)	958 (33%)	492 (17%)
24	DA	2838/2903 (97%)	1000 (35%)	519 (18%)
25	BB	117/118 (99%)	33 (28%)	19 (16%)
55	CA	1530/1530 (100%)	519 (33%)	252 (16%)
56	DB	116/117 (99%)	42 (36%)	18 (15%)
All	All	9025/9150 (98%)	3032 (33%)	1557 (17%)

5 of 3032 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 1557 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	BA	2609	U
55	CA	500	G
24	DA	2287	A
24	BA	2732	G
55	CA	89	U

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	AB	218/241 (90%)	2.10	89 (40%) 1 1	206, 268, 283, 298	0
1	CB	218/241 (90%)	0.99	35 (16%) 2 4	146, 174, 199, 216	0
2	AC	206/233 (88%)	0.53	4 (1%) 64 43	106, 135, 169, 198	0
2	CC	206/233 (88%)	0.43	5 (2%) 56 37	111, 140, 177, 195	0
3	AD	205/206 (99%)	0.35	7 (3%) 43 29	102, 139, 185, 204	0
3	CD	205/206 (99%)	0.01	0 100 100	86, 109, 140, 157	0
4	AE	150/167 (89%)	2.66	75 (50%) 0 1	102, 214, 237, 255	0
4	CE	150/167 (89%)	0.56	8 (5%) 25 18	86, 134, 166, 209	0
5	AF	100/135 (74%)	0.91	19 (19%) 2 3	140, 166, 186, 192	0
5	CF	100/135 (74%)	0.75	7 (7%) 16 13	140, 170, 200, 208	0
6	AG	151/179 (84%)	0.56	6 (3%) 36 25	128, 157, 186, 202	0
6	CG	150/179 (83%)	0.66	17 (11%) 6 7	115, 165, 204, 219	0
7	AH	129/130 (99%)	0.71	13 (10%) 7 8	102, 134, 158, 182	0
7	CH	129/130 (99%)	0.36	1 (0%) 83 64	106, 135, 159, 174	0
8	AI	127/130 (97%)	0.61	8 (6%) 19 14	108, 158, 190, 210	0
8	CI	127/130 (97%)	0.82	15 (11%) 5 6	114, 174, 206, 221	0
9	AJ	98/103 (95%)	0.31	0 100 100	105, 150, 194, 211	0
9	CJ	98/103 (95%)	0.76	10 (10%) 7 8	113, 165, 210, 220	0
10	AK	117/129 (90%)	0.99	13 (11%) 6 7	100, 149, 183, 200	0
10	CK	117/129 (90%)	0.63	4 (3%) 43 29	89, 133, 167, 192	0
11	AL	123/124 (99%)	0.39	2 (1%) 68 47	75, 95, 132, 157	0
11	CL	123/124 (99%)	0.28	1 (0%) 83 64	83, 101, 132, 151	0
12	AM	114/118 (96%)	0.79	13 (11%) 6 7	122, 182, 213, 232	0
12	CM	113/118 (95%)	0.65	9 (7%) 12 11	133, 193, 225, 235	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	AN	96/101 (95%)	0.40	1 (1%) 79 59	111, 142, 184, 210	0
13	CN	95/101 (94%)	0.81	10 (10%) 7 7	117, 149, 199, 207	0
14	AO	88/89 (98%)	0.30	0 100 100	105, 133, 163, 199	0
14	CO	88/89 (98%)	0.37	2 (2%) 57 38	113, 141, 174, 197	0
15	AP	82/82 (100%)	1.00	11 (13%) 4 4	95, 127, 165, 208	0
15	CP	80/82 (97%)	1.01	10 (12%) 5 5	98, 122, 156, 189	0
16	AQ	80/84 (95%)	0.74	3 (3%) 38 27	69, 100, 142, 159	0
16	CQ	80/84 (95%)	0.88	6 (7%) 14 12	72, 111, 142, 159	0
17	AR	55/75 (73%)	0.66	4 (7%) 15 12	129, 148, 180, 190	0
17	CR	55/75 (73%)	0.84	6 (10%) 6 7	131, 150, 170, 182	0
18	AS	79/92 (85%)	0.92	11 (13%) 4 4	140, 176, 210, 235	0
18	CS	79/92 (85%)	1.07	10 (12%) 4 5	151, 182, 215, 230	0
19	AT	85/87 (97%)	0.22	0 100 100	89, 121, 149, 180	0
19	CT	85/87 (97%)	0.69	4 (4%) 30 21	115, 153, 185, 206	0
20	AU	51/71 (71%)	0.78	8 (15%) 3 4	98, 145, 201, 208	0
20	CU	51/71 (71%)	0.74	6 (11%) 5 6	104, 139, 173, 193	0
21	AA	1533/1533 (100%)	-0.48	11 (0%) 84 67	65, 123, 208, 301	0
22	AV	17/17 (100%)	0.01	1 (5%) 22 16	102, 112, 149, 197	0
22	CV	17/17 (100%)	-0.20	1 (5%) 22 16	99, 104, 145, 179	0
23	AW	6/6 (100%)	0.54	1 (16%) 2 3	100, 109, 120, 155	0
23	CW	6/6 (100%)	0.32	0 100 100	98, 105, 123, 130	0
24	BA	2854/2903 (98%)	-0.43	38 (1%) 74 52	36, 66, 188, 342	0
24	DA	2841/2903 (97%)	-0.11	49 (1%) 67 46	79, 132, 236, 340	0
25	BB	118/118 (100%)	-0.65	0 100 100	52, 81, 113, 162	0
26	BC	271/273 (99%)	0.13	3 (1%) 77 56	44, 80, 122, 159	0
26	DC	271/273 (99%)	0.64	13 (4%) 29 21	89, 133, 164, 189	0
27	BD	209/209 (100%)	0.08	0 100 100	37, 59, 105, 146	0
27	DD	209/209 (100%)	0.57	8 (3%) 38 27	83, 131, 164, 186	0
28	BE	201/201 (100%)	0.20	3 (1%) 70 48	38, 84, 131, 164	0
28	DE	201/201 (100%)	0.56	13 (6%) 18 14	95, 171, 212, 250	0
29	BF	177/179 (98%)	0.95	23 (12%) 4 5	90, 148, 201, 218	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
29	DF	178/179 (99%)	2.20	87 (48%) 1 1	250, 278, 301, 305	0
30	BG	176/177 (99%)	0.22	1 (0%) 86 70	66, 91, 135, 160	0
30	DG	176/177 (99%)	0.94	17 (9%) 8 8	120, 148, 177, 204	0
31	BH	149/149 (100%)	2.45	62 (41%) 1 1	89, 262, 290, 299	0
31	DH	149/149 (100%)	1.97	60 (40%) 1 1	156, 244, 279, 286	0
32	BI	141/142 (99%)	2.29	62 (43%) 1 1	237, 306, 364, 376	0
32	DI	141/142 (99%)	2.37	68 (48%) 1 1	277, 331, 367, 378	0
33	BJ	142/142 (100%)	-0.01	0 100 100	41, 57, 102, 157	0
33	DJ	142/142 (100%)	0.47	3 (2%) 60 40	92, 115, 142, 181	0
34	BK	122/123 (99%)	0.13	0 100 100	41, 56, 110, 177	0
34	DK	122/123 (99%)	0.82	7 (5%) 23 16	93, 115, 144, 173	0
35	BL	143/144 (99%)	0.04	1 (0%) 84 67	38, 77, 119, 160	0
35	DL	143/144 (99%)	0.74	10 (6%) 16 13	93, 155, 197, 209	0
36	BM	136/136 (100%)	0.15	2 (1%) 70 48	41, 67, 114, 152	0
36	DM	136/136 (100%)	0.85	10 (7%) 14 12	80, 107, 142, 164	0
37	BN	120/127 (94%)	0.20	0 100 100	46, 63, 84, 138	0
37	DN	120/127 (94%)	1.12	20 (16%) 2 3	122, 154, 180, 217	0
38	BO	116/117 (99%)	0.02	0 100 100	73, 84, 124, 149	0
38	DO	116/117 (99%)	1.85	51 (43%) 1 1	165, 197, 217, 225	0
39	BP	114/115 (99%)	0.14	1 (0%) 81 62	49, 67, 123, 152	0
39	DP	114/115 (99%)	0.78	9 (7%) 13 11	117, 137, 163, 182	0
40	BQ	117/118 (99%)	-0.16	0 100 100	40, 58, 100, 127	0
40	DQ	117/118 (99%)	0.65	5 (4%) 34 23	97, 119, 143, 172	0
41	BR	103/103 (100%)	0.21	0 100 100	39, 70, 116, 158	0
41	DR	103/103 (100%)	0.82	13 (12%) 4 5	96, 133, 157, 164	0
42	BS	110/110 (100%)	-0.03	0 100 100	41, 58, 95, 161	0
42	DS	110/110 (100%)	0.75	8 (7%) 15 12	98, 141, 173, 188	0
43	BT	93/100 (93%)	0.70	6 (6%) 18 14	56, 95, 135, 165	0
43	DT	93/100 (93%)	2.08	43 (46%) 1 1	144, 196, 226, 237	0
44	BU	102/104 (98%)	0.42	2 (1%) 62 41	77, 105, 139, 194	0
44	DU	102/104 (98%)	1.90	43 (42%) 1 1	174, 208, 248, 279	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
45	BV	94/94 (100%)	0.22	0 100 100	60, 81, 115, 143	0
45	DV	94/94 (100%)	1.46	31 (32%) 1 2	125, 188, 226, 239	0
46	BW	79/85 (92%)	0.27	2 (2%) 54 36	50, 75, 131, 168	0
46	DW	79/85 (92%)	1.11	11 (13%) 4 4	88, 134, 164, 184	0
47	BX	77/78 (98%)	0.07	1 (1%) 74 52	50, 84, 126, 147	0
47	DX	77/78 (98%)	0.99	11 (14%) 3 4	110, 157, 187, 203	0
48	BY	63/63 (100%)	0.52	7 (11%) 6 7	87, 109, 154, 163	0
48	DY	63/63 (100%)	0.98	10 (15%) 3 4	196, 218, 251, 257	0
49	BZ	58/59 (98%)	0.25	2 (3%) 43 29	49, 63, 106, 145	0
49	DZ	58/59 (98%)	0.57	4 (6%) 17 13	97, 116, 142, 155	0
50	B0	56/57 (98%)	-0.16	0 100 100	40, 63, 119, 143	0
50	D0	56/57 (98%)	0.68	3 (5%) 25 17	93, 152, 190, 202	0
51	B1	50/55 (90%)	0.61	2 (4%) 36 25	63, 91, 117, 156	0
51	D1	50/55 (90%)	1.31	9 (18%) 2 3	113, 142, 173, 179	0
52	B2	46/46 (100%)	0.05	1 (2%) 59 39	50, 61, 80, 165	0
52	D2	46/46 (100%)	0.45	1 (2%) 59 39	118, 137, 161, 174	0
53	B3	64/65 (98%)	0.11	0 100 100	45, 63, 98, 133	0
53	D3	64/65 (98%)	0.81	4 (6%) 19 14	105, 123, 146, 174	0
54	B4	38/38 (100%)	0.27	0 100 100	54, 68, 100, 118	0
54	D4	38/38 (100%)	0.93	1 (2%) 53 35	95, 117, 138, 142	0
55	CA	1530/1530 (100%)	-0.27	24 (1%) 68 47	77, 126, 214, 305	0
56	DB	117/117 (100%)	-0.42	0 100 100	87, 166, 194, 210	0
All	All	20477/21120 (96%)	0.28	1332 (6%) 18 14	36, 125, 246, 378	0

The worst 5 of 1332 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
29	DF	129	MET	19.6
31	BH	92	GLY	15.2
31	DH	92	GLY	14.5
24	BA	2179	C	14.2
31	BH	116	ARG	13.2

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
57	MG	AA	1627	1/1	0.60	227.00	109,109,109,109	0
57	MG	DA	3065	1/1	2.23	189.73	84,84,84,84	0
57	MG	CA	1619	1/1	0.77	117.80	119,119,119,119	0
57	MG	BB	201	1/1	0.52	90.75	105,105,105,105	0
57	MG	DA	3110	1/1	1.52	77.59	82,82,82,82	0
57	MG	AA	1619	1/1	0.92	75.35	136,136,136,136	0
57	MG	BA	3062	1/1	0.53	57.31	38,38,38,38	0
57	MG	DA	3016	1/1	1.14	57.23	96,96,96,96	0
57	MG	BA	3135	1/1	0.45	56.68	43,43,43,43	0
57	MG	DA	3076	1/1	1.29	40.63	109,109,109,109	0
57	MG	DA	3061	1/1	0.42	39.71	84,84,84,84	0
57	MG	DA	3060	1/1	0.51	39.32	96,96,96,96	0
57	MG	BA	3085	1/1	0.49	37.53	42,42,42,42	0
57	MG	BA	3098	1/1	0.70	33.73	52,52,52,52	0
57	MG	DA	3109	1/1	0.47	33.00	92,92,92,92	0
57	MG	BA	3015	1/1	0.57	30.55	38,38,38,38	0
57	MG	DA	3023	1/1	0.62	30.21	101,101,101,101	0
57	MG	DA	3064	1/1	0.42	29.73	87,87,87,87	0
57	MG	DA	3062	1/1	1.03	28.43	85,85,85,85	0
57	MG	BA	3030	1/1	0.49	26.90	41,41,41,41	0
57	MG	DA	3099	1/1	0.88	26.13	98,98,98,98	0
57	MG	DA	3077	1/1	0.61	26.11	86,86,86,86	0
57	MG	DA	3134	1/1	1.36	24.50	126,126,126,126	0
57	MG	DA	3093	1/1	0.48	23.56	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	DA	3021	1/1	0.68	23.28	132,132,132,132	0
57	MG	DC	301	1/1	0.45	22.98	103,103,103,103	0
57	MG	DA	3100	1/1	0.60	21.95	149,149,149,149	0
57	MG	DJ	201	1/1	0.50	21.25	101,101,101,101	0
57	MG	BA	3077	1/1	0.32	21.17	45,45,45,45	0
57	MG	BA	3014	1/1	0.31	21.05	38,38,38,38	0
57	MG	DA	3017	1/1	0.54	20.82	102,102,102,102	0
57	MG	BA	3058	1/1	0.51	20.61	44,44,44,44	0
57	MG	BA	3011	1/1	0.40	20.56	44,44,44,44	0
57	MG	BA	3071	1/1	0.34	19.18	38,38,38,38	0
57	MG	BA	3061	1/1	0.51	18.04	39,39,39,39	0
57	MG	BA	3131	1/1	0.84	17.86	48,48,48,48	0
57	MG	BA	3037	1/1	0.32	17.50	42,42,42,42	0
57	MG	DA	3096	1/1	0.67	16.48	120,120,120,120	0
57	MG	DA	3120	1/1	0.72	16.18	96,96,96,96	0
57	MG	BA	3084	1/1	0.43	16.16	49,49,49,49	0
57	MG	DA	3028	1/1	1.02	15.45	103,103,103,103	0
57	MG	DA	3040	1/1	0.50	15.35	102,102,102,102	0
57	MG	BA	3102	1/1	0.31	15.31	40,40,40,40	0
57	MG	DA	3080	1/1	0.49	14.44	84,84,84,84	0
57	MG	DA	3128	1/1	0.50	13.98	100,100,100,100	0
57	MG	CA	1602	1/1	0.39	13.71	106,106,106,106	0
57	MG	CA	1603	1/1	0.34	13.06	92,92,92,92	0
57	MG	DA	3090	1/1	0.31	12.59	92,92,92,92	0
57	MG	BA	3119	1/1	0.31	12.22	52,52,52,52	0
57	MG	DA	3066	1/1	0.30	11.72	92,92,92,92	0
57	MG	CA	1640	1/1	0.40	11.28	87,87,87,87	0
57	MG	BA	3057	1/1	0.32	10.99	42,42,42,42	0
57	MG	DA	3126	1/1	0.53	10.86	99,99,99,99	0
57	MG	BA	3056	1/1	0.29	10.76	45,45,45,45	0
57	MG	DA	3032	1/1	0.33	10.51	87,87,87,87	0
57	MG	BA	3026	1/1	0.42	10.46	41,41,41,41	0
57	MG	CA	1615	1/1	0.33	10.36	118,118,118,118	0
57	MG	BA	3095	1/1	0.23	10.18	75,75,75,75	0
57	MG	BA	3041	1/1	0.25	9.94	43,43,43,43	0
57	MG	CA	1624	1/1	0.81	9.83	79,79,79,79	0
57	MG	CA	1612	1/1	0.39	9.77	86,86,86,86	0
57	MG	AA	1636	1/1	0.34	9.32	120,120,120,120	0
57	MG	CA	1625	1/1	0.31	9.00	86,86,86,86	0
57	MG	DA	3133	1/1	0.62	8.97	115,115,115,115	0
57	MG	BA	3016	1/1	0.34	8.90	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	AA	1626	1/1	0.24	8.88	107,107,107,107	0
57	MG	DA	3031	1/1	0.37	8.79	98,98,98,98	0
57	MG	BA	3112	1/1	0.23	8.72	46,46,46,46	0
57	MG	CA	1629	1/1	0.59	8.62	111,111,111,111	0
57	MG	AA	1607	1/1	0.37	8.36	88,88,88,88	0
57	MG	DA	3008	1/1	0.23	7.79	177,177,177,177	0
57	MG	DA	3012	1/1	0.37	7.53	96,96,96,96	0
57	MG	DA	3054	1/1	0.31	7.35	88,88,88,88	0
57	MG	DA	3001	1/1	0.27	7.22	115,115,115,115	0
57	MG	BA	3002	1/1	0.34	7.21	47,47,47,47	0
57	MG	DA	3112	1/1	0.59	7.11	115,115,115,115	0
57	MG	BA	3005	1/1	0.18	6.93	73,73,73,73	0
57	MG	BA	3045	1/1	0.24	6.92	62,62,62,62	0
57	MG	BA	3124	1/1	0.55	6.89	41,41,41,41	0
57	MG	AA	1621	1/1	0.17	6.77	67,67,67,67	0
57	MG	BA	3065	1/1	0.22	6.64	38,38,38,38	0
57	MG	AA	1628	1/1	0.32	6.45	107,107,107,107	0
57	MG	BA	3007	1/1	0.23	6.45	90,90,90,90	0
57	MG	BA	3105	1/1	0.22	6.30	38,38,38,38	0
57	MG	DA	3029	1/1	0.36	6.10	108,108,108,108	0
57	MG	DA	3118	1/1	0.29	5.91	99,99,99,99	0
57	MG	DA	3002	1/1	0.28	5.83	125,125,125,125	0
57	MG	CA	1639	1/1	0.29	5.81	165,165,165,165	0
57	MG	BA	3136	1/1	0.38	5.78	47,47,47,47	0
57	MG	BA	3060	1/1	0.27	5.77	39,39,39,39	0
57	MG	BA	3093	1/1	0.19	5.58	84,84,84,84	0
57	MG	DA	3073	1/1	0.28	5.56	98,98,98,98	0
57	MG	BA	3123	1/1	0.20	5.49	63,63,63,63	0
57	MG	BA	3118	1/1	0.22	5.07	42,42,42,42	0
57	MG	CA	1628	1/1	0.34	5.03	79,79,79,79	0
57	MG	DA	3078	1/1	0.30	4.92	79,79,79,79	0
57	MG	DA	3015	1/1	0.26	4.92	88,88,88,88	0
57	MG	CA	1614	1/1	0.22	4.81	114,114,114,114	0
57	MG	BA	3115	1/1	0.34	4.71	49,49,49,49	0
57	MG	BA	3133	1/1	0.56	4.54	53,53,53,53	0
57	MG	BA	3028	1/1	0.24	4.51	39,39,39,39	0
57	MG	AA	1614	1/1	0.27	4.50	113,113,113,113	0
57	MG	AA	1602	1/1	0.22	4.48	79,79,79,79	0
57	MG	CA	1620	1/1	0.27	4.47	93,93,93,93	0
57	MG	AA	1623	1/1	0.15	4.33	108,108,108,108	0
57	MG	DA	3071	1/1	0.56	4.31	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	1608	1/1	0.24	4.27	86,86,86,86	0
57	MG	DA	3088	1/1	0.23	4.05	101,101,101,101	0
57	MG	CA	1605	1/1	0.22	4.03	89,89,89,89	0
57	MG	DA	3030	1/1	0.52	3.95	101,101,101,101	0
57	MG	DA	3107	1/1	0.25	3.89	130,130,130,130	0
57	MG	DA	3089	1/1	0.23	3.70	110,110,110,110	0
57	MG	DA	3130	1/1	0.66	3.69	85,85,85,85	0
57	MG	DA	3041	1/1	0.28	3.68	113,113,113,113	0
57	MG	BA	3099	1/1	0.20	3.61	41,41,41,41	0
57	MG	AA	1641	1/1	0.34	3.60	89,89,89,89	0
57	MG	BA	3126	1/1	0.25	3.50	57,57,57,57	0
57	MG	AA	1631	1/1	0.24	3.31	98,98,98,98	0
57	MG	BA	3004	1/1	0.26	3.11	69,69,69,69	0
57	MG	BA	3072	1/1	0.20	3.11	38,38,38,38	0
57	MG	CA	1627	1/1	0.26	3.07	106,106,106,106	0
57	MG	DA	3038	1/1	0.20	3.06	108,108,108,108	0
57	MG	DA	3101	1/1	0.25	3.04	82,82,82,82	0
57	MG	BA	3109	1/1	0.20	2.89	42,42,42,42	0
57	MG	BA	3035	1/1	0.18	2.87	55,55,55,55	0
57	MG	DA	3131	1/1	0.90	2.86	103,103,103,103	0
57	MG	AA	1610	1/1	0.14	2.82	125,125,125,125	0
57	MG	CA	1636	1/1	0.58	2.77	88,88,88,88	0
57	MG	CA	1637	1/1	0.29	2.66	83,83,83,83	0
57	MG	BA	3104	1/1	0.19	2.61	38,38,38,38	0
57	MG	AA	1629	1/1	0.20	2.54	129,129,129,129	0
57	MG	AA	1642	1/1	0.17	2.53	74,74,74,74	0
57	MG	BA	3068	1/1	0.20	2.48	52,52,52,52	0
57	MG	DA	3121	1/1	0.24	2.34	97,97,97,97	0
57	MG	AA	1624	1/1	0.18	2.31	94,94,94,94	0
57	MG	BA	3092	1/1	0.16	2.01	108,108,108,108	0
57	MG	DA	3034	1/1	0.21	1.96	89,89,89,89	0
57	MG	CA	1630	1/1	0.32	1.93	79,79,79,79	0
57	MG	BA	3059	1/1	0.22	1.93	50,50,50,50	0
57	MG	AA	1620	1/1	0.20	1.89	144,144,144,144	0
57	MG	CA	1617	1/1	0.39	1.88	130,130,130,130	0
57	MG	CA	1613	1/1	0.23	1.87	79,79,79,79	0
57	MG	DA	3105	1/1	0.19	1.61	91,91,91,91	0
57	MG	DA	3003	1/1	0.26	1.60	94,94,94,94	0
57	MG	DA	3115	1/1	0.20	1.52	84,84,84,84	0
57	MG	DA	3035	1/1	0.20	1.47	88,88,88,88	0
57	MG	DA	3108	1/1	0.23	1.37	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
57	MG	BB	202	1/1	0.17	1.26	114,114,114,114	0
57	MG	CA	1607	1/1	0.22	1.10	89,89,89,89	0
57	MG	CA	1641	1/1	0.18	1.01	91,91,91,91	0
57	MG	AA	1608	1/1	0.18	0.99	82,82,82,82	0
57	MG	BA	3132	1/1	0.49	0.97	42,42,42,42	0
57	MG	BA	3125	1/1	0.18	0.96	40,40,40,40	0
57	MG	DA	3027	1/1	0.19	0.92	87,87,87,87	0
57	MG	BA	3075	1/1	0.41	0.83	40,40,40,40	0
57	MG	DA	3079	1/1	0.22	0.82	90,90,90,90	0
57	MG	DA	3022	1/1	0.21	0.80	105,105,105,105	0
57	MG	DA	3127	1/1	0.21	0.79	104,104,104,104	0
57	MG	DA	3053	1/1	0.21	0.78	101,101,101,101	0
57	MG	DA	3014	1/1	0.31	0.78	90,90,90,90	0
57	MG	CA	1621	1/1	0.19	0.75	85,85,85,85	0
57	MG	DA	3059	1/1	0.48	0.74	88,88,88,88	0
57	MG	DA	3006	1/1	0.19	0.72	149,149,149,149	0
57	MG	DA	3084	1/1	0.18	0.69	157,157,157,157	0
57	MG	DA	3104	1/1	0.21	0.60	107,107,107,107	0
57	MG	DA	3129	1/1	0.31	0.55	83,83,83,83	0
57	MG	BA	3034	1/1	0.18	0.43	40,40,40,40	0
57	MG	DA	3122	1/1	0.23	0.41	142,142,142,142	0
57	MG	CA	1618	1/1	0.19	0.40	108,108,108,108	0
57	MG	AA	1640	1/1	0.13	0.39	132,132,132,132	0
57	MG	DA	3007	1/1	0.35	0.38	192,192,192,192	0
57	MG	BA	3130	1/1	0.16	0.37	49,49,49,49	0
57	MG	BA	3070	1/1	0.23	0.34	140,140,140,140	0
57	MG	AA	1622	1/1	0.16	0.31	85,85,85,85	0
57	MG	BA	3001	1/1	0.15	0.30	45,45,45,45	0
57	MG	DA	3048	1/1	0.18	0.26	131,131,131,131	0
57	MG	DB	201	1/1	0.26	0.25	108,108,108,108	0
57	MG	DA	3094	1/1	0.17	0.21	126,126,126,126	0
57	MG	BA	3108	1/1	0.15	0.20	40,40,40,40	0
57	MG	DA	3072	1/1	0.14	0.16	84,84,84,84	0
57	MG	DA	3124	1/1	0.17	0.12	133,133,133,133	0
57	MG	BA	3101	1/1	0.17	0.11	38,38,38,38	0
57	MG	BA	3128	1/1	0.15	0.11	52,52,52,52	0
57	MG	DA	3025	1/1	0.19	0.09	105,105,105,105	0
57	MG	BA	3111	1/1	0.14	0.09	38,38,38,38	0
57	MG	DA	3116	1/1	0.18	-0.02	98,98,98,98	0
57	MG	BA	3048	1/1	0.14	-0.04	74,74,74,74	0
57	MG	DA	3092	1/1	0.18	-0.04	102,102,102,102	0
57	MG	CA	1622	1/1	0.11	-0.07	138,138,138,138	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	CA	1633	1/1	0.15	-0.09	101,101,101,101	0
57	MG	AA	1637	1/1	0.18	-0.12	87,87,87,87	0
57	MG	DA	3082	1/1	0.21	-0.13	83,83,83,83	0
57	MG	BA	3008	1/1	0.15	-0.17	43,43,43,43	0
57	MG	DA	3051	1/1	0.18	-0.17	177,177,177,177	0
57	MG	BA	3113	1/1	0.14	-0.17	38,38,38,38	0
57	MG	DA	3103	1/1	0.19	-0.18	91,91,91,91	0
57	MG	DA	3047	1/1	0.19	-0.23	148,148,148,148	0
57	MG	DA	3083	1/1	0.21	-0.26	121,121,121,121	0
57	MG	DA	3117	1/1	0.21	-0.31	90,90,90,90	0
57	MG	BA	3038	1/1	0.15	-0.34	42,42,42,42	0
57	MG	AA	1613	1/1	0.14	-0.36	74,74,74,74	0
57	MG	BA	3106	1/1	0.15	-0.36	40,40,40,40	0
57	MG	BA	3107	1/1	0.18	-0.37	49,49,49,49	0
57	MG	DA	3058	1/1	0.15	-0.39	96,96,96,96	0
57	MG	DA	3111	1/1	0.22	-0.44	164,164,164,164	0
57	MG	BA	3081	1/1	0.16	-0.49	40,40,40,40	0
57	MG	AA	1603	1/1	0.12	-0.49	76,76,76,76	0
57	MG	AA	1606	1/1	0.14	-0.49	96,96,96,96	0
57	MG	DA	3046	1/1	0.18	-0.53	142,142,142,142	0
57	MG	BA	3013	1/1	0.15	-0.53	38,38,38,38	0
57	MG	DA	3086	1/1	0.17	-0.58	148,148,148,148	0
57	MG	DA	3049	1/1	0.16	-0.59	150,150,150,150	0
57	MG	AA	1618	1/1	0.17	-0.63	104,104,104,104	0
57	MG	DA	3085	1/1	0.14	-0.66	190,190,190,190	0
57	MG	AA	1625	1/1	0.15	-0.68	90,90,90,90	0
57	MG	DA	3125	1/1	0.18	-0.70	90,90,90,90	0
57	MG	CA	1632	1/1	0.16	-0.75	125,125,125,125	0
57	MG	DA	3050	1/1	0.17	-0.76	148,148,148,148	0
57	MG	DA	3039	1/1	0.16	-0.77	104,104,104,104	0
57	MG	BA	3043	1/1	0.15	-0.78	56,56,56,56	0
57	MG	BA	3051	1/1	0.12	-0.78	39,39,39,39	0
57	MG	CA	1626	1/1	0.14	-0.80	110,110,110,110	0
57	MG	BB	204	1/1	0.12	-0.81	57,57,57,57	0
57	MG	AA	1601	1/1	0.09	-0.83	111,111,111,111	0
57	MG	DA	3045	1/1	0.19	-0.83	141,141,141,141	0
57	MG	BD	301	1/1	0.14	-0.83	39,39,39,39	0
57	MG	BA	3047	1/1	0.16	-0.86	63,63,63,63	0
57	MG	DA	3097	1/1	0.18	-0.88	119,119,119,119	0
57	MG	AA	1630	1/1	0.13	-0.90	79,79,79,79	0
57	MG	CA	1642	1/1	0.12	-0.91	102,102,102,102	0
57	MG	DA	3056	1/1	0.15	-0.94	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3075	1/1	0.12	-0.96	255,255,255,255	0
57	MG	DA	3005	1/1	0.13	-0.97	157,157,157,157	0
57	MG	AA	1617	1/1	0.10	-0.99	123,123,123,123	0
57	MG	BA	3117	1/1	0.15	-1.02	56,56,56,56	0
57	MG	BA	3076	1/1	0.15	-1.02	47,47,47,47	0
57	MG	DA	3009	1/1	0.17	-1.04	121,121,121,121	0
57	MG	BA	3100	1/1	0.09	-1.05	59,59,59,59	0
57	MG	BA	3046	1/1	0.17	-1.11	63,63,63,63	0
57	MG	AA	1633	1/1	0.11	-1.11	107,107,107,107	0
57	MG	DA	3113	1/1	0.15	-1.11	86,86,86,86	0
57	MG	CA	1604	1/1	0.08	-1.13	106,106,106,106	0
57	MG	BA	3121	1/1	0.10	-1.13	45,45,45,45	0
57	MG	BA	3114	1/1	0.12	-1.15	73,73,73,73	0
57	MG	CA	1634	1/1	0.12	-1.16	97,97,97,97	0
57	MG	BB	203	1/1	0.08	-1.18	57,57,57,57	0
57	MG	DA	3033	1/1	0.17	-1.19	94,94,94,94	0
57	MG	BA	3031	1/1	0.13	-1.20	42,42,42,42	0
57	MG	BA	3116	1/1	0.14	-1.21	38,38,38,38	0
57	MG	BA	3122	1/1	0.16	-1.21	40,40,40,40	0
57	MG	DA	3123	1/1	0.15	-1.22	93,93,93,93	0
57	MG	DA	3019	1/1	0.12	-1.23	150,150,150,150	0
57	MG	AA	1611	1/1	0.12	-1.24	91,91,91,91	0
57	MG	BA	3019	1/1	0.10	-1.27	70,70,70,70	0
57	MG	BA	3134	1/1	0.13	-1.30	38,38,38,38	0
57	MG	CA	1610	1/1	0.10	-1.30	129,129,129,129	0
57	MG	DA	3070	1/1	0.14	-1.30	94,94,94,94	0
57	MG	BA	3042	1/1	0.15	-1.34	56,56,56,56	0
57	MG	BA	3052	1/1	0.14	-1.38	38,38,38,38	0
57	MG	DA	3037	1/1	0.15	-1.41	83,83,83,83	0
58	ZN	B4	101	1/1	0.09	-1.46	79,79,79,79	0
57	MG	DA	3020	1/1	0.12	-1.46	153,153,153,153	0
57	MG	BA	3024	1/1	0.12	-1.46	42,42,42,42	0
57	MG	BA	3049	1/1	0.13	-1.52	45,45,45,45	0
57	MG	DA	3068	1/1	0.16	-1.55	86,86,86,86	0
57	MG	DA	3024	1/1	0.14	-1.55	90,90,90,90	0
57	MG	DA	3026	1/1	0.14	-1.59	88,88,88,88	0
57	MG	DA	3010	1/1	0.13	-1.61	108,108,108,108	0
57	MG	BA	3055	1/1	0.13	-1.63	44,44,44,44	0
58	ZN	D4	101	1/1	0.04	-1.66	79,79,79,79	0
57	MG	CA	1616	1/1	0.12	-1.68	136,136,136,136	0
57	MG	CA	1638	1/1	0.12	-1.70	141,141,141,141	0
57	MG	DA	3043	1/1	0.20	-1.74	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3091	1/1	0.11	-1.78	69,69,69,69	0
57	MG	BA	3120	1/1	0.13	-1.81	41,41,41,41	0
57	MG	BA	3094	1/1	0.13	-1.81	75,75,75,75	0
57	MG	BA	3087	1/1	0.11	-1.81	45,45,45,45	0
57	MG	DA	3106	1/1	0.11	-1.82	92,92,92,92	0
57	MG	AA	1643	1/1	0.12	-1.87	81,81,81,81	0
57	MG	DA	3067	1/1	0.15	-1.91	86,86,86,86	0
57	MG	DA	3081	1/1	0.14	-1.93	87,87,87,87	0
57	MG	BA	3018	1/1	0.06	-1.95	67,67,67,67	0
57	MG	BA	3086	1/1	0.13	-1.97	43,43,43,43	0
57	MG	AA	1638	1/1	0.13	-1.98	81,81,81,81	0
57	MG	CA	1609	1/1	0.16	-2.03	96,96,96,96	0
57	MG	BA	3080	1/1	0.13	-2.05	74,74,74,74	0
57	MG	BA	3066	1/1	0.12	-2.11	43,43,43,43	0
57	MG	BA	3110	1/1	0.11	-2.14	50,50,50,50	0
57	MG	BA	3090	1/1	0.11	-2.15	47,47,47,47	0
57	MG	DA	3095	1/1	0.13	-2.18	159,159,159,159	0
57	MG	CA	1601	1/1	0.07	-2.31	142,142,142,142	0
57	MG	DA	3098	1/1	0.13	-2.31	87,87,87,87	0
57	MG	CA	1606	1/1	0.14	-2.36	85,85,85,85	0
57	MG	AA	1632	1/1	0.13	-2.39	95,95,95,95	0
57	MG	DA	3087	1/1	0.14	-2.40	88,88,88,88	0
57	MG	CA	1623	1/1	0.13	-2.42	89,89,89,89	0
57	MG	BA	3103	1/1	0.08	-2.42	64,64,64,64	0
57	MG	BA	3054	1/1	0.12	-2.43	44,44,44,44	0
57	MG	BA	3079	1/1	0.09	-2.44	89,89,89,89	0
57	MG	AA	1634	1/1	0.10	-2.49	102,102,102,102	0
57	MG	DA	3044	1/1	0.13	-2.49	116,116,116,116	0
57	MG	DA	3132	1/1	0.09	-2.51	94,94,94,94	0
57	MG	BA	3040	1/1	0.14	-2.56	41,41,41,41	0
57	MG	AA	1635	1/1	0.09	-2.56	114,114,114,114	0
57	MG	BA	3009	1/1	0.13	-2.60	46,46,46,46	0
57	MG	BA	3006	1/1	0.11	-2.61	88,88,88,88	0
57	MG	BA	3022	1/1	0.10	-2.62	38,38,38,38	0
57	MG	AA	1616	1/1	0.11	-2.66	126,126,126,126	0
57	MG	CA	1631	1/1	0.13	-2.69	91,91,91,91	0
57	MG	BA	3063	1/1	0.11	-2.71	37,37,37,37	0
57	MG	DA	3052	1/1	0.13	-2.72	118,118,118,118	0
57	MG	DA	3114	1/1	0.10	-2.73	98,98,98,98	0
57	MG	DA	3074	1/1	0.11	-2.81	98,98,98,98	0
57	MG	BA	3023	1/1	0.08	-2.84	41,41,41,41	0
57	MG	DA	3036	1/1	0.12	-2.85	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	BA	3050	1/1	0.12	-2.87	40,40,40,40	0
57	MG	DA	3057	1/1	0.13	-2.91	92,92,92,92	0
57	MG	BA	3074	1/1	0.09	-2.97	38,38,38,38	0
57	MG	BA	3096	1/1	0.10	-3.01	45,45,45,45	0
57	MG	BA	3078	1/1	0.08	-3.04	86,86,86,86	0
57	MG	BA	3017	1/1	0.11	-3.06	39,39,39,39	0
57	MG	BA	3032	1/1	0.12	-3.12	40,40,40,40	0
57	MG	CA	1635	1/1	0.10	-3.19	114,114,114,114	0
57	MG	BA	3089	1/1	0.10	-3.25	50,50,50,50	0
57	MG	BA	3025	1/1	0.09	-3.27	41,41,41,41	0
57	MG	DA	3091	1/1	0.12	-3.36	93,93,93,93	0
57	MG	BA	3020	1/1	0.11	-3.40	46,46,46,46	0
57	MG	DA	3018	1/1	0.11	-3.46	106,106,106,106	0
57	MG	BA	3082	1/1	0.11	-3.47	38,38,38,38	0
57	MG	AA	1605	1/1	0.09	-3.54	103,103,103,103	0
57	MG	DA	3102	1/1	0.10	-3.60	84,84,84,84	0
57	MG	BA	3053	1/1	0.12	-3.67	41,41,41,41	0
57	MG	BA	3003	1/1	0.06	-3.74	73,73,73,73	0
57	MG	DA	3069	1/1	0.10	-3.88	86,86,86,86	0
57	MG	BA	3097	1/1	0.11	-4.05	49,49,49,49	0
57	MG	DA	3063	1/1	0.16	-4.11	92,92,92,92	0
57	MG	BA	3067	1/1	0.09	-4.24	40,40,40,40	0
57	MG	DA	3042	1/1	0.14	-4.40	101,101,101,101	0
57	MG	AA	1604	1/1	0.07	-4.57	126,126,126,126	0
57	MG	AA	1639	1/1	0.06	-4.61	119,119,119,119	0
57	MG	BA	3069	1/1	0.08	-4.62	52,52,52,52	0
57	MG	BA	3064	1/1	0.08	-4.68	38,38,38,38	0
57	MG	DA	3013	1/1	0.13	-4.68	93,93,93,93	0
57	MG	BA	3021	1/1	0.09	-4.80	42,42,42,42	0
57	MG	BA	3010	1/1	0.09	-5.51	46,46,46,46	0
57	MG	BA	3012	1/1	0.12	-5.57	38,38,38,38	0
57	MG	AA	1609	1/1	0.11	-5.59	91,91,91,91	0
57	MG	BA	3029	1/1	0.08	-5.62	38,38,38,38	0
57	MG	AA	1615	1/1	0.09	-5.98	117,117,117,117	0
57	MG	BA	3129	1/1	0.09	-6.08	39,39,39,39	0
57	MG	BA	3036	1/1	0.06	-6.34	47,47,47,47	0
57	MG	BA	3073	1/1	0.09	-6.57	43,43,43,43	0
57	MG	BA	3039	1/1	0.10	-6.60	40,40,40,40	0
57	MG	BA	3044	1/1	0.10	-7.01	71,71,71,71	0
57	MG	CA	1611	1/1	0.08	-7.07	93,93,93,93	0
57	MG	BA	3083	1/1	0.06	-7.16	43,43,43,43	0
57	MG	BA	3033	1/1	0.11	-7.84	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
57	MG	DA	3055	1/1	0.14	-8.60	85,85,85,85	0
57	MG	AA	1612	1/1	0.11	-8.89	82,82,82,82	0
57	MG	DA	3119	1/1	0.15	-10.29	138,138,138,138	0
57	MG	BA	3088	1/1	0.06	-12.18	58,58,58,58	0
57	MG	BA	3027	1/1	0.04	-14.53	41,41,41,41	0
57	MG	BA	3127	1/1	0.06	-19.70	40,40,40,40	0
57	MG	DA	3011	1/1	0.54	-	110,110,110,110	0
57	MG	DA	3004	1/1	1.34	-	150,150,150,150	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.