



wwPDB X-ray Structure Validation Summary Report i

Nov 13, 2014 – 01:15 PM EST

PDB ID : 4WF1
Title : Crystal structure of the E. coli ribosome bound to negamycin.
Authors : Olivier, N.B.; Altman, R.B.; Noeske, J.; Basarab, G.S.; Code, E.; Ferguson, A.D.; Gao, N.; Huang, J.; Juetten, M.F.; Livchak, S.; Miller, M.D.; Prince, D.B.; Cate, J.H.D.; Buurman, E.T.; Blanchard, S.C.
Deposited on : 2014-08-31
Resolution : 3.09 Å(reported)

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

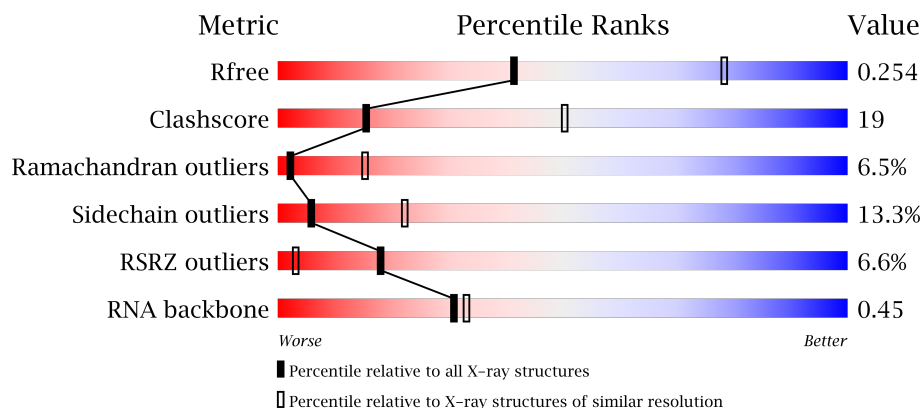
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.16 November 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable24195
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.1.3
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable24195

1 Overall quality at a glance

The reported resolution of this entry is 3.09 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	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)
RNA backbone	1838	1047 (3.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	AA	1539	
1	CA	1539	
2	AB	218	
2	CB	218	
3	AC	206	
3	CC	206	
4	AD	205	
4	CD	205	
5	AE	150	
5	CE	150	
6	AF	100	

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Mol	Chain	Length	Quality of chain
6	CF	100	
7	AG	151	
7	CG	151	
8	AH	129	
8	CH	129	
9	AI	127	
9	CI	127	
10	AJ	98	
10	CJ	98	
11	AK	117	
11	CK	117	
12	AL	123	
12	CL	123	
13	AM	114	
13	CM	114	
14	AN	100	
14	CN	100	
15	AO	88	
15	CO	88	
16	AP	82	
16	CP	82	
17	AQ	80	
17	CQ	80	
18	AR	55	
18	CR	55	
19	AS	79	
19	CS	79	
20	AT	85	
20	CT	85	
21	AU	51	
21	CU	51	
22	BA	2903	
22	DA	2903	
23	BB	119	
23	DB	119	
24	BC	271	
24	DC	271	
25	BD	209	
25	DD	209	
26	BE	201	
26	DE	201	
27	BF	177	

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Mol	Chain	Length	Quality of chain
27	DF	177	
28	BG	176	
28	DG	176	
29	BH	149	
29	DH	149	
30	BI	141	
30	DI	141	
31	BJ	142	
31	DJ	142	
32	BK	122	
32	DK	122	
33	BL	143	
33	DL	143	
34	BM	136	
34	DM	136	
35	BN	120	
35	DN	120	
36	BO	116	
36	DO	116	
37	BP	114	
37	DP	114	
38	BQ	117	
38	DQ	117	
39	BR	103	
39	DR	103	
40	BS	110	
40	DS	110	
41	BT	93	
41	DT	93	
42	BU	102	
42	DU	102	
43	BV	94	
43	DV	94	
44	BW	76	
44	DW	76	
45	BX	77	
45	DX	77	
46	BY	63	
46	DY	63	
47	BZ	58	
47	DZ	58	
48	B0	56	

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Mol	Chain	Length	Quality of chain
48	D0	56	
49	B1	50	
49	D1	50	
50	B2	46	
50	D2	46	
51	B3	64	
51	D3	64	
52	B4	38	
52	D4	38	
53	B5	207	

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

Mol	Type	Chain	Res	Geometry	Electron density
54	MG	AA	1605	-	X
54	MG	AA	1614	-	X
54	MG	AA	1615	-	X
54	MG	AA	1617	-	X
54	MG	AA	1619	-	X
54	MG	AA	1622	-	X
54	MG	AA	1623	-	X
54	MG	AA	1626	-	X
54	MG	AA	1627	-	X
54	MG	AA	1630	-	X
54	MG	AA	1635	-	X
54	MG	AA	1643	-	X
54	MG	AA	1644	-	X
54	MG	AA	1645	-	X
54	MG	AA	1646	-	X
54	MG	AA	1648	-	X
54	MG	AA	1649	-	X
54	MG	AA	1650	-	X
54	MG	AA	1651	-	X
54	MG	AA	1653	-	X
54	MG	AA	1654	-	X
54	MG	AA	1655	-	X
54	MG	AA	1657	-	X
54	MG	AA	1658	-	X
54	MG	AA	1660	-	X
54	MG	AA	1661	-	X
54	MG	AA	1662	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	AA	1663	-	X
54	MG	AA	1664	-	X
54	MG	AA	1665	-	X
54	MG	AA	1666	-	X
54	MG	AA	1667	-	X
54	MG	AA	1668	-	X
54	MG	AA	1669	-	X
54	MG	AA	1670	-	X
54	MG	AA	1671	-	X
54	MG	AM	201	-	X
54	MG	BA	3015	-	X
54	MG	BA	3019	-	X
54	MG	BA	3025	-	X
54	MG	BA	3033	-	X
54	MG	BA	3034	-	X
54	MG	BA	3036	-	X
54	MG	BA	3037	-	X
54	MG	BA	3040	-	X
54	MG	BA	3044	-	X
54	MG	BA	3045	-	X
54	MG	BA	3055	-	X
54	MG	BA	3056	-	X
54	MG	BA	3057	-	X
54	MG	BA	3059	-	X
54	MG	BA	3060	-	X
54	MG	BA	3061	-	X
54	MG	BA	3076	-	X
54	MG	BA	3083	-	X
54	MG	BA	3084	-	X
54	MG	BA	3091	-	X
54	MG	BA	3098	-	X
54	MG	BA	3102	-	X
54	MG	BA	3104	-	X
54	MG	BA	3110	-	X
54	MG	BA	3119	-	X
54	MG	BA	3122	-	X
54	MG	BA	3124	-	X
54	MG	BA	3128	-	X
54	MG	BA	3130	-	X
54	MG	BA	3131	-	X
54	MG	BA	3133	-	X
54	MG	BA	3136	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	BA	3137	-	X
54	MG	BA	3138	-	X
54	MG	BA	3139	-	X
54	MG	BA	3140	-	X
54	MG	BA	3141	-	X
54	MG	BA	3142	-	X
54	MG	BA	3143	-	X
54	MG	BA	3144	-	X
54	MG	BA	3145	-	X
54	MG	BA	3146	-	X
54	MG	BA	3147	-	X
54	MG	BA	3148	-	X
54	MG	BA	3149	-	X
54	MG	BA	3150	-	X
54	MG	BA	3152	-	X
54	MG	BA	3153	-	X
54	MG	BA	3155	-	X
54	MG	BA	3156	-	X
54	MG	BA	3157	-	X
54	MG	BA	3158	-	X
54	MG	BA	3159	-	X
54	MG	BA	3160	-	X
54	MG	BA	3161	-	X
54	MG	BA	3162	-	X
54	MG	BA	3163	-	X
54	MG	BA	3165	-	X
54	MG	BA	3166	-	X
54	MG	BA	3167	-	X
54	MG	BA	3168	-	X
54	MG	BA	3169	-	X
54	MG	BA	3170	-	X
54	MG	BA	3171	-	X
54	MG	BA	3173	-	X
54	MG	BA	3174	-	X
54	MG	BA	3175	-	X
54	MG	BA	3176	-	X
54	MG	BA	3177	-	X
54	MG	BA	3178	-	X
54	MG	BA	3179	-	X
54	MG	BA	3181	-	X
54	MG	BA	3182	-	X
54	MG	BA	3183	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	BA	3185	-	X
54	MG	BA	3186	-	X
54	MG	BA	3187	-	X
54	MG	BA	3188	-	X
54	MG	BA	3189	-	X
54	MG	BA	3190	-	X
54	MG	BA	3191	-	X
54	MG	BA	3193	-	X
54	MG	BB	204	-	X
54	MG	BQ	201	-	X
54	MG	CA	1605	-	X
54	MG	CA	1614	-	X
54	MG	CA	1622	-	X
54	MG	CA	1624	-	X
54	MG	CA	1626	-	X
54	MG	CA	1629	-	X
54	MG	CA	1634	-	X
54	MG	CA	1635	-	X
54	MG	CA	1640	-	X
54	MG	CA	1641	-	X
54	MG	CA	1642	-	X
54	MG	CA	1644	-	X
54	MG	CA	1645	-	X
54	MG	CA	1646	-	X
54	MG	CA	1647	-	X
54	MG	CA	1648	-	X
54	MG	CA	1649	-	X
54	MG	CA	1650	-	X
54	MG	CA	1651	-	X
54	MG	CA	1652	-	X
54	MG	CA	1653	-	X
54	MG	CA	1654	-	X
54	MG	DA	3002	-	X
54	MG	DA	3004	-	X
54	MG	DA	3014	-	X
54	MG	DA	3015	-	X
54	MG	DA	3019	-	X
54	MG	DA	3020	-	X
54	MG	DA	3025	-	X
54	MG	DA	3027	-	X
54	MG	DA	3029	-	X
54	MG	DA	3031	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	DA	3040	-	X
54	MG	DA	3043	-	X
54	MG	DA	3044	-	X
54	MG	DA	3048	-	X
54	MG	DA	3055	-	X
54	MG	DA	3056	-	X
54	MG	DA	3057	-	X
54	MG	DA	3059	-	X
54	MG	DA	3060	-	X
54	MG	DA	3061	-	X
54	MG	DA	3071	-	X
54	MG	DA	3072	-	X
54	MG	DA	3076	-	X
54	MG	DA	3084	-	X
54	MG	DA	3091	-	X
54	MG	DA	3092	-	X
54	MG	DA	3094	-	X
54	MG	DA	3104	-	X
54	MG	DA	3109	-	X
54	MG	DA	3118	-	X
54	MG	DA	3127	-	X
54	MG	DA	3130	-	X
54	MG	DA	3132	-	X
54	MG	DA	3134	-	X
54	MG	DA	3135	-	X
54	MG	DA	3136	-	X
54	MG	DA	3137	-	X
54	MG	DA	3138	-	X
54	MG	DA	3139	-	X
54	MG	DA	3140	-	X
54	MG	DA	3141	-	X
54	MG	DA	3142	-	X
54	MG	DA	3143	-	X
54	MG	DA	3144	-	X
54	MG	DA	3145	-	X
54	MG	DA	3147	-	X
54	MG	DA	3148	-	X
54	MG	DA	3149	-	X
54	MG	DA	3152	-	X
54	MG	DA	3153	-	X
54	MG	DA	3154	-	X
54	MG	DA	3155	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
54	MG	DA	3158	-	X
54	MG	DA	3159	-	X
54	MG	DA	3160	-	X
54	MG	DA	3161	-	X
54	MG	DA	3162	-	X
54	MG	DA	3163	-	X
54	MG	DA	3164	-	X
54	MG	DQ	201	-	X

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 288204 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1538	Total	C	N	O	P	0	0	0
			32995	14716	6050	10691	1538			
1	CA	1539	Total	C	N	O	P	0	0	0
			33015	14725	6052	10699	1539			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			
2	CB	218	Total	C	N	O	S	0	0	0
			1705	1081	305	312	7			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			
3	CC	206	Total	C	N	O	S	0	0	0
			1625	1028	305	289	3			

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			
5	CE	150	Total	C	N	O	S	0	0	0
			1106	687	211	202	6			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			
6	CF	100	Total	C	N	O	S	0	0	0
			818	515	148	149	6			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			
7	CG	151	Total	C	N	O	S	0	0	0
			1182	735	227	216	4			

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	98	Total	C	N	O	S	0	0	0
			787	493	150	143	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			
13	CM	114	Total	C	N	O	S	0	0	0
			884	546	178	157	3			

- Molecule 14 is a protein called 30S ribosomal protein S14.

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

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
15	CO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
16	CP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			
17	CQ	80	Total	C	N	O	S	0	0	0
			649	411	121	114	3			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	55	Total	C	N	O	0	0	0
			456	288	86	82			
18	CR	55	Total	C	N	O	0	0	0
			456	288	86	82			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			
19	CS	79	Total	C	N	O	S	0	0	0
			638	408	120	108	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	AU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			
21	CU	51	Total	C	N	O	S	0	0	0
			426	265	86	74	1			

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	BA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			
22	DA	2897	Total	C	N	O	P	0	0	0
			62195	27745	11446	20107	2897			

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	BB	119	Total	C	N	O	P	0	0	0
			2549	1135	466	829	119			
23	DB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 24 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	BC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			
24	DC	271	Total	C	N	O	S	0	0	0
			2083	1288	423	365	7			

- Molecule 25 is a protein called 50S ribosomal protein L3.

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

- Molecule 26 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 27 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			
27	DF	177	Total	C	N	O	S	0	0	0
			1411	899	249	257	6			

- Molecule 28 is a protein called 50S ribosomal protein L6.

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

- Molecule 29 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	BH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			
29	DH	149	Total	C	N	O	S	0	0	0
			1110	699	197	213	1			

- Molecule 30 is a protein called 50S ribosomal protein L11.

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			
32	DK	122	Total	C	N	O	S	0	0	0
			939	587	180	166	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			
35	DN	120	Total	C	N	O	S	0	0	0
			961	593	196	167	5			

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			
41	DT	93	Total	C	N	O	S	0	0	0
			739	466	139	132	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BU	102	Total	C	N	O	S	0	0	0
			780	492	146	142				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	DU	102	Total	C	N	O			
			780	492	146	142	0	0	0

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BW	76	Total	C	N	O	S		
			580	359	117	103	1	0	0
44	DW	75	Total	C	N	O	S		
			569	353	113	102	1	0	0

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

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

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
49	B1	50	Total	C	N	O	0	0	0
			410	263	75	72			
49	D1	50	Total	C	N	O	0	0	0
			410	263	75	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
53	B5	191	Total	C	N	O	0	0	1
			1142	691	221	230			

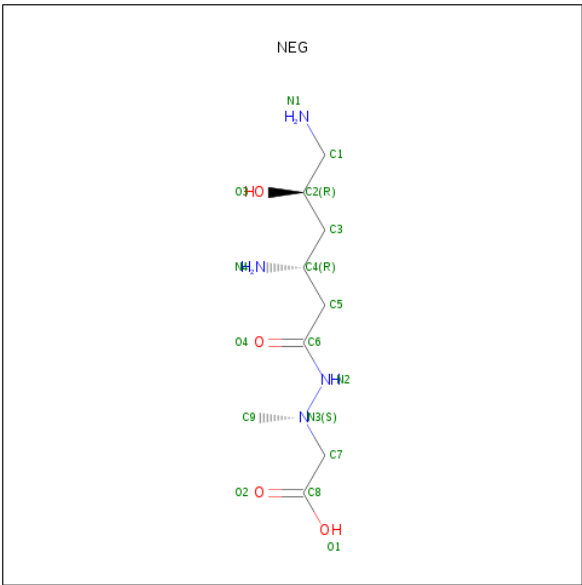
- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BB	4	Total	Mg	0	0
			4	4		
54	DQ	1	Total	Mg	0	0
			1	1		
54	BA	194	Total	Mg	0	0
			194	194		
54	CA	56	Total	Mg	0	0
			56	56		
54	CT	1	Total	Mg	0	0
			1	1		
54	DL	2	Total	Mg	0	0
			2	2		
54	D2	1	Total	Mg	0	0
			1	1		
54	AA	71	Total	Mg	0	0
			71	71		
54	BQ	1	Total	Mg	0	0
			1	1		
54	DA	164	Total	Mg	0	0
			164	164		
54	DB	3	Total	Mg	0	0
			3	3		
54	AM	1	Total	Mg	0	0
			1	1		

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 56 is NEGAMYCIN (three-letter code: NEG) (formula: C₉H₂₀N₄O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
56	CA	1	Total	C	N	O	0	0
			17	9	4	4		

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	AA	196	Total	O	0	0
			196	196		
57	AE	1	Total	O	0	0
			1	1		
57	AL	1	Total	O	0	0
			1	1		
57	AN	3	Total	O	0	0
			3	3		
57	AT	1	Total	O	0	0
			1	1		
57	AU	1	Total	O	0	0
			1	1		
57	BA	620	Total	O	0	0
			620	620		
57	BB	14	Total	O	0	0
			14	14		
57	BC	10	Total	O	0	0
			10	10		
57	BD	4	Total	O	0	0
			4	4		
57	BF	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	BG	1	Total O 1 1	0	0
57	BL	6	Total O 6 6	0	0
57	BN	3	Total O 3 3	0	0
57	BS	1	Total O 1 1	0	0
57	B2	1	Total O 1 1	0	0
57	B3	3	Total O 3 3	0	0
57	B4	2	Total O 2 2	0	0
57	CA	186	Total O 186 186	0	0
57	CL	1	Total O 1 1	0	0
57	CN	3	Total O 3 3	0	0
57	CT	3	Total O 3 3	0	0
57	CU	1	Total O 1 1	0	0
57	DA	611	Total O 611 611	0	0
57	DB	13	Total O 13 13	0	0
57	DC	8	Total O 8 8	0	0
57	DD	3	Total O 3 3	0	0
57	DE	5	Total O 5 5	0	0
57	DJ	1	Total O 1 1	0	0
57	DL	4	Total O 4 4	0	0
57	DN	1	Total O 1 1	0	0
57	DS	1	Total O 1 1	0	0

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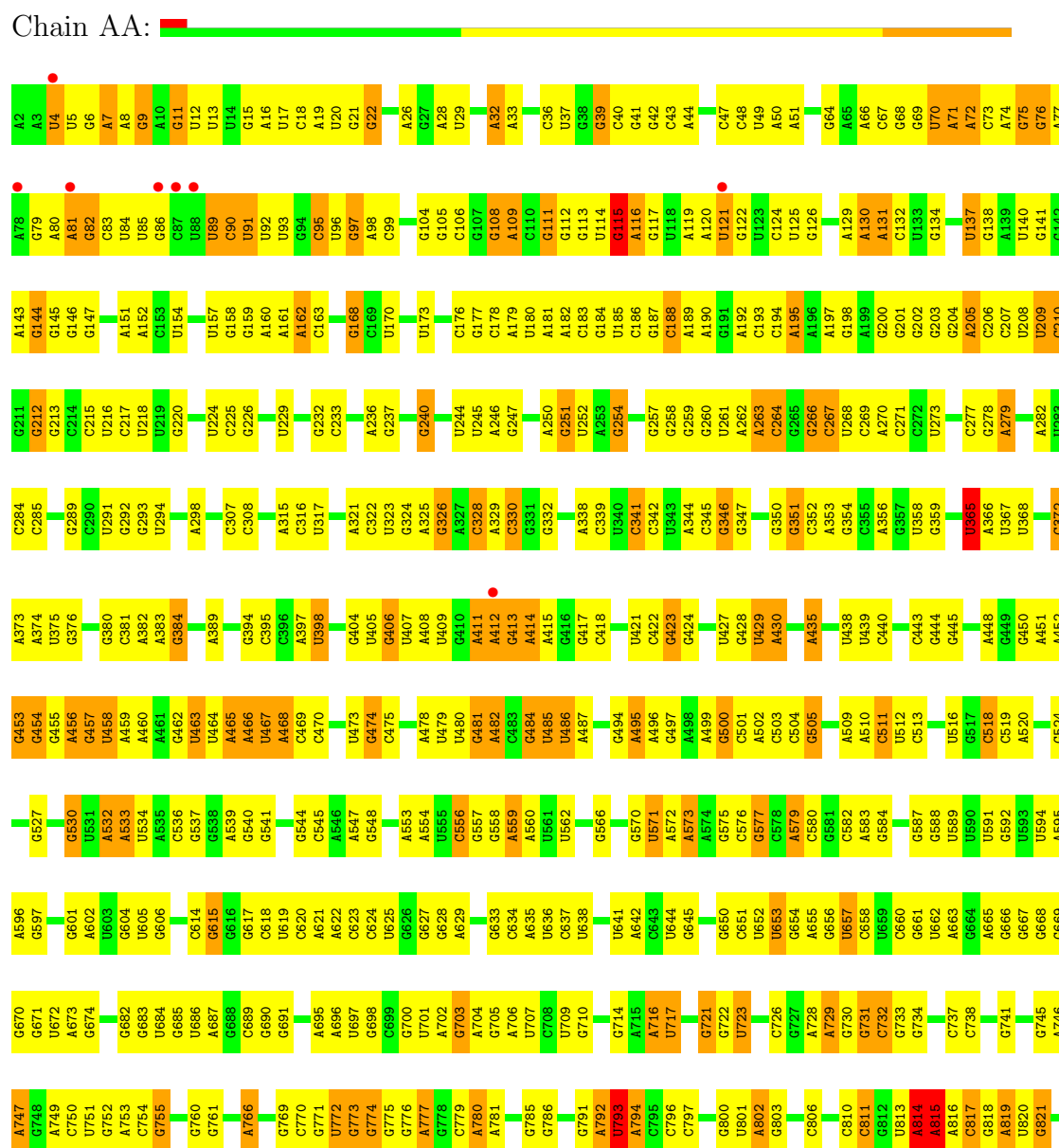
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DT	3	Total 3	O 3	0	0
57	DU	1	Total 1	O 1	0	0
57	DV	1	Total 1	O 1	0	0
57	D2	1	Total 1	O 1	0	0
57	D3	2	Total 2	O 2	0	0
57	D4	1	Total 1	O 1	0	0

3 Residue-property plots

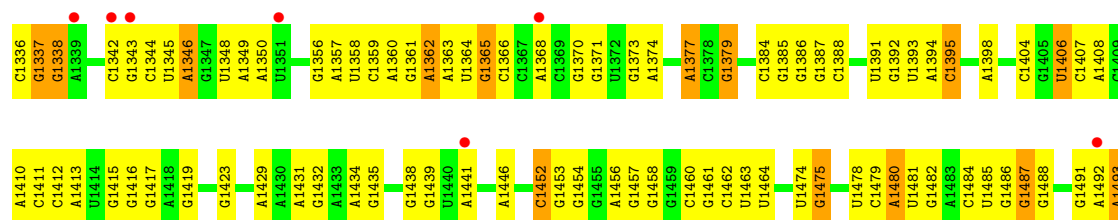
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 16S rRNA



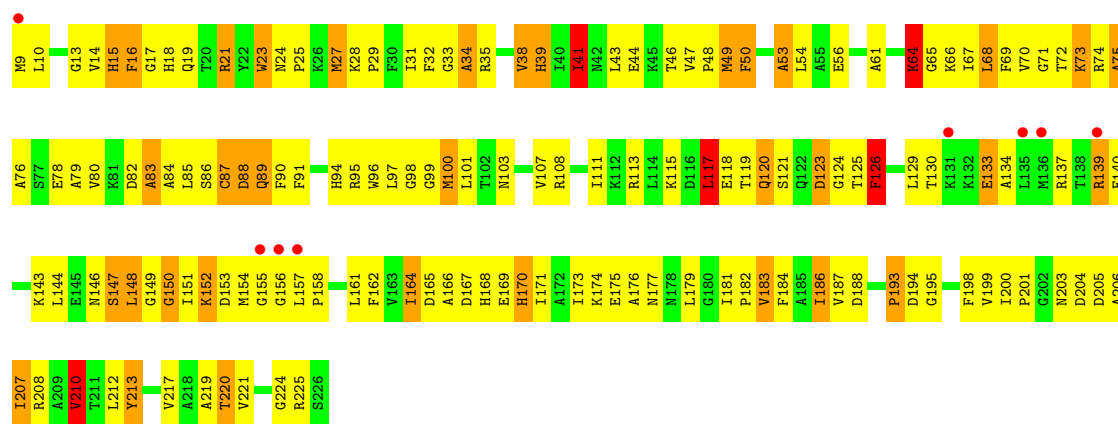


C1273	C1274	A1275	C1276	C1277	C1278	C1279	A1280	C1281	C1282	A1285	A1286	A1287	A1288	C1291	C1292	C1293	C1294	C1295	A1296	C1297	C1298	A1299	C1300	C1301	C1302	C1303	C1304	C1305	A1306	C1307	C1308	C1309	C1310	C1311	C1312	C1313	C1314	C1315	C1316	C1317	A1318	A1319	C1320	C1321	C1322	C1323	C1324	C1325	C1326	C1327	C1328	A1329	C1330	C1331	A1332	C1333	C1334	C1335																																																																																																																																																																																																																																																																																																																																																													
G1208	C1209	C1210	C1211	C1212	A1213	C1214	C1217	C1218	A1219	C1220	C1221	C1222	C1223	A1225	C1226	A1227	C1228	A1229	C1230	C1231	C1234	C1235	C1236	C1237	A1238	C1239	C1240	C1241	C1242	C1243	C1244	C1245	C1246	C1247	C1251	C1252	C1253	C1254	C1255	C1256	C1257	C1260	C1261	C1262	C1263	C1264	C1265	C1266	C1267	C1268	C1269	A1270	C1275	C1276	C1277	C1278	C1279	C1280	C1281	C1282	C1283	C1284	C1285	C1286	C1287																																																																																																																																																																																																																																																																																																																																																						
C1140	C1141	C1142	C1143	C1144	C1145	C1146	C1147	C1148	C1149	C1150	C1151	C1152	C1153	C1154	A1157	C1158	C1159	C1160	C1161	C1162	C1166	C1167	C1168	C1169	C1170	C1171	C1172	C1173	C1174	C1175	C1176	C1177	C1178	C1179	C1180	C1181	C1182	C1183	C1184	C1187	C1188	C1189	C1190	C1191	C1195	C1196	C1197	C1198	C1199	C1200	A1201	C1202	C1203	C1204	C1205	C1206	C1207																																																																																																																																																																																																																																																																																																																																																														
G1072	C1073	C1074	C1075	C1076	C1077	C1078	C1079	C1080	C1081	C1082	C1083	C1084	C1085	C1086	C1087	C1088	C1089	C1090	C1091	C1092	C1093	C1094	C1095	C1096	C1097	C1098	C1099	C1100	C1101	C1102	C1103	C1104	C1105	C1106	C1107	C1108	C1111	C1112	C1113	C1118	C1122	C1123	C1124	C1125	C1126	C1127	C1128	C1132	C1133	C1134	C1135	C1136	C1137	C1138	C1139																																																																																																																																																																																																																																																																																																																																																																
A1004	C1005	C1006	C1007	C1008	C1009	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1054	C1055	C1056	C1057	C1065	C1066	C1067	C1068	C1069	C1070	C1071																																																																																																																																																																																																																																																																																																																																																																
C936	C937	C938	C939	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C962	C965	C966	C967	C968	C969	C970	C971	C972	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C998	C999	C1000	C1001	C1002	C1003																																																																																																																																																																																																																																																																																																																																																														
C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935																																																																																																																																																																																																																																																																																																																																																								
U793	A794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C810	C811	C812	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C840	C841	C842	C843	C844	C845	C846	C849	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866																																																																																																																																																																																																																																																																																																																																																										
G730	C731	C732	C733	C734	C735	C736	C737	C738	C739	C740	C741	C742	C747	C748	C749	C750	C751	C752	C753	C754	C755	C756	C757	C758	C759	C760	C761	C762	C763	C764	C765	C766	C767	C768	C769	C770	C771	C772	C773	C774	C775	C776	C777	C778	C779	C780	C781	C782	C783	C784	C785	C786	C787	C788	C789	C790	C791	C792	C793	C794	C795	C796	C797	C798	C799	C800	C801	C802	C803	C804	C805	C806	C807	C808	C809	C810	C811	C812	C813	C814	C815	C816	C817	C818	C819	C820	C821	C822	C823	C824	C825	C826	C827	C828	C829	C830	C831	C832	C833	C834	C835	C836	C837	C838	C839	C840	C841	C842	C843	C844	C845	C846	C847	C848	C849	C850	C851	C852	C853	C854	C855	C856	C857	C858	C859	C860	C861	C862	C863	C864	C865	C866	C867	C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	C1000	C1001	C1002	C1003	C1004	C1005	C1006	C1007	C1008	C1009	C1010	C1011	C1012	C1013	C1014	C1015	C1016	C1017	C1018	C1019	C1020	C1021	C1022	C1023	C1024	C1025	C1026	C1027	C1028	C1029	C1030	C1031	C1032	C1033	C1034	C1035	C1036	C1037	C1038	C1039	C1040	C1041	C1042	C1043	C1044	C1045	C1046	C1047	C1048	C1049	C1050	C1051	C1052	C1053	C1054	C1055	C1056	C1057	C1058	C1059	C1060	C1061	C1062	C1063	C1064	C1065	C1066	C1067	C1068	C1069	C1070	C1071																																																																						
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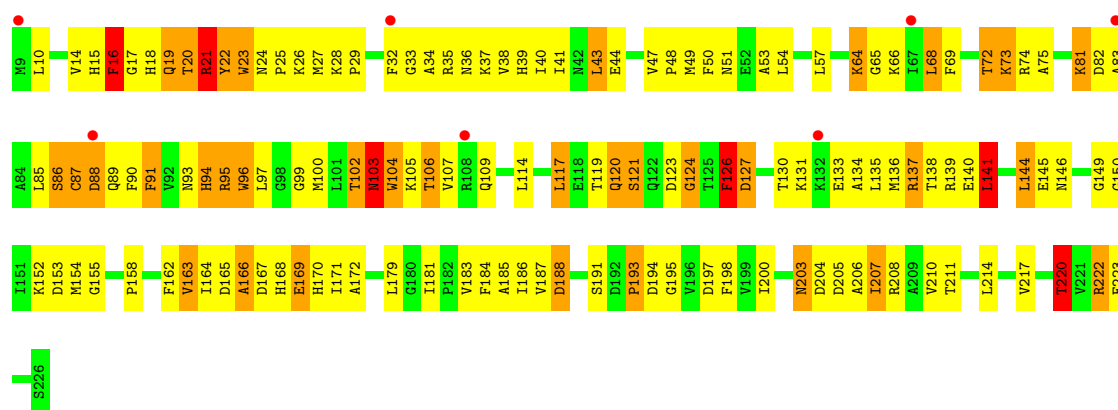
• Molecule 2: 30S ribosomal protein S2

Chain AB:



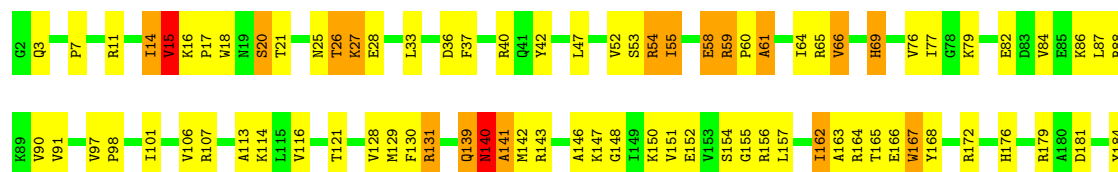
• Molecule 2: 30S ribosomal protein S2

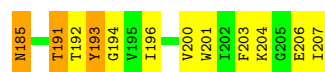
Chain CB:



• Molecule 3: 30S ribosomal protein S3

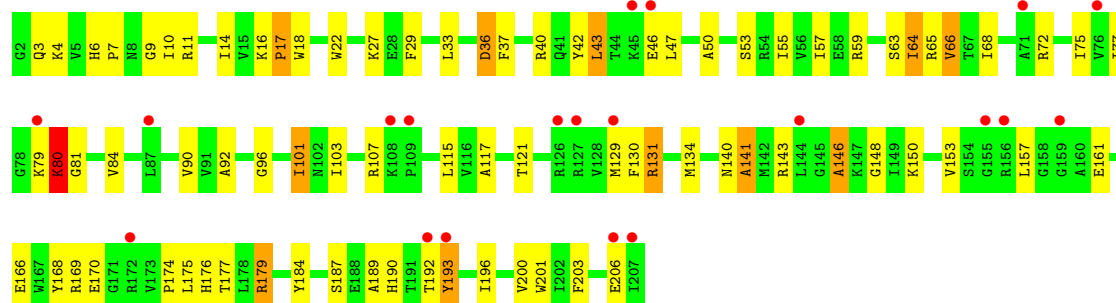
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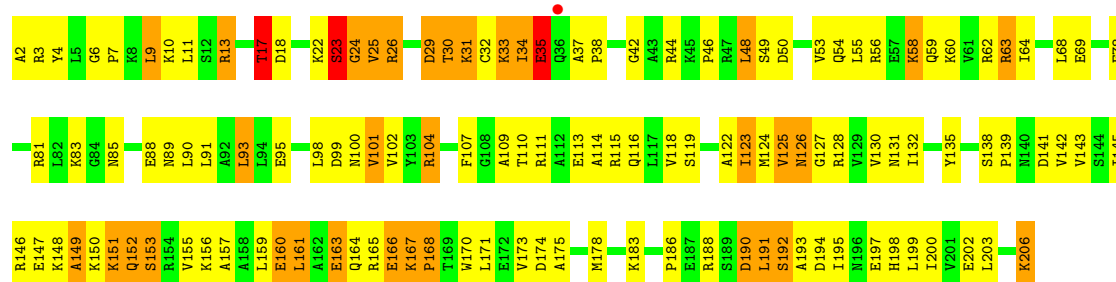
• Molecule 3: 30S ribosomal protein S3

Chain CC:



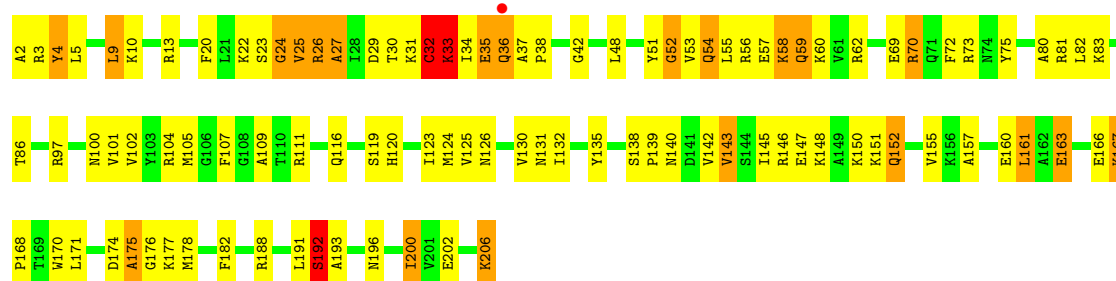
• Molecule 4: 30S ribosomal protein S4

Chain AD:



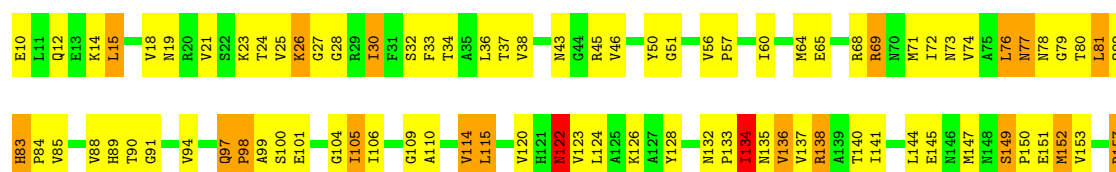
• Molecule 4: 30S ribosomal protein S4

Chain CD:



• Molecule 5: 30S ribosomal protein S5

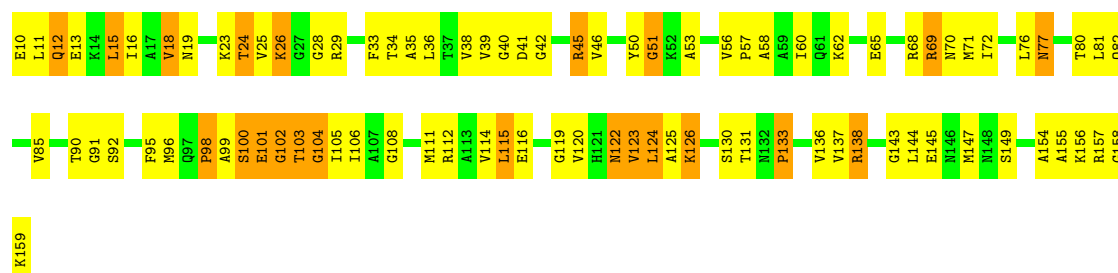
Chain AE:





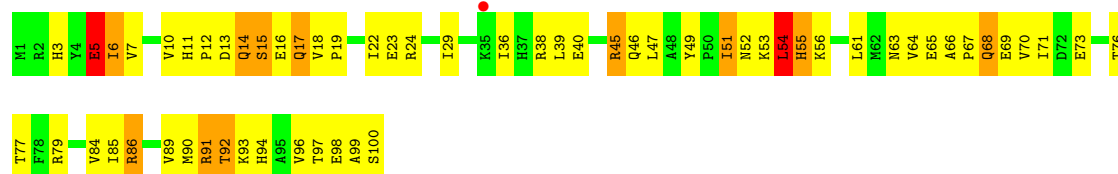
- Molecule 5: 30S ribosomal protein S5

Chain CE:



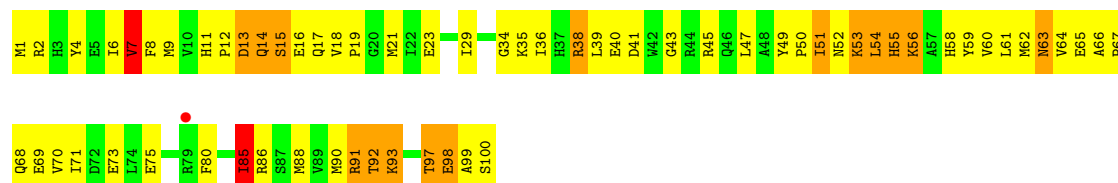
- Molecule 6: 30S ribosomal protein S6

Chain AF:



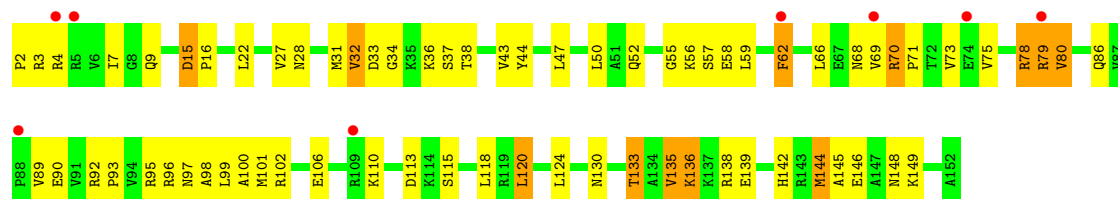
- Molecule 6: 30S ribosomal protein S6

Chain CF:



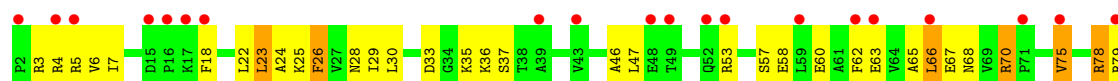
- Molecule 7: 30S ribosomal protein S7

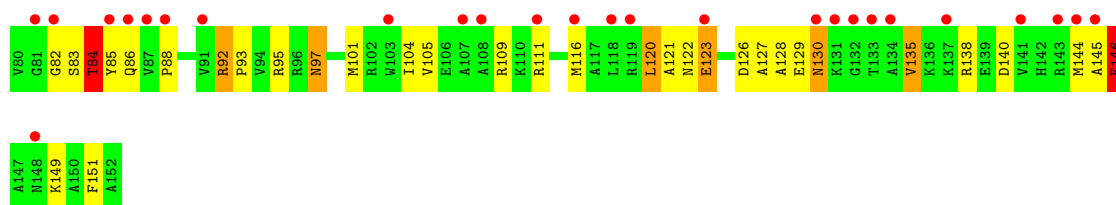
Chain AG:



- Molecule 7: 30S ribosomal protein S7

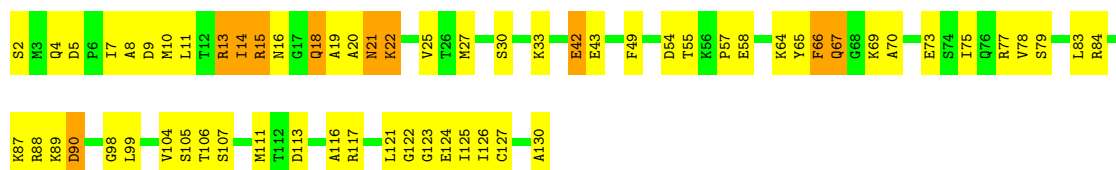
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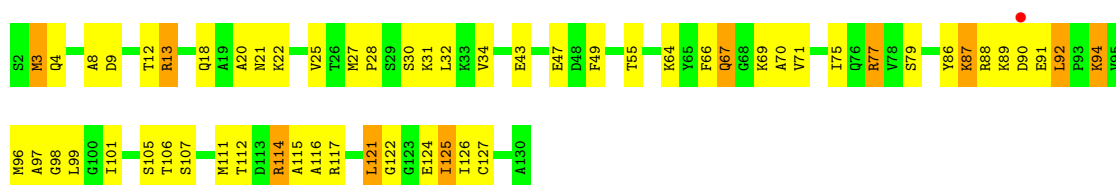
• Molecule 8: 30S ribosomal protein S8

Chain AH:



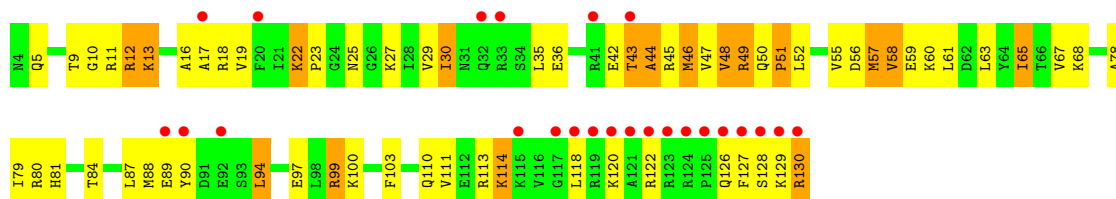
• Molecule 8: 30S ribosomal protein S8

Chain CH:



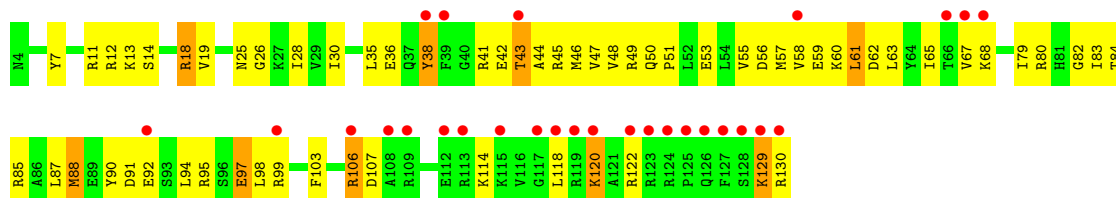
• Molecule 9: 30S ribosomal protein S9

Chain AI:



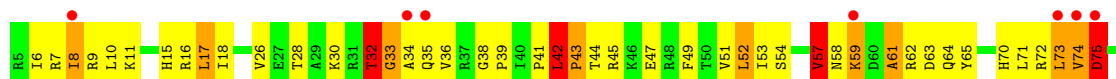
• Molecule 9: 30S ribosomal protein S9

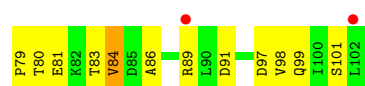
Chain CI:



• Molecule 10: 30S ribosomal protein S10

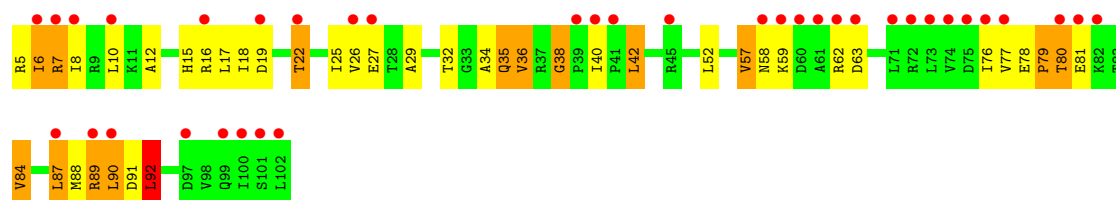
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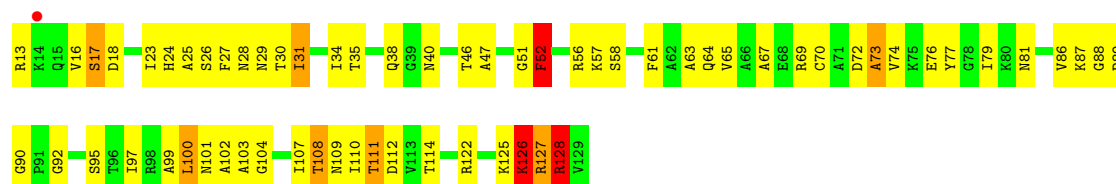
- Molecule 10: 30S ribosomal protein S10

Chain CJ:



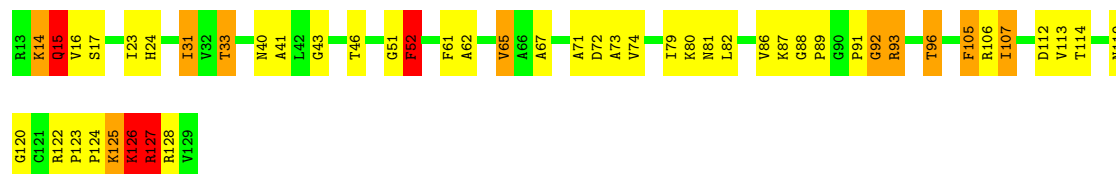
- Molecule 11: 30S ribosomal protein S11

Chain AK:



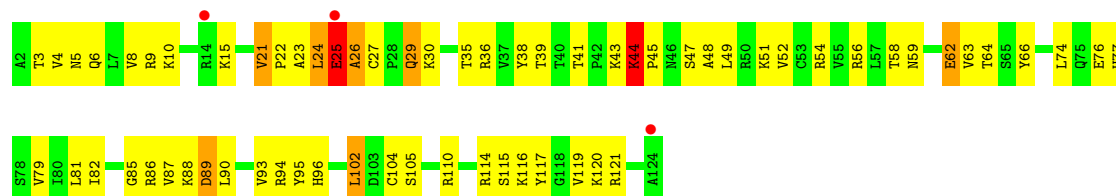
- Molecule 11: 30S ribosomal protein S11

Chain CK:



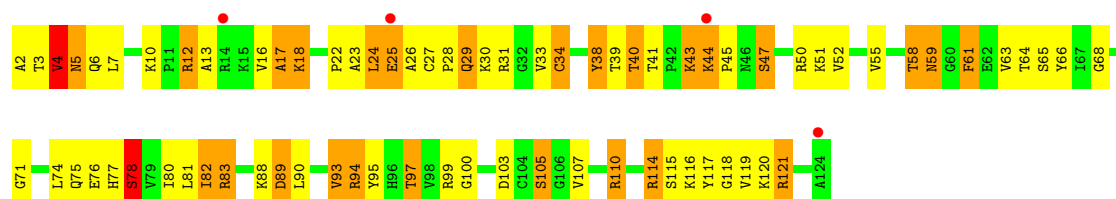
- Molecule 12: 30S ribosomal protein S12

Chain AL:



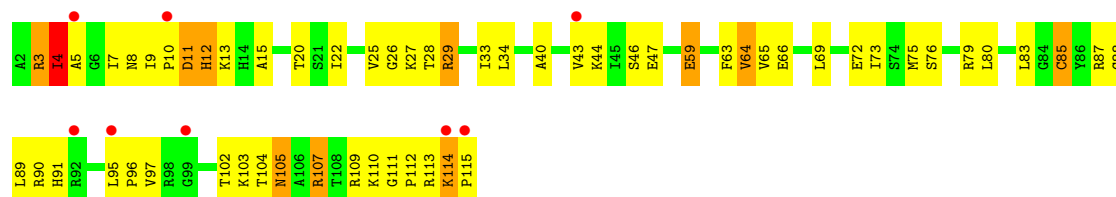
- Molecule 12: 30S ribosomal protein S12

Chain CL:



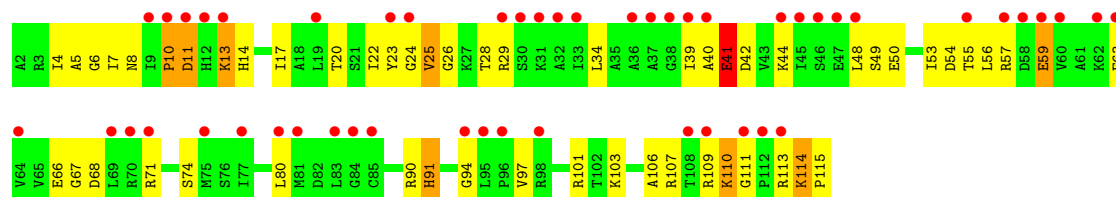
- Molecule 13: 30S ribosomal protein S13

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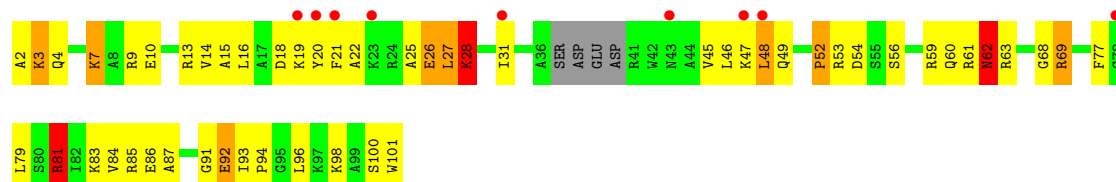
- Molecule 13: 30S ribosomal protein S13

Chain CM:



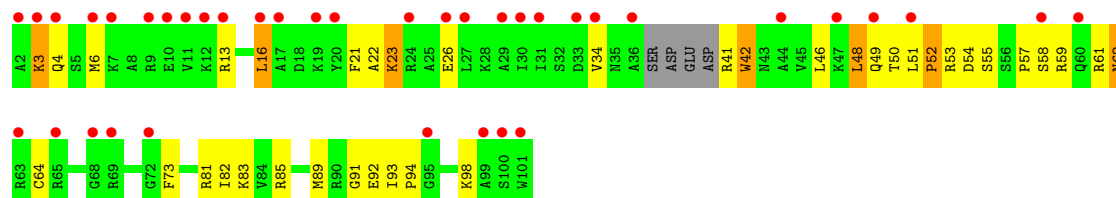
- Molecule 14: 30S ribosomal protein S14

Chain AN:



- Molecule 14: 30S ribosomal protein S14

Chain CN:



- Molecule 15: 30S ribosomal protein S15

Chain AO:



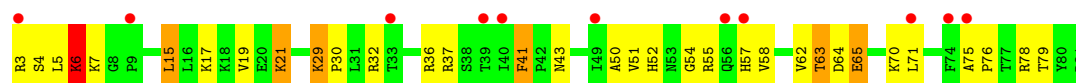
- Molecule 15: 30S ribosomal protein S15

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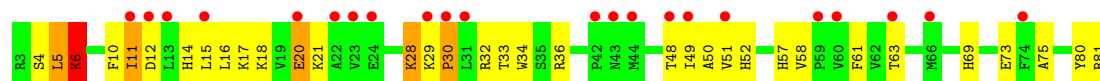
- Molecule 19: 30S ribosomal protein S19

Chain AS:



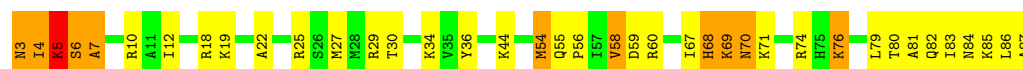
- Molecule 19: 30S ribosomal protein S19

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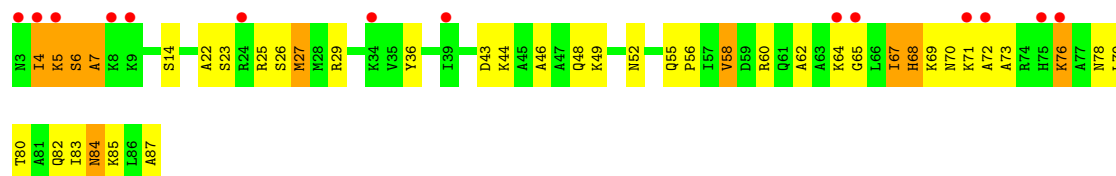
- Molecule 20: 30S ribosomal protein S20

Chain AT:



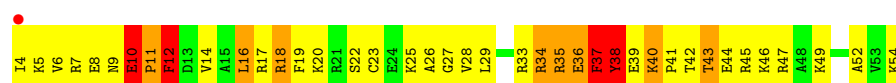
- Molecule 20: 30S ribosomal protein S20

Chain CT:



- Molecule 21: 30S ribosomal protein S21

Chain AU:



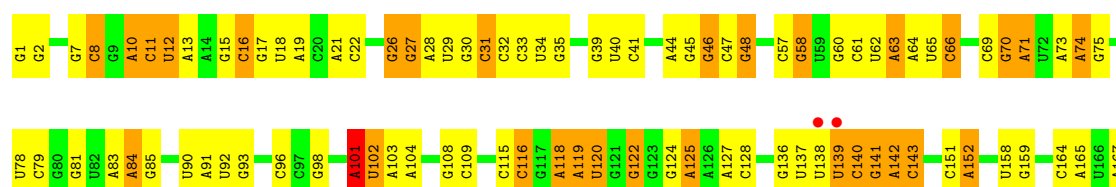
- Molecule 21: 30S ribosomal protein S21

Chain CU:

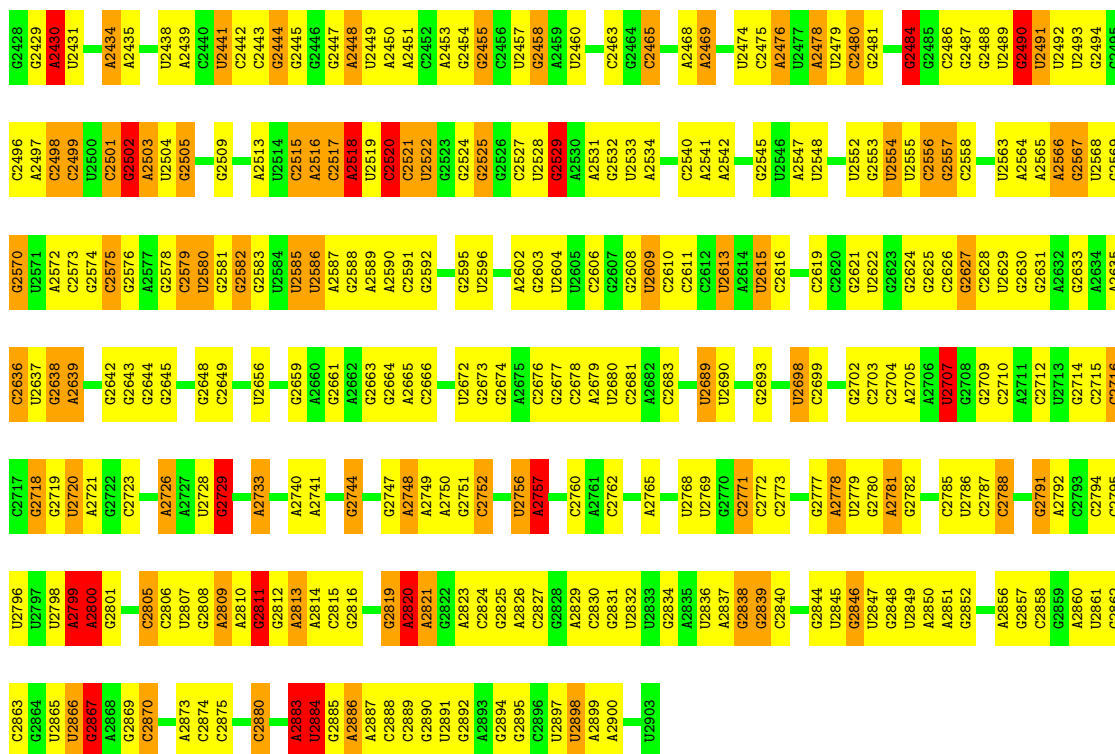


- Molecule 22: 23S rRNA

Chain BA:

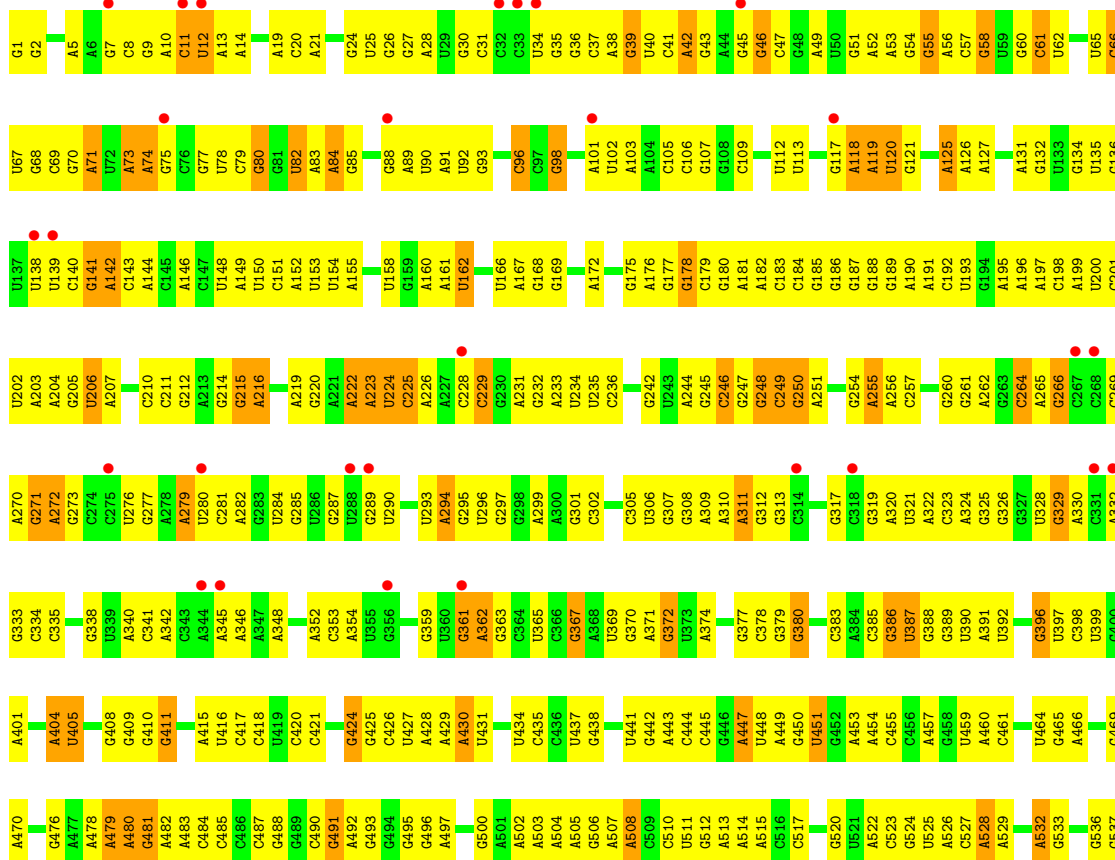


WORLDWIDE
 **PDB**
PROTEIN DATA BANK

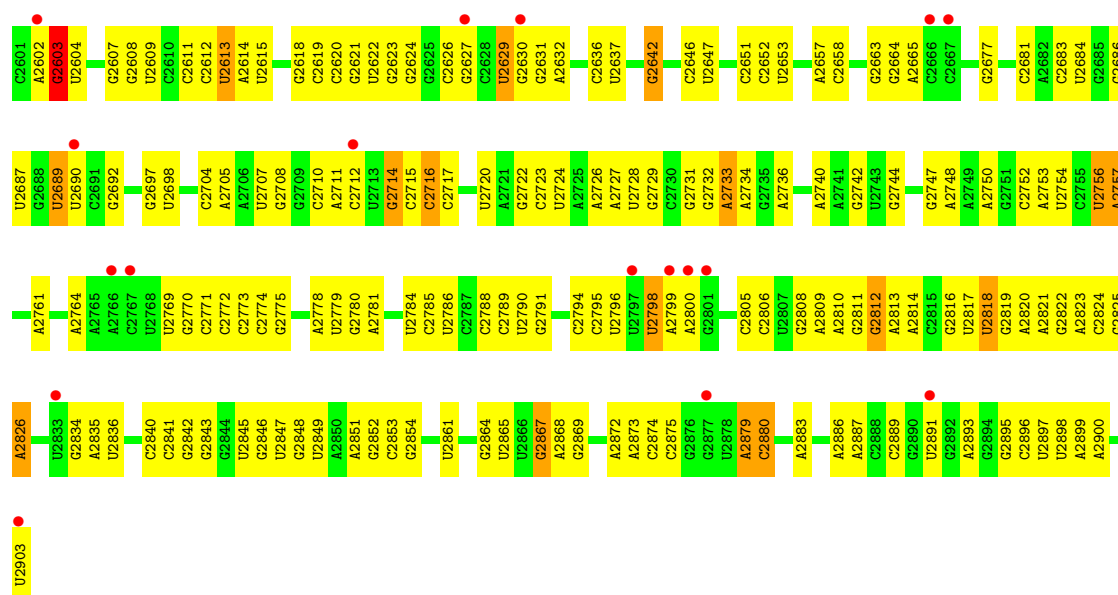


• Molecule 22: 23S rRNA

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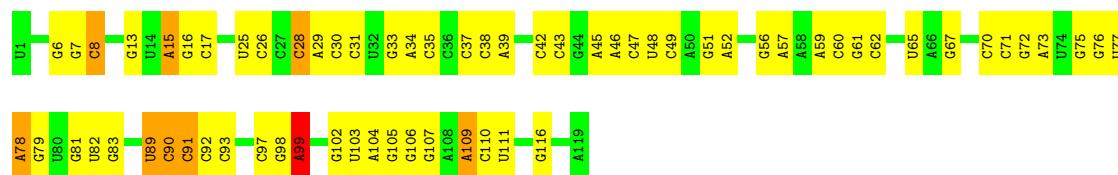


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G2553		U2405	G2330	C2264	A2199	G2127	G2057	C1985	A1918	U1782	A1705	
U2554	U2474	A2406	G2330	C2264	G2200	G2128		C1986	A1919	U1783	A1705	
U2555	C2475	A2407	A2333	A2267	U2202	U2131	A2060		C1920	A1847		
C2556	A2476	U2408	U2334	A2268	U2203	U2132	G2061		G1921	A1848		
A2478	U2477	G2409	G2334	A2288	G2204	G2133	A2062		G1922			
C2558	A2478	G2410	G2334		A2205	G2133	C2063		U1991			
C2559		A2411	C2339	U2271	A2206	A2135	C2064		U1983	U1851	A1713	
A2560	A2482	G2412	A2340	U2272	C2206	A2136	C2065		C1984	C1788	U1714	
U2561	C2483	G2413	G2341	A2273	C2207	G2137	C2066		U1995	A1853	U1715	
U2562	G2484	G2414	C2342	A2274	C2208	U2137	G2067		C1996	C1790	U1716	
U2563	G2415	G2415	U2344	C2275	G2209	G2138	U2068		C1997	U1855	A1717	
A2564	G2416	G2416	G2345	G2276	U2210		G2069		U1998	U1856	U1718	
A2565	C2417	C2417	A2346	G2277	A2211	G2141	A2070		C1999	G1793		
A2566	U2491		A2347	G2277	A2212	C2143	A2071		G2000	A1794	A1722	
A2567	U2492		C2347	G2280	U2213	C2144	C2072		C2001	C1795		
U2493	U2493	C2420	U2348	A2281	C2214	G2144	C2073		G1933	G1860		
U2568		G2421	C2349	A2282	C2215	C2145	U2074		C1934	U1796		
C2569	A2497	C2422	C2350	C2283	G2216	C2146	U2075		G1935	G1797		
C2498	C2498	U2423	G2351	A2284	A2147	U2076	U2076		A1936	U1799		
U2571	C2499	C2424	G2351	C2285	G2218	G2148	A2077		U1865	C1800		
U2500	U2500	A2425	C2354	G2286		U2149	C2078		A1801	G1733		
C2501	C2501	A2426	C2354	A2287		U2150	U2079		A1802	U1736		
G2502	G2502	C2427	G2357	A2288	G2222	U2151	A2080		C1867	C1803		
C2574	G2504	G2428	A2358	A2288	G2223	A2154	G2083		C1868	G1737		
C2575	U2504	G2429	C2359	G2289	G2224	U2155	C2084		G1869	C1738		
G2576	G2505	A2430	C2360	U2291	C2226	G2156	U2085		C1806	A1739		
A2577	U2431	U2431	G2361	U2292	A2227	G2157	U2086		G1807			
C2578				G2293	G2228	A2158			U1402			
C2579	C2512	A2434	C2364	G2294	U2229				U1808			
U2580	A2513	A2435	G2365		U2229				U1809			
C2581	A2516	A2436	A2366	A2297	G2230	C2091	C2091		C1874			
G2582	C2517	G2437	G2367	A2298	U2231	A2162	U2092		A1810			
U2585	A2518	U2438	C2368	U2299	U2232	A2163	A2093		A1745			
U2586	U2519	A2439	C2369	C2300	U2233	C2164	C2094		A1812			
A2587	C2520	C2440	G2370	C2301	U2234	C2165			G1813			
	C2521	U2441	G2371	U2302	U2235	U2166	G2100		U1883			
A2590	U2522	C2442	U2372	G2303	U2236	G2167	A2101		C1817			
C2591	G2523	C2443	G2373	G2304	U2237	G2168			U1818			
	G2524	G2444	C2374	U2305	G2238	A2170	C2104		A1819			
C2594	G2525	G2445		C2306	G2239	A2171	U2105		U1820			
G2595	C2526	G2446	A2378	G2307	U2240	G2172	G2107		A1821			
U2596	U2527	G2447	G2379	G2308	A2241	A2173	G2108		C1822			
C2597	U2528	A2448	C2380	A2309	G2242	U2109	U2034		A1758			
A2598	G2529	U2449	A2381	C2310	G2243	C2175	U2034		G1824			
C2599	A2530	A2450	G2382	U2311	U2244	U2110	U2111		U1825			
G2600	A2531	C2451	C2382	U2312	U2245	C2176	U2112		G1826			



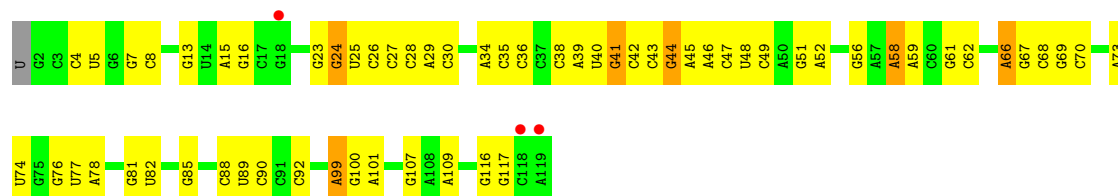
- Molecule 23: 5S rRNA

Chain BB:



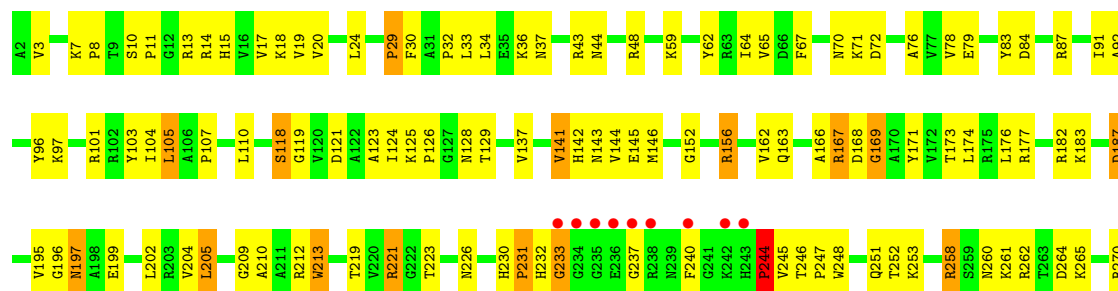
- Molecule 23: 5S rRNA

Chain DB:



- Molecule 24: 50S ribosomal protein L2

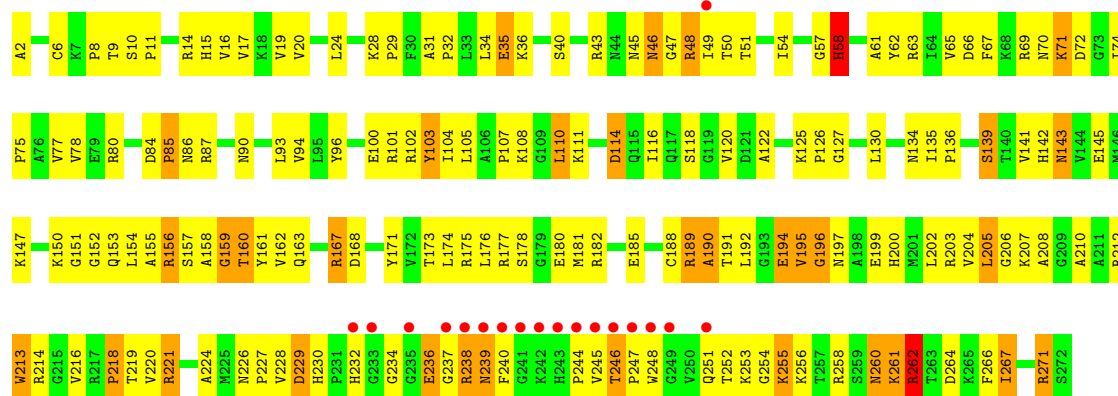
Chain BC:



R271
S272

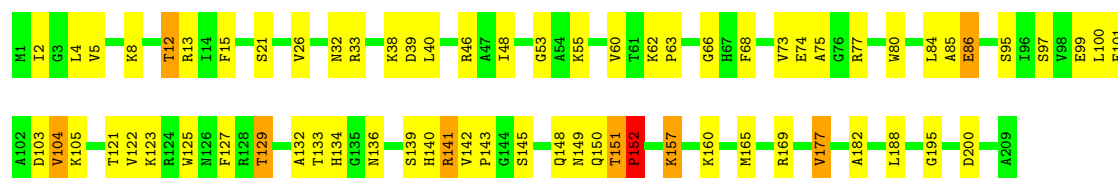
- Molecule 24: 50S ribosomal protein L2

Chain DC:



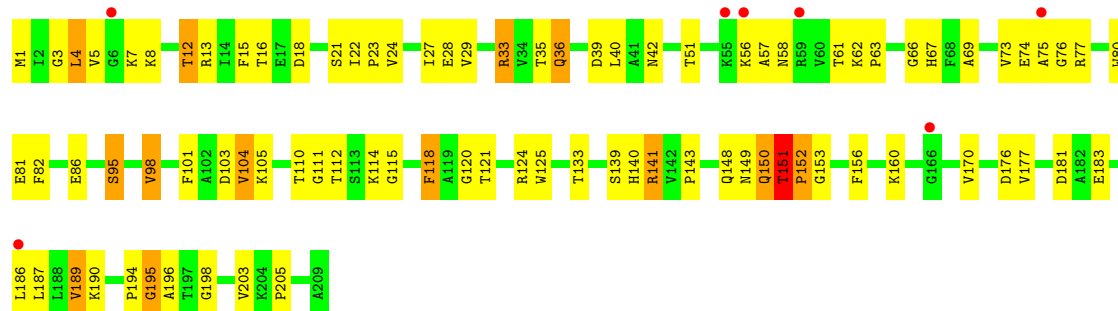
- Molecule 25: 50S ribosomal protein L3

Chain BD:



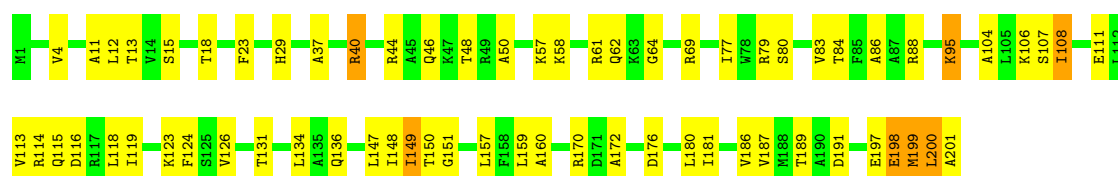
- Molecule 25: 50S ribosomal protein L3

Chain DD:



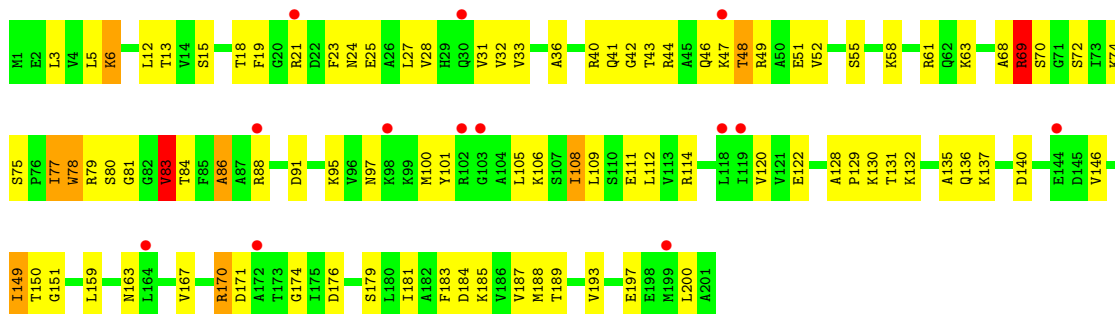
- Molecule 26: 50S ribosomal protein L4

Chain BE:



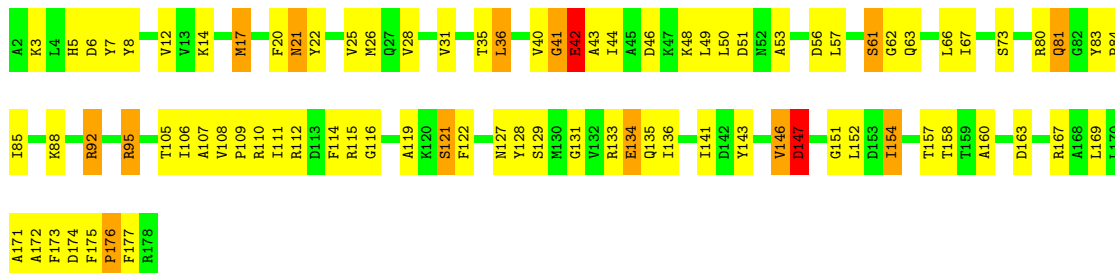
- Molecule 26: 50S ribosomal protein L4

Chain DE:



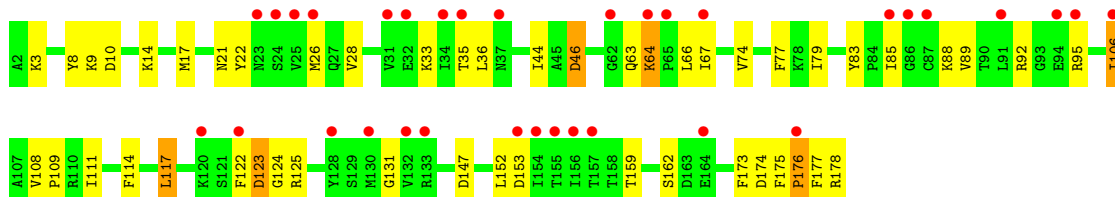
- Molecule 27: 50S ribosomal protein L5

Chain BF:



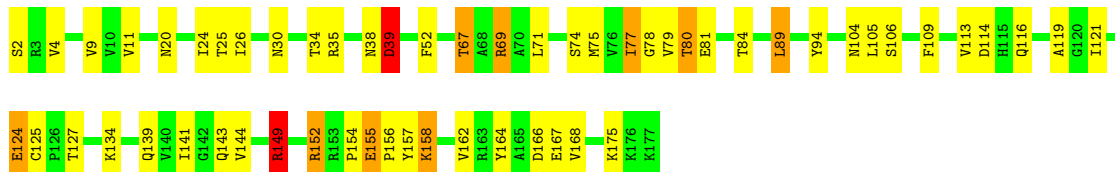
- Molecule 27: 50S ribosomal protein L5

Chain DF:



- Molecule 28: 50S ribosomal protein L6

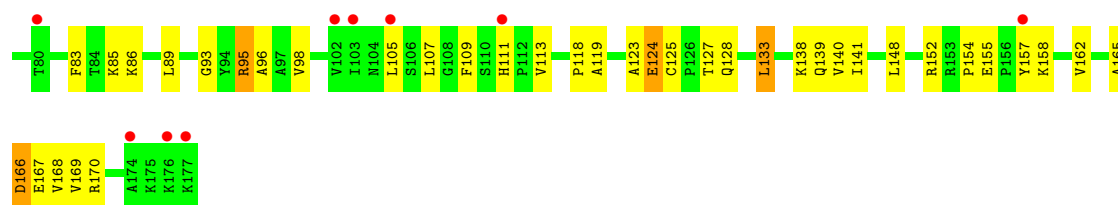
Chain BG:



- Molecule 28: 50S ribosomal protein L6

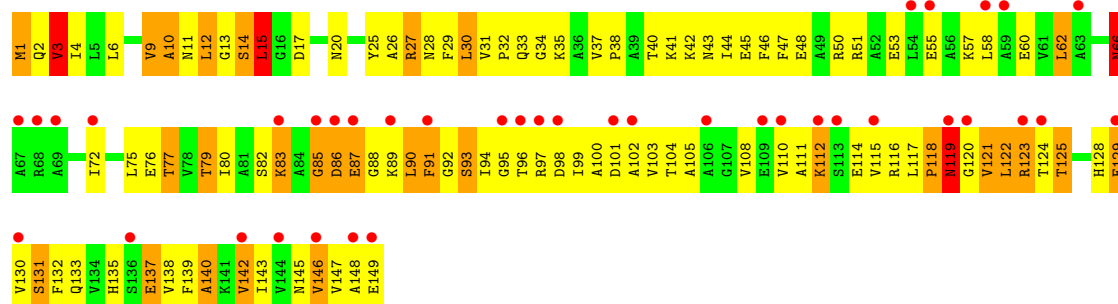
Chain DG:





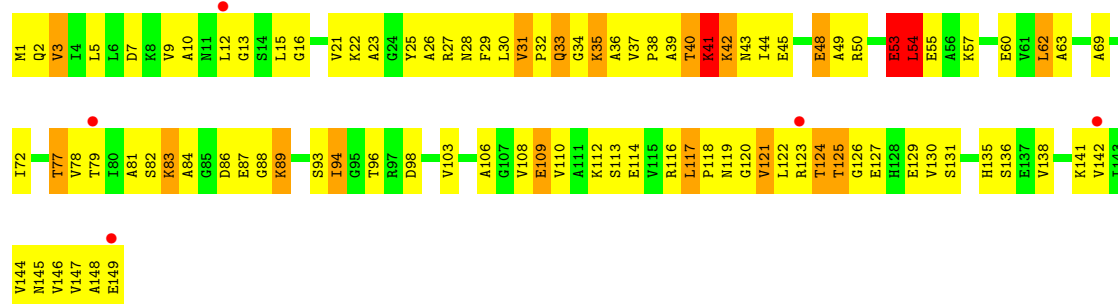
• Molecule 29: 50S ribosomal protein L9

Chain BH:



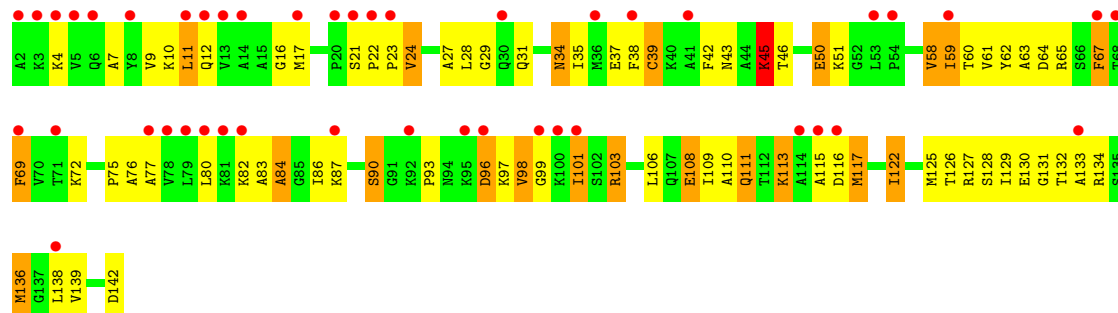
• Molecule 29: 50S ribosomal protein L9

Chain DH:



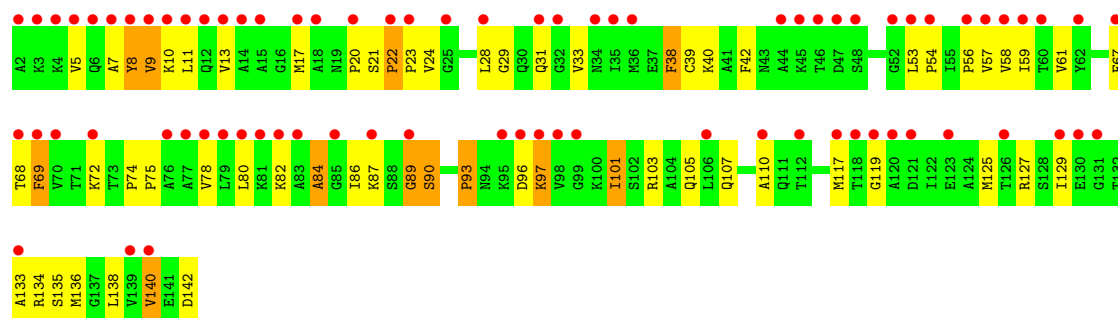
• Molecule 30: 50S ribosomal protein L11

Chain BI:



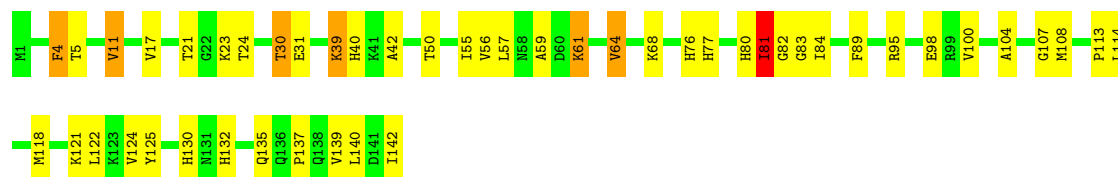
• Molecule 30: 50S ribosomal protein L11

Chain DI:



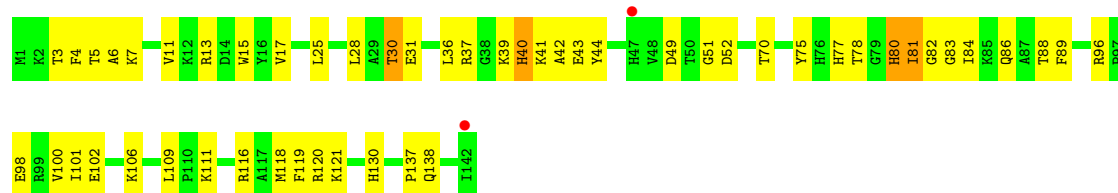
- Molecule 31: 50S ribosomal protein L13

Chain BJ:



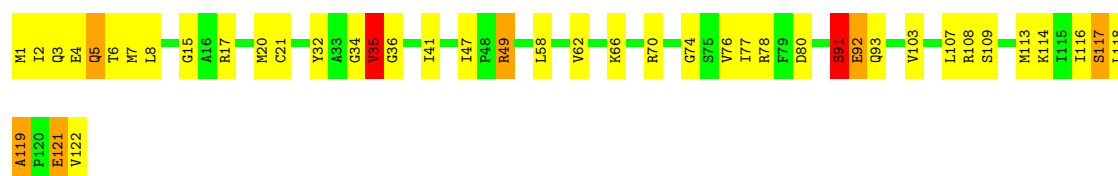
- Molecule 31: 50S ribosomal protein L13

Chain DJ:



- Molecule 32: 50S ribosomal protein L14

Chain BK:



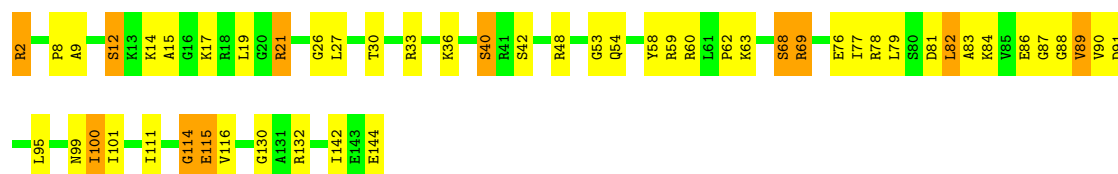
- Molecule 32: 50S ribosomal protein L14

Chain DK:



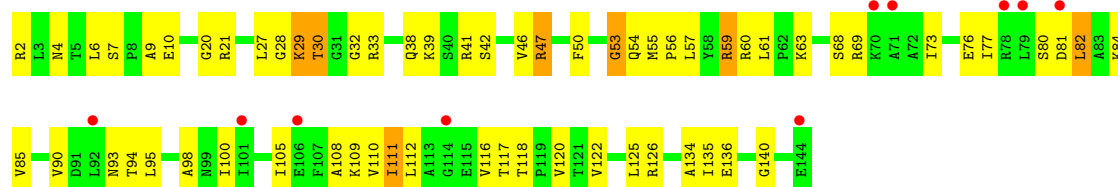
- Molecule 33: 50S ribosomal protein L15

Chain BL:



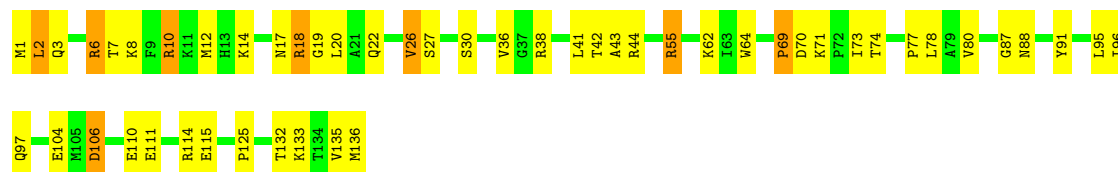
- Molecule 33: 50S ribosomal protein L15

Chain DL:



- Molecule 34: 50S ribosomal protein L16

Chain BM:



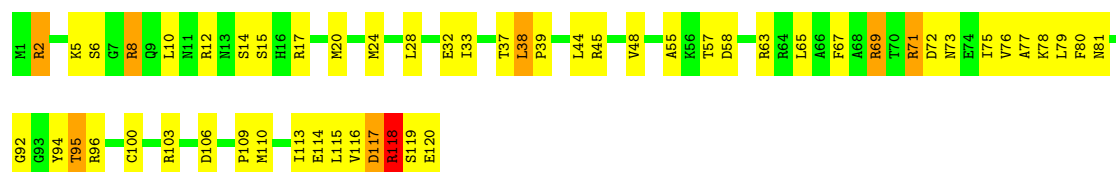
- Molecule 34: 50S ribosomal protein L16

Chain DM:



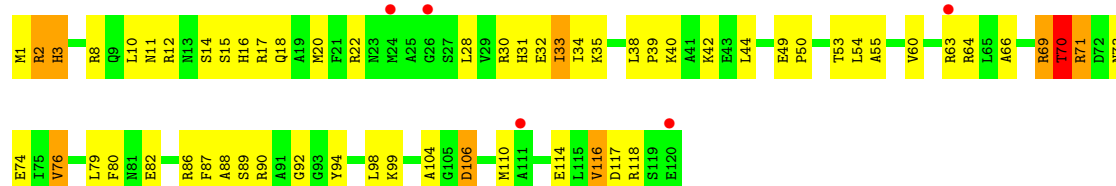
- Molecule 35: 50S ribosomal protein L17

Chain BN:



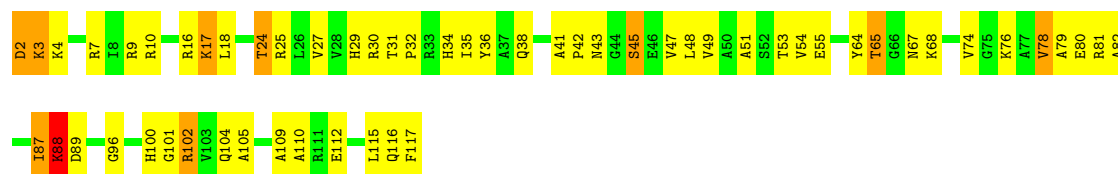
- Molecule 35: 50S ribosomal protein L17

Chain DN:



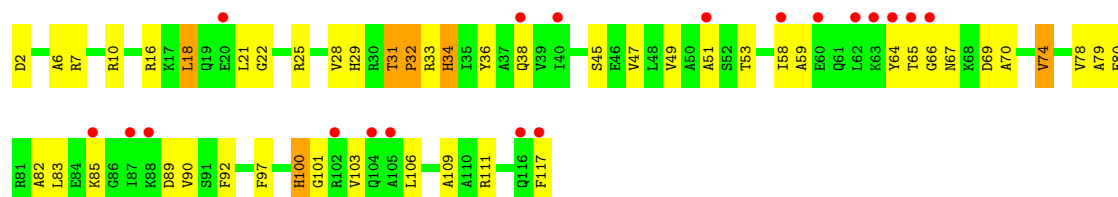
- Molecule 36: 50S ribosomal protein L18

Chain BO:



- Molecule 36: 50S ribosomal protein L18

Chain DO:



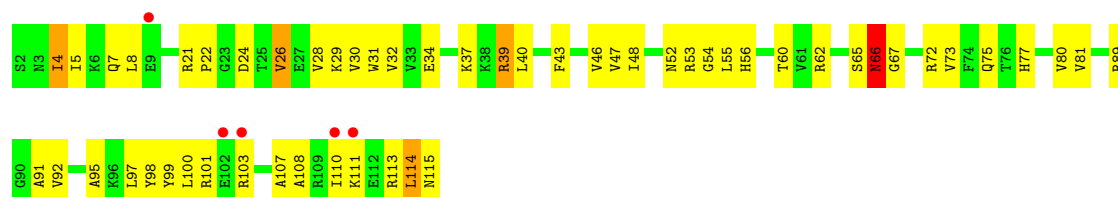
- Molecule 37: 50S ribosomal protein L19

Chain BP:



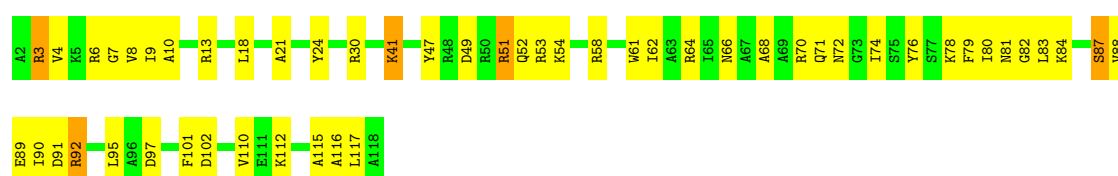
- Molecule 37: 50S ribosomal protein L19

Chain DP:



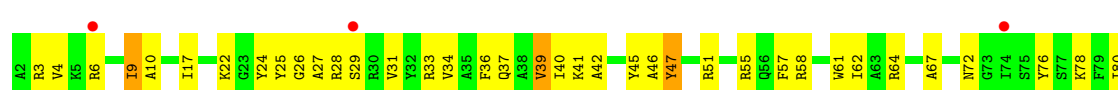
- Molecule 38: 50S ribosomal protein L20

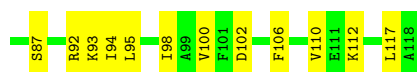
Chain BQ:



- Molecule 38: 50S ribosomal protein L20

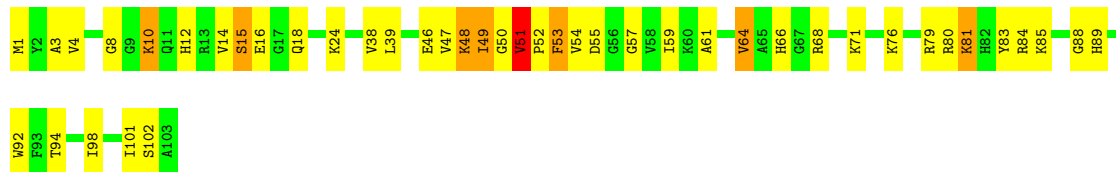
Chain DQ:





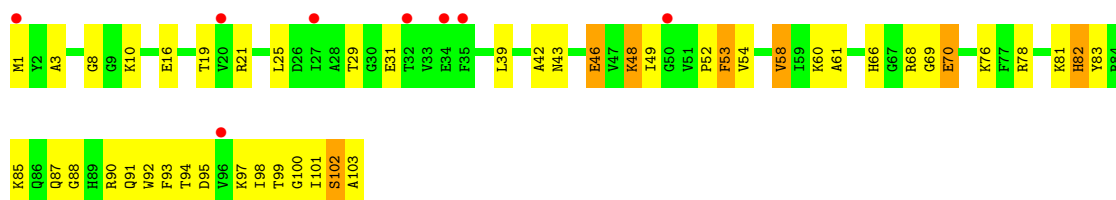
- Molecule 39: 50S ribosomal protein L21

Chain BR:



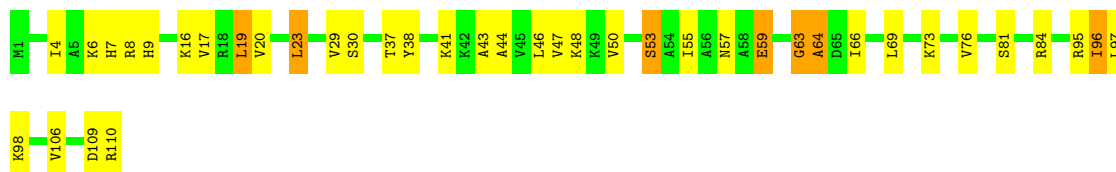
- Molecule 39: 50S ribosomal protein L21

Chain DR:



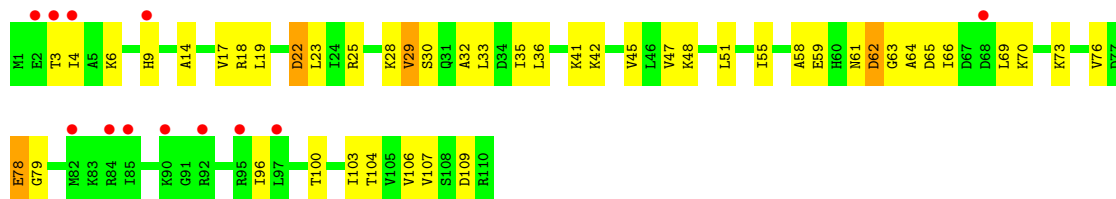
- Molecule 40: 50S ribosomal protein L22

Chain BS:



- Molecule 40: 50S ribosomal protein L22

Chain DS:



- Molecule 41: 50S ribosomal protein L23

Chain BT:



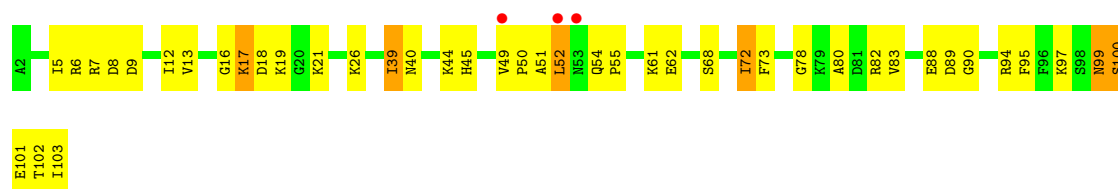
- Molecule 41: 50S ribosomal protein L23

Chain DT:



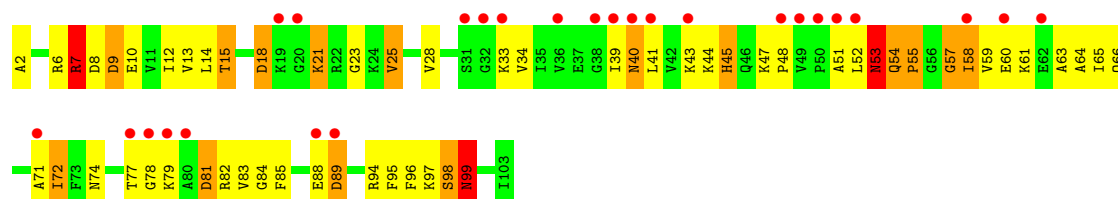
- Molecule 42: 50S ribosomal protein L24

Chain BU:



- Molecule 42: 50S ribosomal protein L24

Chain DU:



- Molecule 43: 50S ribosomal protein L25

Chain BV:



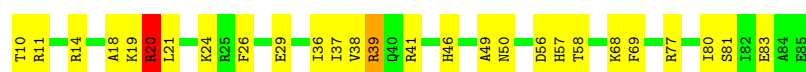
- Molecule 43: 50S ribosomal protein L25

Chain DV:



- Molecule 44: 50S ribosomal protein L27

Chain BW:



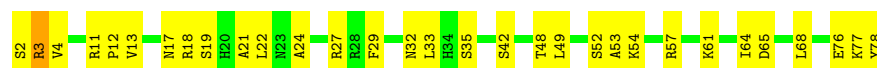
- Molecule 44: 50S ribosomal protein L27

Chain DW:



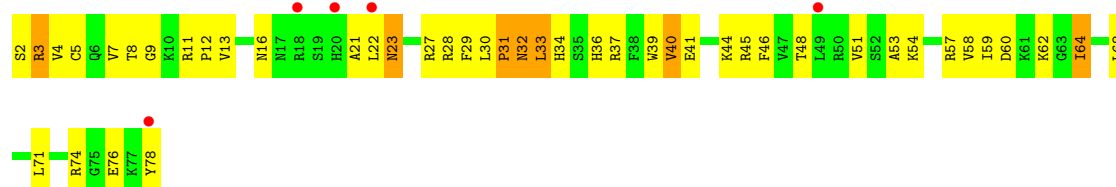
- Molecule 45: 50S ribosomal protein L28

Chain BX:



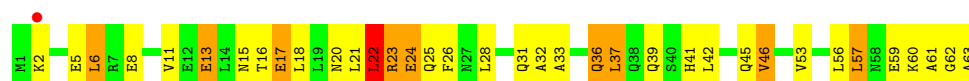
- Molecule 45: 50S ribosomal protein L28

Chain DX:



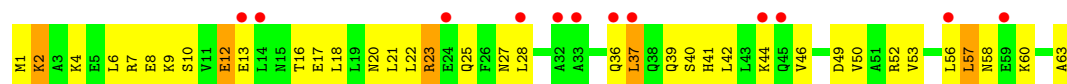
- Molecule 46: 50S ribosomal protein L29

Chain BY:



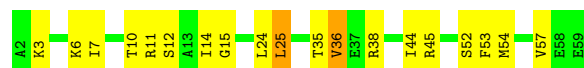
- Molecule 46: 50S ribosomal protein L29

Chain DY:



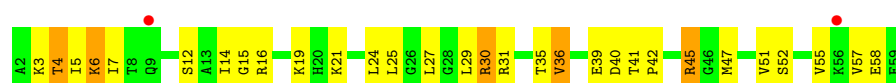
- Molecule 47: 50S ribosomal protein L30

Chain BZ:



- Molecule 47: 50S ribosomal protein L30

Chain DZ:



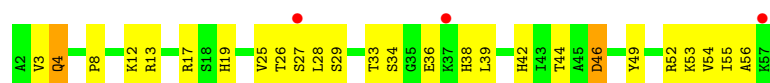
- Molecule 48: 50S ribosomal protein L32

Chain B0:



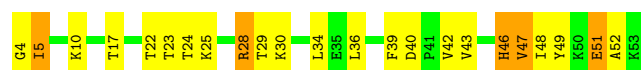
- Molecule 48: 50S ribosomal protein L32

Chain D0: 



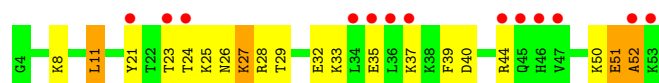
- Molecule 49: 50S ribosomal protein L33

Chain B1: 



- Molecule 49: 50S ribosomal protein L33

Chain D1: 



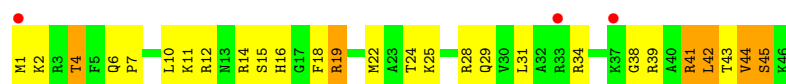
- Molecule 50: 50S ribosomal protein L34

Chain B2: 



- Molecule 50: 50S ribosomal protein L34

Chain D2: 



- Molecule 51: 50S ribosomal protein L35

Chain B3: 



- Molecule 51: 50S ribosomal protein L35

Chain D3: 



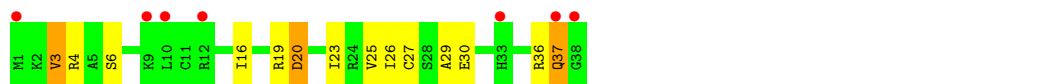
- Molecule 52: 50S ribosomal protein L36

Chain B4: 



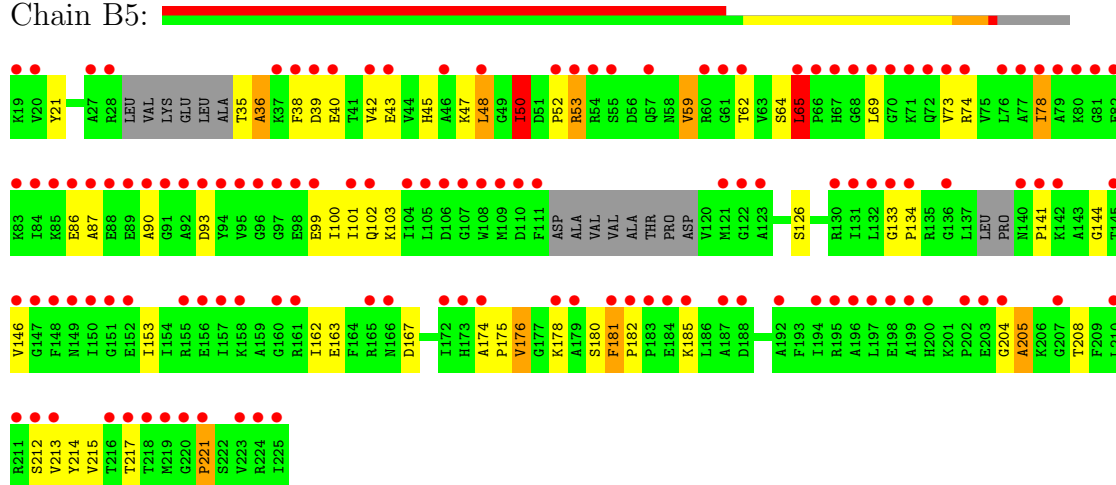
- Molecule 52: 50S ribosomal protein L36

Chain D4:



- Molecule 53: 50S ribosomal protein L1

Chain B5:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.91Å 434.31Å 624.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.14 – 3.09 41.14 – 3.09	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.14-3.09) 99.9 (41.14-3.09)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 3.06Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.202 , 0.244 0.211 , 0.254	Depositor DCC
R_{free} test set	4190 reflections (0.40%)	DCC
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 21.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 1039051 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	288204	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	AA	0.58	3/36944 (0.0%)	1.07	91/57632 (0.2%)
1	CA	0.51	3/36966 (0.0%)	1.00	57/57666 (0.1%)
2	AB	0.42	0/1736	0.60	0/2338
2	CB	0.35	0/1736	0.55	0/2338
3	AC	0.36	0/1652	0.52	0/2225
3	CC	0.36	0/1652	0.48	0/2225
4	AD	0.40	0/1665	0.60	0/2227
4	CD	0.50	0/1665	0.66	0/2227
5	AE	0.46	0/1119	0.71	0/1504
5	CE	0.44	0/1119	0.68	0/1504
6	AF	0.46	0/836	0.63	0/1128
6	CF	0.39	0/836	0.54	0/1128
7	AG	0.37	0/1196	0.53	0/1602
7	CG	0.37	0/1196	0.48	0/1602
8	AH	0.41	0/989	0.59	0/1326
8	CH	0.34	0/989	0.55	0/1326
9	AI	0.35	0/1034	0.54	0/1375
9	CI	0.35	0/1034	0.50	0/1375
10	AJ	0.35	0/797	0.54	0/1077
10	CJ	0.34	0/797	0.51	0/1077
11	AK	0.38	0/893	0.59	0/1205
11	CK	0.35	0/893	0.59	0/1205
12	AL	0.49	0/969	0.73	0/1300
12	CL	0.41	0/969	0.71	0/1300
13	AM	0.36	0/893	0.57	0/1193
13	CM	0.36	0/893	0.54	0/1193
14	AN	0.36	0/785	0.52	0/1043
14	CN	0.34	0/785	0.48	0/1043
15	AO	0.38	0/722	0.60	0/964
15	CO	0.34	0/722	0.54	0/964
16	AP	0.42	0/659	0.59	0/884
16	CP	0.40	0/659	0.62	0/884

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.47	0/658	0.62	0/881
17	CQ	0.37	0/658	0.56	0/881
18	AR	0.39	0/463	0.59	0/621
18	CR	0.37	0/463	0.57	0/621
19	AS	0.37	0/653	0.53	0/877
19	CS	0.35	0/653	0.48	0/877
20	AT	0.44	0/671	0.62	0/888
20	CT	0.37	0/671	0.54	0/888
21	AU	0.58	0/431	0.70	0/570
21	CU	0.57	0/431	0.67	0/570
22	BA	1.11	160/69659 (0.2%)	1.57	1390/108672 (1.3%)
22	DA	0.49	0/69659	0.96	49/108672 (0.0%)
23	BB	0.92	4/2850 (0.1%)	1.50	47/4444 (1.1%)
23	DB	0.39	0/2828	0.83	0/4410
24	BC	0.68	1/2122 (0.0%)	0.79	0/2852
24	DC	0.39	0/2122	0.60	0/2852
25	BD	0.80	1/1586 (0.1%)	0.98	4/2134 (0.2%)
25	DD	0.37	0/1586	0.56	0/2134
26	BE	0.60	0/1571	0.72	0/2113
26	DE	0.37	0/1571	0.53	0/2113
27	BF	0.43	0/1435	0.61	0/1926
27	DF	0.32	0/1435	0.46	0/1926
28	BG	0.50	0/1343	0.70	1/1816 (0.1%)
28	DG	0.32	0/1343	0.46	0/1816
29	BH	0.32	0/1121	0.63	0/1515
29	DH	0.34	0/1121	0.56	0/1515
30	BI	0.39	0/1046	0.51	0/1410
30	DI	0.38	0/1046	0.51	0/1410
31	BJ	0.77	0/1152	0.76	0/1551
31	DJ	0.36	0/1152	0.56	0/1551
32	BK	0.70	0/948	0.86	0/1268
32	DK	0.39	0/948	0.55	0/1268
33	BL	0.66	0/1054	0.80	0/1403
33	DL	0.36	0/1054	0.57	0/1403
34	BM	0.71	0/1093	0.86	1/1460 (0.1%)
34	DM	0.34	0/1093	0.53	0/1460
35	BN	0.71	0/974	0.89	0/1301
35	DN	0.36	0/974	0.53	0/1301
36	BO	0.50	0/902	0.67	0/1209
36	DO	0.32	0/902	0.46	0/1209
37	BP	0.64	0/929	0.74	0/1242
37	DP	0.39	0/929	0.55	0/1242
38	BQ	0.86	0/960	0.92	1/1278 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DQ	0.37	0/960	0.52	0/1278
39	BR	0.82	0/829	0.91	1/1107 (0.1%)
39	DR	0.35	0/829	0.55	0/1107
40	BS	0.85	0/864	0.91	1/1156 (0.1%)
40	DS	0.35	0/864	0.55	0/1156
41	BT	0.67	1/745 (0.1%)	0.77	1/994 (0.1%)
41	DT	0.38	0/745	0.57	0/994
42	BU	0.54	0/788	0.71	0/1051
42	DU	0.41	0/788	0.57	0/1051
43	BV	0.63	0/766	0.70	0/1025
43	DV	0.31	0/766	0.45	0/1025
44	BW	0.70	0/587	0.80	1/776 (0.1%)
44	DW	0.33	0/576	0.48	0/762
45	BX	0.52	0/635	0.71	0/848
45	DX	0.40	0/635	0.60	0/848
46	BY	0.55	0/510	0.74	0/677
46	DY	0.37	0/510	0.54	0/677
47	BZ	0.77	0/453	0.86	0/605
47	DZ	0.34	0/453	0.50	0/605
48	B0	0.77	0/450	0.81	0/599
48	D0	0.36	0/450	0.57	0/599
49	B1	0.50	0/417	0.60	0/554
49	D1	0.36	0/417	0.49	0/554
50	B2	0.77	0/380	0.95	0/498
50	D2	0.39	0/380	0.62	0/498
51	B3	0.63	0/513	0.86	1/676 (0.1%)
51	D3	0.33	0/513	0.53	0/676
52	B4	0.71	0/303	0.87	0/397
52	D4	0.32	0/303	0.51	0/397
53	B5	0.34	0/1145	0.47	0/1556
All	All	0.69	173/310634 (0.1%)	1.09	1646/464376 (0.4%)

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
5	CE	0	2
11	AK	0	1
11	CK	0	1
12	CL	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	BD	0	1
25	DD	0	1
41	BT	0	1
47	BZ	0	1
All	All	0	9

The worst 5 of 173 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	BA	2777	G	N7-C5	15.93	1.48	1.39
22	BA	984	A	N9-C4	-14.44	1.29	1.37
22	BA	2777	G	N9-C8	13.80	1.47	1.37
22	BA	1142	A	N9-C4	-12.51	1.30	1.37
1	CA	500	G	N9-C8	10.22	1.45	1.37

The worst 5 of 1646 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	BD	151	THR	C-N-CD	-21.19	73.98	120.60
22	BA	2777	G	C5-N7-C8	-19.20	94.70	104.30
22	BA	984	A	C2-N3-C4	-18.54	101.33	110.60
22	BA	2777	G	C4-C5-C6	-17.34	108.40	118.80
22	BA	528	A	N1-C6-N6	16.96	128.78	118.60

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	AK	126	LYS	Peptide
25	BD	132	ALA	Peptide
41	BT	2	ILE	Peptide
47	BZ	15	GLY	Peptide
5	CE	102	GLY	Peptide

5.2 Close contacts

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

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32995	0	16607	893	5
1	CA	33015	0	16617	1011	0
2	AB	1705	0	1732	112	0
2	CB	1705	0	1732	107	0
3	AC	1625	0	1696	57	0
3	CC	1625	0	1696	49	0
4	AD	1643	0	1707	117	0
4	CD	1643	0	1707	96	0
5	AE	1106	0	1148	81	0
5	CE	1106	0	1148	88	0
6	AF	818	0	808	47	0
6	CF	818	0	808	47	0
7	AG	1182	0	1238	47	0
7	CG	1182	0	1238	46	0
8	AH	979	0	1031	41	0
8	CH	979	0	1031	36	0
9	AI	1022	0	1070	55	0
9	CI	1022	0	1070	36	0
10	AJ	787	0	828	42	0
10	CJ	787	0	828	32	0
11	AK	877	0	887	59	0
11	CK	877	0	887	52	0
12	AL	955	0	1016	61	0
12	CL	955	0	1016	73	0
13	AM	884	0	941	51	0
13	CM	884	0	941	35	0
14	AN	774	0	824	44	0
14	CN	774	0	824	26	0
15	AO	714	0	734	28	0
15	CO	714	0	734	36	0
16	AP	649	0	666	27	0
16	CP	649	0	666	43	0
17	AQ	649	0	691	46	0
17	CQ	649	0	691	38	0
18	AR	456	0	478	9	0
18	CR	456	0	478	22	0
19	AS	638	0	665	33	0
19	CS	638	0	665	22	0
20	AT	665	0	714	41	0
20	CT	665	0	714	34	0
21	AU	426	0	449	59	0
21	CU	426	0	449	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	BA	62195	0	31278	1182	0
22	DA	62195	0	31280	2055	0
23	BB	2549	0	1291	36	0
23	DB	2529	0	1281	42	0
24	BC	2083	0	2154	81	0
24	DC	2083	0	2154	161	0
25	BD	1565	0	1616	59	0
25	DD	1565	0	1616	69	0
26	BE	1552	0	1619	57	0
26	DE	1552	0	1619	80	0
27	BF	1411	0	1444	66	0
27	DF	1411	0	1444	26	0
28	BG	1323	0	1371	44	0
28	DG	1323	0	1371	41	0
29	BH	1110	0	1148	166	0
29	DH	1110	0	1148	86	5
30	BI	1032	0	1085	54	0
30	DI	1032	0	1085	38	0
31	BJ	1129	0	1162	41	0
31	DJ	1129	0	1162	43	0
32	BK	939	0	1012	29	0
32	DK	939	0	1012	33	0
33	BL	1045	0	1117	54	0
33	DL	1045	0	1117	59	0
34	BM	1074	0	1157	40	0
34	DM	1074	0	1157	23	0
35	BN	961	0	1000	46	0
35	DN	961	0	1000	47	0
36	BO	892	0	923	48	0
36	DO	892	0	923	36	0
37	BP	917	0	962	24	0
37	DP	917	0	962	40	0
38	BQ	947	0	1019	49	0
38	DQ	947	0	1019	47	0
39	BR	816	0	839	59	0
39	DR	816	0	839	45	0
40	BS	857	0	922	29	0
40	DS	857	0	922	29	0
41	BT	739	0	807	49	0
41	DT	739	0	807	27	0
42	BU	780	0	831	33	0
42	DU	780	0	831	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	BV	753	0	780	21	0
43	DV	753	0	780	14	0
44	BW	580	0	594	22	0
44	DW	569	0	581	11	0
45	BX	625	0	652	21	0
45	DX	625	0	652	54	0
46	BY	509	0	543	30	0
46	DY	509	0	543	24	0
47	BZ	449	0	488	12	0
47	DZ	449	0	488	15	0
48	B0	444	0	458	24	0
48	D0	444	0	458	18	0
49	B1	410	0	440	15	0
49	D1	410	0	440	12	0
50	B2	377	0	418	14	0
50	D2	377	0	418	41	0
51	B3	504	0	572	23	0
51	D3	504	0	572	22	0
52	B4	302	0	340	9	0
52	D4	302	0	342	10	0
53	B5	1142	0	865	26	0
54	AA	71	0	0	0	0
54	AM	1	0	0	0	0
54	BA	194	0	0	0	0
54	BB	4	0	0	0	0
54	BQ	1	0	0	0	0
54	CA	56	0	0	0	0
54	CT	1	0	0	0	0
54	D2	1	0	0	0	0
54	DA	164	0	0	0	0
54	DB	3	0	0	0	0
54	DL	2	0	0	0	0
54	DQ	1	0	0	0	0
55	B4	1	0	0	0	0
55	D4	1	0	0	0	0
56	CA	17	0	19	1	0
57	AA	196	0	0	18	0
57	AE	1	0	0	0	0
57	AL	1	0	0	0	0
57	AN	3	0	0	1	0
57	AT	1	0	0	0	0
57	AU	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B2	1	0	0	0	0
57	B3	3	0	0	0	0
57	B4	2	0	0	0	0
57	BA	620	0	0	82	0
57	BB	14	0	0	0	0
57	BC	10	0	0	1	0
57	BD	4	0	0	2	0
57	BF	1	0	0	0	0
57	BG	1	0	0	0	0
57	BL	6	0	0	2	0
57	BN	3	0	0	0	0
57	BS	1	0	0	0	0
57	CA	186	0	0	16	0
57	CL	1	0	0	0	0
57	CN	3	0	0	0	0
57	CT	3	0	0	1	0
57	CU	1	0	0	0	0
57	D2	1	0	0	1	0
57	D3	2	0	0	0	0
57	D4	1	0	0	1	0
57	DA	611	0	0	87	0
57	DB	13	0	0	1	0
57	DC	8	0	0	0	0
57	DD	3	0	0	1	0
57	DE	5	0	0	0	0
57	DJ	1	0	0	0	0
57	DL	4	0	0	0	0
57	DN	1	0	0	0	0
57	DS	1	0	0	0	0
57	DT	3	0	0	0	0
57	DU	1	0	0	0	0
57	DV	1	0	0	0	0
All	All	288204	0	192819	8827	5

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 19.

The worst 5 of 8827 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:BH:94:ILE:H	29:BH:122:LEU:CB	1.08	1.58
29:BH:94:ILE:O	29:BH:122:LEU:CD1	1.69	1.41
29:BH:94:ILE:N	29:BH:122:LEU:CB	1.88	1.34

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
29:BH:94:ILE:N	29:BH:122:LEU:HB3	1.41	1.28
29:BH:122:LEU:HD21	1:CA:368:U:OP2	1.09	1.25

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:AA:368:U:OP2	29:DH:123:ARG:NH2[4_455]	2.03	0.17
1:AA:368:U:OP2	29:DH:123:ARG:NE[4_455]	2.07	0.13
1:AA:368:U:OP1	29:DH:93:SER:OG[4_455]	2.08	0.12
1:AA:368:U:OP2	29:DH:123:ARG:CZ[4_455]	2.18	0.02
1:AA:359:G:OP1	29:DH:89:LYS:NZ[4_455]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	216/218 (99%)	140 (65%)	41 (19%)	35 (16%)	0	0
2	CB	216/218 (99%)	144 (67%)	44 (20%)	28 (13%)	0	3
3	AC	204/206 (99%)	161 (79%)	32 (16%)	11 (5%)	3	20
3	CC	204/206 (99%)	165 (81%)	29 (14%)	10 (5%)	3	23
4	AD	203/205 (99%)	149 (73%)	29 (14%)	25 (12%)	1	3
4	CD	203/205 (99%)	155 (76%)	34 (17%)	14 (7%)	2	13
5	AE	148/150 (99%)	109 (74%)	24 (16%)	15 (10%)	1	6
5	CE	148/150 (99%)	104 (70%)	29 (20%)	15 (10%)	1	6
6	AF	98/100 (98%)	75 (76%)	17 (17%)	6 (6%)	2	16
6	CF	98/100 (98%)	72 (74%)	17 (17%)	9 (9%)	1	7
7	AG	149/151 (99%)	111 (74%)	31 (21%)	7 (5%)	4	23
7	CG	149/151 (99%)	127 (85%)	18 (12%)	4 (3%)	8	39
8	AH	127/129 (98%)	97 (76%)	20 (16%)	10 (8%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	CH	127/129 (98%)	100 (79%)	24 (19%)	3 (2%)	9	43
9	AI	125/127 (98%)	93 (74%)	28 (22%)	4 (3%)	6	35
9	CI	125/127 (98%)	95 (76%)	23 (18%)	7 (6%)	3	19
10	AJ	96/98 (98%)	67 (70%)	13 (14%)	16 (17%)	0	0
10	CJ	96/98 (98%)	69 (72%)	15 (16%)	12 (12%)	1	3
11	AK	115/117 (98%)	91 (79%)	15 (13%)	9 (8%)	1	11
11	CK	115/117 (98%)	87 (76%)	23 (20%)	5 (4%)	4	26
12	AL	121/123 (98%)	84 (69%)	31 (26%)	6 (5%)	3	22
12	CL	121/123 (98%)	90 (74%)	16 (13%)	15 (12%)	1	3
13	AM	112/114 (98%)	84 (75%)	20 (18%)	8 (7%)	2	12
13	CM	112/114 (98%)	83 (74%)	16 (14%)	13 (12%)	1	4
14	AN	92/100 (92%)	65 (71%)	17 (18%)	10 (11%)	1	5
14	CN	92/100 (92%)	71 (77%)	13 (14%)	8 (9%)	1	9
15	AO	86/88 (98%)	72 (84%)	10 (12%)	4 (5%)	4	23
15	CO	86/88 (98%)	69 (80%)	14 (16%)	3 (4%)	6	32
16	AP	80/82 (98%)	49 (61%)	18 (22%)	13 (16%)	0	0
16	CP	80/82 (98%)	61 (76%)	14 (18%)	5 (6%)	2	16
17	AQ	78/80 (98%)	53 (68%)	20 (26%)	5 (6%)	2	15
17	CQ	78/80 (98%)	59 (76%)	12 (15%)	7 (9%)	1	8
18	AR	53/55 (96%)	44 (83%)	8 (15%)	1 (2%)	12	51
18	CR	53/55 (96%)	41 (77%)	8 (15%)	4 (8%)	2	11
19	AS	77/79 (98%)	61 (79%)	13 (17%)	3 (4%)	5	29
19	CS	77/79 (98%)	66 (86%)	6 (8%)	5 (6%)	2	15
20	AT	83/85 (98%)	68 (82%)	8 (10%)	7 (8%)	1	9
20	CT	83/85 (98%)	67 (81%)	10 (12%)	6 (7%)	2	12
21	AU	49/51 (96%)	29 (59%)	11 (22%)	9 (18%)	0	0
21	CU	49/51 (96%)	24 (49%)	11 (22%)	14 (29%)	0	0
24	BC	269/271 (99%)	219 (81%)	38 (14%)	12 (4%)	4	24
24	DC	269/271 (99%)	200 (74%)	43 (16%)	26 (10%)	1	6
25	BD	207/209 (99%)	186 (90%)	18 (9%)	3 (1%)	16	58
25	DD	207/209 (99%)	165 (80%)	32 (16%)	10 (5%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	BE	199/201 (99%)	174 (87%)	22 (11%)	3 (2%)	15	57
26	DE	199/201 (99%)	167 (84%)	24 (12%)	8 (4%)	5	28
27	BF	175/177 (99%)	144 (82%)	19 (11%)	12 (7%)	2	13
27	DF	175/177 (99%)	143 (82%)	24 (14%)	8 (5%)	4	24
28	BG	174/176 (99%)	150 (86%)	18 (10%)	6 (3%)	6	32
28	DG	174/176 (99%)	145 (83%)	21 (12%)	8 (5%)	4	24
29	BH	147/149 (99%)	91 (62%)	35 (24%)	21 (14%)	0	2
29	DH	147/149 (99%)	100 (68%)	32 (22%)	15 (10%)	1	6
30	BI	139/141 (99%)	85 (61%)	37 (27%)	17 (12%)	1	4
30	DI	139/141 (99%)	89 (64%)	39 (28%)	11 (8%)	1	11
31	BJ	140/142 (99%)	127 (91%)	9 (6%)	4 (3%)	7	38
31	DJ	140/142 (99%)	116 (83%)	22 (16%)	2 (1%)	16	58
32	BK	120/122 (98%)	98 (82%)	16 (13%)	6 (5%)	3	22
32	DK	120/122 (98%)	100 (83%)	14 (12%)	6 (5%)	3	22
33	BL	141/143 (99%)	114 (81%)	21 (15%)	6 (4%)	4	26
33	DL	141/143 (99%)	106 (75%)	28 (20%)	7 (5%)	3	22
34	BM	134/136 (98%)	118 (88%)	13 (10%)	3 (2%)	10	46
34	DM	134/136 (98%)	111 (83%)	18 (13%)	5 (4%)	5	31
35	BN	118/120 (98%)	98 (83%)	18 (15%)	2 (2%)	14	54
35	DN	118/120 (98%)	93 (79%)	18 (15%)	7 (6%)	2	17
36	BO	114/116 (98%)	94 (82%)	18 (16%)	2 (2%)	13	52
36	DO	114/116 (98%)	94 (82%)	16 (14%)	4 (4%)	6	32
37	BP	112/114 (98%)	104 (93%)	5 (4%)	3 (3%)	8	39
37	DP	112/114 (98%)	89 (80%)	18 (16%)	5 (4%)	4	24
38	BQ	115/117 (98%)	107 (93%)	5 (4%)	3 (3%)	8	41
38	DQ	115/117 (98%)	97 (84%)	15 (13%)	3 (3%)	8	41
39	BR	101/103 (98%)	90 (89%)	5 (5%)	6 (6%)	2	17
39	DR	101/103 (98%)	79 (78%)	17 (17%)	5 (5%)	3	22
40	BS	108/110 (98%)	99 (92%)	7 (6%)	2 (2%)	12	51
40	DS	108/110 (98%)	91 (84%)	13 (12%)	4 (4%)	5	31
41	BT	91/93 (98%)	73 (80%)	9 (10%)	9 (10%)	1	6

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	DT	91/93 (98%)	65 (71%)	18 (20%)	8 (9%)	1	8
42	BU	100/102 (98%)	79 (79%)	15 (15%)	6 (6%)	2	17
42	DU	100/102 (98%)	74 (74%)	13 (13%)	13 (13%)	0	3
43	BV	92/94 (98%)	86 (94%)	5 (5%)	1 (1%)	21	65
43	DV	92/94 (98%)	83 (90%)	7 (8%)	2 (2%)	10	46
44	BW	74/76 (97%)	66 (89%)	7 (10%)	1 (1%)	16	58
44	DW	73/76 (96%)	61 (84%)	11 (15%)	1 (1%)	16	58
45	BX	75/77 (97%)	68 (91%)	6 (8%)	1 (1%)	18	60
45	DX	75/77 (97%)	54 (72%)	17 (23%)	4 (5%)	3	21
46	BY	61/63 (97%)	47 (77%)	5 (8%)	9 (15%)	0	2
46	DY	61/63 (97%)	50 (82%)	8 (13%)	3 (5%)	3	23
47	BZ	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
47	DZ	56/58 (97%)	49 (88%)	5 (9%)	2 (4%)	5	31
48	B0	54/56 (96%)	44 (82%)	8 (15%)	2 (4%)	5	31
48	D0	54/56 (96%)	37 (68%)	14 (26%)	3 (6%)	3	19
49	B1	48/50 (96%)	39 (81%)	7 (15%)	2 (4%)	4	27
49	D1	48/50 (96%)	35 (73%)	9 (19%)	4 (8%)	1	9
50	B2	44/46 (96%)	39 (89%)	3 (7%)	2 (4%)	4	24
50	D2	44/46 (96%)	38 (86%)	3 (7%)	3 (7%)	2	14
51	B3	62/64 (97%)	57 (92%)	4 (6%)	1 (2%)	14	55
51	D3	62/64 (97%)	54 (87%)	6 (10%)	2 (3%)	6	35
52	B4	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
52	D4	36/38 (95%)	31 (86%)	3 (8%)	2 (6%)	3	19
53	B5	183/207 (88%)	100 (55%)	58 (32%)	25 (14%)	0	2
All	All	11418/11651 (98%)	8949 (78%)	1727 (15%)	742 (6%)	2	15

5 of 742 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	16	PHE
2	AB	34	ALA
2	AB	73	LYS
2	AB	74	ARG
2	AB	120	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	180/180 (100%)	142 (79%)	38 (21%)	1	7
2	CB	180/180 (100%)	141 (78%)	39 (22%)	1	6
3	AC	170/170 (100%)	138 (81%)	32 (19%)	2	9
3	CC	170/170 (100%)	150 (88%)	20 (12%)	8	29
4	AD	172/172 (100%)	148 (86%)	24 (14%)	5	21
4	CD	172/172 (100%)	149 (87%)	23 (13%)	6	22
5	AE	113/113 (100%)	89 (79%)	24 (21%)	1	7
5	CE	113/113 (100%)	94 (83%)	19 (17%)	3	11
6	AF	87/87 (100%)	71 (82%)	16 (18%)	2	9
6	CF	87/87 (100%)	67 (77%)	20 (23%)	1	5
7	AG	124/124 (100%)	103 (83%)	21 (17%)	3	11
7	CG	124/124 (100%)	102 (82%)	22 (18%)	3	10
8	AH	104/104 (100%)	92 (88%)	12 (12%)	8	31
8	CH	104/104 (100%)	88 (85%)	16 (15%)	4	15
9	AI	105/105 (100%)	82 (78%)	23 (22%)	1	6
9	CI	105/105 (100%)	84 (80%)	21 (20%)	2	8
10	AJ	86/86 (100%)	71 (83%)	15 (17%)	3	11
10	CJ	86/86 (100%)	75 (87%)	11 (13%)	6	24
11	AK	90/90 (100%)	73 (81%)	17 (19%)	2	9
11	CK	90/90 (100%)	75 (83%)	15 (17%)	3	11
12	AL	103/103 (100%)	90 (87%)	13 (13%)	7	24
12	CL	103/103 (100%)	81 (79%)	22 (21%)	1	7
13	AM	92/92 (100%)	82 (89%)	10 (11%)	9	34
13	CM	92/92 (100%)	82 (89%)	10 (11%)	9	34
14	AN	79/83 (95%)	71 (90%)	8 (10%)	11	38
14	CN	79/83 (95%)	74 (94%)	5 (6%)	25	66
15	AO	76/76 (100%)	66 (87%)	10 (13%)	6	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	CO	76/76 (100%)	61 (80%)	15 (20%)	2	8
16	AP	65/65 (100%)	54 (83%)	11 (17%)	3	11
16	CP	65/65 (100%)	55 (85%)	10 (15%)	4	15
17	AQ	74/74 (100%)	58 (78%)	16 (22%)	1	6
17	CQ	74/74 (100%)	59 (80%)	15 (20%)	2	8
18	AR	48/48 (100%)	44 (92%)	4 (8%)	16	53
18	CR	48/48 (100%)	43 (90%)	5 (10%)	10	36
19	AS	70/70 (100%)	63 (90%)	7 (10%)	11	38
19	CS	70/70 (100%)	63 (90%)	7 (10%)	11	38
20	AT	65/65 (100%)	55 (85%)	10 (15%)	4	15
20	CT	65/65 (100%)	55 (85%)	10 (15%)	4	15
21	AU	44/44 (100%)	29 (66%)	15 (34%)	0	0
21	CU	44/44 (100%)	31 (70%)	13 (30%)	0	1
24	BC	216/216 (100%)	195 (90%)	21 (10%)	12	41
24	DC	216/216 (100%)	191 (88%)	25 (12%)	8	30
25	BD	164/164 (100%)	154 (94%)	10 (6%)	26	67
25	DD	164/164 (100%)	147 (90%)	17 (10%)	10	36
26	BE	165/165 (100%)	152 (92%)	13 (8%)	18	55
26	DE	165/165 (100%)	152 (92%)	13 (8%)	18	55
27	BF	148/148 (100%)	127 (86%)	21 (14%)	5	20
27	DF	148/148 (100%)	131 (88%)	17 (12%)	8	31
28	BG	137/137 (100%)	122 (89%)	15 (11%)	9	34
28	DG	137/137 (100%)	124 (90%)	13 (10%)	12	42
29	BH	114/114 (100%)	89 (78%)	25 (22%)	1	6
29	DH	114/114 (100%)	89 (78%)	25 (22%)	1	6
30	BI	109/109 (100%)	86 (79%)	23 (21%)	1	7
30	DI	109/109 (100%)	91 (84%)	18 (16%)	3	12
31	BJ	116/116 (100%)	106 (91%)	10 (9%)	15	51
31	DJ	116/116 (100%)	110 (95%)	6 (5%)	32	73
32	BK	103/103 (100%)	93 (90%)	10 (10%)	12	41
32	DK	103/103 (100%)	96 (93%)	7 (7%)	22	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	BL	102/102 (100%)	88 (86%)	14 (14%)	5	21
33	DL	102/102 (100%)	94 (92%)	8 (8%)	18	57
34	BM	109/109 (100%)	98 (90%)	11 (10%)	11	38
34	DM	109/109 (100%)	104 (95%)	5 (5%)	37	78
35	BN	100/100 (100%)	87 (87%)	13 (13%)	6	23
35	DN	100/100 (100%)	89 (89%)	11 (11%)	9	34
36	BO	86/86 (100%)	72 (84%)	14 (16%)	3	12
36	DO	86/86 (100%)	78 (91%)	8 (9%)	13	44
37	BP	99/99 (100%)	89 (90%)	10 (10%)	11	38
37	DP	99/99 (100%)	89 (90%)	10 (10%)	11	38
38	BQ	89/89 (100%)	81 (91%)	8 (9%)	14	47
38	DQ	89/89 (100%)	84 (94%)	5 (6%)	30	70
39	BR	84/84 (100%)	71 (84%)	13 (16%)	4	14
39	DR	84/84 (100%)	79 (94%)	5 (6%)	27	67
40	BS	93/93 (100%)	80 (86%)	13 (14%)	5	21
40	DS	93/93 (100%)	86 (92%)	7 (8%)	19	58
41	BT	80/80 (100%)	68 (85%)	12 (15%)	4	17
41	DT	80/80 (100%)	68 (85%)	12 (15%)	4	17
42	BU	83/83 (100%)	74 (89%)	9 (11%)	9	34
42	DU	83/83 (100%)	73 (88%)	10 (12%)	7	27
43	BV	78/78 (100%)	68 (87%)	10 (13%)	6	24
43	DV	78/78 (100%)	71 (91%)	7 (9%)	14	47
44	BW	57/58 (98%)	55 (96%)	2 (4%)	48	86
44	DW	56/58 (97%)	52 (93%)	4 (7%)	21	61
45	BX	67/67 (100%)	64 (96%)	3 (4%)	38	78
45	DX	67/67 (100%)	61 (91%)	6 (9%)	14	47
46	BY	55/55 (100%)	47 (86%)	8 (14%)	5	18
46	DY	55/55 (100%)	46 (84%)	9 (16%)	3	12
47	BZ	48/48 (100%)	41 (85%)	7 (15%)	5	18
47	DZ	48/48 (100%)	40 (83%)	8 (17%)	3	11
48	B0	47/47 (100%)	40 (85%)	7 (15%)	4	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	D0	47/47 (100%)	42 (89%)	5 (11%)	10	35
49	B1	45/45 (100%)	39 (87%)	6 (13%)	6	22
49	D1	45/45 (100%)	43 (96%)	2 (4%)	39	79
50	B2	38/38 (100%)	34 (90%)	4 (10%)	10	35
50	D2	38/38 (100%)	32 (84%)	6 (16%)	4	14
51	B3	51/51 (100%)	47 (92%)	4 (8%)	18	57
51	D3	51/51 (100%)	48 (94%)	3 (6%)	28	68
52	B4	34/34 (100%)	29 (85%)	5 (15%)	4	18
52	D4	34/34 (100%)	31 (91%)	3 (9%)	14	49
53	B5	61/161 (38%)	50 (82%)	11 (18%)	2	10
All	All	9388/9499 (99%)	8137 (87%)	1251 (13%)	6	22

5 of 1251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	BS	59	GLU
3	CC	27	LYS
37	DP	80	VAL
42	BU	9	ASP
50	B2	25	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
27	BF	21	ASN
6	CF	37	HIS
40	DS	7	HIS
36	BO	29	HIS
15	CO	46	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1537/1539 (99%)	304 (19%)	13 (0%)
1	CA	1538/1539 (99%)	303 (19%)	7 (0%)
22	BA	2895/2903 (99%)	518 (17%)	34 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	DA	2895/2903 (99%)	536 (18%)	22 (0%)
23	BB	118/119 (99%)	16 (13%)	1 (0%)
23	DB	117/119 (98%)	18 (15%)	0
All	All	9100/9122 (99%)	1695 (18%)	77 (0%)

5 of 1695 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	4	U
1	AA	5	U
1	AA	7	A
1	AA	9	G
1	AA	13	U

5 of 77 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
22	BA	1610	A
22	BA	2425	A
22	DA	2225	A
22	BA	1738	G
22	BA	2286	G

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 502 ligands modelled in this entry, 501 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected

value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	NEG	CA	1657	54	16,16,16	0.95	1 (6%)	20,20,20	0.82	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	NEG	CA	1657	54	-	0/18/18/18	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	CA	1657	NEG	C6-N2	2.82	1.37	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	CA	1657	NEG	C5-C4-N4	2.05	115.39	110.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	AA	1538/1539 (99%)	-0.21	44 (2%)	49	7	12, 56, 146, 187	0
1	CA	1539/1539 (100%)	0.19	102 (6%)	18	3	24, 78, 151, 182	0
2	AB	218/218 (100%)	0.12	8 (3%)	39	6	38, 79, 106, 130	0
2	CB	218/218 (100%)	0.25	7 (3%)	45	7	62, 97, 114, 127	0
3	AC	206/206 (100%)	0.16	0	100	100	57, 83, 97, 110	0
3	CC	206/206 (100%)	0.80	20 (9%)	8	2	83, 101, 112, 120	0
4	AD	205/205 (100%)	-0.09	1 (0%)	88	39	39, 64, 88, 106	0
4	CD	205/205 (100%)	-0.17	1 (0%)	88	39	21, 41, 70, 92	0
5	AE	150/150 (100%)	-0.10	1 (0%)	84	32	31, 50, 83, 105	0
5	CE	150/150 (100%)	-0.10	0	100	100	28, 58, 89, 109	0
6	AF	100/100 (100%)	0.06	1 (1%)	79	23	36, 60, 80, 92	0
6	CF	100/100 (100%)	0.01	1 (1%)	79	23	48, 81, 103, 108	0
7	AG	151/151 (100%)	0.42	8 (5%)	25	4	68, 93, 106, 116	0
7	CG	151/151 (100%)	1.52	46 (30%)	1	0	95, 117, 127, 130	0
8	AH	129/129 (100%)	-0.17	0	100	100	31, 52, 72, 90	0
8	CH	129/129 (100%)	-0.01	1 (0%)	83	28	55, 75, 93, 105	0
9	AI	127/127 (100%)	0.92	24 (18%)	2	0	70, 95, 110, 122	0
9	CI	127/127 (100%)	1.26	28 (22%)	1	0	100, 112, 123, 131	0
10	AJ	98/98 (100%)	0.56	9 (9%)	9	2	76, 90, 107, 127	0
10	CJ	98/98 (100%)	1.85	37 (37%)	1	0	97, 114, 122, 133	0
11	AK	117/117 (100%)	0.02	1 (0%)	81	25	26, 70, 98, 117	0
11	CK	117/117 (100%)	-0.02	0	100	100	36, 75, 94, 98	0
12	AL	123/123 (100%)	-0.08	3 (2%)	56	9	23, 39, 70, 100	0
12	CL	123/123 (100%)	0.14	4 (3%)	44	6	34, 56, 84, 108	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	114/114 (100%)	0.58	8 (7%) 16 3	70, 87, 104, 111	0
13	CM	114/114 (100%)	1.94	50 (43%) 1 0	105, 122, 130, 134	0
14	AN	96/100 (96%)	0.66	9 (9%) 9 2	79, 91, 108, 117	0
14	CN	96/100 (96%)	1.58	38 (39%) 1 0	98, 112, 125, 129	0
15	AO	88/88 (100%)	-0.11	0 100 100	30, 51, 72, 92	0
15	CO	88/88 (100%)	0.10	2 (2%) 57 9	45, 71, 89, 106	0
16	AP	82/82 (100%)	0.06	1 (1%) 75 20	34, 51, 92, 108	0
16	CP	82/82 (100%)	0.45	0 100 100	52, 73, 105, 117	0
17	AQ	80/80 (100%)	0.10	1 (1%) 74 19	30, 53, 77, 120	0
17	CQ	80/80 (100%)	0.50	2 (2%) 54 9	48, 88, 102, 109	0
18	AR	55/55 (100%)	0.13	2 (3%) 41 6	44, 57, 87, 108	0
18	CR	55/55 (100%)	0.12	3 (5%) 24 4	41, 58, 85, 109	0
19	AS	79/79 (100%)	0.86	11 (13%) 4 1	78, 95, 107, 113	0
19	CS	79/79 (100%)	1.47	22 (27%) 1 0	105, 123, 130, 133	0
20	AT	85/85 (100%)	0.12	0 100 100	35, 52, 79, 98	0
20	CT	85/85 (100%)	0.90	14 (16%) 2 1	61, 86, 102, 106	0
21	AU	51/51 (100%)	0.18	1 (1%) 62 12	39, 73, 105, 115	0
21	CU	51/51 (100%)	0.16	0 100 100	46, 73, 101, 107	0
22	BA	2897/2903 (99%)	-0.08	124 (4%) 34 5	1, 14, 135, 195	0
22	DA	2897/2903 (99%)	0.33	162 (5%) 24 3	38, 91, 152, 183	0
23	BB	119/119 (100%)	-0.51	0 100 100	2, 25, 59, 89	0
23	DB	118/119 (99%)	0.23	3 (2%) 54 9	80, 119, 136, 145	0
24	BC	271/271 (100%)	-0.14	9 (3%) 44 6	2, 21, 52, 65	0
24	DC	271/271 (100%)	0.26	18 (6%) 18 3	45, 70, 90, 96	0
25	BD	209/209 (100%)	-0.27	0 100 100	1, 12, 38, 77	0
25	DD	209/209 (100%)	0.45	7 (3%) 44 6	56, 82, 97, 107	0
26	BE	201/201 (100%)	-0.26	0 100 100	1, 27, 64, 92	0
26	DE	201/201 (100%)	0.63	13 (6%) 18 3	63, 98, 114, 122	0
27	BF	177/177 (100%)	-0.12	0 100 100	20, 51, 84, 100	0
27	DF	177/177 (100%)	1.13	33 (18%) 2 0	100, 119, 131, 137	0
28	BG	176/176 (100%)	-0.22	0 100 100	12, 38, 66, 79	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	DG	176/176 (100%)	0.95	21 (11%) 5 1	87, 105, 116, 126	0
29	BH	149/149 (100%)	1.29	39 (26%) 1 0	25, 102, 121, 129	0
29	DH	149/149 (100%)	0.48	5 (3%) 43 6	25, 92, 107, 115	0
30	BI	141/141 (100%)	1.65	44 (31%) 1 0	103, 122, 132, 139	0
30	DI	141/141 (100%)	2.44	77 (54%) 0 0	109, 130, 140, 149	0
31	BJ	142/142 (100%)	-0.27	0 100 100	1, 8, 28, 41	0
31	DJ	142/142 (100%)	0.24	2 (1%) 72 17	57, 79, 92, 103	0
32	BK	122/122 (100%)	-0.29	0 100 100	4, 13, 35, 66	0
32	DK	122/122 (100%)	0.32	0 100 100	56, 75, 94, 106	0
33	BL	143/143 (100%)	-0.26	0 100 100	1, 22, 52, 87	0
33	DL	143/143 (100%)	0.79	10 (6%) 16 3	58, 92, 106, 127	0
34	BM	136/136 (100%)	-0.32	0 100 100	1, 11, 34, 82	0
34	DM	136/136 (100%)	0.21	2 (1%) 70 16	50, 79, 94, 113	0
35	BN	120/120 (100%)	-0.31	0 100 100	2, 10, 21, 70	0
35	DN	120/120 (100%)	0.49	5 (4%) 35 5	65, 88, 100, 123	0
36	BO	116/116 (100%)	-0.26	0 100 100	12, 30, 47, 57	0
36	DO	116/116 (100%)	1.09	19 (16%) 2 1	91, 106, 114, 121	0
37	BP	114/114 (100%)	-0.26	0 100 100	5, 18, 46, 67	0
37	DP	114/114 (100%)	0.52	5 (4%) 33 5	65, 81, 94, 103	0
38	BQ	117/117 (100%)	-0.23	0 100 100	1, 4, 15, 52	0
38	DQ	117/117 (100%)	0.48	3 (2%) 53 8	62, 79, 89, 94	0
39	BR	103/103 (100%)	-0.33	0 100 100	1, 13, 35, 67	0
39	DR	103/103 (100%)	0.75	8 (7%) 13 2	67, 91, 101, 103	0
40	BS	110/110 (100%)	-0.30	0 100 100	1, 5, 27, 79	0
40	DS	110/110 (100%)	0.79	12 (10%) 6 1	68, 88, 105, 112	0
41	BT	93/93 (100%)	-0.03	2 (2%) 59 11	8, 27, 77, 106	0
41	DT	93/93 (100%)	1.02	14 (15%) 3 1	80, 98, 117, 125	0
42	BU	102/102 (100%)	0.00	3 (2%) 49 7	13, 32, 67, 96	0
42	DU	102/102 (100%)	1.37	26 (25%) 1 0	88, 106, 122, 129	0
43	BV	94/94 (100%)	-0.29	0 100 100	7, 23, 51, 63	0
43	DV	94/94 (100%)	0.25	1 (1%) 77 22	74, 95, 107, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BW	76/76 (100%)	-0.21	0 100 100	3, 13, 32, 61	0
44	DW	75/76 (98%)	0.91	11 (14%) 3 1	60, 90, 99, 114	0
45	BX	77/77 (100%)	-0.23	0 100 100	5, 26, 54, 77	0
45	DX	77/77 (100%)	0.43	5 (6%) 18 3	57, 80, 94, 101	0
46	BY	63/63 (100%)	-0.02	1 (1%) 68 15	17, 40, 74, 92	0
46	DY	63/63 (100%)	1.01	12 (19%) 2 0	89, 105, 112, 115	0
47	BZ	58/58 (100%)	-0.23	0 100 100	2, 8, 35, 48	0
47	DZ	58/58 (100%)	0.34	2 (3%) 43 6	64, 81, 96, 102	0
48	B0	56/56 (100%)	-0.34	0 100 100	1, 11, 44, 65	0
48	D0	56/56 (100%)	0.61	3 (5%) 25 4	58, 89, 102, 109	0
49	B1	50/50 (100%)	0.15	0 100 100	25, 38, 63, 84	0
49	D1	50/50 (100%)	1.50	13 (26%) 1 0	79, 99, 108, 112	0
50	B2	46/46 (100%)	-0.17	0 100 100	3, 8, 17, 80	0
50	D2	46/46 (100%)	0.64	3 (6%) 18 3	58, 80, 89, 105	0
51	B3	64/64 (100%)	-0.24	0 100 100	5, 11, 20, 33	0
51	D3	64/64 (100%)	0.66	4 (6%) 19 3	66, 82, 93, 98	0
52	B4	38/38 (100%)	-0.14	0 100 100	4, 13, 33, 51	0
52	D4	38/38 (100%)	1.05	7 (18%) 2 0	65, 84, 99, 109	0
53	B5	191/207 (92%)	2.81	129 (67%) 0 0	108, 127, 138, 143	0
All	All	20734/20773 (99%)	0.25	1368 (6%) 18 3	1, 73, 130, 195	0

The worst 5 of 1368 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
22	BA	2184	A	18.5
22	BA	2101	A	14.5
22	BA	2100	G	12.5
30	BI	3	LYS	11.8
22	BA	2174	C	11.6

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
54	MG	DA	3130	1/1	1.58	266.53	108,108,108,108	0
54	MG	DA	3076	1/1	0.54	237.67	114,114,114,114	0
54	MG	DA	3145	1/1	1.19	120.91	60,60,60,60	0
54	MG	BA	3076	1/1	0.27	112.00	60,60,60,60	0
54	MG	BA	3102	1/1	0.36	107.67	68,68,68,68	0
54	MG	BA	3176	1/1	0.44	94.05	37,37,37,37	0
54	MG	BA	3055	1/1	0.72	93.77	89,89,89,89	0
54	MG	BA	3142	1/1	0.61	90.40	17,17,17,17	0
54	MG	CA	1626	1/1	1.08	78.12	125,125,125,125	0
54	MG	AA	1668	1/1	0.23	77.67	39,39,39,39	0
54	MG	AA	1644	1/1	0.66	73.14	60,60,60,60	0
54	MG	BA	3148	1/1	0.66	66.69	44,44,44,44	0
54	MG	BA	3140	1/1	0.27	62.94	34,34,34,34	0
54	MG	BA	3156	1/1	0.84	59.17	40,40,40,40	0
54	MG	DA	3139	1/1	0.57	58.49	49,49,49,49	0
54	MG	BA	3178	1/1	0.74	52.18	41,41,41,41	0
54	MG	AA	1660	1/1	0.35	51.40	72,72,72,72	0
54	MG	BA	3163	1/1	0.96	50.40	36,36,36,36	0
54	MG	AA	1665	1/1	0.61	46.44	61,61,61,61	0
54	MG	BA	3159	1/1	0.41	45.22	18,18,18,18	0
54	MG	DA	3025	1/1	1.67	45.07	120,120,120,120	0
54	MG	BA	3179	1/1	1.45	44.60	29,29,29,29	0
54	MG	BA	3144	1/1	0.47	42.69	34,34,34,34	0
54	MG	AA	1643	1/1	0.69	40.44	7,7,7,7	0
54	MG	BA	3137	1/1	0.56	40.30	11,11,11,11	0
54	MG	BA	3181	1/1	0.42	40.10	33,33,33,33	0
54	MG	AA	1650	1/1	0.74	38.45	49,49,49,49	0
54	MG	DA	3061	1/1	1.28	37.46	91,91,91,91	0
54	MG	BA	3174	1/1	0.87	37.43	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3055	1/1	0.67	35.32	109,109,109,109	0
54	MG	BA	3145	1/1	0.59	34.10	35,35,35,35	0
54	MG	AA	1645	1/1	0.86	33.61	52,52,52,52	0
54	MG	BA	3057	1/1	0.56	33.49	40,40,40,40	0
54	MG	BA	3173	1/1	0.22	33.41	40,40,40,40	0
54	MG	AA	1663	1/1	0.66	33.21	36,36,36,36	0
54	MG	AA	1614	1/1	0.69	32.95	97,97,97,97	0
54	MG	CA	1649	1/1	0.65	32.65	50,50,50,50	0
54	MG	DA	3094	1/1	0.37	32.52	99,99,99,99	0
54	MG	DA	3155	1/1	0.72	31.71	51,51,51,51	0
54	MG	AA	1669	1/1	0.74	31.36	83,83,83,83	0
54	MG	BA	3138	1/1	0.51	30.02	1,1,1,1	0
54	MG	BA	3139	1/1	0.48	29.44	1,1,1,1	0
54	MG	CA	1640	1/1	0.31	29.35	29,29,29,29	0
54	MG	AA	1646	1/1	0.55	29.04	49,49,49,49	0
54	MG	CA	1648	1/1	0.42	28.99	47,47,47,47	0
54	MG	CA	1646	1/1	0.78	28.95	21,21,21,21	0
54	MG	AA	1651	1/1	0.78	27.45	52,52,52,52	0
54	MG	BA	3168	1/1	0.75	27.18	43,43,43,43	0
54	MG	AM	201	1/1	1.30	26.19	63,63,63,63	0
54	MG	BA	3147	1/1	0.37	25.83	13,13,13,13	0
54	MG	BA	3153	1/1	0.58	25.42	33,33,33,33	0
54	MG	DA	3135	1/1	0.60	25.14	112,112,112,112	0
54	MG	BA	3036	1/1	0.50	25.02	20,20,20,20	0
54	MG	AA	1655	1/1	0.44	24.02	55,55,55,55	0
54	MG	DA	3057	1/1	0.89	23.74	99,99,99,99	0
54	MG	BA	3060	1/1	0.65	23.63	72,72,72,72	0
54	MG	AA	1653	1/1	0.36	23.48	27,27,27,27	0
54	MG	BA	3146	1/1	0.37	23.37	32,32,32,32	0
54	MG	AA	1649	1/1	0.64	23.33	52,52,52,52	0
54	MG	CA	1622	1/1	0.57	23.08	84,84,84,84	0
54	MG	DA	3029	1/1	0.18	23.00	83,83,83,83	0
54	MG	BA	3157	1/1	0.21	22.00	26,26,26,26	0
54	MG	AA	1658	1/1	0.51	21.97	71,71,71,71	0
54	MG	AA	1661	1/1	0.56	21.54	40,40,40,40	0
54	MG	BA	3141	1/1	0.63	19.98	2,2,2,2	0
54	MG	BA	3034	1/1	0.45	19.83	39,39,39,39	0
54	MG	BA	3025	1/1	0.32	19.13	38,38,38,38	0
54	MG	BA	3056	1/1	0.36	19.06	27,27,27,27	0
54	MG	BA	3143	1/1	0.47	19.02	18,18,18,18	0
54	MG	BA	3161	1/1	0.41	18.93	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1667	1/1	0.46	18.68	54,54,54,54	0
54	MG	BA	3167	1/1	0.41	18.67	25,25,25,25	0
54	MG	BB	204	1/1	0.65	18.48	6,6,6,6	0
54	MG	AA	1627	1/1	0.51	18.16	68,68,68,68	0
54	MG	DA	3091	1/1	0.72	17.98	128,128,128,128	0
54	MG	DA	3060	1/1	0.64	17.96	92,92,92,92	0
54	MG	BA	3015	1/1	0.33	17.94	62,62,62,62	0
54	MG	CA	1644	1/1	1.59	17.89	86,86,86,86	0
54	MG	AA	1670	1/1	0.41	17.47	49,49,49,49	0
54	MG	BA	3166	1/1	0.42	17.23	36,36,36,36	0
54	MG	DA	3040	1/1	0.63	16.98	94,94,94,94	0
54	MG	BA	3128	1/1	0.41	16.95	1,1,1,1	0
54	MG	CA	1654	1/1	0.45	16.86	70,70,70,70	0
54	MG	BA	3044	1/1	0.34	16.73	1,1,1,1	0
54	MG	DA	3153	1/1	0.43	16.48	58,58,58,58	0
54	MG	BA	3083	1/1	0.31	16.22	44,44,44,44	0
54	MG	AA	1662	1/1	0.82	15.93	76,76,76,76	0
54	MG	BA	3040	1/1	0.46	15.78	1,1,1,1	0
54	MG	DA	3118	1/1	0.64	15.69	113,113,113,113	0
54	MG	CA	1650	1/1	0.40	15.61	85,85,85,85	0
54	MG	DA	3020	1/1	0.73	15.59	76,76,76,76	0
54	MG	DA	3137	1/1	0.49	15.36	38,38,38,38	0
54	MG	DA	3164	1/1	0.44	14.78	60,60,60,60	0
54	MG	CA	1645	1/1	0.37	14.76	52,52,52,52	0
54	MG	CA	1635	1/1	0.99	14.53	99,99,99,99	0
54	MG	BA	3189	1/1	0.16	14.50	43,43,43,43	0
54	MG	AA	1666	1/1	0.34	14.39	55,55,55,55	0
54	MG	BA	3019	1/1	0.40	14.27	1,1,1,1	0
54	MG	BA	3160	1/1	0.34	13.85	7,7,7,7	0
54	MG	CA	1647	1/1	0.60	13.73	72,72,72,72	0
54	MG	DA	3136	1/1	0.55	13.72	46,46,46,46	0
54	MG	AA	1671	1/1	0.47	13.58	52,52,52,52	0
54	MG	CA	1653	1/1	0.36	12.20	54,54,54,54	0
54	MG	BA	3152	1/1	0.45	12.02	1,1,1,1	0
54	MG	CA	1624	1/1	0.28	11.79	4,4,4,4	0
54	MG	DA	3056	1/1	0.64	11.75	103,103,103,103	0
54	MG	CA	1651	1/1	0.44	11.68	70,70,70,70	0
54	MG	AA	1626	1/1	0.25	11.61	1,1,1,1	0
54	MG	BA	3119	1/1	0.30	11.60	40,40,40,40	0
54	MG	DA	3004	1/1	0.49	11.59	112,112,112,112	0
54	MG	BA	3059	1/1	0.43	11.39	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1654	1/1	0.43	11.36	46,46,46,46	0
54	MG	DA	3140	1/1	0.53	11.00	51,51,51,51	0
54	MG	AA	1622	1/1	0.25	10.98	21,21,21,21	0
54	MG	BA	3182	1/1	0.30	10.47	25,25,25,25	0
54	MG	BA	3104	1/1	0.28	10.42	1,1,1,1	0
54	MG	CA	1652	1/1	0.46	10.18	73,73,73,73	0
54	MG	BA	3098	1/1	0.36	10.14	41,41,41,41	0
54	MG	CA	1642	1/1	0.32	10.03	53,53,53,53	0
54	MG	DA	3027	1/1	0.49	9.96	106,106,106,106	0
54	MG	DA	3142	1/1	0.42	9.78	53,53,53,53	0
54	MG	BA	3183	1/1	0.41	9.72	35,35,35,35	0
54	MG	DA	3132	1/1	1.00	9.65	123,123,123,123	0
54	MG	BA	3061	1/1	0.34	9.30	56,56,56,56	0
54	MG	BA	3165	1/1	0.29	9.28	29,29,29,29	0
54	MG	BA	3170	1/1	0.25	9.27	44,44,44,44	0
54	MG	BA	3091	1/1	0.26	9.11	53,53,53,53	0
54	MG	BA	3185	1/1	0.27	8.84	17,17,17,17	0
54	MG	BQ	201	1/1	0.30	8.82	17,17,17,17	0
54	MG	AA	1657	1/1	0.44	8.73	42,42,42,42	0
54	MG	DA	3043	1/1	0.30	8.68	104,104,104,104	0
54	MG	BA	3175	1/1	0.21	8.55	38,38,38,38	0
54	MG	DA	3084	1/1	0.45	8.14	104,104,104,104	0
54	MG	BA	3193	1/1	0.27	7.85	46,46,46,46	0
54	MG	DA	3162	1/1	0.50	7.82	66,66,66,66	0
54	MG	DA	3044	1/1	0.31	7.78	51,51,51,51	0
54	MG	BA	3133	1/1	0.59	7.74	63,63,63,63	0
54	MG	DA	3161	1/1	0.31	7.53	65,65,65,65	0
54	MG	AA	1615	1/1	0.24	7.49	52,52,52,52	0
54	MG	BA	3150	1/1	0.31	7.21	23,23,23,23	0
54	MG	DA	3154	1/1	0.41	7.19	63,63,63,63	0
54	MG	AA	1630	1/1	0.27	6.88	78,78,78,78	0
54	MG	BA	3162	1/1	0.35	6.85	30,30,30,30	0
54	MG	AA	1648	1/1	0.28	6.85	34,34,34,34	0
54	MG	BA	3084	1/1	0.22	6.82	33,33,33,33	0
54	MG	AA	1635	1/1	0.28	6.71	73,73,73,73	0
54	MG	DA	3092	1/1	0.45	6.49	123,123,123,123	0
54	MG	BA	3191	1/1	0.30	6.48	17,17,17,17	0
54	MG	DA	3143	1/1	0.42	6.34	63,63,63,63	0
54	MG	DA	3031	1/1	0.54	6.10	95,95,95,95	0
54	MG	DA	3147	1/1	0.41	5.96	49,49,49,49	0
54	MG	BA	3149	1/1	0.20	5.81	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1617	1/1	0.94	5.80	124,124,124,124	0
54	MG	BA	3155	1/1	0.24	5.73	21,21,21,21	0
54	MG	DA	3134	1/1	0.30	5.61	112,112,112,112	0
54	MG	DA	3148	1/1	0.28	5.54	53,53,53,53	0
54	MG	DA	3141	1/1	0.58	5.28	45,45,45,45	0
54	MG	DA	3002	1/1	0.48	4.89	94,94,94,94	0
54	MG	DA	3163	1/1	0.25	4.78	45,45,45,45	0
54	MG	BA	3177	1/1	0.20	4.77	24,24,24,24	0
54	MG	BA	3110	1/1	0.24	4.61	61,61,61,61	0
54	MG	DA	3071	1/1	0.34	4.59	99,99,99,99	0
54	MG	BA	3131	1/1	0.29	4.58	49,49,49,49	0
54	MG	BA	3187	1/1	0.21	4.57	41,41,41,41	0
54	MG	BA	3037	1/1	0.23	4.42	1,1,1,1	0
54	MG	DA	3104	1/1	0.47	4.35	97,97,97,97	0
54	MG	AA	1623	1/1	0.20	4.30	60,60,60,60	0
54	MG	DA	3072	1/1	0.27	4.28	78,78,78,78	0
54	MG	CA	1614	1/1	0.28	3.98	60,60,60,60	0
54	MG	AA	1664	1/1	0.27	3.80	58,58,58,58	0
54	MG	BA	3190	1/1	0.26	3.74	46,46,46,46	0
54	MG	BA	3158	1/1	0.24	3.73	15,15,15,15	0
54	MG	BA	3171	1/1	0.21	3.70	29,29,29,29	0
54	MG	BA	3186	1/1	0.35	3.66	29,29,29,29	0
54	MG	DA	3127	1/1	0.39	3.60	91,91,91,91	0
54	MG	DA	3160	1/1	0.29	3.53	86,86,86,86	0
54	MG	BA	3130	1/1	0.28	3.51	7,7,7,7	0
54	MG	DA	3059	1/1	0.33	3.50	87,87,87,87	0
54	MG	DA	3152	1/1	0.27	3.42	59,59,59,59	0
54	MG	DA	3014	1/1	0.29	3.39	86,86,86,86	0
54	MG	DA	3109	1/1	0.36	3.31	64,64,64,64	0
54	MG	BA	3136	1/1	0.25	3.13	50,50,50,50	0
54	MG	DA	3019	1/1	0.32	3.10	38,38,38,38	0
54	MG	DA	3138	1/1	0.40	3.09	41,41,41,41	0
54	MG	BA	3045	1/1	0.24	3.00	5,5,5,5	0
54	MG	CA	1605	1/1	0.20	2.98	110,110,110,110	0
54	MG	BA	3124	1/1	0.33	2.86	44,44,44,44	0
54	MG	BA	3033	1/1	0.23	2.84	1,1,1,1	0
54	MG	AA	1619	1/1	0.24	2.79	57,57,57,57	0
54	MG	AA	1605	1/1	0.18	2.78	35,35,35,35	0
54	MG	DA	3144	1/1	0.28	2.72	96,96,96,96	0
54	MG	BA	3122	1/1	0.22	2.57	1,1,1,1	0
54	MG	DA	3158	1/1	0.32	2.48	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3188	1/1	0.21	2.47	5,5,5,5	0
54	MG	DA	3048	1/1	0.34	2.39	109,109,109,109	0
54	MG	DA	3015	1/1	0.34	2.28	90,90,90,90	0
54	MG	DA	3159	1/1	0.50	2.25	71,71,71,71	0
54	MG	BA	3169	1/1	0.18	2.18	33,33,33,33	0
54	MG	DA	3149	1/1	0.33	2.11	77,77,77,77	0
54	MG	BA	3125	1/1	0.20	1.92	4,4,4,4	0
54	MG	DA	3039	1/1	0.21	1.87	96,96,96,96	0
54	MG	DA	3151	1/1	0.24	1.87	42,42,42,42	0
54	MG	DA	3124	1/1	0.25	1.86	55,55,55,55	0
54	MG	AA	1652	1/1	0.22	1.84	63,63,63,63	0
54	MG	DL	201	1/1	0.48	1.75	95,95,95,95	0
54	MG	CA	1631	1/1	0.26	1.69	85,85,85,85	0
54	MG	DA	3051	1/1	0.20	1.68	51,51,51,51	0
54	MG	DA	3037	1/1	0.25	1.68	66,66,66,66	0
54	MG	BA	3108	1/1	0.21	1.66	1,1,1,1	0
54	MG	CA	1607	1/1	0.19	1.51	96,96,96,96	0
54	MG	DA	3115	1/1	0.24	1.46	79,79,79,79	0
54	MG	BA	3090	1/1	0.18	1.42	13,13,13,13	0
54	MG	DA	3157	1/1	0.37	1.37	61,61,61,61	0
54	MG	DA	3007	1/1	0.28	1.32	114,114,114,114	0
54	MG	BA	3154	1/1	0.24	1.31	18,18,18,18	0
54	MG	DA	3096	1/1	0.23	1.23	81,81,81,81	0
54	MG	BA	3151	1/1	0.23	1.13	7,7,7,7	0
54	MG	BA	3109	1/1	0.21	1.11	1,1,1,1	0
54	MG	CA	1641	1/1	0.53	1.08	49,49,49,49	0
54	MG	DA	3083	1/1	0.30	1.08	116,116,116,116	0
54	MG	BA	3053	1/1	0.21	1.03	1,1,1,1	0
54	MG	CA	1638	1/1	0.18	0.96	28,28,28,28	0
54	MG	DA	3035	1/1	0.25	0.94	54,54,54,54	0
54	MG	DA	3110	1/1	0.26	0.91	89,89,89,89	0
54	MG	DA	3112	1/1	0.34	0.86	78,78,78,78	0
54	MG	CA	1612	1/1	0.18	0.82	20,20,20,20	0
54	MG	BA	3013	1/1	0.20	0.81	1,1,1,1	0
54	MG	DA	3075	1/1	0.23	0.80	78,78,78,78	0
54	MG	DA	3125	1/1	0.24	0.79	83,83,83,83	0
54	MG	BA	3105	1/1	0.21	0.74	10,10,10,10	0
54	MG	BA	3035	1/1	0.20	0.72	1,1,1,1	0
54	MG	CA	1634	1/1	0.62	0.69	143,143,143,143	0
54	MG	DA	3080	1/1	0.25	0.69	74,74,74,74	0
54	MG	CA	1621	1/1	0.18	0.68	75,75,75,75	0
54	MG	BA	3184	1/1	0.18	0.68	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3046	1/1	0.20	0.65	5,5,5,5	0
54	MG	CA	1629	1/1	0.57	0.63	123,123,123,123	0
54	MG	CA	1611	1/1	0.11	0.60	42,42,42,42	0
54	MG	DA	3008	1/1	0.26	0.57	96,96,96,96	0
54	MG	AA	1638	1/1	0.15	0.57	88,88,88,88	0
54	MG	DA	3108	1/1	0.24	0.52	22,22,22,22	0
54	MG	CA	1643	1/1	0.23	0.50	43,43,43,43	0
54	MG	BA	3012	1/1	0.23	0.49	1,1,1,1	0
54	MG	DA	3119	1/1	0.23	0.43	83,83,83,83	0
54	MG	DA	3114	1/1	0.43	0.40	126,126,126,126	0
54	MG	BA	3049	1/1	0.20	0.38	3,3,3,3	0
54	MG	DA	3116	1/1	0.19	0.34	106,106,106,106	0
54	MG	DA	3013	1/1	0.24	0.33	72,72,72,72	0
54	MG	BA	3004	1/1	0.17	0.32	55,55,55,55	0
54	MG	CA	1636	1/1	0.16	0.29	93,93,93,93	0
54	MG	DQ	201	1/1	0.68	0.28	51,51,51,51	0
54	MG	BA	3017	1/1	0.21	0.18	1,1,1,1	0
54	MG	DA	3088	1/1	0.23	0.17	81,81,81,81	0
54	MG	DL	202	1/1	0.41	0.17	116,116,116,116	0
54	MG	DA	3011	1/1	0.26	0.10	98,98,98,98	0
54	MG	BA	3132	1/1	0.41	0.09	45,45,45,45	0
54	MG	DA	3070	1/1	0.21	0.01	105,105,105,105	0
54	MG	BA	3194	1/1	0.15	-0.01	42,42,42,42	0
54	MG	BA	3006	1/1	0.15	-0.02	29,29,29,29	0
54	MG	DA	3123	1/1	0.23	-0.05	88,88,88,88	0
54	MG	DA	3024	1/1	0.23	-0.11	77,77,77,77	0
54	MG	CA	1633	1/1	0.33	-0.11	134,134,134,134	0
54	MG	DA	3033	1/1	0.20	-0.11	77,77,77,77	0
54	MG	CT	101	1/1	0.18	-0.13	91,91,91,91	0
54	MG	DA	3005	1/1	0.18	-0.17	113,113,113,113	0
54	MG	BB	201	1/1	0.15	-0.19	32,32,32,32	0
54	MG	DA	3093	1/1	0.24	-0.22	119,119,119,119	0
54	MG	DA	3131	1/1	0.31	-0.26	79,79,79,79	0
54	MG	BA	3047	1/1	0.12	-0.33	43,43,43,43	0
54	MG	AA	1647	1/1	0.19	-0.35	51,51,51,51	0
54	MG	BA	3164	1/1	0.17	-0.36	13,13,13,13	0
54	MG	AA	1636	1/1	0.18	-0.37	46,46,46,46	0
54	MG	BA	3048	1/1	0.17	-0.38	10,10,10,10	0
54	MG	BA	3117	1/1	0.20	-0.39	1,1,1,1	0
54	MG	DA	3101	1/1	0.20	-0.41	85,85,85,85	0
54	MG	CA	1639	1/1	0.20	-0.45	59,59,59,59	0
54	MG	AA	1629	1/1	0.22	-0.45	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3120	1/1	0.22	-0.48	82,82,82,82	0
54	MG	DA	3117	1/1	0.21	-0.51	79,79,79,79	0
54	MG	AA	1610	1/1	0.10	-0.52	64,64,64,64	0
54	MG	DA	3102	1/1	0.20	-0.56	77,77,77,77	0
54	MG	DA	3017	1/1	0.25	-0.59	71,71,71,71	0
54	MG	BA	3041	1/1	0.14	-0.60	3,3,3,3	0
54	MG	BA	3079	1/1	0.17	-0.61	29,29,29,29	0
54	MG	BA	3008	1/1	0.16	-0.61	3,3,3,3	0
54	MG	BA	3106	1/1	0.18	-0.67	1,1,1,1	0
54	MG	DA	3023	1/1	0.20	-0.70	57,57,57,57	0
54	MG	DA	3074	1/1	0.18	-0.70	96,96,96,96	0
54	MG	CA	1632	1/1	0.17	-0.71	85,85,85,85	0
54	MG	DA	3067	1/1	0.16	-0.72	70,70,70,70	0
54	MG	BA	3116	1/1	0.18	-0.72	1,1,1,1	0
54	MG	BA	3121	1/1	0.14	-0.74	50,50,50,50	0
55	ZN	B4	101	1/1	0.16	-0.75	28,28,28,28	0
54	MG	DA	3006	1/1	0.13	-0.79	127,127,127,127	0
54	MG	AA	1608	1/1	0.17	-0.79	26,26,26,26	0
54	MG	DA	3086	1/1	0.20	-0.82	81,81,81,81	0
54	MG	AA	1632	1/1	0.09	-0.84	60,60,60,60	0
54	MG	D2	101	1/1	0.18	-0.87	111,111,111,111	0
54	MG	BA	3075	1/1	0.16	-0.88	3,3,3,3	0
54	MG	AA	1641	1/1	0.14	-0.88	12,12,12,12	0
54	MG	AA	1656	1/1	0.13	-0.89	46,46,46,46	0
54	MG	DA	3030	1/1	0.17	-0.90	71,71,71,71	0
54	MG	DA	3018	1/1	0.10	-0.92	88,88,88,88	0
54	MG	BA	3022	1/1	0.14	-0.94	1,1,1,1	0
54	MG	BA	3074	1/1	0.07	-0.94	24,24,24,24	0
54	MG	CA	1613	1/1	0.10	-0.95	51,51,51,51	0
54	MG	DA	3156	1/1	0.18	-0.95	72,72,72,72	0
54	MG	BA	3115	1/1	0.16	-0.96	58,58,58,58	0
54	MG	DA	3041	1/1	0.16	-0.98	96,96,96,96	0
54	MG	DA	3077	1/1	0.13	-0.98	114,114,114,114	0
54	MG	AA	1607	1/1	0.06	-0.99	48,48,48,48	0
54	MG	AA	1620	1/1	0.12	-0.99	100,100,100,100	0
54	MG	BA	3023	1/1	0.18	-1.03	1,1,1,1	0
54	MG	CA	1628	1/1	0.22	-1.06	137,137,137,137	0
54	MG	DA	3107	1/1	0.17	-1.08	70,70,70,70	0
54	MG	CA	1637	1/1	0.13	-1.08	35,35,35,35	0
54	MG	DA	3121	1/1	0.18	-1.09	62,62,62,62	0
54	MG	BA	3097	1/1	0.17	-1.11	1,1,1,1	0
54	MG	DA	3047	1/1	0.14	-1.12	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	NEG	CA	1657	17/17	0.13	-1.16	62,88,103,104	0
54	MG	BA	3042	1/1	0.13	-1.17	1,1,1,1	0
54	MG	DA	3087	1/1	0.10	-1.20	84,84,84,84	0
54	MG	DA	3100	1/1	0.16	-1.20	74,74,74,74	0
54	MG	CA	1615	1/1	0.16	-1.22	39,39,39,39	0
54	MG	DA	3085	1/1	0.14	-1.23	71,71,71,71	0
54	MG	BA	3032	1/1	0.18	-1.26	4,4,4,4	0
54	MG	DA	3012	1/1	0.20	-1.30	46,46,46,46	0
54	MG	CA	1602	1/1	0.11	-1.30	93,93,93,93	0
54	MG	DA	3129	1/1	0.18	-1.30	93,93,93,93	0
54	MG	DA	3036	1/1	0.12	-1.33	114,114,114,114	0
54	MG	DB	202	1/1	0.08	-1.37	89,89,89,89	0
54	MG	DA	3001	1/1	0.13	-1.43	93,93,93,93	0
54	MG	BA	3069	1/1	0.09	-1.43	72,72,72,72	0
55	ZN	D4	101	1/1	0.09	-1.44	95,95,95,95	0
54	MG	BA	3039	1/1	0.18	-1.54	1,1,1,1	0
54	MG	BA	3086	1/1	0.17	-1.62	2,2,2,2	0
54	MG	AA	1628	1/1	0.13	-1.66	84,84,84,84	0
54	MG	DA	3042	1/1	0.12	-1.67	67,67,67,67	0
54	MG	BA	3113	1/1	0.15	-1.73	4,4,4,4	0
54	MG	AA	1616	1/1	0.08	-1.73	94,94,94,94	0
54	MG	BA	3107	1/1	0.15	-1.73	3,3,3,3	0
54	MG	DA	3066	1/1	0.17	-1.74	58,58,58,58	0
54	MG	AA	1602	1/1	0.11	-1.81	37,37,37,37	0
54	MG	AA	1624	1/1	0.13	-1.83	36,36,36,36	0
54	MG	DA	3046	1/1	0.14	-1.84	80,80,80,80	0
54	MG	AA	1639	1/1	0.12	-1.89	60,60,60,60	0
54	MG	BA	3123	1/1	0.14	-1.92	6,6,6,6	0
54	MG	DA	3010	1/1	0.15	-1.94	60,60,60,60	0
54	MG	CA	1656	1/1	0.09	-1.95	88,88,88,88	0
54	MG	BA	3030	1/1	0.17	-1.99	4,4,4,4	0
54	MG	BA	3100	1/1	0.15	-2.11	4,4,4,4	0
54	MG	DA	3021	1/1	0.11	-2.13	69,69,69,69	0
54	MG	BA	3001	1/1	0.13	-2.15	39,39,39,39	0
54	MG	DA	3003	1/1	0.10	-2.16	83,83,83,83	0
54	MG	BA	3009	1/1	0.14	-2.26	1,1,1,1	0
54	MG	DA	3097	1/1	0.09	-2.32	67,67,67,67	0
54	MG	CA	1608	1/1	0.16	-2.33	86,86,86,86	0
54	MG	AA	1634	1/1	0.13	-2.34	58,58,58,58	0
54	MG	DA	3105	1/1	0.16	-2.34	77,77,77,77	0
54	MG	BA	3018	1/1	0.09	-2.37	14,14,14,14	0
54	MG	CA	1604	1/1	0.06	-2.38	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	DA	3078	1/1	0.09	-2.39	103,103,103,103	0
54	MG	AA	1601	1/1	0.09	-2.40	59,59,59,59	0
54	MG	DA	3053	1/1	0.18	-2.40	49,49,49,49	0
54	MG	DA	3122	1/1	0.10	-2.44	51,51,51,51	0
54	MG	DA	3089	1/1	0.15	-2.44	106,106,106,106	0
54	MG	BA	3103	1/1	0.12	-2.49	2,2,2,2	0
54	MG	CA	1619	1/1	0.12	-2.50	85,85,85,85	0
54	MG	BA	3062	1/1	0.12	-2.56	4,4,4,4	0
54	MG	CA	1630	1/1	0.06	-2.59	79,79,79,79	0
54	MG	DA	3016	1/1	0.20	-2.60	103,103,103,103	0
54	MG	DA	3103	1/1	0.10	-2.61	85,85,85,85	0
54	MG	BA	3192	1/1	0.14	-2.61	30,30,30,30	0
54	MG	BA	3067	1/1	0.15	-2.63	2,2,2,2	0
54	MG	BA	3027	1/1	0.15	-2.63	10,10,10,10	0
54	MG	BB	202	1/1	0.09	-2.65	10,10,10,10	0
54	MG	BA	3099	1/1	0.16	-2.65	1,1,1,1	0
54	MG	BA	3114	1/1	0.14	-2.68	14,14,14,14	0
54	MG	DA	3095	1/1	0.07	-2.71	77,77,77,77	0
54	MG	AA	1642	1/1	0.10	-2.71	23,23,23,23	0
54	MG	BA	3134	1/1	0.16	-2.72	3,3,3,3	0
54	MG	DA	3022	1/1	0.10	-2.73	74,74,74,74	0
54	MG	DA	3150	1/1	0.14	-2.75	86,86,86,86	0
54	MG	AA	1618	1/1	0.09	-2.78	89,89,89,89	0
54	MG	CA	1617	1/1	0.14	-2.78	38,38,38,38	0
54	MG	BA	3077	1/1	0.11	-2.79	16,16,16,16	0
54	MG	BA	3064	1/1	0.12	-2.81	5,5,5,5	0
54	MG	BA	3126	1/1	0.15	-2.82	3,3,3,3	0
54	MG	DA	3128	1/1	0.13	-2.88	60,60,60,60	0
54	MG	BA	3050	1/1	0.11	-2.89	7,7,7,7	0
54	MG	DB	203	1/1	0.08	-2.97	106,106,106,106	0
54	MG	BA	3011	1/1	0.08	-2.98	16,16,16,16	0
54	MG	DA	3026	1/1	0.13	-3.01	93,93,93,93	0
54	MG	DA	3050	1/1	0.10	-3.13	41,41,41,41	0
54	MG	CA	1610	1/1	0.04	-3.17	57,57,57,57	0
54	MG	DA	3133	1/1	0.14	-3.17	78,78,78,78	0
54	MG	BA	3094	1/1	0.08	-3.19	19,19,19,19	0
54	MG	BA	3051	1/1	0.14	-3.20	2,2,2,2	0
54	MG	BA	3007	1/1	0.07	-3.22	29,29,29,29	0
54	MG	BA	3028	1/1	0.16	-3.29	1,1,1,1	0
54	MG	DA	3058	1/1	0.10	-3.31	64,64,64,64	0
54	MG	DA	3069	1/1	0.06	-3.33	121,121,121,121	0
54	MG	BA	3010	1/1	0.12	-3.35	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3063	1/1	0.12	-3.39	6,6,6,6	0
54	MG	BA	3092	1/1	0.10	-3.42	33,33,33,33	0
54	MG	DA	3099	1/1	0.12	-3.44	69,69,69,69	0
54	MG	AA	1611	1/1	0.10	-3.45	32,32,32,32	0
54	MG	BA	3101	1/1	0.11	-3.49	14,14,14,14	0
54	MG	CA	1609	1/1	0.10	-3.55	56,56,56,56	0
54	MG	CA	1616	1/1	0.11	-3.58	43,43,43,43	0
54	MG	DA	3073	1/1	0.12	-3.66	69,69,69,69	0
54	MG	AA	1637	1/1	0.10	-3.68	13,13,13,13	0
54	MG	BA	3135	1/1	0.15	-3.70	23,23,23,23	0
54	MG	DA	3034	1/1	0.11	-3.71	90,90,90,90	0
54	MG	BA	3065	1/1	0.14	-3.72	1,1,1,1	0
54	MG	DA	3038	1/1	0.15	-3.73	68,68,68,68	0
54	MG	AA	1631	1/1	0.07	-3.75	32,32,32,32	0
54	MG	CA	1603	1/1	0.06	-3.77	40,40,40,40	0
54	MG	BA	3078	1/1	0.07	-3.80	48,48,48,48	0
54	MG	DA	3111	1/1	0.12	-3.80	71,71,71,71	0
54	MG	BA	3016	1/1	0.12	-3.85	13,13,13,13	0
54	MG	DA	3009	1/1	0.08	-3.86	91,91,91,91	0
54	MG	DA	3062	1/1	0.12	-3.88	67,67,67,67	0
54	MG	DA	3068	1/1	0.07	-3.92	81,81,81,81	0
54	MG	CA	1620	1/1	0.10	-3.97	81,81,81,81	0
54	MG	BA	3003	1/1	0.09	-3.99	29,29,29,29	0
54	MG	BA	3112	1/1	0.11	-4.01	25,25,25,25	0
54	MG	AA	1633	1/1	0.10	-4.05	25,25,25,25	0
54	MG	AA	1604	1/1	0.08	-4.08	81,81,81,81	0
54	MG	BA	3054	1/1	0.12	-4.14	4,4,4,4	0
54	MG	BA	3096	1/1	0.08	-4.26	2,2,2,2	0
54	MG	BA	3002	1/1	0.09	-4.28	11,11,11,11	0
54	MG	BA	3072	1/1	0.13	-4.28	1,1,1,1	0
54	MG	DA	3052	1/1	0.09	-4.28	50,50,50,50	0
54	MG	BA	3080	1/1	0.14	-4.28	24,24,24,24	0
54	MG	BA	3066	1/1	0.12	-4.29	3,3,3,3	0
54	MG	DA	3113	1/1	0.13	-4.33	54,54,54,54	0
54	MG	CA	1606	1/1	0.10	-4.35	61,61,61,61	0
54	MG	CA	1601	1/1	0.12	-4.40	45,45,45,45	0
54	MG	DA	3082	1/1	0.08	-4.40	80,80,80,80	0
54	MG	AA	1621	1/1	0.08	-4.45	32,32,32,32	0
54	MG	CA	1618	1/1	0.10	-4.52	35,35,35,35	0
54	MG	BA	3068	1/1	0.11	-4.63	1,1,1,1	0
54	MG	DA	3028	1/1	0.13	-4.69	83,83,83,83	0
54	MG	DA	3064	1/1	0.11	-4.70	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	BA	3073	1/1	0.11	-4.75	16,16,16,16	0
54	MG	DA	3063	1/1	0.14	-4.77	64,64,64,64	0
54	MG	BA	3129	1/1	0.15	-4.79	1,1,1,1	0
54	MG	DA	3065	1/1	0.14	-4.83	44,44,44,44	0
54	MG	BA	3111	1/1	0.09	-4.84	40,40,40,40	0
54	MG	BA	3024	1/1	0.10	-4.99	13,13,13,13	0
54	MG	DA	3079	1/1	0.11	-5.00	91,91,91,91	0
54	MG	BA	3093	1/1	0.11	-5.01	11,11,11,11	0
54	MG	CA	1627	1/1	0.08	-5.04	116,116,116,116	0
54	MG	AA	1613	1/1	0.07	-5.13	13,13,13,13	0
54	MG	DA	3090	1/1	0.09	-5.30	85,85,85,85	0
54	MG	DB	201	1/1	0.10	-5.46	118,118,118,118	0
54	MG	BA	3081	1/1	0.13	-5.53	1,1,1,1	0
54	MG	DA	3146	1/1	0.22	-5.55	68,68,68,68	0
54	MG	BA	3020	1/1	0.05	-5.58	1,1,1,1	0
54	MG	AA	1606	1/1	0.07	-5.68	42,42,42,42	0
54	MG	BA	3021	1/1	0.12	-5.91	1,1,1,1	0
54	MG	BA	3058	1/1	0.08	-5.92	14,14,14,14	0
54	MG	DA	3032	1/1	0.06	-5.92	67,67,67,67	0
54	MG	AA	1625	1/1	0.08	-6.25	47,47,47,47	0
54	MG	CA	1655	1/1	0.07	-6.26	85,85,85,85	0
54	MG	BB	203	1/1	0.08	-6.28	12,12,12,12	0
54	MG	CA	1623	1/1	0.06	-6.30	48,48,48,48	0
54	MG	DA	3106	1/1	0.10	-6.31	60,60,60,60	0
54	MG	BA	3071	1/1	0.07	-6.54	13,13,13,13	0
54	MG	BA	3038	1/1	0.14	-6.65	1,1,1,1	0
54	MG	DA	3054	1/1	0.14	-6.74	64,64,64,64	0
54	MG	DA	3081	1/1	0.12	-7.27	75,75,75,75	0
54	MG	BA	3005	1/1	0.06	-7.41	44,44,44,44	0
54	MG	DA	3049	1/1	0.11	-7.43	61,61,61,61	0
54	MG	CA	1625	1/1	0.04	-7.67	44,44,44,44	0
54	MG	BA	3087	1/1	0.07	-7.83	18,18,18,18	0
54	MG	DA	3126	1/1	0.12	-7.87	58,58,58,58	0
54	MG	BA	3082	1/1	0.07	-7.99	8,8,8,8	0
54	MG	BA	3029	1/1	0.09	-8.10	20,20,20,20	0
54	MG	BA	3085	1/1	0.13	-8.25	9,9,9,9	0
54	MG	AA	1640	1/1	0.06	-8.53	39,39,39,39	0
54	MG	AA	1609	1/1	0.05	-8.78	23,23,23,23	0
54	MG	BA	3127	1/1	0.12	-8.88	3,3,3,3	0
54	MG	BA	3014	1/1	0.12	-9.50	8,8,8,8	0
54	MG	DA	3045	1/1	0.12	-9.85	74,74,74,74	0
54	MG	BA	3043	1/1	0.08	-10.15	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
54	MG	AA	1603	1/1	0.04	-11.01	30,30,30,30	0
54	MG	BA	3120	1/1	0.14	-11.60	10,10,10,10	0
54	MG	BA	3088	1/1	0.12	-12.30	25,25,25,25	0
54	MG	BA	3089	1/1	0.07	-12.88	8,8,8,8	0
54	MG	BA	3052	1/1	0.08	-12.88	1,1,1,1	0
54	MG	BA	3070	1/1	0.10	-13.20	6,6,6,6	0
54	MG	AA	1612	1/1	0.11	-14.09	42,42,42,42	0
54	MG	BA	3118	1/1	0.09	-14.99	14,14,14,14	0
54	MG	BA	3095	1/1	0.07	-15.90	6,6,6,6	0
54	MG	BA	3026	1/1	0.07	-16.55	2,2,2,2	0
54	MG	BA	3031	1/1	0.04	-25.80	11,11,11,11	0
54	MG	AA	1659	1/1	0.41	-	68,68,68,68	0
54	MG	DA	3098	1/1	0.17	-	89,89,89,89	0
54	MG	BA	3172	1/1	0.17	-	29,29,29,29	0
54	MG	BA	3180	1/1	0.22	-	45,45,45,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.