



wwPDB X-ray Structure Validation Summary Report

Jun 16, 2014 – 07:47 PM BST

PDB ID : 4V8X
Title : Structure of Thermus thermophilus 30s ribosome
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Deposited on : 2013-07-19
Resolution : 3.35 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

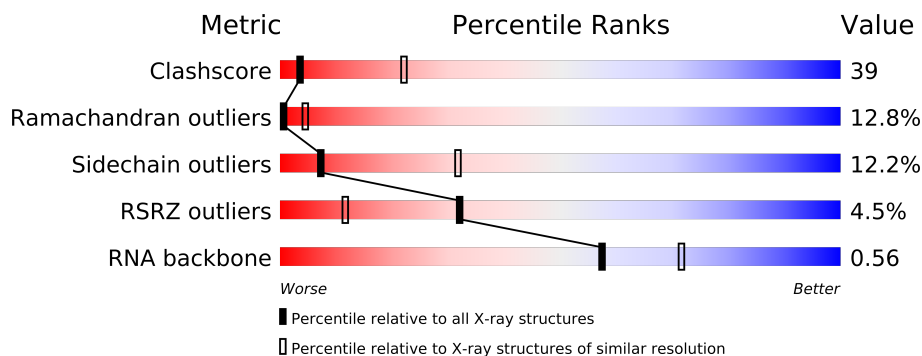
The following versions of software and data (see [references](#)) were used in the production of this report:

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

1 Overall quality at a glance

The reported resolution of this entry is 3.35 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))
Clashscore	79885	1030 (3.48-3.24)
Ramachandran outliers	78287	1008 (3.48-3.24)
Sidechain outliers	78261	1007 (3.48-3.24)
RSRZ outliers	66119	1141 (3.50-3.22)
RNA backbone	1838	1005 (4.00-2.72)

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	1504	
1	CA	1504	
2	AB	256	
2	CB	256	
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	

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Mol	Chain	Length	Quality of chain
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
23	AW	77	
23	CV	77	
23	CW	77	
24	AX	25	
25	AY	84	
25	AZ	84	
25	CY	84	
25	CZ	84	
26	B0	85	
26	D0	85	
27	B1	98	
27	D1	98	
28	B2	72	

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Mol	Chain	Length	Quality of chain
28	D2	72	
29	B3	60	
29	D3	60	
30	B4	71	
30	D4	71	
31	B5	60	
31	D5	60	
32	B6	54	
32	D6	54	
33	B7	49	
33	D7	49	
34	B8	65	
34	D8	65	
35	B9	37	
35	D9	37	
36	BA	2848	
36	DA	2848	
37	BB	119	
37	DB	119	
38	BC	229	
38	DC	229	
39	BD	276	
39	DD	276	
40	BE	206	
40	DE	206	
41	BF	210	
41	DF	210	
42	BG	182	
42	DG	182	
43	BH	180	
43	DH	180	
44	BI	148	
44	DI	148	
45	BJ	130	
45	DJ	130	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	

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Mol	Chain	Length	Quality of chain
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	
59	CX	10	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 298206 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 RNA (1504-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O	0	0	0
			1010	639	197	174			
9	CI	127	Total	C	N	O	0	0	0
			1010	639	197	174			

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			
13	CM	119	Total	C	N	O	S	0	0	1
			938	579	194	163	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- 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
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- 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	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 23 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CV	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
23	CW	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 24 is a RNA chain called 5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*AP*AP*AP*AP*AP*UP*G U2M A2M A2MP*AP*AP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	11	Total	C	N	O	P	0	0	0
			239	111	49	69	10			

- Molecule 25 is a protein called TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	AZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			
25	CY	84	Total	C	N	O	S	0	0	0
			722	464	126	130	2			
25	CZ	84	Total	C	N	O	S	0	0	0
			723	464	126	131	2			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
26	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			
27	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
28	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
29	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			
30	D4	58	Total	C	N	O	S	0	0	1
			451	285	78	83	5			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	B5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	D5	56	Total	C	N	O	S	0	0	1
			428	267	87	69	5			

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	B6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			
32	D6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	B7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			
33	D7	48	Total	C	N	O	S	0	0	1
			410	251	103	54	2			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
34	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	B9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			
35	D9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 36 is a RNA chain called RNA (2848-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			
36	DA	2848	Total	C	N	O	P	0	0	0
			61341	27300	11478	19716	2847			

- Molecule 37 is a RNA chain called RNA (119-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
37	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			
38	DC	120	Total	C	N	O	S	0	0	0
			937	590	174	172	1			

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
39	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
40	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
41	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
42	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			
43	DH	165	Total	C	N	O	S	0	0	1
			1260	800	234	225	1			

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
44	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BJ	130	Total	C	N	O		0	0	0
			651	390	130	131				
45	DJ	130	Total	C	N	O		0	0	0
			651	390	130	131				

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
46	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
48	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			
49	DQ	141	Total	C	N	O	S	0	0	1
			1113	710	211	185	7			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
50	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				
51	DS	99	Total	C	N	O		0	0	1
			771	486	155	130				

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			
52	DT	136	Total	C	N	O	S	0	0	1
			1124	699	231	193	1			

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
53	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
54	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
55	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
56	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
57	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	BZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1
58	DZ	185	Total 1468	C 936	N 262	O 268	S 2	0	0	1

- Molecule 59 is a RNA chain called BACTERIAL TOXIN YOEB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	10	Total 217	C 101	N 44	O 63	P 9	0	0	0

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	236	Total 236	Mg 236	0	0
60	CA	103	Total 103	Mg 103	0	0
60	DF	1	Total 1	Mg 1	0	0
60	CV	2	Total 2	Mg 2	0	0
60	B1	2	Total 2	Mg 2	0	0
60	BP	1	Total 1	Mg 1	0	0
60	AX	1	Total 1	Mg 1	0	0
60	DR	1	Total 1	Mg 1	0	0
60	B5	2	Total 2	Mg 2	0	0
60	BB	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	AV	1	Total 1	Mg 1	0	0
60	BX	1	Total 1	Mg 1	0	0
60	AA	103	Total 103	Mg 103	0	0
60	CG	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DX	1	Total 1	Mg 1	0	0
60	DA	242	Total 242	Mg 242	0	0
60	AL	1	Total 1	Mg 1	0	0
60	D1	1	Total 1	Mg 1	0	0
60	D5	1	Total 1	Mg 1	0	0
60	B0	1	Total 1	Mg 1	0	0
60	CL	1	Total 1	Mg 1	0	0
60	DB	1	Total 1	Mg 1	0	0

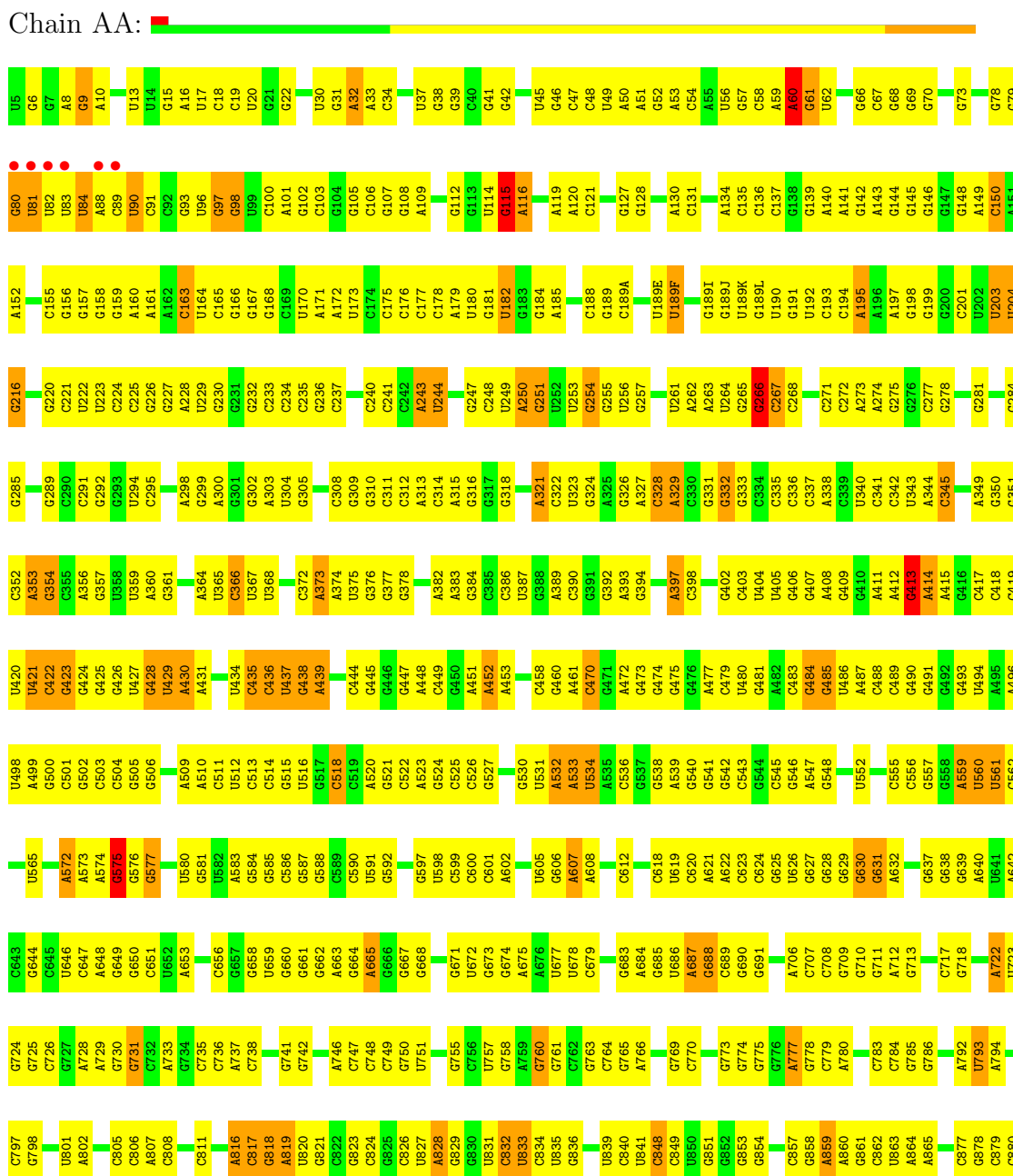
- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

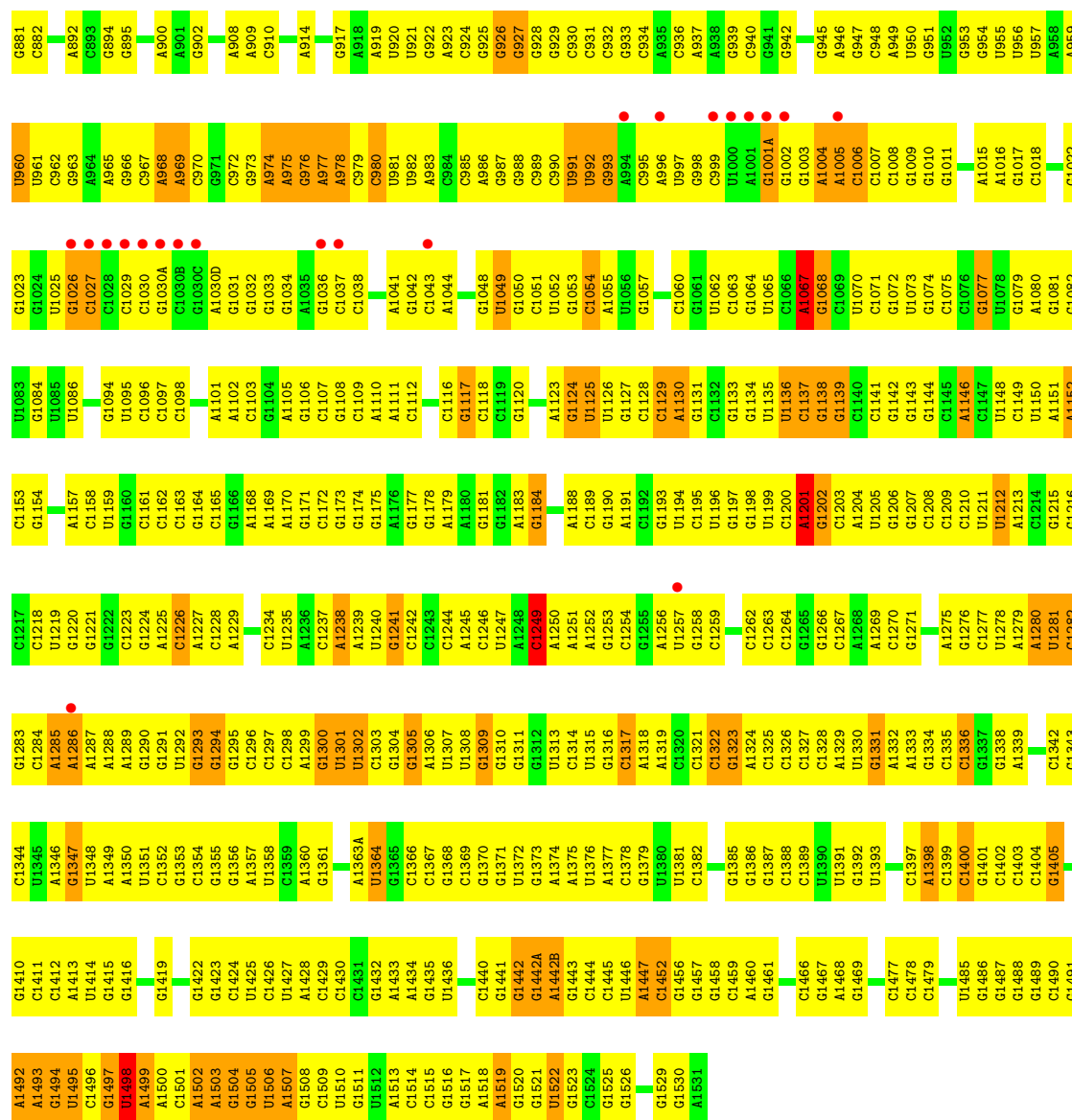
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
61	CN	1	Total 1	Zn 1	0	0
61	AD	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	AN	1	Total 1	Zn 1	0	0

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.

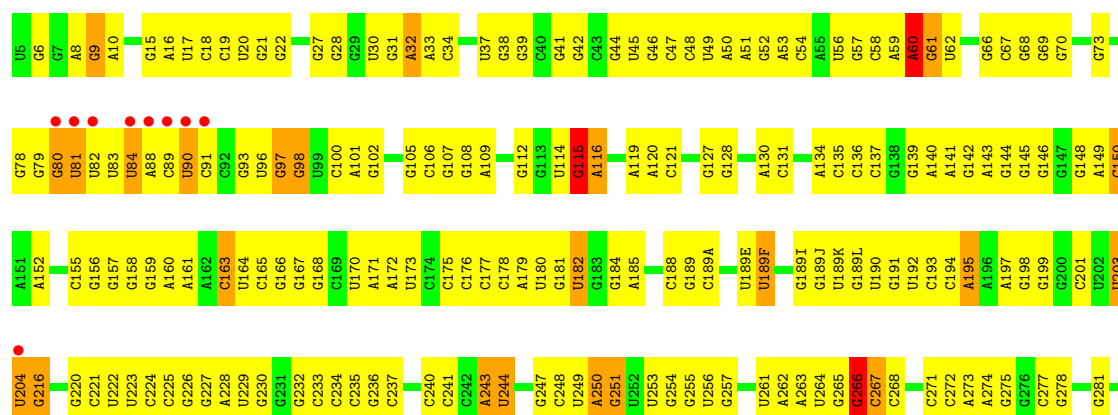
• Molecule 1: RNA (1504-MER)



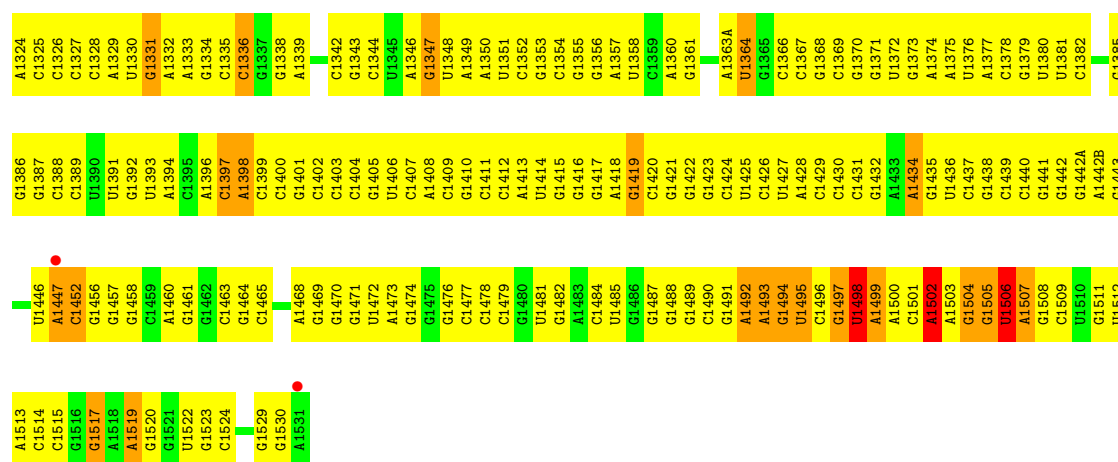


• Molecule 1: RNA (1504-MER)

Chain CA:

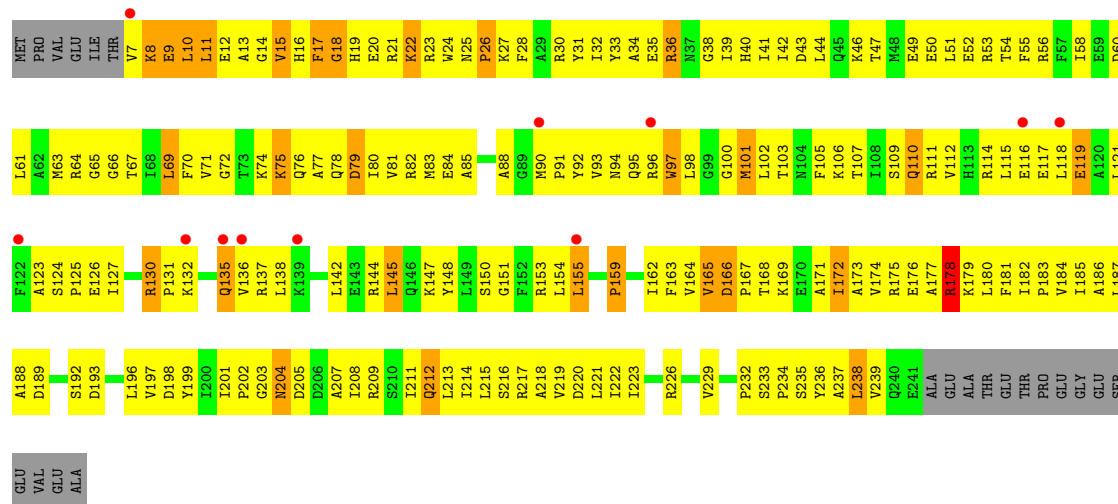






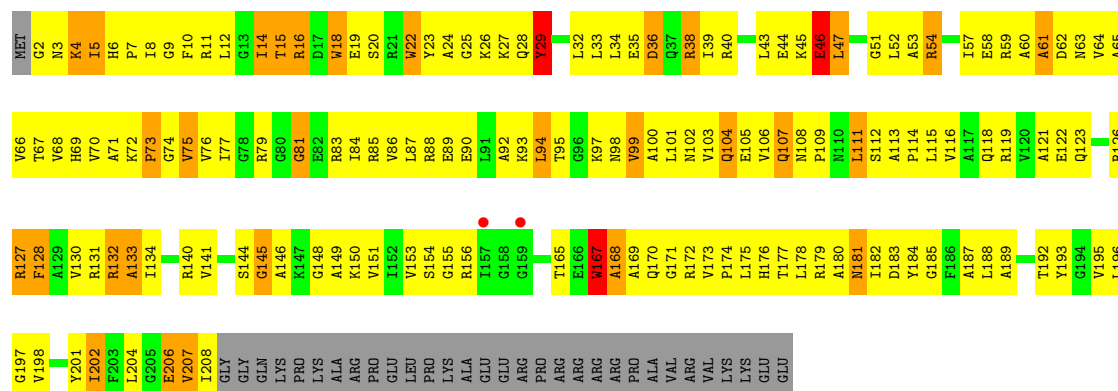
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain AB:



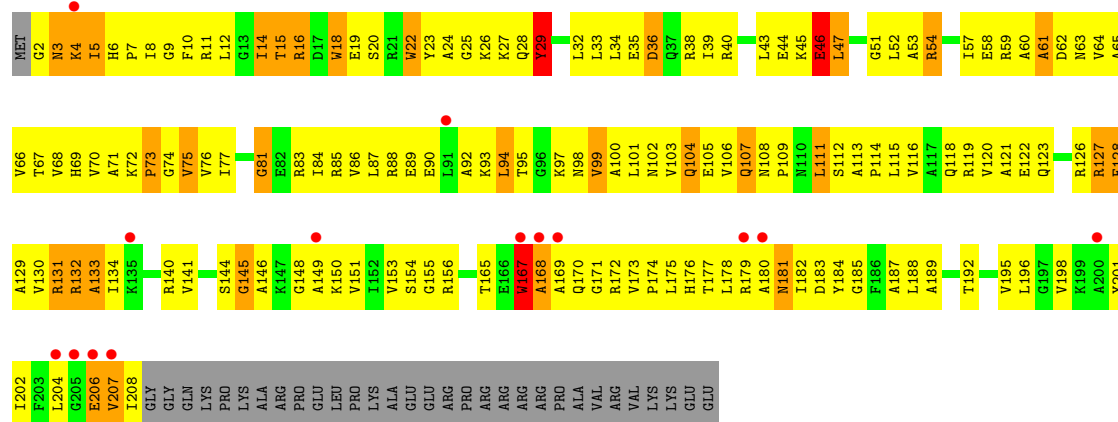
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain AC:



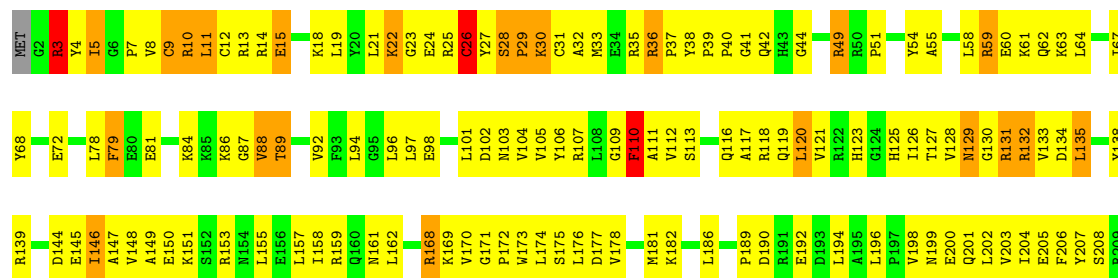
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain CC:



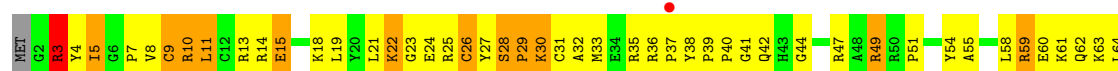
- Molecule 4: 30S RIBOSOMAL PROTEIN S4

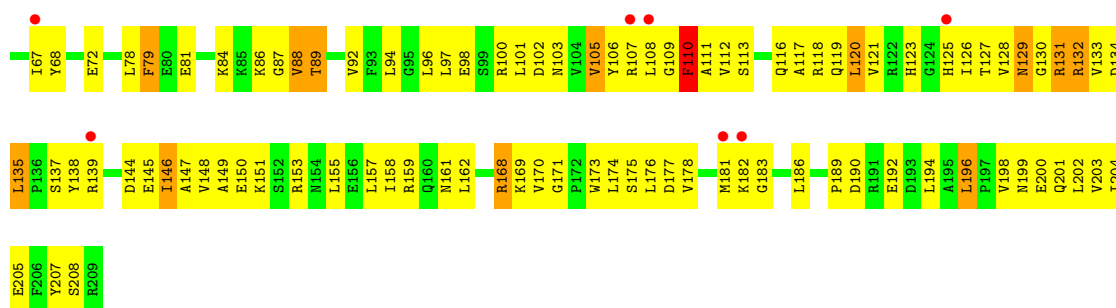
Chain AD:



- Molecule 4: 30S RIBOSOMAL PROTEIN S4

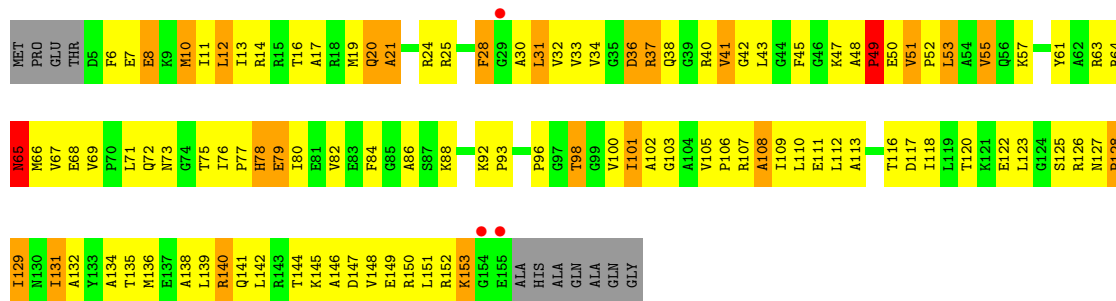
Chain CD:





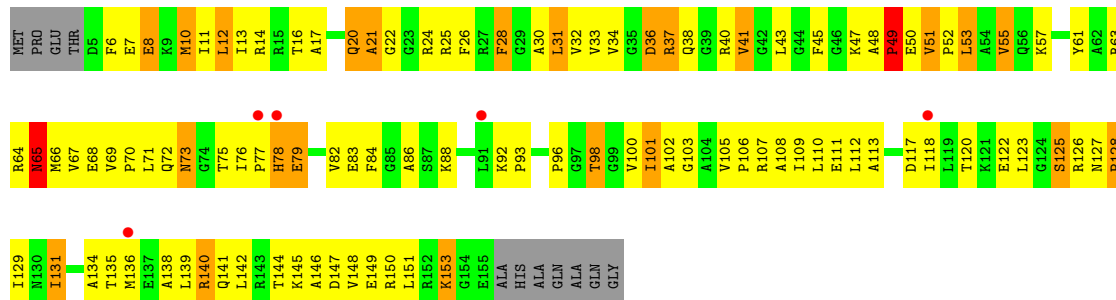
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain AE:



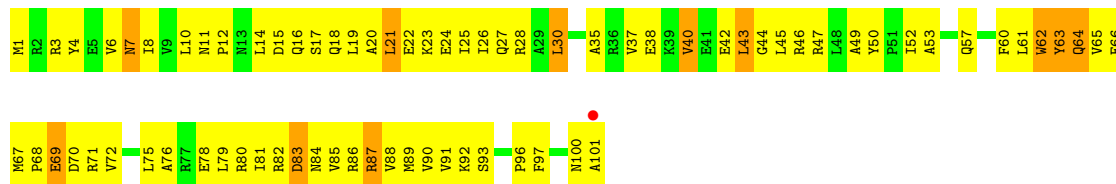
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain CE:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain AF:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

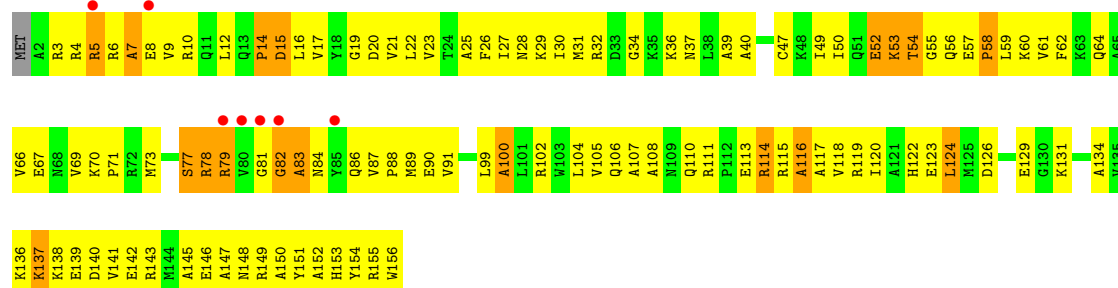
Chain CF:





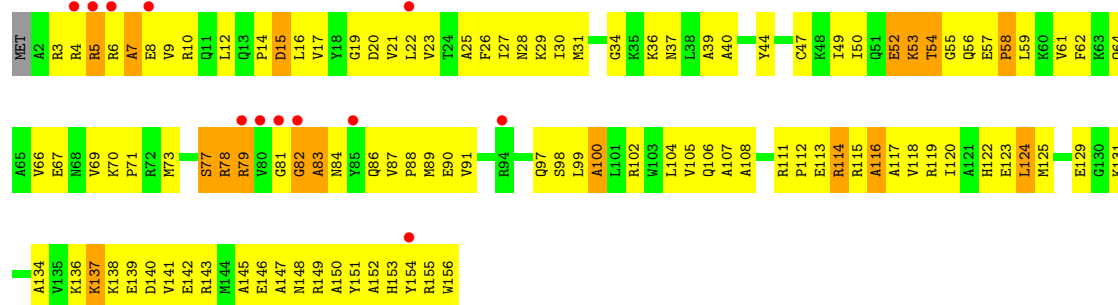
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain AG:



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain CG:



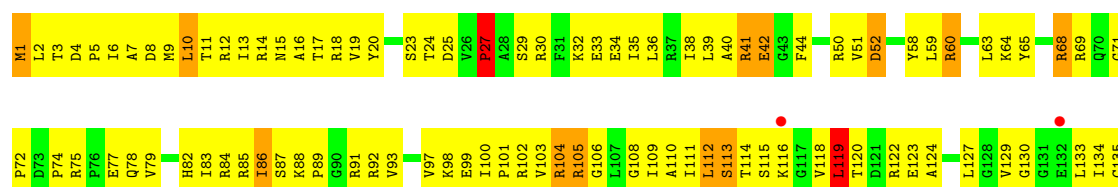
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain AH:



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

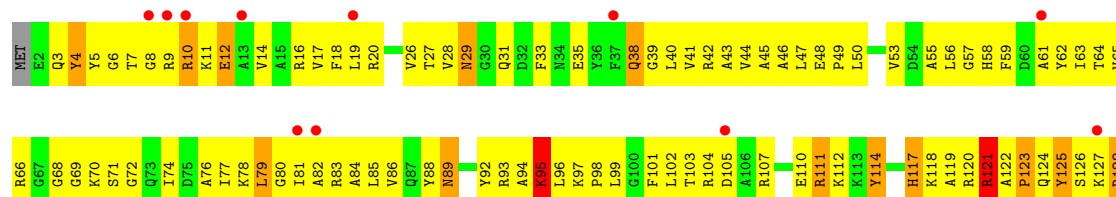
Chain CH:





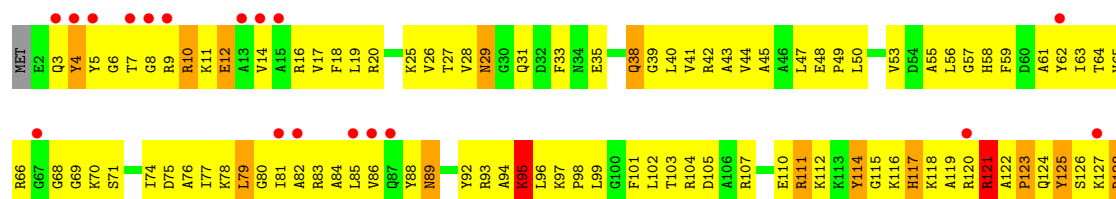
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain AI:



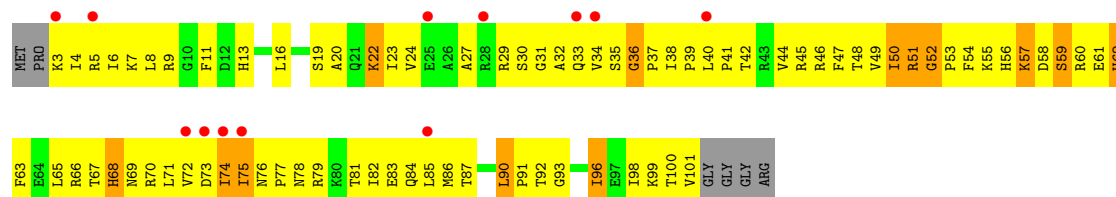
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain CI:



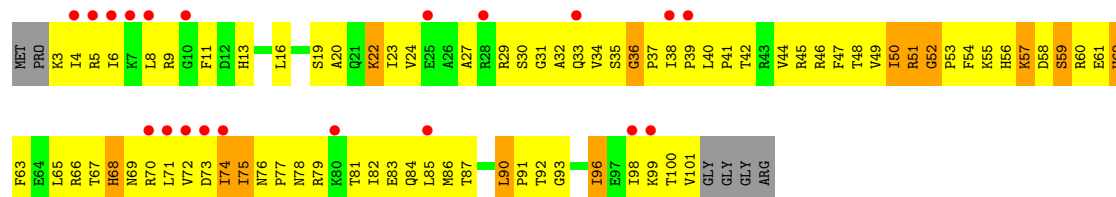
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain AJ:



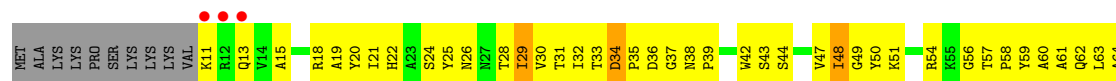
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

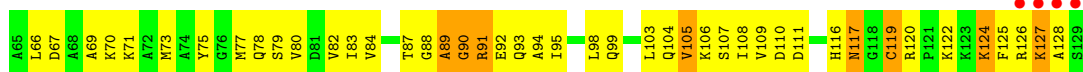
Chain CJ:



• Molecule 11: 30S RIBOSOMAL PROTEIN S11

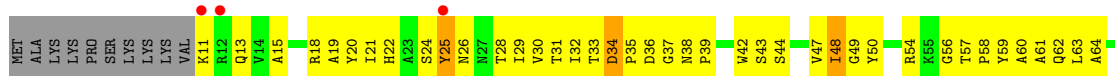
Chain AK:





• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain CK:



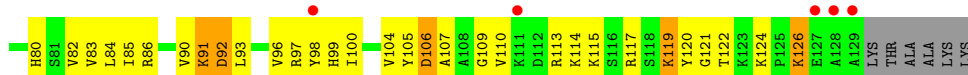
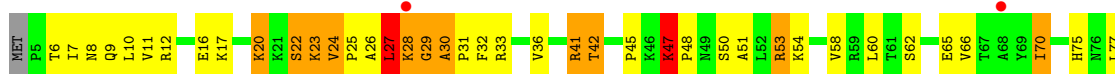
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain AL:



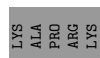
• Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain CL:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

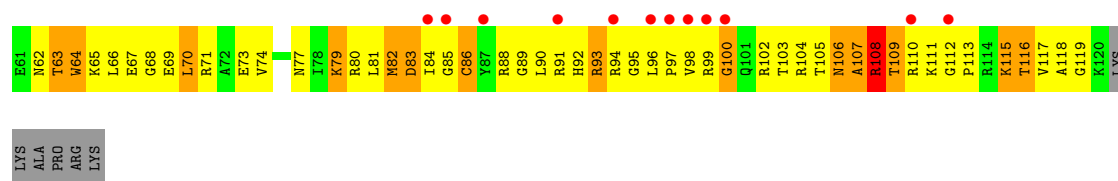
Chain AM:



• Molecule 13: 30S RIBOSOMAL PROTEIN S13

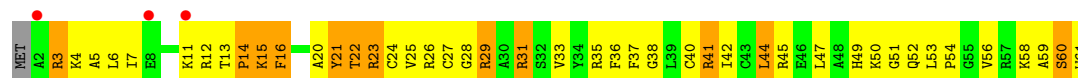
Chain CM:





• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain AN:



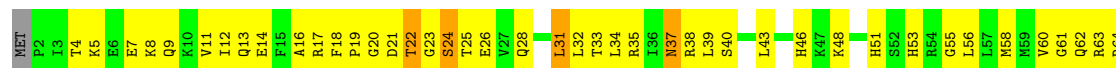
• Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain CN:



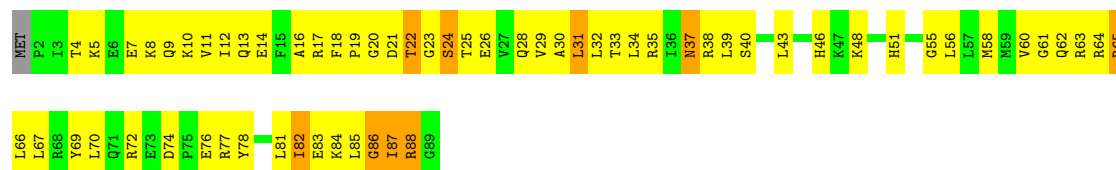
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain AO:



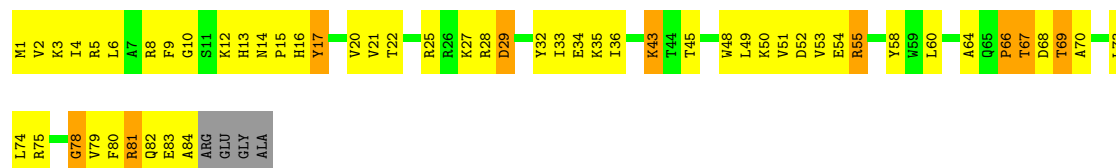
• Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain CO:



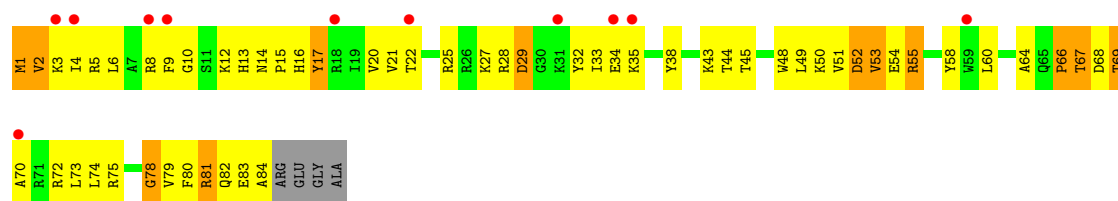
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain AP:



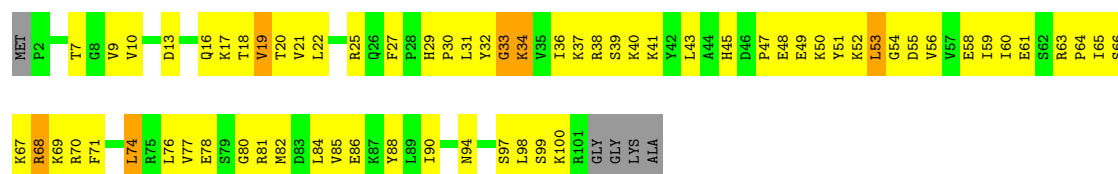
• Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain CP:



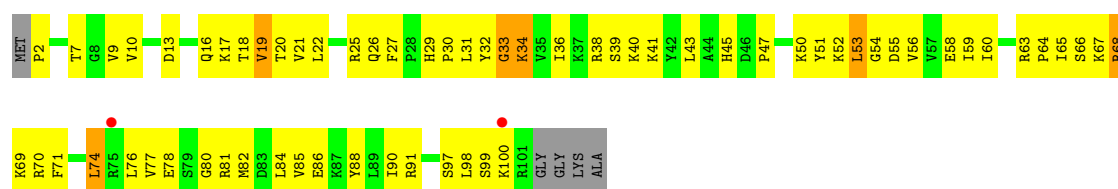
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain AQ:



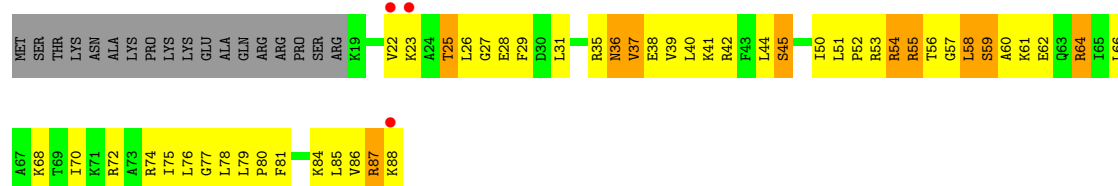
• Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain CQ:



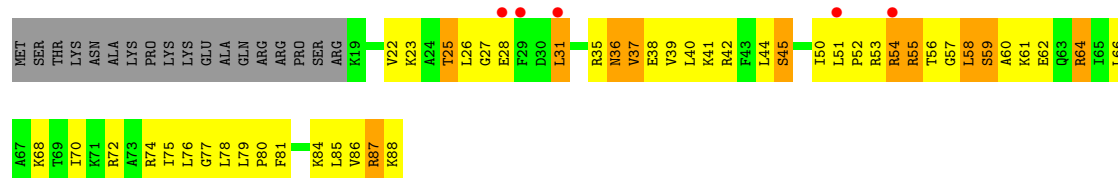
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR:



• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR:



• Molecule 19: 30S RIBOSOMAL PROTEIN S19

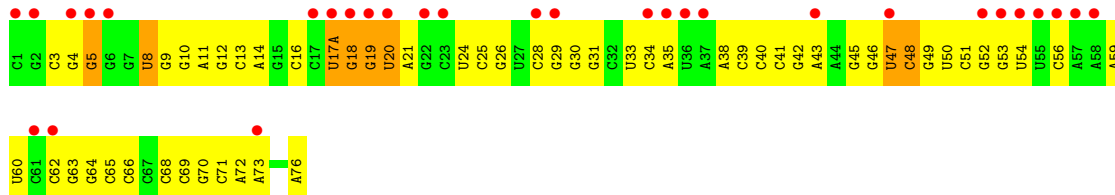
Chain AS:





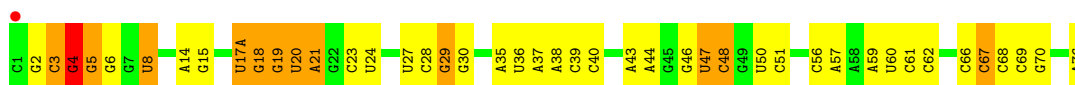
- Molecule 23: RNA (77-MER)

Chain AW:



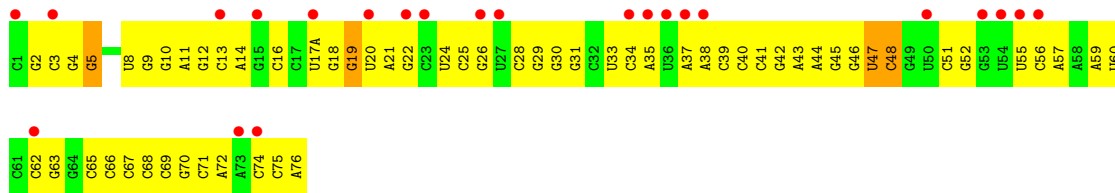
- Molecule 23: RNA (77-MER)

Chain CV:



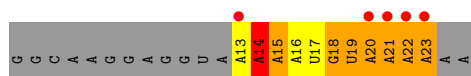
- Molecule 23: RNA (77-MER)

Chain CW:



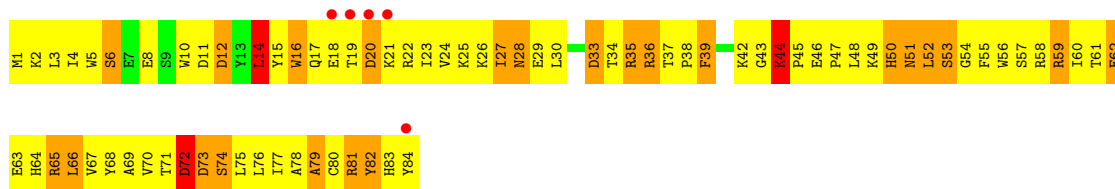
- Molecule 24: 5'-R(*GP*GP*CP*AP*AP*GP*GP*AP*GP*GP*UP*AP*AP*AP*AP*AP*UP*GU2M A2M A2MP*AP*AP*AP*A)-3'

Chain AX:



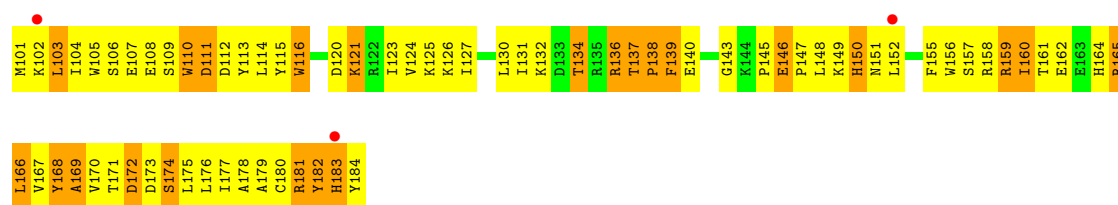
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

Chain AY:



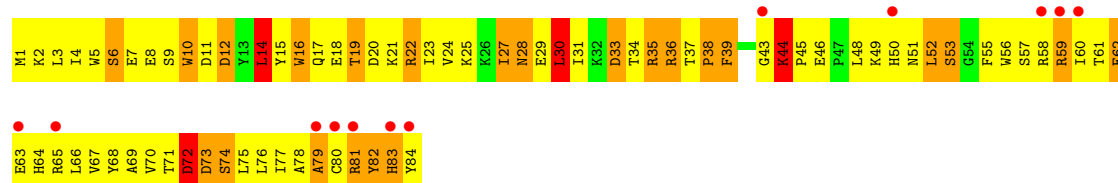
- Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

Chain AZ:



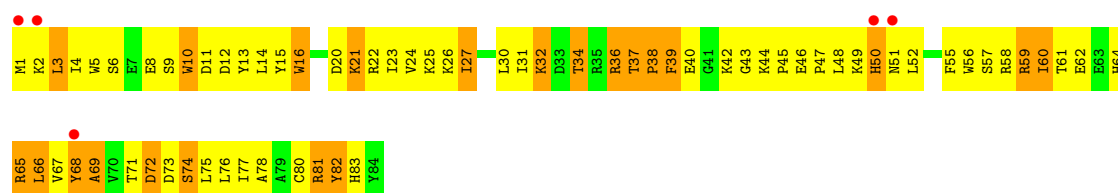
● Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

Chain CY:



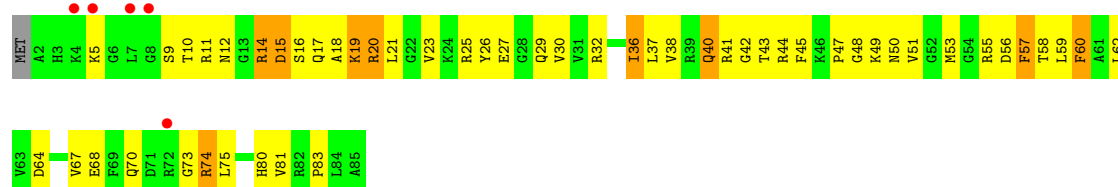
● Molecule 25: TOXIN OF THE YOEB-YEFM TOXIN-ANTITOXIN SYSTEM

Chain CZ:



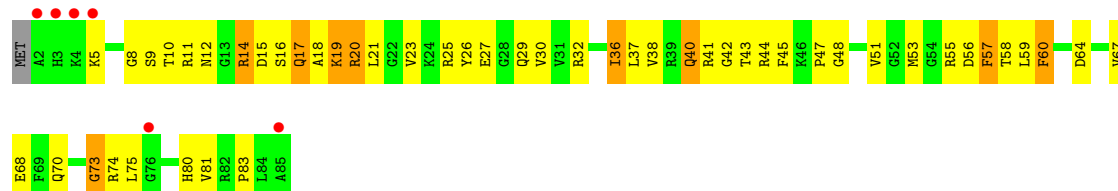
● Molecule 26: 50S RIBOSOMAL PROTEIN L27

Chain B0:



● Molecule 26: 50S RIBOSOMAL PROTEIN L27

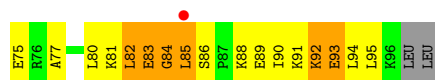
Chain D0:



● Molecule 27: 50S RIBOSOMAL PROTEIN L28

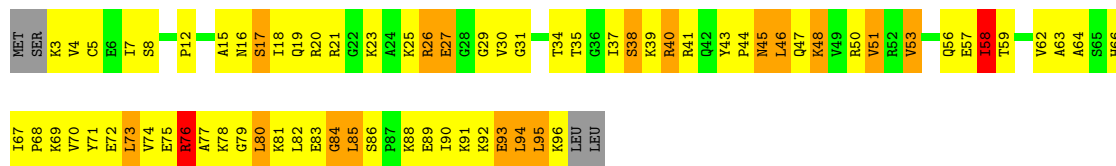
Chain B1:





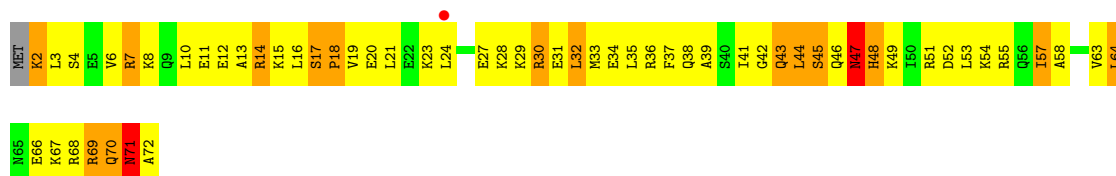
• Molecule 27: 50S RIBOSOMAL PROTEIN L28

Chain D1:



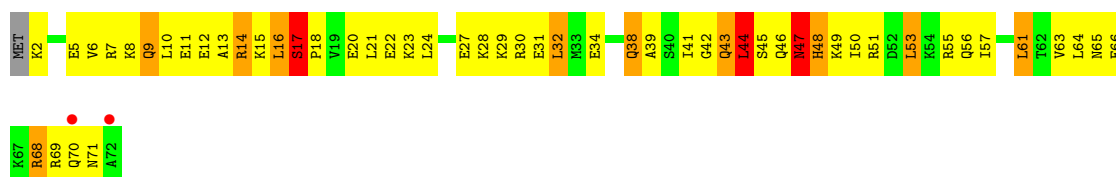
• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain B2:



• Molecule 28: 50S RIBOSOMAL PROTEIN L29

Chain D2:



• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain B3:



• Molecule 29: 50S RIBOSOMAL PROTEIN L30

Chain D3:



• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain B4:



ARG
ARG
TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 30: 50S RIBOSOMAL PROTEIN L31

Chain D4:

ARG
ARG
TYR
GLY
ASP
SER
TYR
ARG
LYS
GLY
ARG

• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain B5:

• Molecule 31: 50S RIBOSOMAL PROTEIN L32

Chain D5:

• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain B6:

• Molecule 32: 50S RIBOSOMAL PROTEIN L33

Chain D6:

• Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain B7:

• Molecule 33: 50S RIBOSOMAL PROTEIN L34

Chain D7:

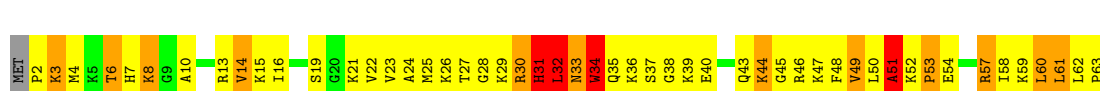
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain B8:



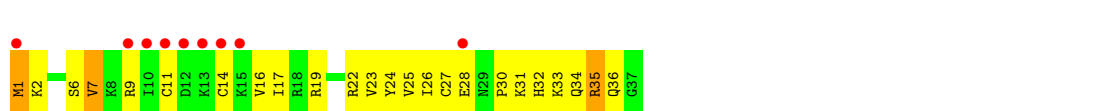
- Molecule 34: 50S RIBOSOMAL PROTEIN L35

Chain D8:



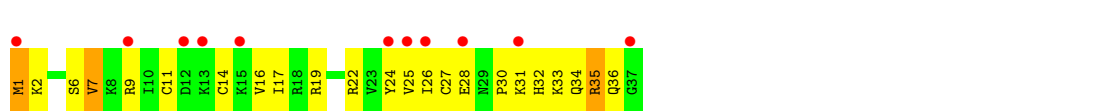
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain B9:



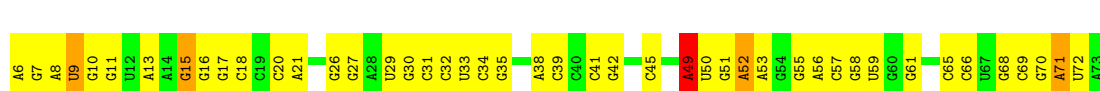
- Molecule 35: 50S RIBOSOMAL PROTEIN L36

Chain D9:



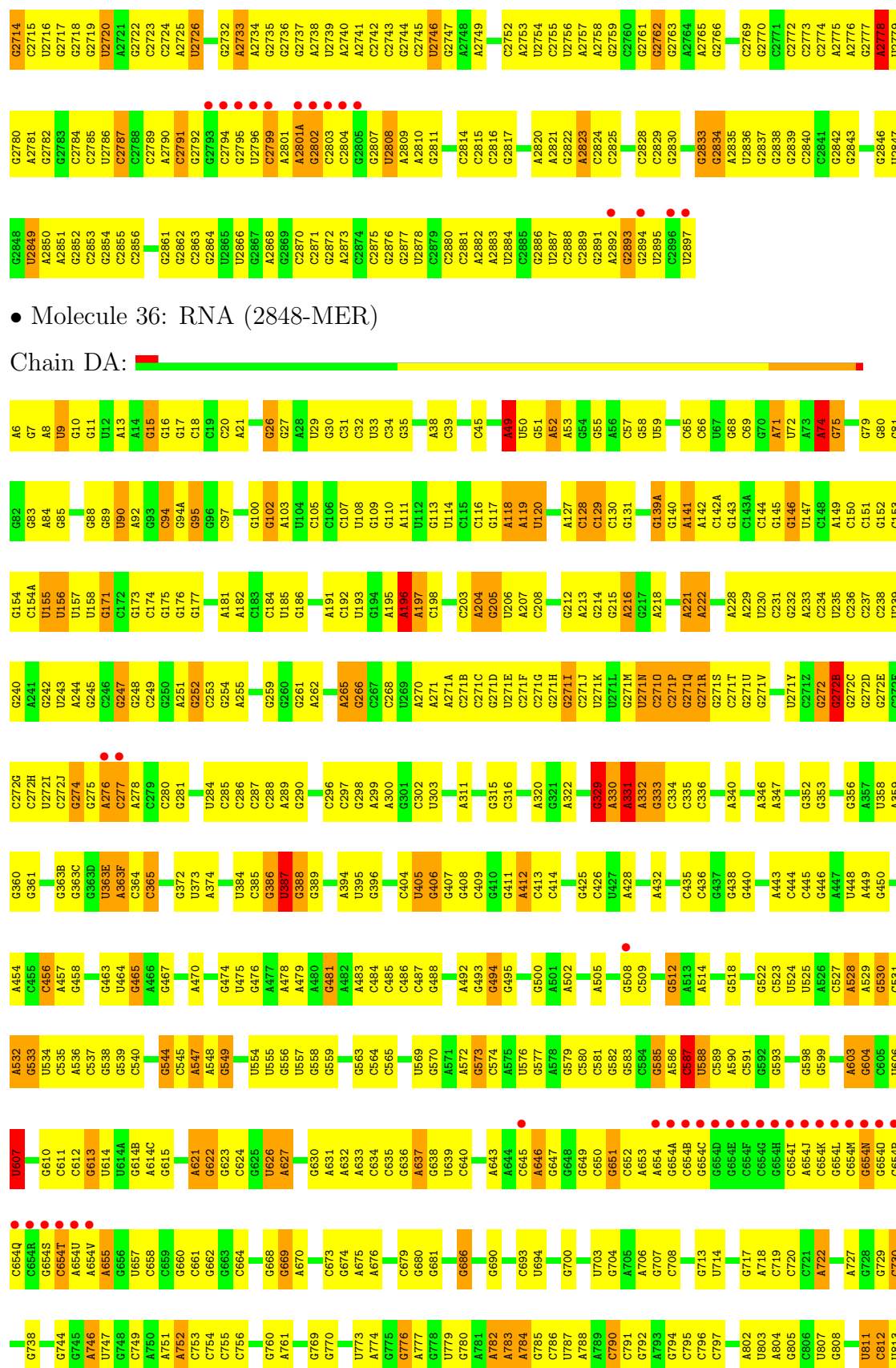
- Molecule 36: RNA (2848-MER)

Chain BA:



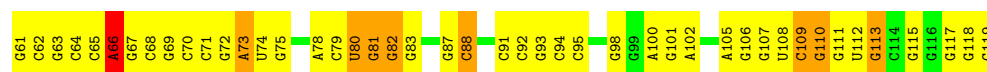






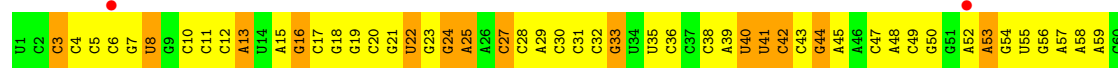
C1920	G1835	C1765	C1684	U1802	G1538	G1470	G1400	U1326	G1248	G1163	G1039	U958	C886	C814
G1921	C1836	U1766	C1685	A1603	G1539	A1471	G1401	C1527	C1251	G1164	C1040	A959	A857	C815
G1922	C1837	C1767	C1686		U1540	A1472	C1402	G1328		U1165	C1041	A960	C888	C816
G1923	C1838		G1687	C1607	G1541	G1473	C1403	U1329	G1252	C1166	G1042	C961	C889	C817
C1924	G1839	G1771	C1688	A1608	A1542	C1474	C1404	U1330	A1253	U1167	C1043	G962	A890	A819
G1925	G1840	G1772	A1689	A1609	C1543	G1475	U1405	A1331		G1168	G1044	U963	G892	A818
U1926	U1841	A1773	A1690	A1610	A1544		U1406		G1256	G1169	A1045	C964	C893	
A1927	G1842	C1774	C1691		A1545	G1478	C1407		C1257	G1170	A1046	C965	C894	G823
A1928		U1775	U1692	A1614	C1546		C1408		C1258	G1171	G1047		U895	A824
G1929	G1845		C1693	C1615	C1547	U1481	C1409		G1259	G1173	A1048	U969	A896	C825
G1930	G1846	U1778	C1694	A1616	C1548	U1482	G1410		G1260	A1174	C1049	C897	C897	U826
	A1847	U1779	G1695	C1617	C1549	G1484	C1411			U1175	A1050	C971	C898	U827
G1935	A1848	U1780	G1696	A1618	C1550	G1485	A1412		G1264	G1176	G1051	G972	A899	U828
A1936			C1697		C1551	A1486		G1344	A1265	A1177	C1052	A973	A900	A829
A1937	A1853	C1782	A1698	G1623		A1487				C1178	C1053	A901	A901	G830
A1938	G1854	A1783	G1699	G1624	A1554	G1488	C1416	G1348	A1268	C1179	A1106	C975	C902	G831
U1939	G1855	C1623		C1625	G1555	U1489	G1418	A1349	A1269	U1187	G1112	C975	C908	C844
U1940	G1856	A1784	A1700	G1626	G1556	A1490	A1419	C1350	C1270	U1188	U1113		A909	G845
	G1857	A1786	A1701		C1557	G1491	U1420	C1351	G1271	C1181	U1108	G979	C904	U832
	G1858	A1787	G1702	G1833	C1558	G1492	G1421	U1352	U1282	A1182	C1109	A980	U905	U833
U1946			G1703		C1559	C1493	G1422	U1353	U1273		G1110		G896	C834
C1947	G1862	C1790	G1705	C1638	G1560	A1494		A1354	U1274	G1186	A1111	A983	U907	G843
G1948	G1863	A1791	U1706	U1639	G1561	A1495		G1355	A1275	U1187	G1112		C908	C844
A1952	U1864			C1640	A1562	A1496	C1428	U1356		U1188	U1113	G987	A909	G845
A1953	G1865	U1794	G1710	A1641	G1563	U1497	G1429	U1357	A1278	A1189	G1114	C981	A910	C846
G1954	C1866	C1795	C1711	G1842	C1564	C1498	C1430	G1358	G1279	G1190	G1115	C992	A911	U847
U1955	A1876	U1796	C1712	G1643	G1565	C1499	U1431	G1359	G1280	G1191	C1116	G993	C912	G848
U1956	A1877	C1797	U1713	C1644	A1566	G1500	C1432	A1360	G1281	G1192	G1117		U913	A849
C1957	G1878	U1798	G1714		G1567	C1501	U1433	A1361	U1282	G1193			C914	C850
C1958	G1879	G1799	G1715	C1648	G1568	C1502	U1434	C1362	U1283	A1194	G1120	A996	C915	U851
G1959		C1800	G1718		A1569	U1503	G1435	G1363	U1285	G1195	C1121	C998	C916	C852
	C1882		G1719	A1852	A1570	C1504	G1436	G1364	A1286		G1125	U999	A917	G853
C1962	G1883	A1803	U1720	C1653	A1571	C1505	U1437	A1287	C1202	C1201			G918	G854
U1963	A1884	C1804	G1721	A1854	A1572	C1506	U1438	A1366	G1203	G1202	U1130	C1005	C923	G855
G1964	C1885		A1722	A1855	C1573	A1507	A1439	C1289	A1204	G1203	G1131	C1006	C924	C856
	G1886	U1807	U1739	A1856	C1574	A1508	G1440	G1368	U1290	U1205			C925	U858
C1967	G1887	U1808	G1740	C1657	G1575	C1509	G1441	C1291	C1291	A1210	G1135	A1009	C926	G859
G1968	G1888	A1809	A1741	C1658	U1576	A1509A	G1442	U1292	U1292	U1211	G1136	A1010	A926	U860
A1969			G1742		C1577	A1509B	G1443	G1373	U1293	U1212			G927	A861
A1970		A1810	C1743	C1662	U1578	G1510	U1444	G1374	U1294	G1212	C1140	G1011	G928	G862
A1971	G1899	A1812	G1744	C1663	A1579	C1511	A1445	C1375			U1141	G1012		A863
A1972	A1900	G1813	C1745	A1664	A1580		A1445A	C1376		G1215	U1142	G1013	G932	G864
G1973	G1891	G1814	G1746	A1665	C1581	C1516	C1446	A1379	C1297	G1216	A1142A	G1015	A933	C865
C1974	C1902	A1815	G1746	C1666	C1582	G1517	G1447	A1384	G1298		A1143	G1016	G934	A866
	G1903	G1816	G1747	G1667	A1583	U1518	G1448	A1380	C1299	C1221	G1144			
G1980		G1817	G1747A	A1668	C1584	G1519	G1449	G1381	U1300	C1221A	G1145	U1019	G939	G869
A1981	G1906	U1818	G1748	A1669	A1586	G1520	G1450	G1382	A1301	C1222	C1146	A1020	G940	A870
C1982	G1907	A1819	A1749	C1670	A1587	U1523		G1310		G1223	C1147	A1021	A941	U871
C1983	C1908	U1820	G1750		C1588	G1524	U1453			C1224	A1148	G1022	G942	
G1984		A1821	C1751	U1673	C1589		G1455	U1313		G1225	G1149	U1023	U943	G875
	G1910			G1674	U1590	A1528		C1385		A1226	C1150	G1024	G944	C876
G1987	G1911	G1826	C1764	C1675	G1591	A1528A	A1460	C1386	U1314	G1227	C1151	G1025	A945	C877
C1988	A1912	C1827	A1755	A1676	C1592	G1529	G1461	C1387	C1315		G1152	U1026	G946	A878
G1989	G1989	A1677	G1756	A1677		C1530		G1388	A1317	C1153	C1153	A1027	G947	G879
C1990	C1914	G1678	U1757	U1679	G1595	C1531	G1464	G1389		G1231	G1154	A1028		G880
U1991	U1915	U1830	U1757	U1679			G1465	U1394	G1319	G1232	A1155	A1029	G952	G881
G1992		G1831		U1880	C1598	U1534	G1466	A1395	C1320	U1240	A1156		A953	G882
C1993	U1917	G1681	A1762	G1681	C1599	A1535	G1468	U1396	A1321	A1241			G954	G883
U1994	U1918	U1833	G1763	G1682	C1600	C1536	C1467		A1322	A1242	C1161		C955	C884
C1996		A1919	G1764	C1683	G1601	G1537	A1469	C1399			G1162			C885





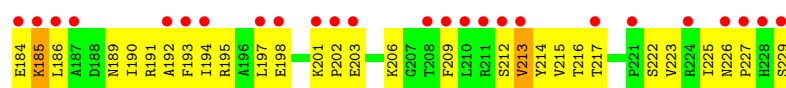
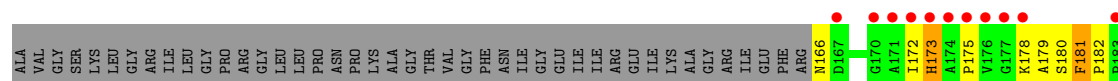
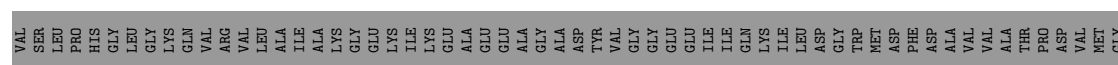
• Molecule 37: RNA (119-MER)

Chain DB:



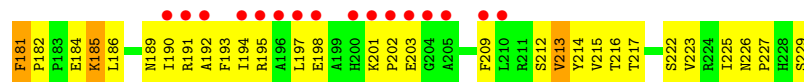
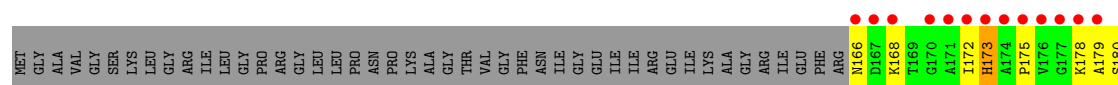
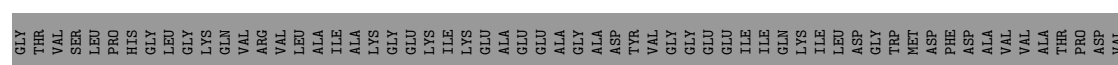
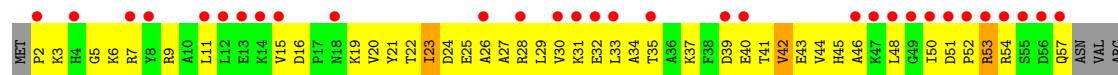
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

Chain BC:



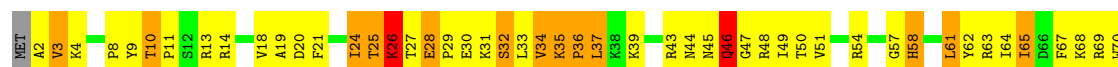
• Molecule 38: 50S RIBOSOMAL PROTEIN L1

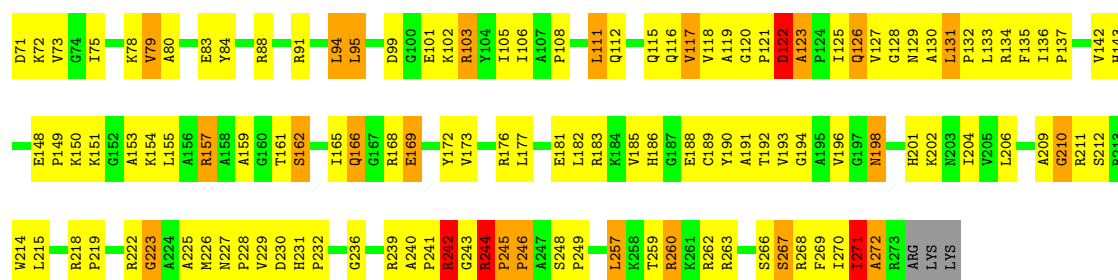
Chain DC:



• Molecule 39: 50S RIBOSOMAL PROTEIN L2

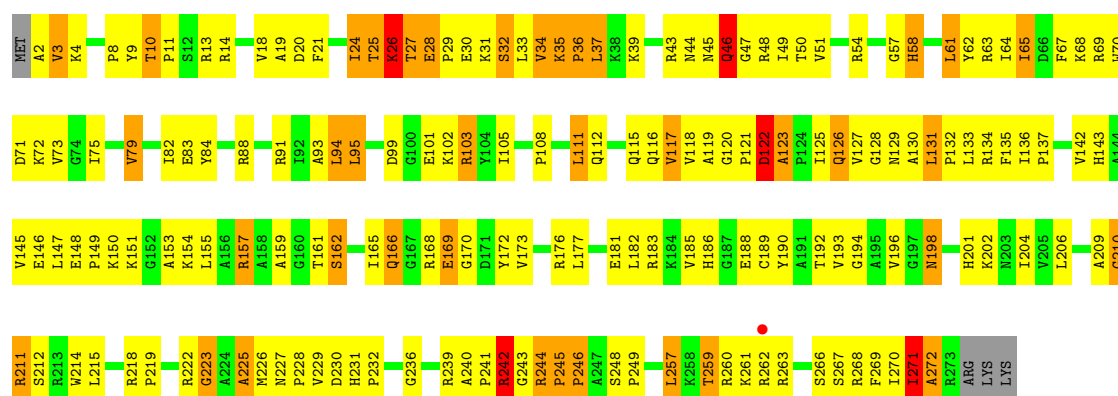
Chain BD:





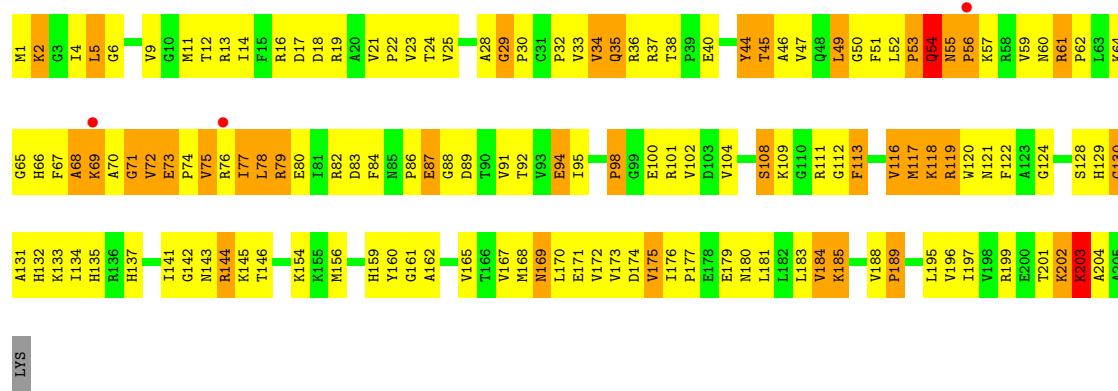
• Molecule 39: 50S RIBOSOMAL PROTEIN L2

Chain DD:



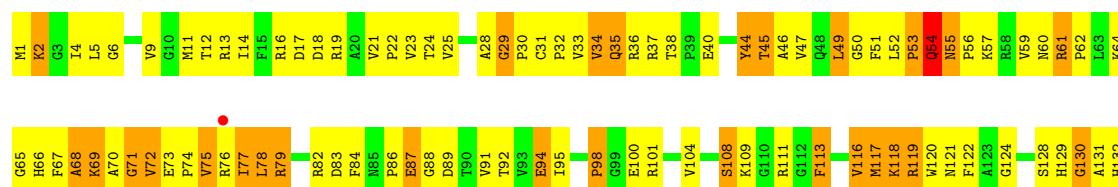
• Molecule 40: 50S RIBOSOMAL PROTEIN L3

Chain BE:



• Molecule 40: 50S RIBOSOMAL PROTEIN L3

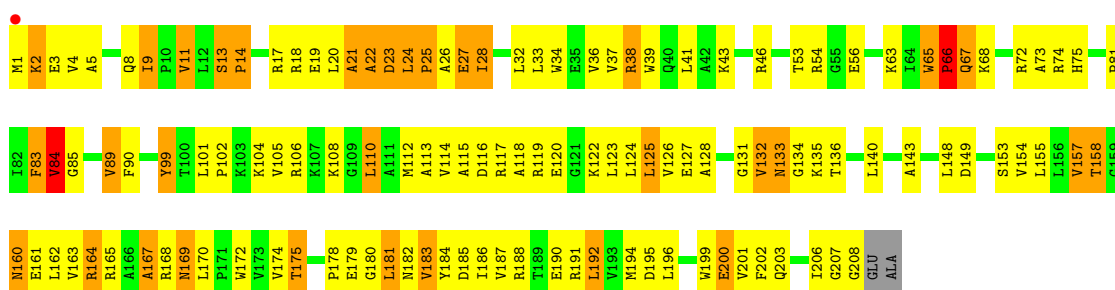
Chain DE:





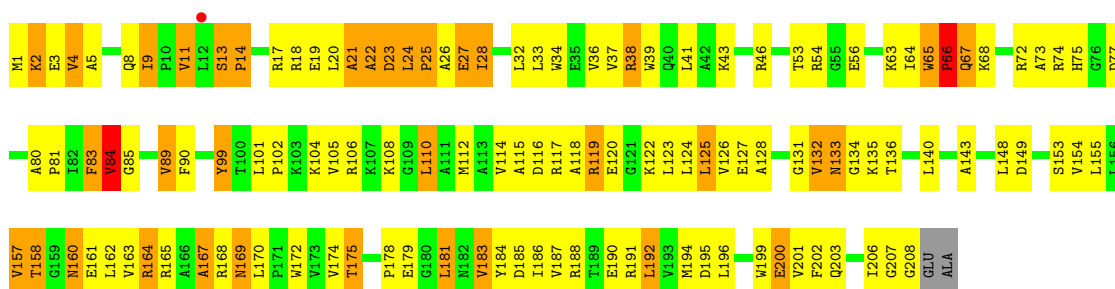
• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain BF:



• Molecule 41: 50S RIBOSOMAL PROTEIN L4

Chain DF:



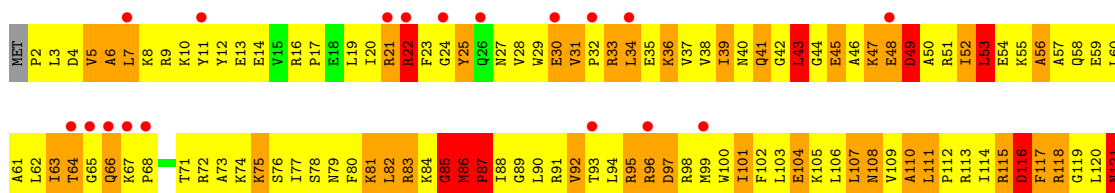
• Molecule 42: 50S RIBOSOMAL PROTEIN L5

Chain BG:



• Molecule 42: 50S RIBOSOMAL PROTEIN L5

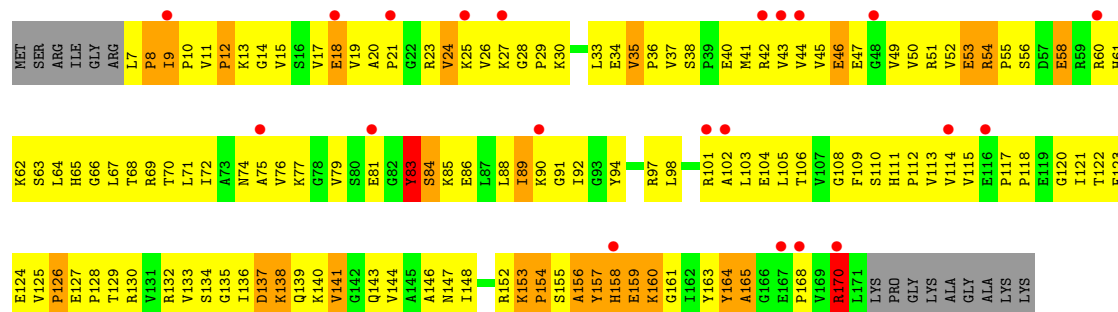
Chain DG:





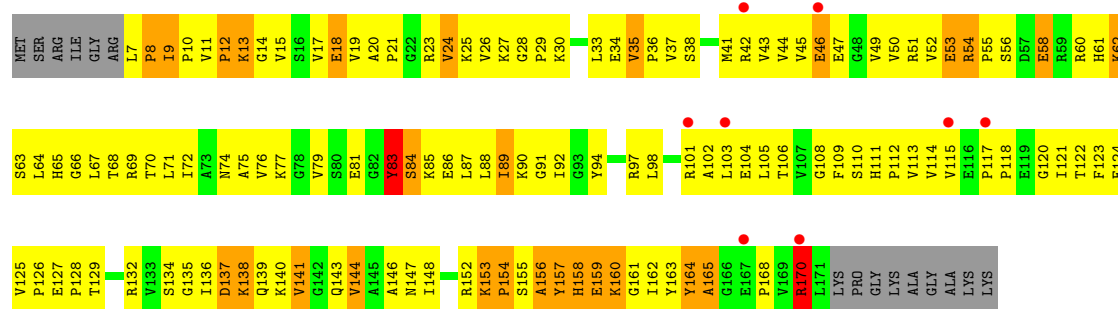
• Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain BH:



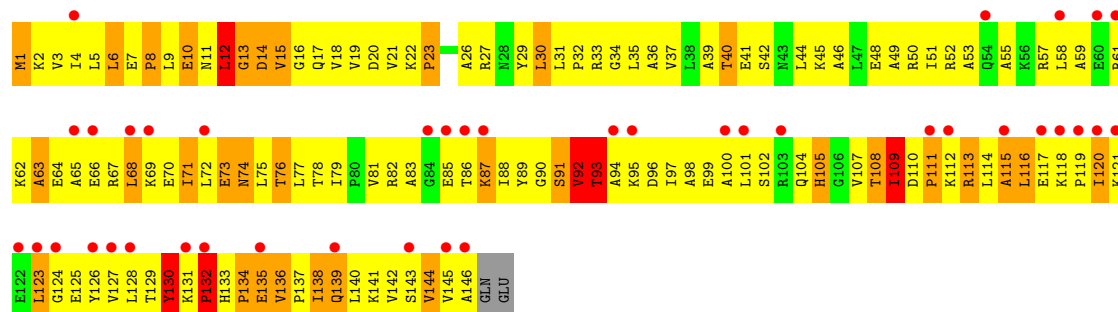
• Molecule 43: 50S RIBOSOMAL PROTEIN L6

Chain DH:



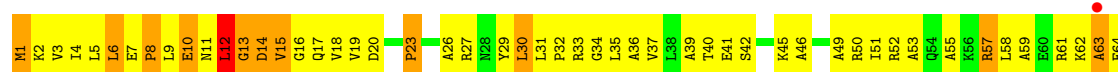
• Molecule 44: 50S RIBOSOMAL PROTEIN L9

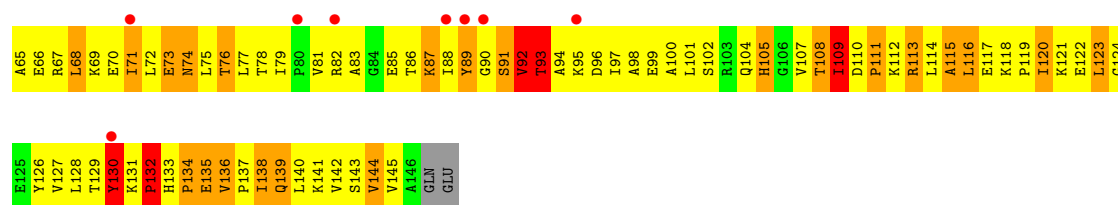
Chain BI:



• Molecule 44: 50S RIBOSOMAL PROTEIN L9

Chain DI:





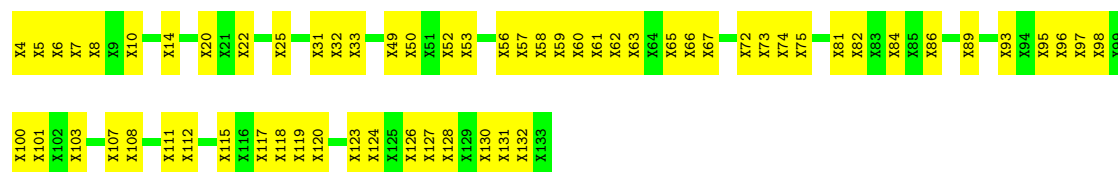
• Molecule 45: 50S RIBOSOMAL PROTEIN L10

Chain BJ:



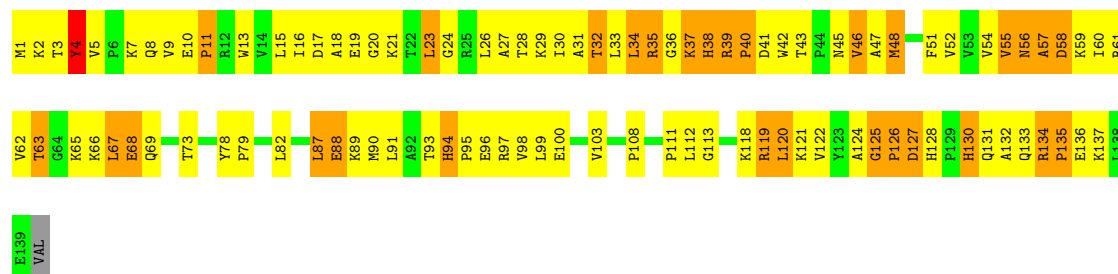
• Molecule 45: 50S RIBOSOMAL PROTEIN L10

Chain DJ:



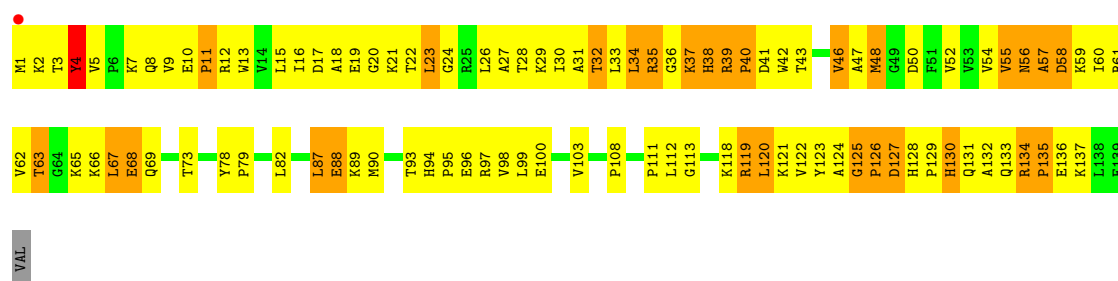
• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain BN:



• Molecule 46: 50S RIBOSOMAL PROTEIN L13

Chain DN:



• Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain BO:



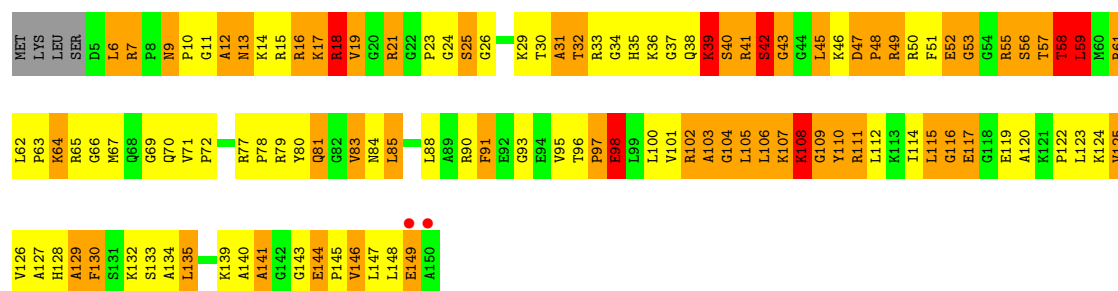
- Molecule 47: 50S RIBOSOMAL PROTEIN L14

Chain DO:



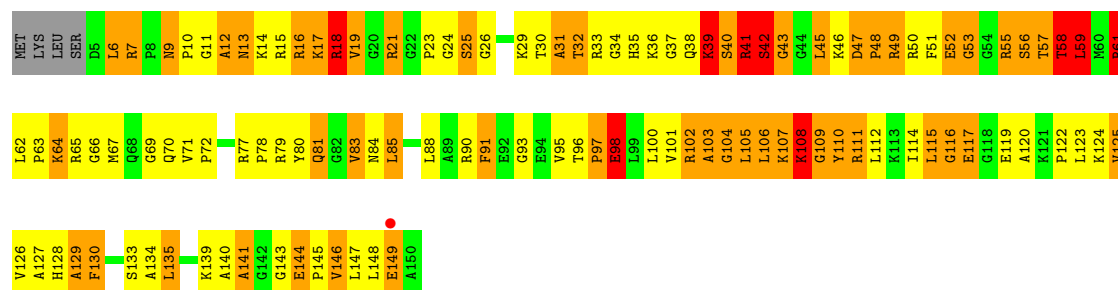
- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain BP:



- Molecule 48: 50S RIBOSOMAL PROTEIN L15

Chain DP:



- Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain BQ:

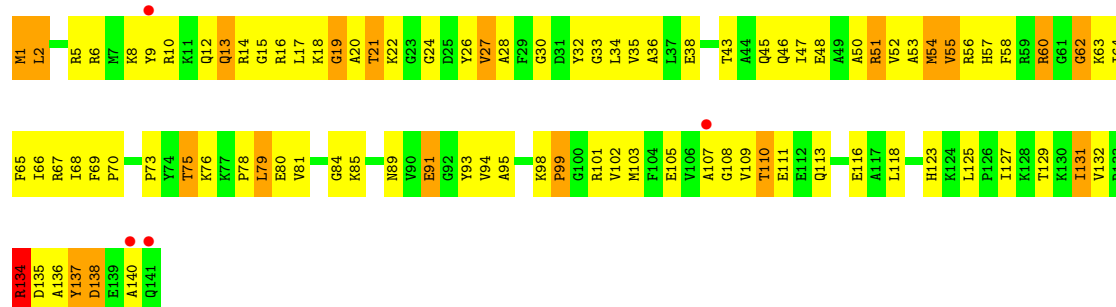




Q141

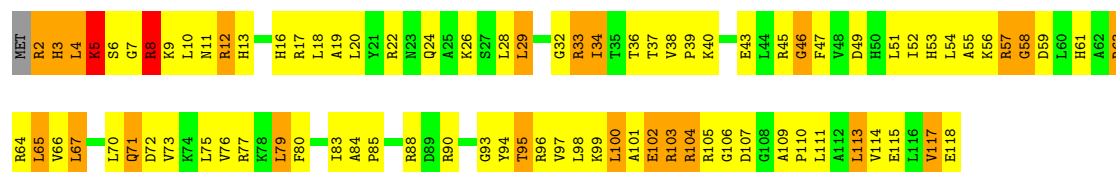
• Molecule 49: 50S RIBOSOMAL PROTEIN L16

Chain DQ: 



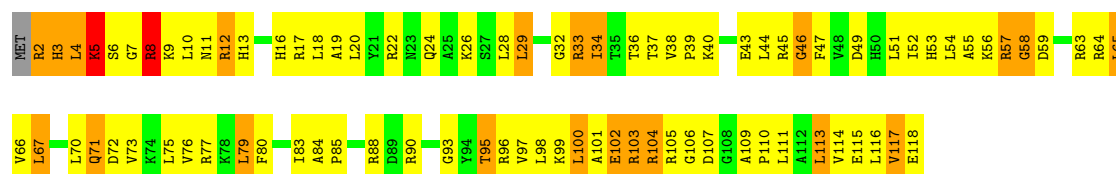
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain BR: 



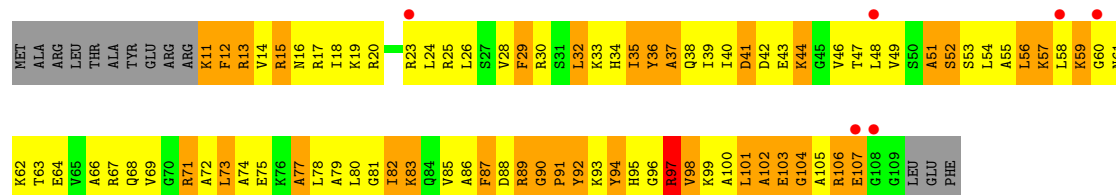
• Molecule 50: 50S RIBOSOMAL PROTEIN L17

Chain DR: 



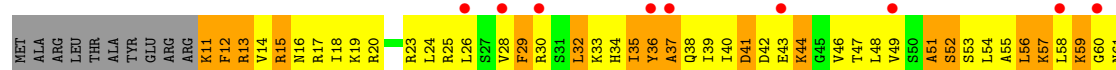
• Molecule 51: 50S RIBOSOMAL PROTEIN L18

Chain BS: 



• Molecule 51: 50S RIBOSOMAL PROTEIN L18

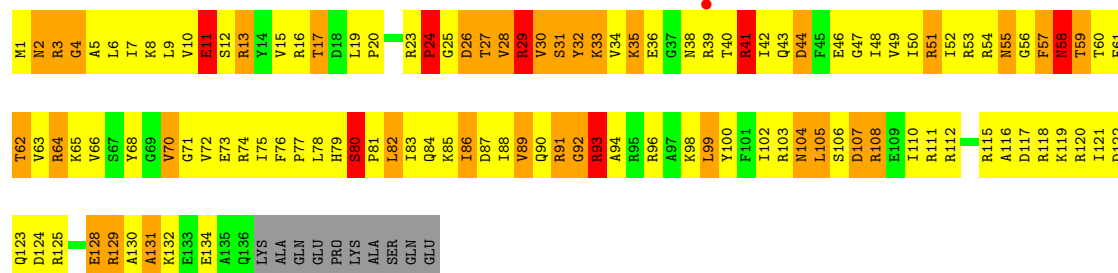
Chain DS: 





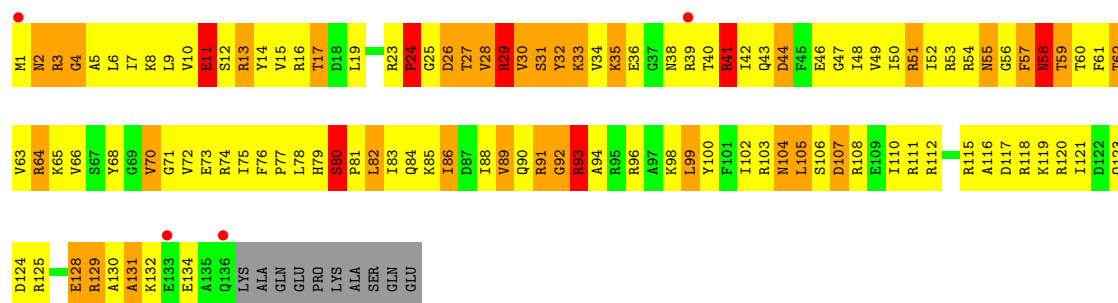
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain BT:



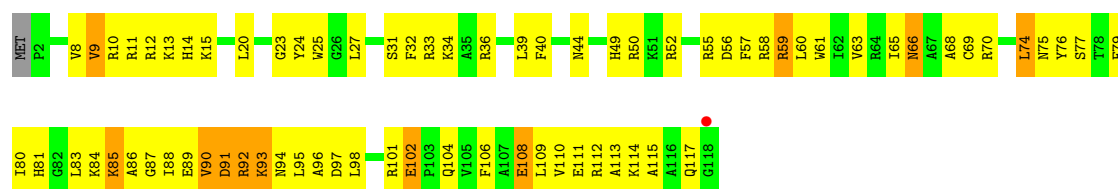
• Molecule 52: 50S RIBOSOMAL PROTEIN L19

Chain DT:



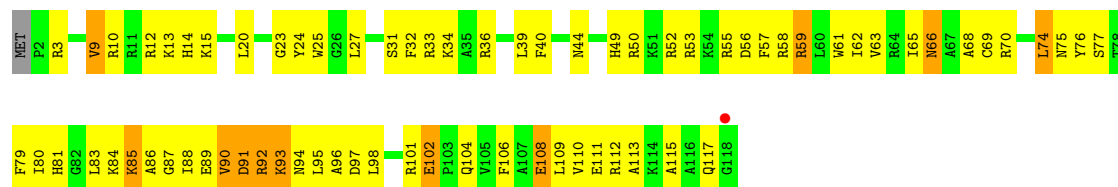
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain BU:



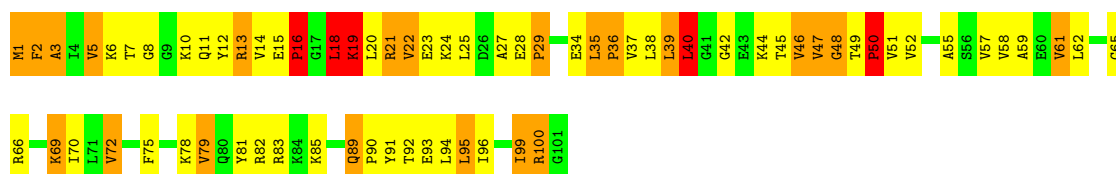
• Molecule 53: 50S RIBOSOMAL PROTEIN L20

Chain DU:



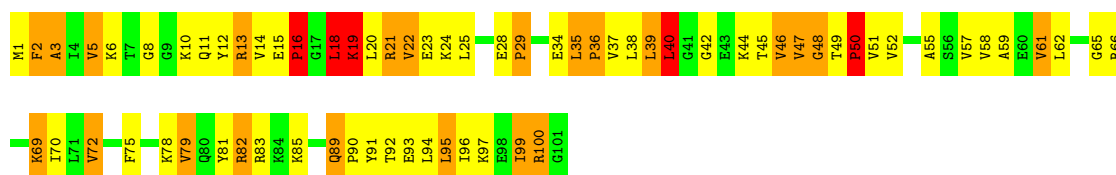
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain BV:



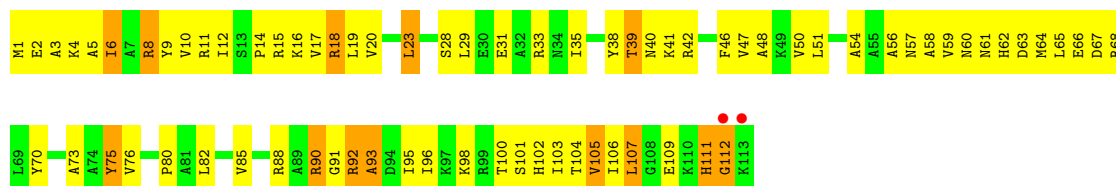
• Molecule 54: 50S RIBOSOMAL PROTEIN L21

Chain DV:



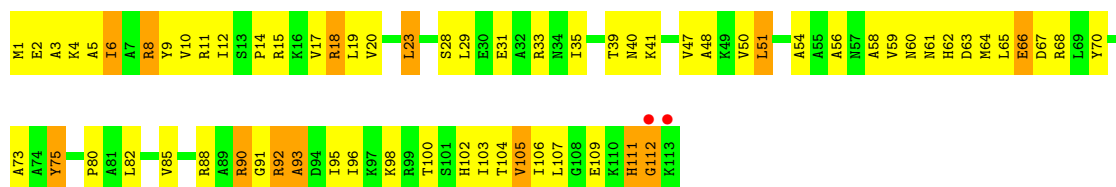
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain BW:



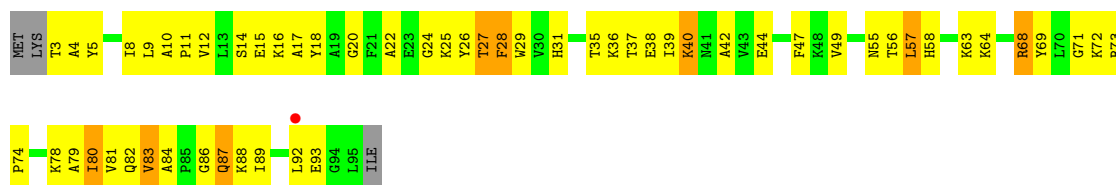
• Molecule 55: 50S RIBOSOMAL PROTEIN L22

Chain DW:



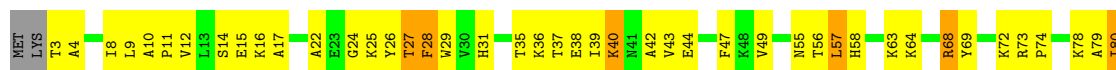
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

Chain BX:



• Molecule 56: 50S RIBOSOMAL PROTEIN L23

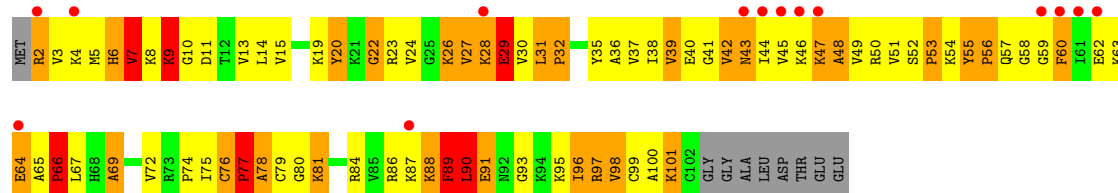
Chain DX:





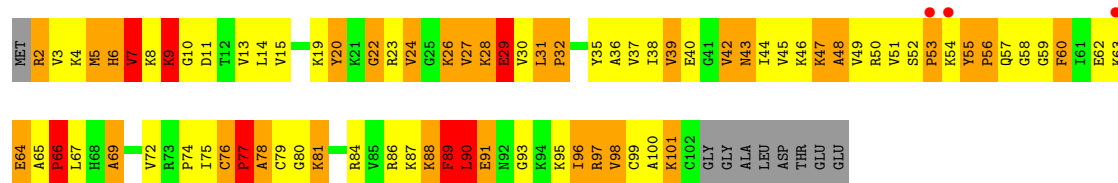
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain BY:



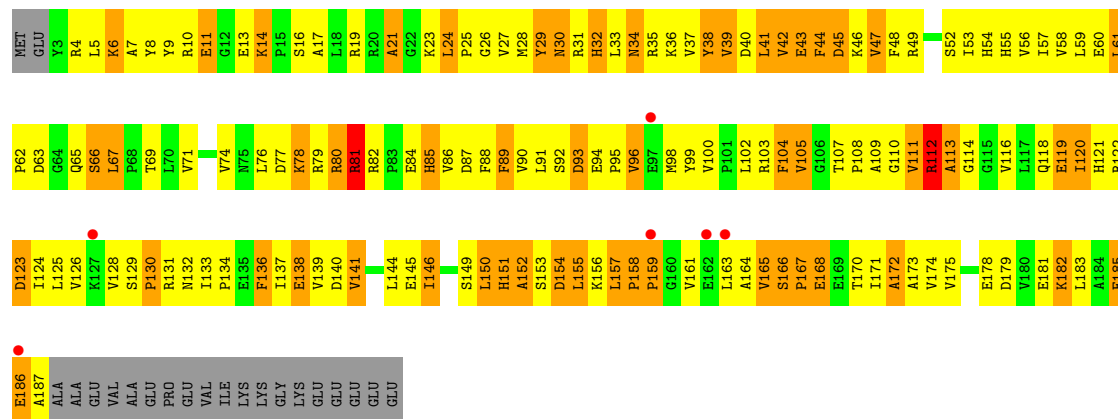
• Molecule 57: 50S RIBOSOMAL PROTEIN L24

Chain DY:



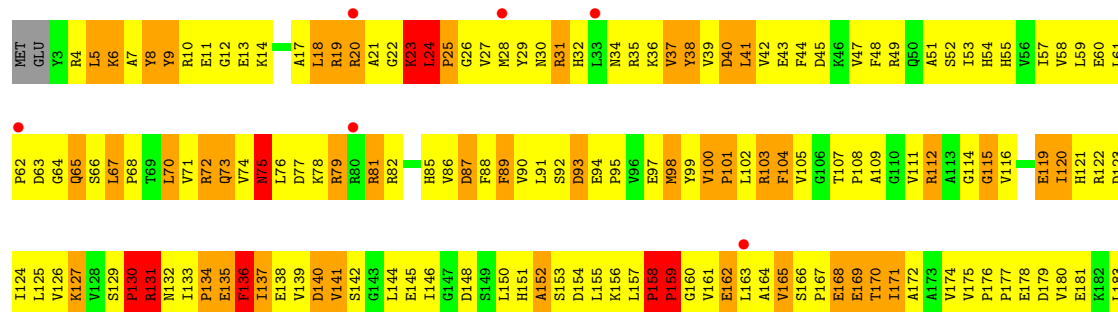
• Molecule 58: 50S RIBOSOMAL PROTEIN L25

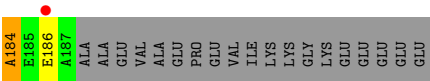
Chain BZ:



• Molecule 58: 50S RIBOSOMAL PROTEIN L25

Chain DZ:





● Molecule 59: BACTERIAL TOXIN YOEB

Chain CX: A horizontal bar representing the sequence of Chain CX. The bar is mostly orange, with a red segment at the beginning.



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.59Å 455.43Å 616.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.79 – 3.35 49.79 – 3.35	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.79-3.35) 99.7 (49.79-3.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 3.33Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.261 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	96.2	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 842969 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	298206	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.56% 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: 5MU, ZN, MG, OMU, A2M

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	0.43	1/36190 (0.0%)	0.69	13/56486 (0.0%)
1	CA	0.41	1/36190 (0.0%)	0.70	15/56486 (0.0%)
2	AB	0.33	0/1936	0.62	0/2611
2	CB	0.33	0/1936	0.61	0/2611
3	AC	0.33	0/1637	0.59	0/2207
3	CC	0.33	0/1637	0.59	0/2207
4	AD	0.38	0/1733	0.67	1/2318 (0.0%)
4	CD	0.35	0/1733	0.64	0/2318
5	AE	0.38	0/1163	0.67	0/1566
5	CE	0.37	0/1163	0.65	0/1566
6	AF	0.34	0/856	0.64	0/1154
6	CF	0.35	0/856	0.64	0/1154
7	AG	0.32	0/1276	0.55	0/1709
7	CG	0.30	0/1276	0.55	0/1709
8	AH	0.35	0/1136	0.69	0/1527
8	CH	0.33	0/1136	0.68	0/1527
9	AI	0.33	0/1027	0.60	0/1373
9	CI	0.32	0/1027	0.61	0/1373
10	AJ	0.35	0/808	0.62	0/1087
10	CJ	0.33	0/808	0.61	0/1087
11	AK	0.33	0/900	0.61	0/1213
11	CK	0.35	0/900	0.61	0/1213
12	AL	0.42	0/987	0.75	0/1322
12	CL	0.43	0/987	0.74	1/1322 (0.1%)
13	AM	0.33	0/943	0.84	3/1256 (0.2%)
13	CM	0.33	0/943	0.85	3/1256 (0.2%)
14	AN	0.36	0/501	0.94	3/664 (0.5%)
14	CN	0.37	0/501	0.92	3/664 (0.5%)
15	AO	0.36	0/745	0.61	0/992
15	CO	0.38	0/745	0.61	0/992
16	AP	0.39	0/717	0.63	0/965
16	CP	0.36	0/717	0.61	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.39	0/837	0.66	0/1119
17	CQ	0.37	0/837	0.65	0/1119
18	AR	0.37	0/579	1.06	3/768 (0.4%)
18	CR	0.36	0/579	0.97	3/768 (0.4%)
19	AS	0.43	0/643	0.92	3/867 (0.3%)
19	CS	0.51	0/643	0.98	3/867 (0.3%)
20	AT	0.35	0/765	0.61	0/1007
20	CT	0.32	0/765	0.60	0/1007
21	AU	0.46	0/213	0.61	0/279
21	CU	0.48	0/213	0.61	0/279
22	AV	0.49	0/1810	0.70	0/2821
23	AW	0.39	0/1832	0.69	0/2855
23	CV	0.44	0/1832	0.72	1/2855 (0.0%)
23	CW	0.37	0/1832	0.69	0/2855
24	AX	0.41	0/194	0.65	0/301
25	AY	0.41	0/742	0.63	1/1002 (0.1%)
25	AZ	0.40	0/743	0.63	0/1002
25	CY	0.48	0/742	0.69	2/1002 (0.2%)
25	CZ	0.47	0/743	0.64	0/1002
26	B0	0.39	0/671	0.68	0/892
26	D0	0.39	0/671	0.69	0/892
27	B1	0.43	0/739	0.81	1/983 (0.1%)
27	D1	0.47	0/739	0.78	0/983
28	B2	0.38	0/600	0.68	0/793
28	D2	0.47	0/600	0.76	1/793 (0.1%)
29	B3	0.38	0/473	0.65	0/636
29	D3	0.40	0/473	0.66	0/636
30	B4	0.39	0/461	0.70	0/623
30	D4	0.40	0/461	0.69	0/623
31	B5	0.51	0/442	0.86	0/598
31	D5	0.54	0/442	0.85	0/598
32	B6	0.46	0/440	0.83	0/586
32	D6	0.51	0/440	0.85	0/586
33	B7	0.48	0/418	0.68	0/552
33	D7	0.54	0/418	0.69	0/552
34	B8	0.57	0/516	0.97	4/681 (0.6%)
34	D8	0.56	0/516	0.97	5/681 (0.7%)
35	B9	0.36	0/310	0.61	0/407
35	D9	0.36	0/310	0.62	0/407
36	BA	0.53	5/68704 (0.0%)	0.74	50/107260 (0.0%)
36	DA	0.56	3/68704 (0.0%)	0.75	57/107260 (0.1%)
37	BB	0.39	0/2853	0.69	0/4451
37	DB	0.41	0/2853	0.70	0/4451

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	BC	0.31	0/956	0.55	0/1288
38	DC	0.31	0/956	0.55	0/1288
39	BD	0.47	0/2155	0.82	2/2907 (0.1%)
39	DD	0.51	0/2155	0.83	3/2907 (0.1%)
40	BE	0.46	0/1597	0.78	1/2155 (0.0%)
40	DE	0.47	0/1597	0.78	1/2155 (0.0%)
41	BF	0.46	0/1659	0.76	1/2246 (0.0%)
41	DF	0.48	0/1659	0.76	1/2246 (0.0%)
42	BG	0.36	0/1498	0.66	0/2013
42	DG	0.42	0/1498	0.79	1/2013 (0.0%)
43	BH	0.38	0/1285	0.71	0/1741
43	DH	0.40	0/1285	0.72	0/1741
44	BI	0.37	0/1147	0.87	3/1553 (0.2%)
44	DI	0.39	0/1147	0.88	3/1553 (0.2%)
46	BN	0.42	0/1132	0.74	1/1527 (0.1%)
46	DN	0.43	0/1132	0.75	1/1527 (0.1%)
47	BO	0.45	0/943	0.69	0/1269
47	DO	0.41	0/943	0.67	0/1269
48	BP	0.53	0/1131	1.06	6/1504 (0.4%)
48	DP	0.55	0/1131	1.08	7/1504 (0.5%)
49	BQ	0.44	0/1134	0.68	0/1517
49	DQ	0.42	0/1134	0.68	0/1517
50	BR	0.42	0/974	0.77	2/1302 (0.2%)
50	DR	0.44	0/974	0.79	2/1302 (0.2%)
51	BS	0.40	0/779	0.69	0/1038
51	DS	0.41	0/779	0.69	0/1038
52	BT	0.48	0/1138	0.83	3/1521 (0.2%)
52	DT	0.45	0/1138	0.81	3/1521 (0.2%)
53	BU	0.44	0/975	0.75	0/1297
53	DU	0.47	0/975	0.75	0/1297
54	BV	0.42	0/790	0.73	0/1057
54	DV	0.46	0/790	0.75	0/1057
55	BW	0.44	0/907	0.72	0/1216
55	DW	0.46	0/907	0.74	0/1216
56	BX	0.44	0/740	0.69	0/995
56	DX	0.47	0/740	0.71	0/995
57	BY	0.51	0/789	0.79	1/1053 (0.1%)
57	DY	0.55	0/789	0.80	1/1053 (0.1%)
58	BZ	0.38	0/1500	0.71	0/2037
58	DZ	0.40	0/1500	0.74	1/2037 (0.0%)
59	CX	0.44	0/169	0.70	0/262
All	All	0.48	10/321535 (0.0%)	0.73	220/480333 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	1	15
1	CA	0	13
22	AV	0	1
23	CV	0	2
24	AX	0	1
36	BA	7	51
36	DA	7	58
37	BB	0	2
37	DB	0	2
59	CX	0	1
All	All	15	146

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	BA	975(A)	G	O3'-P	-12.04	1.46	1.61
1	AA	413	G	O3'-P	-8.20	1.51	1.61
1	CA	413	G	O3'-P	-7.59	1.52	1.61
36	BA	783	A	C5-C6	-5.78	1.35	1.41
36	BA	2506	U	N1-C2	5.66	1.43	1.38

The worst 5 of 220 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	AR	64	ARG	NE-CZ-NH2	-15.72	112.44	120.30
19	CS	81	ARG	NE-CZ-NH1	15.12	127.86	120.30
18	AR	64	ARG	NE-CZ-NH1	14.85	127.73	120.30
13	CM	29	ARG	NE-CZ-NH2	-13.53	113.53	120.30
13	CM	29	ARG	NE-CZ-NH1	13.37	126.99	120.30

5 of 15 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	AA	115	G	C3'
36	BA	49	A	C3'
36	BA	331	A	C3'
36	BA	752	A	C3'
36	BA	1799	G	C3'

5 of 146 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	13	U	Sidechain
1	AA	254	G	Sidechain
1	AA	318	G	Sidechain
1	AA	436	C	Sidechain
1	AA	575	G	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16317	1250	0
1	CA	32329	0	16317	1322	1
2	AB	1901	0	1951	294	0
2	CB	1901	0	1951	300	0
3	AC	1613	0	1677	234	0
3	CC	1613	0	1677	234	0
4	AD	1703	0	1766	193	0
4	CD	1703	0	1764	192	0
5	AE	1147	0	1207	140	0
5	CE	1147	0	1207	133	0
6	AF	843	0	857	109	0
6	CF	843	0	857	111	0
7	AG	1257	0	1296	134	0
7	CG	1257	0	1296	136	0
8	AH	1116	0	1177	129	0
8	CH	1116	0	1177	125	0
9	AI	1010	0	1035	149	0
9	CI	1010	0	1035	152	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	162	0
11	AK	885	0	904	107	0
11	CK	885	0	904	106	0
12	AL	971	0	1057	109	0
12	CL	971	0	1057	112	0
13	AM	938	0	991	143	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	CM	938	0	991	152	0
14	AN	492	0	530	70	0
14	CN	492	0	531	70	0
15	AO	734	0	771	75	0
15	CO	734	0	771	70	0
16	AP	701	0	720	69	0
16	CP	701	0	720	78	0
17	AQ	824	0	891	75	0
17	CQ	824	0	891	73	0
18	AR	574	0	644	84	0
18	CR	574	0	644	82	0
19	AS	630	0	652	109	0
19	CS	630	0	652	106	0
20	AT	763	0	861	85	0
20	CT	763	0	861	95	0
21	AU	209	0	221	23	0
21	CU	209	0	221	25	0
22	AV	1641	0	839	55	0
23	AW	1640	0	837	57	0
23	CV	1640	0	837	55	0
23	CW	1640	0	837	66	0
24	AX	239	0	127	94	0
25	AY	722	0	713	147	0
25	AZ	723	0	710	110	0
25	CY	722	0	713	149	0
25	CZ	723	0	713	103	0
26	B0	662	0	688	79	0
26	D0	662	0	688	75	0
27	B1	732	0	808	87	0
27	D1	732	0	808	91	0
28	B2	598	0	653	88	0
28	D2	598	0	653	67	0
29	B3	468	0	523	27	0
29	D3	468	0	523	27	0
30	B4	451	0	449	126	0
30	D4	451	0	449	109	0
31	B5	428	0	445	65	0
31	D5	428	0	445	65	0
32	B6	433	0	461	109	0
32	D6	433	0	461	110	0
33	B7	410	0	454	29	0
33	D7	410	0	454	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	B8	508	0	576	119	0
34	D8	508	0	576	120	0
35	B9	307	0	338	34	0
35	D9	307	0	338	31	0
36	BA	61341	0	30927	1970	0
36	DA	61341	0	30928	1950	0
37	BB	2551	0	1295	125	0
37	DB	2551	0	1295	119	0
38	BC	937	0	957	96	0
38	DC	937	0	957	101	0
39	BD	2105	0	2182	253	0
39	DD	2105	0	2182	266	0
40	BE	1564	0	1629	215	0
40	DE	1564	0	1629	213	0
41	BF	1624	0	1677	185	0
41	DF	1624	0	1677	168	0
42	BG	1474	0	1534	329	0
42	DG	1474	0	1534	389	0
43	BH	1260	0	1326	180	0
43	DH	1260	0	1326	175	0
44	BI	1132	0	1218	282	1
44	DI	1132	0	1218	279	0
45	BJ	651	0	177	28	0
45	DJ	651	0	174	64	0
46	BN	1105	0	1180	154	0
46	DN	1105	0	1180	160	0
47	BO	933	0	996	86	0
47	DO	933	0	996	97	0
48	BP	1114	0	1187	297	0
48	DP	1114	0	1187	294	0
49	BQ	1113	0	1171	105	0
49	DQ	1113	0	1171	112	0
50	BR	960	0	1021	139	0
50	DR	960	0	1021	130	0
51	BS	771	0	832	166	0
51	DS	771	0	832	173	0
52	BT	1124	0	1181	226	0
52	DT	1124	0	1181	211	0
53	BU	958	0	1014	125	0
53	DU	958	0	1015	123	0
54	BV	779	0	852	135	0
54	DV	779	0	852	139	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	BW	896	0	953	90	0
55	DW	896	0	953	82	0
56	BX	726	0	778	74	0
56	DX	726	0	778	71	0
57	BY	776	0	870	182	0
57	DY	776	0	870	176	0
58	BZ	1468	0	1492	253	0
58	DZ	1468	0	1492	348	0
59	CX	217	0	116	77	0
60	AA	103	0	0	0	0
60	AL	1	0	0	0	0
60	AV	1	0	0	0	0
60	AX	1	0	0	0	0
60	B0	1	0	0	0	0
60	B1	2	0	0	0	0
60	B5	2	0	0	0	0
60	BA	236	0	0	0	0
60	BB	2	0	0	0	0
60	BF	1	0	0	0	0
60	BP	1	0	0	0	0
60	BX	1	0	0	0	0
60	CA	103	0	0	0	0
60	CG	1	0	0	0	0
60	CL	1	0	0	0	0
60	CV	2	0	0	0	0
60	D1	1	0	0	0	0
60	D5	1	0	0	0	0
60	DA	242	0	0	0	0
60	DB	1	0	0	0	0
60	DF	1	0	0	0	0
60	DR	1	0	0	0	0
60	DX	1	0	0	0	0
61	AD	1	0	0	2	0
61	AN	1	0	0	0	0
61	CD	1	0	0	1	0
61	CN	1	0	0	1	0
All	All	298206	0	202858	19519	1

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 39.

The worst 5 of 19519 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:AX:19:OMU:CM2	25:AY:51:ASN:HD21	1.10	1.58
4:CD:26:CYS:SG	61:CD:301:ZN:ZN	1.01	1.49
1:AA:1493:A:C8	24:AX:20:A2M:HM'3	1.49	1.48
1:AA:1493:A:C8	24:AX:20:A2M:CM'	1.98	1.46
1:AA:1493:A:N7	24:AX:20:A2M:CM'	1.89	1.34

All (1) 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)
44:BI:121:LYS:NZ	1:CA:358:U:OP1[4_555]	2.13	0.07

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	233/256 (91%)	128 (55%)	77 (33%)	28 (12%)	1	6
2	CB	233/256 (91%)	129 (55%)	75 (32%)	29 (12%)	1	5
3	AC	205/239 (86%)	123 (60%)	54 (26%)	28 (14%)	0	4
3	CC	205/239 (86%)	125 (61%)	53 (26%)	27 (13%)	0	4
4	AD	206/209 (99%)	138 (67%)	52 (25%)	16 (8%)	1	16
4	CD	206/209 (99%)	139 (68%)	51 (25%)	16 (8%)	1	16
5	AE	149/162 (92%)	106 (71%)	31 (21%)	12 (8%)	1	15
5	CE	149/162 (92%)	107 (72%)	29 (20%)	13 (9%)	1	13
6	AF	99/101 (98%)	74 (75%)	18 (18%)	7 (7%)	2	19
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	2	19
7	AG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	1	7
7	CG	153/156 (98%)	106 (69%)	30 (20%)	17 (11%)	1	7
8	AH	136/138 (99%)	99 (73%)	25 (18%)	12 (9%)	1	13
8	CH	136/138 (99%)	98 (72%)	25 (18%)	13 (10%)	1	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	AI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	12
9	CI	121/128 (94%)	82 (68%)	28 (23%)	11 (9%)	1	12
10	AJ	97/105 (92%)	69 (71%)	21 (22%)	7 (7%)	2	19
10	CJ	97/105 (92%)	72 (74%)	18 (19%)	7 (7%)	2	19
11	AK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	1	11
11	CK	117/129 (91%)	84 (72%)	22 (19%)	11 (9%)	1	11
12	AL	123/132 (93%)	87 (71%)	26 (21%)	10 (8%)	1	15
12	CL	123/132 (93%)	88 (72%)	25 (20%)	10 (8%)	1	15
13	AM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	3
13	CM	107/126 (85%)	71 (66%)	20 (19%)	16 (15%)	0	3
14	AN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	2
14	CN	58/61 (95%)	37 (64%)	11 (19%)	10 (17%)	0	2
15	AO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	2	20
15	CO	86/89 (97%)	60 (70%)	20 (23%)	6 (7%)	2	20
16	AP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	2	18
16	CP	82/88 (93%)	59 (72%)	17 (21%)	6 (7%)	2	18
17	AQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	3	29
17	CQ	98/105 (93%)	74 (76%)	19 (19%)	5 (5%)	3	29
18	AR	68/88 (77%)	41 (60%)	17 (25%)	10 (15%)	0	3
18	CR	68/88 (77%)	42 (62%)	16 (24%)	10 (15%)	0	3
19	AS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	2
19	CS	77/93 (83%)	45 (58%)	19 (25%)	13 (17%)	0	2
20	AT	97/106 (92%)	59 (61%)	26 (27%)	12 (12%)	1	5
20	CT	97/106 (92%)	58 (60%)	26 (27%)	13 (13%)	0	4
21	AU	23/27 (85%)	14 (61%)	6 (26%)	3 (13%)	0	4
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	2
25	AY	82/84 (98%)	53 (65%)	13 (16%)	16 (20%)	0	1
25	AZ	82/84 (98%)	54 (66%)	20 (24%)	8 (10%)	1	10
25	CY	82/84 (98%)	50 (61%)	16 (20%)	16 (20%)	0	1
25	CZ	82/84 (98%)	59 (72%)	15 (18%)	8 (10%)	1	10
26	B0	82/85 (96%)	67 (82%)	11 (13%)	4 (5%)	3	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	D0	82/85 (96%)	67 (82%)	10 (12%)	5 (6%)	2	24
27	B1	92/98 (94%)	67 (73%)	12 (13%)	13 (14%)	0	3
27	D1	92/98 (94%)	66 (72%)	14 (15%)	12 (13%)	0	4
28	B2	69/72 (96%)	44 (64%)	14 (20%)	11 (16%)	0	2
28	D2	69/72 (96%)	45 (65%)	16 (23%)	8 (12%)	1	6
29	B3	58/60 (97%)	48 (83%)	8 (14%)	2 (3%)	6	43
29	D3	58/60 (97%)	47 (81%)	9 (16%)	2 (3%)	6	43
30	B4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
30	D4	56/71 (79%)	17 (30%)	24 (43%)	15 (27%)	0	0
31	B5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	4
31	D5	54/60 (90%)	39 (72%)	8 (15%)	7 (13%)	0	4
32	B6	48/54 (89%)	25 (52%)	7 (15%)	16 (33%)	0	0
32	D6	48/54 (89%)	26 (54%)	7 (15%)	15 (31%)	0	0
33	B7	46/49 (94%)	43 (94%)	2 (4%)	1 (2%)	10	56
33	D7	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
34	B8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	2
34	D8	62/65 (95%)	36 (58%)	16 (26%)	10 (16%)	0	2
35	B9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	14
35	D9	35/37 (95%)	26 (74%)	6 (17%)	3 (9%)	1	14
38	BC	116/229 (51%)	84 (72%)	26 (22%)	6 (5%)	3	28
38	DC	116/229 (51%)	85 (73%)	25 (22%)	6 (5%)	3	28
39	BD	270/276 (98%)	205 (76%)	37 (14%)	28 (10%)	1	8
39	DD	270/276 (98%)	202 (75%)	41 (15%)	27 (10%)	1	9
40	BE	203/206 (98%)	146 (72%)	34 (17%)	23 (11%)	1	7
40	DE	203/206 (98%)	145 (71%)	35 (17%)	23 (11%)	1	7
41	BF	206/210 (98%)	155 (75%)	29 (14%)	22 (11%)	1	8
41	DF	206/210 (98%)	157 (76%)	26 (13%)	23 (11%)	1	7
42	BG	177/182 (97%)	105 (59%)	33 (19%)	39 (22%)	0	1
42	DG	177/182 (97%)	80 (45%)	47 (27%)	50 (28%)	0	0
43	BH	163/180 (91%)	98 (60%)	39 (24%)	26 (16%)	0	2
43	DH	163/180 (91%)	98 (60%)	38 (23%)	27 (17%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	BI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	1
44	DI	144/148 (97%)	76 (53%)	37 (26%)	31 (22%)	0	1
46	BN	137/140 (98%)	96 (70%)	23 (17%)	18 (13%)	0	4
46	DN	137/140 (98%)	95 (69%)	25 (18%)	17 (12%)	1	5
47	BO	120/122 (98%)	107 (89%)	10 (8%)	3 (2%)	9	52
47	DO	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	9	52
48	BP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
48	DP	144/150 (96%)	71 (49%)	35 (24%)	38 (26%)	0	0
49	BQ	139/141 (99%)	109 (78%)	17 (12%)	13 (9%)	1	11
49	DQ	139/141 (99%)	107 (77%)	20 (14%)	12 (9%)	1	14
50	BR	115/118 (98%)	89 (77%)	14 (12%)	12 (10%)	1	8
50	DR	115/118 (98%)	89 (77%)	13 (11%)	13 (11%)	1	7
51	BS	97/112 (87%)	51 (53%)	23 (24%)	23 (24%)	0	1
51	DS	97/112 (87%)	50 (52%)	23 (24%)	24 (25%)	0	1
52	BT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	1
52	DT	134/146 (92%)	79 (59%)	28 (21%)	27 (20%)	0	1
53	BU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	3	28
53	DU	115/118 (98%)	87 (76%)	22 (19%)	6 (5%)	3	28
54	BV	99/101 (98%)	63 (64%)	21 (21%)	15 (15%)	0	3
54	DV	99/101 (98%)	63 (64%)	22 (22%)	14 (14%)	0	3
55	BW	111/113 (98%)	91 (82%)	14 (13%)	6 (5%)	3	27
55	DW	111/113 (98%)	96 (86%)	9 (8%)	6 (5%)	3	27
56	BX	91/96 (95%)	71 (78%)	17 (19%)	3 (3%)	6	44
56	DX	91/96 (95%)	72 (79%)	16 (18%)	3 (3%)	6	44
57	BY	99/110 (90%)	42 (42%)	25 (25%)	32 (32%)	0	0
57	DY	99/110 (90%)	41 (41%)	26 (26%)	32 (32%)	0	0
58	BZ	183/206 (89%)	102 (56%)	40 (22%)	41 (22%)	0	1
58	DZ	183/206 (89%)	85 (46%)	58 (32%)	40 (22%)	0	1
All	All	11928/12922 (92%)	7972 (67%)	2431 (20%)	1525 (13%)	0	4

5 of 1525 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	10	LEU
2	AB	75	LYS
2	AB	123	ALA
2	AB	155	LEU

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	202/220 (92%)	189 (94%)	13 (6%)	25	69
2	CB	202/220 (92%)	191 (95%)	11 (5%)	31	74
3	AC	160/188 (85%)	146 (91%)	14 (9%)	14	52
3	CC	160/188 (85%)	147 (92%)	13 (8%)	17	57
4	AD	180/181 (99%)	162 (90%)	18 (10%)	11	43
4	CD	180/181 (99%)	162 (90%)	18 (10%)	11	43
5	AE	115/123 (94%)	98 (85%)	17 (15%)	4	22
5	CE	115/123 (94%)	98 (85%)	17 (15%)	4	22
6	AF	90/90 (100%)	84 (93%)	6 (7%)	23	67
6	CF	90/90 (100%)	84 (93%)	6 (7%)	23	67
7	AG	126/127 (99%)	120 (95%)	6 (5%)	35	78
7	CG	126/127 (99%)	121 (96%)	5 (4%)	42	82
8	AH	119/119 (100%)	109 (92%)	10 (8%)	16	55
8	CH	119/119 (100%)	108 (91%)	11 (9%)	13	49
9	AI	98/99 (99%)	89 (91%)	9 (9%)	13	49
9	CI	98/99 (99%)	89 (91%)	9 (9%)	13	49
10	AJ	88/92 (96%)	81 (92%)	7 (8%)	17	58
10	CJ	88/92 (96%)	81 (92%)	7 (8%)	17	58
11	AK	90/99 (91%)	87 (97%)	3 (3%)	50	86
11	CK	90/99 (91%)	87 (97%)	3 (3%)	50	86
12	AL	104/109 (95%)	95 (91%)	9 (9%)	15	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	CL	104/109 (95%)	95 (91%)	9 (9%)	15	53
13	AM	94/101 (93%)	83 (88%)	11 (12%)	8	34
13	CM	94/101 (93%)	83 (88%)	11 (12%)	8	34
14	AN	49/50 (98%)	46 (94%)	3 (6%)	26	71
14	CN	49/50 (98%)	46 (94%)	3 (6%)	26	71
15	AO	79/80 (99%)	73 (92%)	6 (8%)	19	61
15	CO	79/80 (99%)	73 (92%)	6 (8%)	19	61
16	AP	72/74 (97%)	65 (90%)	7 (10%)	12	45
16	CP	72/74 (97%)	65 (90%)	7 (10%)	12	45
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	32	75
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	32	75
18	AR	61/77 (79%)	61 (100%)	0	100	100
18	CR	61/77 (79%)	60 (98%)	1 (2%)	75	94
19	AS	69/80 (86%)	60 (87%)	9 (13%)	6	28
19	CS	69/80 (86%)	61 (88%)	8 (12%)	8	35
20	AT	76/82 (93%)	68 (90%)	8 (10%)	10	40
20	CT	76/82 (93%)	69 (91%)	7 (9%)	13	49
21	AU	19/22 (86%)	17 (90%)	2 (10%)	10	40
21	CU	19/22 (86%)	17 (90%)	2 (10%)	10	40
25	AY	78/78 (100%)	65 (83%)	13 (17%)	3	17
25	AZ	78/78 (100%)	57 (73%)	21 (27%)	1	3
25	CY	78/78 (100%)	64 (82%)	14 (18%)	2	13
25	CZ	78/78 (100%)	56 (72%)	22 (28%)	0	2
26	B0	66/67 (98%)	56 (85%)	10 (15%)	4	21
26	D0	66/67 (98%)	56 (85%)	10 (15%)	4	21
27	B1	78/83 (94%)	69 (88%)	9 (12%)	8	35
27	D1	78/83 (94%)	66 (85%)	12 (15%)	4	21
28	B2	66/67 (98%)	56 (85%)	10 (15%)	4	21
28	D2	66/67 (98%)	56 (85%)	10 (15%)	4	21
29	B3	51/52 (98%)	46 (90%)	5 (10%)	12	45
29	D3	51/52 (98%)	46 (90%)	5 (10%)	12	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	B4	51/63 (81%)	39 (76%)	12 (24%)	1	5
30	D4	51/63 (81%)	39 (76%)	12 (24%)	1	5
31	B5	47/52 (90%)	42 (89%)	5 (11%)	10	40
31	D5	47/52 (90%)	42 (89%)	5 (11%)	10	40
32	B6	49/52 (94%)	38 (78%)	11 (22%)	1	5
32	D6	49/52 (94%)	36 (74%)	13 (26%)	1	3
33	B7	40/42 (95%)	36 (90%)	4 (10%)	11	43
33	D7	40/42 (95%)	36 (90%)	4 (10%)	11	43
34	B8	53/55 (96%)	42 (79%)	11 (21%)	2	7
34	D8	53/55 (96%)	43 (81%)	10 (19%)	2	11
35	B9	34/34 (100%)	32 (94%)	2 (6%)	28	72
35	D9	34/34 (100%)	32 (94%)	2 (6%)	28	72
38	BC	99/181 (55%)	96 (97%)	3 (3%)	53	87
38	DC	99/181 (55%)	96 (97%)	3 (3%)	53	87
39	BD	213/218 (98%)	188 (88%)	25 (12%)	8	34
39	DD	213/218 (98%)	187 (88%)	26 (12%)	7	32
40	BE	165/166 (99%)	143 (87%)	22 (13%)	6	27
40	DE	165/166 (99%)	144 (87%)	21 (13%)	6	29
41	BF	165/166 (99%)	145 (88%)	20 (12%)	7	32
41	DF	165/166 (99%)	145 (88%)	20 (12%)	7	32
42	BG	155/156 (99%)	137 (88%)	18 (12%)	8	35
42	DG	155/156 (99%)	121 (78%)	34 (22%)	1	6
43	BH	137/148 (93%)	127 (93%)	10 (7%)	20	63
43	DH	137/148 (93%)	127 (93%)	10 (7%)	20	63
44	BI	122/124 (98%)	105 (86%)	17 (14%)	5	25
44	DI	122/124 (98%)	105 (86%)	17 (14%)	5	25
46	BN	117/119 (98%)	98 (84%)	19 (16%)	3	18
46	DN	117/119 (98%)	98 (84%)	19 (16%)	3	18
47	BO	100/100 (100%)	94 (94%)	6 (6%)	27	71
47	DO	100/100 (100%)	94 (94%)	6 (6%)	27	71
48	BP	112/116 (97%)	84 (75%)	28 (25%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	DP	112/116 (97%)	84 (75%)	28 (25%)	1	3
49	BQ	110/111 (99%)	95 (86%)	15 (14%)	5	26
49	DQ	110/111 (99%)	95 (86%)	15 (14%)	5	26
50	BR	100/101 (99%)	83 (83%)	17 (17%)	3	16
50	DR	100/101 (99%)	83 (83%)	17 (17%)	3	16
51	BS	77/88 (88%)	60 (78%)	17 (22%)	1	6
51	DS	77/88 (88%)	60 (78%)	17 (22%)	1	6
52	BT	118/127 (93%)	98 (83%)	20 (17%)	3	16
52	DT	118/127 (93%)	99 (84%)	19 (16%)	3	18
53	BU	92/94 (98%)	83 (90%)	9 (10%)	12	45
53	DU	92/94 (98%)	83 (90%)	9 (10%)	12	45
54	BV	82/82 (100%)	61 (74%)	21 (26%)	1	3
54	DV	82/82 (100%)	62 (76%)	20 (24%)	1	4
55	BW	91/92 (99%)	78 (86%)	13 (14%)	5	24
55	DW	91/92 (99%)	77 (85%)	14 (15%)	4	21
56	BX	74/78 (95%)	68 (92%)	6 (8%)	17	57
56	DX	74/78 (95%)	68 (92%)	6 (8%)	17	57
57	BY	84/91 (92%)	67 (80%)	17 (20%)	2	8
57	DY	84/91 (92%)	67 (80%)	17 (20%)	2	8
58	BZ	162/179 (90%)	137 (85%)	25 (15%)	4	21
58	DZ	162/179 (90%)	131 (81%)	31 (19%)	2	10
All	All	10102/10740 (94%)	8871 (88%)	1231 (12%)	7	32

5 of 1231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
56	BX	27	THR
9	CI	95	LYS
53	DU	74	LEU
57	BY	60	PHE
3	CC	131	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 309 such sidechains are listed below:

Mol	Chain	Res	Type
53	BU	14	HIS
4	CD	123	HIS
50	DR	61	HIS
54	BV	11	GLN
2	CB	76	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1504 (99%)	214 (14%)	30 (1%)
1	CA	1503/1504 (99%)	209 (13%)	31 (2%)
22	AV	76/77 (98%)	15 (19%)	0
23	AW	76/77 (98%)	10 (13%)	1 (1%)
23	CV	76/77 (98%)	12 (15%)	0
23	CW	76/77 (98%)	10 (13%)	1 (1%)
24	AX	10/25 (40%)	8 (80%)	1 (10%)
36	BA	2847/2848 (99%)	500 (17%)	49 (1%)
36	DA	2847/2848 (99%)	498 (17%)	47 (1%)
37	BB	118/119 (99%)	25 (21%)	2 (1%)
37	DB	118/119 (99%)	25 (21%)	2 (1%)
59	CX	9/10 (90%)	6 (66%)	2 (22%)
All	All	9259/9285 (99%)	1532 (16%)	166 (1%)

5 of 1532 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	22	G
1	AA	30	U
1	AA	31	G
1	AA	32	A

5 of 166 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
36	BA	2439	A
1	CA	366	C
36	DA	2191	G
36	BA	2481	G
1	CA	60	A

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

7 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
22	5MU	AV	54	22	20,22,23	1.08	2 (10%)	25,32,35	1.31	2 (8%)
24	OMU	AX	19	24	20,22,23	1.69	2 (10%)	24,31,34	1.14	1 (4%)
24	A2M	AX	20	60,24	23,25,26	0.65	0	33,36,39	1.03	1 (3%)
24	A2M	AX	21	24	23,25,26	0.66	0	33,36,39	1.30	1 (3%)
59	OMU	CX	19	59	20,22,23	1.69	1 (5%)	24,31,34	0.99	1 (4%)
59	A2M	CX	20	59	23,25,26	0.65	0	33,36,39	0.97	1 (3%)
59	A2M	CX	21	59	23,25,26	0.66	0	33,36,39	0.68	0

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
22	5MU	AV	54	22	-	0/6/25/26	0/2/2/2
24	OMU	AX	19	24	-	0/8/27/28	0/2/2/2
24	A2M	AX	20	60,24	-	0/10/27/28	0/3/3/3
24	A2M	AX	21	24	-	0/10/27/28	0/3/3/3
59	OMU	CX	19	59	-	1/8/27/28	0/2/2/2
59	A2M	CX	20	59	-	0/10/27/28	0/3/3/3
59	A2M	CX	21	59	-	0/10/27/28	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	CX	19	OMU	C5-C4	6.33	1.44	1.37
24	AX	19	OMU	C5-C4	6.30	1.44	1.37
22	AV	54	5MU	C6-N1	2.32	1.38	1.34
22	AV	54	5MU	C6-C5	-2.12	1.34	1.40
24	AX	19	OMU	O2'-CM2	-2.06	1.34	1.42

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	21	A2M	CM'-O2'-C2'	-6.56	96.81	114.53
24	AX	20	A2M	CM'-O2'-C2'	-4.73	101.75	114.53
22	AV	54	5MU	C6-N1-C2	-4.47	121.14	122.41
59	CX	20	A2M	CM'-O2'-C2'	-4.31	102.89	114.53
24	AX	19	OMU	CM2-O2'-C2'	-4.22	103.14	114.53

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	CX	19	OMU	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 711 ligands modelled in this entry, 711 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
13	CM	5
13	AM	5
9	AI	2
9	CI	2
42	DG	1
42	BG	1

The worst 5 of 16 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	DG	112:PRO	C	113:ARG	N	5.57
1	CM	69:GLU	C	70:LEU	N	4.17
1	AM	69:GLU	C	70:LEU	N	4.16
1	CM	112:GLY	C	113:PRO	N	3.94
1	AM	112:GLY	C	113:PRO	N	3.93

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	1504/1504 (100%)	-0.08	27 (1%) 65 28	63, 109, 201, 216	0
1	CA	1504/1504 (100%)	0.11	41 (2%) 52 19	65, 139, 211, 216	0
2	AB	235/256 (91%)	0.28	11 (4%) 30 11	87, 146, 195, 216	0
2	CB	235/256 (91%)	0.32	8 (3%) 43 16	86, 165, 206, 216	0
3	AC	207/239 (86%)	0.25	2 (0%) 79 42	83, 143, 188, 216	0
3	CC	207/239 (86%)	0.60	14 (6%) 17 7	100, 164, 200, 216	0
4	AD	208/209 (99%)	0.03	0 100 100	70, 104, 147, 167	0
4	CD	208/209 (99%)	0.48	8 (3%) 38 14	95, 151, 199, 216	0
5	AE	151/162 (93%)	0.14	3 (1%) 62 25	62, 102, 142, 216	0
5	CE	151/162 (93%)	0.53	5 (3%) 44 16	60, 125, 168, 210	0
6	AF	101/101 (100%)	0.06	1 (0%) 79 42	73, 128, 164, 183	0
6	CF	101/101 (100%)	-0.06	0 100 100	63, 112, 156, 181	0
7	AG	155/156 (99%)	0.23	7 (4%) 32 11	91, 136, 181, 210	0
7	CG	155/156 (99%)	0.47	12 (7%) 13 6	91, 153, 194, 216	0
8	AH	138/138 (100%)	0.18	0 100 100	73, 108, 147, 193	0
8	CH	138/138 (100%)	0.35	2 (1%) 72 33	89, 132, 183, 213	0
9	AI	127/128 (99%)	0.68	11 (8%) 10 5	95, 155, 190, 216	0
9	CI	127/128 (99%)	1.09	18 (14%) 3 2	113, 170, 211, 216	0
10	AJ	99/105 (94%)	0.89	12 (12%) 5 3	88, 159, 208, 216	0
10	CJ	99/105 (94%)	1.25	20 (20%) 2 2	122, 174, 215, 216	0
11	AK	119/129 (92%)	0.52	7 (5%) 22 8	70, 120, 170, 212	0
11	CK	119/129 (92%)	0.22	6 (5%) 28 10	70, 120, 167, 195	0
12	AL	125/132 (94%)	0.26	5 (4%) 36 13	60, 89, 139, 216	0
12	CL	125/132 (94%)	0.55	7 (5%) 24 9	77, 113, 157, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	119/126 (94%)	0.29	4 (3%) 43 16	80, 143, 183, 216	0
13	CM	119/126 (94%)	0.62	15 (12%) 4 2	97, 167, 210, 216	0
14	AN	60/61 (98%)	0.51	3 (5%) 28 10	84, 136, 187, 204	0
14	CN	60/61 (98%)	0.40	0 100 100	92, 154, 192, 206	0
15	AO	88/89 (98%)	0.17	0 100 100	66, 108, 148, 177	0
15	CO	88/89 (98%)	0.04	0 100 100	70, 114, 149, 174	0
16	AP	84/88 (95%)	0.27	0 100 100	70, 94, 143, 199	0
16	CP	84/88 (95%)	1.09	11 (13%) 4 2	99, 138, 175, 208	0
17	AQ	100/105 (95%)	0.08	0 100 100	70, 99, 129, 161	0
17	CQ	100/105 (95%)	0.32	2 (2%) 62 25	90, 125, 158, 179	0
18	AR	70/88 (79%)	0.54	3 (4%) 34 12	87, 128, 170, 181	0
18	CR	70/88 (79%)	0.52	5 (7%) 16 6	77, 118, 168, 186	0
19	AS	79/93 (84%)	0.87	7 (8%) 10 5	111, 163, 209, 216	0
19	CS	79/93 (84%)	1.33	17 (21%) 1 2	122, 169, 213, 216	0
20	AT	99/106 (93%)	0.31	0 100 100	71, 107, 163, 187	0
20	CT	99/106 (93%)	0.69	7 (7%) 16 6	93, 143, 181, 216	0
21	AU	25/27 (92%)	1.72	7 (28%) 1 1	99, 143, 176, 193	0
21	CU	25/27 (92%)	2.44	12 (48%) 1 0	102, 155, 182, 191	0
22	AV	77/77 (100%)	-0.31	1 (1%) 74 35	71, 108, 162, 206	0
23	AW	77/77 (100%)	1.98	30 (38%) 1 1	151, 218, 220, 221	0
23	CV	77/77 (100%)	-0.22	1 (1%) 74 35	76, 126, 184, 211	0
23	CW	77/77 (100%)	1.58	23 (29%) 1 1	151, 218, 220, 221	0
24	AX	11/25 (44%)	2.27	5 (45%) 1 0	52, 137, 174, 180	0
25	AY	84/84 (100%)	0.69	5 (5%) 21 8	105, 142, 171, 199	0
25	AZ	84/84 (100%)	0.48	3 (3%) 41 14	121, 166, 197, 200	0
25	CY	84/84 (100%)	1.18	12 (14%) 3 2	103, 160, 194, 200	0
25	CZ	84/84 (100%)	0.76	5 (5%) 21 8	132, 182, 200, 200	0
26	B0	84/85 (98%)	0.36	5 (5%) 21 8	69, 103, 160, 207	0
26	D0	84/85 (98%)	0.61	6 (7%) 16 6	76, 107, 163, 198	0
27	B1	94/98 (95%)	0.22	1 (1%) 77 38	55, 87, 144, 208	0
27	D1	94/98 (95%)	0.15	0 100 100	53, 83, 132, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	B2	71/72 (98%)	0.18	1 (1%) 72 33	81, 122, 156, 205	0
28	D2	71/72 (98%)	-0.10	2 (2%) 50 19	51, 84, 123, 188	0
29	B3	60/60 (100%)	0.63	3 (5%) 28 10	66, 97, 144, 212	0
29	D3	60/60 (100%)	0.10	1 (1%) 67 28	61, 93, 159, 199	0
30	B4	58/71 (81%)	0.11	1 (1%) 67 28	104, 171, 212, 216	0
30	D4	58/71 (81%)	0.58	3 (5%) 26 10	145, 180, 214, 216	0
31	B5	56/60 (93%)	0.04	1 (1%) 65 28	49, 92, 147, 216	0
31	D5	56/60 (93%)	-0.07	1 (1%) 65 28	49, 83, 151, 216	0
32	B6	50/54 (92%)	1.09	9 (18%) 2 2	89, 132, 180, 183	0
32	D6	50/54 (92%)	0.74	6 (12%) 5 3	97, 140, 188, 210	0
33	B7	48/49 (97%)	0.07	0 100 100	50, 73, 123, 163	0
33	D7	48/49 (97%)	0.09	1 (2%) 60 24	42, 57, 101, 161	0
34	B8	64/65 (98%)	0.31	1 (1%) 68 30	57, 85, 144, 170	0
34	D8	64/65 (98%)	0.29	1 (1%) 68 30	48, 85, 142, 210	0
35	B9	37/37 (100%)	1.66	9 (24%) 1 2	94, 118, 163, 186	0
35	D9	37/37 (100%)	1.73	11 (29%) 1 1	93, 119, 162, 173	0
36	BA	2848/2848 (100%)	-0.05	90 (3%) 45 17	46, 88, 203, 216	0
36	DA	2848/2848 (100%)	-0.04	79 (2%) 50 19	43, 82, 203, 216	0
37	BB	119/119 (100%)	-0.18	1 (0%) 83 47	88, 144, 195, 212	0
37	DB	119/119 (100%)	0.19	3 (2%) 54 20	90, 173, 210, 216	0
38	BC	120/229 (52%)	2.43	65 (54%) 0 0	139, 202, 216, 216	0
38	DC	120/229 (52%)	2.13	60 (50%) 0 0	145, 202, 216, 216	0
39	BD	272/276 (98%)	0.03	0 100 100	45, 83, 120, 188	0
39	DD	272/276 (98%)	0.02	1 (0%) 90 66	45, 77, 113, 185	0
40	BE	205/206 (99%)	0.07	3 (1%) 70 31	50, 89, 166, 201	0
40	DE	205/206 (99%)	0.22	2 (0%) 79 42	37, 89, 146, 194	0
41	BF	208/210 (99%)	-0.07	1 (0%) 88 59	49, 88, 164, 216	0
41	DF	208/210 (99%)	-0.00	1 (0%) 88 59	36, 82, 164, 211	0
42	BG	181/182 (99%)	0.30	6 (3%) 44 16	100, 143, 188, 212	0
42	DG	181/182 (99%)	0.75	25 (13%) 4 2	109, 171, 215, 216	0
43	BH	165/180 (91%)	0.98	21 (12%) 4 2	98, 166, 214, 216	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	DH	165/180 (91%)	0.40	8 (4%) 29 11	67, 127, 186, 216	0
44	BI	146/148 (98%)	1.72	40 (27%) 1 1	84, 172, 216, 216	0
44	DI	146/148 (98%)	0.63	9 (6%) 20 8	69, 144, 211, 216	0
45	BJ	0/130	-	-	-	-
45	DJ	0/130	-	-	-	-
46	BN	139/140 (99%)	0.23	0 100 100	63, 97, 149, 192	0
46	DN	139/140 (99%)	0.01	1 (0%) 84 50	54, 90, 144, 175	0
47	BO	122/122 (100%)	-0.06	0 100 100	48, 78, 111, 141	0
47	DO	122/122 (100%)	0.13	0 100 100	60, 89, 121, 138	0
48	BP	146/150 (97%)	0.35	2 (1%) 72 33	51, 103, 161, 216	0
48	DP	146/150 (97%)	0.25	1 (0%) 84 50	51, 105, 162, 210	0
49	BQ	141/141 (100%)	0.01	1 (0%) 84 50	65, 96, 134, 209	0
49	DQ	141/141 (100%)	0.27	4 (2%) 50 19	67, 103, 149, 208	0
50	BR	117/118 (99%)	0.03	0 100 100	55, 89, 123, 137	0
50	DR	117/118 (99%)	0.20	0 100 100	51, 84, 121, 145	0
51	BS	99/112 (88%)	0.61	6 (6%) 21 8	93, 141, 189, 208	0
51	DS	99/112 (88%)	0.81	11 (11%) 6 3	91, 154, 199, 216	0
52	BT	136/146 (93%)	0.11	1 (0%) 84 50	64, 97, 176, 216	0
52	DT	136/146 (93%)	0.20	4 (2%) 49 18	68, 110, 189, 215	0
53	BU	117/118 (99%)	-0.02	1 (0%) 81 45	53, 86, 139, 210	0
53	DU	117/118 (99%)	-0.08	1 (0%) 81 45	45, 75, 122, 215	0
54	BV	101/101 (100%)	0.14	0 100 100	53, 109, 158, 206	0
54	DV	101/101 (100%)	0.01	0 100 100	38, 93, 133, 216	0
55	BW	113/113 (100%)	0.16	2 (1%) 65 28	55, 80, 132, 199	0
55	DW	113/113 (100%)	0.07	2 (1%) 65 28	40, 72, 121, 209	0
56	BX	93/96 (96%)	0.17	1 (1%) 77 38	63, 106, 136, 155	0
56	DX	93/96 (96%)	0.05	0 100 100	55, 79, 117, 164	0
57	BY	101/110 (91%)	0.88	14 (13%) 4 2	62, 114, 180, 206	0
57	DY	101/110 (91%)	0.47	3 (2%) 48 18	56, 102, 168, 211	0
58	BZ	185/206 (89%)	0.30	6 (3%) 45 17	85, 131, 186, 216	0
58	DZ	185/206 (89%)	0.25	7 (3%) 38 14	88, 144, 202, 215	0
59	CX	10/10 (100%)	1.73	4 (40%) 1 1	110, 173, 193, 194	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	21443/22467 (95%)	0.23	955 (4%) 32 11	36, 111, 202, 221	0

The worst 5 of 955 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CA	89	C	14.0
36	DA	654(L)	G	12.4
36	DA	654(K)	C	11.8
12	AL	129	ALA	11.7
36	DA	654(N)	G	11.4

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

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
24	A2M	AX	20	23/24	0.45	-	158,164,194,194	0
59	A2M	CX	21	23/24	0.32	-	177,179,187,190	0
24	A2M	AX	21	23/24	0.39	-	140,147,161,184	0
22	5MU	AV	54	21/22	0.23	-	114,133,152,153	0
59	OMU	CX	19	21/22	0.29	-	117,161,200,200	0
24	OMU	AX	19	21/22	0.30	-	99,130,198,198	0
59	A2M	CX	20	23/24	0.36	-	168,174,200,200	0

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(\AA^2)	Q<0.9
60	MG	BA	2911	1/1	0.74	-	74,74,74,74	0
60	MG	DA	2934	1/1	0.42	-	86,86,86,86	0
60	MG	DA	3085	1/1	0.50	-	86,86,86,86	0
60	MG	CA	1689	1/1	0.71	-	75,75,75,75	0
60	MG	B5	102	1/1	0.56	-	79,79,79,79	0
61	ZN	CD	301	1/1	0.10	-	106,106,106,106	0
60	MG	CA	1658	1/1	0.36	-	93,93,93,93	0
60	MG	BA	3128	1/1	0.76	-	117,117,117,117	0
60	MG	CA	1644	1/1	0.67	-	94,94,94,94	0
60	MG	BA	2947	1/1	0.64	-	88,88,88,88	0
60	MG	CA	1648	1/1	0.13	-	71,71,71,71	0
60	MG	DA	3094	1/1	0.44	-	87,87,87,87	0
60	MG	DA	2922	1/1	0.40	-	59,59,59,59	0
60	MG	AA	1682	1/1	0.41	-	98,98,98,98	0
60	MG	AA	1643	1/1	0.63	-	106,106,106,106	0
60	MG	DA	3120	1/1	0.51	-	71,71,71,71	0
60	MG	CA	1684	1/1	0.37	-	101,101,101,101	0
60	MG	AA	1685	1/1	0.29	-	66,66,66,66	0
60	MG	DA	2933	1/1	0.50	-	53,53,53,53	0
60	MG	DA	2963	1/1	0.55	-	70,70,70,70	0
60	MG	DA	2944	1/1	0.40	-	74,74,74,74	0
60	MG	DA	3057	1/1	0.44	-	92,92,92,92	0
60	MG	AA	1601	1/1	0.88	-	100,100,100,100	0
60	MG	BA	3015	1/1	0.53	-	94,94,94,94	0
60	MG	BA	2954	1/1	0.34	-	66,66,66,66	0
60	MG	BA	3006	1/1	0.42	-	91,91,91,91	0
60	MG	DA	3133	1/1	0.77	-	87,87,87,87	0
60	MG	AA	1656	1/1	0.24	-	140,140,140,140	0
60	MG	DA	2961	1/1	0.66	-	90,90,90,90	0
60	MG	BA	2936	1/1	0.76	-	58,58,58,58	0
60	MG	BA	2925	1/1	0.34	-	97,97,97,97	0
60	MG	DB	201	1/1	0.44	-	69,69,69,69	0
60	MG	DA	2956	1/1	0.46	-	63,63,63,63	0
60	MG	DA	3039	1/1	0.60	-	85,85,85,85	0
60	MG	BA	3084	1/1	1.05	-	126,126,126,126	0
60	MG	DA	2948	1/1	0.59	-	60,60,60,60	0
60	MG	AA	1608	1/1	0.48	-	81,81,81,81	0
60	MG	AA	1695	1/1	0.36	-	105,105,105,105	0
60	MG	AA	1618	1/1	0.27	-	121,121,121,121	0
60	MG	AA	1657	1/1	0.37	-	121,121,121,121	0
60	MG	BA	2960	1/1	0.54	-	105,105,105,105	0
60	MG	DA	2992	1/1	0.42	-	75,75,75,75	0
60	MG	AA	1620	1/1	0.23	-	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3078	1/1	0.74	-	122,122,122,122	0
60	MG	AA	1627	1/1	1.10	-	101,101,101,101	0
60	MG	DA	2994	1/1	0.58	-	52,52,52,52	0
60	MG	DA	3061	1/1	0.48	-	94,94,94,94	0
60	MG	DA	3134	1/1	0.69	-	89,89,89,89	0
60	MG	CA	1619	1/1	0.10	-	67,67,67,67	0
60	MG	DA	2904	1/1	0.84	-	49,49,49,49	0
60	MG	BA	2962	1/1	0.73	-	64,64,64,64	0
60	MG	AA	1605	1/1	0.33	-	66,66,66,66	0
60	MG	CA	1666	1/1	0.56	-	137,137,137,137	1
60	MG	BA	2989	1/1	0.71	-	87,87,87,87	0
60	MG	CA	1661	1/1	0.44	-	81,81,81,81	0
60	MG	CA	1685	1/1	0.31	-	115,115,115,115	0
60	MG	DA	2907	1/1	0.63	-	51,51,51,51	0
60	MG	BA	3115	1/1	0.85	-	85,85,85,85	0
60	MG	AA	1603	1/1	1.35	-	94,94,94,94	0
60	MG	BA	2958	1/1	0.18	-	76,76,76,76	0
60	MG	DA	3064	1/1	0.25	-	66,66,66,66	0
60	MG	AA	1667	1/1	0.91	-	118,118,118,118	0
60	MG	BA	3090	1/1	1.34	-	123,123,123,123	0
60	MG	DA	2909	1/1	0.67	-	55,55,55,55	0
60	MG	DA	2968	1/1	0.45	-	43,43,43,43	0
60	MG	DA	3118	1/1	0.71	-	73,73,73,73	0
60	MG	B1	101	1/1	0.51	-	113,113,113,113	0
60	MG	DA	3055	1/1	0.30	-	106,106,106,106	0
60	MG	AA	1634	1/1	1.59	-	120,120,120,120	0
60	MG	BA	3060	1/1	0.86	-	83,83,83,83	0
60	MG	AA	1645	1/1	1.23	-	99,99,99,99	0
60	MG	DA	3008	1/1	0.23	-	92,92,92,92	0
60	MG	BA	2902	1/1	0.39	-	155,155,155,155	0
60	MG	CA	1647	1/1	0.28	-	97,97,97,97	0
60	MG	BA	2991	1/1	0.49	-	122,122,122,122	0
60	MG	CA	1674	1/1	0.23	-	137,137,137,137	0
60	MG	CA	1627	1/1	0.58	-	162,162,162,162	0
60	MG	BA	3022	1/1	0.40	-	125,125,125,125	0
60	MG	AA	1642	1/1	0.63	-	102,102,102,102	0
60	MG	DA	2921	1/1	0.44	-	49,49,49,49	0
60	MG	DA	3128	1/1	1.22	-	92,92,92,92	0
60	MG	CA	1672	1/1	0.86	-	109,109,109,109	0
60	MG	BA	3052	1/1	0.23	-	99,99,99,99	0
60	MG	AA	1636	1/1	0.78	-	142,142,142,142	0
60	MG	AA	1674	1/1	1.04	-	87,87,87,87	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1679	1/1	0.54	-	79,79,79,79	0
60	MG	CA	1703	1/1	0.41	-	107,107,107,107	0
60	MG	DA	3022	1/1	0.30	-	81,81,81,81	0
60	MG	AA	1654	1/1	0.51	-	139,139,139,139	0
60	MG	BA	2963	1/1	0.64	-	103,103,103,103	0
60	MG	DA	2938	1/1	0.35	-	45,45,45,45	0
60	MG	DA	2957	1/1	0.55	-	66,66,66,66	0
60	MG	DA	3089	1/1	1.25	-	92,92,92,92	0
60	MG	BA	3066	1/1	0.98	-	113,113,113,113	0
60	MG	BA	2901	1/1	0.31	-	145,145,145,145	0
60	MG	DA	3142	1/1	0.21	-	81,81,81,81	0
60	MG	BA	3136	1/1	0.55	-	106,106,106,106	0
60	MG	DA	3032	1/1	0.49	-	67,67,67,67	0
60	MG	DA	3003	1/1	0.88	-	69,69,69,69	1
60	MG	D1	101	1/1	0.89	-	92,92,92,92	0
60	MG	DA	3054	1/1	0.77	-	80,80,80,80	0
60	MG	DA	3053	1/1	0.43	-	71,71,71,71	0
60	MG	AA	1619	1/1	0.15	-	72,72,72,72	0
60	MG	BA	2904	1/1	0.76	-	56,56,56,56	0
60	MG	DA	3065	1/1	0.88	-	75,75,75,75	0
60	MG	CA	1688	1/1	0.93	-	103,103,103,103	0
60	MG	DA	3043	1/1	0.32	-	96,96,96,96	0
60	MG	CA	1694	1/1	0.93	-	112,112,112,112	0
60	MG	DA	3024	1/1	0.79	-	106,106,106,106	0
60	MG	BA	3027	1/1	0.54	-	51,51,51,51	0
60	MG	CV	101	1/1	0.38	-	67,67,67,67	0
60	MG	BA	2957	1/1	0.38	-	63,63,63,63	0
60	MG	BA	2940	1/1	0.53	-	64,64,64,64	0
60	MG	BA	3028	1/1	0.44	-	89,89,89,89	0
60	MG	BA	2994	1/1	0.29	-	77,77,77,77	0
60	MG	AA	1613	1/1	1.42	-	114,114,114,114	0
60	MG	DA	3082	1/1	0.77	-	77,77,77,77	0
60	MG	DA	3068	1/1	1.06	-	102,102,102,102	0
60	MG	BA	3096	1/1	0.33	-	84,84,84,84	0
60	MG	BA	2916	1/1	0.29	-	71,71,71,71	0
60	MG	CA	1655	1/1	0.56	-	111,111,111,111	0
60	MG	BA	2909	1/1	0.50	-	64,64,64,64	0
60	MG	BA	2998	1/1	0.69	-	88,88,88,88	0
60	MG	AA	1611	1/1	0.22	-	82,82,82,82	0
60	MG	BA	2949	1/1	0.49	-	77,77,77,77	0
60	MG	BA	2959	1/1	0.45	-	59,59,59,59	0
60	MG	DA	3131	1/1	0.82	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1690	1/1	0.81	-	96,96,96,96	0
60	MG	DA	2973	1/1	0.61	-	51,51,51,51	0
60	MG	DA	2910	1/1	0.34	-	57,57,57,57	0
60	MG	CA	1618	1/1	0.59	-	83,83,83,83	0
60	MG	BA	3042	1/1	0.43	-	78,78,78,78	0
60	MG	BA	2977	1/1	1.12	-	107,107,107,107	0
60	MG	DA	2954	1/1	0.25	-	57,57,57,57	0
60	MG	DA	3088	1/1	0.79	-	110,110,110,110	0
60	MG	CA	1680	1/1	0.66	-	148,148,148,148	0
60	MG	AA	1672	1/1	1.81	-	136,136,136,136	0
60	MG	AA	1699	1/1	0.61	-	109,109,109,109	0
60	MG	CA	1660	1/1	0.81	-	95,95,95,95	0
60	MG	BA	3053	1/1	0.81	-	122,122,122,122	0
60	MG	DA	2949	1/1	0.88	-	102,102,102,102	0
60	MG	DA	2931	1/1	0.45	-	52,52,52,52	0
60	MG	BA	2978	1/1	0.80	-	134,134,134,134	0
60	MG	DA	3111	1/1	1.00	-	62,62,62,62	0
60	MG	BA	3065	1/1	1.00	-	122,122,122,122	0
60	MG	DA	3018	1/1	0.45	-	114,114,114,114	0
60	MG	CA	1629	1/1	0.99	-	95,95,95,95	0
60	MG	DA	3092	1/1	0.41	-	86,86,86,86	0
60	MG	DA	3086	1/1	0.47	-	78,78,78,78	0
60	MG	BA	2931	1/1	0.40	-	72,72,72,72	0
60	MG	BA	3010	1/1	0.43	-	88,88,88,88	0
60	MG	AX	101	1/1	0.72	-	96,96,96,96	0
60	MG	BA	2930	1/1	1.30	-	117,117,117,117	0
60	MG	BA	3055	1/1	0.63	-	87,87,87,87	0
60	MG	DA	3106	1/1	0.74	-	143,143,143,143	0
60	MG	DA	2950	1/1	0.37	-	55,55,55,55	0
60	MG	BA	3087	1/1	0.98	-	112,112,112,112	0
60	MG	CA	1649	1/1	0.10	-	82,82,82,82	0
60	MG	DA	3098	1/1	0.63	-	107,107,107,107	0
60	MG	DA	2983	1/1	0.33	-	93,93,93,93	0
60	MG	CA	1601	1/1	0.92	-	86,86,86,86	0
60	MG	BA	2938	1/1	0.31	-	67,67,67,67	0
60	MG	CA	1673	1/1	0.49	-	116,116,116,116	0
60	MG	DA	2998	1/1	0.53	-	91,91,91,91	0
60	MG	CA	1663	1/1	0.39	-	121,121,121,121	0
60	MG	DA	2926	1/1	0.71	-	47,47,47,47	0
60	MG	DA	3080	1/1	0.77	-	130,130,130,130	0
60	MG	AA	1665	1/1	2.48	-	121,121,121,121	0
60	MG	AA	1612	1/1	1.06	-	102,102,102,102	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1683	1/1	0.12	-	93,93,93,93	0
60	MG	AA	1639	1/1	0.47	-	98,98,98,98	1
60	MG	DA	3067	1/1	0.49	-	52,52,52,52	0
60	MG	CA	1614	1/1	0.33	-	87,87,87,87	0
60	MG	BA	3002	1/1	1.11	-	97,97,97,97	0
60	MG	CA	1606	1/1	0.47	-	118,118,118,118	0
60	MG	CA	1636	1/1	0.53	-	90,90,90,90	0
60	MG	AA	1625	1/1	0.49	-	85,85,85,85	0
60	MG	DA	3010	1/1	0.59	-	92,92,92,92	0
60	MG	DA	3015	1/1	0.48	-	76,76,76,76	0
60	MG	BA	2986	1/1	0.63	-	81,81,81,81	0
60	MG	BA	3094	1/1	0.93	-	100,100,100,100	0
60	MG	DA	2991	1/1	0.43	-	126,126,126,126	0
60	MG	BA	3012	1/1	1.17	-	91,91,91,91	0
60	MG	DA	3020	1/1	0.22	-	50,50,50,50	0
60	MG	BA	3118	1/1	1.62	-	110,110,110,110	0
60	MG	BA	3070	1/1	0.86	-	118,118,118,118	0
60	MG	DA	2952	1/1	0.45	-	56,56,56,56	0
60	MG	BA	3079	1/1	0.79	-	72,72,72,72	0
60	MG	DA	3074	1/1	0.70	-	96,96,96,96	0
60	MG	AA	1668	1/1	0.60	-	109,109,109,109	0
60	MG	BA	3102	1/1	0.49	-	108,108,108,108	0
60	MG	DA	2913	1/1	0.49	-	70,70,70,70	0
60	MG	AA	1687	1/1	0.20	-	74,74,74,74	0
60	MG	AA	1683	1/1	0.44	-	89,89,89,89	0
60	MG	CA	1611	1/1	0.45	-	97,97,97,97	0
60	MG	BA	2985	1/1	0.31	-	87,87,87,87	0
60	MG	DA	3077	1/1	0.48	-	96,96,96,96	0
60	MG	BA	2943	1/1	0.78	-	56,56,56,56	0
60	MG	DA	2930	1/1	0.47	-	55,55,55,55	0
60	MG	DA	3129	1/1	0.26	-	113,113,113,113	0
60	MG	DA	2976	1/1	0.65	-	53,53,53,53	0
60	MG	DA	3034	1/1	0.31	-	72,72,72,72	0
60	MG	BA	3093	1/1	0.77	-	99,99,99,99	0
60	MG	BA	3047	1/1	0.21	-	105,105,105,105	0
60	MG	BA	3114	1/1	1.54	-	130,130,130,130	0
60	MG	AA	1606	1/1	1.03	-	98,98,98,98	0
60	MG	CA	1699	1/1	0.42	-	134,134,134,134	0
60	MG	BA	3068	1/1	1.35	-	103,103,103,103	0
60	MG	BA	3081	1/1	0.77	-	103,103,103,103	0
60	MG	CA	1610	1/1	0.19	-	116,116,116,116	0
60	MG	DA	3130	1/1	1.38	-	115,115,115,115	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	2985	1/1	0.28	-	85,85,85,85	0
60	MG	BA	3116	1/1	0.27	-	91,91,91,91	0
60	MG	DA	2920	1/1	0.17	-	75,75,75,75	0
60	MG	DA	3127	1/1	1.20	-	112,112,112,112	0
60	MG	BA	2950	1/1	0.94	-	81,81,81,81	0
60	MG	CA	1634	1/1	0.38	-	122,122,122,122	0
60	MG	DA	3027	1/1	0.90	-	92,92,92,92	0
60	MG	AA	1694	1/1	0.54	-	102,102,102,102	0
60	MG	CA	1654	1/1	0.51	-	107,107,107,107	0
60	MG	BA	2997	1/1	0.17	-	79,79,79,79	0
60	MG	BA	2995	1/1	0.44	-	105,105,105,105	0
60	MG	BA	3064	1/1	0.50	-	86,86,86,86	0
60	MG	AA	1652	1/1	0.37	-	103,103,103,103	1
60	MG	DA	3045	1/1	0.91	-	104,104,104,104	0
60	MG	DA	2967	1/1	0.61	-	51,51,51,51	0
60	MG	DA	3028	1/1	0.50	-	123,123,123,123	0
60	MG	DA	2916	1/1	0.79	-	53,53,53,53	0
60	MG	BA	3000	1/1	0.47	-	52,52,52,52	1
60	MG	BA	3103	1/1	1.13	-	107,107,107,107	0
60	MG	AA	1686	1/1	1.30	-	99,99,99,99	0
60	MG	CA	1664	1/1	0.98	-	112,112,112,112	0
60	MG	DA	3107	1/1	0.67	-	59,59,59,59	0
60	MG	BA	3086	1/1	0.63	-	114,114,114,114	0
60	MG	CA	1632	1/1	0.14	-	79,79,79,79	0
60	MG	AA	1650	1/1	0.88	-	111,111,111,111	0
60	MG	CV	102	1/1	1.60	-	132,132,132,132	1
60	MG	DA	3059	1/1	1.07	-	110,110,110,110	0
60	MG	CA	1625	1/1	0.57	-	96,96,96,96	0
60	MG	DA	3141	1/1	0.58	-	92,92,92,92	0
60	MG	BA	2913	1/1	0.54	-	59,59,59,59	0
60	MG	DA	2905	1/1	0.45	-	59,59,59,59	0
60	MG	DA	3042	1/1	0.35	-	81,81,81,81	0
60	MG	DA	3104	1/1	0.69	-	118,118,118,118	0
60	MG	DA	3091	1/1	0.36	-	107,107,107,107	0
60	MG	BA	2974	1/1	0.93	-	68,68,68,68	0
60	MG	CA	1681	1/1	0.30	-	113,113,113,113	1
60	MG	DA	3124	1/1	1.88	-	98,98,98,98	0
60	MG	AA	1670	1/1	1.39	-	130,130,130,130	0
60	MG	BA	3024	1/1	0.53	-	96,96,96,96	0
60	MG	BA	3036	1/1	0.29	-	97,97,97,97	0
60	MG	BA	3035	1/1	0.18	-	86,86,86,86	0
60	MG	DA	3081	1/1	0.59	-	104,104,104,104	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3057	1/1	0.52	-	73,73,73,73	0
60	MG	DA	3046	1/1	0.79	-	76,76,76,76	0
60	MG	DA	2925	1/1	0.43	-	58,58,58,58	0
60	MG	CA	1692	1/1	0.62	-	117,117,117,117	0
60	MG	CA	1605	1/1	0.19	-	104,104,104,104	0
60	MG	DA	3050	1/1	1.44	-	105,105,105,105	0
60	MG	DA	3093	1/1	0.48	-	86,86,86,86	0
60	MG	BA	2903	1/1	0.76	-	97,97,97,97	0
60	MG	DA	3110	1/1	0.73	-	63,63,63,63	0
60	MG	BA	2973	1/1	0.61	-	92,92,92,92	0
60	MG	DA	3023	1/1	0.40	-	103,103,103,103	0
60	MG	DA	3030	1/1	0.31	-	101,101,101,101	0
60	MG	DA	3063	1/1	0.93	-	94,94,94,94	0
60	MG	AA	1646	1/1	0.96	-	125,125,125,125	0
60	MG	DA	3087	1/1	0.69	-	68,68,68,68	0
60	MG	AA	1673	1/1	0.10	-	79,79,79,79	0
60	MG	DA	3016	1/1	0.16	-	83,83,83,83	0
60	MG	CA	1696	1/1	1.19	-	162,162,162,162	0
60	MG	DA	3121	1/1	0.63	-	104,104,104,104	0
60	MG	BA	3072	1/1	0.81	-	89,89,89,89	0
60	MG	BA	2961	1/1	0.73	-	78,78,78,78	0
60	MG	AA	1615	1/1	0.89	-	84,84,84,84	0
60	MG	BA	2988	1/1	0.69	-	117,117,117,117	0
60	MG	AA	1693	1/1	0.96	-	119,119,119,119	0
60	MG	CA	1603	1/1	0.79	-	113,113,113,113	0
60	MG	AA	1676	1/1	0.28	-	104,104,104,104	0
60	MG	DA	2953	1/1	0.34	-	65,65,65,65	0
60	MG	DA	2918	1/1	0.67	-	59,59,59,59	0
60	MG	B5	101	1/1	0.41	-	76,76,76,76	0
60	MG	DA	3006	1/1	0.54	-	65,65,65,65	0
60	MG	BA	3091	1/1	0.41	-	79,79,79,79	0
60	MG	CA	1617	1/1	0.13	-	93,93,93,93	0
60	MG	DA	3132	1/1	0.57	-	120,120,120,120	0
60	MG	BA	2992	1/1	0.54	-	61,61,61,61	0
60	MG	CA	1643	1/1	0.26	-	105,105,105,105	0
60	MG	CA	1633	1/1	0.65	-	93,93,93,93	0
60	MG	CA	1638	1/1	0.36	-	81,81,81,81	0
60	MG	BA	3104	1/1	0.26	-	115,115,115,115	0
60	MG	AA	1696	1/1	0.81	-	90,90,90,90	0
60	MG	BB	201	1/1	1.02	-	84,84,84,84	0
60	MG	BA	3130	1/1	0.30	-	111,111,111,111	0
60	MG	BA	3110	1/1	1.08	-	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3040	1/1	0.97	-	99,99,99,99	0
60	MG	AA	1700	1/1	1.31	-	111,111,111,111	0
60	MG	DA	2942	1/1	0.88	-	90,90,90,90	0
60	MG	BA	2928	1/1	0.97	-	63,63,63,63	0
60	MG	DA	3048	1/1	0.62	-	129,129,129,129	0
60	MG	DA	2923	1/1	0.30	-	52,52,52,52	0
60	MG	DA	3102	1/1	0.39	-	80,80,80,80	0
60	MG	BA	3013	1/1	0.30	-	72,72,72,72	0
60	MG	AA	1628	1/1	0.50	-	87,87,87,87	0
60	MG	DA	2917	1/1	0.85	-	58,58,58,58	0
60	MG	BA	2917	1/1	0.83	-	58,58,58,58	0
60	MG	BA	2969	1/1	0.45	-	61,61,61,61	0
60	MG	BA	3083	1/1	0.56	-	87,87,87,87	0
60	MG	BA	3018	1/1	1.67	-	109,109,109,109	0
60	MG	AA	1658	1/1	0.63	-	92,92,92,92	0
60	MG	AA	1617	1/1	0.46	-	104,104,104,104	0
60	MG	AV	101	1/1	0.57	-	83,83,83,83	1
60	MG	DA	2941	1/1	0.21	-	45,45,45,45	0
60	MG	BA	2929	1/1	0.69	-	65,65,65,65	0
60	MG	AA	1647	1/1	0.46	-	104,104,104,104	0
60	MG	BA	2920	1/1	1.14	-	98,98,98,98	0
60	MG	DA	3116	1/1	0.91	-	104,104,104,104	0
60	MG	B1	102	1/1	0.66	-	83,83,83,83	0
60	MG	BA	2933	1/1	0.64	-	77,77,77,77	0
60	MG	AA	1703	1/1	1.31	-	102,102,102,102	0
60	MG	BA	3071	1/1	0.45	-	61,61,61,61	0
60	MG	BA	3020	1/1	0.65	-	103,103,103,103	0
60	MG	AA	1630	1/1	0.07	-	109,109,109,109	1
60	MG	DA	2914	1/1	0.40	-	49,49,49,49	0
60	MG	DA	3026	1/1	0.36	-	78,78,78,78	0
60	MG	BA	3026	1/1	0.31	-	85,85,85,85	0
60	MG	BA	2945	1/1	0.93	-	73,73,73,73	0
60	MG	AA	1649	1/1	0.72	-	124,124,124,124	0
60	MG	DA	3035	1/1	0.49	-	105,105,105,105	0
60	MG	AA	1669	1/1	0.28	-	96,96,96,96	0
60	MG	CA	1635	1/1	0.10	-	98,98,98,98	0
60	MG	DA	2975	1/1	1.21	-	138,138,138,138	0
60	MG	DA	2936	1/1	0.23	-	59,59,59,59	0
60	MG	DA	3060	1/1	0.53	-	107,107,107,107	0
60	MG	BA	3029	1/1	0.35	-	139,139,139,139	0
60	MG	BA	3132	1/1	0.52	-	116,116,116,116	0
60	MG	BA	2976	1/1	0.47	-	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3046	1/1	0.48	-	112,112,112,112	0
60	MG	CA	1657	1/1	0.32	-	56,56,56,56	1
60	MG	BA	3016	1/1	0.27	-	102,102,102,102	0
60	MG	AA	1633	1/1	0.58	-	78,78,78,78	0
60	MG	BA	3063	1/1	0.64	-	136,136,136,136	0
60	MG	DA	3047	1/1	0.23	-	112,112,112,112	0
60	MG	AA	1691	1/1	0.37	-	96,96,96,96	0
60	MG	DA	3044	1/1	0.24	-	79,79,79,79	0
60	MG	DA	3058	1/1	0.49	-	104,104,104,104	0
60	MG	BA	3014	1/1	0.36	-	74,74,74,74	0
61	ZN	CN	101	1/1	0.05	-	153,153,153,153	0
60	MG	CA	1624	1/1	1.63	-	119,119,119,119	0
60	MG	AA	1688	1/1	1.12	-	113,113,113,113	0
60	MG	DA	3069	1/1	0.59	-	73,73,73,73	0
60	MG	BA	3077	1/1	0.39	-	84,84,84,84	0
60	MG	BA	3058	1/1	0.50	-	88,88,88,88	0
60	MG	DA	2939	1/1	0.51	-	41,41,41,41	0
60	MG	BA	2939	1/1	0.44	-	50,50,50,50	0
60	MG	DA	3119	1/1	0.87	-	75,75,75,75	0
61	ZN	AN	101	1/1	0.04	-	153,153,153,153	0
60	MG	DA	2969	1/1	0.83	-	84,84,84,84	0
60	MG	BA	2955	1/1	1.10	-	109,109,109,109	0
60	MG	AA	1702	1/1	0.77	-	74,74,74,74	0
60	MG	DA	3025	1/1	0.54	-	51,51,51,51	0
60	MG	DA	3019	1/1	0.89	-	112,112,112,112	0
60	MG	AA	1698	1/1	1.37	-	80,80,80,80	0
60	MG	AA	1681	1/1	0.94	-	99,99,99,99	0
60	MG	CA	1662	1/1	0.73	-	113,113,113,113	0
60	MG	BA	2952	1/1	0.79	-	87,87,87,87	0
60	MG	BA	2905	1/1	0.43	-	58,58,58,58	0
60	MG	BA	3044	1/1	0.57	-	108,108,108,108	0
60	MG	BA	2934	1/1	0.46	-	55,55,55,55	0
61	ZN	AD	301	1/1	0.16	-	106,106,106,106	0
60	MG	DA	3017	1/1	0.09	-	97,97,97,97	0
60	MG	CA	1686	1/1	0.53	-	94,94,94,94	0
60	MG	BA	3074	1/1	0.20	-	104,104,104,104	0
60	MG	AA	1635	1/1	0.30	-	111,111,111,111	0
60	MG	BA	2915	1/1	0.35	-	51,51,51,51	0
60	MG	CA	1698	1/1	1.53	-	145,145,145,145	0
60	MG	DA	2982	1/1	0.80	-	75,75,75,75	0
60	MG	BA	2983	1/1	0.35	-	108,108,108,108	0
60	MG	CA	1671	1/1	0.57	-	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	3126	1/1	0.79	-	76,76,76,76	0
60	MG	AA	1610	1/1	0.30	-	84,84,84,84	0
60	MG	DA	3072	1/1	0.43	-	102,102,102,102	0
60	MG	AA	1623	1/1	0.67	-	100,100,100,100	0
60	MG	CA	1651	1/1	0.14	-	144,144,144,144	0
60	MG	BA	3037	1/1	0.82	-	79,79,79,79	0
60	MG	DA	3004	1/1	0.54	-	113,113,113,113	0
60	MG	CA	1621	1/1	0.12	-	96,96,96,96	0
60	MG	BA	3082	1/1	0.47	-	101,101,101,101	0
60	MG	BA	3127	1/1	0.40	-	84,84,84,84	0
60	MG	AA	1697	1/1	1.11	-	127,127,127,127	0
60	MG	DA	3099	1/1	0.64	-	108,108,108,108	0
60	MG	DA	2958	1/1	0.26	-	96,96,96,96	0
60	MG	DA	2940	1/1	0.71	-	72,72,72,72	0
60	MG	BA	3119	1/1	1.01	-	99,99,99,99	0
60	MG	AA	1640	1/1	0.52	-	64,64,64,64	1
60	MG	BA	2927	1/1	0.64	-	59,59,59,59	0
60	MG	BA	2953	1/1	1.12	-	113,113,113,113	0
60	MG	DA	2987	1/1	0.20	-	86,86,86,86	0
60	MG	DA	3005	1/1	0.59	-	53,53,53,53	0
60	MG	DA	2924	1/1	0.23	-	87,87,87,87	0
60	MG	BA	2980	1/1	0.62	-	82,82,82,82	0
60	MG	BA	2967	1/1	0.65	-	57,57,57,57	0
60	MG	DA	2974	1/1	0.70	-	92,92,92,92	0
60	MG	BA	2979	1/1	0.21	-	103,103,103,103	0
60	MG	AA	1663	1/1	0.77	-	83,83,83,83	0
60	MG	BA	3124	1/1	1.21	-	120,120,120,120	0
60	MG	CA	1656	1/1	0.61	-	90,90,90,90	0
60	MG	DA	3014	1/1	0.74	-	77,77,77,77	0
60	MG	AA	1679	1/1	0.57	-	100,100,100,100	0
60	MG	BA	3112	1/1	0.62	-	47,47,47,47	0
60	MG	BA	2932	1/1	0.36	-	61,61,61,61	0
60	MG	BA	3092	1/1	0.55	-	82,82,82,82	0
60	MG	BA	3034	1/1	0.13	-	82,82,82,82	0
60	MG	BA	3041	1/1	0.52	-	71,71,71,71	0
60	MG	DA	2903	1/1	1.00	-	85,85,85,85	0
60	MG	DA	2981	1/1	0.81	-	105,105,105,105	0
60	MG	DA	2912	1/1	0.51	-	45,45,45,45	0
60	MG	CA	1615	1/1	0.67	-	127,127,127,127	0
60	MG	BA	2993	1/1	0.75	-	92,92,92,92	0
60	MG	AA	1660	1/1	0.30	-	105,105,105,105	0
60	MG	DA	2960	1/1	0.63	-	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	2946	1/1	0.29	-	66,66,66,66	0
60	MG	BF	301	1/1	0.50	-	100,100,100,100	0
60	MG	DA	2978	1/1	0.51	-	85,85,85,85	0
60	MG	CA	1677	1/1	0.71	-	88,88,88,88	0
60	MG	DA	3114	1/1	0.75	-	96,96,96,96	0
60	MG	DA	3062	1/1	0.34	-	49,49,49,49	0
60	MG	AA	1602	1/1	0.60	-	131,131,131,131	0
60	MG	BA	3019	1/1	0.39	-	74,74,74,74	0
60	MG	AA	1684	1/1	0.85	-	103,103,103,103	0
60	MG	BA	2908	1/1	1.19	-	103,103,103,103	0
60	MG	DA	2990	1/1	0.64	-	88,88,88,88	0
60	MG	BA	2984	1/1	0.87	-	95,95,95,95	0
60	MG	DA	2955	1/1	0.26	-	54,54,54,54	0
60	MG	AL	201	1/1	0.40	-	125,125,125,125	1
60	MG	BA	3025	1/1	0.67	-	95,95,95,95	0
60	MG	DA	2935	1/1	0.81	-	68,68,68,68	0
60	MG	BA	2944	1/1	0.39	-	58,58,58,58	0
60	MG	AA	1671	1/1	1.00	-	96,96,96,96	0
60	MG	BA	2975	1/1	0.31	-	92,92,92,92	0
60	MG	BA	3117	1/1	0.48	-	72,72,72,72	0
60	MG	BA	3098	1/1	0.68	-	89,89,89,89	0
60	MG	BA	3100	1/1	0.48	-	117,117,117,117	0
60	MG	AA	1648	1/1	0.73	-	92,92,92,92	0
60	MG	AA	1638	1/1	0.13	-	139,139,139,139	1
60	MG	DA	3117	1/1	0.94	-	123,123,123,123	0
60	MG	BA	3125	1/1	0.47	-	91,91,91,91	0
60	MG	BA	3089	1/1	0.56	-	155,155,155,155	0
60	MG	AA	1641	1/1	0.62	-	93,93,93,93	0
60	MG	BA	3050	1/1	0.93	-	116,116,116,116	0
60	MG	DA	2951	1/1	0.99	-	91,91,91,91	0
60	MG	CA	1637	1/1	0.58	-	141,141,141,141	0
60	MG	D5	101	1/1	0.32	-	56,56,56,56	0
60	MG	AA	1653	1/1	0.40	-	94,94,94,94	0
60	MG	DA	3052	1/1	0.27	-	57,57,57,57	0
60	MG	DA	3112	1/1	0.78	-	83,83,83,83	0
60	MG	DA	3083	1/1	1.14	-	112,112,112,112	0
60	MG	BA	3080	1/1	0.61	-	115,115,115,115	0
60	MG	DA	2929	1/1	0.66	-	94,94,94,94	0
60	MG	BA	3059	1/1	0.52	-	95,95,95,95	0
60	MG	BA	2910	1/1	0.26	-	75,75,75,75	0
60	MG	AA	1689	1/1	0.26	-	98,98,98,98	0
60	MG	DA	3041	1/1	2.25	-	154,154,154,154	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	AA	1632	1/1	0.75	-	75,75,75,75	0
60	MG	DA	3105	1/1	0.34	-	93,93,93,93	0
60	MG	CA	1608	1/1	0.21	-	113,113,113,113	0
60	MG	CA	1602	1/1	0.13	-	92,92,92,92	0
60	MG	CA	1669	1/1	0.24	-	113,113,113,113	0
60	MG	DA	3079	1/1	0.14	-	131,131,131,131	0
60	MG	BA	3005	1/1	0.67	-	85,85,85,85	0
60	MG	DA	3122	1/1	1.22	-	79,79,79,79	0
60	MG	DA	3137	1/1	0.61	-	121,121,121,121	0
60	MG	BA	3095	1/1	0.18	-	97,97,97,97	0
60	MG	DA	2993	1/1	0.34	-	79,79,79,79	0
60	MG	BA	2996	1/1	1.06	-	106,106,106,106	0
60	MG	BA	2981	1/1	0.15	-	88,88,88,88	0
60	MG	CA	1702	1/1	1.17	-	96,96,96,96	0
60	MG	BA	2982	1/1	0.25	-	100,100,100,100	0
60	MG	DA	2959	1/1	0.64	-	61,61,61,61	0
60	MG	AA	1666	1/1	0.27	-	84,84,84,84	0
60	MG	CA	1641	1/1	1.45	-	94,94,94,94	0
60	MG	AA	1622	1/1	0.31	-	128,128,128,128	0
60	MG	CA	1668	1/1	0.28	-	93,93,93,93	0
60	MG	CA	1653	1/1	0.65	-	127,127,127,127	0
60	MG	BA	2922	1/1	0.48	-	53,53,53,53	0
60	MG	BA	3075	1/1	0.22	-	100,100,100,100	0
60	MG	DA	3073	1/1	0.53	-	87,87,87,87	0
60	MG	CA	1622	1/1	0.55	-	93,93,93,93	0
60	MG	BA	3078	1/1	0.32	-	104,104,104,104	0
60	MG	CA	1665	1/1	0.65	-	111,111,111,111	1
60	MG	AA	1659	1/1	1.10	-	113,113,113,113	0
60	MG	BA	3069	1/1	0.20	-	87,87,87,87	0
60	MG	BA	3038	1/1	0.36	-	90,90,90,90	0
60	MG	DA	3031	1/1	0.82	-	92,92,92,92	0
60	MG	BA	3049	1/1	0.45	-	65,65,65,65	0
60	MG	DA	2971	1/1	0.61	-	66,66,66,66	0
60	MG	BA	3134	1/1	0.70	-	75,75,75,75	0
60	MG	AA	1621	1/1	0.36	-	95,95,95,95	0
60	MG	BA	2987	1/1	0.70	-	100,100,100,100	0
60	MG	DA	3095	1/1	0.38	-	98,98,98,98	0
60	MG	DA	2977	1/1	0.12	-	104,104,104,104	0
60	MG	DA	2980	1/1	1.15	-	111,111,111,111	0
60	MG	BA	3109	1/1	0.63	-	101,101,101,101	0
60	MG	BA	2907	1/1	0.56	-	55,55,55,55	0
60	MG	DA	2919	1/1	0.84	-	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3017	1/1	0.61	-	117,117,117,117	0
60	MG	DA	3051	1/1	0.29	-	56,56,56,56	0
60	MG	BA	2935	1/1	0.49	-	110,110,110,110	0
60	MG	DA	3109	1/1	0.64	-	45,45,45,45	0
60	MG	DA	2901	1/1	0.78	-	136,136,136,136	0
60	MG	DA	3040	1/1	0.37	-	64,64,64,64	0
60	MG	BA	3009	1/1	1.00	-	117,117,117,117	0
60	MG	DA	2908	1/1	0.89	-	83,83,83,83	0
60	MG	DA	3108	1/1	0.59	-	61,61,61,61	0
60	MG	DA	2984	1/1	0.63	-	120,120,120,120	0
60	MG	CA	1642	1/1	1.30	-	97,97,97,97	0
60	MG	DA	3123	1/1	0.62	-	82,82,82,82	0
60	MG	BA	3122	1/1	0.76	-	84,84,84,84	0
60	MG	DA	3033	1/1	0.19	-	100,100,100,100	0
60	MG	CA	1687	1/1	0.44	-	119,119,119,119	0
60	MG	DA	3096	1/1	1.03	-	124,124,124,124	0
60	MG	BA	3033	1/1	0.36	-	92,92,92,92	0
60	MG	DA	3100	1/1	0.81	-	113,113,113,113	0
60	MG	BA	2951	1/1	0.23	-	63,63,63,63	0
60	MG	DA	3021	1/1	0.28	-	81,81,81,81	0
60	MG	BA	3135	1/1	0.48	-	83,83,83,83	0
60	MG	DA	2966	1/1	0.67	-	48,48,48,48	0
60	MG	BA	2956	1/1	0.59	-	64,64,64,64	0
60	MG	BA	3004	1/1	0.31	-	63,63,63,63	0
60	MG	CA	1675	1/1	0.31	-	122,122,122,122	0
60	MG	BA	3067	1/1	0.27	-	93,93,93,93	0
60	MG	CA	1616	1/1	0.18	-	105,105,105,105	0
60	MG	DA	3002	1/1	0.36	-	95,95,95,95	0
60	MG	AA	1614	1/1	0.60	-	98,98,98,98	0
60	MG	BA	2970	1/1	1.22	-	86,86,86,86	0
60	MG	AA	1662	1/1	1.10	-	127,127,127,127	0
60	MG	BB	202	1/1	0.89	-	117,117,117,117	0
60	MG	BA	3023	1/1	1.12	-	79,79,79,79	0
60	MG	BA	3054	1/1	0.39	-	94,94,94,94	0
60	MG	AA	1677	1/1	0.25	-	114,114,114,114	0
60	MG	BA	3073	1/1	0.31	-	100,100,100,100	0
60	MG	DA	3007	1/1	0.24	-	82,82,82,82	0
60	MG	DA	3138	1/1	0.39	-	113,113,113,113	0
60	MG	DA	3000	1/1	0.59	-	77,77,77,77	0
60	MG	DA	2996	1/1	0.36	-	63,63,63,63	0
60	MG	DA	2937	1/1	0.33	-	45,45,45,45	0
60	MG	DA	2962	1/1	0.50	-	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	BA	3043	1/1	0.26	-	83,83,83,83	0
60	MG	DF	301	1/1	0.30	-	100,100,100,100	0
60	MG	BA	3088	1/1	0.43	-	105,105,105,105	0
60	MG	DA	3075	1/1	0.38	-	75,75,75,75	0
60	MG	DA	3090	1/1	0.74	-	106,106,106,106	0
60	MG	AA	1626	1/1	0.15	-	99,99,99,99	0
60	MG	DA	2965	1/1	0.57	-	96,96,96,96	0
60	MG	AA	1631	1/1	0.68	-	87,87,87,87	0
60	MG	BA	2999	1/1	0.79	-	121,121,121,121	0
60	MG	BA	3108	1/1	0.50	-	102,102,102,102	0
60	MG	CA	1701	1/1	0.53	-	58,58,58,58	0
60	MG	BA	2968	1/1	1.09	-	72,72,72,72	0
60	MG	DA	2902	1/1	0.14	-	152,152,152,152	0
60	MG	BA	2912	1/1	0.74	-	71,71,71,71	0
60	MG	CG	201	1/1	0.56	-	83,83,83,83	1
60	MG	BA	2964	1/1	0.43	-	80,80,80,80	0
60	MG	CA	1613	1/1	0.40	-	89,89,89,89	0
60	MG	CA	1652	1/1	0.88	-	148,148,148,148	0
60	MG	BA	2948	1/1	0.34	-	67,67,67,67	0
60	MG	AA	1624	1/1	0.55	-	111,111,111,111	0
60	MG	BA	3062	1/1	0.68	-	89,89,89,89	0
60	MG	CA	1691	1/1	1.40	-	105,105,105,105	0
60	MG	BA	3097	1/1	0.37	-	88,88,88,88	0
60	MG	BA	2926	1/1	0.41	-	58,58,58,58	0
60	MG	DA	3136	1/1	0.18	-	94,94,94,94	0
60	MG	CA	1678	1/1	0.61	-	86,86,86,86	1
60	MG	BA	3120	1/1	0.68	-	111,111,111,111	0
60	MG	DA	3038	1/1	0.60	-	77,77,77,77	0
60	MG	BA	2965	1/1	0.41	-	111,111,111,111	0
60	MG	CA	1646	1/1	0.51	-	119,119,119,119	0
60	MG	DA	3013	1/1	0.96	-	89,89,89,89	0
60	MG	CA	1609	1/1	0.16	-	84,84,84,84	0
60	MG	AA	1609	1/1	0.99	-	106,106,106,106	0
60	MG	AA	1616	1/1	0.42	-	84,84,84,84	0
60	MG	AA	1655	1/1	0.38	-	94,94,94,94	1
60	MG	DA	3066	1/1	0.53	-	102,102,102,102	0
60	MG	BA	3105	1/1	0.13	-	68,68,68,68	0
60	MG	BA	3129	1/1	0.62	-	84,84,84,84	0
60	MG	DA	2932	1/1	0.60	-	64,64,64,64	0
60	MG	BA	3045	1/1	0.23	-	88,88,88,88	0
60	MG	DA	3103	1/1	0.31	-	82,82,82,82	0
60	MG	DA	2947	1/1	0.18	-	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DX	101	1/1	0.69	-	72,72,72,72	1
60	MG	DA	2988	1/1	0.22	-	111,111,111,111	0
60	MG	DA	3139	1/1	0.84	-	69,69,69,69	0
60	MG	DA	3070	1/1	0.80	-	79,79,79,79	0
60	MG	BA	3113	1/1	0.40	-	126,126,126,126	0
60	MG	DA	2946	1/1	0.32	-	57,57,57,57	0
60	MG	DA	2928	1/1	0.39	-	42,42,42,42	0
60	MG	B0	101	1/1	0.46	-	98,98,98,98	0
60	MG	CA	1682	1/1	0.16	-	151,151,151,151	0
60	MG	BA	3111	1/1	0.95	-	103,103,103,103	0
60	MG	BA	3099	1/1	0.24	-	117,117,117,117	0
60	MG	BP	201	1/1	0.22	-	71,71,71,71	0
60	MG	BA	2914	1/1	0.38	-	83,83,83,83	0
60	MG	CA	1607	1/1	0.41	-	101,101,101,101	0
60	MG	AA	1629	1/1	0.57	-	65,65,65,65	1
60	MG	BA	3133	1/1	1.13	-	73,73,73,73	0
60	MG	DA	2986	1/1	0.74	-	87,87,87,87	0
60	MG	BA	3048	1/1	0.27	-	87,87,87,87	0
60	MG	DA	2970	1/1	0.15	-	47,47,47,47	0
60	MG	DA	3115	1/1	0.53	-	162,162,162,162	0
60	MG	BA	2906	1/1	0.41	-	100,100,100,100	0
60	MG	AA	1678	1/1	0.59	-	121,121,121,121	0
60	MG	BA	2966	1/1	0.41	-	92,92,92,92	0
60	MG	CA	1623	1/1	0.21	-	82,82,82,82	0
60	MG	CA	1690	1/1	0.80	-	100,100,100,100	0
60	MG	DA	2911	1/1	0.54	-	62,62,62,62	0
60	MG	CA	1659	1/1	0.38	-	104,104,104,104	1
60	MG	DA	3084	1/1	0.21	-	103,103,103,103	0
60	MG	BA	3008	1/1	0.66	-	96,96,96,96	0
60	MG	DA	3036	1/1	0.51	-	59,59,59,59	0
60	MG	BA	3021	1/1	0.14	-	79,79,79,79	0
60	MG	CA	1670	1/1	0.09	-	153,153,153,153	0
60	MG	AA	1604	1/1	0.40	-	132,132,132,132	0
60	MG	BA	3123	1/1	0.51	-	80,80,80,80	0
60	MG	BA	3003	1/1	0.68	-	68,68,68,68	0
60	MG	BA	2921	1/1	0.34	-	98,98,98,98	0
60	MG	BA	3031	1/1	0.93	-	108,108,108,108	0
60	MG	AA	1680	1/1	0.33	-	75,75,75,75	0
60	MG	DA	3001	1/1	0.30	-	69,69,69,69	0
60	MG	CA	1640	1/1	1.14	-	102,102,102,102	0
60	MG	BA	3131	1/1	0.59	-	79,79,79,79	0
60	MG	CA	1650	1/1	1.27	-	127,127,127,127	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	CA	1604	1/1	0.72	-	115,115,115,115	0
60	MG	DA	3125	1/1	0.40	-	72,72,72,72	0
60	MG	DA	3097	1/1	0.53	-	112,112,112,112	0
60	MG	BA	2919	1/1	0.50	-	75,75,75,75	0
60	MG	CA	1630	1/1	0.19	-	105,105,105,105	0
60	MG	AA	1661	1/1	0.92	-	94,94,94,94	0
60	MG	BA	2924	1/1	0.26	-	52,52,52,52	0
60	MG	BX	101	1/1	1.25	-	110,110,110,110	1
60	MG	BA	3030	1/1	0.74	-	96,96,96,96	0
60	MG	BA	3011	1/1	0.71	-	106,106,106,106	0
60	MG	DA	2906	1/1	0.33	-	67,67,67,67	0
60	MG	BA	3056	1/1	0.27	-	55,55,55,55	0
60	MG	BA	3085	1/1	0.56	-	118,118,118,118	0
60	MG	DA	3076	1/1	0.30	-	119,119,119,119	0
60	MG	CL	201	1/1	0.52	-	87,87,87,87	1
60	MG	DA	2989	1/1	0.59	-	79,79,79,79	0
60	MG	DA	2999	1/1	0.22	-	94,94,94,94	0
60	MG	CA	1626	1/1	1.49	-	102,102,102,102	0
60	MG	BA	3001	1/1	0.20	-	157,157,157,157	0
60	MG	AA	1644	1/1	0.10	-	141,141,141,141	0
60	MG	DR	201	1/1	0.98	-	117,117,117,117	0
60	MG	DA	2997	1/1	0.17	-	79,79,79,79	0
60	MG	CA	1693	1/1	0.53	-	65,65,65,65	0
60	MG	DA	2927	1/1	0.76	-	52,52,52,52	0
60	MG	AA	1692	1/1	1.12	-	101,101,101,101	0
60	MG	DA	3009	1/1	0.87	-	168,168,168,168	0
60	MG	BA	2990	1/1	0.36	-	81,81,81,81	0
60	MG	DA	3049	1/1	0.47	-	85,85,85,85	0
60	MG	CA	1645	1/1	0.18	-	68,68,68,68	0
60	MG	BA	3126	1/1	1.67	-	131,131,131,131	0
60	MG	BA	3107	1/1	0.56	-	87,87,87,87	0
60	MG	DA	3056	1/1	0.47	-	126,126,126,126	0
60	MG	AA	1607	1/1	0.16	-	107,107,107,107	0
60	MG	AA	1651	1/1	0.33	-	113,113,113,113	0
60	MG	CA	1639	1/1	0.37	-	99,99,99,99	0
60	MG	BA	2942	1/1	0.83	-	107,107,107,107	0
60	MG	DA	3071	1/1	0.76	-	123,123,123,123	0
60	MG	BA	2971	1/1	0.14	-	52,52,52,52	0
60	MG	CA	1631	1/1	0.95	-	111,111,111,111	0
60	MG	CA	1667	1/1	1.48	-	83,83,83,83	1
60	MG	AA	1675	1/1	0.44	-	93,93,93,93	0
60	MG	AA	1637	1/1	0.57	-	99,99,99,99	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
60	MG	DA	2995	1/1	0.76	-	75,75,75,75	0
60	MG	DA	3029	1/1	0.65	-	99,99,99,99	0
60	MG	DA	3037	1/1	0.43	-	74,74,74,74	0
60	MG	BA	3032	1/1	0.72	-	98,98,98,98	0
60	MG	CA	1676	1/1	0.27	-	119,119,119,119	0
60	MG	DA	3140	1/1	0.70	-	77,77,77,77	0
60	MG	BA	2937	1/1	0.79	-	70,70,70,70	0
60	MG	CA	1697	1/1	1.05	-	126,126,126,126	0
60	MG	DA	2945	1/1	0.22	-	57,57,57,57	0
60	MG	DA	3135	1/1	1.52	-	103,103,103,103	0
60	MG	CA	1628	1/1	0.42	-	66,66,66,66	0
60	MG	BA	2941	1/1	0.59	-	49,49,49,49	0
60	MG	DA	2964	1/1	1.18	-	109,109,109,109	0
60	MG	BA	3007	1/1	0.32	-	125,125,125,125	0
60	MG	AA	1664	1/1	0.24	-	90,90,90,90	0
60	MG	BA	2923	1/1	0.46	-	78,78,78,78	0
60	MG	DA	3011	1/1	0.35	-	88,88,88,88	0
60	MG	CA	1612	1/1	0.57	-	102,102,102,102	0
60	MG	BA	3039	1/1	0.47	-	67,67,67,67	0
60	MG	BA	3061	1/1	0.57	-	71,71,71,71	0
60	MG	BA	3076	1/1	0.55	-	108,108,108,108	0
60	MG	BA	2918	1/1	0.85	-	64,64,64,64	0
60	MG	BA	3101	1/1	0.84	-	123,123,123,123	0
60	MG	DA	3101	1/1	0.14	-	88,88,88,88	0
60	MG	BA	3051	1/1	0.73	-	72,72,72,72	0
60	MG	DA	2979	1/1	0.31	-	57,57,57,57	0
60	MG	BA	2972	1/1	0.73	-	76,76,76,76	0
60	MG	BA	3106	1/1	0.79	-	97,97,97,97	0
60	MG	AA	1701	1/1	0.56	-	71,71,71,71	0
60	MG	DA	2972	1/1	0.67	-	100,100,100,100	0
60	MG	CA	1620	1/1	1.14	-	115,115,115,115	0
60	MG	DA	2943	1/1	0.25	-	59,59,59,59	0
60	MG	CA	1700	1/1	0.60	-	113,113,113,113	0
60	MG	BA	3121	1/1	0.47	-	112,112,112,112	0
60	MG	DA	3012	1/1	0.30	-	53,53,53,53	0
60	MG	DA	2915	1/1	0.42	-	64,64,64,64	0
60	MG	CA	1695	1/1	0.73	-	80,80,80,80	0
60	MG	DA	3113	1/1	0.49	-	96,96,96,96	0

6.5 Other polymers ⓘ

There are no such residues in this entry.