



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 20, 2025 – 08:03 AM EDT

PDB ID : 4V7M
Title : The structures of Capreomycin bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-11-12
Resolution : 3.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

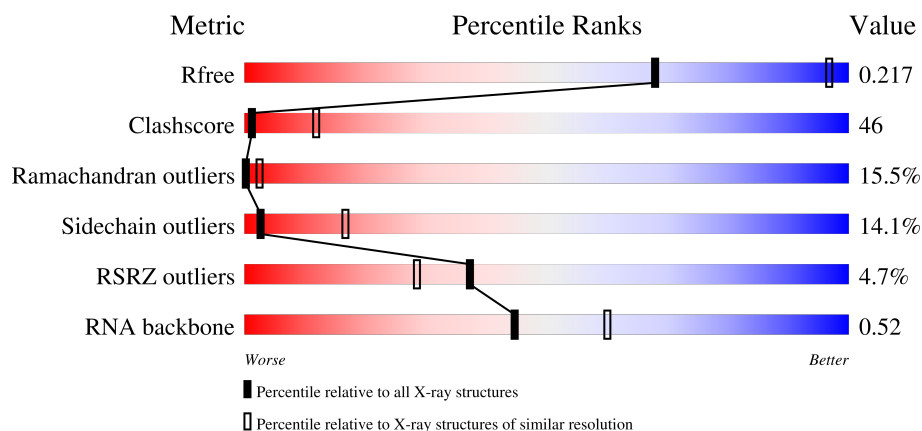
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	1597 (3.52-3.40)
Clashscore	180529	1041 (3.50-3.42)
Ramachandran outliers	177936	1026 (3.50-3.42)
Sidechain outliers	177891	1027 (3.50-3.42)
RSRZ outliers	164620	1596 (3.52-3.40)
RNA backbone	3690	1057 (3.92-3.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	AA	1508	<div> <div>2%</div> <div>22% 62% 13% ..</div> </div>
1	CA	1508	<div> <div>3%</div> <div>20% 63% 14% ..</div> </div>
2	AB	256	<div> <div>5%</div> <div>13% 61% 16% • 8%</div> </div>
2	CB	256	<div> <div>5%</div> <div>17% 58% 14% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
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	
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	

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Mol	Chain	Length	Quality of chain
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	30	
22	CV	30	
23	AW	75	
23	CW	75	
24	AX	77	
25	AY	75	
25	CY	75	
26	AZ	6	
26	CZ	6	
27	BA	2915	
27	DA	2915	
28	BB	122	

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Mol	Chain	Length	Quality of chain
28	DB	122	
29	BC	229	
29	DC	229	
30	BD	276	
30	DD	276	
31	BE	206	
31	DE	206	
32	BF	210	
32	DF	210	
33	BG	182	
33	DG	182	
34	BH	180	
34	DH	180	
35	BI	148	
35	DI	148	
36	BN	140	
36	DN	140	
37	BO	122	
37	DO	122	
38	BP	150	
38	DP	150	
39	BQ	141	
39	DQ	141	
40	BR	118	
40	DR	118	

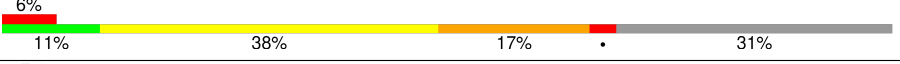
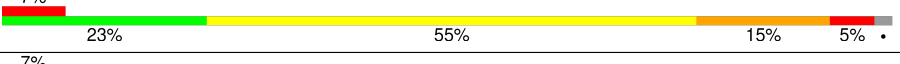
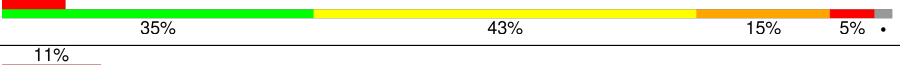

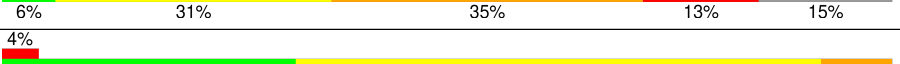
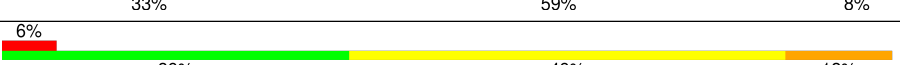
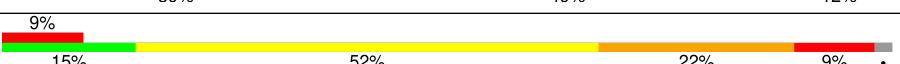
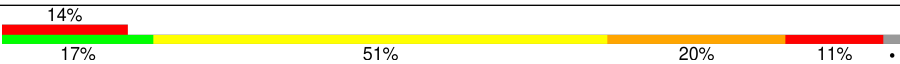

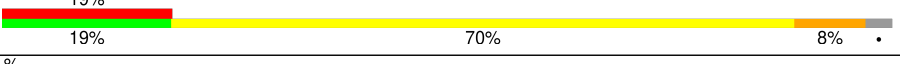
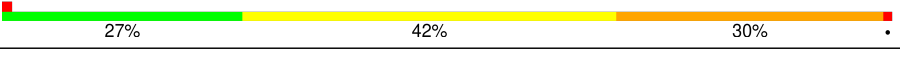

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Mol	Chain	Length	Quality of chain
41	BS	112	
41	DS	112	
42	BT	146	
42	DT	146	
43	BU	118	
43	DU	118	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	96	
46	DX	96	
47	BY	110	
47	DY	110	
48	BZ	206	
48	DZ	206	
49	B0	85	
49	D0	85	
50	B1	98	
50	D1	98	
51	B2	72	
51	D2	72	
52	B3	60	
52	D3	60	
53	B4	71	

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Mol	Chain	Length	Quality of chain
53	D4	71	
54	B5	60	
54	D5	60	
55	B6	54	
55	D6	54	
56	B7	49	
56	D7	49	
57	B8	65	
57	D8	65	
58	B9	37	
58	D9	37	
59	CX	77	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	DPP	AZ	2	-	-	X	-
26	KBE	CZ	1	-	-	X	-
26	DPP	CZ	2	-	-	X	-
60	MG	AA	1630	-	-	-	X
60	MG	AA	1648	-	-	-	X
60	MG	BA	3201	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 293848 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1495	Total	C	N	O	P	0	0	0
			32132	14303	5953	10382	1494			
1	CA	1493	Total	C	N	O	P	0	0	0
			32098	14287	5956	10363	1492			

- 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	206	Total	C	N	O	S	0	0	1
			1604	1011	314	278	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	154	Total	C	N	O	S	0	0	0
			1249	776	251	217	5			

- 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
			1006	637	195	174				
9	CI	127	Total	C	N	O		0	0	0
			1006	637	195	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	116	Total	C	N	O	S	0	0	0
			864	537	164	160	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	122	Total	C	N	O	S	0	0	1
			965	597	200	166	2			
13	CM	118	Total	C	N	O	S	0	0	0
			937	579	193	163	2			

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

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 (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			205	93	40	63	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

- Molecule 23 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			
23	CW	74	Total	C	N	O	P	0	0	0
			1573	702	279	518	74			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1639	732	297	534	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	conflict	GB CP001790.1
AY	44	U	A	conflict	GB CP001790.1
CY	33	G	C	conflict	GB CP001790.1
CY	44	U	A	conflict	GB CP001790.1

- Molecule 26 is a protein called capreomycin IA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			47	25	14	8			
26	CZ	6	Total	C	N	O	0	0	0
			47	25	14	8			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2789	Total	C	N	O	P	0	0	0
			60072	26734	11238	19312	2788			
27	DA	2775	Total	C	N	O	P	0	0	0
			59767	26598	11176	19219	2774			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
29	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 30 is a protein called 50S ribosomal protein L2.

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

- Molecule 31 is a protein called 50S ribosomal protein L3.

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

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BF	206	Total	C	N	O	S	0	0	1
			1607	1024	301	280	2			
32	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 33 is a protein called 50S ribosomal protein L5.

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

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	161	Total	C	N	O	S	0	0	0
			1233	783	227	222	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

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

- Molecule 36 is a protein called 50S ribosomal protein L13.

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

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

- Molecule 37 is a protein called 50S ribosomal protein L14.

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

- Molecule 38 is a protein called 50S ribosomal protein L15.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			
39	DQ	138	Total	C	N	O	S	0	0	0
			1094	697	205	185	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

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

- Molecule 41 is a protein called 50S ribosomal protein L18.

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

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			
42	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

- Molecule 43 is a protein called 50S ribosomal protein L20.

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

- Molecule 44 is a protein called 50S ribosomal protein L21.

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

- Molecule 45 is a protein called 50S ribosomal protein L22.

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

- Molecule 46 is a protein called 50S ribosomal protein L23.

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

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	88	Total	C	N	O	S	0	0	1
			672	432	131	105	4			
47	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
48	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L29.

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

- Molecule 52 is a protein called 50S ribosomal protein L30.

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

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

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			
53	D4	49	Total	C	N	O	S	0	0	1
			344	215	60	65	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	48	Total	C	N	O	S	0	0	1
			402	249	83	66	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
56	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 57 is a protein called 50S ribosomal protein L35.

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

- Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
58	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 59 is a RNA chain called RNA (77-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CX	46	G	A	conflict	GB CP001637.1

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	114	Total	Mg	0	0
			114	114		
60	AG	1	Total	Mg	0	0
			1	1		
60	AW	4	Total	Mg	0	0
			4	4		
60	AX	9	Total	Mg	0	0
			9	9		
60	BA	334	Total	Mg	0	0
			334	334		
60	BB	5	Total	Mg	0	0
			5	5		
60	BD	1	Total	Mg	0	0
			1	1		
60	BE	3	Total	Mg	0	0
			3	3		
60	BF	1	Total	Mg	0	0
			1	1		
60	BG	1	Total	Mg	0	0
			1	1		
60	BP	2	Total	Mg	0	0
			2	2		

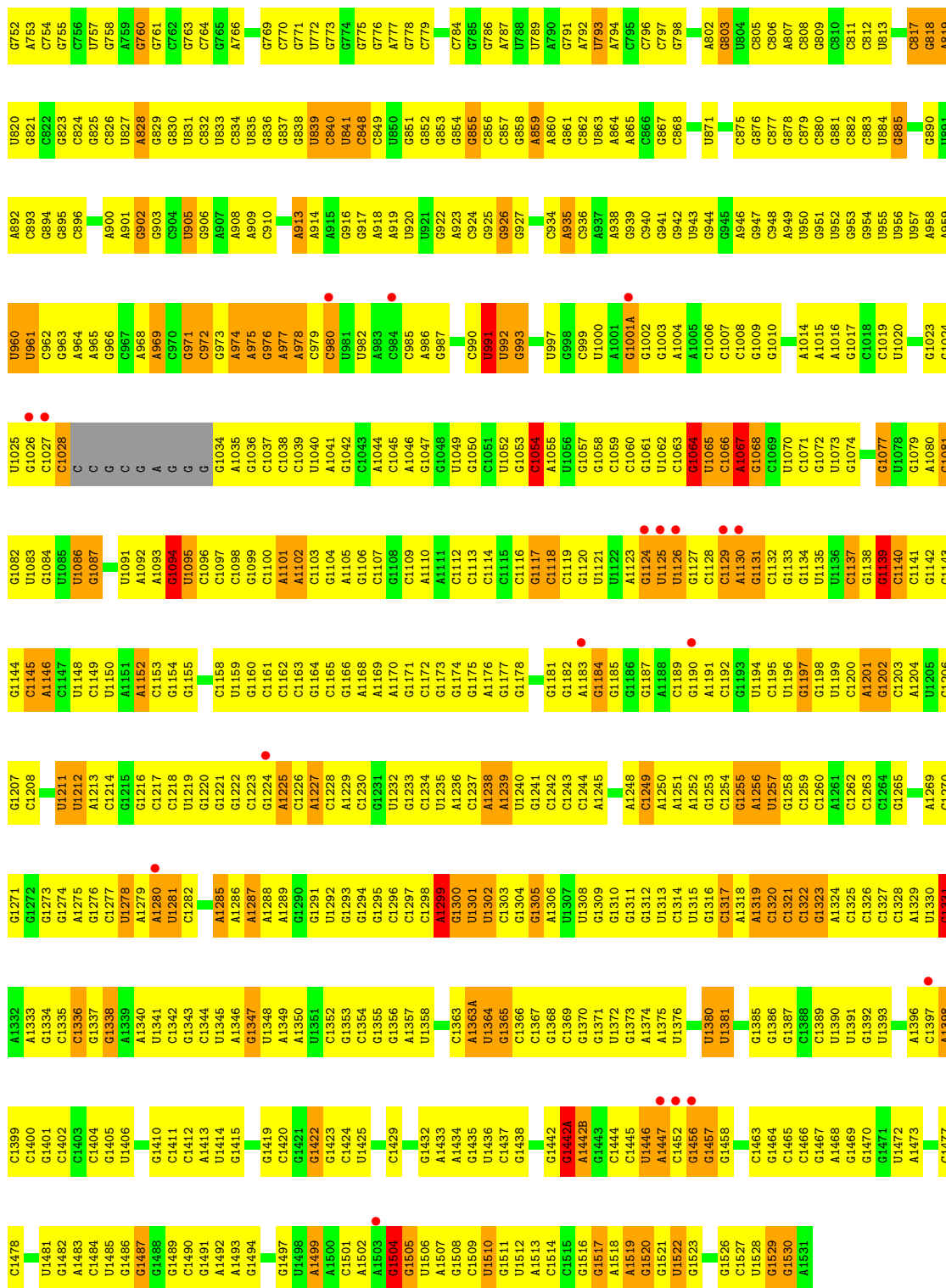
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BR	1	Total 1	Mg 1	0	0
60	BU	2	Total 2	Mg 2	0	0
60	BX	1	Total 1	Mg 1	0	0
60	B0	3	Total 3	Mg 3	0	0
60	B5	1	Total 1	Mg 1	0	0
60	CA	102	Total 102	Mg 102	0	0
60	CE	1	Total 1	Mg 1	0	0
60	CK	1	Total 1	Mg 1	0	0
60	CV	1	Total 1	Mg 1	0	0
60	CW	4	Total 4	Mg 4	0	0
60	DA	239	Total 239	Mg 239	0	0
60	DB	3	Total 3	Mg 3	0	0
60	DD	2	Total 2	Mg 2	0	0
60	DE	1	Total 1	Mg 1	0	0
60	DF	1	Total 1	Mg 1	0	0
60	DO	1	Total 1	Mg 1	0	0
60	D0	1	Total 1	Mg 1	0	0
60	D5	1	Total 1	Mg 1	0	0
60	D7	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	AD	1	Total 1	Zn 1	0	0
61	B4	1	Total 1	Zn 1	0	0
61	B5	1	Total 1	Zn 1	0	0
61	B9	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	D4	1	Total 1	Zn 1	0	0
61	D5	1	Total 1	Zn 1	0	0
61	D9	1	Total 1	Zn 1	0	0

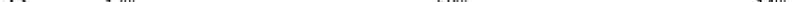


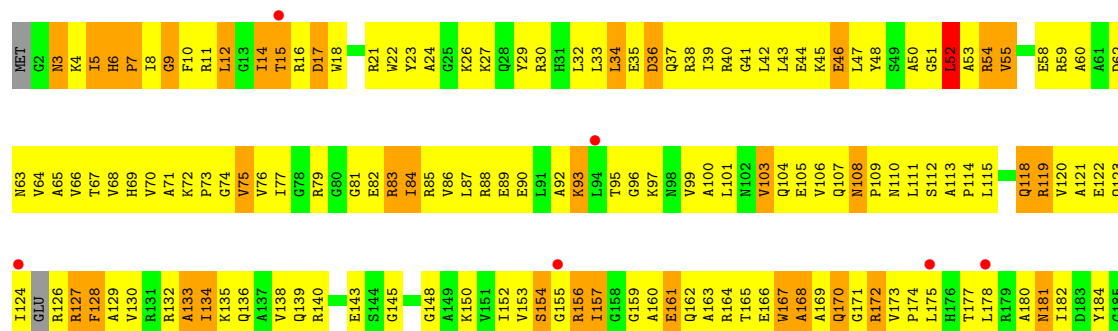
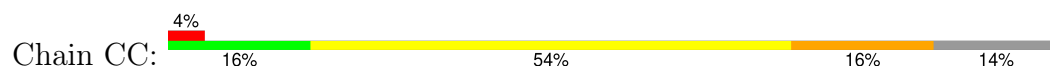
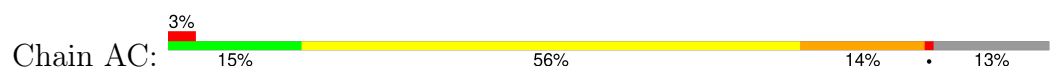
- Molecule 1: 16S ribosomal RNA

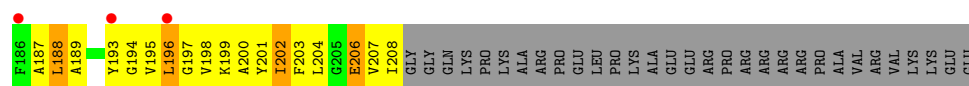


A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038	A1039	A1040	A1041	A1042	A1043	A1044	A1045	A1046	A1047	A1048	A1049	A1050																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																
G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
C868	C869	C870	C871	C872	C873	C874	C875	C876	C877	C878	C879	C880	C881	C882	C883	C884	C885	C886	C887	C888	C889	C890	C891	C892	C893	C894	C895	C896	C897	C898	C899	C900	C901	C902	C903	C904	C905	C906	C907	C908	C909	C910	C911	C912	C913	C914	C915	C916	C917	C918	C919	C920	C921	C922	C923	C924	C925	C926	C927	C928	C929	C930	C931	C932	C933	C934	C935	C936	C937	C938	C939	C940	C941	C942	C943	C944	C945	C946	C947	C948	C949	C950	C951	C952	C953	C954	C955	C956	C957	C958	C959	C960	C961	C962	C963	C964	C965	C966	C967	C968	C969	C970	C971	C972	C973	C974	C975	C976	C977	C978	C979	C980	C981	C982	C983	C984	C985	C986	C987	C988	C989	C990	C991	C992	C993	C994	C995	C996	C997	C998	C999	G1000																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G258	G259	G260	G261	G262	G263	G264	G265	G266	G267	G268	G269	A270	C271	G272	A273	G274	G275	G276	C277	G278	A279	C280	G281	G282	G283	G284	G285	G286	G287	G288	G289	G290	G291	G292	G293	G294	G295	G296	G297	G298	G299	A300	G301	G302	G303	G304	G305	G306	G307	G308	G309	G310	G311	G312	G313	G314	G315	G316	G317	G318	G319	G320	G321	G322	G323	G324	G325	G326	G327	G328	G329	G330	G331	G332	G333	G334	G335	G336	G337	G338	G339	G340	G341	G342	G343	G344	G345	G346	G347	G348	G349	G350	G351	G352	G353	G354	G355	G356	G357	G358	G359	G360	G361	G362	G363	G364	G365	G366	G367	G368	G369	G370	G371	G372	G373	G374	G375	G376	G377	G378	G379	G380	G381	G382	G383	G384	G385	G386	G387	G388	G389	G390	G391	G392	G393	G394	G395	G396	G397	G398	G399	G400	G401	G402	G403	G404	G405	G406	G407	G408	G409	G410	G411	G412	G413	G414	G415	G416	G417	G418	G419	G420	G421	G422	G423	G424	G425	G426	G427	G428	G429	G430	G431	G432	G433	G434	G435	G436	G437	G438	G439	G440	G441	G442	G443	G444	G445	G446	G447	G448	G449	G450	G451	G452	G453	G454	G455	G456	G457	G458	G459	G460	G461	G462	G463	G464	G465	G466	G467	G468	G469	G470	G471	G472	G473	G474	G475	G476	G477	G478	G479	G480	G481	G482	G483	G484	G485	G486	G487	G488	G489	G490	G491	G492	G493	G494	G495	G496	G497	G498	G499	G500	G501	G502	G503	G504	G505	G506	G507	G508	G509	G510	G511	G512	G513	G514	G515	G516	G517	G518	G519	G520	G521	G522	G523	G524	G525	G526	G527	G528	G529	G530	G531	G532	G533	G534	G535	G536	G537	G538	G539	G540	G541	G542	G543	G544	G545	G546	G547	G548	G549	G550	G551	G552	G553	G554	G555	G556	G557	G558	G559	G560	G561	G562	G563	G564	G565	G566	G567	G568	G569	G570	G571	G572	G573	G574	G575	G576	G577	G578	G579	G580	G581	G582	G583	G584	G585	G586	G587	G588	G589	G590	G591	G592	G593	G594	G595	G596	G597	G598	G599	G600	G601	G602	G603	G604	G605	G606	G607	G608	G609	G610	G611	G612	G613	G614	G615	G616	G617	G618	G619	G620	G621	G622	G623	G624	G625	G626	G627	G628	G629	G630	G631	G632	G633	G634	G635	G636	G637	G638	G639	G640	G641	G642	G643	G644	G645	G646	G647	G648	G649	G650	G651	G652	G653	G654	G655	G656	G657	G658	G659	G660	G661	G662	G663	G664	G665	G666	G667	G668	G669	G670	G671	G672	G673	G674	G675	G676	G677	G678	G679	G680	G681	G682	G683	G684	G685	G686	G687	G688	G689	G690	G691	G692	G693	G694	G695	G696	G697	G698	G699	G700	G701	G702	G703	G704	G705	G706	G707	G708	G709	G710	G711	G712	G713	G714	G715	G716	G717	G718	G719	G720	G721	G722	G723	G724	G725	G726	G727	G728	G729	G730	G731	G732	G733	G734	G735	G736	G737	G738	G739	G740	G741	G742	G743	G744	G745	G746	G747	G748	G749	G750	G751	G752	G753	G754	G755	G756	G757	G758	G759	G760	G761	G762	G763	G764	G765	G766	G767	G768	G769	G770	G771	G772	G773	G774	G775	G776	G777	G778	G779	G780	G781	G782	G783	G784	G785	G786	G787	G788	G789	G790	G791	G792	G793	G794	G795	G796	G797	G798	G799	G800	G801	G802	G803	G804	G805	G806	G807	G808	G809	G810	G811	G812	G813	G814	G815	G816	G817	G818	G819	G820	G821	G822	G823	G824	G825	G826	G827	G828	G829	G830	G831	G832	G833	G834	G835	G836	G837	G838	G839	G840	G841	G842	G843	G844	G845	G846	G847	G848	G849	G850	G851	G852	G853	G854	G855	G856	G857	G858	G859	G860	G861	G862	G863	G864	G865	G866	G867	G868	G869	G870	G871	G872	G873	G874	G875	G876	G877	G878	G879	G880	G881	G882	G883	G884	G885	G886	G887	G888	G889	G890	G891	G892	G893	G894	G895	G896	G897	G898	G899	G900	G901	G902	G903	G904	G905	G906	G907	G908	G909	G910	G911	G912	G913	G914	G915	G916	G917	G918	G919	G920	G921	G922	G923	G924	G925	G926	G927	G928	G929	G930	G931	G932	G933	G934	G935	G936	G937	G938	G939	G940	G941	G942	G943	G944	G945	G946	G947	G948	G949	G950	G951	G952	G953	G954	G955	G956	G957	G958	G959	G960	G961	G962	G963	G964	G965	G966	G967	G968	G969	G970	G971	G972	G973	G974	G975	G976	G977	G978	G979	G980	G981	G982	G983	G984	G985	G986	G987	G988	G989	G990	G991	G992	G993	G994	G995	G996	G997	G998	G999	G1000
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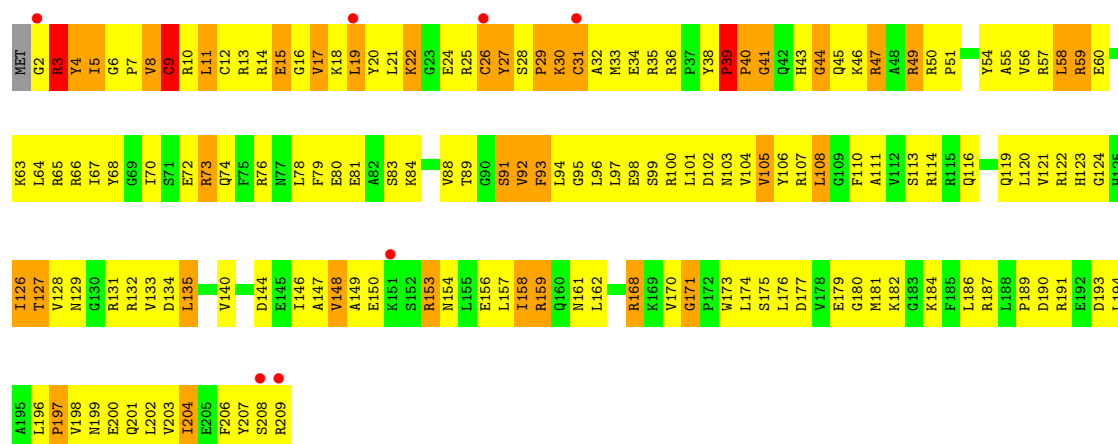


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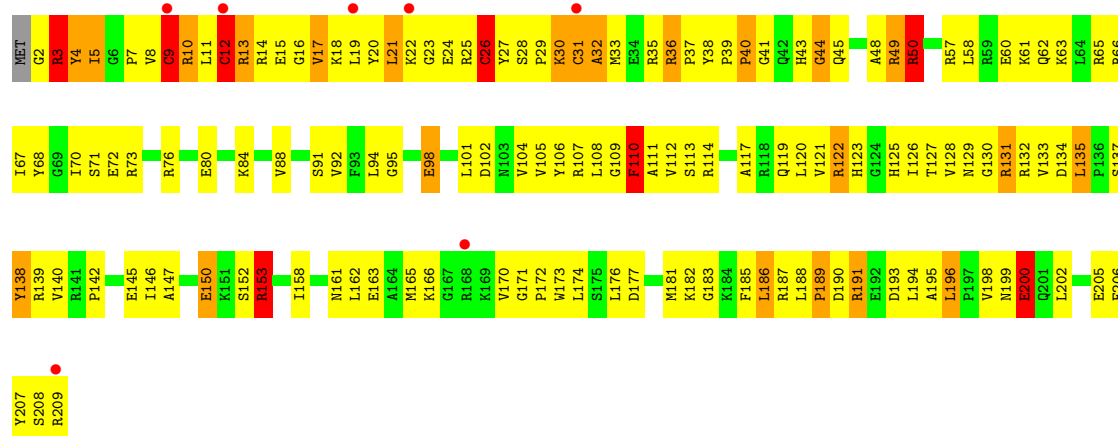




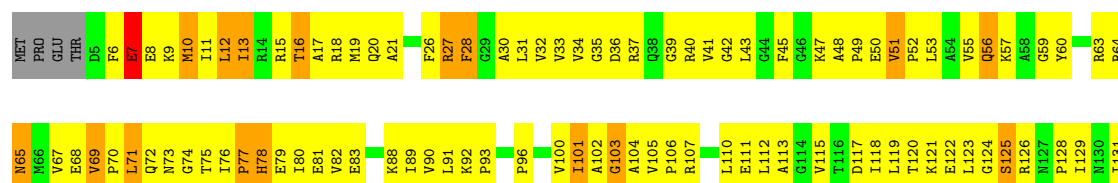
• Molecule 4: 30S ribosomal protein S4

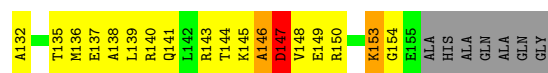


• Molecule 4: 30S ribosomal protein S4

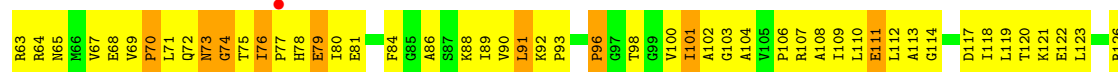
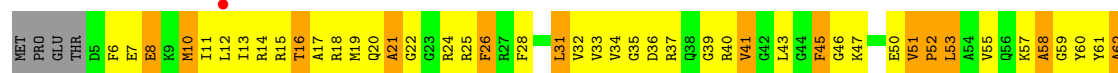


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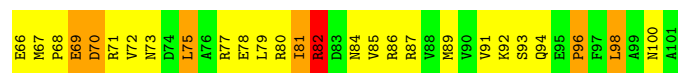




• Molecule 5: 30S ribosomal protein S5



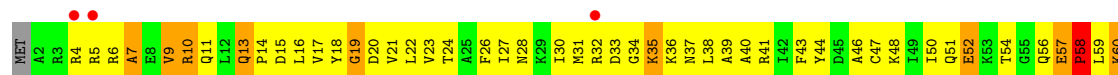
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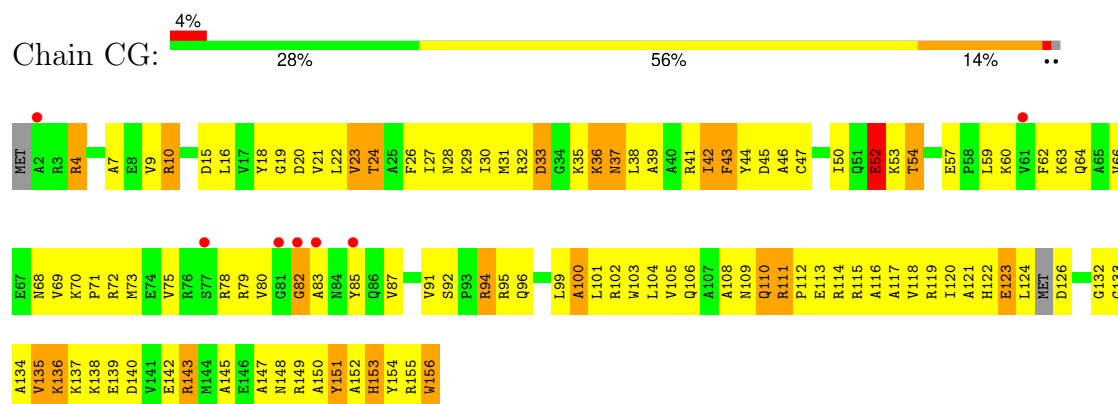
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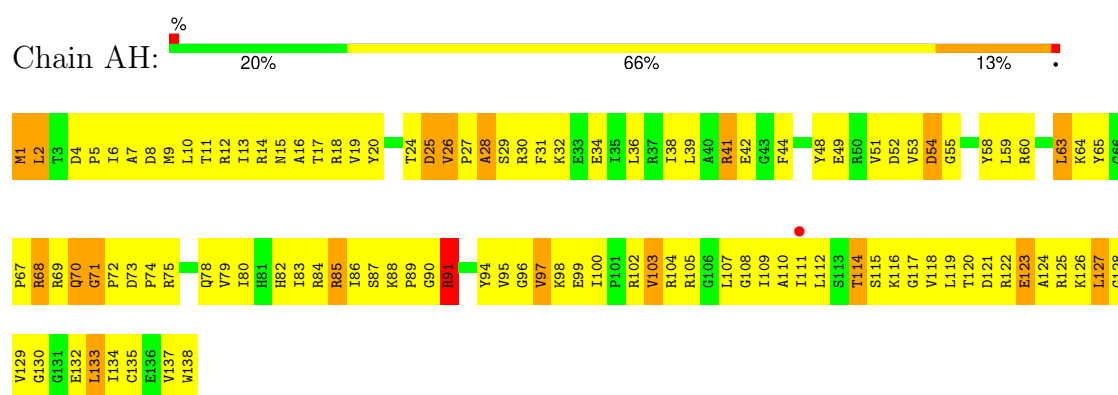
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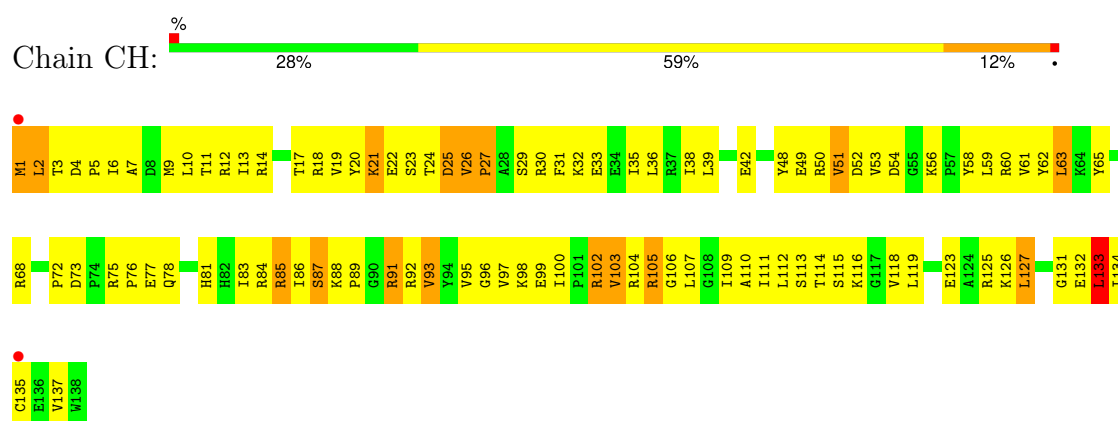
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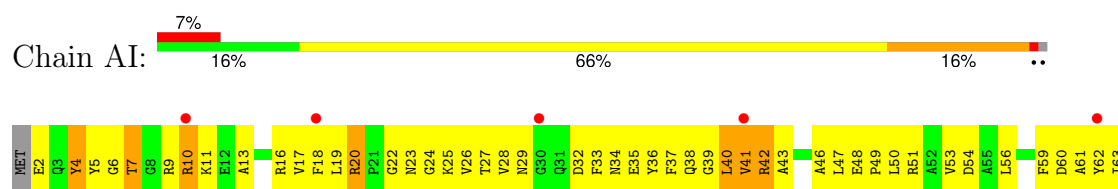
- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

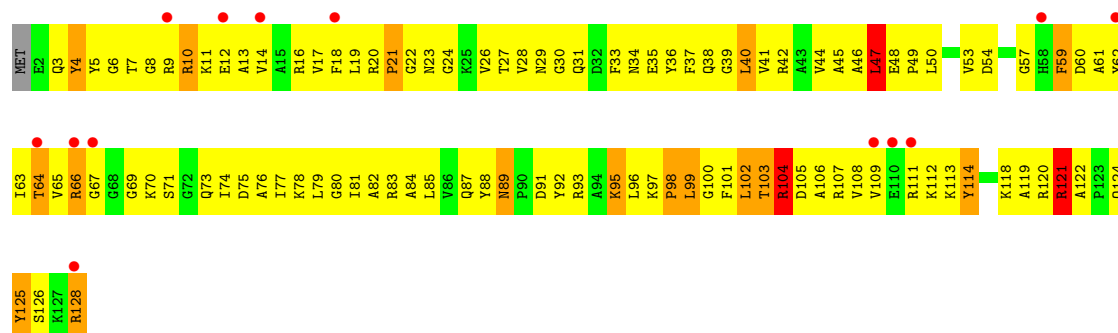


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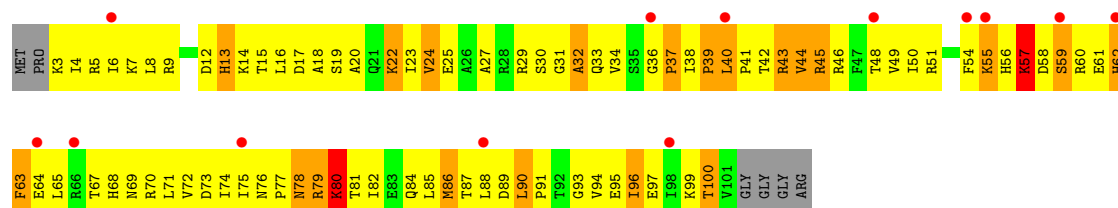
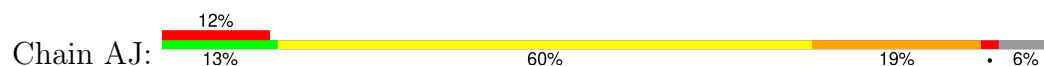




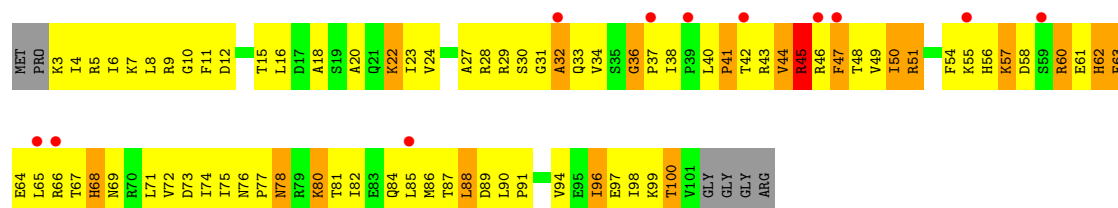
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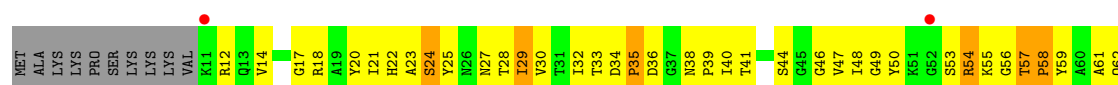
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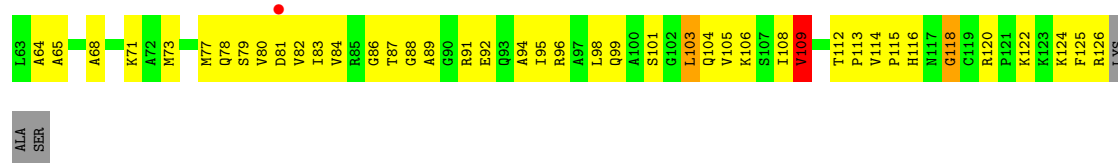


• Molecule 10: 30S ribosomal protein S10



• Molecule 11: 30S ribosomal protein S11

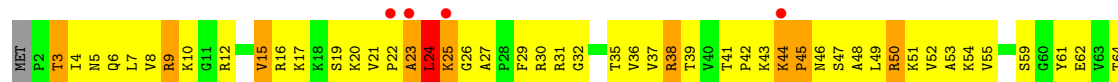




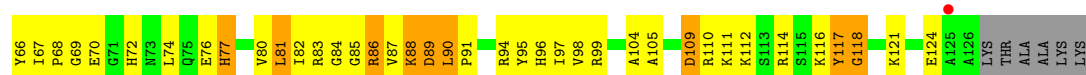
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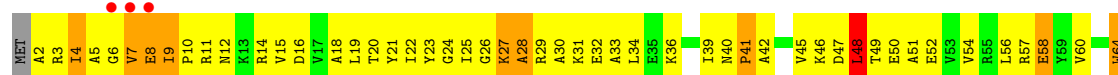
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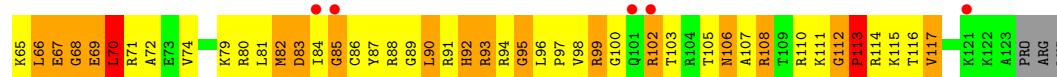


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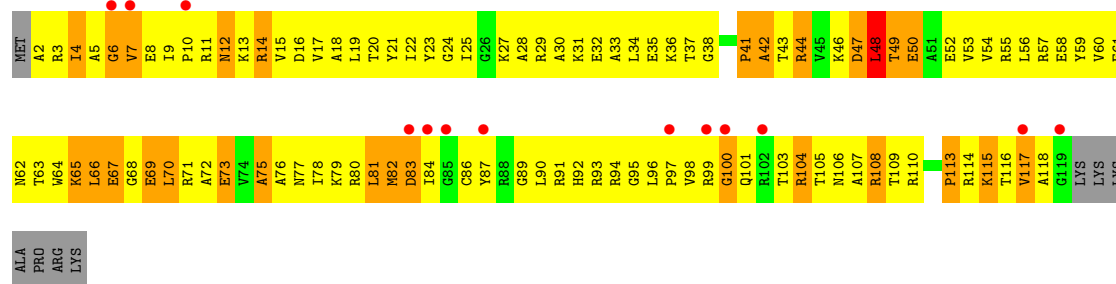
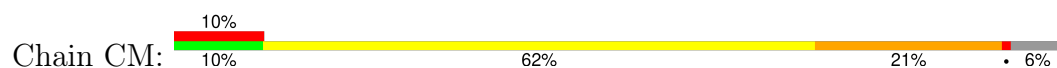


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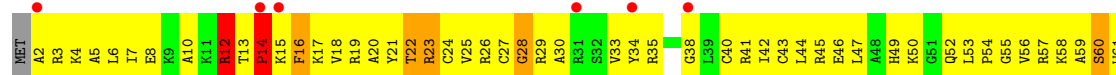
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- Molecule 14: 30S ribosomal protein S14



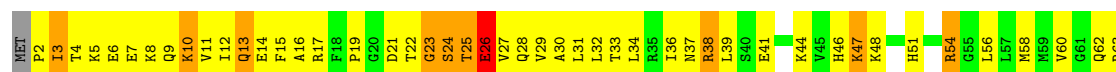
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- Molecule 15: 30S ribosomal protein S15

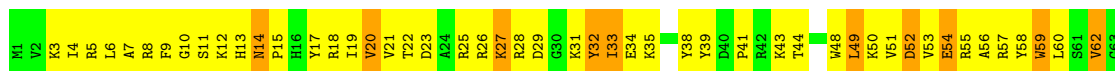


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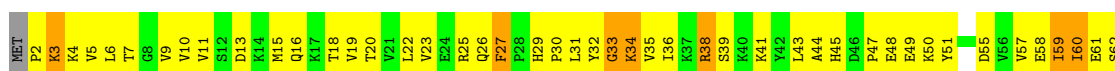
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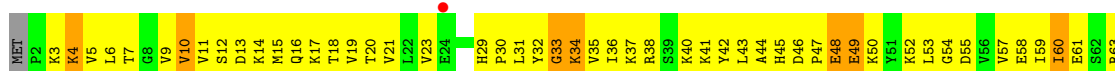
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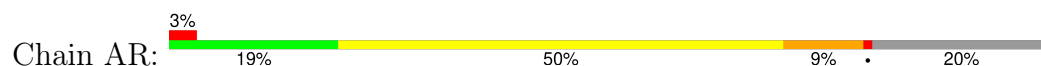
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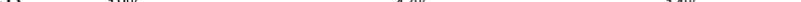
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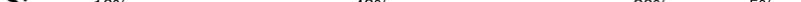
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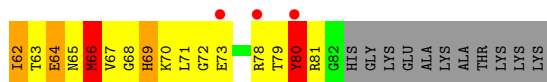


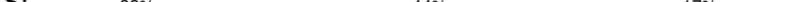


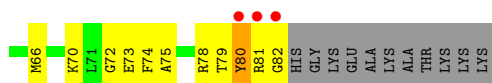
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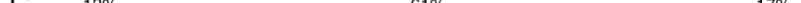


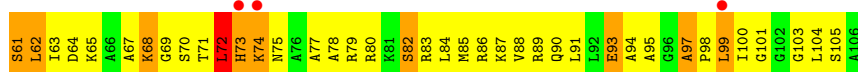
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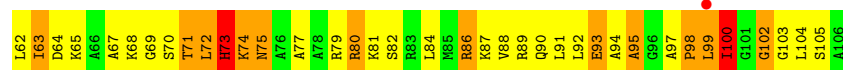
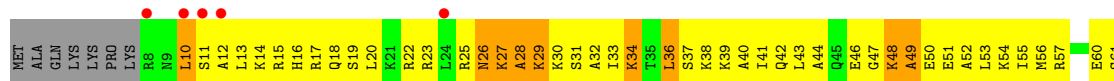
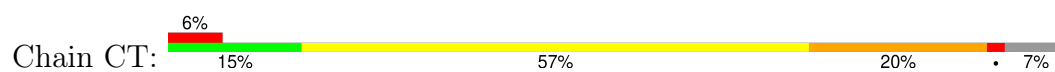


Chain CS: 



Chain AT: 





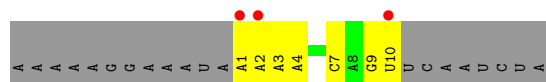
- Molecule 21: 30S ribosomal protein Thx



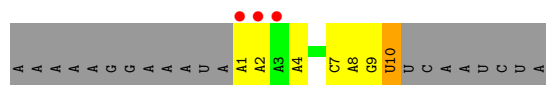
- Molecule 21: 30S ribosomal protein Thx



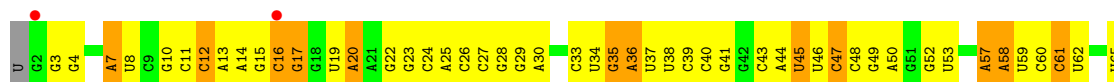
- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')



- Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')

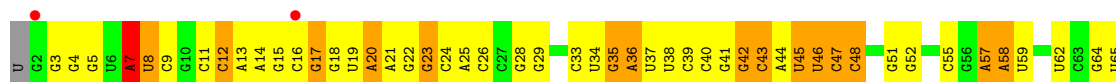


- Molecule 23: tRNA-Gln

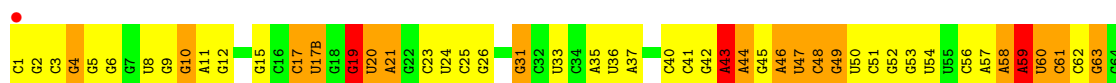




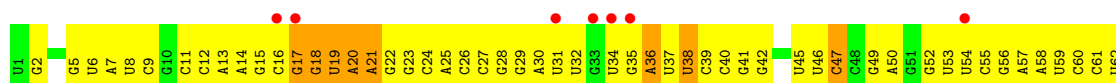
- Molecule 23: tRNA-Gln



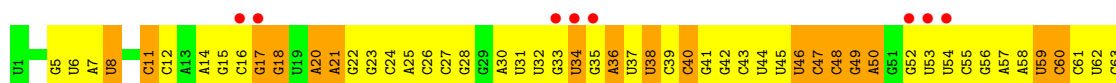
- Molecule 24: tRNA-Met



- Molecule 25: tRNA-Gln



- Molecule 25: tRNA-Gln

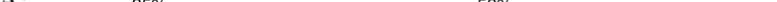


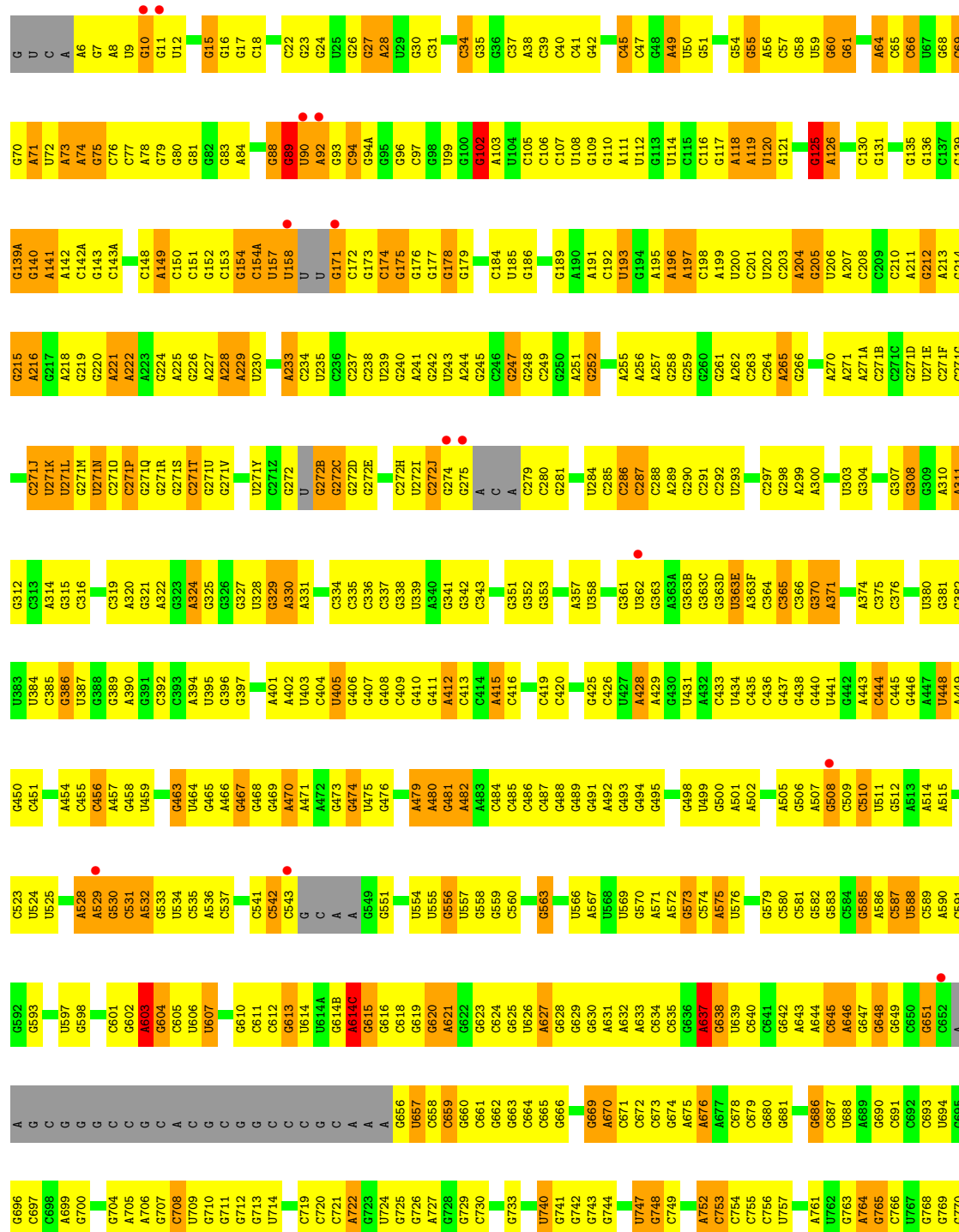
- Molecule 26: capreomycin IA



- Molecule 26: capreomycin IA

KBE1	A2	UAL3	MYN4	A5	S6
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Chain BA: 



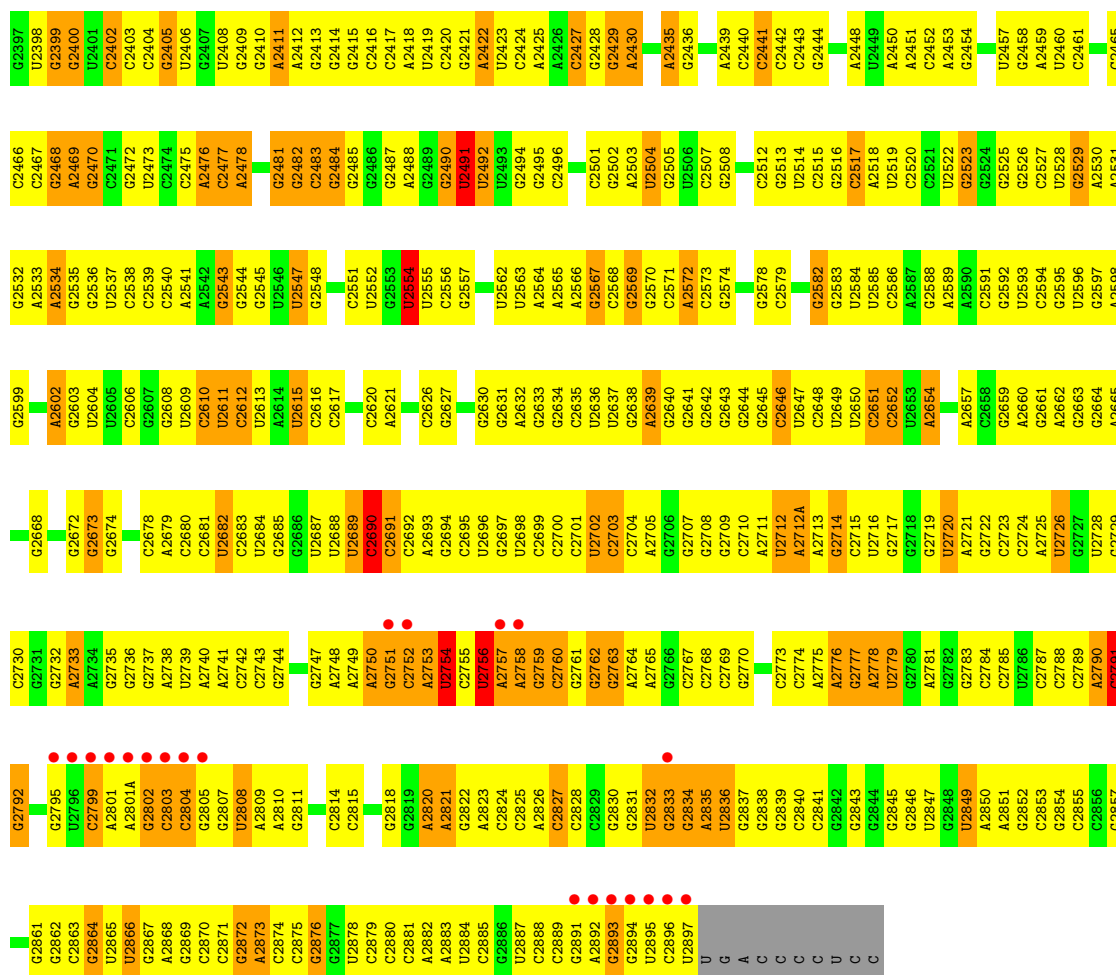




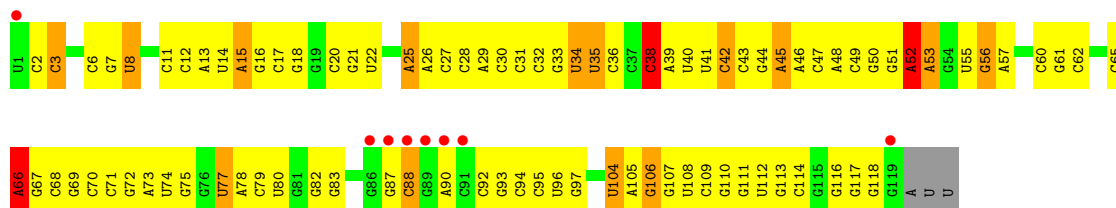




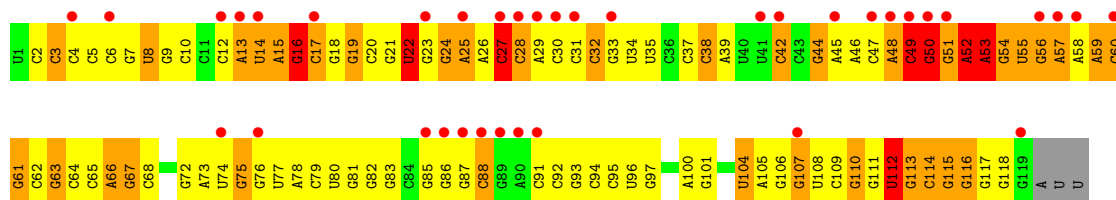
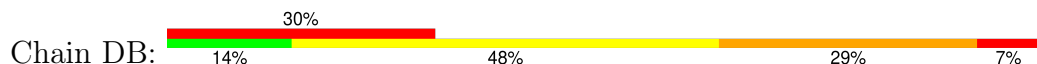
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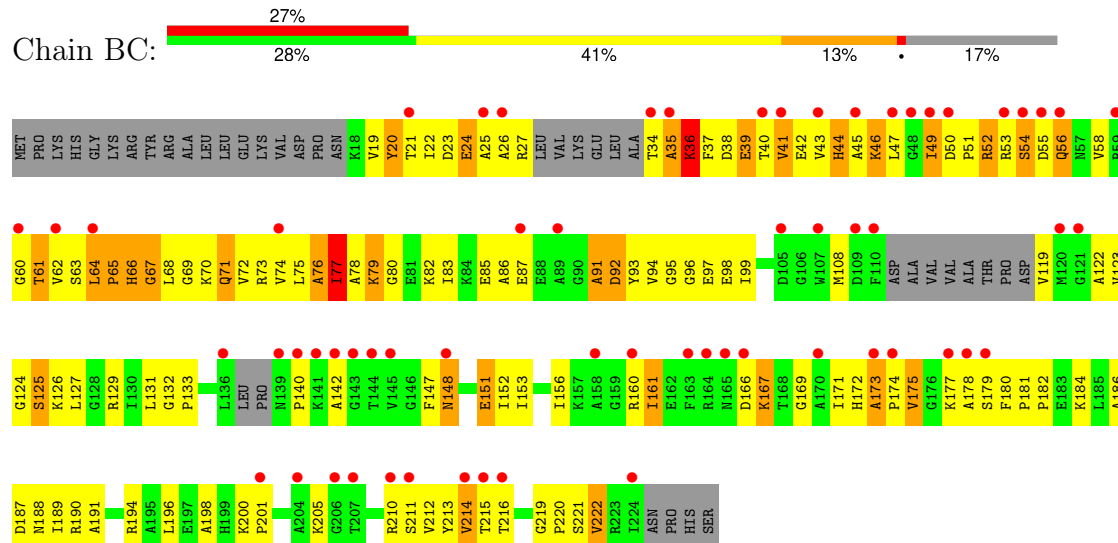
• Molecule 28: 5S ribosomal RNA



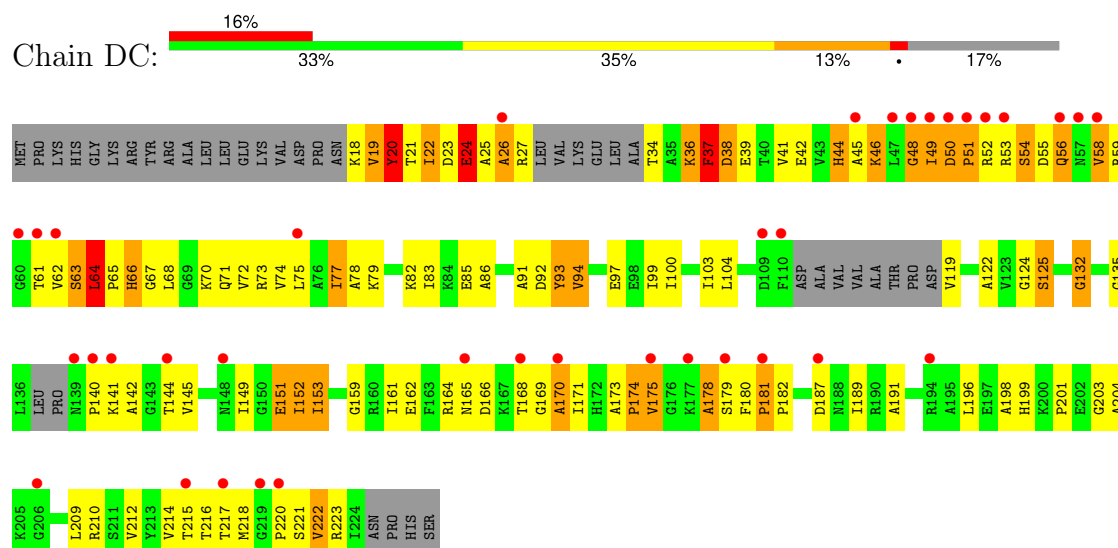
• Molecule 28: 5S ribosomal RNA



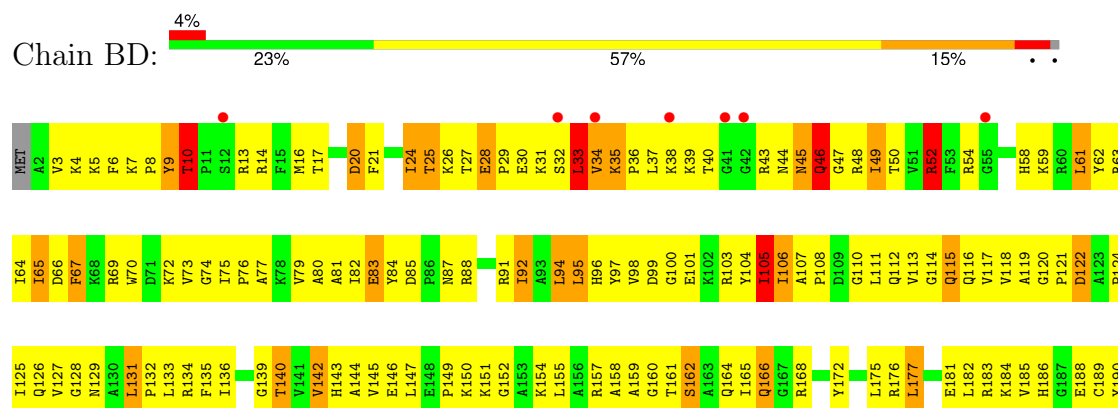
- Molecule 29: 50S ribosomal protein L1

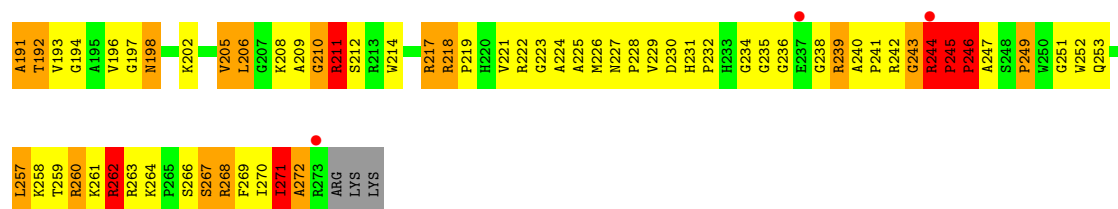


- Molecule 29: 50S ribosomal protein L1

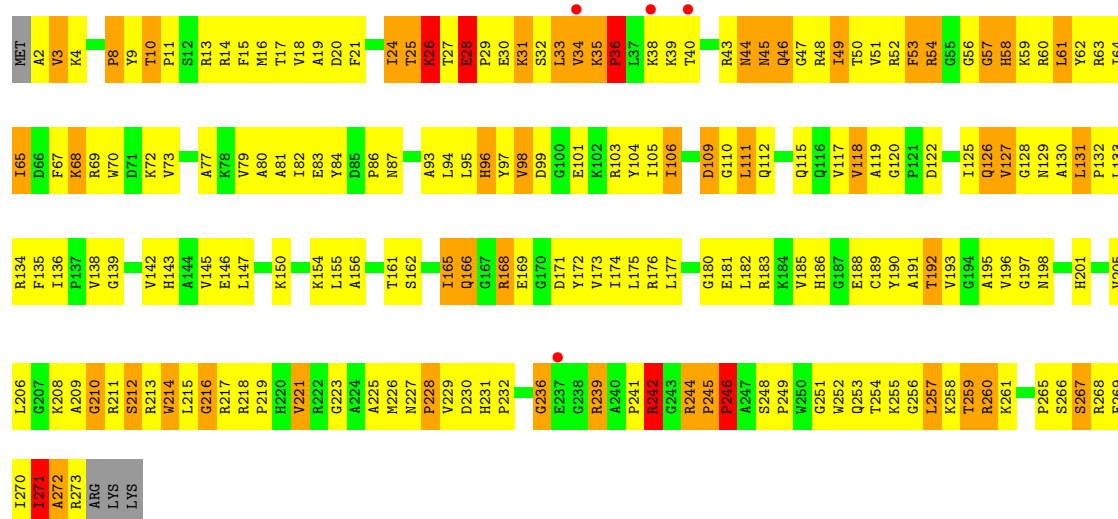


- Molecule 30: 50S ribosomal protein L2

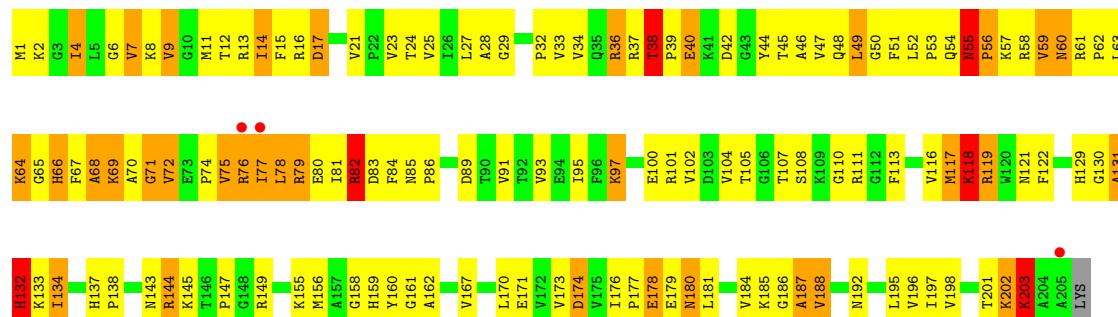




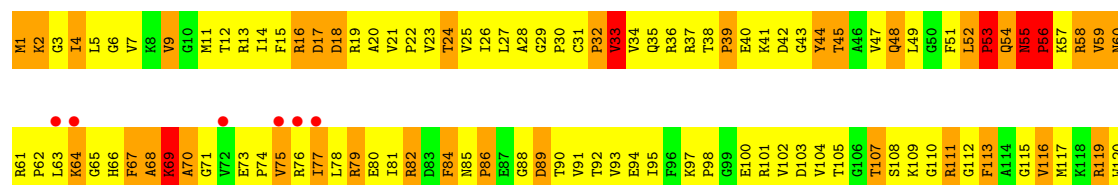
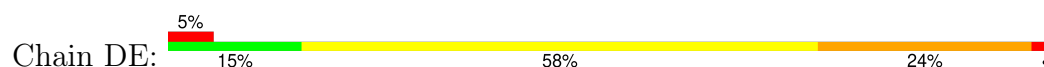
• Molecule 30: 50S ribosomal protein L2

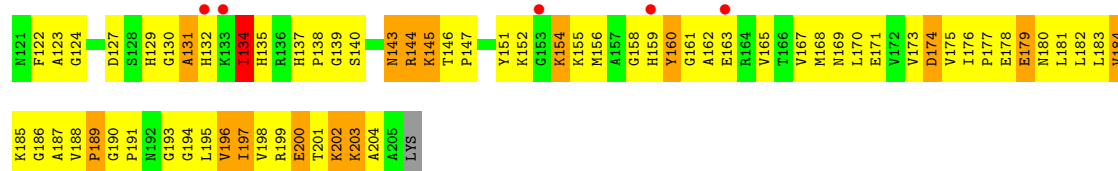


• Molecule 31: 50S ribosomal protein L3

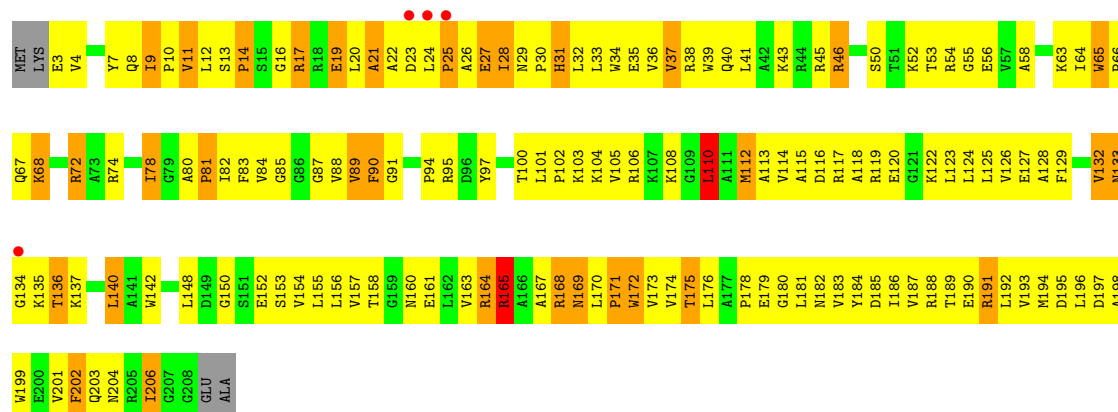


• Molecule 31: 50S ribosomal protein L3

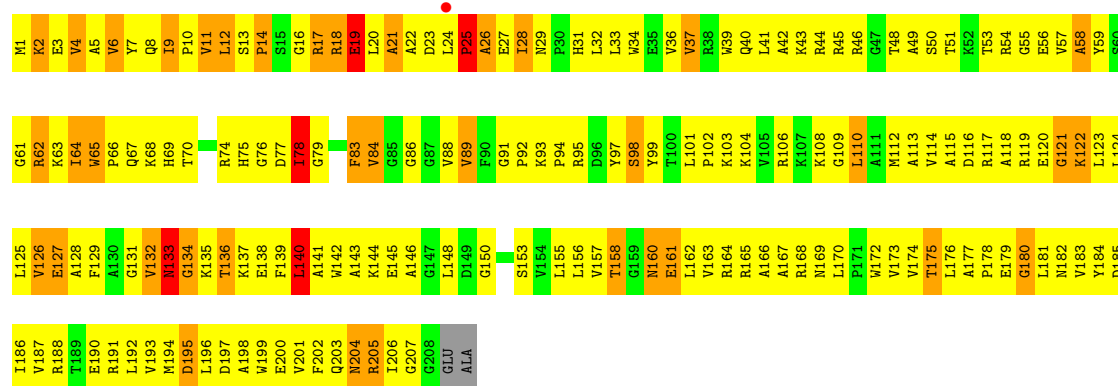




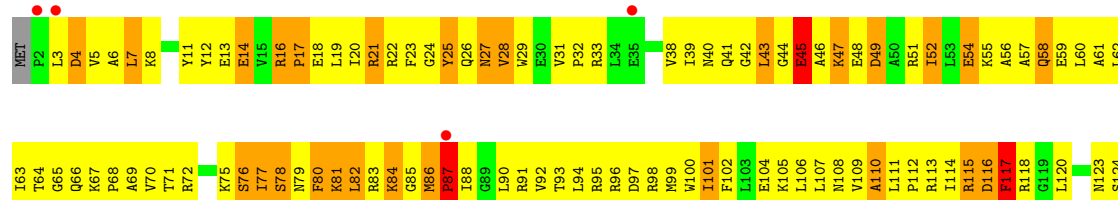
• Molecule 32: 50S ribosomal protein L4

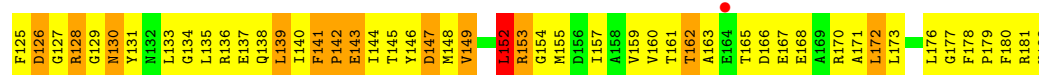


• Molecule 32: 50S ribosomal protein L4

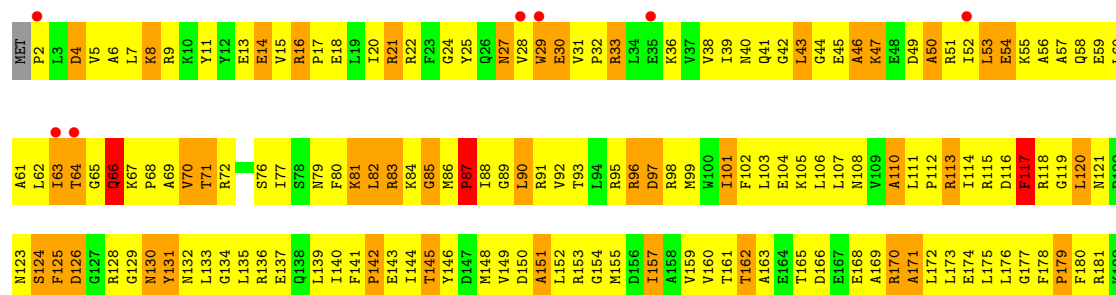
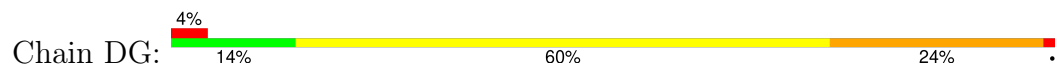


• Molecule 33: 50S ribosomal protein L5

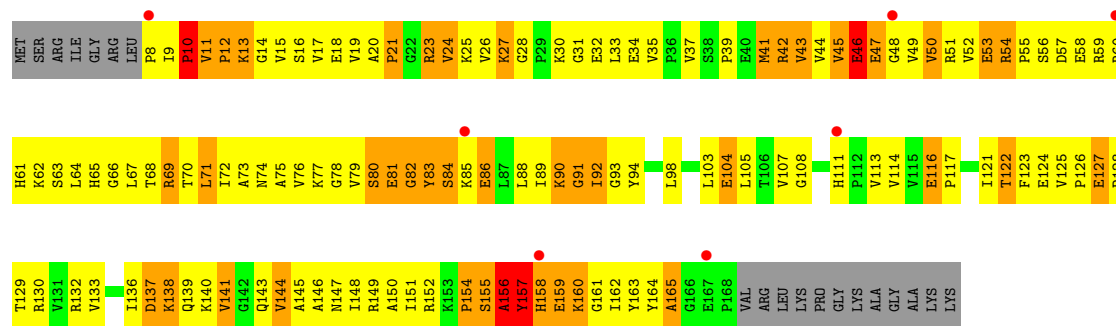
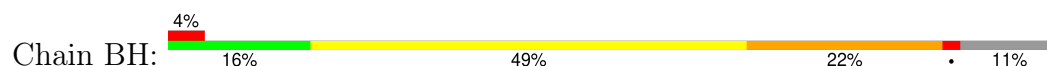




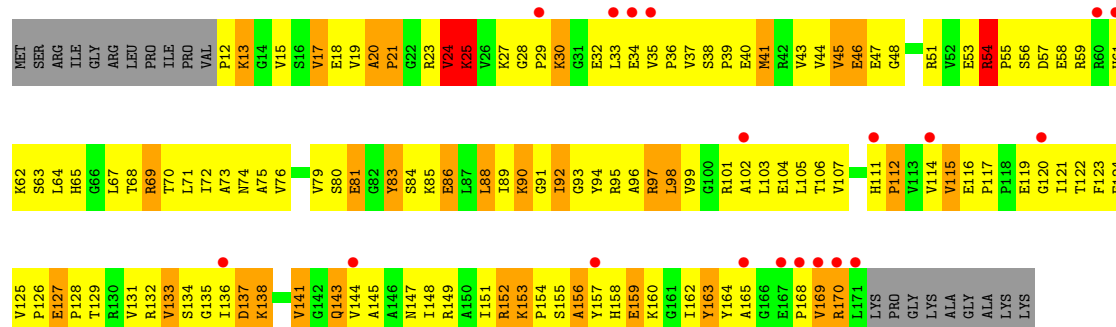
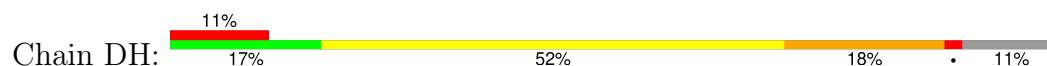
- Molecule 33: 50S ribosomal protein L5



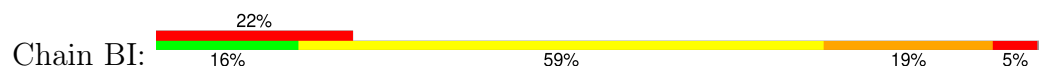
- Molecule 34: 50S ribosomal protein L6

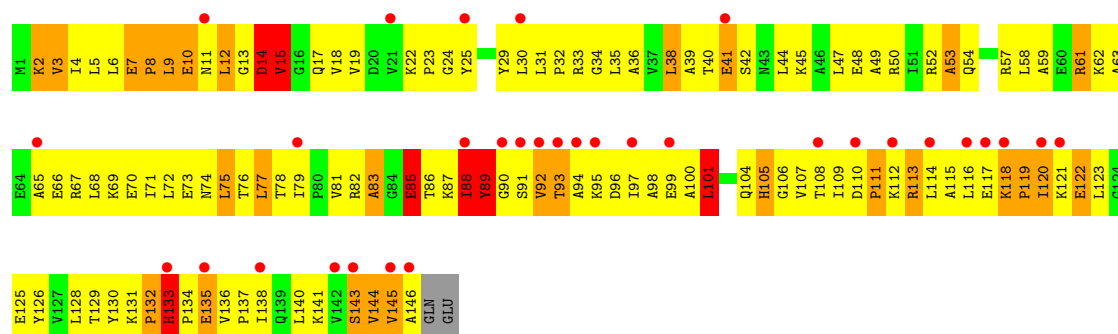


- Molecule 34: 50S ribosomal protein L6

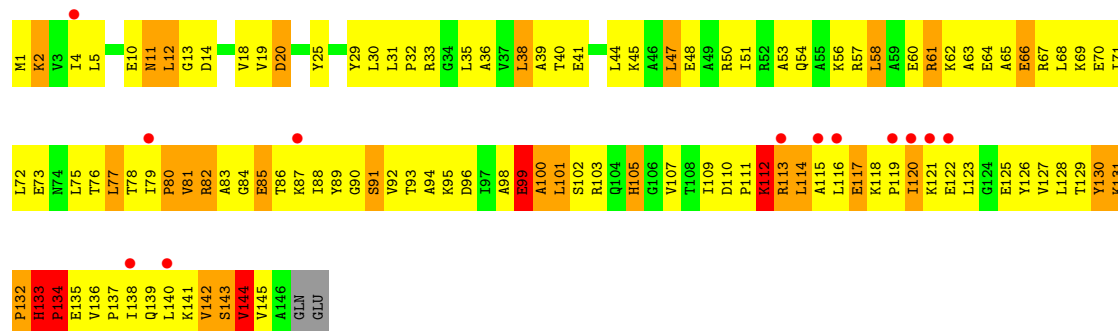


- Molecule 35: 50S ribosomal protein L9

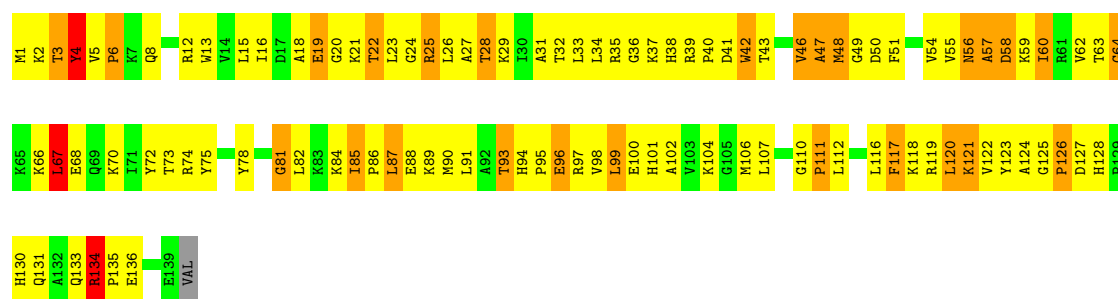




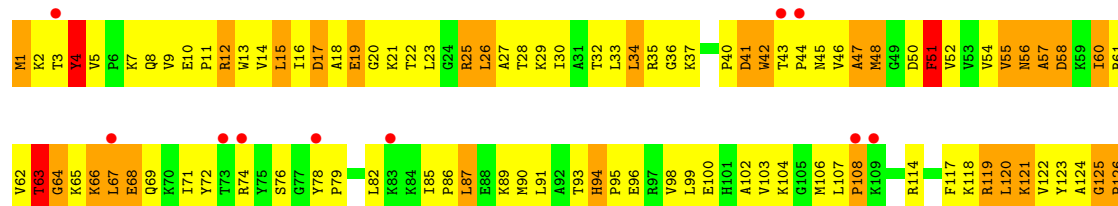
• Molecule 35: 50S ribosomal protein L9



• Molecule 36: 50S ribosomal protein L13

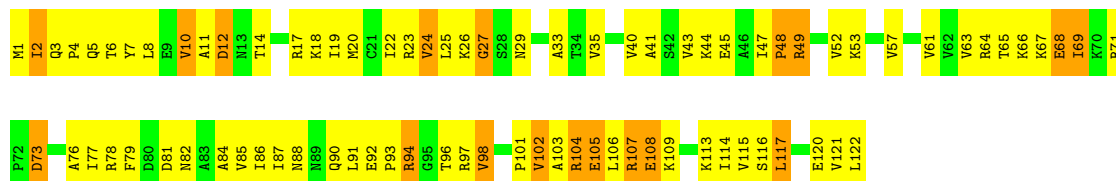


• Molecule 36: 50S ribosomal protein L13

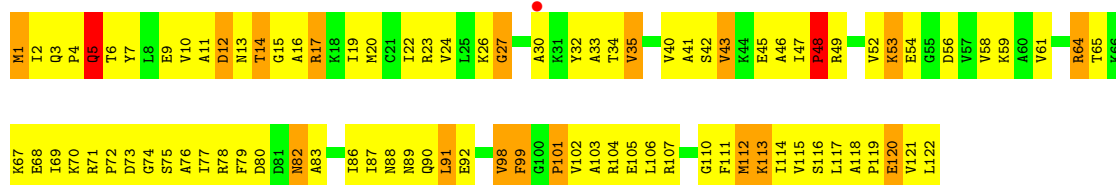




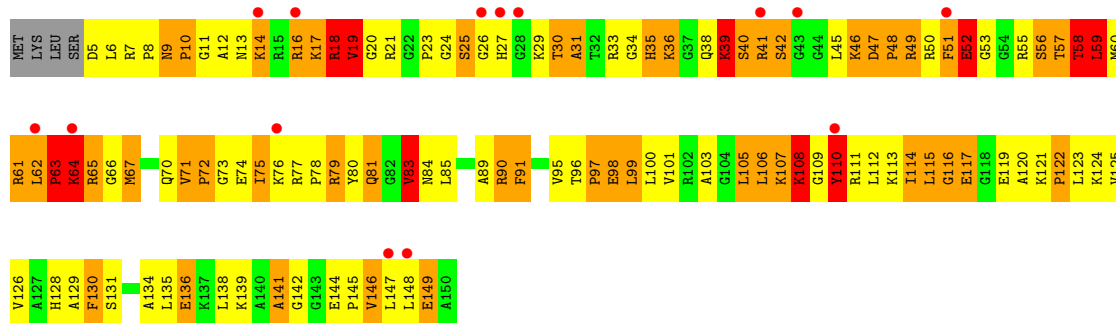
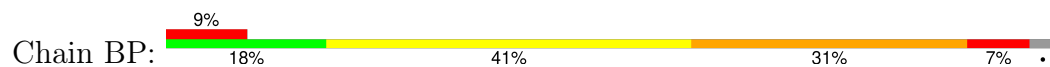
- Molecule 37: 50S ribosomal protein L14



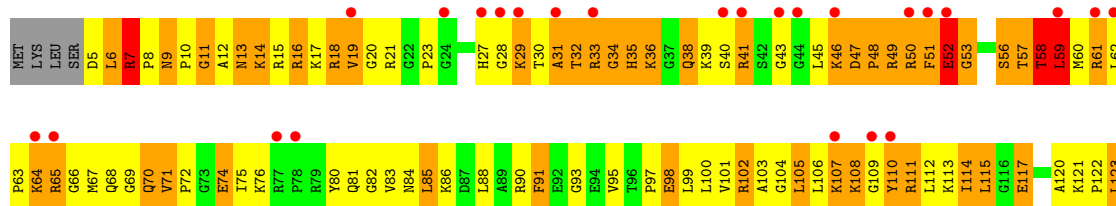
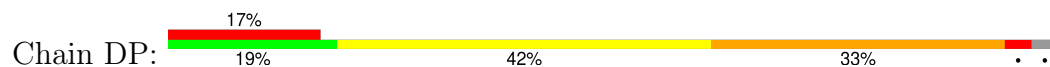
- Molecule 37: 50S ribosomal protein L14



- Molecule 38: 50S ribosomal protein L15

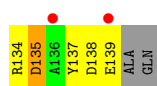


- Molecule 38: 50S ribosomal protein L15

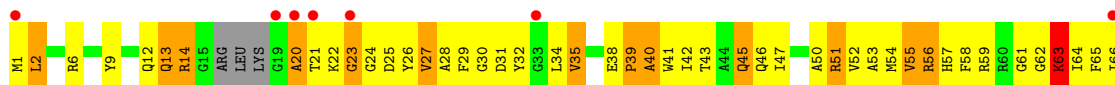




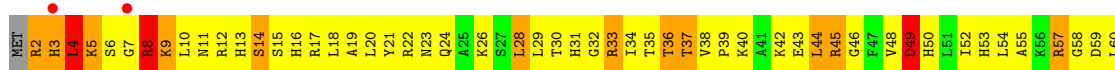
• Molecule 39: 50S ribosomal protein L16



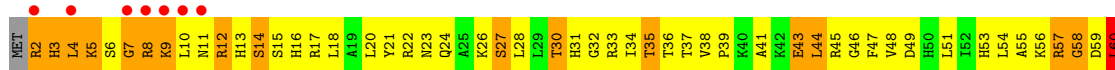
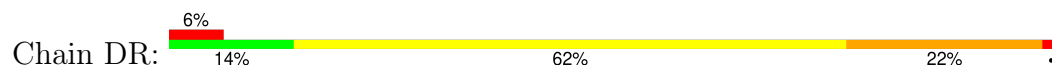
• Molecule 39: 50S ribosomal protein L16



• Molecule 40: 50S ribosomal protein L17

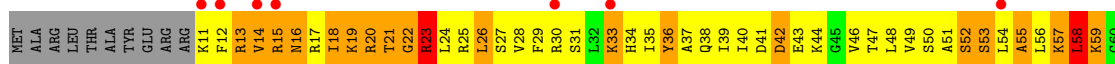


• Molecule 40: 50S ribosomal protein L17

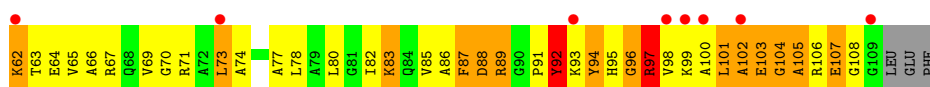
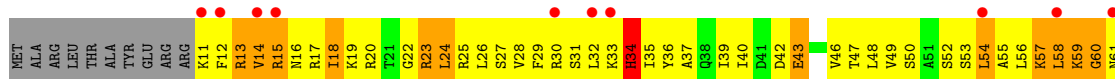
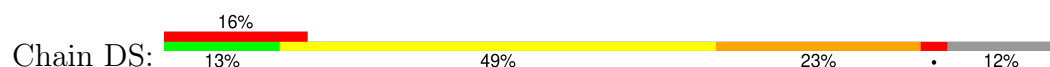




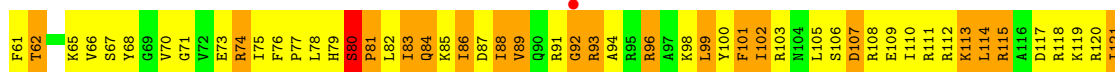
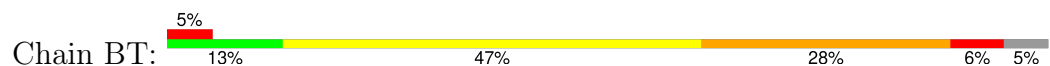
• Molecule 41: 50S ribosomal protein L18



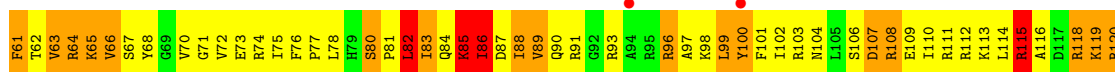
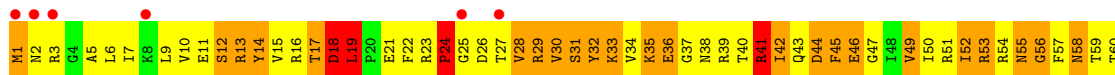
• Molecule 41: 50S ribosomal protein L18



• Molecule 42: 50S ribosomal protein L19

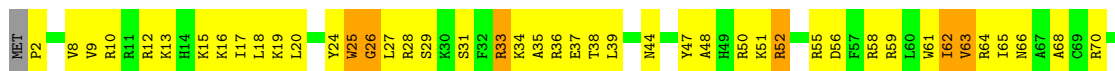


• Molecule 42: 50S ribosomal protein L19

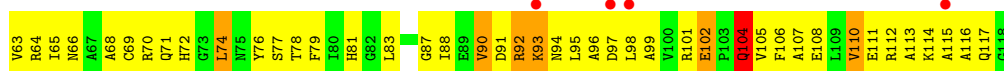
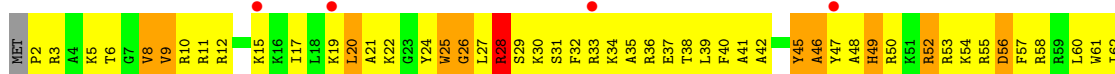




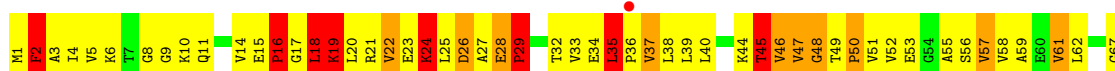
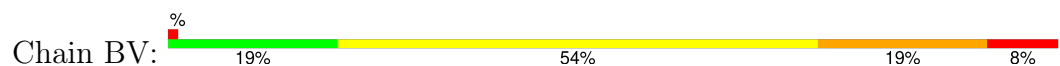
- Molecule 43: 50S ribosomal protein L20



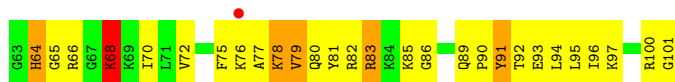
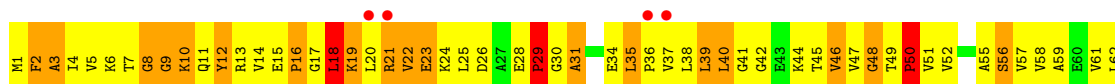
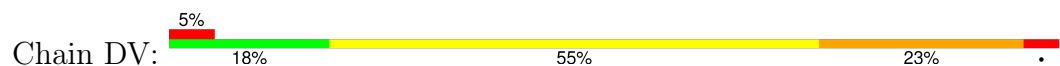
- Molecule 43: 50S ribosomal protein L20



- Molecule 44: 50S ribosomal protein L21

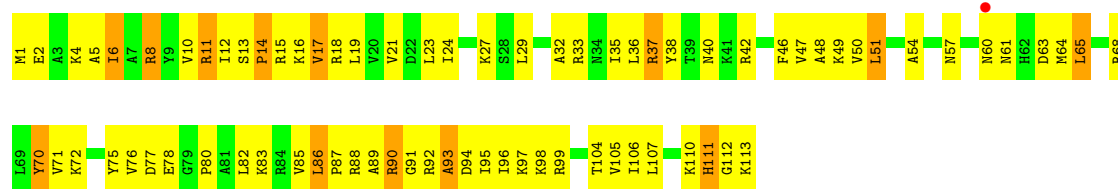


- Molecule 44: 50S ribosomal protein L21

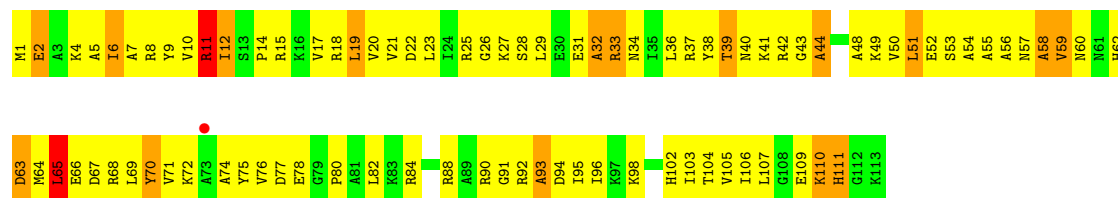


- Molecule 45: 50S ribosomal protein L22

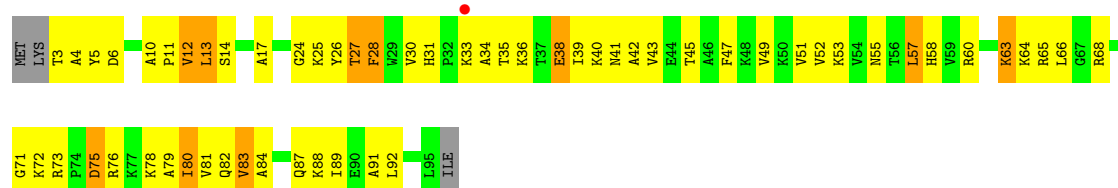




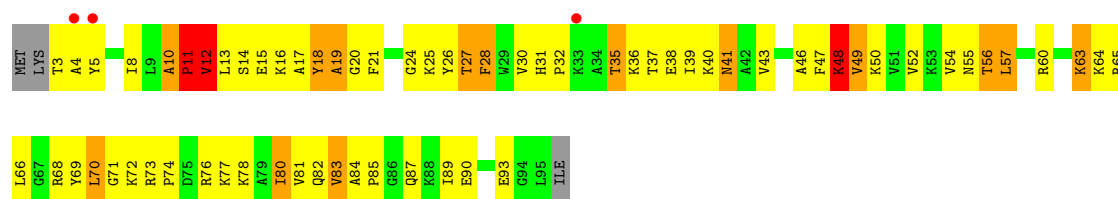
• Molecule 45: 50S ribosomal protein L22



• Molecule 46: 50S ribosomal protein L23



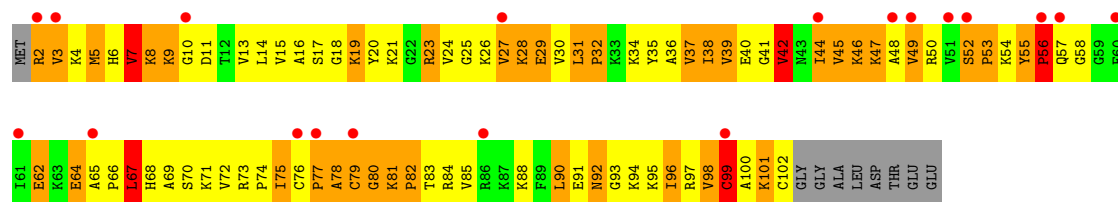
• Molecule 46: 50S ribosomal protein L23



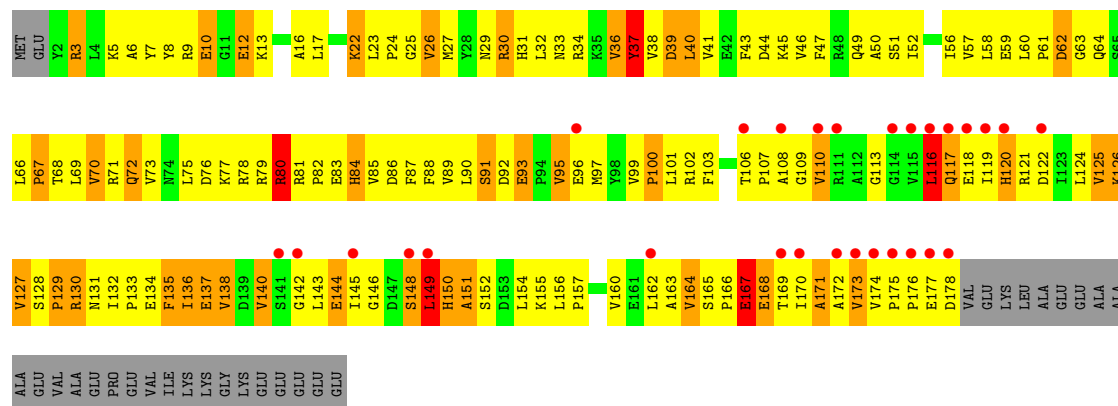
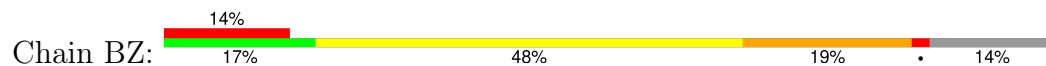
• Molecule 47: 50S ribosomal protein L24



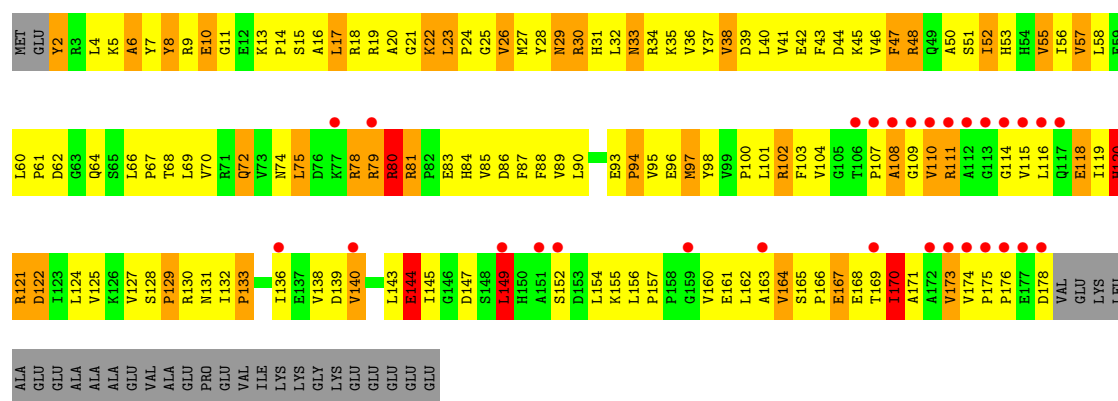
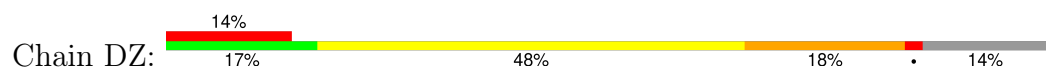
• Molecule 47: 50S ribosomal protein L24



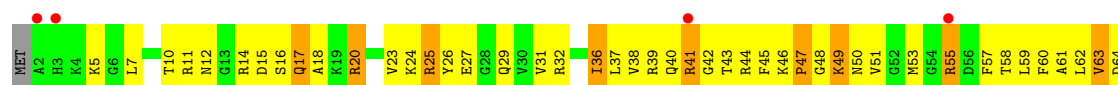
• Molecule 48: 50S ribosomal protein L25

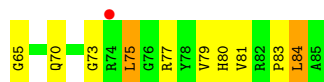


• Molecule 48: 50S ribosomal protein L25

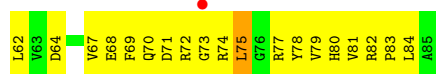


• Molecule 49: 50S ribosomal protein L27

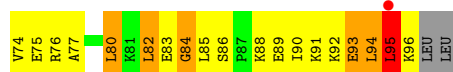




• Molecule 49: 50S ribosomal protein L27



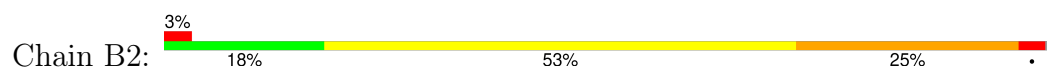
• Molecule 50: 50S ribosomal protein L28



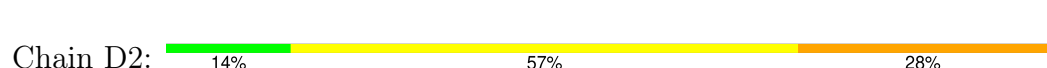
• Molecule 50: 50S ribosomal protein L28

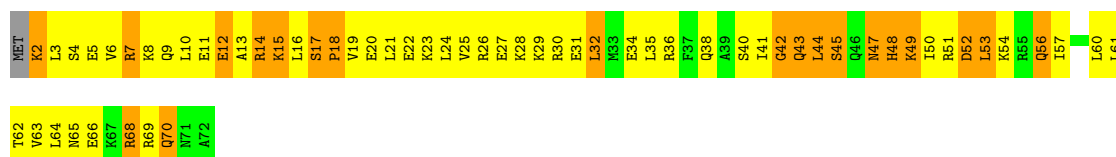


• Molecule 51: 50S ribosomal protein L29



• Molecule 51: 50S ribosomal protein L29





- Molecule 52: 50S ribosomal protein L30

Chain B3: 22% 67% 12%



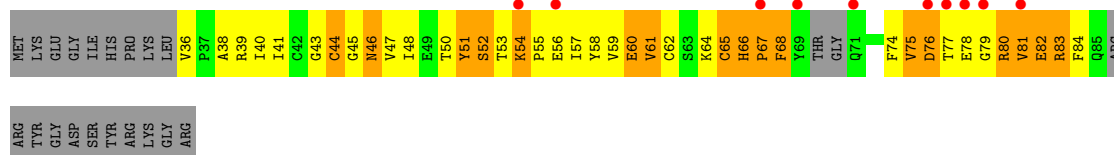
- Molecule 52: 50S ribosomal protein L30

Chain D3: 2% 20% 68% 10%



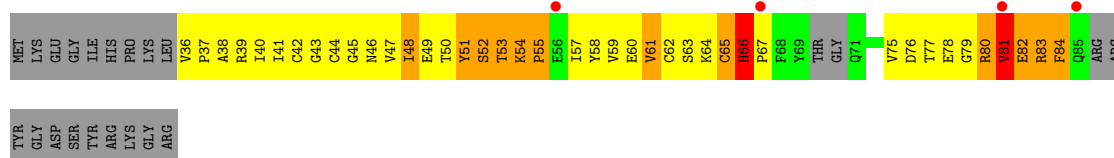
- Molecule 53: 50S ribosomal protein L31

Chain B4: 14% 13% 32% 24% 31%



- Molecule 53: 50S ribosomal protein L31

Chain D4: 6% 11% 38% 17% 31%



- Molecule 54: 50S ribosomal protein L32

Chain B5: 7% 23% 55% 15% 5%



- Molecule 54: 50S ribosomal protein L32

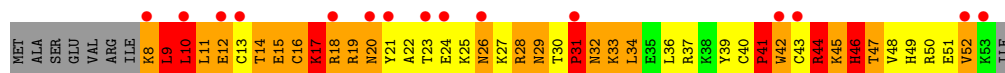
Chain D5: 7% 35% 43% 15% 5%



- Molecule 55: 50S ribosomal protein L33



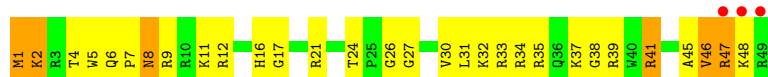
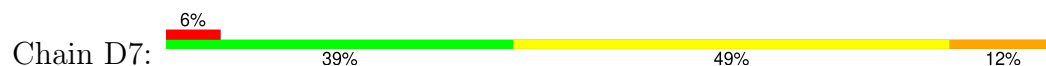
- Molecule 55: 50S ribosomal protein L33



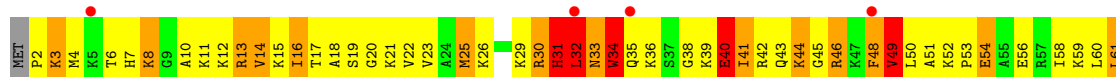
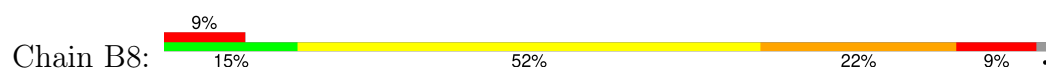
- Molecule 56: 50S ribosomal protein L34



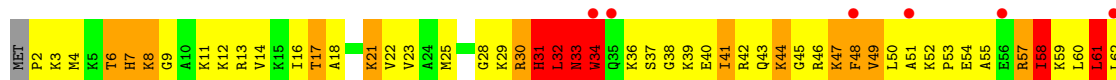
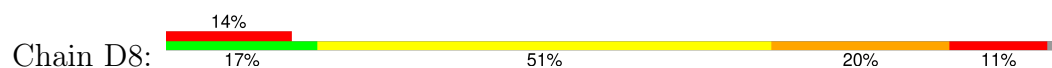
- Molecule 56: 50S ribosomal protein L34



- Molecule 57: 50S ribosomal protein L35

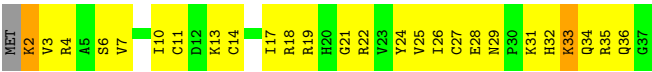
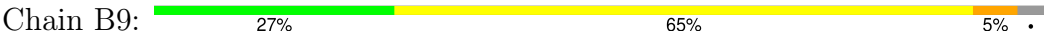


- Molecule 57: 50S ribosomal protein L35

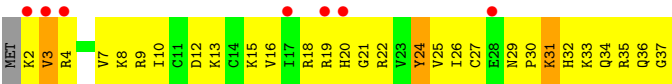




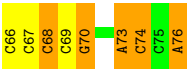
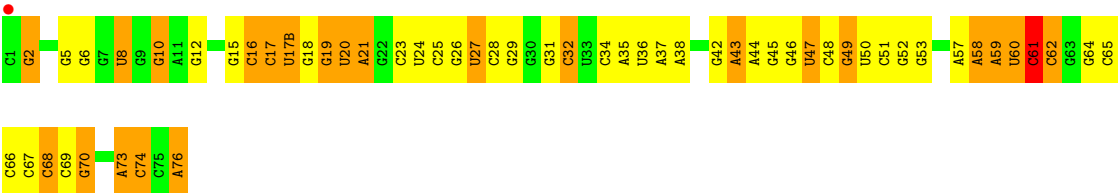
● Molecule 58: 50S ribosomal protein L36



● Molecule 58: 50S ribosomal protein L36



● Molecule 59: RNA (77-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.35Å 448.24Å 631.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.45 50.00 – 3.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.45) 85.3 (50.00-3.45)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.268 0.218 , 0.217	Depositor DCC
R_{free} test set	33186 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	293848	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.48	0/35968	0.74	23/56136 (0.0%)
1	CA	0.50	9/35932 (0.0%)	0.75	27/56082 (0.0%)
2	AB	0.39	0/1936	0.68	0/2611
2	CB	0.37	0/1936	0.66	0/2611
3	AC	0.38	0/1637	0.65	0/2207
3	CC	0.37	0/1627	0.67	0/2192
4	AD	0.42	0/1733	0.71	0/2318
4	CD	0.44	0/1733	0.72	1/2318 (0.0%)
5	AE	0.41	0/1163	0.68	0/1566
5	CE	0.42	0/1163	0.68	0/1566
6	AF	0.44	0/856	0.75	1/1154 (0.1%)
6	CF	0.43	0/856	0.71	0/1154
7	AG	0.38	0/1276	0.61	0/1709
7	CG	0.39	0/1267	0.62	0/1696
8	AH	0.40	0/1136	0.72	0/1527
8	CH	0.38	0/1136	0.70	0/1527
9	AI	0.38	0/1024	0.68	0/1372
9	CI	0.36	0/1024	0.67	0/1372
10	AJ	0.36	0/808	0.66	0/1087
10	CJ	0.36	0/808	0.67	0/1087
11	AK	0.41	0/879	0.75	0/1187
11	CK	0.39	0/900	0.68	0/1213
12	AL	0.44	0/987	0.80	0/1322
12	CL	0.44	0/987	0.74	0/1322
13	AM	0.37	0/975	0.75	2/1305 (0.2%)
13	CM	0.36	0/947	0.72	0/1270
14	AN	0.41	0/501	0.69	0/664
14	CN	0.45	0/501	0.67	0/664
15	AO	0.39	0/745	0.64	0/992
15	CO	0.37	0/745	0.64	0/992
16	AP	0.40	0/717	0.70	0/965
16	CP	0.43	0/717	0.74	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	0/837	0.67	0/1119
17	CQ	0.40	0/837	0.68	0/1119
18	AR	0.48	0/579	0.75	0/768
18	CR	0.41	0/579	0.72	0/768
19	AS	0.40	0/643	0.70	1/867 (0.1%)
19	CS	0.37	0/643	0.66	0/867
20	AT	0.38	0/765	0.72	1/1007 (0.1%)
20	CT	0.37	0/765	0.70	0/1007
21	AU	0.42	0/213	0.60	0/279
21	CU	0.34	0/213	0.62	0/279
22	AV	0.48	0/230	0.65	0/357
22	CV	0.45	0/239	0.69	0/371
23	AW	0.47	0/1756	0.78	0/2734
23	CW	0.46	0/1756	0.75	2/2734 (0.1%)
24	AX	0.58	2/1831 (0.1%)	0.87	6/2853 (0.2%)
25	AY	0.37	0/1776	0.71	0/2766
25	CY	0.36	0/1776	0.71	0/2766
26	AZ	0.91	0/5	0.51	0/5
26	CZ	0.51	0/5	0.85	0/5
27	BA	0.61	3/67273 (0.0%)	0.79	62/105005 (0.1%)
27	DA	0.51	1/66930 (0.0%)	0.77	45/104469 (0.0%)
28	BB	0.57	0/2853	0.81	6/4451 (0.1%)
28	DB	0.79	6/2853 (0.2%)	0.95	13/4451 (0.3%)
29	BC	0.31	0/1145	0.60	0/1556
29	DC	0.30	0/1145	0.61	0/1556
30	BD	0.54	0/2155	0.86	3/2907 (0.1%)
30	DD	0.51	0/2155	0.82	2/2907 (0.1%)
31	BE	0.56	0/1597	0.87	2/2155 (0.1%)
31	DE	0.42	0/1597	0.75	0/2155
32	BF	0.50	0/1642	0.82	1/2225 (0.0%)
32	DF	0.42	0/1659	0.75	1/2246 (0.0%)
33	BG	0.44	0/1499	0.78	0/2016
33	DG	0.40	0/1499	0.72	0/2016
34	BH	0.59	0/1258	0.91	2/1703 (0.1%)
34	DH	0.33	0/1246	0.67	0/1684
35	BI	0.39	0/1147	0.74	0/1553
35	DI	0.37	0/1147	0.75	0/1553
36	BN	0.54	0/1132	0.91	2/1527 (0.1%)
36	DN	0.41	0/1132	0.77	1/1527 (0.1%)
37	BO	0.54	0/943	0.80	0/1269
37	DO	0.44	0/943	0.69	0/1269
38	BP	0.59	0/1131	1.16	5/1504 (0.3%)
38	DP	0.48	0/1131	1.00	5/1504 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	BQ	0.53	0/1128	0.77	0/1508
39	DQ	0.42	0/1114	0.68	0/1488
40	BR	0.55	0/974	0.92	2/1302 (0.2%)
40	DR	0.43	0/974	0.81	0/1302
41	BS	0.55	0/779	0.97	2/1038 (0.2%)
41	DS	0.43	0/779	0.75	0/1038
42	BT	0.57	0/1156	0.96	5/1544 (0.3%)
42	DT	0.46	0/1156	0.83	1/1544 (0.1%)
43	BU	0.57	0/975	0.85	0/1297
43	DU	0.38	0/975	0.69	0/1297
44	BV	0.58	0/790	0.95	2/1057 (0.2%)
44	DV	0.41	0/790	0.72	0/1057
45	BW	0.53	0/907	0.77	0/1216
45	DW	0.41	0/907	0.72	0/1216
46	BX	0.51	0/740	0.78	0/995
46	DX	0.48	0/740	0.73	0/995
47	BY	0.61	0/680	0.93	1/904 (0.1%)
47	DY	0.46	0/789	0.82	1/1053 (0.1%)
48	BZ	0.41	0/1436	0.72	0/1951
48	DZ	0.36	0/1436	0.70	0/1951
49	B0	0.47	0/671	0.74	0/892
49	D0	0.41	0/671	0.67	0/892
50	B1	0.49	0/739	0.76	1/983 (0.1%)
50	D1	0.43	0/739	0.76	0/983
51	B2	0.45	0/600	0.74	0/793
51	D2	0.39	0/600	0.67	0/793
52	B3	0.48	0/473	0.76	0/636
52	D3	0.34	0/473	0.63	0/636
53	B4	0.43	0/349	0.71	0/474
53	D4	0.39	0/349	0.64	0/474
54	B5	0.62	0/473	1.04	2/639 (0.3%)
54	D5	0.50	0/473	0.82	0/639
55	B6	0.72	0/409	1.07	0/548
55	D6	0.70	0/397	1.12	4/531 (0.8%)
56	B7	0.55	0/427	0.80	0/563
56	D7	0.48	0/427	0.73	0/563
57	B8	0.63	0/516	1.02	2/681 (0.3%)
57	D8	0.51	0/516	0.87	1/681 (0.1%)
58	B9	0.53	0/302	0.80	0/397
58	D9	0.39	0/302	0.70	0/397
59	CX	0.47	0/1832	0.75	1/2855 (0.0%)
All	All	0.51	21/318243 (0.0%)	0.77	239/475835 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	35
1	CA	1	31
19	AS	0	1
23	AW	0	1
23	CW	0	1
24	AX	0	1
27	BA	4	96
27	DA	0	63
28	BB	0	3
28	DB	0	6
42	BT	0	1
59	CX	0	2
All	All	5	241

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AX	46	A	C6-N6	-11.79	1.24	1.33
1	CA	101	A	C6-N6	-8.09	1.27	1.33
1	CA	1458	G	C5-C6	-7.73	1.34	1.42
1	CA	70	G	C5-C6	-7.36	1.34	1.42
1	CA	1446	U	N1-C2	-7.30	1.31	1.38

The worst 5 of 239 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AX	46	A	C5-C6-N1	-12.54	111.43	117.70
28	DB	53	A	O5'-P-OP2	11.96	125.06	110.70
24	AX	46	A	C6-N1-C2	10.83	125.10	118.60
24	AX	46	A	N1-C2-N3	-10.72	123.94	129.30
27	BA	1992	G	C2'-C3'-O3'	10.30	132.16	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	BA	1378	A	C3'
27	BA	1799	G	C3'
27	BA	1992	G	C3'

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Mol	Chain	Res	Type	Atom
27	BA	2497	A	C3'
1	CA	533	A	C3'

5 of 241 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	181	G	Sidechain
1	AA	298	A	Sidechain
1	AA	37	U	Sidechain
1	AA	388	G	Sidechain
1	AA	490	G	Sidechain

5.2 Too-close contacts [i](#)

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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32132	0	16219	1429	0
1	CA	32098	0	16199	1614	0
2	AB	1901	0	1951	312	0
2	CB	1901	0	1951	269	0
3	AC	1613	0	1677	278	0
3	CC	1604	0	1670	270	0
4	AD	1703	0	1763	264	0
4	CD	1703	0	1763	197	0
5	AE	1147	0	1207	160	0
5	CE	1147	0	1207	172	0
6	AF	843	0	857	91	0
6	CF	843	0	857	99	0
7	AG	1257	0	1296	161	0
7	CG	1249	0	1286	155	0
8	AH	1116	0	1177	165	0
8	CH	1116	0	1177	143	0
9	AI	1006	0	1034	176	0
9	CI	1006	0	1034	201	0
10	AJ	795	0	840	159	0
10	CJ	795	0	840	175	0
11	AK	864	0	881	94	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	CK	885	0	904	117	0
12	AL	971	0	1057	122	0
12	CL	971	0	1057	128	0
13	AM	965	0	1034	166	0
13	CM	937	0	995	162	0
14	AN	492	0	533	77	0
14	CN	492	0	533	108	0
15	AO	734	0	771	94	0
15	CO	734	0	771	99	0
16	AP	701	0	720	107	0
16	CP	701	0	720	96	0
17	AQ	824	0	891	114	0
17	CQ	824	0	891	125	0
18	AR	574	0	644	87	0
18	CR	574	0	644	83	0
19	AS	630	0	652	126	0
19	CS	630	0	652	110	0
20	AT	763	0	861	134	0
20	CT	763	0	861	131	0
21	AU	209	0	221	26	0
21	CU	209	0	221	24	0
22	AV	205	0	106	7	0
22	CV	213	0	110	11	0
23	AW	1573	0	800	86	0
23	CW	1573	0	800	72	0
24	AX	1639	0	835	72	0
25	AY	1591	0	810	72	0
25	CY	1591	0	810	81	0
26	AZ	47	0	40	11	0
26	CZ	47	0	40	14	0
27	BA	60072	0	30294	2481	0
27	DA	59767	0	30140	2934	0
28	BB	2551	0	1295	107	0
28	DB	2551	0	1295	201	0
29	BC	1142	0	865	119	0
29	DC	1142	0	865	116	0
30	BD	2105	0	2182	345	0
30	DD	2105	0	2182	317	0
31	BE	1564	0	1629	250	0
31	DE	1564	0	1629	346	0
32	BF	1607	0	1652	226	0
32	DF	1624	0	1677	293	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	BG	1474	0	1535	250	0
33	DG	1474	0	1535	310	0
34	BH	1233	0	1294	217	0
34	DH	1223	0	1282	184	0
35	BI	1132	0	1218	207	0
35	DI	1132	0	1218	223	0
36	BN	1105	0	1180	153	0
36	DN	1105	0	1180	195	0
37	BO	933	0	996	114	0
37	DO	933	0	996	145	0
38	BP	1114	0	1187	303	0
38	DP	1114	0	1187	329	0
39	BQ	1107	0	1166	179	0
39	DQ	1094	0	1141	150	0
40	BR	960	0	1021	148	0
40	DR	960	0	1021	182	0
41	BS	771	0	832	185	0
41	DS	771	0	832	188	0
42	BT	1142	0	1202	236	0
42	DT	1142	0	1202	303	0
43	BU	958	0	1014	151	0
43	DU	958	0	1015	187	0
44	BV	779	0	852	162	0
44	DV	779	0	852	141	0
45	BW	896	0	953	108	0
45	DW	896	0	953	135	0
46	BX	726	0	778	75	0
46	DX	726	0	778	87	0
47	BY	672	0	766	190	0
47	DY	776	0	870	211	0
48	BZ	1404	0	1432	215	0
48	DZ	1404	0	1432	266	0
49	B0	662	0	688	83	0
49	D0	662	0	688	92	0
50	B1	732	0	808	97	0
50	D1	732	0	808	98	0
51	B2	598	0	653	75	0
51	D2	598	0	653	95	0
52	B3	468	0	523	46	0
52	D3	468	0	523	71	0
53	B4	344	0	305	69	0
53	D4	344	0	305	62	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	B5	459	0	476	80	0
54	D5	459	0	477	62	0
55	B6	402	0	413	109	0
55	D6	390	0	404	135	0
56	B7	419	0	467	46	0
56	D7	419	0	467	41	0
57	B8	508	0	576	130	0
57	D8	508	0	576	138	0
58	B9	299	0	323	34	0
58	D9	299	0	323	57	0
59	CX	1640	0	837	62	0
60	AA	114	0	0	0	0
60	AG	1	0	0	0	0
60	AW	4	0	0	0	0
60	AX	9	0	0	0	0
60	B0	3	0	0	0	0
60	B5	1	0	0	0	0
60	BA	334	0	0	0	0
60	BB	5	0	0	0	0
60	BD	1	0	0	0	0
60	BE	3	0	0	0	0
60	BF	1	0	0	0	0
60	BG	1	0	0	0	0
60	BP	2	0	0	0	0
60	BR	1	0	0	0	0
60	BU	2	0	0	0	0
60	BX	1	0	0	0	0
60	CA	102	0	0	0	0
60	CE	1	0	0	0	0
60	CK	1	0	0	0	0
60	CV	1	0	0	0	0
60	CW	4	0	0	0	0
60	D0	1	0	0	0	0
60	D5	1	0	0	0	0
60	D7	1	0	0	0	0
60	DA	239	0	0	0	0
60	DB	3	0	0	0	0
60	DD	2	0	0	0	0
60	DE	1	0	0	0	0
60	DF	1	0	0	0	0
60	DO	1	0	0	0	0
61	AD	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
61	B4	1	0	0	0	0
61	B5	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	D4	1	0	0	0	0
61	D5	1	0	0	0	0
61	D9	1	0	0	0	0
All	All	293848	0	198788	22560	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 46.

The worst 5 of 22560 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:B6:15:GLU:CD	55:B6:18:ARG:HE	1.41	1.22
4:AD:19:LEU:HD11	4:AD:67:ILE:HG13	1.24	1.19
1:CA:1321:C:H3'	1:CA:1322:C:H5''	1.21	1.19
13:AM:90:LEU:HD23	13:AM:93:ARG:HG2	1.23	1.18
2:AB:166:ASP:HB3	2:AB:169:LYS:HB2	1.24	1.18

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	147 (63%)	57 (24%)	29 (12%)	0	4
2	CB	233/256 (91%)	144 (62%)	56 (24%)	33 (14%)	0	3
3	AC	205/239 (86%)	122 (60%)	53 (26%)	30 (15%)	0	3
3	CC	202/239 (84%)	116 (57%)	48 (24%)	38 (19%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AD	206/209 (99%)	138 (67%)	39 (19%)	29 (14%)	0	3
4	CD	206/209 (99%)	141 (68%)	39 (19%)	26 (13%)	0	4
5	AE	149/162 (92%)	98 (66%)	34 (23%)	17 (11%)	0	5
5	CE	149/162 (92%)	107 (72%)	27 (18%)	15 (10%)	0	6
6	AF	99/101 (98%)	74 (75%)	16 (16%)	9 (9%)	0	7
6	CF	99/101 (98%)	71 (72%)	21 (21%)	7 (7%)	1	10
7	AG	153/156 (98%)	108 (71%)	28 (18%)	17 (11%)	0	5
7	CG	150/156 (96%)	93 (62%)	39 (26%)	18 (12%)	0	5
8	AH	136/138 (99%)	87 (64%)	37 (27%)	12 (9%)	0	7
8	CH	136/138 (99%)	92 (68%)	37 (27%)	7 (5%)	1	16
9	AI	125/128 (98%)	86 (69%)	26 (21%)	13 (10%)	0	6
9	CI	125/128 (98%)	72 (58%)	43 (34%)	10 (8%)	1	8
10	AJ	97/105 (92%)	59 (61%)	27 (28%)	11 (11%)	0	5
10	CJ	97/105 (92%)	52 (54%)	34 (35%)	11 (11%)	0	5
11	AK	114/129 (88%)	82 (72%)	26 (23%)	6 (5%)	1	15
11	CK	117/129 (91%)	81 (69%)	25 (21%)	11 (9%)	0	7
12	AL	123/132 (93%)	78 (63%)	29 (24%)	16 (13%)	0	4
12	CL	123/132 (93%)	82 (67%)	19 (15%)	22 (18%)	0	2
13	AM	120/126 (95%)	69 (58%)	28 (23%)	23 (19%)	0	1
13	CM	116/126 (92%)	66 (57%)	24 (21%)	26 (22%)	0	1
14	AN	58/61 (95%)	33 (57%)	17 (29%)	8 (14%)	0	3
14	CN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	5
15	AO	86/89 (97%)	61 (71%)	16 (19%)	9 (10%)	0	6
15	CO	86/89 (97%)	62 (72%)	15 (17%)	9 (10%)	0	6
16	AP	82/88 (93%)	54 (66%)	19 (23%)	9 (11%)	0	5
16	CP	82/88 (93%)	56 (68%)	24 (29%)	2 (2%)	5	30
17	AQ	98/105 (93%)	76 (78%)	13 (13%)	9 (9%)	0	7
17	CQ	98/105 (93%)	64 (65%)	23 (24%)	11 (11%)	0	5
18	AR	68/88 (77%)	48 (71%)	14 (21%)	6 (9%)	0	7
18	CR	68/88 (77%)	50 (74%)	11 (16%)	7 (10%)	0	6
19	AS	77/93 (83%)	46 (60%)	13 (17%)	18 (23%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	CS	77/93 (83%)	49 (64%)	18 (23%)	10 (13%)	0	4
20	AT	97/106 (92%)	57 (59%)	25 (26%)	15 (16%)	0	2
20	CT	97/106 (92%)	64 (66%)	18 (19%)	15 (16%)	0	2
21	AU	23/27 (85%)	15 (65%)	7 (30%)	1 (4%)	2	19
21	CU	23/27 (85%)	19 (83%)	1 (4%)	3 (13%)	0	4
29	BC	183/229 (80%)	67 (37%)	66 (36%)	50 (27%)	0	0
29	DC	183/229 (80%)	62 (34%)	69 (38%)	52 (28%)	0	0
30	BD	270/276 (98%)	175 (65%)	54 (20%)	41 (15%)	0	2
30	DD	270/276 (98%)	180 (67%)	51 (19%)	39 (14%)	0	3
31	BE	203/206 (98%)	133 (66%)	38 (19%)	32 (16%)	0	2
31	DE	203/206 (98%)	115 (57%)	49 (24%)	39 (19%)	0	1
32	BF	204/210 (97%)	141 (69%)	40 (20%)	23 (11%)	0	5
32	DF	206/210 (98%)	126 (61%)	44 (21%)	36 (18%)	0	2
33	BG	179/182 (98%)	114 (64%)	31 (17%)	34 (19%)	0	1
33	DG	179/182 (98%)	98 (55%)	53 (30%)	28 (16%)	0	2
34	BH	159/180 (88%)	92 (58%)	31 (20%)	36 (23%)	0	1
34	DH	158/180 (88%)	96 (61%)	30 (19%)	32 (20%)	0	1
35	BI	144/148 (97%)	72 (50%)	37 (26%)	35 (24%)	0	0
35	DI	144/148 (97%)	73 (51%)	48 (33%)	23 (16%)	0	2
36	BN	137/140 (98%)	98 (72%)	23 (17%)	16 (12%)	0	5
36	DN	137/140 (98%)	83 (61%)	30 (22%)	24 (18%)	0	2
37	BO	120/122 (98%)	95 (79%)	19 (16%)	6 (5%)	1	16
37	DO	120/122 (98%)	84 (70%)	23 (19%)	13 (11%)	0	6
38	BP	144/150 (96%)	68 (47%)	33 (23%)	43 (30%)	0	0
38	DP	144/150 (96%)	69 (48%)	38 (26%)	37 (26%)	0	0
39	BQ	137/141 (97%)	99 (72%)	25 (18%)	13 (10%)	0	7
39	DQ	134/141 (95%)	86 (64%)	28 (21%)	20 (15%)	0	3
40	BR	115/118 (98%)	73 (64%)	24 (21%)	18 (16%)	0	2
40	DR	115/118 (98%)	69 (60%)	29 (25%)	17 (15%)	0	3
41	BS	97/112 (87%)	46 (47%)	25 (26%)	26 (27%)	0	0
41	DS	97/112 (87%)	44 (45%)	28 (29%)	25 (26%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	BT	136/146 (93%)	81 (60%)	25 (18%)	30 (22%)	0	1
42	DT	136/146 (93%)	71 (52%)	28 (21%)	37 (27%)	0	0
43	BU	115/118 (98%)	79 (69%)	27 (24%)	9 (8%)	1	8
43	DU	115/118 (98%)	63 (55%)	36 (31%)	16 (14%)	0	3
44	BV	99/101 (98%)	59 (60%)	18 (18%)	22 (22%)	0	1
44	DV	99/101 (98%)	56 (57%)	25 (25%)	18 (18%)	0	1
45	BW	111/113 (98%)	86 (78%)	20 (18%)	5 (4%)	2	18
45	DW	111/113 (98%)	74 (67%)	23 (21%)	14 (13%)	0	4
46	BX	91/96 (95%)	71 (78%)	19 (21%)	1 (1%)	12	44
46	DX	91/96 (95%)	63 (69%)	16 (18%)	12 (13%)	0	4
47	BY	84/110 (76%)	30 (36%)	25 (30%)	29 (34%)	0	0
47	DY	99/110 (90%)	36 (36%)	27 (27%)	36 (36%)	0	0
48	BZ	175/206 (85%)	94 (54%)	46 (26%)	35 (20%)	0	1
48	DZ	175/206 (85%)	85 (49%)	52 (30%)	38 (22%)	0	1
49	B0	82/85 (96%)	66 (80%)	11 (13%)	5 (6%)	1	13
49	D0	82/85 (96%)	64 (78%)	14 (17%)	4 (5%)	2	16
50	B1	92/98 (94%)	72 (78%)	13 (14%)	7 (8%)	1	9
50	D1	92/98 (94%)	70 (76%)	11 (12%)	11 (12%)	0	5
51	B2	69/72 (96%)	43 (62%)	13 (19%)	13 (19%)	0	1
51	D2	69/72 (96%)	41 (59%)	16 (23%)	12 (17%)	0	2
52	B3	58/60 (97%)	49 (84%)	4 (7%)	5 (9%)	0	8
52	D3	58/60 (97%)	46 (79%)	6 (10%)	6 (10%)	0	6
53	B4	45/71 (63%)	18 (40%)	10 (22%)	17 (38%)	0	0
53	D4	45/71 (63%)	19 (42%)	11 (24%)	15 (33%)	0	0
54	B5	57/60 (95%)	41 (72%)	8 (14%)	8 (14%)	0	3
54	D5	57/60 (95%)	42 (74%)	8 (14%)	7 (12%)	0	5
55	B6	46/54 (85%)	18 (39%)	9 (20%)	19 (41%)	0	0
55	D6	44/54 (82%)	15 (34%)	12 (27%)	17 (39%)	0	0
56	B7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	1	12
56	D7	47/49 (96%)	40 (85%)	5 (11%)	2 (4%)	2	19
57	B8	62/65 (95%)	30 (48%)	19 (31%)	13 (21%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
57	D8	62/65 (95%)	33 (53%)	17 (27%)	12 (19%)	0	1
58	B9	34/37 (92%)	27 (79%)	5 (15%)	2 (6%)	1	13
58	D9	34/37 (92%)	24 (71%)	7 (21%)	3 (9%)	0	7
All	All	11692/12586 (93%)	7260 (62%)	2616 (22%)	1816 (16%)	0	2

5 of 1816 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	24	TRP
2	AB	122	PHE
2	AB	128	GLU
2	AB	154	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%)	177 (88%)	25 (12%)	4	20
2	CB	202/220 (92%)	177 (88%)	25 (12%)	4	20
3	AC	160/188 (85%)	144 (90%)	16 (10%)	6	27
3	CC	159/188 (85%)	142 (89%)	17 (11%)	5	25
4	AD	180/181 (99%)	159 (88%)	21 (12%)	4	22
4	CD	180/181 (99%)	162 (90%)	18 (10%)	6	27
5	AE	115/123 (94%)	103 (90%)	12 (10%)	5	26
5	CE	115/123 (94%)	99 (86%)	16 (14%)	3	17
6	AF	90/90 (100%)	82 (91%)	8 (9%)	8	31
6	CF	90/90 (100%)	79 (88%)	11 (12%)	4	20
7	AG	126/127 (99%)	109 (86%)	17 (14%)	3	18
7	CG	125/127 (98%)	115 (92%)	10 (8%)	10	34
8	AH	119/119 (100%)	106 (89%)	13 (11%)	5	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	CH	119/119 (100%)	105 (88%)	14 (12%)	4	21
9	AI	97/99 (98%)	85 (88%)	12 (12%)	4	20
9	CI	97/99 (98%)	82 (84%)	15 (16%)	2	13
10	AJ	88/92 (96%)	73 (83%)	15 (17%)	1	10
10	CJ	88/92 (96%)	77 (88%)	11 (12%)	3	20
11	AK	88/99 (89%)	82 (93%)	6 (7%)	13	41
11	CK	90/99 (91%)	83 (92%)	7 (8%)	10	35
12	AL	104/109 (95%)	92 (88%)	12 (12%)	4	22
12	CL	104/109 (95%)	92 (88%)	12 (12%)	4	22
13	AM	97/101 (96%)	84 (87%)	13 (13%)	3	18
13	CM	94/101 (93%)	82 (87%)	12 (13%)	3	19
14	AN	49/50 (98%)	43 (88%)	6 (12%)	4	20
14	CN	49/50 (98%)	47 (96%)	2 (4%)	26	56
15	AO	79/80 (99%)	71 (90%)	8 (10%)	6	27
15	CO	79/80 (99%)	69 (87%)	10 (13%)	3	19
16	AP	72/74 (97%)	62 (86%)	10 (14%)	3	17
16	CP	72/74 (97%)	65 (90%)	7 (10%)	6	28
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	8	33
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	19	48
18	AR	61/77 (79%)	57 (93%)	4 (7%)	14	42
18	CR	61/77 (79%)	53 (87%)	8 (13%)	3	18
19	AS	69/80 (86%)	55 (80%)	14 (20%)	1	5
19	CS	69/80 (86%)	55 (80%)	14 (20%)	1	5
20	AT	76/82 (93%)	63 (83%)	13 (17%)	1	10
20	CT	76/82 (93%)	66 (87%)	10 (13%)	3	18
21	AU	19/22 (86%)	17 (90%)	2 (10%)	5	26
21	CU	19/22 (86%)	17 (90%)	2 (10%)	5	26
26	AZ	1/1 (100%)	1 (100%)	0	100	100
26	CZ	1/1 (100%)	1 (100%)	0	100	100
29	BC	61/181 (34%)	55 (90%)	6 (10%)	6	28
29	DC	61/181 (34%)	52 (85%)	9 (15%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BD	213/218 (98%)	184 (86%)	29 (14%)	3	18
30	DD	213/218 (98%)	183 (86%)	30 (14%)	3	17
31	BE	165/166 (99%)	142 (86%)	23 (14%)	3	17
31	DE	165/166 (99%)	133 (81%)	32 (19%)	1	6
32	BF	163/166 (98%)	142 (87%)	21 (13%)	3	19
32	DF	165/166 (99%)	143 (87%)	22 (13%)	3	18
33	BG	155/156 (99%)	136 (88%)	19 (12%)	4	20
33	DG	155/156 (99%)	133 (86%)	22 (14%)	2	16
34	BH	134/148 (90%)	116 (87%)	18 (13%)	3	18
34	DH	132/148 (89%)	119 (90%)	13 (10%)	6	28
35	BI	122/124 (98%)	107 (88%)	15 (12%)	4	20
35	DI	122/124 (98%)	104 (85%)	18 (15%)	2	15
36	BN	117/119 (98%)	94 (80%)	23 (20%)	1	6
36	DN	117/119 (98%)	98 (84%)	19 (16%)	2	11
37	BO	100/100 (100%)	84 (84%)	16 (16%)	2	12
37	DO	100/100 (100%)	88 (88%)	12 (12%)	4	21
38	BP	112/116 (97%)	86 (77%)	26 (23%)	0	3
38	DP	112/116 (97%)	90 (80%)	22 (20%)	1	6
39	BQ	110/111 (99%)	89 (81%)	21 (19%)	1	6
39	DQ	108/111 (97%)	96 (89%)	12 (11%)	5	24
40	BR	100/101 (99%)	83 (83%)	17 (17%)	1	10
40	DR	100/101 (99%)	84 (84%)	16 (16%)	2	12
41	BS	77/88 (88%)	53 (69%)	24 (31%)	0	2
41	DS	77/88 (88%)	67 (87%)	10 (13%)	3	19
42	BT	120/127 (94%)	88 (73%)	32 (27%)	0	3
42	DT	120/127 (94%)	87 (72%)	33 (28%)	0	2
43	BU	92/94 (98%)	78 (85%)	14 (15%)	2	14
43	DU	92/94 (98%)	82 (89%)	10 (11%)	5	24
44	BV	82/82 (100%)	64 (78%)	18 (22%)	1	4
44	DV	82/82 (100%)	65 (79%)	17 (21%)	1	5
45	BW	91/92 (99%)	78 (86%)	13 (14%)	2	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	DW	91/92 (99%)	84 (92%)	7 (8%)	10	36
46	BX	74/78 (95%)	63 (85%)	11 (15%)	2	15
46	DX	74/78 (95%)	58 (78%)	16 (22%)	1	4
47	BY	73/91 (80%)	59 (81%)	14 (19%)	1	6
47	DY	84/91 (92%)	69 (82%)	15 (18%)	1	8
48	BZ	155/179 (87%)	131 (84%)	24 (16%)	2	13
48	DZ	155/179 (87%)	138 (89%)	17 (11%)	5	24
49	B0	66/67 (98%)	60 (91%)	6 (9%)	7	30
49	D0	66/67 (98%)	58 (88%)	8 (12%)	4	20
50	B1	78/83 (94%)	65 (83%)	13 (17%)	2	10
50	D1	78/83 (94%)	72 (92%)	6 (8%)	10	36
51	B2	66/67 (98%)	52 (79%)	14 (21%)	1	4
51	D2	66/67 (98%)	58 (88%)	8 (12%)	4	20
52	B3	51/52 (98%)	44 (86%)	7 (14%)	3	17
52	D3	51/52 (98%)	46 (90%)	5 (10%)	6	28
53	B4	34/63 (54%)	30 (88%)	4 (12%)	4	21
53	D4	34/63 (54%)	28 (82%)	6 (18%)	1	8
54	B5	51/52 (98%)	42 (82%)	9 (18%)	1	8
54	D5	51/52 (98%)	41 (80%)	10 (20%)	1	6
55	B6	44/52 (85%)	27 (61%)	17 (39%)	0	1
55	D6	44/52 (85%)	30 (68%)	14 (32%)	0	2
56	B7	41/42 (98%)	37 (90%)	4 (10%)	6	28
56	D7	41/42 (98%)	35 (85%)	6 (15%)	2	16
57	B8	53/55 (96%)	40 (76%)	13 (24%)	0	3
57	D8	53/55 (96%)	39 (74%)	14 (26%)	0	3
58	B9	33/34 (97%)	32 (97%)	1 (3%)	36	65
58	D9	33/34 (97%)	31 (94%)	2 (6%)	15	44
All	All	9644/10430 (92%)	8280 (86%)	1364 (14%)	3	17

5 of 1364 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
20	CT	75	ASN

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Mol	Chain	Res	Type
40	DR	8	ARG
30	DD	96	HIS
20	CT	73	HIS
33	DG	113	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 345 such sidechains are listed below:

Mol	Chain	Res	Type
15	CO	71	GLN
38	DP	9	ASN
19	CS	47	HIS
32	DF	8	GLN
42	DT	43	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1508 (99%)	234 (15%)	56 (3%)
1	CA	1491/1508 (98%)	248 (16%)	61 (4%)
22	AV	9/30 (30%)	1 (11%)	0
22	CV	9/30 (30%)	2 (22%)	0
23	AW	73/75 (97%)	15 (20%)	3 (4%)
23	CW	73/75 (97%)	20 (27%)	3 (4%)
24	AX	76/77 (98%)	24 (31%)	4 (5%)
25	AY	74/75 (98%)	19 (25%)	0
25	CY	74/75 (98%)	20 (27%)	0
27	BA	2779/2915 (95%)	539 (19%)	96 (3%)
27	DA	2765/2915 (94%)	555 (20%)	114 (4%)
28	BB	118/122 (96%)	16 (13%)	3 (2%)
28	DB	118/122 (96%)	40 (33%)	5 (4%)
59	CX	76/77 (98%)	21 (27%)	2 (2%)
All	All	9228/9604 (96%)	1754 (19%)	347 (3%)

5 of 1754 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	28	G
1	AA	31	G
1	AA	32	A

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Mol	Chain	Res	Type
1	AA	39	G

5 of 347 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
27	DA	100	G
27	DA	1653	G
27	DA	301	G
27	DA	995	C
27	DA	2111	C

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

10 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	$\# Z > 2$
26	UAL	AZ	3	26	6,8,9	2.68	2 (33%)	4,9,11	1.96	1 (25%)
26	DPP	CZ	2	26	4,5,6	0.85	0	1,5,7	0.30	0
26	MYN	CZ	4	26	8,11,12	1.97	1 (12%)	6,14,16	1.67	2 (33%)
26	DPP	AZ	5	26	4,5,6	0.50	0	1,5,7	0.25	0
26	DPP	AZ	2	26	4,5,6	0.54	0	1,5,7	0.55	0
26	KBE	CZ	1	26	8,8,9	1.33	1 (12%)	6,8,10	2.26	2 (33%)
26	UAL	CZ	3	26	6,8,9	2.67	2 (33%)	4,9,11	1.48	1 (25%)
26	MYN	AZ	4	26	8,11,12	2.47	1 (12%)	6,14,16	1.49	0
26	KBE	AZ	1	26	8,8,9	1.61	1 (12%)	6,8,10	2.62	2 (33%)
26	DPP	CZ	5	26	4,5,6	0.74	0	1,5,7	0.31	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
26	UAL	AZ	3	26	-	0/3/7/9	-
26	DPP	CZ	2	26	-	1/2/4/6	-
26	MYN	CZ	4	26	-	0/1/16/18	0/1/1/1
26	DPP	AZ	5	26	-	0/2/4/6	-
26	DPP	AZ	2	26	-	2/2/4/6	-
26	KBE	CZ	1	26	-	1/7/7/8	-
26	UAL	CZ	3	26	-	0/3/7/9	-
26	MYN	AZ	4	26	-	0/1/16/18	0/1/1/1
26	KBE	AZ	1	26	-	1/7/7/8	-
26	DPP	CZ	5	26	-	0/2/4/6	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	AZ	4	MYN	CZ-NE	6.81	1.41	1.34
26	CZ	4	MYN	CZ-NE	5.07	1.39	1.34
26	CZ	3	UAL	C-CA	4.76	1.53	1.45
26	AZ	3	UAL	C1-N1	-4.51	1.33	1.40
26	AZ	3	UAL	C-CA	4.47	1.52	1.45

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	AZ	1	KBE	CB-CA-C	5.71	121.39	112.17
26	CZ	1	KBE	CB-CA-C	4.86	120.02	112.17
26	AZ	3	UAL	O-C-CA	-3.72	120.72	125.39
26	AZ	1	KBE	O-C-CA	-2.80	117.22	125.38
26	CZ	3	UAL	O-C-CA	-2.73	121.97	125.39

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	AZ	1	KBE	C-CA-CB-N
26	CZ	1	KBE	C-CA-CB-N
26	AZ	2	DPP	N-CA-CB-NG
26	AZ	2	DPP	C-CA-CB-NG
26	CZ	2	DPP	N-CA-CB-NG

There are no ring outliers.

8 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	AZ	3	UAL	3	0
26	CZ	2	DPP	4	0
26	CZ	4	MYN	1	0
26	AZ	2	DPP	4	0
26	CZ	1	KBE	10	0
26	CZ	3	UAL	2	0
26	AZ	4	MYN	3	0
26	AZ	1	KBE	5	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 850 ligands modelled in this entry, 850 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.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1495/1508 (99%)	-0.08	25 (1%) 69 52	32, 72, 154, 200	0
1	CA	1493/1508 (99%)	0.14	49 (3%) 49 36	38, 81, 158, 200	0
2	AB	235/256 (91%)	0.28	12 (5%) 34 27	69, 98, 133, 148	0
2	CB	235/256 (91%)	0.47	12 (5%) 34 27	74, 103, 147, 165	0
3	AC	207/239 (86%)	0.08	6 (2%) 54 40	66, 86, 109, 114	0
3	CC	206/239 (86%)	0.45	9 (4%) 39 30	76, 98, 123, 136	0
4	AD	208/209 (99%)	0.07	7 (3%) 48 35	52, 73, 87, 92	0
4	CD	208/209 (99%)	0.08	7 (3%) 48 35	47, 68, 85, 89	0
5	AE	151/162 (93%)	-0.22	0 100 100	49, 67, 94, 107	0
5	CE	151/162 (93%)	0.10	2 (1%) 74 59	53, 75, 94, 100	0
6	AF	101/101 (100%)	-0.19	0 100 100	54, 69, 84, 98	0
6	CF	101/101 (100%)	-0.11	0 100 100	49, 73, 83, 98	0
7	AG	155/156 (99%)	0.24	9 (5%) 30 24	62, 82, 107, 124	0
7	CG	154/156 (98%)	0.32	7 (4%) 39 29	69, 92, 116, 124	0
8	AH	138/138 (100%)	-0.10	1 (0%) 84 71	54, 71, 82, 96	0
8	CH	138/138 (100%)	0.11	2 (1%) 73 57	55, 75, 87, 97	0
9	AI	127/128 (99%)	0.55	9 (7%) 23 20	57, 99, 123, 126	0
9	CI	127/128 (99%)	0.79	13 (10%) 13 12	72, 106, 123, 129	0
10	AJ	99/105 (94%)	1.03	13 (13%) 8 9	69, 108, 130, 130	0
10	CJ	99/105 (94%)	0.84	11 (11%) 12 11	79, 115, 136, 143	0
11	AK	116/129 (89%)	-0.07	3 (2%) 57 42	53, 67, 89, 107	0
11	CK	119/129 (92%)	0.04	6 (5%) 35 27	56, 76, 99, 114	0
12	AL	125/132 (94%)	0.24	4 (3%) 50 37	49, 63, 80, 103	0
12	CL	125/132 (94%)	0.22	5 (4%) 43 32	51, 71, 83, 99	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	122/126 (96%)	0.37	8 (6%) 26 21	63, 87, 97, 102	0
13	CM	118/126 (93%)	0.71	13 (11%) 12 11	77, 100, 114, 120	0
14	AN	60/61 (98%)	0.50	4 (6%) 25 21	52, 77, 91, 97	0
14	CN	60/61 (98%)	1.12	6 (10%) 14 13	75, 92, 101, 105	0
15	AO	88/89 (98%)	-0.01	0 100 100	47, 65, 82, 93	0
15	CO	88/89 (98%)	-0.05	1 (1%) 77 62	50, 70, 87, 92	0
16	AP	84/88 (95%)	0.06	0 100 100	50, 68, 95, 109	0
16	CP	84/88 (95%)	0.30	3 (3%) 46 34	55, 66, 85, 109	0
17	AQ	100/105 (95%)	0.03	0 100 100	53, 69, 84, 88	0
17	CQ	100/105 (95%)	0.11	2 (2%) 64 48	59, 73, 91, 94	0
18	AR	70/88 (79%)	0.24	3 (4%) 40 30	49, 68, 94, 100	0
18	CR	70/88 (79%)	-0.07	1 (1%) 73 57	56, 74, 99, 104	0
19	AS	79/93 (84%)	0.57	6 (7%) 21 18	63, 90, 110, 115	0
19	CS	79/93 (84%)	0.87	9 (11%) 11 11	91, 111, 132, 138	0
20	AT	99/106 (93%)	0.58	7 (7%) 23 20	54, 75, 104, 110	0
20	CT	99/106 (93%)	0.57	6 (6%) 28 23	63, 76, 111, 114	0
21	AU	25/27 (92%)	0.86	1 (4%) 43 32	74, 82, 90, 95	0
21	CU	25/27 (92%)	0.85	2 (8%) 20 17	72, 93, 105, 109	0
22	AV	10/30 (33%)	1.02	3 (30%) 1 2	51, 66, 125, 128	0
22	CV	10/30 (33%)	0.95	3 (30%) 1 2	65, 81, 134, 138	0
23	AW	74/75 (98%)	0.08	3 (4%) 42 31	49, 117, 149, 154	0
23	CW	74/75 (98%)	0.33	2 (2%) 56 41	79, 129, 148, 165	0
24	AX	77/77 (100%)	-0.07	1 (1%) 74 59	35, 85, 115, 128	0
25	AY	75/75 (100%)	0.39	7 (9%) 16 14	62, 157, 189, 191	0
25	CY	75/75 (100%)	0.62	8 (10%) 12 12	76, 170, 192, 197	0
26	AZ	1/6 (16%)	-0.07	0 100 100	64, 64, 64, 64	0
26	CZ	1/6 (16%)	-0.42	0 100 100	91, 91, 91, 91	0
27	BA	2789/2915 (95%)	-0.39	50 (1%) 67 51	19, 44, 164, 200	0
27	DA	2775/2915 (95%)	0.04	69 (2%) 58 43	30, 72, 170, 200	0
28	BB	119/122 (97%)	0.13	8 (6%) 25 21	36, 70, 127, 168	0
28	DB	119/122 (97%)	1.71	37 (31%) 1 2	109, 142, 170, 179	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
29	BC	191/229 (83%)	1.53	61 (31%) 1 2	103, 169, 180, 186	0
29	DC	191/229 (83%)	1.22	37 (19%) 4 4	125, 170, 183, 186	0
30	BD	272/276 (98%)	-0.16	10 (3%) 45 33	18, 41, 61, 73	0
30	DD	272/276 (98%)	-0.04	4 (1%) 71 55	31, 52, 69, 81	0
31	BE	205/206 (99%)	-0.20	3 (1%) 71 55	16, 42, 76, 94	0
31	DE	205/206 (99%)	0.41	11 (5%) 32 25	44, 80, 112, 119	0
32	BF	206/210 (98%)	-0.23	4 (1%) 66 50	17, 46, 110, 129	0
32	DF	208/210 (99%)	0.18	1 (0%) 87 77	40, 69, 120, 132	0
33	BG	181/182 (99%)	0.14	5 (2%) 55 40	49, 74, 102, 119	0
33	DG	181/182 (99%)	0.47	7 (3%) 44 33	75, 101, 117, 125	0
34	BH	161/180 (89%)	0.20	7 (4%) 40 30	39, 65, 81, 95	0
34	DH	160/180 (88%)	1.00	19 (11%) 10 10	106, 129, 153, 161	0
35	BI	146/148 (98%)	1.22	32 (21%) 3 4	57, 134, 150, 159	0
35	DI	146/148 (98%)	0.63	12 (8%) 19 17	62, 107, 139, 150	0
36	BN	139/140 (99%)	-0.16	0 100 100	23, 43, 67, 73	0
36	DN	139/140 (99%)	0.55	11 (7%) 20 17	69, 86, 106, 108	0
37	BO	122/122 (100%)	-0.40	0 100 100	22, 44, 60, 67	0
37	DO	122/122 (100%)	0.17	1 (0%) 82 69	47, 72, 80, 86	0
38	BP	146/150 (97%)	0.49	14 (9%) 15 13	17, 60, 91, 121	0
38	DP	146/150 (97%)	0.89	25 (17%) 5 6	45, 82, 103, 126	0
39	BQ	139/141 (98%)	-0.13	2 (1%) 73 57	29, 47, 70, 82	0
39	DQ	138/141 (97%)	0.85	16 (11%) 11 11	58, 88, 107, 136	0
40	BR	117/118 (99%)	-0.09	2 (1%) 69 52	17, 37, 59, 66	0
40	DR	117/118 (99%)	0.30	7 (5%) 29 23	39, 64, 81, 88	0
41	BS	99/112 (88%)	0.48	11 (11%) 12 11	40, 65, 82, 91	0
41	DS	99/112 (88%)	1.07	18 (18%) 4 5	71, 93, 106, 109	0
42	BT	138/146 (94%)	0.24	7 (5%) 34 27	27, 53, 108, 143	0
42	DT	138/146 (94%)	0.53	10 (7%) 23 20	64, 79, 136, 142	0
43	BU	117/118 (99%)	-0.24	1 (0%) 81 66	20, 37, 59, 86	0
43	DU	117/118 (99%)	0.33	8 (6%) 25 21	48, 80, 111, 120	0
44	BV	101/101 (100%)	-0.14	1 (0%) 79 64	18, 49, 68, 74	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	DV	101/101 (100%)	0.29	5 (4%)	35	27	54, 100, 114, 122	0
45	BW	113/113 (100%)	-0.40	1 (0%)	81	66	21, 34, 64, 102	0
45	DW	113/113 (100%)	-0.03	1 (0%)	81	66	39, 61, 93, 118	0
46	BX	93/96 (96%)	-0.15	1 (1%)	77	62	31, 45, 69, 76	0
46	DX	93/96 (96%)	0.16	3 (3%)	50	37	39, 66, 79, 85	0
47	BY	88/110 (80%)	0.48	7 (7%)	20	17	41, 58, 79, 87	0
47	DY	101/110 (91%)	1.20	19 (18%)	4	5	62, 83, 144, 153	0
48	BZ	177/206 (85%)	0.63	28 (15%)	6	7	52, 85, 159, 164	0
48	DZ	177/206 (85%)	1.17	29 (16%)	5	6	93, 123, 178, 184	0
49	B0	84/85 (98%)	0.14	5 (5%)	29	23	27, 49, 71, 85	0
49	D0	84/85 (98%)	0.68	4 (4%)	36	28	66, 82, 96, 104	0
50	B1	94/98 (95%)	-0.03	2 (2%)	63	47	28, 49, 80, 91	0
50	D1	94/98 (95%)	0.28	2 (2%)	63	47	40, 62, 94, 101	0
51	B2	71/72 (98%)	-0.01	2 (2%)	55	40	37, 62, 93, 106	0
51	D2	71/72 (98%)	0.05	0	100	100	59, 78, 98, 117	0
52	B3	60/60 (100%)	-0.06	0	100	100	27, 44, 69, 103	0
52	D3	60/60 (100%)	0.56	1 (1%)	69	52	70, 88, 111, 119	0
53	B4	49/71 (69%)	0.73	10 (20%)	3	4	72, 97, 116, 119	0
53	D4	49/71 (69%)	0.78	4 (8%)	19	17	100, 115, 120, 121	0
54	B5	59/60 (98%)	0.20	4 (6%)	25	21	21, 38, 93, 115	0
54	D5	59/60 (98%)	0.38	4 (6%)	25	21	46, 62, 116, 136	0
55	B6	48/54 (88%)	0.95	6 (12%)	9	9	29, 58, 71, 90	0
55	D6	46/54 (85%)	1.56	15 (32%)	1	2	50, 81, 91, 101	0
56	B7	49/49 (100%)	-0.14	2 (4%)	42	31	20, 32, 77, 90	0
56	D7	49/49 (100%)	0.05	3 (6%)	28	23	36, 47, 84, 92	0
57	B8	64/65 (98%)	0.55	6 (9%)	15	14	26, 44, 62, 99	0
57	D8	64/65 (98%)	1.09	9 (14%)	7	8	51, 66, 85, 109	0
58	B9	36/37 (97%)	-0.17	0	100	100	15, 45, 57, 59	0
58	D9	36/37 (97%)	1.11	7 (19%)	4	4	79, 94, 99, 102	0
59	CX	77/77 (100%)	0.07	1 (1%)	74	59	63, 100, 127, 140	0
All	All	21180/22202 (95%)	0.16	1003 (4%)	37	28	15, 72, 152, 200	0

The worst 5 of 1003 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
57	D8	65	GLU	10.0
35	BI	94	ALA	9.8
54	D5	2	ALA	9.3
28	DB	49	C	8.7
34	DH	170	ARG	8.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	UAL	CZ	3	9/10	0.81	0.15	91,92,93,93	0
26	KBE	CZ	1	9/10	0.82	0.23	95,98,100,100	0
26	UAL	AZ	3	9/10	0.85	0.12	63,66,70,71	0
26	DPP	AZ	5	6/7	0.85	0.15	62,64,65,65	0
26	DPP	CZ	2	6/7	0.87	0.12	92,93,95,98	0
26	KBE	AZ	1	9/10	0.87	0.19	71,74,78,79	0
26	MYN	CZ	4	11/12	0.91	0.12	88,89,91,92	0
26	DPP	CZ	5	6/7	0.92	0.14	88,89,89,90	0
26	MYN	AZ	4	11/12	0.93	0.12	61,64,65,65	0
26	DPP	AZ	2	6/7	0.93	0.12	66,67,69,71	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	CA	1683	1/1	0.43	0.33	53,53,53,53	0
60	MG	DB	202	1/1	0.51	0.21	80,80,80,80	0
60	MG	CW	103	1/1	0.52	0.17	73,73,73,73	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3164	1/1	0.53	0.25	64,64,64,64	0
60	MG	DA	3190	1/1	0.54	0.20	43,43,43,43	0
60	MG	CA	1652	1/1	0.59	0.26	61,61,61,61	0
60	MG	AA	1684	1/1	0.61	0.34	69,69,69,69	0
60	MG	CA	1696	1/1	0.62	0.19	91,91,91,91	0
60	MG	CA	1611	1/1	0.62	0.37	66,66,66,66	0
60	MG	DA	3053	1/1	0.62	0.28	32,32,32,32	0
60	MG	DA	3176	1/1	0.65	0.23	54,54,54,54	0
60	MG	BA	3283	1/1	0.65	0.30	38,38,38,38	0
60	MG	AA	1626	1/1	0.65	0.20	51,51,51,51	0
60	MG	CA	1633	1/1	0.66	0.19	62,62,62,62	0
60	MG	AW	103	1/1	0.66	0.20	72,72,72,72	0
60	MG	DA	3235	1/1	0.67	0.22	61,61,61,61	0
60	MG	AA	1640	1/1	0.67	0.14	70,70,70,70	0
60	MG	BA	3195	1/1	0.68	0.34	49,49,49,49	0
60	MG	AA	1646	1/1	0.68	0.16	71,71,71,71	0
60	MG	DA	3162	1/1	0.69	0.26	44,44,44,44	0
60	MG	BA	3104	1/1	0.69	0.15	42,42,42,42	0
60	MG	CA	1664	1/1	0.69	0.22	83,83,83,83	0
60	MG	DA	3128	1/1	0.70	0.29	24,24,24,24	0
60	MG	DA	3167	1/1	0.70	0.16	36,36,36,36	0
60	MG	DA	3148	1/1	0.71	0.19	42,42,42,42	0
60	MG	DA	3188	1/1	0.71	0.22	72,72,72,72	0
60	MG	BA	3109	1/1	0.71	0.32	58,58,58,58	0
60	MG	CA	1641	1/1	0.71	0.34	66,66,66,66	0
60	MG	BA	3201	1/1	0.71	0.55	53,53,53,53	0
60	MG	DA	3175	1/1	0.72	0.33	72,72,72,72	0
60	MG	DA	3095	1/1	0.72	0.22	61,61,61,61	0
60	MG	BA	3085	1/1	0.72	0.36	70,70,70,70	0
60	MG	DA	3122	1/1	0.73	0.19	40,40,40,40	0
60	MG	BA	3213	1/1	0.73	0.24	49,49,49,49	0
60	MG	DA	3225	1/1	0.73	0.23	39,39,39,39	0
60	MG	AA	1681	1/1	0.73	0.13	58,58,58,58	0
60	MG	BA	3190	1/1	0.73	0.15	39,39,39,39	0
60	MG	AA	1637	1/1	0.74	0.18	44,44,44,44	0
60	MG	DA	3189	1/1	0.74	0.15	57,57,57,57	0
60	MG	AX	103	1/1	0.75	0.19	51,51,51,51	0
60	MG	BA	3162	1/1	0.75	0.23	56,56,56,56	0
60	MG	DA	3231	1/1	0.75	0.30	49,49,49,49	0
60	MG	BA	3189	1/1	0.75	0.18	40,40,40,40	0
60	MG	DA	3171	1/1	0.75	0.30	52,52,52,52	0
60	MG	BA	3144	1/1	0.76	0.32	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1645	1/1	0.76	0.39	56,56,56,56	0
60	MG	DA	3090	1/1	0.76	0.20	21,21,21,21	0
60	MG	CA	1647	1/1	0.76	0.34	44,44,44,44	0
60	MG	AA	1651	1/1	0.76	0.31	53,53,53,53	0
60	MG	AA	1690	1/1	0.76	0.26	23,23,23,23	0
60	MG	CA	1677	1/1	0.76	0.20	51,51,51,51	0
60	MG	AA	1702	1/1	0.76	0.24	41,41,41,41	0
60	MG	CA	1685	1/1	0.76	0.31	59,59,59,59	0
60	MG	AA	1644	1/1	0.76	0.33	39,39,39,39	0
60	MG	DF	301	1/1	0.76	0.14	53,53,53,53	0
60	MG	DA	3134	1/1	0.77	0.18	59,59,59,59	0
60	MG	DA	3027	1/1	0.77	0.36	38,38,38,38	0
60	MG	AA	1630	1/1	0.77	0.44	62,62,62,62	0
60	MG	AA	1632	1/1	0.77	0.27	48,48,48,48	0
60	MG	BA	3313	1/1	0.78	0.29	45,45,45,45	0
60	MG	CA	1701	1/1	0.78	0.16	53,53,53,53	0
60	MG	AA	1638	1/1	0.78	0.40	76,76,76,76	0
60	MG	CA	1624	1/1	0.78	0.33	40,40,40,40	0
60	MG	AA	1648	1/1	0.78	0.42	68,68,68,68	0
60	MG	DA	3001	1/1	0.79	0.24	51,51,51,51	0
60	MG	DA	3227	1/1	0.79	0.19	36,36,36,36	0
60	MG	BA	3187	1/1	0.80	0.18	17,17,17,17	0
60	MG	DA	3221	1/1	0.80	0.27	52,52,52,52	0
60	MG	BB	203	1/1	0.80	0.21	35,35,35,35	0
60	MG	BA	3289	1/1	0.80	0.26	42,42,42,42	0
60	MG	DA	3091	1/1	0.81	0.28	55,55,55,55	0
60	MG	BA	3204	1/1	0.81	0.30	25,25,25,25	0
60	MG	CA	1649	1/1	0.81	0.24	54,54,54,54	0
60	MG	AA	1608	1/1	0.81	0.27	22,22,22,22	0
60	MG	DA	3131	1/1	0.81	0.47	63,63,63,63	0
60	MG	AA	1680	1/1	0.81	0.34	70,70,70,70	0
60	MG	DA	3136	1/1	0.81	0.23	31,31,31,31	0
60	MG	DA	3144	1/1	0.81	0.26	53,53,53,53	0
60	MG	DA	3021	1/1	0.81	0.18	27,27,27,27	0
60	MG	BA	3165	1/1	0.81	0.26	48,48,48,48	0
60	MG	BA	3050	1/1	0.81	0.25	1,1,1,1	0
60	MG	BA	3328	1/1	0.81	0.21	34,34,34,34	0
60	MG	DA	3168	1/1	0.81	0.29	55,55,55,55	0
60	MG	DO	201	1/1	0.81	0.09	65,65,65,65	0
60	MG	AW	101	1/1	0.82	0.22	48,48,48,48	0
60	MG	BA	3084	1/1	0.82	0.12	27,27,27,27	0
60	MG	AA	1601	1/1	0.82	0.21	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3138	1/1	0.82	0.26	63,63,63,63	0
60	MG	AG	201	1/1	0.82	0.12	42,42,42,42	0
60	MG	CA	1675	1/1	0.82	0.31	31,31,31,31	0
60	MG	AX	104	1/1	0.82	0.11	57,57,57,57	0
60	MG	CA	1679	1/1	0.82	0.14	43,43,43,43	0
60	MG	CA	1640	1/1	0.83	0.15	41,41,41,41	0
60	MG	CA	1655	1/1	0.83	0.19	29,29,29,29	0
60	MG	BA	3191	1/1	0.83	0.15	6,6,6,6	0
60	MG	AX	108	1/1	0.83	0.17	34,34,34,34	0
60	MG	BA	3164	1/1	0.83	0.19	33,33,33,33	0
60	MG	BA	3329	1/1	0.83	0.18	45,45,45,45	0
60	MG	DA	3115	1/1	0.83	0.23	36,36,36,36	0
60	MG	DA	3117	1/1	0.83	0.27	49,49,49,49	0
60	MG	DA	3155	1/1	0.83	0.30	31,31,31,31	0
60	MG	AA	1705	1/1	0.84	0.11	4,4,4,4	0
60	MG	AA	1704	1/1	0.84	0.23	13,13,13,13	0
60	MG	BA	3222	1/1	0.84	0.16	26,26,26,26	0
60	MG	DA	3198	1/1	0.84	0.17	32,32,32,32	0
60	MG	DA	3214	1/1	0.84	0.31	21,21,21,21	0
60	MG	DA	3159	1/1	0.84	0.23	32,32,32,32	0
60	MG	CA	1602	1/1	0.84	0.23	26,26,26,26	0
60	MG	CA	1603	1/1	0.84	0.20	38,38,38,38	0
60	MG	BA	3120	1/1	0.84	0.38	87,87,87,87	0
60	MG	CA	1616	1/1	0.84	0.32	52,52,52,52	0
60	MG	BA	3167	1/1	0.84	0.21	22,22,22,22	0
60	MG	AX	101	1/1	0.84	0.11	41,41,41,41	0
60	MG	BA	3316	1/1	0.84	0.25	35,35,35,35	0
60	MG	BA	3312	1/1	0.85	0.16	22,22,22,22	0
60	MG	AA	1671	1/1	0.85	0.12	49,49,49,49	0
60	MG	DA	3181	1/1	0.85	0.21	50,50,50,50	0
60	MG	CW	101	1/1	0.85	0.07	55,55,55,55	0
60	MG	BA	3107	1/1	0.85	0.39	65,65,65,65	0
60	MG	CA	1618	1/1	0.85	0.20	14,14,14,14	0
60	MG	BA	3281	1/1	0.85	0.19	21,21,21,21	0
60	MG	DA	3200	1/1	0.85	0.21	42,42,42,42	0
60	MG	DA	3204	1/1	0.85	0.27	67,67,67,67	0
60	MG	CA	1665	1/1	0.85	0.16	33,33,33,33	0
60	MG	DA	3040	1/1	0.85	0.26	19,19,19,19	0
60	MG	CA	1626	1/1	0.85	0.13	31,31,31,31	0
60	MG	AA	1707	1/1	0.85	0.36	52,52,52,52	0
60	MG	BB	202	1/1	0.85	0.18	9,9,9,9	0
60	MG	CA	1682	1/1	0.85	0.30	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3239	1/1	0.85	0.11	34,34,34,34	0
60	MG	DA	3114	1/1	0.85	0.11	34,34,34,34	0
60	MG	AA	1700	1/1	0.85	0.17	74,74,74,74	0
60	MG	BA	3294	1/1	0.85	0.49	90,90,90,90	0
60	MG	DA	3143	1/1	0.86	0.31	54,54,54,54	0
60	MG	BA	3171	1/1	0.86	0.15	36,36,36,36	0
60	MG	DA	3145	1/1	0.86	0.15	35,35,35,35	0
60	MG	CA	1686	1/1	0.86	0.07	37,37,37,37	0
60	MG	BA	3186	1/1	0.86	0.20	60,60,60,60	0
60	MG	DA	3111	1/1	0.86	0.29	64,64,64,64	0
60	MG	BA	3117	1/1	0.86	0.29	1,1,1,1	0
60	MG	BA	3305	1/1	0.86	0.18	32,32,32,32	0
60	MG	B0	102	1/1	0.86	0.34	40,40,40,40	0
60	MG	CA	1638	1/1	0.86	0.26	31,31,31,31	0
60	MG	DA	3008	1/1	0.86	0.24	13,13,13,13	0
60	MG	BA	3059	1/1	0.86	0.16	25,25,25,25	0
60	MG	BA	3001	1/1	0.86	0.29	43,43,43,43	0
60	MG	CA	1609	1/1	0.86	0.20	50,50,50,50	0
60	MG	BA	3159	1/1	0.86	0.20	20,20,20,20	0
60	MG	BA	3251	1/1	0.87	0.24	1,1,1,1	0
60	MG	BA	3270	1/1	0.87	0.23	32,32,32,32	0
60	MG	DA	3076	1/1	0.87	0.19	25,25,25,25	0
60	MG	DA	3084	1/1	0.87	0.23	71,71,71,71	0
60	MG	AA	1642	1/1	0.87	0.21	41,41,41,41	0
60	MG	AA	1689	1/1	0.87	0.11	2,2,2,2	0
60	MG	BA	3101	1/1	0.87	0.19	31,31,31,31	0
60	MG	BA	3293	1/1	0.87	0.30	45,45,45,45	0
60	MG	AA	1643	1/1	0.87	0.15	29,29,29,29	0
60	MG	DA	3186	1/1	0.87	0.36	53,53,53,53	0
60	MG	BA	3297	1/1	0.87	0.20	42,42,42,42	0
60	MG	BA	3304	1/1	0.87	0.15	36,36,36,36	0
60	MG	DA	3121	1/1	0.87	0.19	34,34,34,34	0
60	MG	BA	3033	1/1	0.87	0.28	1,1,1,1	0
60	MG	DA	3124	1/1	0.87	0.25	36,36,36,36	0
60	MG	CA	1629	1/1	0.87	0.19	16,16,16,16	0
60	MG	AA	1669	1/1	0.87	0.15	35,35,35,35	0
60	MG	BA	3056	1/1	0.87	0.18	1,1,1,1	0
60	MG	BA	3210	1/1	0.87	0.30	33,33,33,33	0
60	MG	BA	3177	1/1	0.87	0.26	41,41,41,41	0
60	MG	CA	1643	1/1	0.87	0.15	7,7,7,7	0
60	MG	BA	3215	1/1	0.87	0.36	60,60,60,60	0
60	MG	DA	3237	1/1	0.87	0.21	10,10,10,10	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BB	201	1/1	0.87	0.18	46,46,46,46	0
60	MG	DA	3147	1/1	0.87	0.11	26,26,26,26	0
60	MG	AA	1708	1/1	0.87	0.25	41,41,41,41	0
60	MG	DA	3037	1/1	0.87	0.09	24,24,24,24	0
60	MG	BA	3125	1/1	0.88	0.07	1,1,1,1	0
60	MG	CA	1630	1/1	0.88	0.10	57,57,57,57	0
60	MG	DA	3146	1/1	0.88	0.18	17,17,17,17	0
60	MG	DA	3005	1/1	0.88	0.27	28,28,28,28	0
60	MG	AA	1692	1/1	0.88	0.16	19,19,19,19	0
60	MG	BA	3309	1/1	0.88	0.09	1,1,1,1	0
60	MG	AA	1696	1/1	0.88	0.24	20,20,20,20	0
60	MG	DA	3160	1/1	0.88	0.24	27,27,27,27	0
60	MG	DA	3029	1/1	0.88	0.18	1,1,1,1	0
60	MG	BA	3205	1/1	0.88	0.28	30,30,30,30	0
60	MG	AA	1673	1/1	0.88	0.12	39,39,39,39	0
60	MG	AA	1620	1/1	0.88	0.26	31,31,31,31	0
60	MG	DA	3063	1/1	0.88	0.20	24,24,24,24	0
60	MG	BA	3093	1/1	0.88	0.24	1,1,1,1	0
60	MG	DA	3080	1/1	0.88	0.15	36,36,36,36	0
60	MG	BA	3094	1/1	0.88	0.09	11,11,11,11	0
60	MG	DA	3182	1/1	0.88	0.23	23,23,23,23	0
60	MG	DA	3184	1/1	0.88	0.38	35,35,35,35	0
60	MG	DA	3087	1/1	0.88	0.17	32,32,32,32	0
60	MG	BA	3229	1/1	0.88	0.31	49,49,49,49	0
60	MG	BA	3241	1/1	0.88	0.55	80,80,80,80	0
60	MG	BX	101	1/1	0.88	0.10	31,31,31,31	0
60	MG	DA	3098	1/1	0.88	0.17	27,27,27,27	0
60	MG	BA	3169	1/1	0.88	0.18	16,16,16,16	0
60	MG	AA	1654	1/1	0.88	0.21	68,68,68,68	0
60	MG	AA	1683	1/1	0.88	0.13	16,16,16,16	0
60	MG	CA	1606	1/1	0.88	0.33	45,45,45,45	0
60	MG	AA	1664	1/1	0.88	0.20	46,46,46,46	0
60	MG	BA	3108	1/1	0.88	0.25	2,2,2,2	0
60	MG	DA	3228	1/1	0.88	0.23	34,34,34,34	0
60	MG	CA	1684	1/1	0.88	0.13	33,33,33,33	0
60	MG	BA	3014	1/1	0.88	0.30	1,1,1,1	0
60	MG	CA	1617	1/1	0.88	0.16	1,1,1,1	0
60	MG	CA	1694	1/1	0.88	0.43	51,51,51,51	0
60	MG	AA	1610	1/1	0.88	0.17	36,36,36,36	0
60	MG	BA	3296	1/1	0.88	0.25	26,26,26,26	0
60	MG	AA	1618	1/1	0.88	0.32	22,22,22,22	0
60	MG	D7	101	1/1	0.88	0.13	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3143	1/1	0.89	0.11	32,32,32,32	0
60	MG	AA	1652	1/1	0.89	0.22	28,28,28,28	0
60	MG	DA	3161	1/1	0.89	0.15	33,33,33,33	0
60	MG	DA	3078	1/1	0.89	0.09	26,26,26,26	0
60	MG	AA	1613	1/1	0.89	0.17	36,36,36,36	0
60	MG	BA	3115	1/1	0.89	0.21	1,1,1,1	0
60	MG	BA	3291	1/1	0.89	0.22	14,14,14,14	0
60	MG	CA	1631	1/1	0.89	0.09	19,19,19,19	0
60	MG	BA	3036	1/1	0.89	0.26	8,8,8,8	0
60	MG	BD	301	1/1	0.89	0.28	12,12,12,12	0
60	MG	DA	3177	1/1	0.89	0.13	13,13,13,13	0
60	MG	AA	1670	1/1	0.89	0.15	54,54,54,54	0
60	MG	DA	3103	1/1	0.89	0.17	26,26,26,26	0
60	MG	DA	3109	1/1	0.89	0.15	50,50,50,50	0
60	MG	BA	3091	1/1	0.89	0.20	1,1,1,1	0
60	MG	CA	1700	1/1	0.89	0.22	36,36,36,36	0
60	MG	B0	103	1/1	0.89	0.19	22,22,22,22	0
60	MG	DA	3116	1/1	0.89	0.27	47,47,47,47	0
60	MG	CA	1702	1/1	0.89	0.18	27,27,27,27	0
60	MG	CA	1644	1/1	0.89	0.48	67,67,67,67	0
60	MG	BA	3237	1/1	0.89	0.17	1,1,1,1	0
60	MG	DA	3211	1/1	0.89	0.16	23,23,23,23	0
60	MG	BA	3302	1/1	0.89	0.11	11,11,11,11	0
60	MG	DA	3217	1/1	0.89	0.16	27,27,27,27	0
60	MG	DA	3220	1/1	0.89	0.24	30,30,30,30	0
60	MG	DA	3003	1/1	0.89	0.15	17,17,17,17	0
60	MG	BA	3238	1/1	0.89	0.22	29,29,29,29	0
60	MG	BA	3168	1/1	0.89	0.36	60,60,60,60	0
60	MG	DA	3013	1/1	0.89	0.16	30,30,30,30	0
60	MG	BA	3247	1/1	0.89	0.20	35,35,35,35	0
60	MG	CA	1656	1/1	0.89	0.19	39,39,39,39	0
60	MG	BA	3128	1/1	0.89	0.19	16,16,16,16	0
60	MG	DA	3238	1/1	0.89	0.39	42,42,42,42	0
60	MG	DA	3035	1/1	0.89	0.21	1,1,1,1	0
60	MG	BA	3258	1/1	0.89	0.22	32,32,32,32	0
60	MG	CA	1670	1/1	0.89	0.20	26,26,26,26	0
60	MG	DA	3048	1/1	0.89	0.18	23,23,23,23	0
60	MG	CA	1672	1/1	0.89	0.19	21,21,21,21	0
60	MG	BA	3029	1/1	0.90	0.22	36,36,36,36	0
60	MG	BA	3310	1/1	0.90	0.24	38,38,38,38	0
60	MG	CA	1607	1/1	0.90	0.27	29,29,29,29	0
60	MG	AA	1665	1/1	0.90	0.13	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3274	1/1	0.90	0.15	21,21,21,21	0
60	MG	CA	1690	1/1	0.90	0.20	31,31,31,31	0
60	MG	DA	3185	1/1	0.90	0.13	10,10,10,10	0
60	MG	DA	3042	1/1	0.90	0.12	46,46,46,46	0
60	MG	CA	1692	1/1	0.90	0.24	32,32,32,32	0
60	MG	DA	3049	1/1	0.90	0.21	36,36,36,36	0
60	MG	BA	3172	1/1	0.90	0.12	18,18,18,18	0
60	MG	BA	3158	1/1	0.90	0.34	35,35,35,35	0
60	MG	DA	3199	1/1	0.90	0.15	35,35,35,35	0
60	MG	DA	3075	1/1	0.90	0.29	1,1,1,1	0
60	MG	DA	3141	1/1	0.90	0.20	36,36,36,36	0
60	MG	AA	1647	1/1	0.90	0.20	39,39,39,39	0
60	MG	BA	3160	1/1	0.90	0.34	29,29,29,29	0
60	MG	DA	3216	1/1	0.90	0.14	24,24,24,24	0
60	MG	DA	3079	1/1	0.90	0.20	19,19,19,19	0
60	MG	DA	3218	1/1	0.90	0.31	50,50,50,50	0
60	MG	AA	1682	1/1	0.90	0.13	48,48,48,48	0
60	MG	BA	3236	1/1	0.90	0.21	11,11,11,11	0
60	MG	DA	3086	1/1	0.90	0.33	58,58,58,58	0
60	MG	CA	1669	1/1	0.90	0.13	16,16,16,16	0
60	MG	DA	3156	1/1	0.90	0.09	47,47,47,47	0
60	MG	AA	1605	1/1	0.90	0.10	35,35,35,35	0
60	MG	DA	3234	1/1	0.90	0.21	40,40,40,40	0
60	MG	AA	1657	1/1	0.90	0.21	37,37,37,37	0
60	MG	AA	1604	1/1	0.90	0.19	14,14,14,14	0
60	MG	BA	3200	1/1	0.90	0.22	14,14,14,14	0
60	MG	DA	3009	1/1	0.90	0.16	12,12,12,12	0
60	MG	DA	3166	1/1	0.90	0.28	36,36,36,36	0
60	MG	DA	3104	1/1	0.90	0.26	42,42,42,42	0
60	MG	BA	3141	1/1	0.90	0.21	17,17,17,17	0
60	MG	DA	3016	1/1	0.90	0.17	12,12,12,12	0
60	MG	DA	3178	1/1	0.91	0.13	22,22,22,22	0
60	MG	AA	1661	1/1	0.91	0.13	21,21,21,21	0
60	MG	CA	1621	1/1	0.91	0.20	30,30,30,30	0
60	MG	AA	1603	1/1	0.91	0.13	32,32,32,32	0
60	MG	BA	3243	1/1	0.91	0.42	45,45,45,45	0
60	MG	BA	3096	1/1	0.91	0.24	34,34,34,34	0
60	MG	BA	3149	1/1	0.91	0.14	14,14,14,14	0
60	MG	BA	3151	1/1	0.91	0.17	22,22,22,22	0
60	MG	DA	3072	1/1	0.91	0.11	8,8,8,8	0
60	MG	DA	3073	1/1	0.91	0.21	58,58,58,58	0
60	MG	DA	3142	1/1	0.91	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3259	1/1	0.91	0.32	16,16,16,16	0
60	MG	DA	3201	1/1	0.91	0.19	36,36,36,36	0
60	MG	DA	3203	1/1	0.91	0.34	38,38,38,38	0
60	MG	AX	106	1/1	0.91	0.26	25,25,25,25	0
60	MG	BA	3051	1/1	0.91	0.24	14,14,14,14	0
60	MG	DA	3213	1/1	0.91	0.28	31,31,31,31	0
60	MG	BA	3276	1/1	0.91	0.22	16,16,16,16	0
60	MG	BA	3053	1/1	0.91	0.19	1,1,1,1	0
60	MG	AA	1656	1/1	0.91	0.22	10,10,10,10	0
60	MG	DA	3153	1/1	0.91	0.15	13,13,13,13	0
60	MG	DA	3154	1/1	0.91	0.15	38,38,38,38	0
60	MG	BA	3284	1/1	0.91	0.15	21,21,21,21	0
60	MG	DA	3222	1/1	0.91	0.13	24,24,24,24	0
60	MG	AA	1678	1/1	0.91	0.25	29,29,29,29	0
60	MG	CW	104	1/1	0.91	0.11	57,57,57,57	0
60	MG	BA	3114	1/1	0.91	0.14	14,14,14,14	0
60	MG	BA	3211	1/1	0.91	0.38	36,36,36,36	0
60	MG	BA	3071	1/1	0.91	0.17	1,1,1,1	0
60	MG	BA	3082	1/1	0.91	0.23	44,44,44,44	0
60	MG	CA	1608	1/1	0.91	0.14	24,24,24,24	0
60	MG	AA	1679	1/1	0.91	0.12	36,36,36,36	0
60	MG	BA	3026	1/1	0.91	0.19	7,7,7,7	0
60	MG	CA	1612	1/1	0.91	0.39	35,35,35,35	0
60	MG	CA	1613	1/1	0.91	0.33	36,36,36,36	0
60	MG	BA	3127	1/1	0.91	0.18	1,1,1,1	0
60	MG	AA	1621	1/1	0.91	0.24	28,28,28,28	0
60	MG	DA	3088	1/1	0.92	0.21	22,22,22,22	0
60	MG	BA	3007	1/1	0.92	0.24	1,1,1,1	0
60	MG	DA	3170	1/1	0.92	0.19	33,33,33,33	0
60	MG	BA	3074	1/1	0.92	0.15	4,4,4,4	0
60	MG	DA	3174	1/1	0.92	0.23	6,6,6,6	0
60	MG	BA	3075	1/1	0.92	0.11	2,2,2,2	0
60	MG	BA	3240	1/1	0.92	0.38	75,75,75,75	0
60	MG	BA	3080	1/1	0.92	0.24	15,15,15,15	0
60	MG	CA	1662	1/1	0.92	0.15	38,38,38,38	0
60	MG	DA	3107	1/1	0.92	0.15	37,37,37,37	0
60	MG	AA	1685	1/1	0.92	0.25	69,69,69,69	0
60	MG	BA	3043	1/1	0.92	0.22	1,1,1,1	0
60	MG	BA	3250	1/1	0.92	0.12	12,12,12,12	0
60	MG	BA	3021	1/1	0.92	0.21	1,1,1,1	0
60	MG	BA	3022	1/1	0.92	0.23	19,19,19,19	0
60	MG	DA	3026	1/1	0.92	0.14	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1673	1/1	0.92	0.10	15,15,15,15	0
60	MG	CA	1619	1/1	0.92	0.24	20,20,20,20	0
60	MG	DA	3123	1/1	0.92	0.30	40,40,40,40	0
60	MG	CA	1676	1/1	0.92	0.07	25,25,25,25	0
60	MG	AA	1709	1/1	0.92	0.16	36,36,36,36	0
60	MG	DA	3130	1/1	0.92	0.08	27,27,27,27	0
60	MG	DA	3039	1/1	0.92	0.10	53,53,53,53	0
60	MG	DA	3205	1/1	0.92	0.09	2,2,2,2	0
60	MG	BA	3266	1/1	0.92	0.21	12,12,12,12	0
60	MG	CA	1680	1/1	0.92	0.07	44,44,44,44	0
60	MG	DA	3047	1/1	0.92	0.20	29,29,29,29	0
60	MG	BA	3027	1/1	0.92	0.28	1,1,1,1	0
60	MG	BA	3330	1/1	0.92	0.10	12,12,12,12	0
60	MG	AA	1713	1/1	0.92	0.16	43,43,43,43	0
60	MG	DA	3054	1/1	0.92	0.11	21,21,21,21	0
60	MG	DA	3055	1/1	0.92	0.16	17,17,17,17	0
60	MG	DA	3057	1/1	0.92	0.07	32,32,32,32	0
60	MG	BA	3133	1/1	0.92	0.24	1,1,1,1	0
60	MG	DA	3071	1/1	0.92	0.14	19,19,19,19	0
60	MG	BA	3140	1/1	0.92	0.35	26,26,26,26	0
60	MG	CA	1636	1/1	0.92	0.25	26,26,26,26	0
60	MG	CA	1691	1/1	0.92	0.11	21,21,21,21	0
60	MG	BA	3097	1/1	0.92	0.28	44,44,44,44	0
60	MG	DA	3157	1/1	0.92	0.30	58,58,58,58	0
60	MG	BA	3173	1/1	0.92	0.20	50,50,50,50	0
60	MG	CA	1695	1/1	0.92	0.18	40,40,40,40	0
60	MG	DB	201	1/1	0.92	0.18	51,51,51,51	0
60	MG	BA	3287	1/1	0.92	0.09	7,7,7,7	0
60	MG	DD	301	1/1	0.92	0.13	21,21,21,21	0
60	MG	BA	3226	1/1	0.92	0.23	39,39,39,39	0
60	MG	BA	3062	1/1	0.92	0.20	1,1,1,1	0
60	MG	BA	3231	1/1	0.92	0.14	2,2,2,2	0
60	MG	BA	3142	1/1	0.93	0.07	30,30,30,30	0
60	MG	DA	3052	1/1	0.93	0.17	14,14,14,14	0
60	MG	BA	3197	1/1	0.93	0.15	24,24,24,24	0
60	MG	AA	1691	1/1	0.93	0.28	23,23,23,23	0
60	MG	DA	3158	1/1	0.93	0.15	49,49,49,49	0
60	MG	BA	3018	1/1	0.93	0.18	1,1,1,1	0
60	MG	BA	3147	1/1	0.93	0.14	8,8,8,8	0
60	MG	DA	3059	1/1	0.93	0.21	6,6,6,6	0
60	MG	DA	3060	1/1	0.93	0.16	23,23,23,23	0
60	MG	BA	3285	1/1	0.93	0.13	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3064	1/1	0.93	0.15	12,12,12,12	0
60	MG	DA	3065	1/1	0.93	0.16	28,28,28,28	0
60	MG	DA	3066	1/1	0.93	0.30	40,40,40,40	0
60	MG	CA	1610	1/1	0.93	0.13	48,48,48,48	0
60	MG	AA	1710	1/1	0.93	0.32	29,29,29,29	0
60	MG	DA	3172	1/1	0.93	0.18	6,6,6,6	0
60	MG	AA	1660	1/1	0.93	0.28	49,49,49,49	0
60	MG	AA	1625	1/1	0.93	0.15	21,21,21,21	0
60	MG	CA	1614	1/1	0.93	0.37	50,50,50,50	0
60	MG	AA	1699	1/1	0.93	0.07	21,21,21,21	0
60	MG	CA	1688	1/1	0.93	0.11	37,37,37,37	0
60	MG	BA	3064	1/1	0.93	0.32	45,45,45,45	0
60	MG	BA	3106	1/1	0.93	0.15	3,3,3,3	0
60	MG	BA	3223	1/1	0.93	0.31	42,42,42,42	0
60	MG	BA	3301	1/1	0.93	0.15	16,16,16,16	0
60	MG	BA	3066	1/1	0.93	0.10	1,1,1,1	0
60	MG	BA	3069	1/1	0.93	0.17	1,1,1,1	0
60	MG	CA	1697	1/1	0.93	0.15	27,27,27,27	0
60	MG	DA	3094	1/1	0.93	0.17	16,16,16,16	0
60	MG	DA	3196	1/1	0.93	0.21	1,1,1,1	0
60	MG	CA	1698	1/1	0.93	0.20	29,29,29,29	0
60	MG	AW	102	1/1	0.93	0.07	36,36,36,36	0
60	MG	BA	3006	1/1	0.93	0.31	37,37,37,37	0
60	MG	BA	3034	1/1	0.93	0.23	1,1,1,1	0
60	MG	BA	3077	1/1	0.93	0.19	1,1,1,1	0
60	MG	CW	102	1/1	0.93	0.07	40,40,40,40	0
60	MG	BA	3078	1/1	0.93	0.20	1,1,1,1	0
60	MG	CA	1637	1/1	0.93	0.54	57,57,57,57	0
60	MG	BA	3122	1/1	0.93	0.21	12,12,12,12	0
60	MG	CA	1639	1/1	0.93	0.18	16,16,16,16	0
60	MG	BA	3325	1/1	0.93	0.10	19,19,19,19	0
60	MG	BA	3176	1/1	0.93	0.13	1,1,1,1	0
60	MG	BA	3245	1/1	0.93	0.14	25,25,25,25	0
60	MG	BA	3079	1/1	0.93	0.14	7,7,7,7	0
60	MG	BA	3332	1/1	0.93	0.20	1,1,1,1	0
60	MG	DA	3020	1/1	0.93	0.28	40,40,40,40	0
60	MG	DA	3129	1/1	0.93	0.09	20,20,20,20	0
60	MG	BA	3334	1/1	0.93	0.12	1,1,1,1	0
60	MG	DA	3025	1/1	0.93	0.17	1,1,1,1	0
60	MG	DA	3229	1/1	0.93	0.12	20,20,20,20	0
60	MG	BA	3249	1/1	0.93	0.34	13,13,13,13	0
60	MG	AA	1633	1/1	0.93	0.13	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3081	1/1	0.93	0.09	19,19,19,19	0
60	MG	BA	3040	1/1	0.93	0.22	1,1,1,1	0
60	MG	CA	1660	1/1	0.93	0.13	21,21,21,21	0
60	MG	BE	302	1/1	0.93	0.17	1,1,1,1	0
60	MG	BG	201	1/1	0.93	0.15	30,30,30,30	0
60	MG	BA	3042	1/1	0.93	0.06	1,1,1,1	0
60	MG	DB	203	1/1	0.93	0.05	54,54,54,54	0
60	MG	DA	3043	1/1	0.93	0.14	9,9,9,9	0
60	MG	DA	3046	1/1	0.93	0.10	28,28,28,28	0
60	MG	BA	3008	1/1	0.93	0.08	4,4,4,4	0
60	MG	BA	3194	1/1	0.93	0.38	54,54,54,54	0
60	MG	CA	1653	1/1	0.94	0.18	36,36,36,36	0
60	MG	BA	3248	1/1	0.94	0.21	34,34,34,34	0
60	MG	DA	3036	1/1	0.94	0.10	5,5,5,5	0
60	MG	AA	1686	1/1	0.94	0.37	34,34,34,34	0
60	MG	AA	1687	1/1	0.94	0.17	20,20,20,20	0
60	MG	AA	1672	1/1	0.94	0.13	53,53,53,53	0
60	MG	CA	1663	1/1	0.94	0.05	31,31,31,31	0
60	MG	DA	3149	1/1	0.94	0.23	39,39,39,39	0
60	MG	BA	3253	1/1	0.94	0.23	39,39,39,39	0
60	MG	BA	3256	1/1	0.94	0.20	23,23,23,23	0
60	MG	BB	204	1/1	0.94	0.14	21,21,21,21	0
60	MG	BA	3193	1/1	0.94	0.29	22,22,22,22	0
60	MG	CA	1671	1/1	0.94	0.13	24,24,24,24	0
60	MG	BA	3068	1/1	0.94	0.07	11,11,11,11	0
60	MG	BA	3263	1/1	0.94	0.29	47,47,47,47	0
60	MG	BU	201	1/1	0.94	0.17	23,23,23,23	0
60	MG	BA	3264	1/1	0.94	0.34	32,32,32,32	0
60	MG	BA	3265	1/1	0.94	0.14	13,13,13,13	0
60	MG	BA	3146	1/1	0.94	0.09	13,13,13,13	0
60	MG	BA	3037	1/1	0.94	0.24	33,33,33,33	0
60	MG	BA	3198	1/1	0.94	0.11	5,5,5,5	0
60	MG	BA	3016	1/1	0.94	0.16	1,1,1,1	0
60	MG	BA	3279	1/1	0.94	0.15	29,29,29,29	0
60	MG	BA	3105	1/1	0.94	0.09	8,8,8,8	0
60	MG	DA	3067	1/1	0.94	0.13	23,23,23,23	0
60	MG	DA	3069	1/1	0.94	0.17	6,6,6,6	0
60	MG	BA	3203	1/1	0.94	0.17	17,17,17,17	0
60	MG	BA	3073	1/1	0.94	0.19	1,1,1,1	0
60	MG	BA	3041	1/1	0.94	0.20	1,1,1,1	0
60	MG	AA	1659	1/1	0.94	0.13	23,23,23,23	0
60	MG	AA	1649	1/1	0.94	0.11	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	CA	1693	1/1	0.94	0.10	20,20,20,20	0
60	MG	BA	3044	1/1	0.94	0.19	1,1,1,1	0
60	MG	BA	3292	1/1	0.94	0.18	27,27,27,27	0
60	MG	DA	3082	1/1	0.94	0.14	15,15,15,15	0
60	MG	DA	3083	1/1	0.94	0.39	35,35,35,35	0
60	MG	BA	3046	1/1	0.94	0.19	10,10,10,10	0
60	MG	BA	3116	1/1	0.94	0.19	26,26,26,26	0
60	MG	DA	3192	1/1	0.94	0.17	10,10,10,10	0
60	MG	DA	3195	1/1	0.94	0.17	18,18,18,18	0
60	MG	BA	3295	1/1	0.94	0.15	41,41,41,41	0
60	MG	CA	1699	1/1	0.94	0.10	30,30,30,30	0
60	MG	AA	1636	1/1	0.94	0.20	28,28,28,28	0
60	MG	BA	3224	1/1	0.94	0.11	20,20,20,20	0
60	MG	BA	3300	1/1	0.94	0.14	22,22,22,22	0
60	MG	CE	201	1/1	0.94	0.12	56,56,56,56	0
60	MG	DA	3096	1/1	0.94	0.14	16,16,16,16	0
60	MG	BA	3003	1/1	0.94	0.21	64,64,64,64	0
60	MG	DA	3100	1/1	0.94	0.12	18,18,18,18	0
60	MG	BA	3227	1/1	0.94	0.13	33,33,33,33	0
60	MG	BA	3303	1/1	0.94	0.27	32,32,32,32	0
60	MG	DA	3215	1/1	0.94	0.17	23,23,23,23	0
60	MG	BA	3004	1/1	0.94	0.17	8,8,8,8	0
60	MG	BA	3083	1/1	0.94	0.24	1,1,1,1	0
60	MG	DA	3002	1/1	0.94	0.12	9,9,9,9	0
60	MG	AA	1629	1/1	0.94	0.31	51,51,51,51	0
60	MG	BA	3174	1/1	0.94	0.06	7,7,7,7	0
60	MG	BA	3058	1/1	0.94	0.11	1,1,1,1	0
60	MG	BA	3088	1/1	0.94	0.13	1,1,1,1	0
60	MG	DA	3120	1/1	0.94	0.18	3,3,3,3	0
60	MG	BA	3314	1/1	0.94	0.12	35,35,35,35	0
60	MG	DA	3015	1/1	0.94	0.10	1,1,1,1	0
60	MG	BA	3178	1/1	0.94	0.19	1,1,1,1	0
60	MG	DA	3018	1/1	0.94	0.09	15,15,15,15	0
60	MG	DA	3125	1/1	0.94	0.06	49,49,49,49	0
60	MG	DA	3127	1/1	0.94	0.14	20,20,20,20	0
60	MG	DA	3019	1/1	0.94	0.05	6,6,6,6	0
60	MG	BA	3320	1/1	0.94	0.12	23,23,23,23	0
60	MG	BA	3322	1/1	0.94	0.16	10,10,10,10	0
60	MG	DA	3024	1/1	0.94	0.10	5,5,5,5	0
60	MG	BA	3184	1/1	0.94	0.32	40,40,40,40	0
60	MG	BA	3135	1/1	0.94	0.15	20,20,20,20	0
60	MG	BA	3032	1/1	0.94	0.16	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3139	1/1	0.94	0.14	1,1,1,1	0
60	MG	DA	3028	1/1	0.94	0.17	1,1,1,1	0
61	ZN	B5	102	1/1	0.94	0.07	51,51,51,51	0
60	MG	CA	1601	1/1	0.95	0.21	1,1,1,1	0
60	MG	BA	3134	1/1	0.95	0.19	12,12,12,12	0
60	MG	DA	3152	1/1	0.95	0.17	8,8,8,8	0
60	MG	BA	3286	1/1	0.95	0.24	18,18,18,18	0
60	MG	CA	1604	1/1	0.95	0.17	1,1,1,1	0
60	MG	BA	3225	1/1	0.95	0.13	9,9,9,9	0
60	MG	BA	3010	1/1	0.95	0.21	2,2,2,2	0
60	MG	BA	3137	1/1	0.95	0.20	1,1,1,1	0
60	MG	BA	3228	1/1	0.95	0.22	52,52,52,52	0
60	MG	BA	3139	1/1	0.95	0.14	1,1,1,1	0
60	MG	CA	1687	1/1	0.95	0.16	17,17,17,17	0
60	MG	BA	3230	1/1	0.95	0.15	19,19,19,19	0
60	MG	BA	3179	1/1	0.95	0.11	17,17,17,17	0
60	MG	DA	3163	1/1	0.95	0.23	32,32,32,32	0
60	MG	BA	3013	1/1	0.95	0.17	1,1,1,1	0
60	MG	AA	1695	1/1	0.95	0.16	30,30,30,30	0
60	MG	BA	3299	1/1	0.95	0.12	13,13,13,13	0
60	MG	AA	1614	1/1	0.95	0.09	22,22,22,22	0
60	MG	BA	3188	1/1	0.95	0.18	30,30,30,30	0
60	MG	BA	3102	1/1	0.95	0.12	1,1,1,1	0
60	MG	AA	1645	1/1	0.95	0.17	22,22,22,22	0
60	MG	CA	1623	1/1	0.95	0.27	33,33,33,33	0
60	MG	AA	1658	1/1	0.95	0.10	1,1,1,1	0
60	MG	CA	1625	1/1	0.95	0.15	3,3,3,3	0
60	MG	BA	3246	1/1	0.95	0.12	1,1,1,1	0
60	MG	CA	1628	1/1	0.95	0.08	12,12,12,12	0
60	MG	BA	3308	1/1	0.95	0.18	30,30,30,30	0
60	MG	BA	3076	1/1	0.95	0.19	1,1,1,1	0
60	MG	BA	3049	1/1	0.95	0.15	1,1,1,1	0
60	MG	DA	3093	1/1	0.95	0.22	31,31,31,31	0
60	MG	AA	1712	1/1	0.95	0.30	36,36,36,36	0
60	MG	DA	3187	1/1	0.95	0.04	27,27,27,27	0
60	MG	CA	1634	1/1	0.95	0.14	16,16,16,16	0
60	MG	BA	3155	1/1	0.95	0.14	14,14,14,14	0
60	MG	DA	3097	1/1	0.95	0.07	51,51,51,51	0
60	MG	DA	3191	1/1	0.95	0.21	31,31,31,31	0
60	MG	AA	1677	1/1	0.95	0.20	30,30,30,30	0
60	MG	DA	3099	1/1	0.95	0.05	14,14,14,14	0
60	MG	AA	1703	1/1	0.95	0.19	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	1653	1/1	0.95	0.17	38,38,38,38	0
60	MG	BA	3202	1/1	0.95	0.13	1,1,1,1	0
60	MG	BA	3323	1/1	0.95	0.15	2,2,2,2	0
60	MG	CA	1642	1/1	0.95	0.10	28,28,28,28	0
60	MG	DA	3202	1/1	0.95	0.13	18,18,18,18	0
60	MG	DA	3110	1/1	0.95	0.13	48,48,48,48	0
60	MG	BA	3057	1/1	0.95	0.10	3,3,3,3	0
60	MG	DA	3112	1/1	0.95	0.17	7,7,7,7	0
60	MG	DA	3207	1/1	0.95	0.11	1,1,1,1	0
60	MG	BA	3326	1/1	0.95	0.17	21,21,21,21	0
60	MG	BA	3260	1/1	0.95	0.57	65,65,65,65	0
60	MG	BA	3261	1/1	0.95	0.16	16,16,16,16	0
60	MG	CA	1648	1/1	0.95	0.13	24,24,24,24	0
60	MG	DA	3118	1/1	0.95	0.28	22,22,22,22	0
60	MG	BA	3005	1/1	0.95	0.35	1,1,1,1	0
60	MG	CA	1651	1/1	0.95	0.35	35,35,35,35	0
60	MG	DA	3219	1/1	0.95	0.06	19,19,19,19	0
60	MG	AA	1612	1/1	0.95	0.13	15,15,15,15	0
60	MG	BA	3061	1/1	0.95	0.13	17,17,17,17	0
60	MG	CA	1654	1/1	0.95	0.08	44,44,44,44	0
60	MG	DA	3223	1/1	0.95	0.10	13,13,13,13	0
60	MG	AA	1706	1/1	0.95	0.08	28,28,28,28	0
60	MG	DA	3226	1/1	0.95	0.06	30,30,30,30	0
60	MG	DA	3126	1/1	0.95	0.16	7,7,7,7	0
60	MG	BA	3268	1/1	0.95	0.12	1,1,1,1	0
60	MG	CA	1658	1/1	0.95	0.25	30,30,30,30	0
60	MG	BA	3212	1/1	0.95	0.12	11,11,11,11	0
60	MG	BA	3271	1/1	0.95	0.18	28,28,28,28	0
60	MG	DA	3038	1/1	0.95	0.13	8,8,8,8	0
60	MG	BA	3089	1/1	0.95	0.11	12,12,12,12	0
60	MG	AW	104	1/1	0.95	0.15	31,31,31,31	0
60	MG	BA	3217	1/1	0.95	0.05	1,1,1,1	0
60	MG	CA	1668	1/1	0.95	0.19	30,30,30,30	0
60	MG	BA	3221	1/1	0.95	0.28	35,35,35,35	0
60	MG	BU	202	1/1	0.95	0.20	1,1,1,1	0
60	MG	BA	3282	1/1	0.95	0.19	20,20,20,20	0
60	MG	DD	302	1/1	0.95	0.19	6,6,6,6	0
60	MG	B0	101	1/1	0.95	0.19	4,4,4,4	0
60	MG	DA	3051	1/1	0.95	0.11	18,18,18,18	0
60	MG	D0	101	1/1	0.95	0.19	12,12,12,12	0
60	MG	BA	3132	1/1	0.95	0.19	1,1,1,1	0
60	MG	BA	3009	1/1	0.95	0.20	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3112	1/1	0.96	0.06	11,11,11,11	0
60	MG	BA	3207	1/1	0.96	0.20	21,21,21,21	0
60	MG	CA	1674	1/1	0.96	0.27	55,55,55,55	0
60	MG	B5	101	1/1	0.96	0.08	16,16,16,16	0
60	MG	BA	3113	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3278	1/1	0.96	0.07	15,15,15,15	0
60	MG	AA	1617	1/1	0.96	0.11	13,13,13,13	0
60	MG	BA	3035	1/1	0.96	0.11	1,1,1,1	0
60	MG	CA	1681	1/1	0.96	0.27	44,44,44,44	0
60	MG	BA	3161	1/1	0.96	0.29	24,24,24,24	0
60	MG	AA	1655	1/1	0.96	0.21	2,2,2,2	0
60	MG	DA	3068	1/1	0.96	0.06	9,9,9,9	0
60	MG	BA	3216	1/1	0.96	0.13	25,25,25,25	0
60	MG	BA	3163	1/1	0.96	0.07	12,12,12,12	0
60	MG	BA	3219	1/1	0.96	0.05	15,15,15,15	0
60	MG	DA	3165	1/1	0.96	0.12	14,14,14,14	0
60	MG	BA	3220	1/1	0.96	0.12	1,1,1,1	0
60	MG	AX	109	1/1	0.96	0.06	16,16,16,16	0
60	MG	BA	3118	1/1	0.96	0.31	46,46,46,46	0
60	MG	BA	3166	1/1	0.96	0.16	8,8,8,8	0
60	MG	CA	1615	1/1	0.96	0.20	28,28,28,28	0
60	MG	BA	3119	1/1	0.96	0.14	91,91,91,91	0
60	MG	BA	3039	1/1	0.96	0.20	1,1,1,1	0
60	MG	BA	3086	1/1	0.96	0.10	4,4,4,4	0
60	MG	BA	3170	1/1	0.96	0.32	55,55,55,55	0
60	MG	BA	3123	1/1	0.96	0.12	6,6,6,6	0
60	MG	AA	1607	1/1	0.96	0.48	51,51,51,51	0
60	MG	DA	3180	1/1	0.96	0.23	5,5,5,5	0
60	MG	BA	3126	1/1	0.96	0.11	5,5,5,5	0
60	MG	BA	3065	1/1	0.96	0.13	2,2,2,2	0
60	MG	BA	3234	1/1	0.96	0.13	15,15,15,15	0
60	MG	DA	3092	1/1	0.96	0.05	17,17,17,17	0
60	MG	BA	3235	1/1	0.96	0.12	1,1,1,1	0
60	MG	BA	3002	1/1	0.96	0.24	17,17,17,17	0
60	MG	CV	601	1/1	0.96	0.23	16,16,16,16	0
60	MG	BA	3129	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3131	1/1	0.96	0.26	1,1,1,1	0
60	MG	CA	1632	1/1	0.96	0.16	6,6,6,6	0
60	MG	BA	3239	1/1	0.96	0.14	2,2,2,2	0
60	MG	DA	3193	1/1	0.96	0.13	29,29,29,29	0
60	MG	DA	3194	1/1	0.96	0.27	44,44,44,44	0
60	MG	BA	3092	1/1	0.96	0.21	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3101	1/1	0.96	0.18	20,20,20,20	0
60	MG	DA	3102	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3311	1/1	0.96	0.31	40,40,40,40	0
60	MG	BA	3180	1/1	0.96	0.14	40,40,40,40	0
60	MG	DA	3105	1/1	0.96	0.11	59,59,59,59	0
60	MG	BA	3242	1/1	0.96	0.30	49,49,49,49	0
60	MG	BA	3182	1/1	0.96	0.10	1,1,1,1	0
60	MG	BA	3244	1/1	0.96	0.22	34,34,34,34	0
60	MG	DA	3012	1/1	0.96	0.10	1,1,1,1	0
60	MG	BA	3319	1/1	0.96	0.14	31,31,31,31	0
60	MG	DA	3209	1/1	0.96	0.12	5,5,5,5	0
60	MG	DA	3113	1/1	0.96	0.18	2,2,2,2	0
60	MG	DA	3212	1/1	0.96	0.04	4,4,4,4	0
60	MG	AA	1631	1/1	0.96	0.25	12,12,12,12	0
60	MG	AA	1628	1/1	0.96	0.14	10,10,10,10	0
60	MG	BA	3025	1/1	0.96	0.27	31,31,31,31	0
60	MG	BA	3072	1/1	0.96	0.06	6,6,6,6	0
60	MG	AA	1697	1/1	0.96	0.05	27,27,27,27	0
60	MG	DA	3119	1/1	0.96	0.15	5,5,5,5	0
60	MG	BA	3047	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3103	1/1	0.96	0.14	1,1,1,1	0
60	MG	BA	3192	1/1	0.96	0.26	31,31,31,31	0
60	MG	BA	3048	1/1	0.96	0.16	1,1,1,1	0
60	MG	BA	3333	1/1	0.96	0.21	1,1,1,1	0
60	MG	AA	1698	1/1	0.96	0.09	23,23,23,23	0
60	MG	AA	1688	1/1	0.96	0.06	49,49,49,49	0
60	MG	BA	3196	1/1	0.96	0.12	21,21,21,21	0
60	MG	CA	1657	1/1	0.96	0.27	23,23,23,23	0
60	MG	BA	3145	1/1	0.96	0.12	31,31,31,31	0
60	MG	CA	1659	1/1	0.96	0.36	46,46,46,46	0
60	MG	BA	3031	1/1	0.96	0.22	1,1,1,1	0
60	MG	CA	1661	1/1	0.96	0.08	9,9,9,9	0
60	MG	DA	3135	1/1	0.96	0.13	11,11,11,11	0
60	MG	DA	3041	1/1	0.96	0.22	1,1,1,1	0
60	MG	DA	3137	1/1	0.96	0.34	39,39,39,39	0
60	MG	AA	1674	1/1	0.96	0.11	32,32,32,32	0
60	MG	AA	1711	1/1	0.96	0.05	15,15,15,15	0
60	MG	DA	3140	1/1	0.96	0.12	24,24,24,24	0
60	MG	BE	303	1/1	0.96	0.28	58,58,58,58	0
60	MG	BA	3110	1/1	0.96	0.23	6,6,6,6	0
60	MG	BA	3267	1/1	0.96	0.09	6,6,6,6	0
60	MG	BA	3152	1/1	0.96	0.17	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3050	1/1	0.96	0.06	38,38,38,38	0
60	MG	D5	101	1/1	0.96	0.10	10,10,10,10	0
60	MG	BA	3269	1/1	0.96	0.24	12,12,12,12	0
60	MG	BA	3154	1/1	0.96	0.05	16,16,16,16	0
60	MG	BP	201	1/1	0.97	0.23	11,11,11,11	0
60	MG	BA	3055	1/1	0.97	0.11	1,1,1,1	0
60	MG	BA	3157	1/1	0.97	0.17	10,10,10,10	0
60	MG	AA	1675	1/1	0.97	0.16	4,4,4,4	0
60	MG	BA	3017	1/1	0.97	0.18	1,1,1,1	0
60	MG	CA	1646	1/1	0.97	0.07	1,1,1,1	0
60	MG	AA	1701	1/1	0.97	0.11	11,11,11,11	0
60	MG	AA	1662	1/1	0.97	0.06	21,21,21,21	0
60	MG	BA	3130	1/1	0.97	0.22	1,1,1,1	0
60	MG	CA	1650	1/1	0.97	0.20	1,1,1,1	0
60	MG	DA	3058	1/1	0.97	0.13	1,1,1,1	0
60	MG	BA	3307	1/1	0.97	0.16	19,19,19,19	0
60	MG	BA	3060	1/1	0.97	0.13	4,4,4,4	0
60	MG	DA	3062	1/1	0.97	0.12	8,8,8,8	0
60	MG	AA	1663	1/1	0.97	0.28	14,14,14,14	0
60	MG	AA	1616	1/1	0.97	0.20	32,32,32,32	0
60	MG	CA	1605	1/1	0.97	0.22	6,6,6,6	0
60	MG	DA	3197	1/1	0.97	0.17	21,21,21,21	0
60	MG	AA	1609	1/1	0.97	0.12	1,1,1,1	0
60	MG	AA	1627	1/1	0.97	0.17	22,22,22,22	0
60	MG	DA	3133	1/1	0.97	0.12	16,16,16,16	0
60	MG	BA	3272	1/1	0.97	0.22	15,15,15,15	0
60	MG	BA	3136	1/1	0.97	0.32	42,42,42,42	0
60	MG	BA	3315	1/1	0.97	0.23	29,29,29,29	0
60	MG	DA	3004	1/1	0.97	0.12	7,7,7,7	0
60	MG	BA	3111	1/1	0.97	0.09	1,1,1,1	0
60	MG	DA	3074	1/1	0.97	0.28	48,48,48,48	0
60	MG	DA	3006	1/1	0.97	0.26	4,4,4,4	0
60	MG	DA	3210	1/1	0.97	0.06	2,2,2,2	0
60	MG	BA	3028	1/1	0.97	0.08	1,1,1,1	0
60	MG	BA	3067	1/1	0.97	0.04	1,1,1,1	0
60	MG	DA	3010	1/1	0.97	0.19	1,1,1,1	0
60	MG	DA	3011	1/1	0.97	0.05	4,4,4,4	0
60	MG	DA	3081	1/1	0.97	0.12	3,3,3,3	0
60	MG	BA	3321	1/1	0.97	0.19	1,1,1,1	0
60	MG	BA	3280	1/1	0.97	0.08	7,7,7,7	0
60	MG	AA	1606	1/1	0.97	0.18	1,1,1,1	0
60	MG	AX	102	1/1	0.97	0.13	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	DA	3150	1/1	0.97	0.08	28,28,28,28	0
60	MG	DA	3151	1/1	0.97	0.21	26,26,26,26	0
60	MG	DA	3017	1/1	0.97	0.09	1,1,1,1	0
60	MG	BA	3209	1/1	0.97	0.18	24,24,24,24	0
60	MG	DA	3089	1/1	0.97	0.07	27,27,27,27	0
60	MG	AA	1619	1/1	0.97	0.03	10,10,10,10	0
60	MG	AA	1611	1/1	0.97	0.07	33,33,33,33	0
60	MG	AA	1615	1/1	0.97	0.06	18,18,18,18	0
60	MG	BA	3331	1/1	0.97	0.28	35,35,35,35	0
60	MG	DA	3230	1/1	0.97	0.04	17,17,17,17	0
60	MG	BA	3095	1/1	0.97	0.19	47,47,47,47	0
60	MG	BA	3288	1/1	0.97	0.16	29,29,29,29	0
60	MG	AA	1622	1/1	0.97	0.15	12,12,12,12	0
60	MG	BA	3148	1/1	0.97	0.05	1,1,1,1	0
60	MG	BA	3121	1/1	0.97	0.26	23,23,23,23	0
60	MG	DA	3033	1/1	0.97	0.10	4,4,4,4	0
60	MG	BA	3183	1/1	0.97	0.13	1,1,1,1	0
60	MG	BA	3054	1/1	0.97	0.08	6,6,6,6	0
60	MG	BB	205	1/1	0.97	0.13	1,1,1,1	0
60	MG	BA	3255	1/1	0.97	0.07	19,19,19,19	0
60	MG	CA	1635	1/1	0.97	0.11	20,20,20,20	0
60	MG	BE	301	1/1	0.97	0.09	1,1,1,1	0
60	MG	BA	3100	1/1	0.97	0.06	10,10,10,10	0
60	MG	BA	3124	1/1	0.97	0.11	13,13,13,13	0
60	MG	BF	301	1/1	0.97	0.04	14,14,14,14	0
60	MG	DA	3044	1/1	0.97	0.09	1,1,1,1	0
60	MG	BA	3298	1/1	0.97	0.18	13,13,13,13	0
61	ZN	D4	101	1/1	0.97	0.04	113,113,113,113	0
61	ZN	D5	102	1/1	0.97	0.04	75,75,75,75	0
60	MG	BA	3199	1/1	0.98	0.11	1,1,1,1	0
60	MG	BA	3327	1/1	0.98	0.18	17,17,17,17	0
60	MG	DA	3014	1/1	0.98	0.14	4,4,4,4	0
60	MG	BA	3019	1/1	0.98	0.19	1,1,1,1	0
60	MG	CA	1622	1/1	0.98	0.12	12,12,12,12	0
60	MG	BA	3020	1/1	0.98	0.20	1,1,1,1	0
60	MG	AA	1694	1/1	0.98	0.13	5,5,5,5	0
60	MG	AA	1650	1/1	0.98	0.12	15,15,15,15	0
60	MG	BA	3045	1/1	0.98	0.11	2,2,2,2	0
60	MG	BA	3023	1/1	0.98	0.06	1,1,1,1	0
60	MG	DA	3022	1/1	0.98	0.07	11,11,11,11	0
60	MG	DA	3023	1/1	0.98	0.06	14,14,14,14	0
60	MG	CA	1678	1/1	0.98	0.27	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	AA	1634	1/1	0.98	0.11	1,1,1,1	0
60	MG	BA	3208	1/1	0.98	0.16	1,1,1,1	0
60	MG	BA	3175	1/1	0.98	0.13	26,26,26,26	0
60	MG	BA	3290	1/1	0.98	0.17	24,24,24,24	0
60	MG	AA	1666	1/1	0.98	0.06	9,9,9,9	0
60	MG	DA	3208	1/1	0.98	0.08	12,12,12,12	0
60	MG	DA	3030	1/1	0.98	0.04	8,8,8,8	0
60	MG	DA	3031	1/1	0.98	0.06	9,9,9,9	0
60	MG	BA	3098	1/1	0.98	0.32	1,1,1,1	0
60	MG	AA	1667	1/1	0.98	0.05	15,15,15,15	0
60	MG	BA	3150	1/1	0.98	0.20	9,9,9,9	0
60	MG	BA	3214	1/1	0.98	0.09	54,54,54,54	0
60	MG	BA	3252	1/1	0.98	0.04	4,4,4,4	0
60	MG	AA	1639	1/1	0.98	0.03	29,29,29,29	0
60	MG	BA	3181	1/1	0.98	0.21	16,16,16,16	0
60	MG	AA	1635	1/1	0.98	0.09	23,23,23,23	0
60	MG	BP	202	1/1	0.98	0.14	1,1,1,1	0
60	MG	BA	3257	1/1	0.98	0.05	22,22,22,22	0
60	MG	BA	3218	1/1	0.98	0.08	9,9,9,9	0
60	MG	BA	3153	1/1	0.98	0.27	16,16,16,16	0
60	MG	BA	3052	1/1	0.98	0.20	1,1,1,1	0
60	MG	DA	3224	1/1	0.98	0.04	18,18,18,18	0
60	MG	BA	3185	1/1	0.98	0.05	3,3,3,3	0
60	MG	BA	3262	1/1	0.98	0.14	3,3,3,3	0
60	MG	AX	105	1/1	0.98	0.03	12,12,12,12	0
60	MG	BA	3156	1/1	0.98	0.07	7,7,7,7	0
60	MG	BA	3011	1/1	0.98	0.10	1,1,1,1	0
60	MG	DA	3169	1/1	0.98	0.19	16,16,16,16	0
60	MG	BA	3012	1/1	0.98	0.21	1,1,1,1	0
60	MG	DA	3233	1/1	0.98	0.12	1,1,1,1	0
60	MG	AA	1641	1/1	0.98	0.11	13,13,13,13	0
60	MG	AA	1623	1/1	0.98	0.19	10,10,10,10	0
60	MG	DA	3236	1/1	0.98	0.08	39,39,39,39	0
60	MG	DA	3173	1/1	0.98	0.10	10,10,10,10	0
60	MG	BA	3015	1/1	0.98	0.04	5,5,5,5	0
60	MG	AA	1714	1/1	0.98	0.12	6,6,6,6	0
60	MG	BA	3038	1/1	0.98	0.18	1,1,1,1	0
60	MG	AA	1602	1/1	0.98	0.05	1,1,1,1	0
60	MG	BA	3317	1/1	0.98	0.11	22,22,22,22	0
60	MG	DA	3179	1/1	0.98	0.04	19,19,19,19	0
60	MG	BA	3318	1/1	0.98	0.05	20,20,20,20	0
60	MG	DE	301	1/1	0.98	0.04	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3233	1/1	0.98	0.08	1,1,1,1	0
60	MG	BA	3275	1/1	0.98	0.10	7,7,7,7	0
60	MG	DA	3183	1/1	0.98	0.11	9,9,9,9	0
60	MG	AA	1693	1/1	0.98	0.06	31,31,31,31	0
60	MG	BA	3277	1/1	0.98	0.05	1,1,1,1	0
61	ZN	AD	301	1/1	0.98	0.17	46,46,46,46	0
61	ZN	B4	101	1/1	0.98	0.04	89,89,89,89	0
60	MG	BA	3138	1/1	0.98	0.08	1,1,1,1	0
60	MG	CA	1667	1/1	0.98	0.14	5,5,5,5	0
60	MG	BA	3063	1/1	0.98	0.12	1,1,1,1	0
61	ZN	D9	101	1/1	0.98	0.04	93,93,93,93	0
60	MG	BA	3306	1/1	0.99	0.11	5,5,5,5	0
60	MG	DA	3045	1/1	0.99	0.04	11,11,11,11	0
60	MG	DA	3132	1/1	0.99	0.06	6,6,6,6	0
60	MG	BA	3232	1/1	0.99	0.18	1,1,1,1	0
60	MG	AA	1624	1/1	0.99	0.19	1,1,1,1	0
60	MG	CA	1689	1/1	0.99	0.03	7,7,7,7	0
60	MG	BA	3024	1/1	0.99	0.07	11,11,11,11	0
60	MG	DA	3106	1/1	0.99	0.03	23,23,23,23	0
60	MG	DA	3232	1/1	0.99	0.08	3,3,3,3	0
60	MG	DA	3077	1/1	0.99	0.06	13,13,13,13	0
60	MG	DA	3108	1/1	0.99	0.09	18,18,18,18	0
60	MG	BA	3324	1/1	0.99	0.04	1,1,1,1	0
60	MG	BA	3087	1/1	0.99	0.05	6,6,6,6	0
60	MG	BA	3030	1/1	0.99	0.10	7,7,7,7	0
60	MG	BA	3206	1/1	0.99	0.20	6,6,6,6	0
60	MG	DA	3206	1/1	0.99	0.05	12,12,12,12	0
60	MG	DA	3007	1/1	0.99	0.06	1,1,1,1	0
60	MG	CA	1620	1/1	0.99	0.10	32,32,32,32	0
60	MG	DA	3056	1/1	0.99	0.03	2,2,2,2	0
60	MG	BA	3273	1/1	0.99	0.03	1,1,1,1	0
60	MG	AA	1676	1/1	0.99	0.18	11,11,11,11	0
60	MG	DA	3034	1/1	0.99	0.06	1,1,1,1	0
60	MG	BA	3099	1/1	0.99	0.23	8,8,8,8	0
60	MG	DA	3061	1/1	0.99	0.03	21,21,21,21	0
60	MG	AA	1668	1/1	0.99	0.07	24,24,24,24	0
60	MG	AX	107	1/1	0.99	0.06	8,8,8,8	0
60	MG	BR	201	1/1	0.99	0.04	1,1,1,1	0
60	MG	CA	1627	1/1	0.99	0.04	9,9,9,9	0
60	MG	BA	3070	1/1	0.99	0.31	1,1,1,1	0
60	MG	CK	201	1/1	0.99	0.03	19,19,19,19	0
61	ZN	CD	301	1/1	0.99	0.19	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
60	MG	BA	3254	1/1	0.99	0.08	72,72,72,72	0
60	MG	CA	1666	1/1	0.99	0.07	9,9,9,9	0
60	MG	DA	3070	1/1	0.99	0.09	14,14,14,14	0
60	MG	BA	3090	1/1	1.00	0.04	13,13,13,13	0
60	MG	DA	3032	1/1	1.00	0.02	1,1,1,1	0
60	MG	DA	3085	1/1	1.00	0.21	1,1,1,1	0
61	ZN	B9	101	1/1	1.00	0.02	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.