wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 14, 2023 – 07:12 PM EDT

PDB ID	:	4V97
Title	:	Crystal structure of the bacterial ribosome ram mutation G299A.
Authors	:	Fagan, C.E.; Dunkle, J.A.; Maehigashi, T.; Dunham, C.M.
Deposited on	:	2012-04-06
Resolution	:	3.52 Å(reported)

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

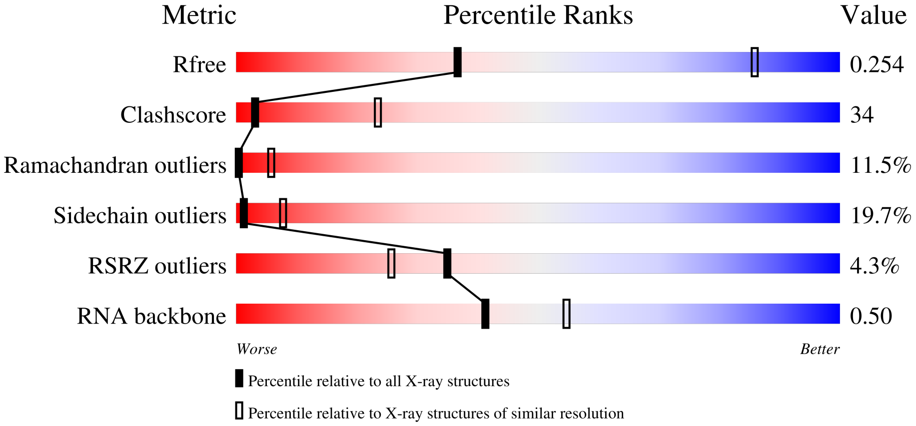
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

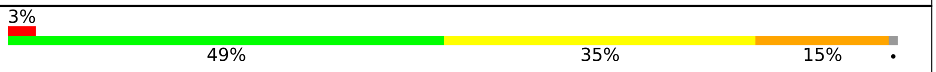
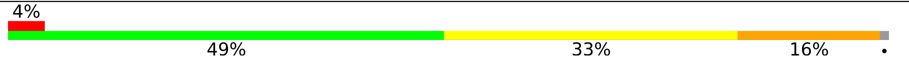
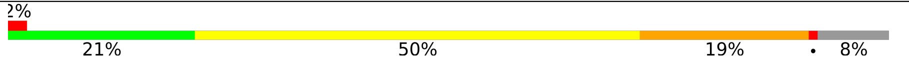
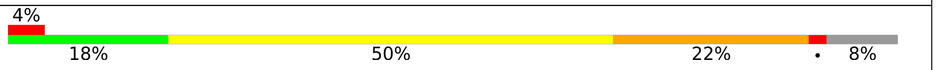
The reported resolution of this entry is 3.52 Å.

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}	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)
RNA backbone	3102	1003 (4.02-3.00)

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 <=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	1522	
1	CA	1522	
2	AB	256	
2	CB	256	

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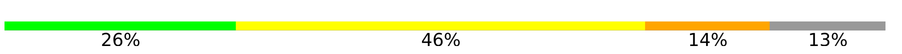
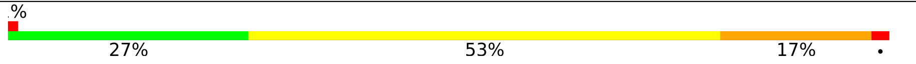
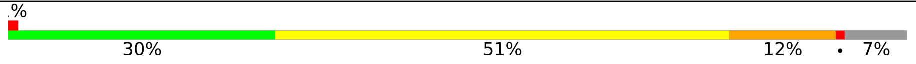
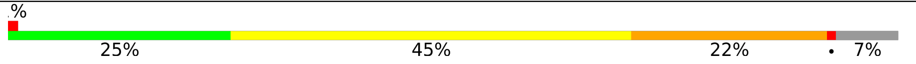
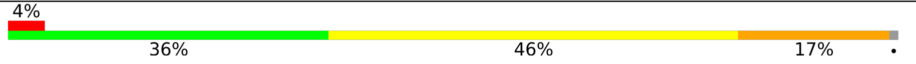
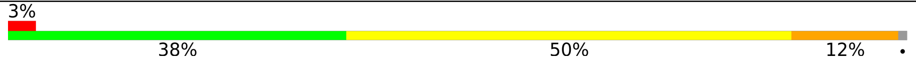
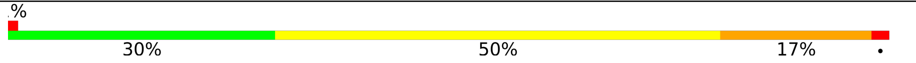
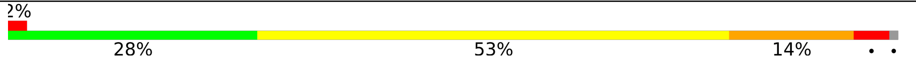
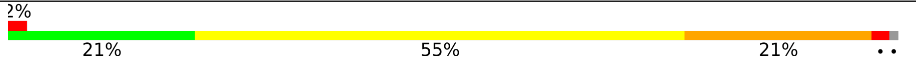
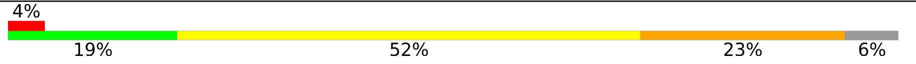
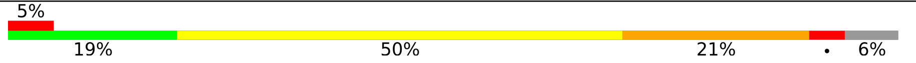
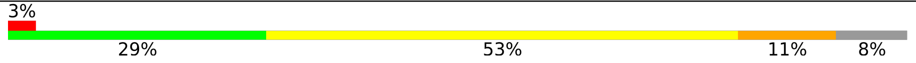
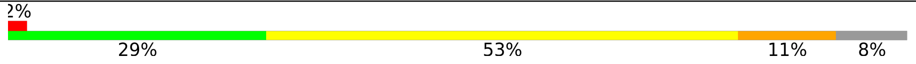
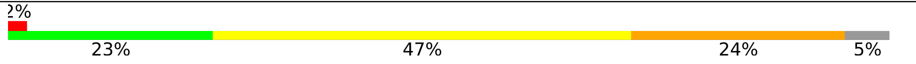
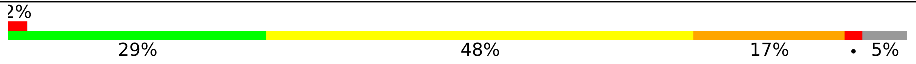
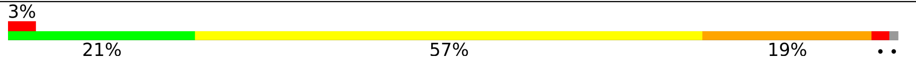
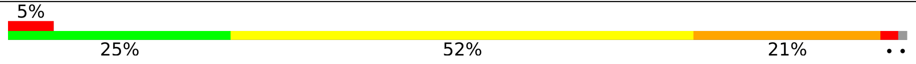
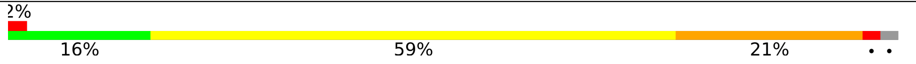
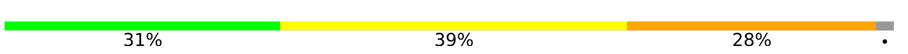
Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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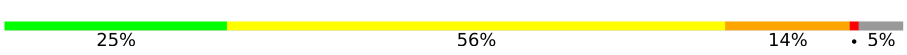
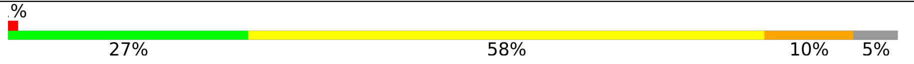
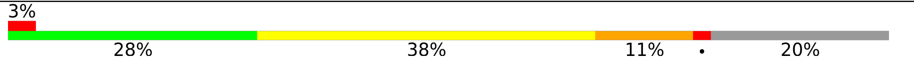
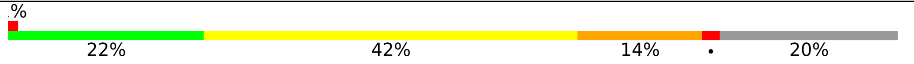
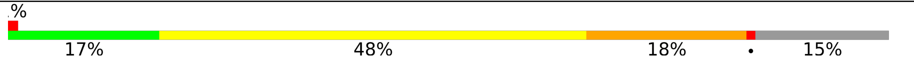
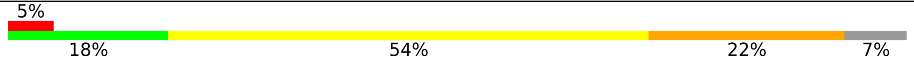
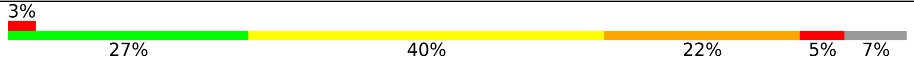
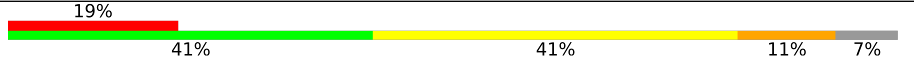
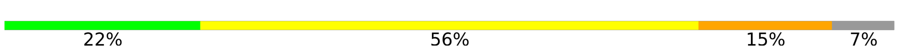
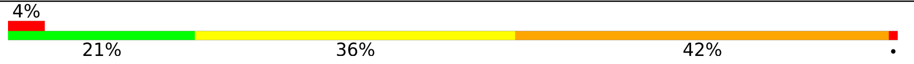
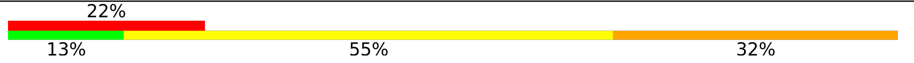
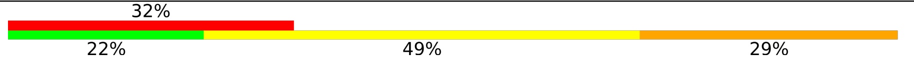
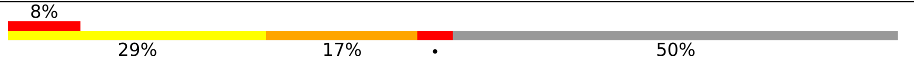
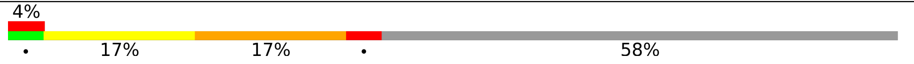
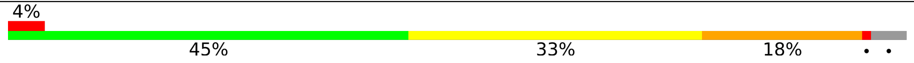
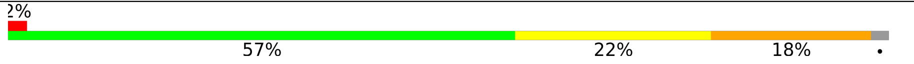
Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	77	
22	CV	77	
23	AW	76	
23	AY	76	
23	CW	76	
23	CY	76	
24	AX	24	
24	CX	24	
25	BA	2915	
25	DA	2915	
26	BB	122	
26	DB	122	

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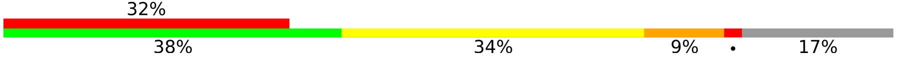
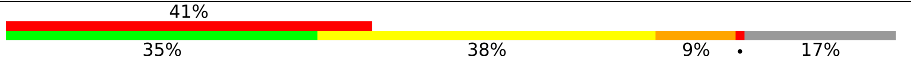
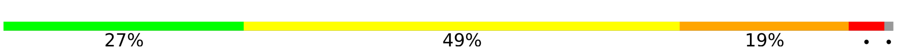
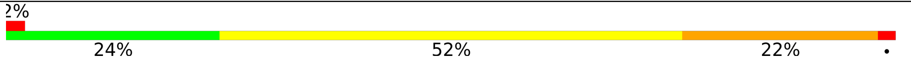
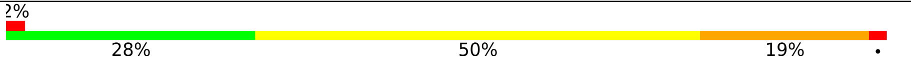
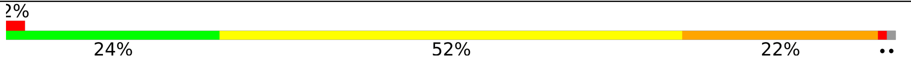
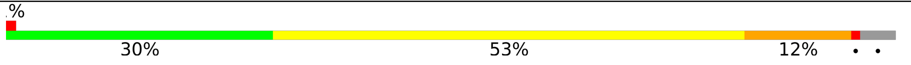
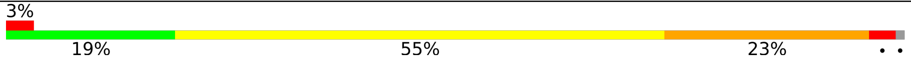
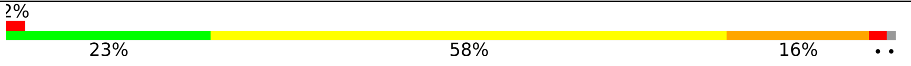
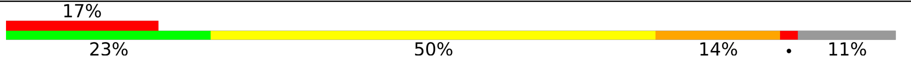
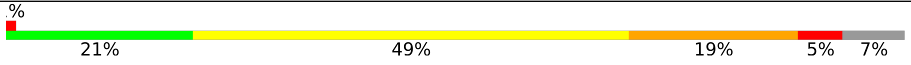
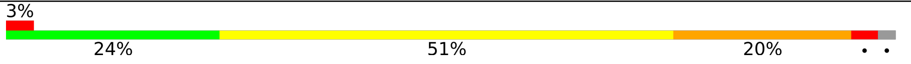
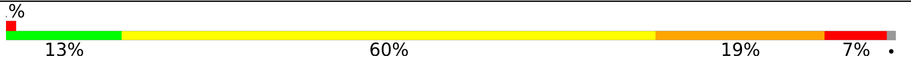
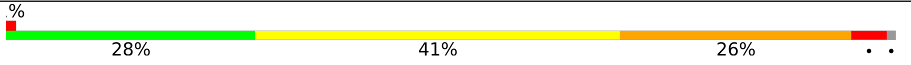
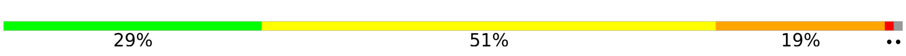
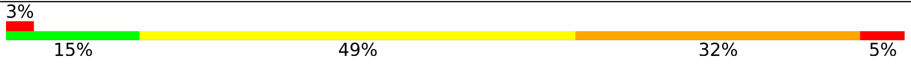
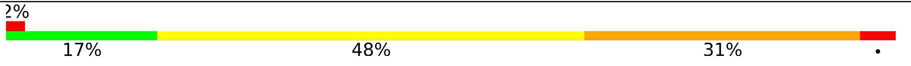
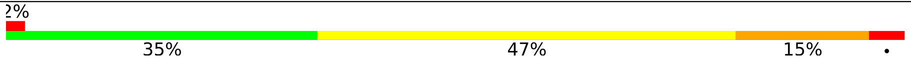
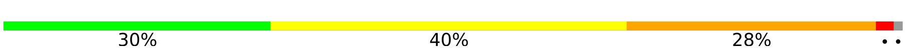
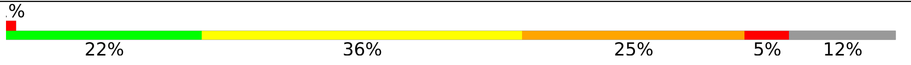
Mol	Chain	Length	Quality of chain
27	BC	229	
27	DC	229	
28	BD	276	
28	DD	276	
29	BE	206	
29	DE	206	
30	BF	210	
30	DF	210	
31	BG	182	
31	DG	182	
32	BH	180	
32	DH	180	
33	BI	148	
33	DI	148	
34	BN	140	
34	DN	140	
35	BO	122	
35	DO	122	
36	BP	150	
36	DP	150	
37	BQ	141	
37	DQ	141	
38	BR	118	
38	DR	118	
39	BS	112	

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Mol	Chain	Length	Quality of chain
39	DS	112	2% 21% 57% 18% • •
40	BT	146	4% 18% 50% 24% • 5%
40	DT	146	5% 14% 53% 21% 6% 5%
41	BU	118	% 25% 52% 22% ••
41	DU	118	% 26% 58% 14% •
42	BV	101	27% 42% 28% •
42	DV	101	% 25% 54% 19% •
43	BW	113	2% 27% 52% 20% •
43	DW	113	37% 48% 15%
44	BX	96	40% 38% 19% • •
44	DX	96	40% 46% 11% •
45	BY	110	18% 20% 36% 32% • 8%
45	DY	110	3% 20% 41% 27% 5% 7%
46	BZ	206	8% 23% 47% 13% • 14%
46	DZ	206	9% 18% 50% 16% • 14%
47	B0	85	7% 39% 49% 9% ••
47	D0	85	8% 39% 52% 7% ••
48	B1	98	% 28% 52% 14% • •
48	D1	98	37% 42% 15% • •
49	B2	72	3% 26% 56% 15% ••
49	D2	72	26% 56% 14% • •
50	B3	60	3% 40% 40% 17% •
50	D3	60	2% 37% 57% 7%
51	B4	71	• 23% 15% • 56%
51	D4	71	3% 14% 34% 7% • 44%

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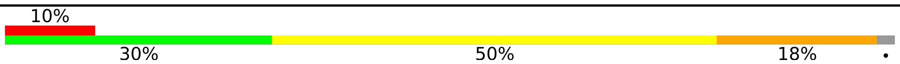
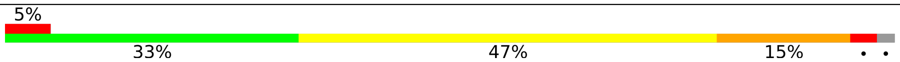
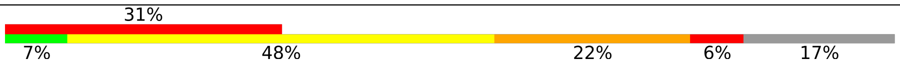
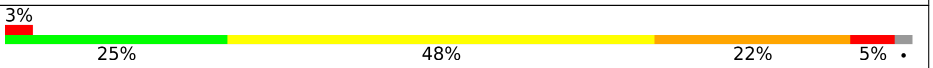
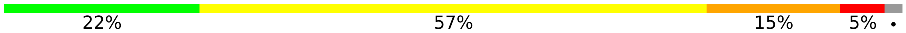
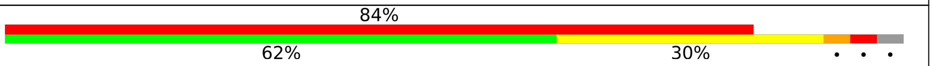
Mol	Chain	Length	Quality of chain
52	B5	60	
52	D5	60	
53	B6	54	
53	D6	54	
54	B7	49	
54	D7	49	
55	B8	65	
55	D8	65	
56	B9	37	
56	D9	37	

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
57	MG	AA	7002	-	-	-	X
57	MG	AA	7027	-	-	-	X
57	MG	AA	7046	-	-	-	X
57	MG	AA	7055	-	-	-	X
57	MG	AA	7069	-	-	-	X
57	MG	AA	7071	-	-	-	X
57	MG	AA	7074	-	-	-	X
57	MG	AA	7076	-	-	-	X
57	MG	AA	7080	-	-	-	X
57	MG	AA	7086	-	-	-	X
57	MG	AA	7097	-	-	-	X
57	MG	BA	3021	-	-	-	X
57	MG	BA	3026	-	-	-	X
57	MG	BA	3028	-	-	-	X
57	MG	BA	3052	-	-	-	X
57	MG	BA	3063	-	-	-	X
57	MG	BA	3074	-	-	-	X
57	MG	BA	3095	-	-	-	X
57	MG	BA	3107	-	-	-	X
57	MG	BA	3110	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	BA	3117	-	-	-	X
57	MG	BA	3120	-	-	-	X
57	MG	BA	3126	-	-	-	X
57	MG	BA	3155	-	-	-	X
57	MG	BA	3164	-	-	-	X
57	MG	BA	3173	-	-	-	X
57	MG	BA	3196	-	-	-	X
57	MG	BA	3203	-	-	-	X
57	MG	BA	3216	-	-	-	X
57	MG	BA	3227	-	-	-	X
57	MG	BA	3242	-	-	-	X
57	MG	BA	3245	-	-	-	X
57	MG	BA	3246	-	-	-	X
57	MG	BA	3248	-	-	-	X
57	MG	BA	3262	-	-	-	X
57	MG	BA	3271	-	-	-	X
57	MG	BA	3277	-	-	-	X
57	MG	BA	3278	-	-	-	X
57	MG	BA	3290	-	-	-	X
57	MG	BA	3297	-	-	-	X
57	MG	BA	3306	-	-	-	X
57	MG	BA	3315	-	-	-	X
57	MG	BA	3317	-	-	-	X
57	MG	BA	3318	-	-	-	X
57	MG	BA	3320	-	-	-	X
57	MG	BB	203	-	-	-	X
57	MG	CA	1609	-	-	-	X
57	MG	CA	1610	-	-	-	X
57	MG	CA	1639	-	-	-	X
57	MG	CA	1651	-	-	-	X
57	MG	CA	1674	-	-	-	X
57	MG	CA	1691	-	-	-	X
57	MG	CA	1694	-	-	-	X
57	MG	CA	1704	-	-	-	X
57	MG	CA	1708	-	-	-	X
57	MG	CA	1713	-	-	-	X
57	MG	CA	1714	-	-	-	X
57	MG	CA	1716	-	-	-	X
57	MG	CA	1739	-	-	-	X
57	MG	D1	101	-	-	-	X
57	MG	DA	9329	-	-	-	X
57	MG	DA	9399	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	DA	9429	-	-	-	X
57	MG	DA	9432	-	-	-	X
57	MG	DA	9434	-	-	-	X
57	MG	DA	9440	-	-	-	X
57	MG	DA	9441	-	-	-	X
57	MG	DA	9450	-	-	-	X
57	MG	DA	9458	-	-	-	X
57	MG	DA	9550	-	-	-	X
57	MG	DA	9552	-	-	-	X
57	MG	DA	9559	-	-	-	X
57	MG	DA	9569	-	-	-	X
57	MG	DA	9573	-	-	-	X
57	MG	DA	9595	-	-	-	X
57	MG	DA	9602	-	-	-	X
57	MG	DA	9603	-	-	-	X
57	MG	DA	9615	-	-	-	X
57	MG	DA	9620	-	-	-	X
57	MG	DA	9622	-	-	-	X
57	MG	DA	9643	-	-	-	X
57	MG	DA	9645	-	-	-	X
57	MG	DA	9655	-	-	-	X
57	MG	DA	9665	-	-	-	X
57	MG	DA	9674	-	-	-	X
57	MG	DA	9677	-	-	-	X
57	MG	DA	9685	-	-	-	X
57	MG	DA	9694	-	-	-	X
59	ZN	CN	101	-	-	X	-

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 293977 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	AA	1504	32328	14390	5992	10443	1503	0	0	0
1	CA	1504	32328	14390	5992	10443	1503	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AA	299	A	G	engineered mutation	GB AP008226.1
CA	299	A	G	engineered mutation	GB AP008226.1

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

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

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

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

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

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

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

- 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 1147 724 218 201 4	0	0	1
5	CE	151	Total C N O S 1147 724 218 201 4	0	0	1

- 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 843 531 155 154 3	0	0	0
6	CF	101	Total C N O S 843 531 155 154 3	0	0	0

- 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 1257 781 252 218 6	0	0	0
7	CG	155	Total C N O S 1257 781 252 218 6	0	0	0

- 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 1116 705 215 193 3	0	0	0
8	CH	138	Total C N O S 1116 705 215 193 3	0	0	0

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

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

- 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			
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			
13	CM	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	AO	88	734	459	147	126	2	0	0	0
15	CO	88	734	459	147	126	2	0	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
19	AS	79	630	403	115	110	2	0	0	1
19	CS	79	630	403	115	110	2	0	0	1

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

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

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

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

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

- Molecule 22 is a RNA chain called P-SITE tRNA fMet.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	AV	77	Total C N O P 1644 732 297 538 77	0	0	0
22	CV	77	Total C N O P 1643 732 297 537 77	0	0	0

- Molecule 23 is a RNA chain called E-SITE TRNA PHE OR A-SITE tRNA Phe.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	AW	76	Total C N O P 1619 723 290 531 75	0	0	0
23	AY	17	Total C N O P 365 163 68 117 17	0	0	0
23	CW	76	Total C N O P 1619 723 290 531 75	0	0	0
23	CY	17	Total C N O P 365 163 68 117 17	0	0	0

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	AX	12	Total C N O P 255 115 46 82 12	0	0	0
24	CX	10	Total C N O P 210 96 39 66 9	0	0	0

- Molecule 25 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	BA	2810	Total	C	N	O	P	0	0	0
			60527	26937	11326	19455	2809			
25	DA	2824	Total	C	N	O	P	0	0	0
			60827	27071	11381	19552	2823			

- Molecule 26 is a RNA chain called 5S rRNA.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	DF	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
32	DH	168	Total	C	N	O	S	0	0	0
			1290	820	240	229	1			

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BI	145	Total	C	N	O	S	0	0	0
			1131	723	200	207	1			
33	DI	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 35 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 36 is a protein called 50S RIBOSOMAL PROTEIN L15.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	BP	150	Total C N O S 1145 712 232 198 3	0	0	0
36	DP	150	Total C N O S 1145 712 232 198 3	0	0	0

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
37	BQ	141	Total C N O S 1122 715 212 188 7	0	0	0
37	DQ	141	Total C N O S 1122 715 212 188 7	0	0	0

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L17.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
38	BR	117	Total C N O 960 599 202 159	0	0	0
38	DR	118	Total C N O S 968 604 203 160 1	0	0	0

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L18.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
39	BS	99	Total C N O 771 486 155 130	0	0	1
39	DS	111	Total C N O 882 556 176 150	0	0	0

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BU	117	Total 964	C 610	N 202	O 151	S 1	0	0	0
41	DU	117	Total 958	C 604	N 202	O 151	S 1	0	0	0

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BY	101	Total 776	C 500	N 149	O 123	S 4	0	0	1
45	DY	102	Total 785	C 505	N 150	O 125	S 5	0	0	0

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L27.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

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

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B4	31	Total 226	C 142	N 37	O 43	S 4	0	0	1
51	D4	40	Total 298	C 189	N 50	O 54	S 5	0	0	1

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L33.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
53	B6	45	Total C N O S 381 235 78 64 4	0	0	1
53	D6	45	Total C N O S 381 235 78 64 4	0	0	1

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	110	Total Mg 110 110	0	0
57	AE	1	Total Mg 1 1	0	0
57	AV	5	Total Mg 5 5	0	0
57	AX	1	Total Mg 1 1	0	0
57	BA	323	Total Mg 323 323	0	0
57	BB	5	Total Mg 5 5	0	0
57	BD	2	Total Mg 2 2	0	0
57	BE	3	Total Mg 3 3	0	0
57	BF	1	Total Mg 1 1	0	0
57	BN	1	Total Mg 1 1	0	0
57	BO	1	Total Mg 1 1	0	0
57	BP	1	Total Mg 1 1	0	0
57	BU	1	Total Mg 1 1	0	0
57	B5	1	Total Mg 1 1	0	0
57	B7	1	Total Mg 1 1	0	0
57	CA	141	Total Mg 141 141	0	0
57	CE	2	Total Mg 2 2	0	0
57	CV	5	Total Mg 5 5	0	0
57	CW	1	Total Mg 1 1	0	0
57	CX	1	Total Mg 1 1	0	0
57	CY	1	Total Mg 1 1	0	0
57	DA	397	Total Mg 397 397	0	0

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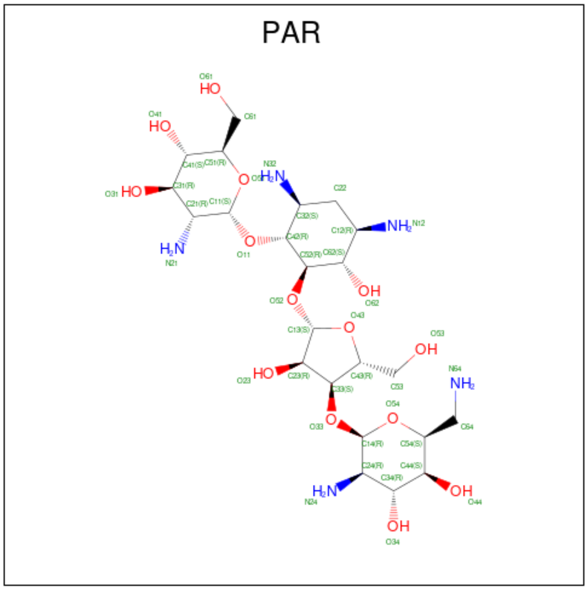
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	DB	5	Total Mg 5 5	0	0
57	DD	3	Total Mg 3 3	0	0
57	DE	2	Total Mg 2 2	0	0
57	DF	1	Total Mg 1 1	0	0
57	DP	3	Total Mg 3 3	0	0
57	DQ	1	Total Mg 1 1	0	0
57	DU	3	Total Mg 3 3	0	0
57	DW	1	Total Mg 1 1	0	0
57	DX	1	Total Mg 1 1	0	0
57	D0	2	Total Mg 2 2	0	0
57	D1	2	Total Mg 2 2	0	0
57	D2	1	Total Mg 1 1	0	0
57	D5	2	Total Mg 2 2	0	0
57	D8	1	Total Mg 1 1	0	0

- Molecule 58 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
58	AA	1	Total C N O 42 23 5 14	0	0
58	CA	1	Total C N O 42 23 5 14	0	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

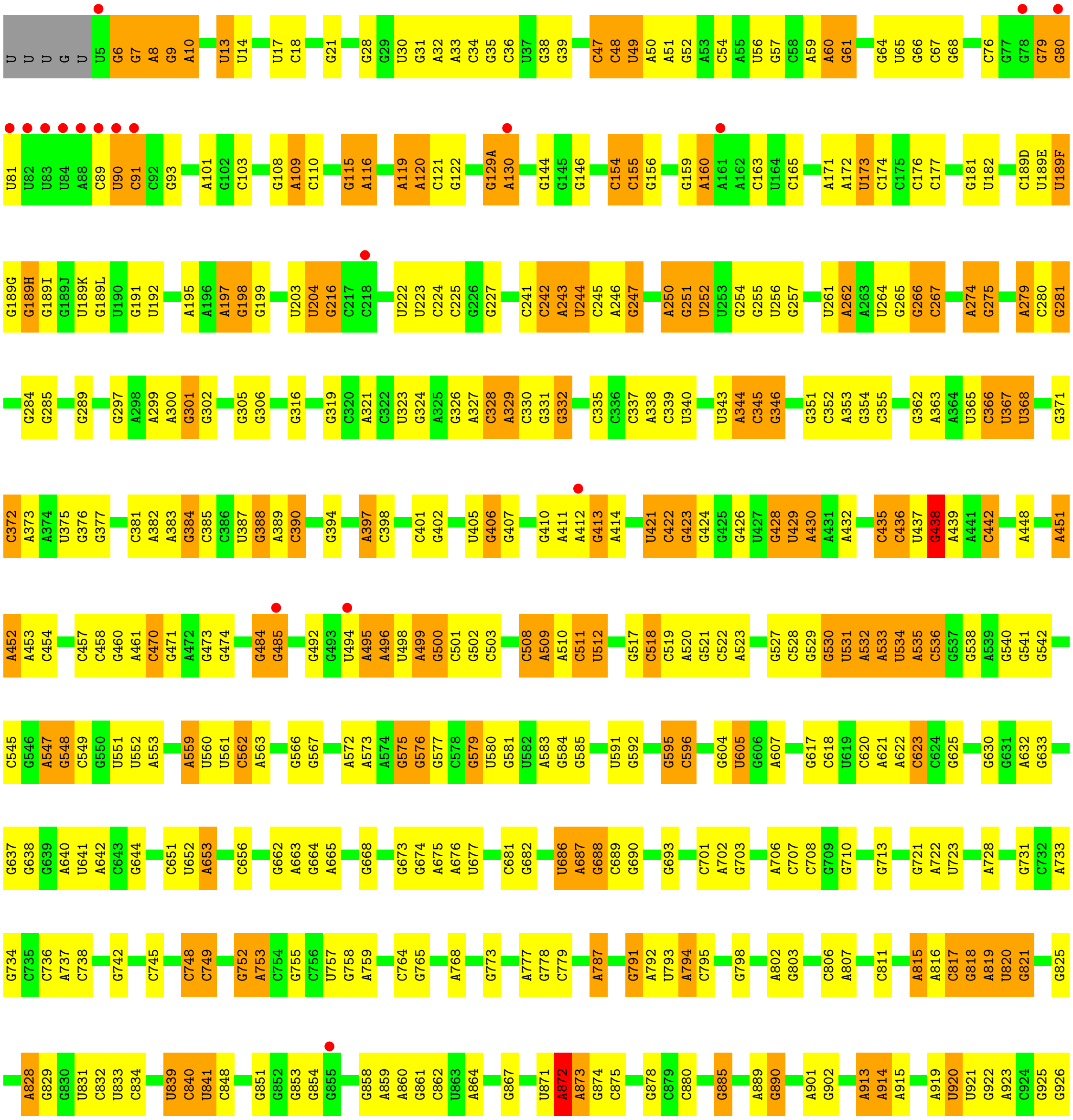
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
59	AD	1	Total Zn 1 1	0	0
59	AN	1	Total Zn 1 1	0	0
59	CD	1	Total Zn 1 1	0	0
59	CN	1	Total Zn 1 1	0	0

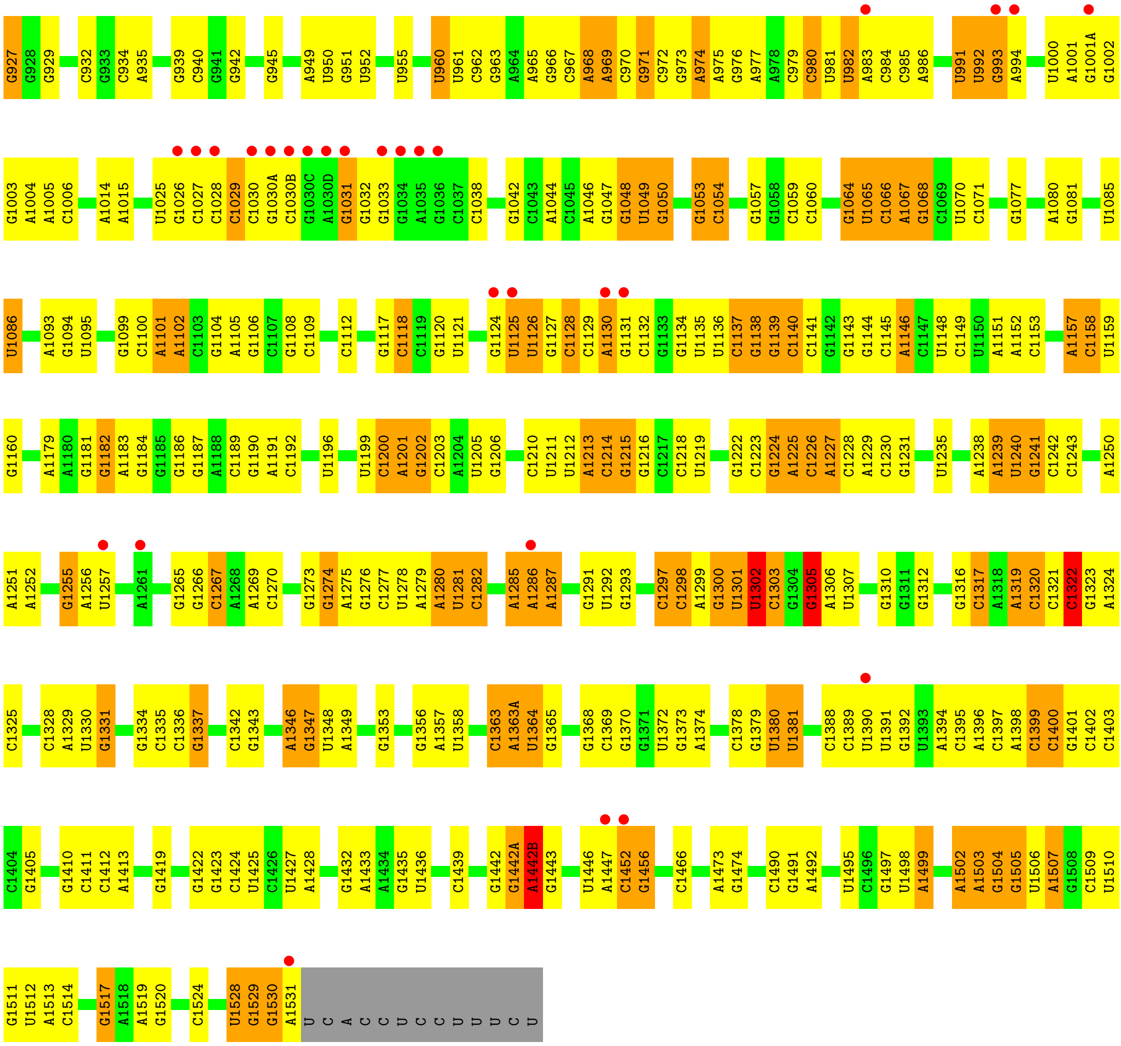
3 Residue-property plots ⓘ

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

- Molecule 1: 16S rRNA

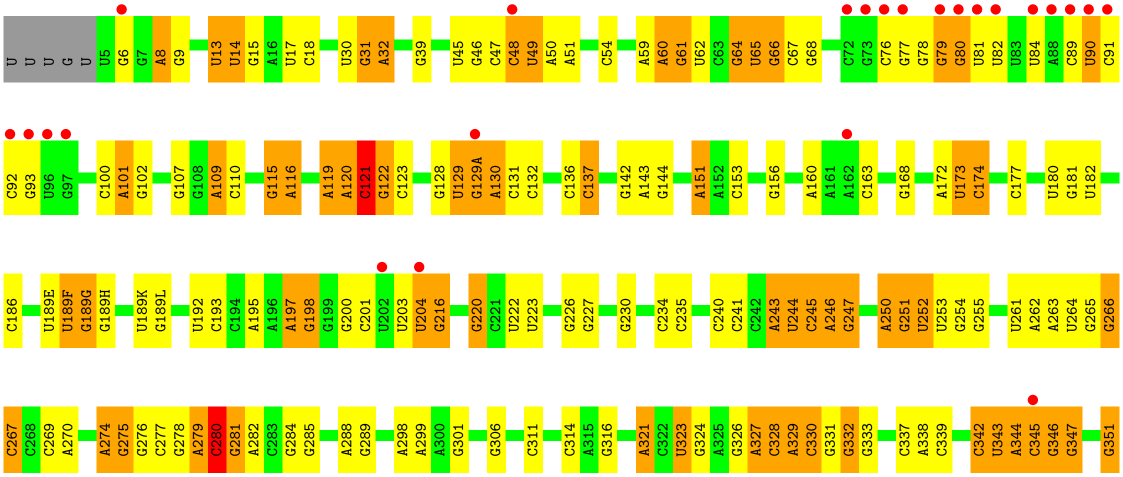
Chain AA:

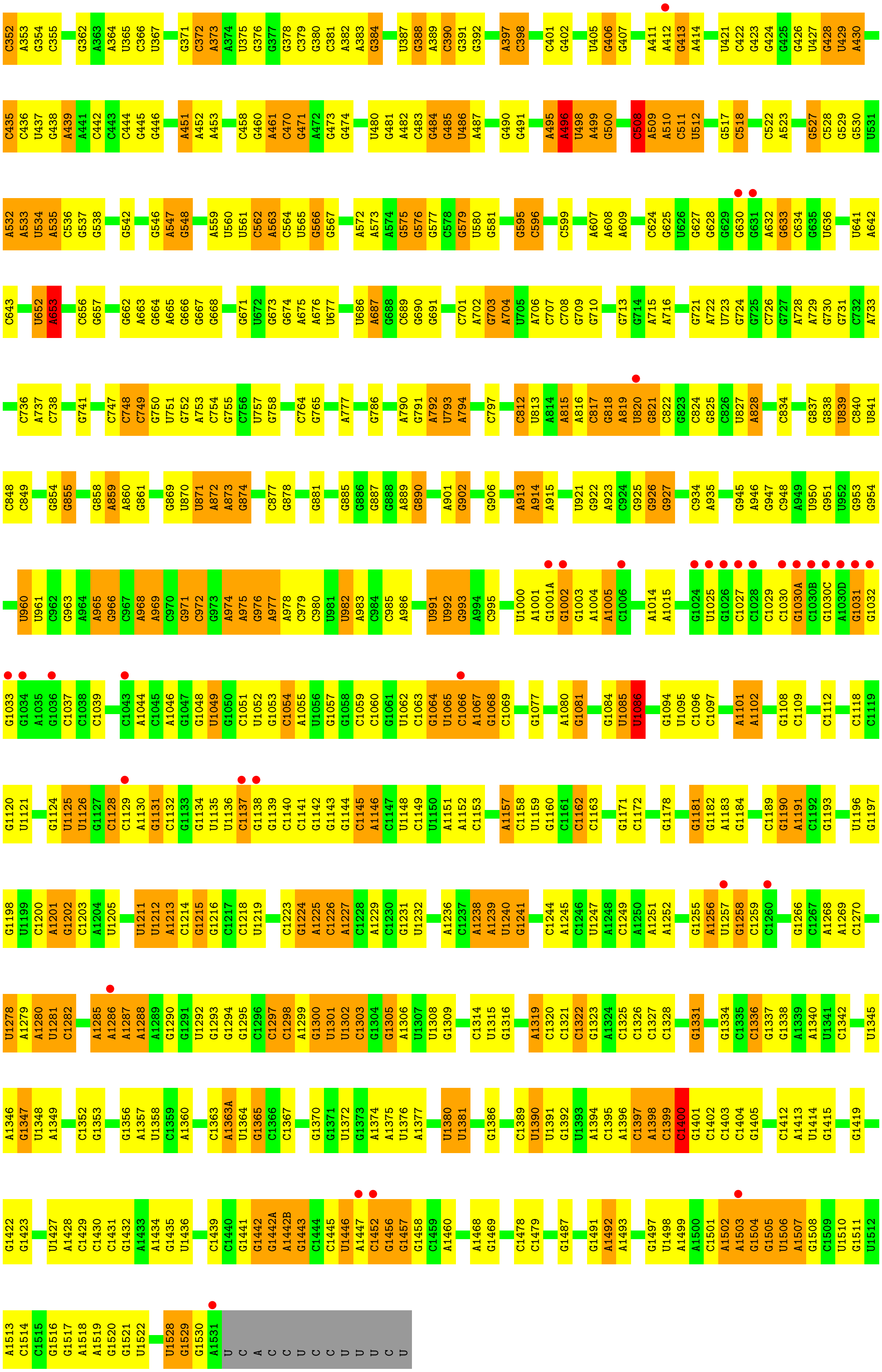




- Molecule 1: 16S rRNA

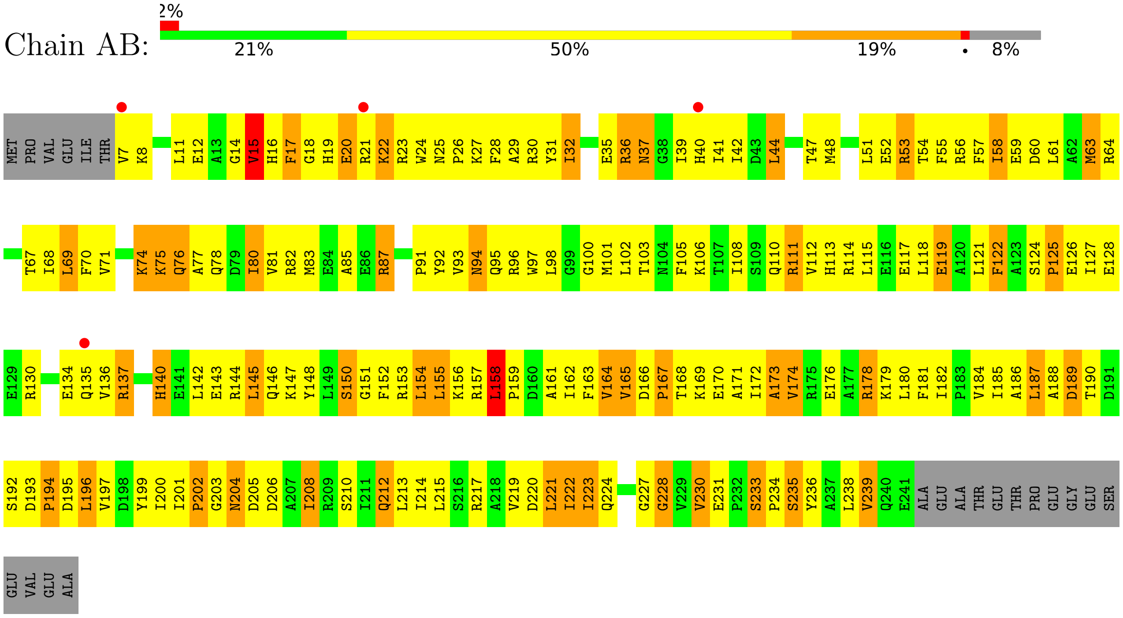
Chain CA:




C352 A353 G354 C355 G362 A363 A364 U365 C366 U367 G371 C372 A373 A374 U375 G376 G377 C378 C379 G380 C381 A382 A383 G384 U387 G388 A389 C390 G391 G392 A397 C398 C401 G402 U405 G406 G407 A411 A412 G413 A414 U421 C422 G423 G424 G425 C426 U427 G428 U429 A430
C435 C436 U437 G438 A439 A441 C442 C443 C444 G445 G446 A451 A452 A453 C458 G460 A461 C470 G471 A472 G473 G474 U480 G481 A482 C483 G484 G485 U486 A487 G490 G491 A495 A496 U498 A499 G500 C508 A509 A510 C511 U512 G517 C518 C522 A523 G527 C528 G529 G530 U531
A532 A533 U534 A535 C536 G537 G538 G542 G546 A547 G548 A559 U560 U561 C562 A563 C564 U565 G566 G567 A572 A573 A574 G575 G576 G577 C578 G579 U580 G581 G595 C596 C599 A607 A608 A609 C624 G625 U626 G627 G628 G629 G630 G631 A632 G633 C634 G635 U636 U641 A642
C643 U652 A653 C656 G657 G662 A663 G664 A665 G666 G667 G668 G671 U672 G673 G674 A675 A676 U677 U686 A687 G688 C689 G690 G691 C701 A702 G703 A704 U705 A706 C707 C708 G709 G710 G713 G714 A715 A716 G721 A722 U723 G724 G725 C726 G727 A728 A729 G730 G731 C732 A733
C736 A737 C738 G741 C747 C748 C749 G750 U751 G752 A753 C754 G755 C756 U757 G758 C764 G765 A777 G786 A790 G791 A792 U793 A794 C797 C812 U813 A814 A815 A816 C817 G818 A819 U820 G821 C822 G823 C824 G825 C826 U827 A828 C834 G837 G838 U839 C840 U841
C848 C849 G854 G855 G858 A859 A860 G861 G869 U870 U871 A872 A873 G874 C877 G878 G881 G885 G886 G887 G888 A889 G890 A901 G902 G906 A913 A914 A915 U921 G922 A923 C924 G925 G926 G927 C934 A935 G945 A946 G947 C948 A949 U950 G951 U952 G953 G954
U960 U961 C962 G963 A964 A965 G966 C967 A968 A969 C970 G971 C972 G973 A974 A975 G976 A977 A978 C979 C980 U981 U982 A983 C984 C985 A986 U991 U992 G993 A994 C995 U1000 A1001 G1001A G1002 G1003 A1004 A1005 C1006 A1014 A1015 G1024 U1025 G1026 C1027 C1028 C1029 C1030 G1030A C1030B G1030C A1030D G1031 G1032
G1033 G1034 A1035 G1036 C1037 C1038 C1039 C1043 A1044 C1045 A1046 G1047 G1048 U1049 G1050 C1051 U1052 G1053 C1054 A1055 U1056 G1057 G1058 C1059 C1060 G1061 U1062 C1063 G1064 U1065 C1066 A1067 G1068 C1069 G1077 A1080 G1081 G1084 U1085 U1086 G1094 U1095 C1096 C1097 A1101 A1102 G1108 C1109 C1112 C1118 C1119
G1120 U1121 G1124 U1125 U1126 G1127 C1128 C1129 A1130 G1131 C1132 G1133 G1134 U1135 U1136 C1137 G1138 G1139 C1140 C1141 G1142 G1143 G1144 C1145 A1146 C1147 U1148 C1149 U1150 A1151 A1152 C1153 A1157 C1158 U1159 G1160 C1161 C1162 C1163 G1171 C1172 G1178 G1181 G1182 A1183 G1184 C1189 G1190 A1191 C1192 G1193 U1196 G1197
G1198 U1199 C1200 A1201 G1202 C1203 A1204 U1205 U1211 U1212 A1213 C1214 G1215 G1216 C1217 C1218 U1219 C1223 G1224 A1225 C1226 A1227 C1228 A1229 C1230 G1231 U1232 A1236 C1237 A1238 A1239 U1240 G1241 C1244 A1245 C1246 U1247 A1248 C1249 A1250 A1251 A1252 G1255 A1256 U1257 G1258 C1259 C1260 G1266 C1267 A1268 A1269 C1270
U1278 A1279 A1280 U1281 C1282 A1285 A1286 A1287 A1288 A1289 G1290 G1291 U1292 G1293 G1294 G1295 C1296 C1297 C1298 A1299 G1300 U1301 U1302 C1303 G1304 G1305 A1306 U1307 U1308 G1309 C1314 U1315 G1316 A1319 C1320 C1321 C1322 G1323 A1324 C1325 C1326 C1327 C1328 G1331 G1334 C1335 C1336 G1337 G1338 A1339 A1340 U1341 C1342 U1345
A1346 G1347 U1348 A1349 C1352 G1353 G1356 A1357 U1358 C1359 A1360 C1363 A1363A U1364 G1365 C1366 C1367 G1370 G1371 U1372 G1373 A1374 A1375 U1376 A1377 U1380 U1381 G1386 C1389 U1390 U1391 G1392 U1393 A1394 C1395 A1396 C1397 A1398 C1399 C1400 G1401 C1402 C1403 C1404 G1405 C1412 A1413 U1414 G1415 G1419
G1422 G1423 U1427 A1428 C1429 C1430 C1431 G1432 A1433 A1434 G1435 U1436 C1439 C1440 G1441 G1442 G1442A A1442B G1443 C1444 C1445 U1446 A1447 C1452 G1456 G1457 G1458 C1459 A1460 A1468 G1469 C1478 C1479 G1487 G1491 A1492 A1493 G1497 U1498 A1499 A1500 C1501 A1502 A1503 G1504 G1505 U1506 A1507 G1508 C1509 U1510 G1511 U1512
A1513 C1514 C1515 G1516 G1517 A1518 A1519 G1520 G1521 U1522 U1528 G1529 G1530 A1531 U C A C U C C U U U C U

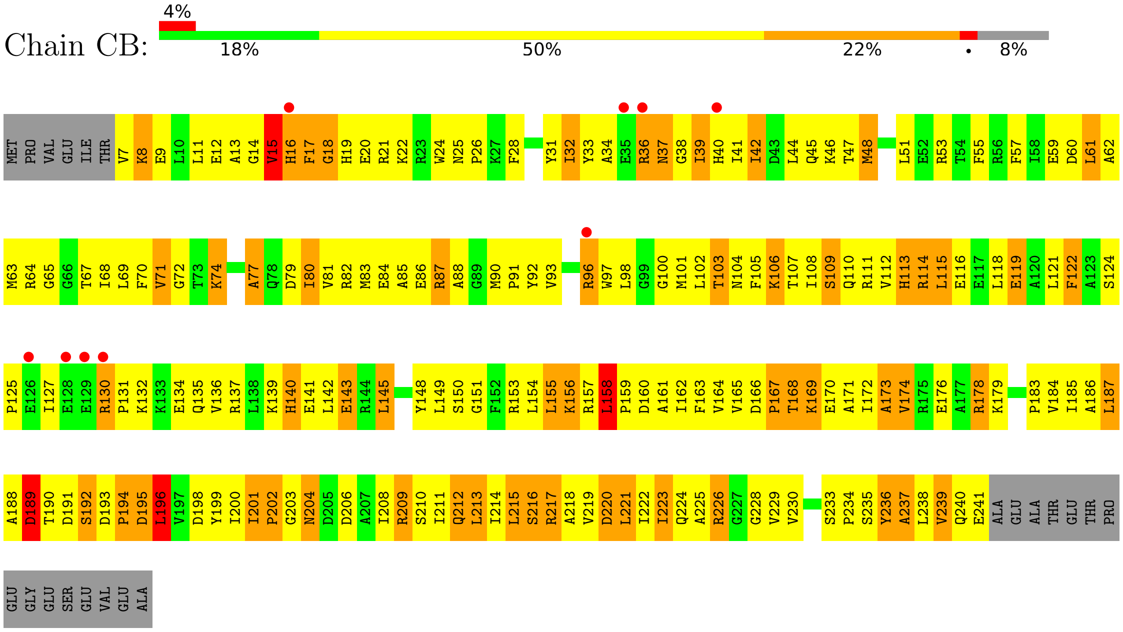
- Molecule 2: 30S ribosomal protein S2

Chain AB:



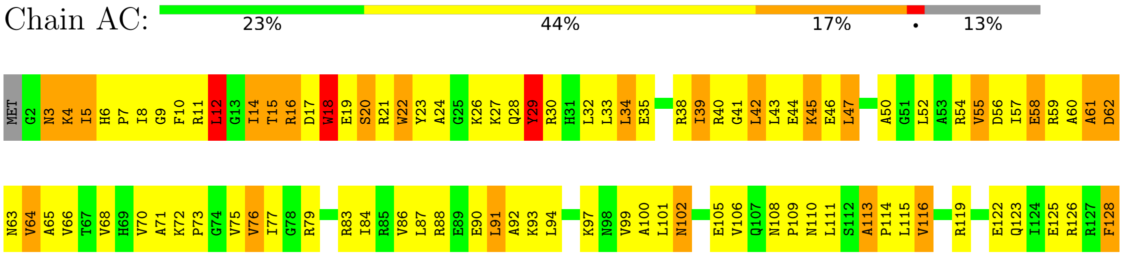
- Molecule 2: 30S ribosomal protein S2

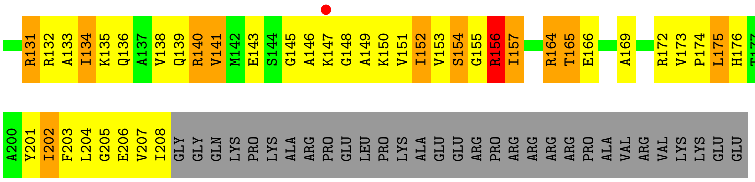
Chain CB:



- Molecule 3: 30S ribosomal protein S3

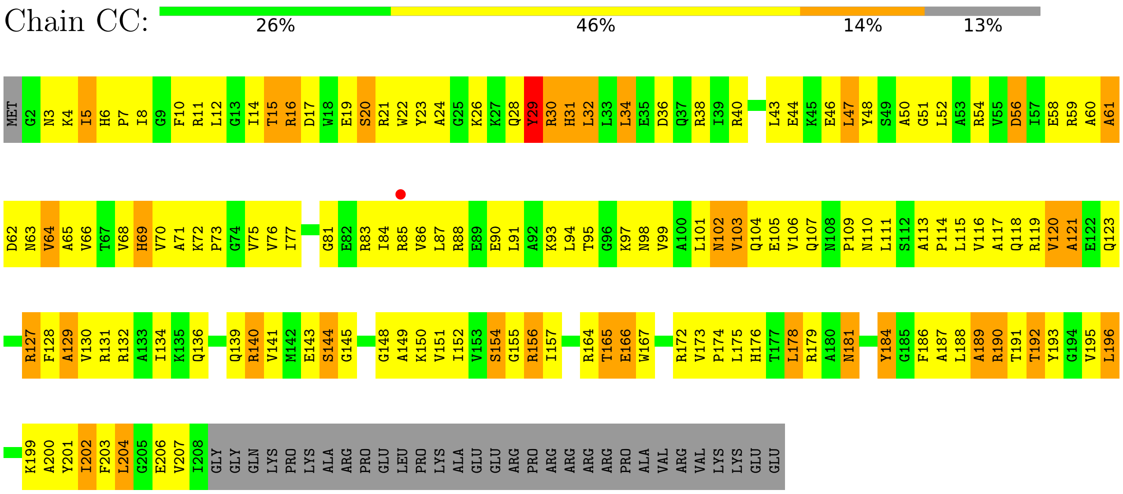
Chain AC:





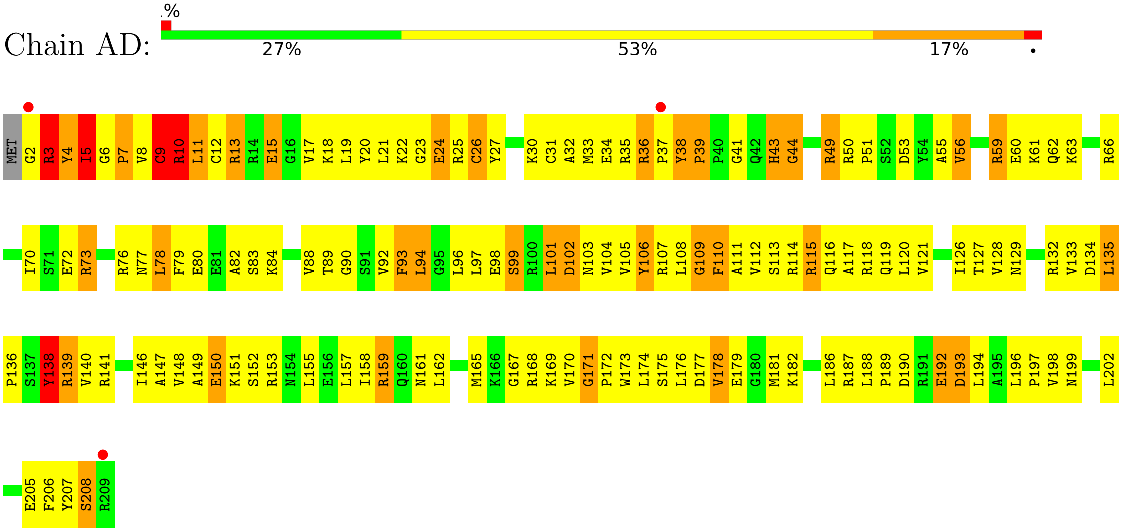
- Molecule 3: 30S ribosomal protein S3

Chain CC:



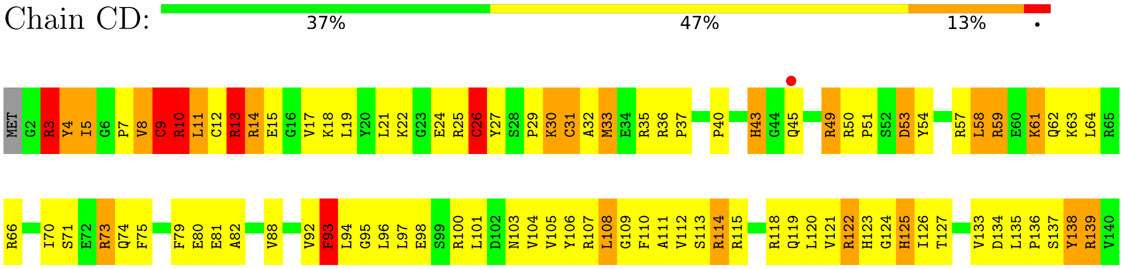
- Molecule 4: 30S ribosomal protein S4

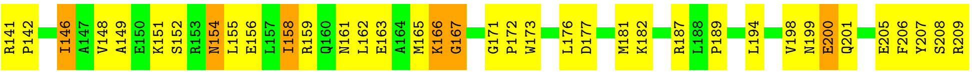
Chain AD:



- Molecule 4: 30S ribosomal protein S4

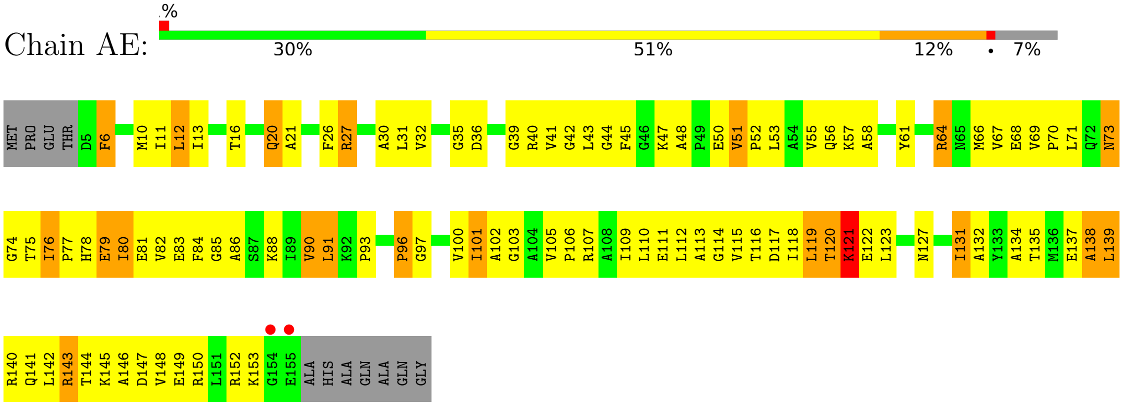
Chain CD:





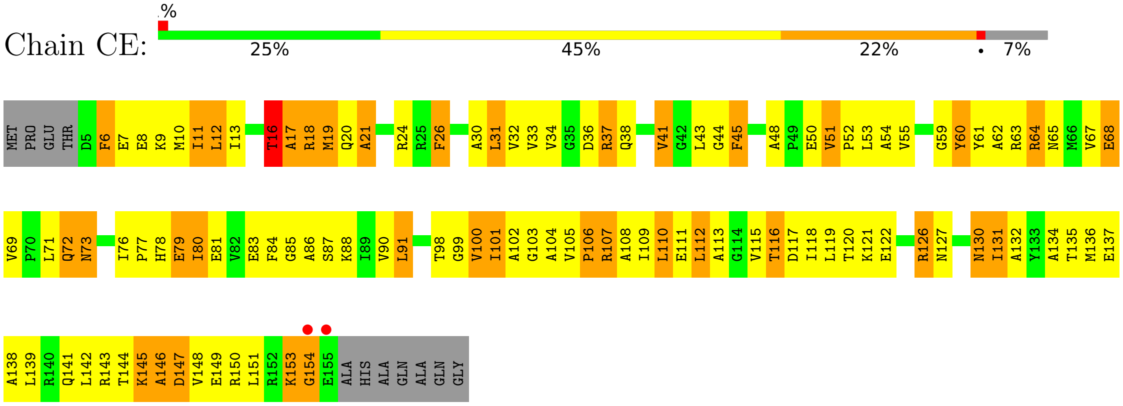
- Molecule 5: 30S ribosomal protein S5

Chain AE:



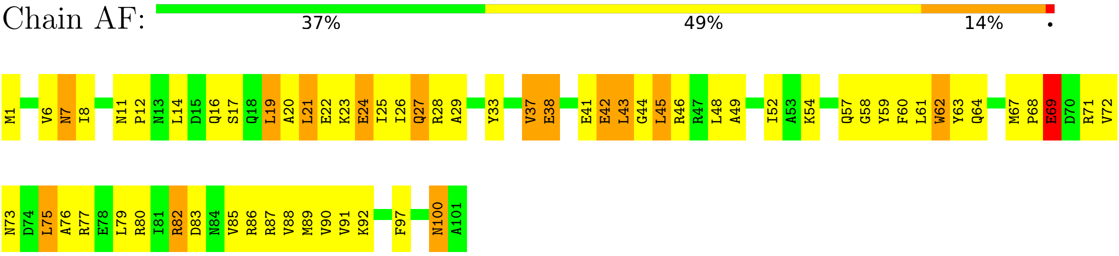
- Molecule 5: 30S ribosomal protein S5

Chain CE:



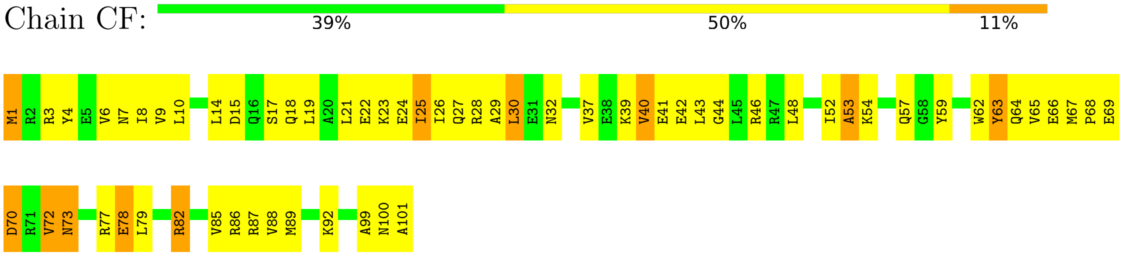
- Molecule 6: 30S ribosomal protein S6

Chain AF:

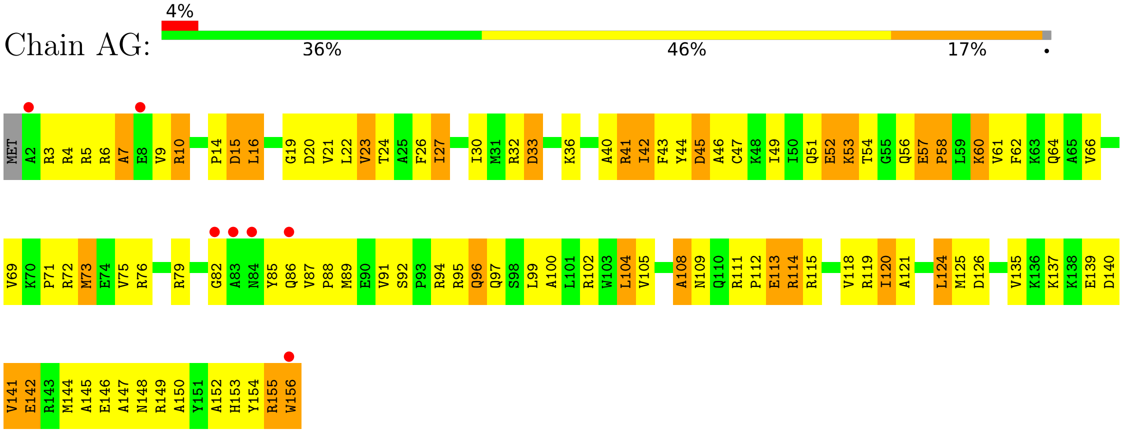


- Molecule 6: 30S ribosomal protein S6

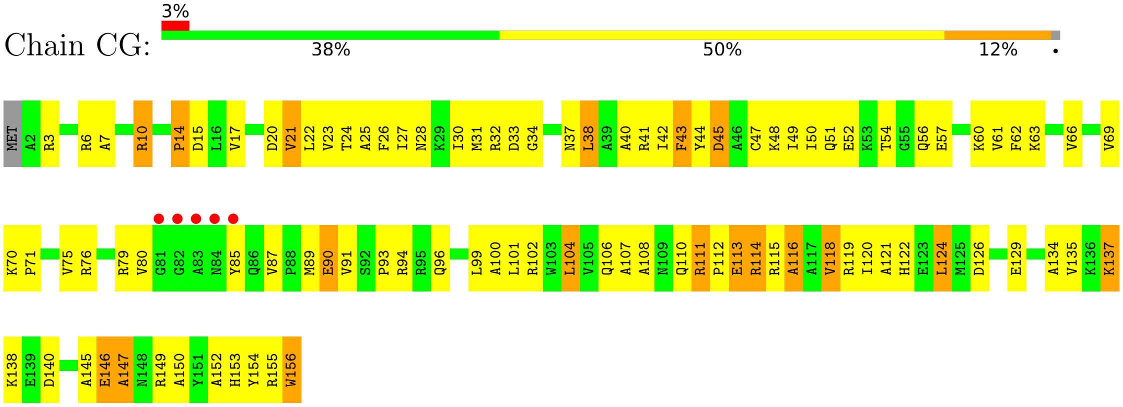
Chain CF:



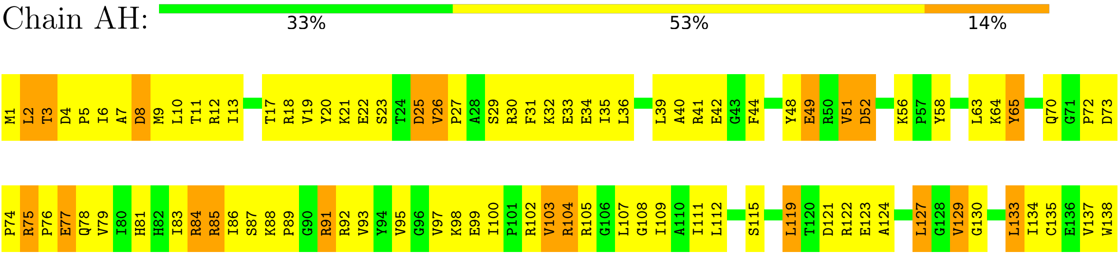
- Molecule 7: 30S ribosomal protein S7



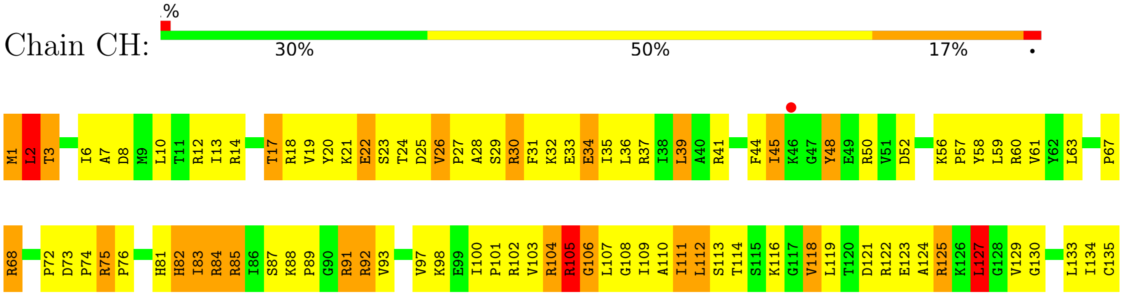
- Molecule 7: 30S ribosomal protein S7



- Molecule 8: 30S ribosomal protein S8



- Molecule 8: 30S ribosomal protein S8

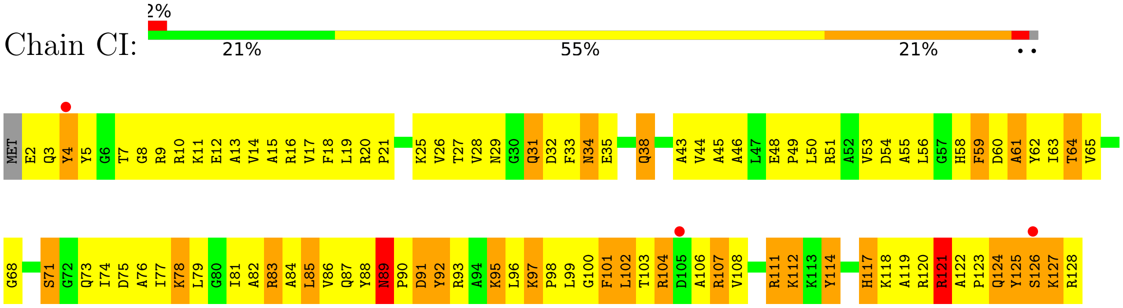


- Molecule 9: 30S ribosomal protein S9

Chain AI:

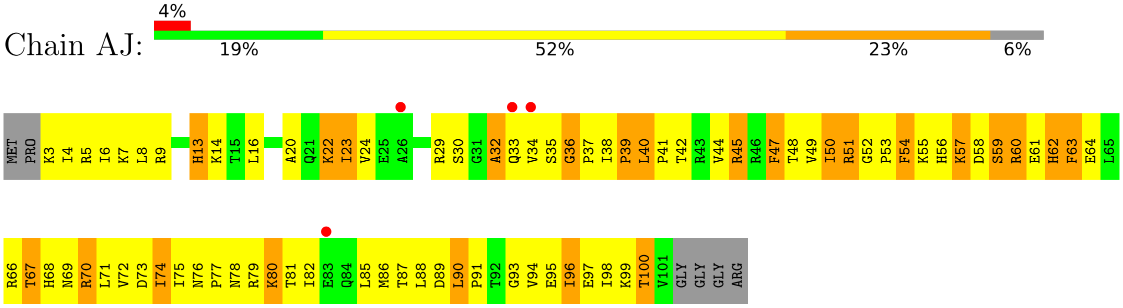
- Molecule 9: 30S ribosomal protein S9

Chain CI:



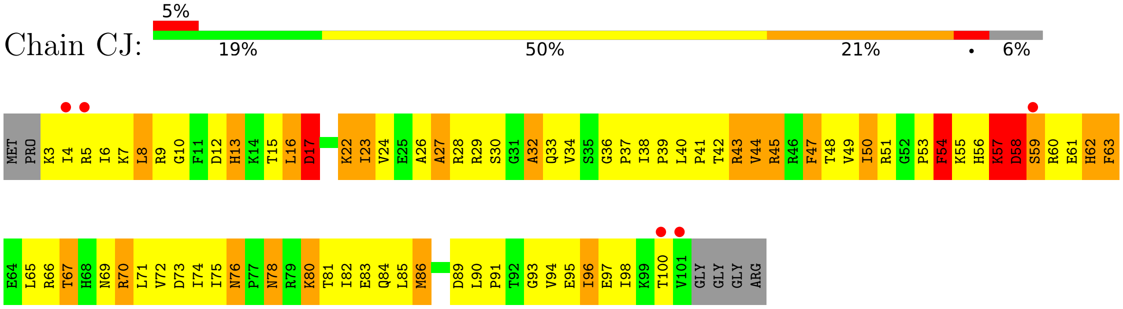
- Molecule 10: 30S ribosomal protein S10

Chain AJ:



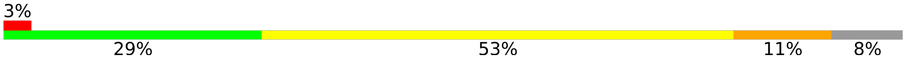
- Molecule 10: 30S ribosomal protein S10

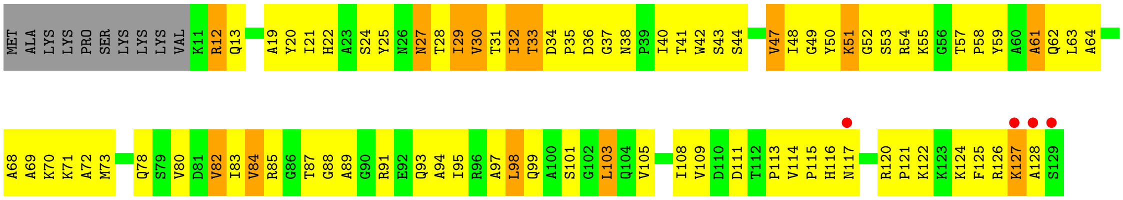
Chain CJ:



- Molecule 11: 30S ribosomal protein S11

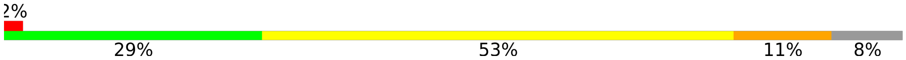
Chain AK:

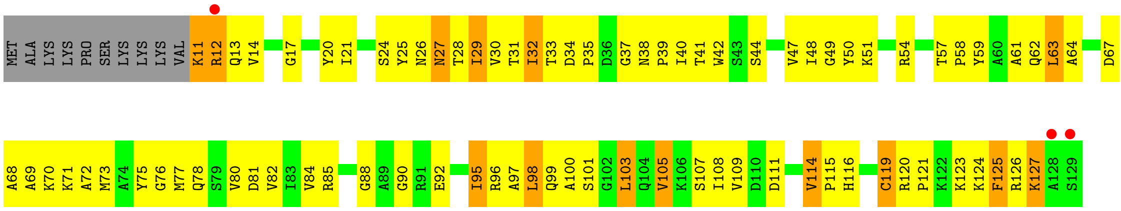




- Molecule 11: 30S ribosomal protein S11

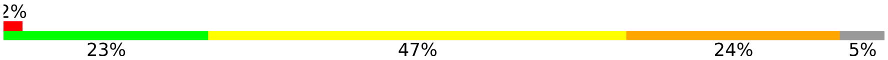
Chain CK:

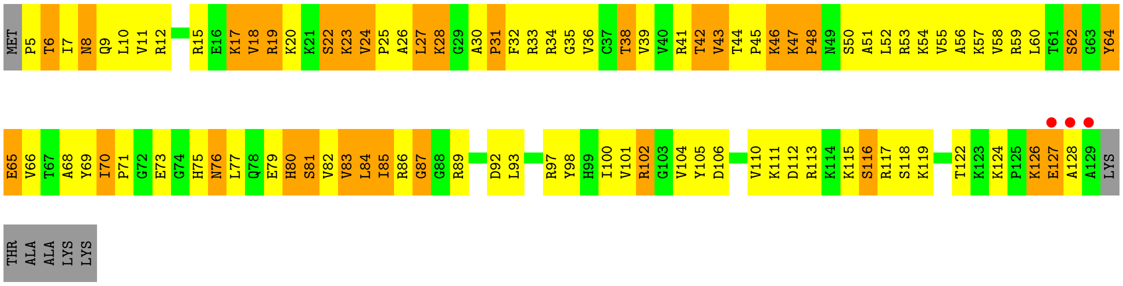




- Molecule 12: 30S ribosomal protein S12

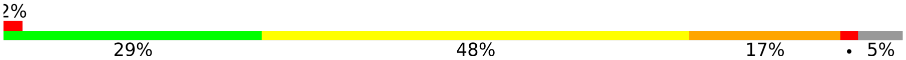
Chain AL:





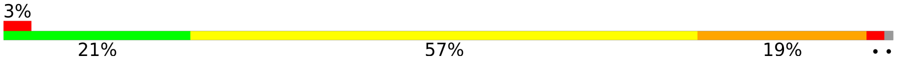
- Molecule 12: 30S ribosomal protein S12

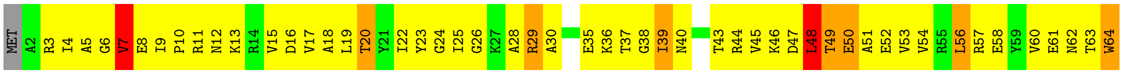
Chain CL:



- Molecule 13: 30S ribosomal protein S13

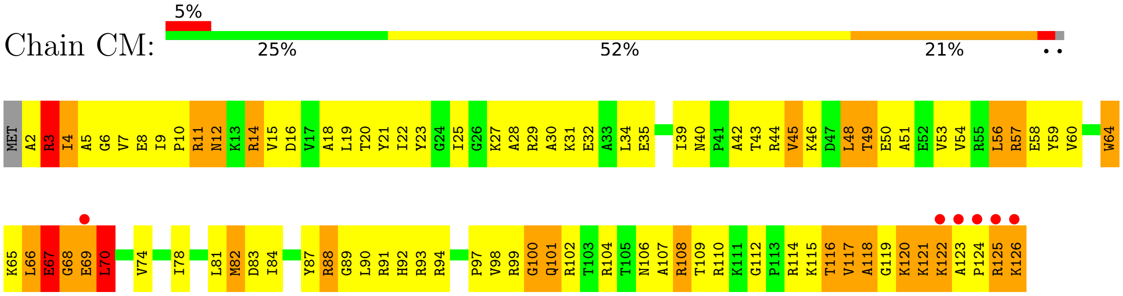
Chain AM:





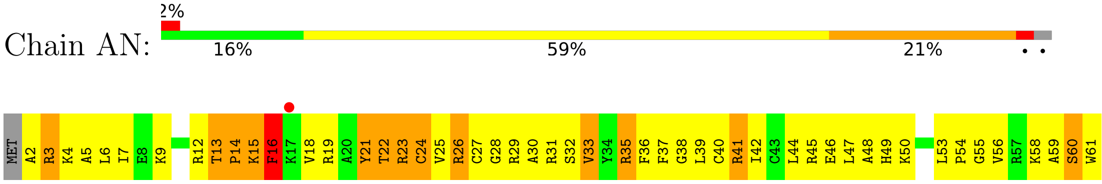
- Molecule 13: 30S ribosomal protein S13

Chain CM:



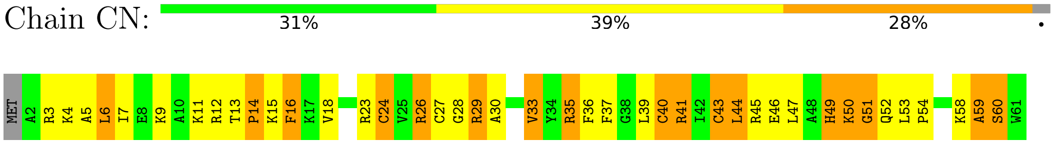
- Molecule 14: 30S ribosomal protein S14 type Z

Chain AN:



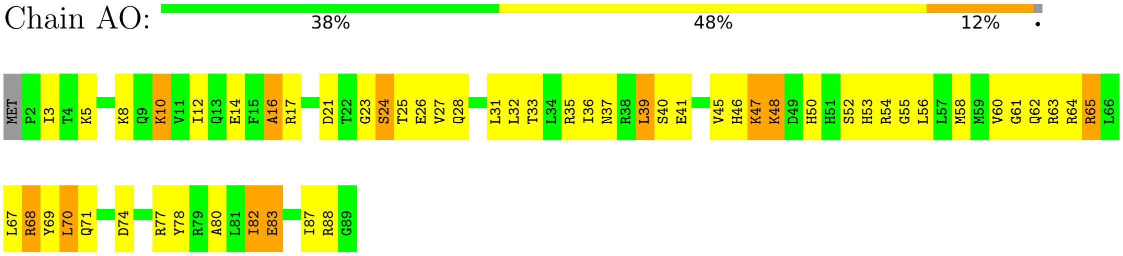
- Molecule 14: 30S ribosomal protein S14 type Z

Chain CN:



- Molecule 15: 30S ribosomal protein S15

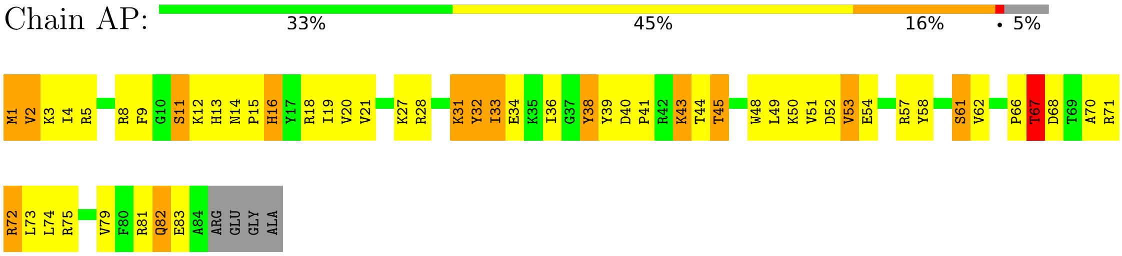
Chain AO:



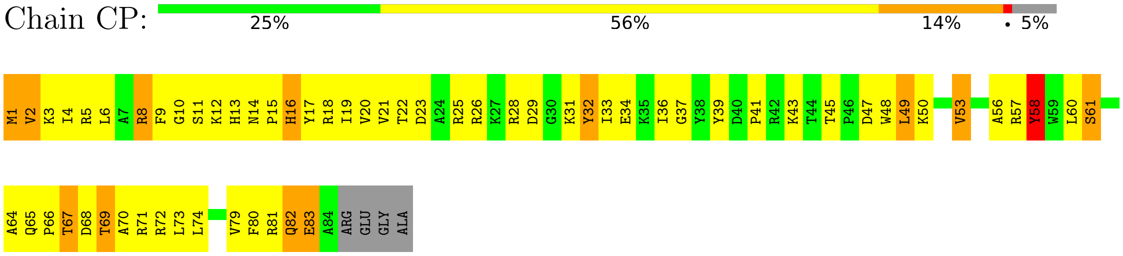
- Molecule 15: 30S ribosomal protein S15

Chain CO:

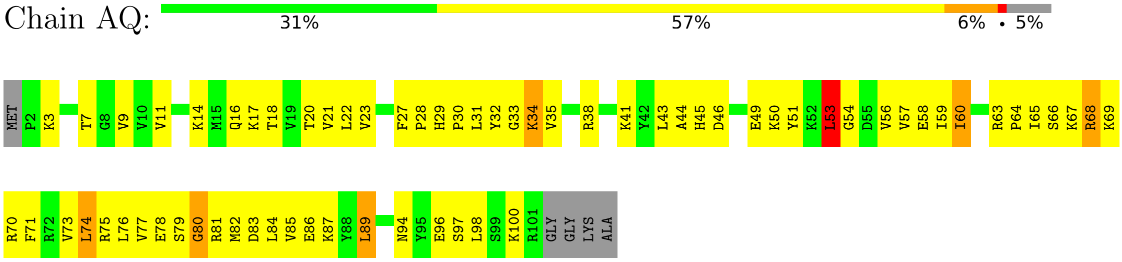
- Molecule 16: 30S ribosomal protein S16



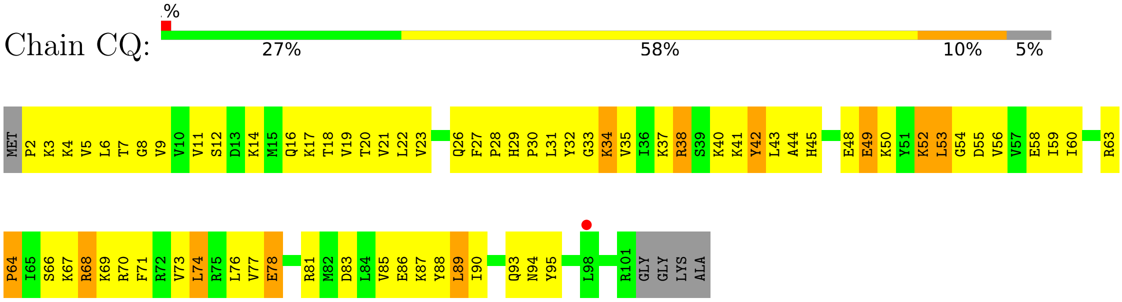
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 17: 30S ribosomal protein S17



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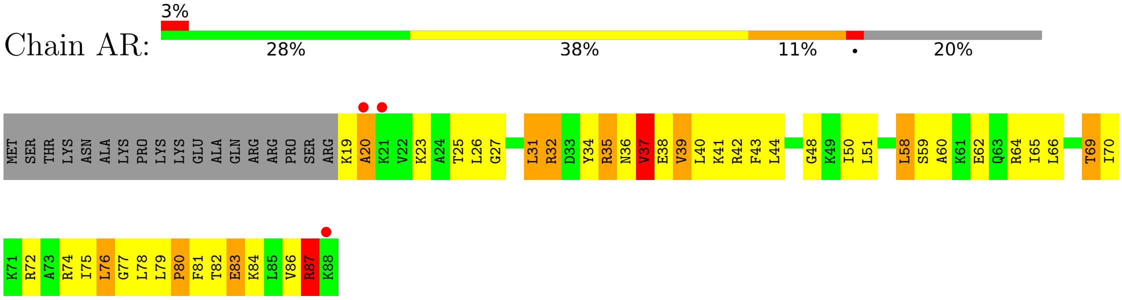

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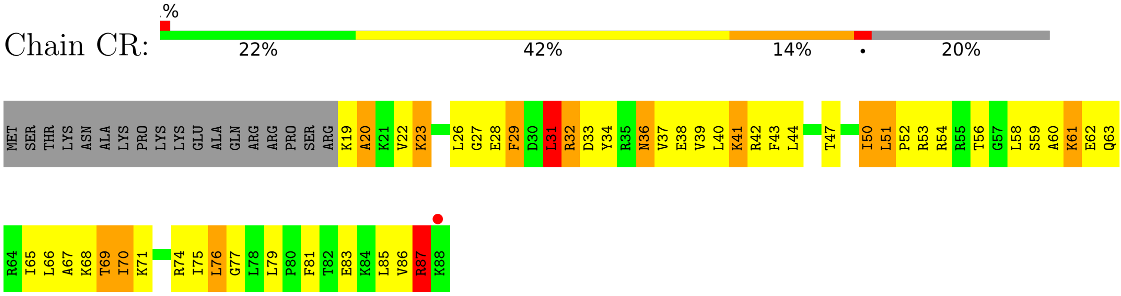

- Molecule 19: 30S ribosomal protein S19

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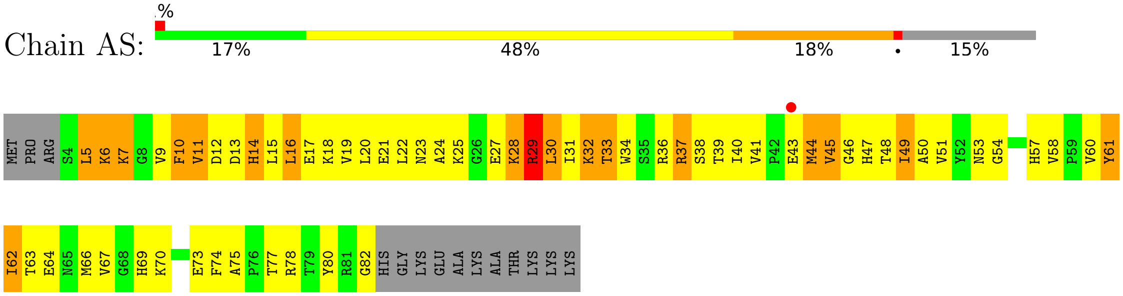

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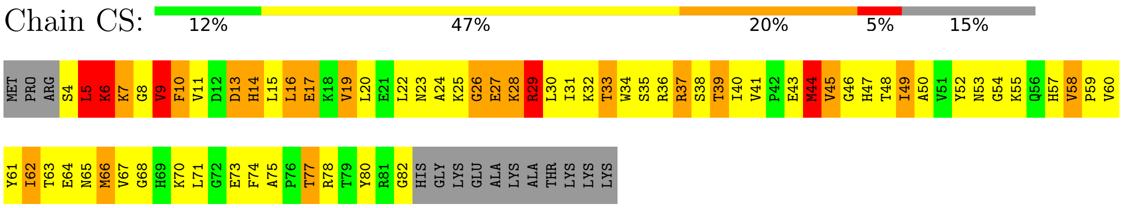

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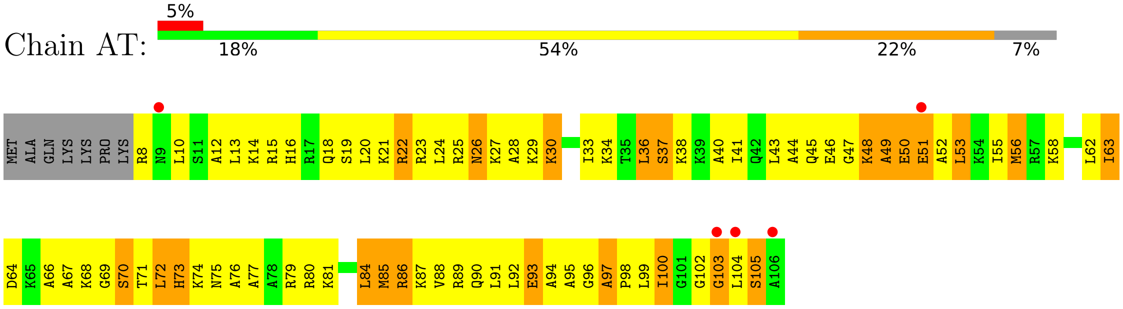

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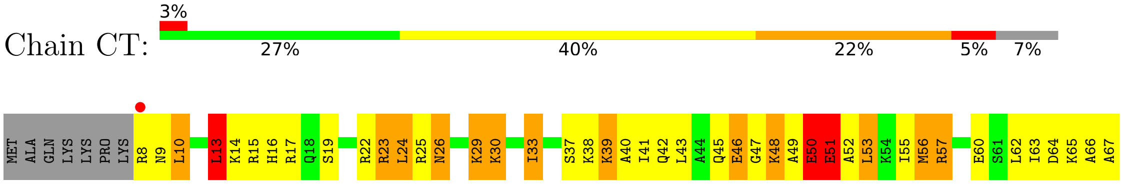

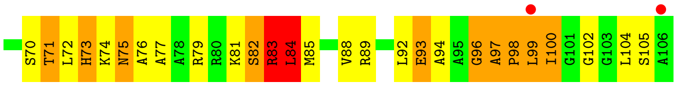

- Molecule 21: 30S ribosomal protein Thx

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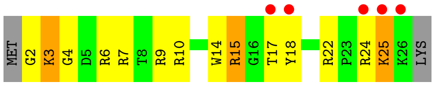

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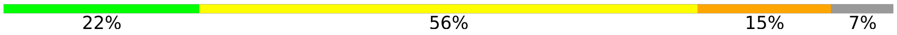

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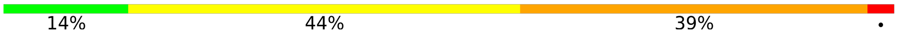

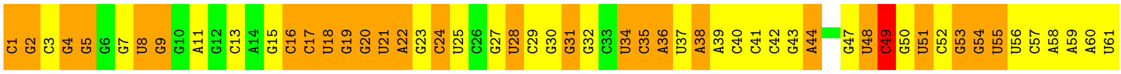

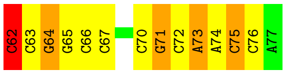

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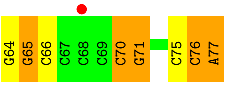

- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

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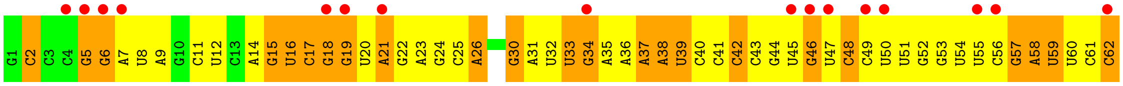

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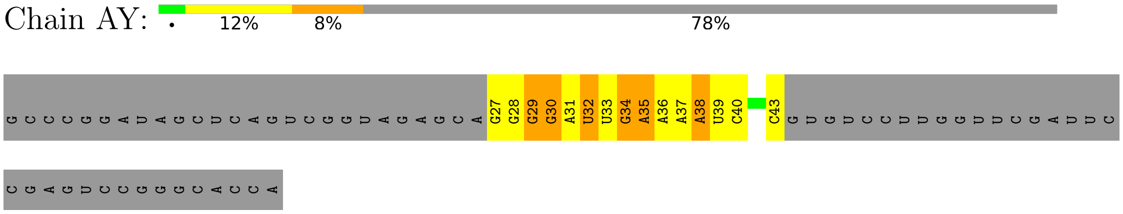

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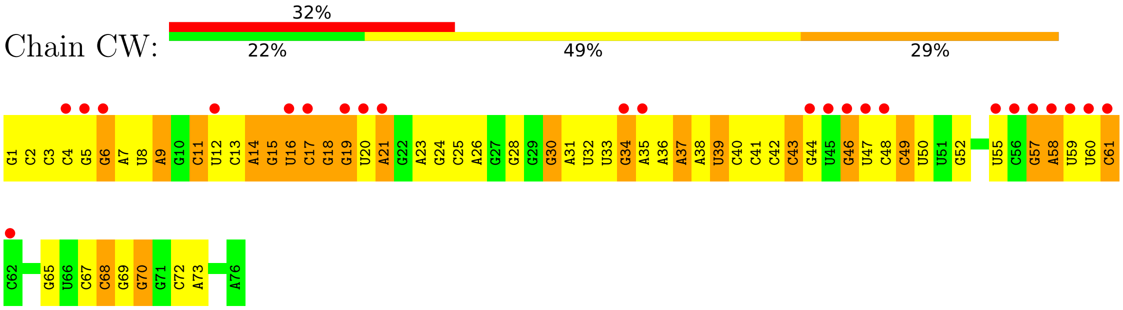

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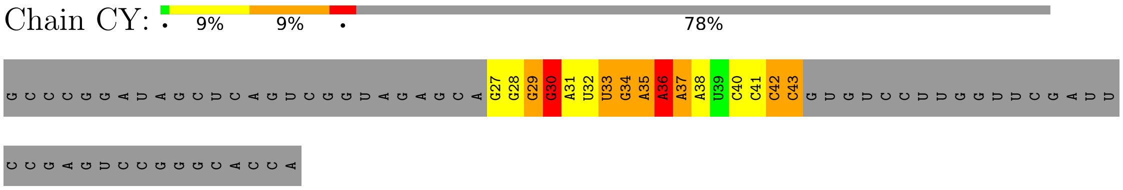
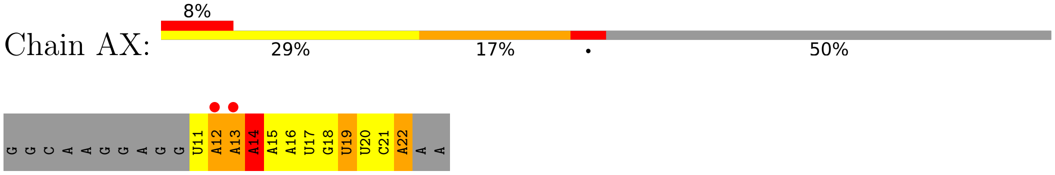


- Molecule 24: mRNA



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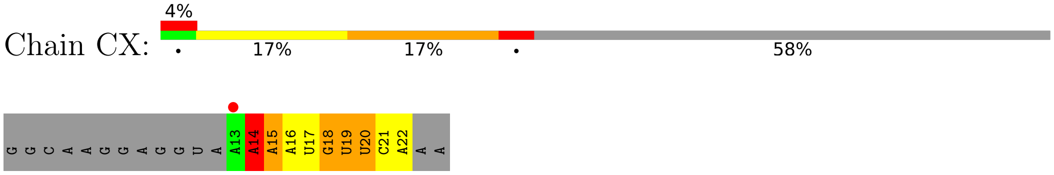
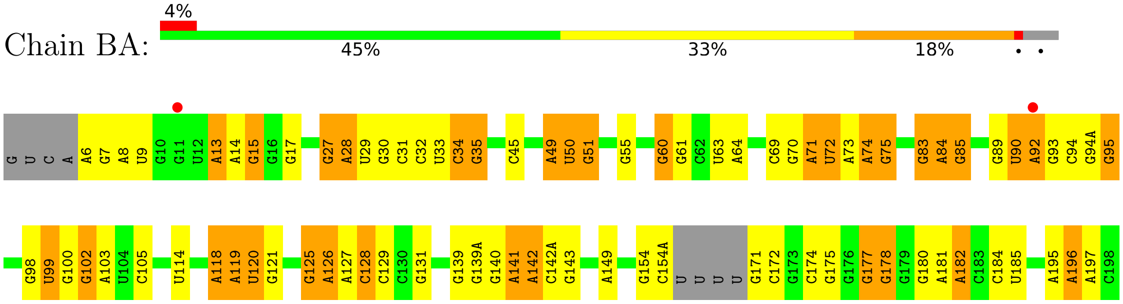
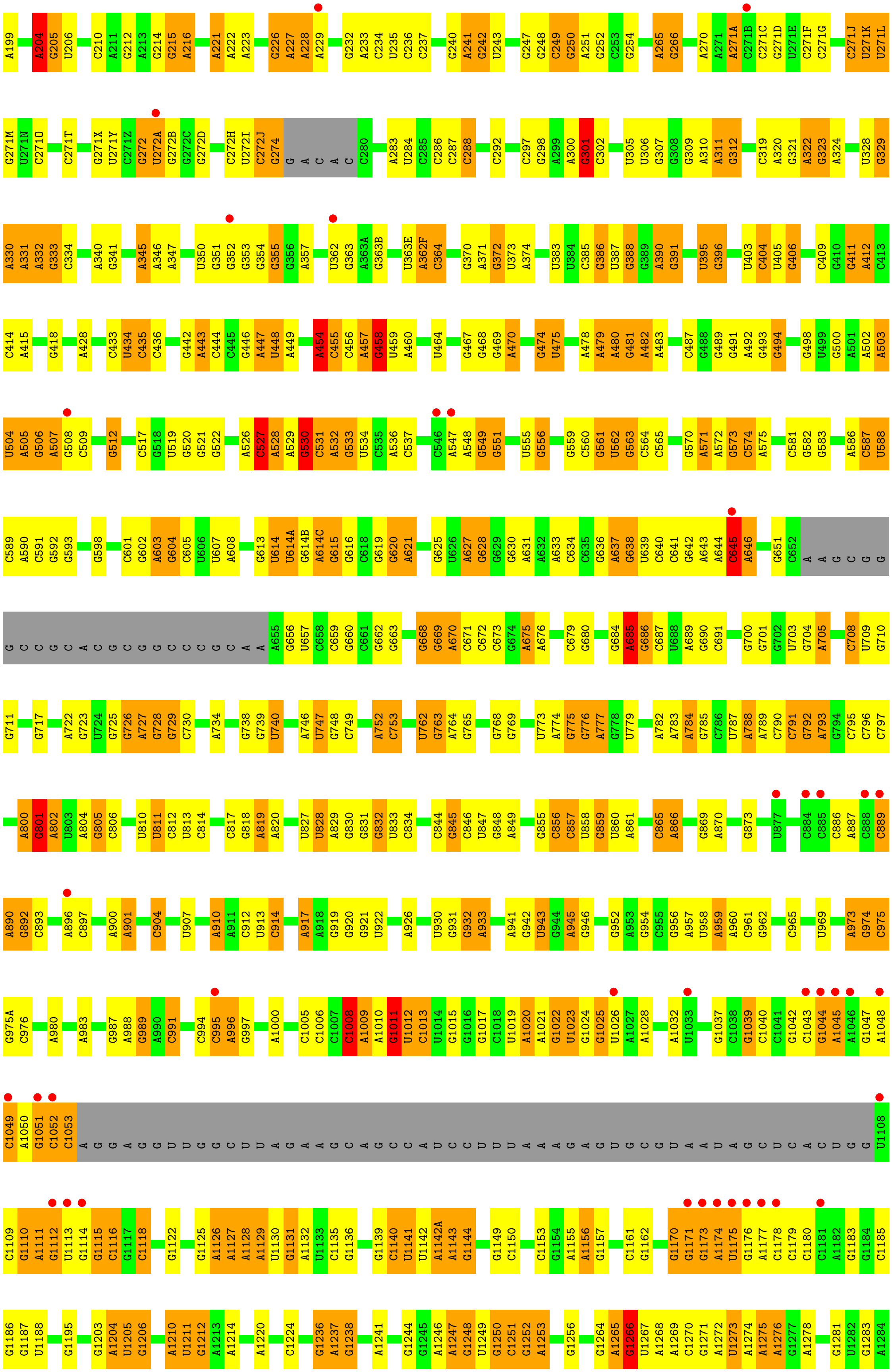


- Molecule 25: 23S rRNA

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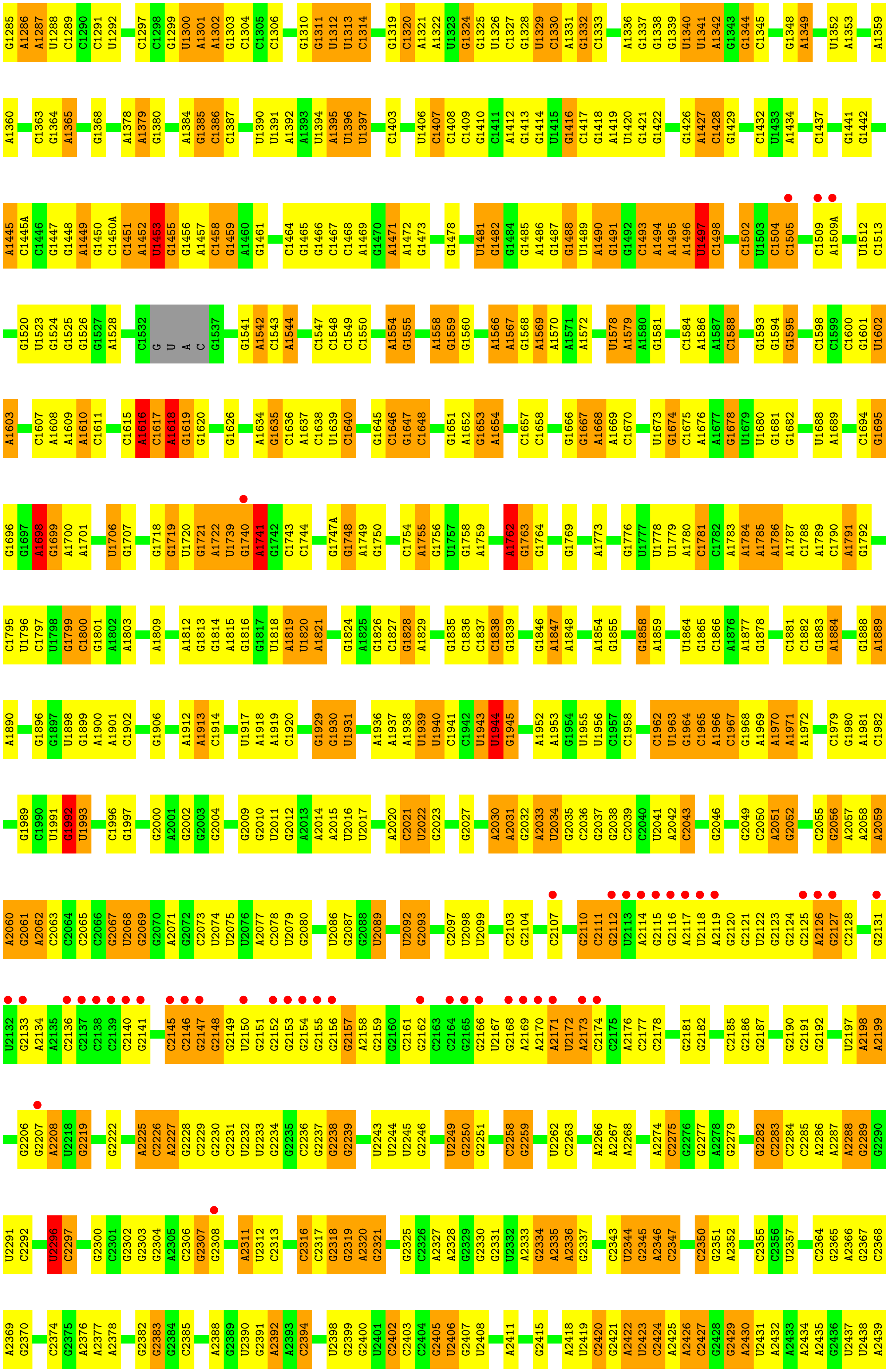
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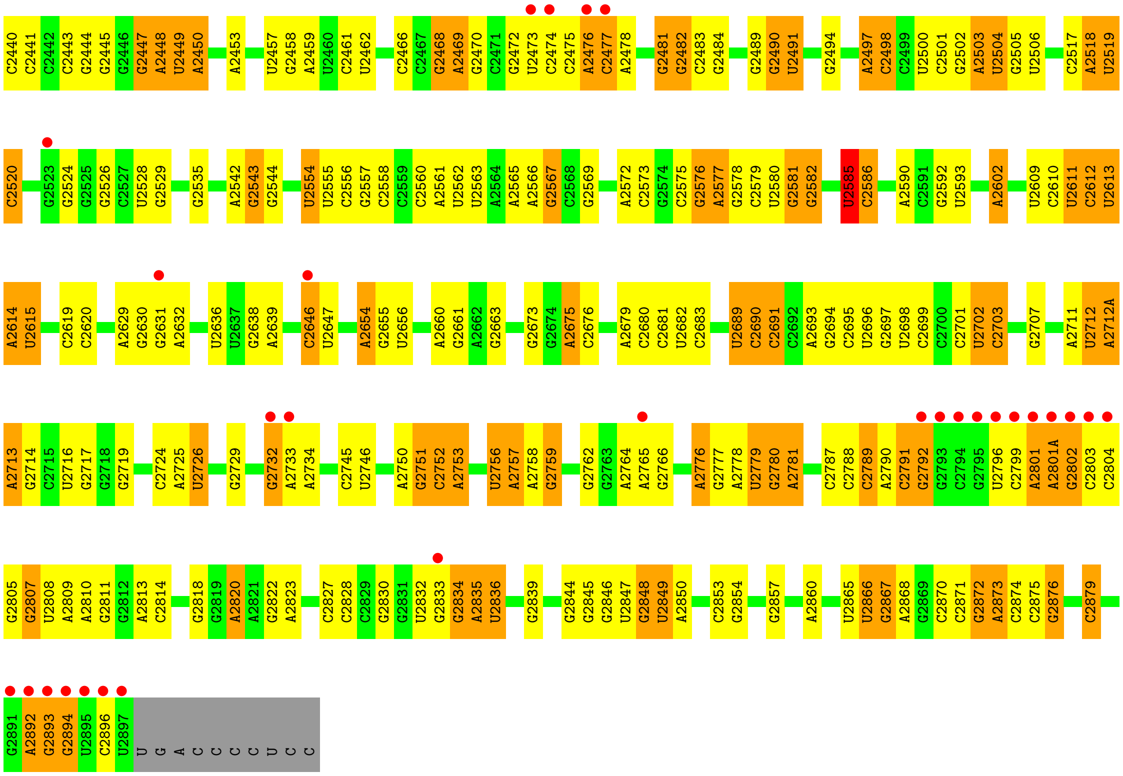
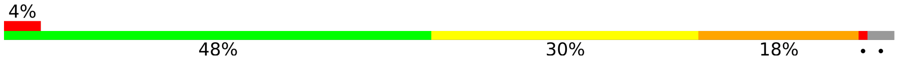
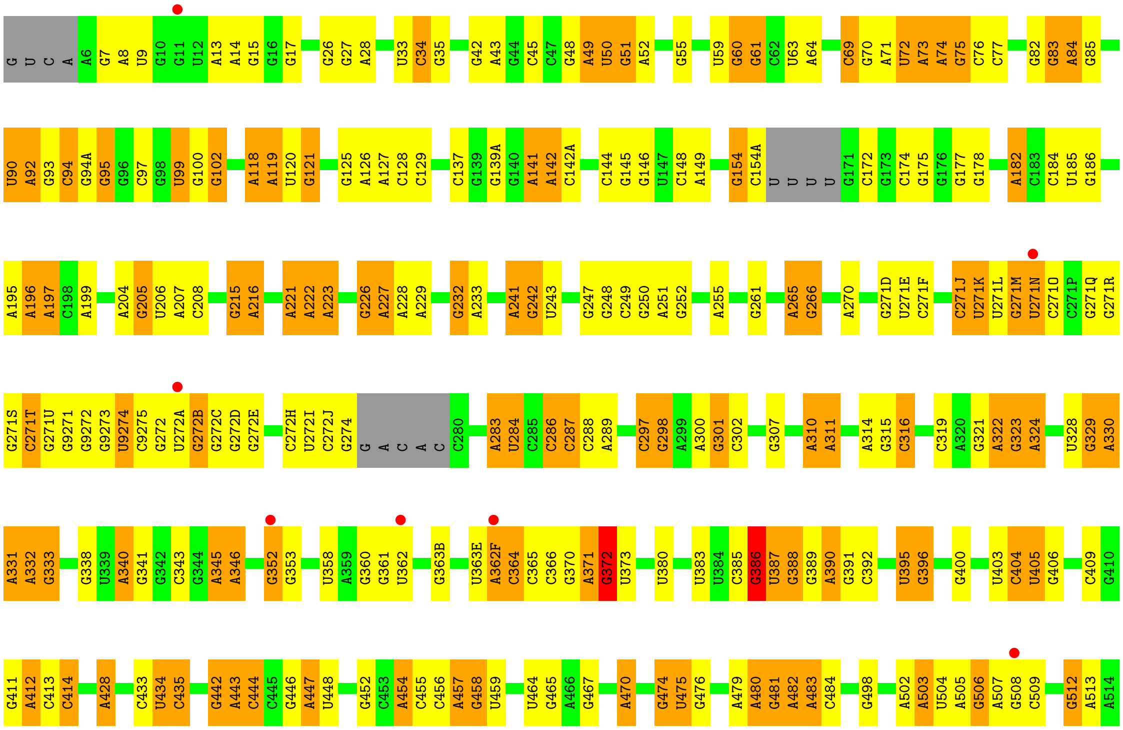
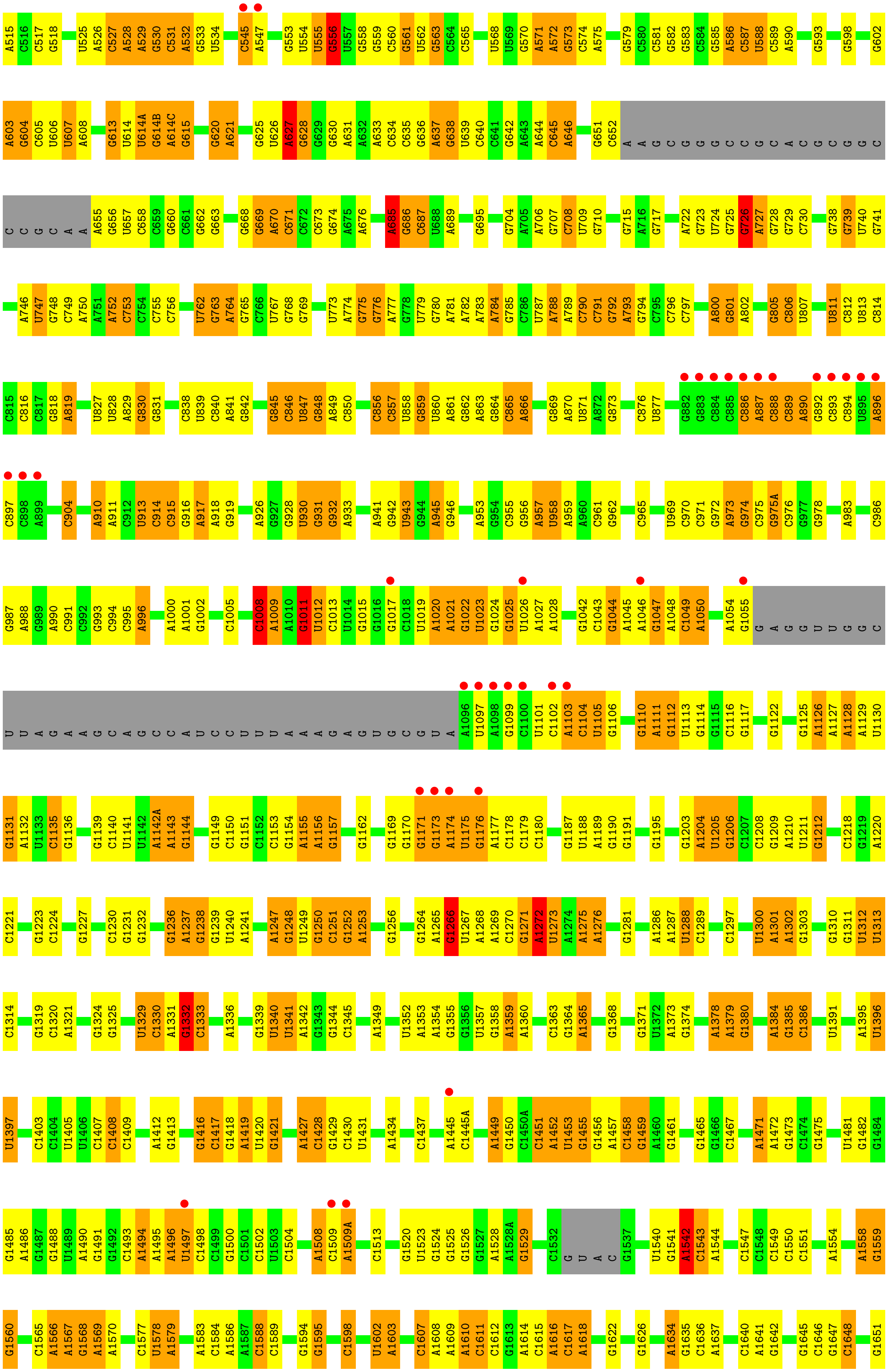


- Molecule 25: 23S rRNA

Chain DA:



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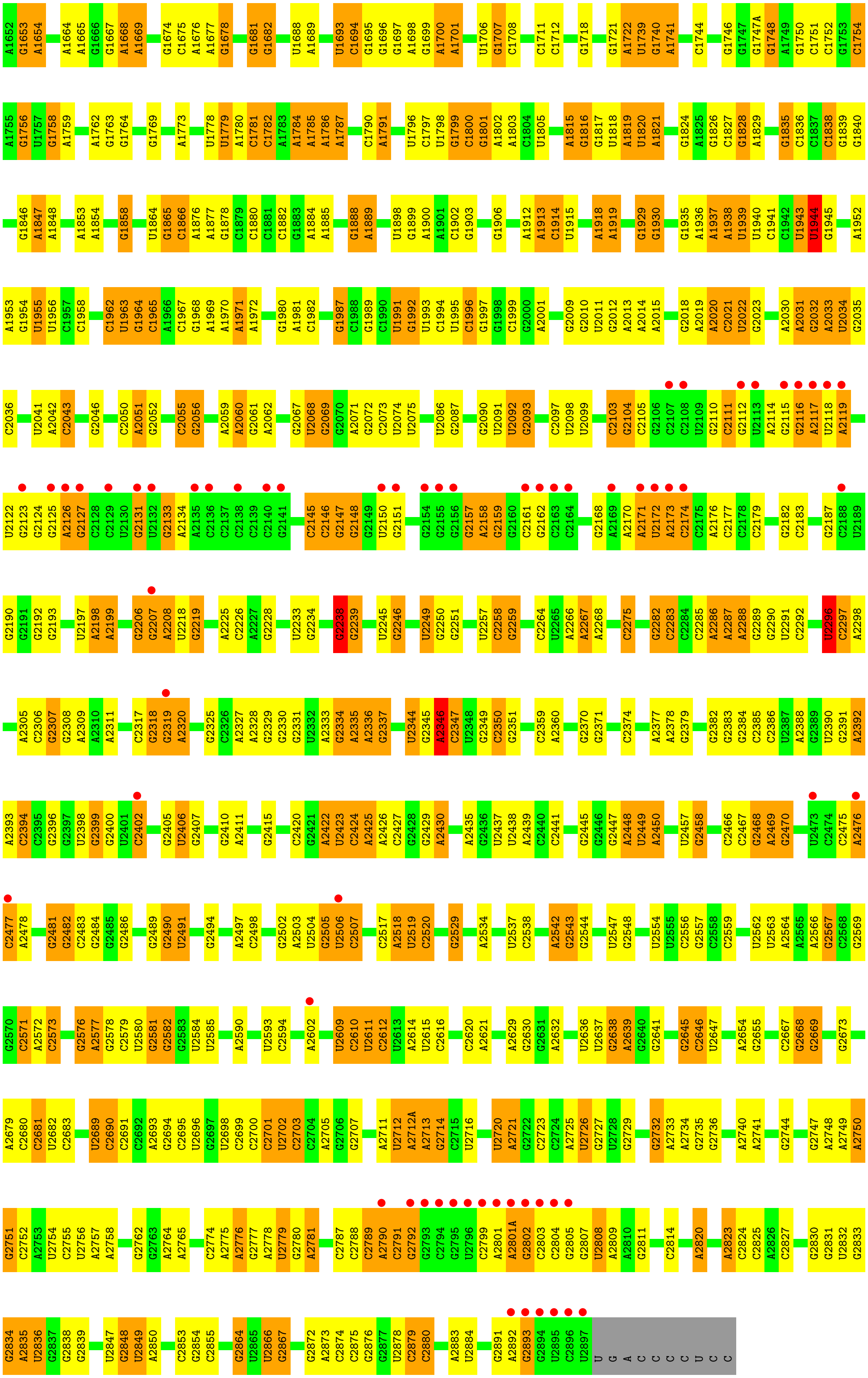
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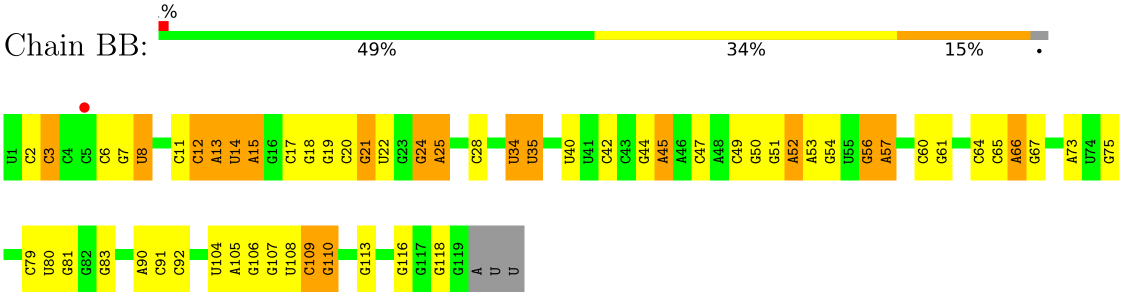
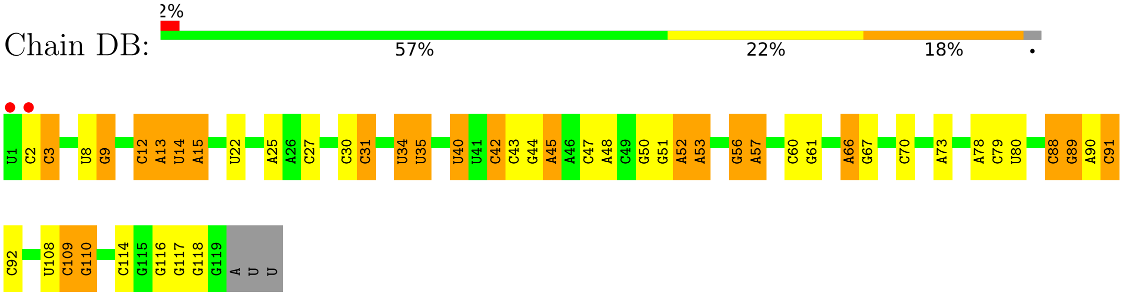
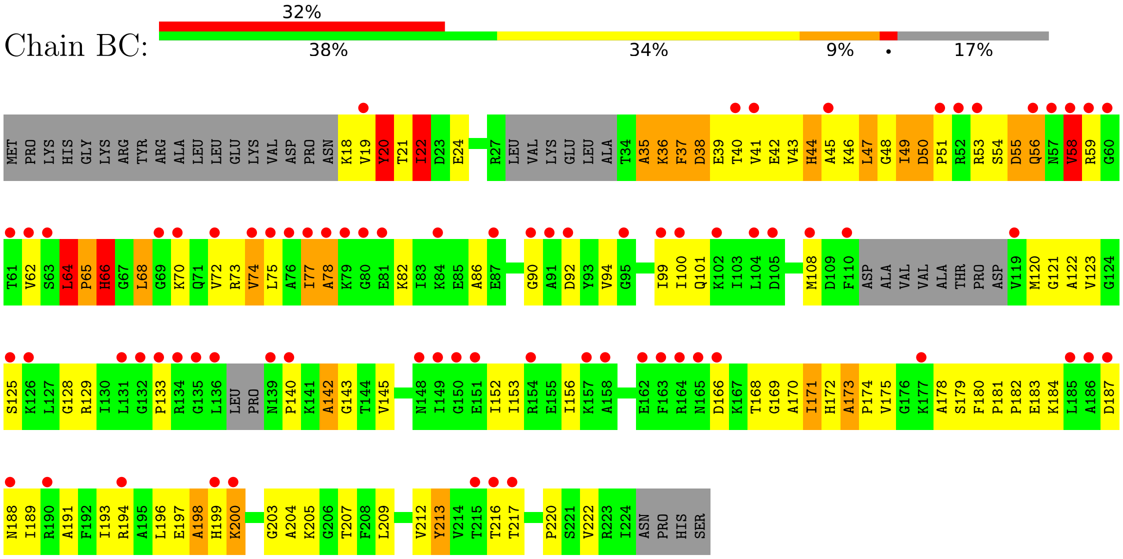
- Molecule 26: 5S rRNA



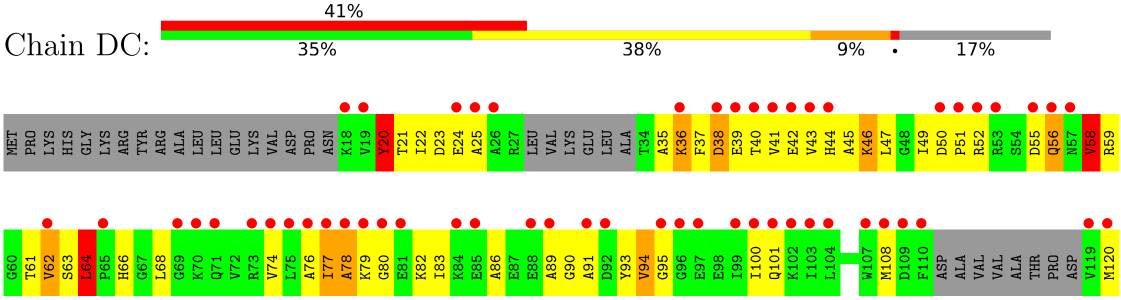
- Molecule 26: 5S rRNA

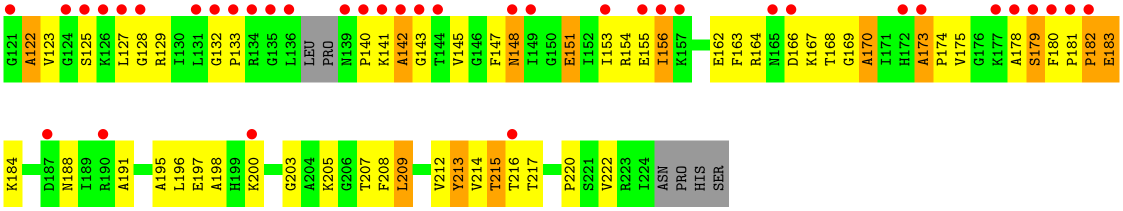


- Molecule 27: 50S RIBOSOMAL PROTEIN L1



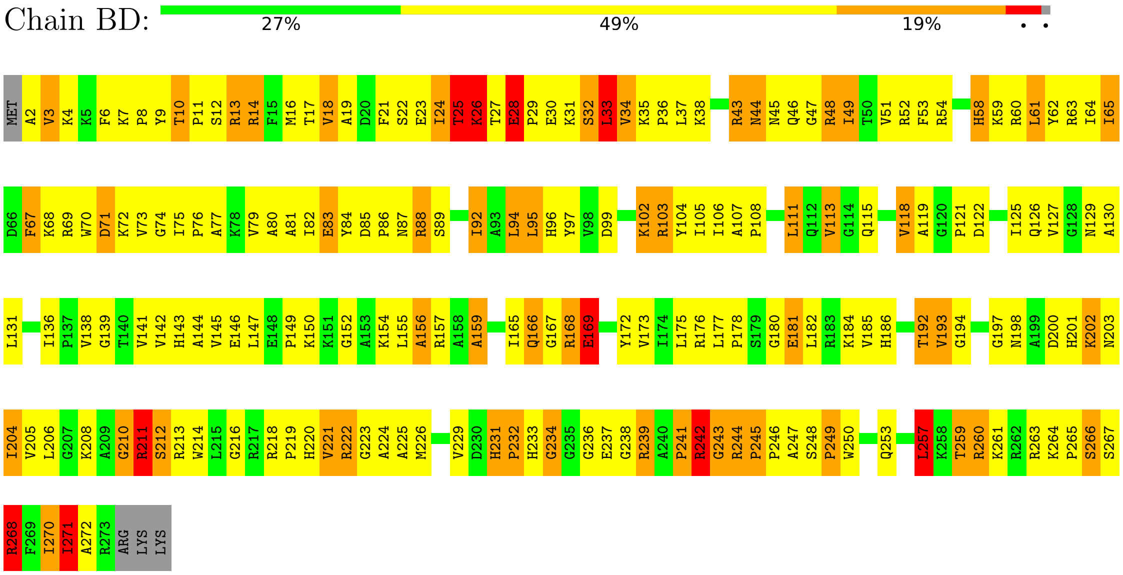
- Molecule 27: 50S RIBOSOMAL PROTEIN L1





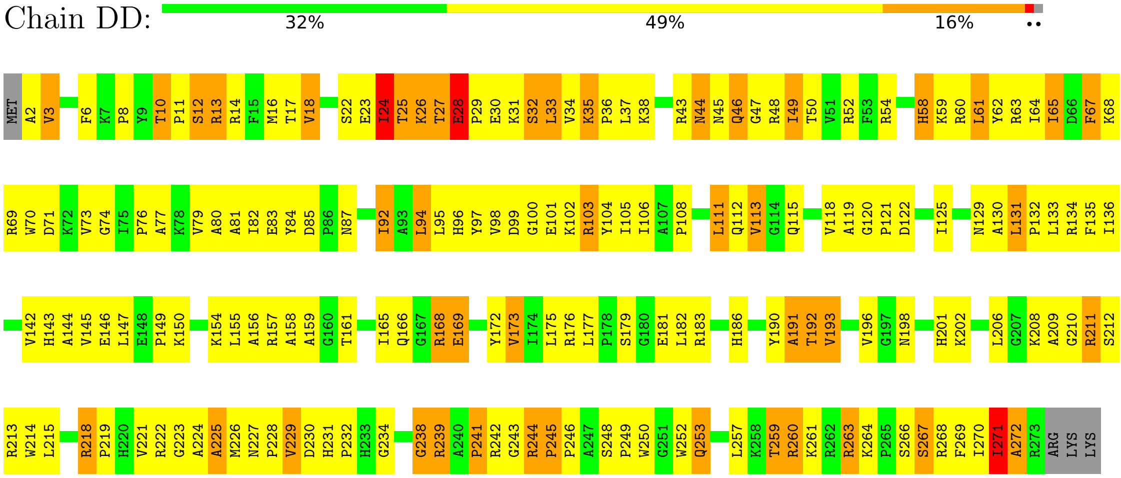
- Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain BD:



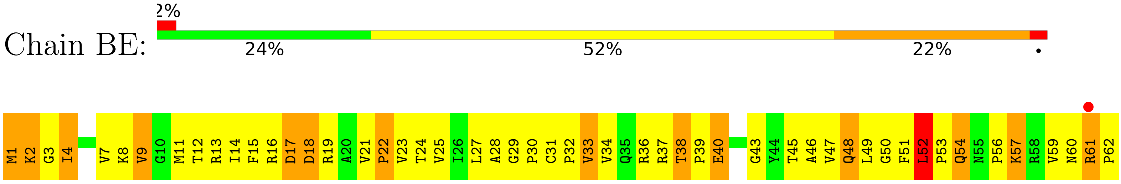
- Molecule 28: 50S RIBOSOMAL PROTEIN L2

Chain DD:



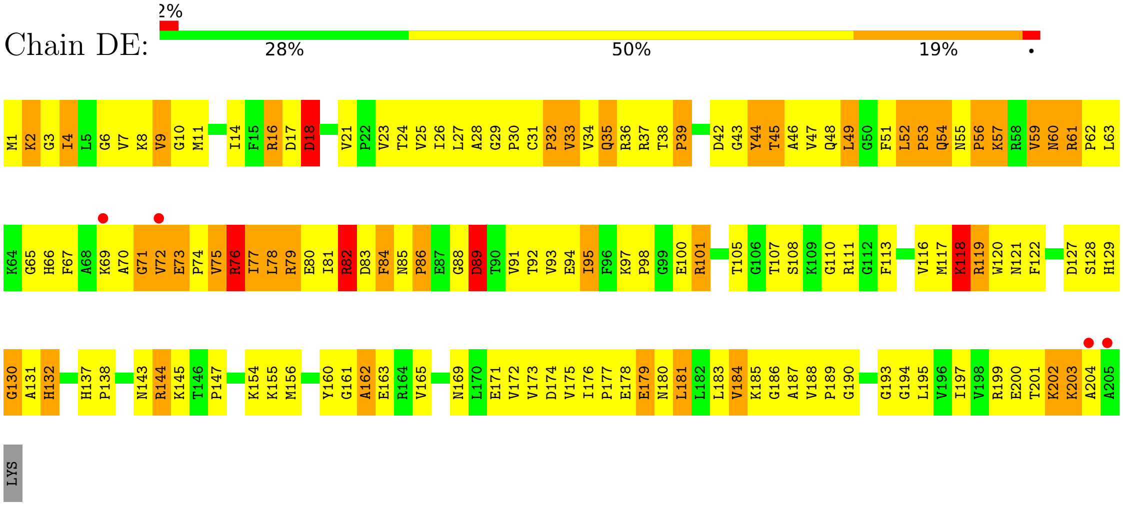
- Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain BE:



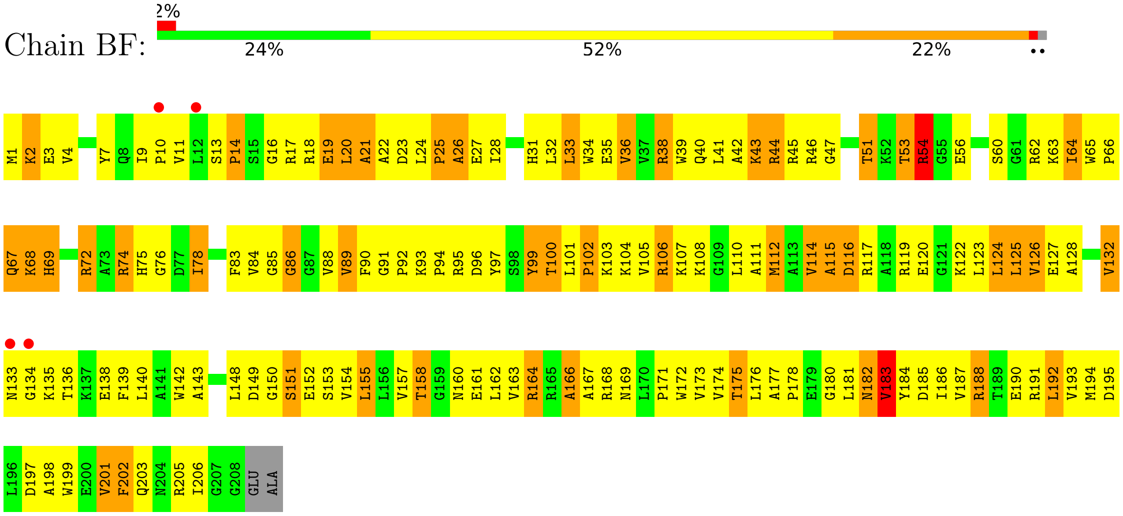
- Molecule 29: 50S RIBOSOMAL PROTEIN L3

Chain DE:



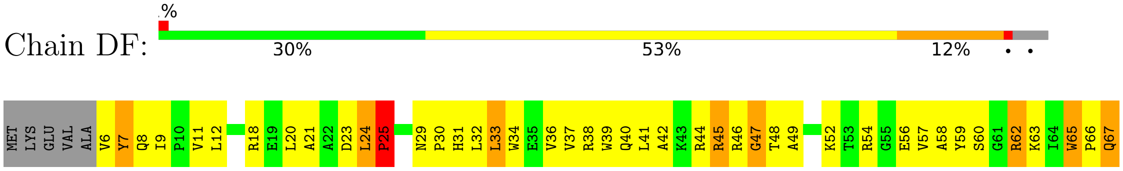
- Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain BF:



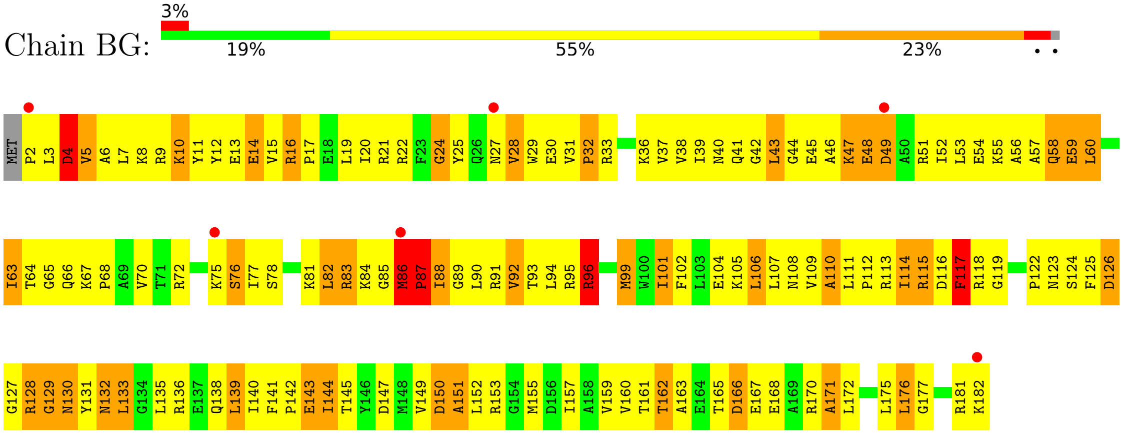
- Molecule 30: 50S RIBOSOMAL PROTEIN L4

Chain DF:



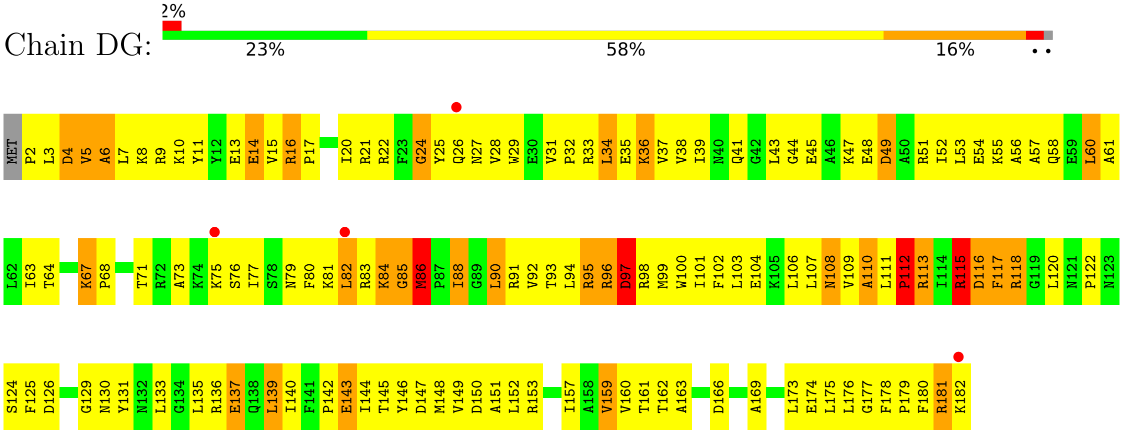
- Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain BG:



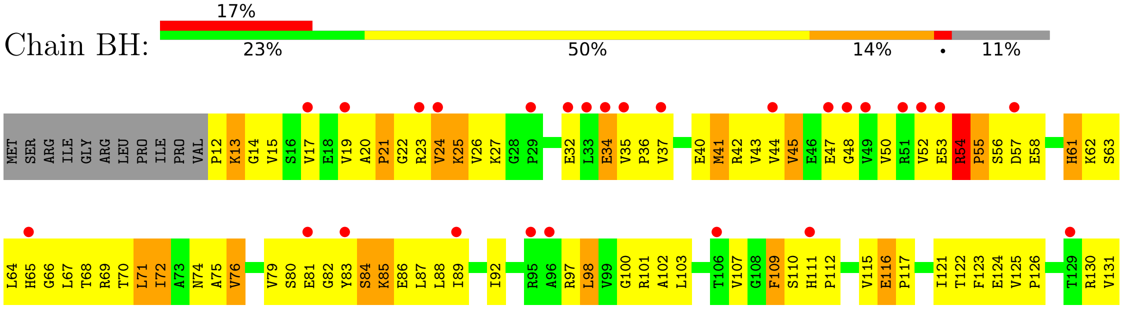
- Molecule 31: 50S RIBOSOMAL PROTEIN L5

Chain DG:

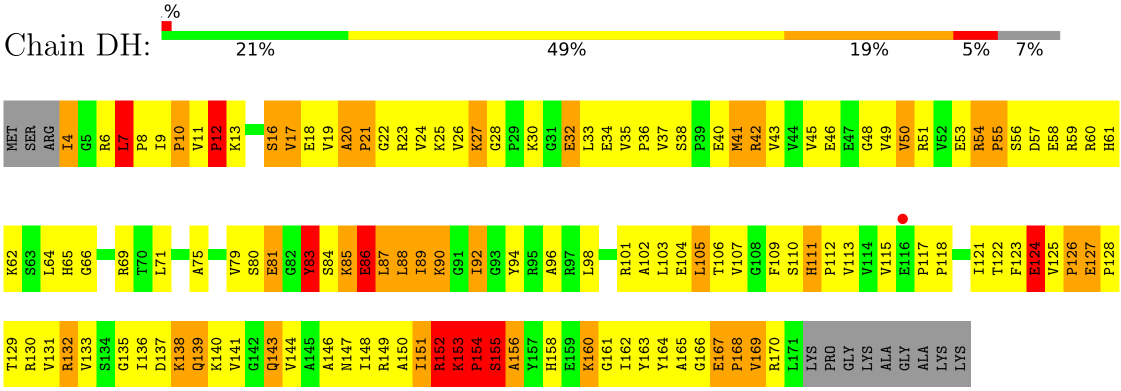


- Molecule 32: 50S RIBOSOMAL PROTEIN L6

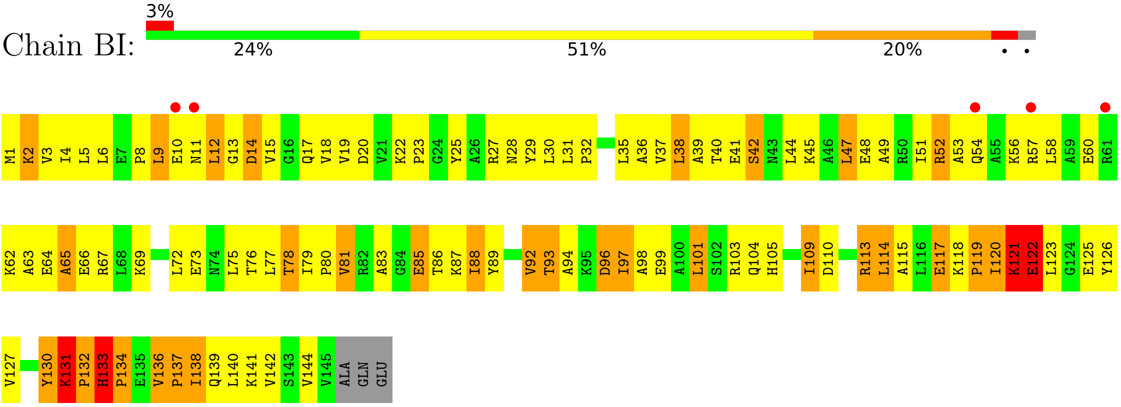
Chain BH:



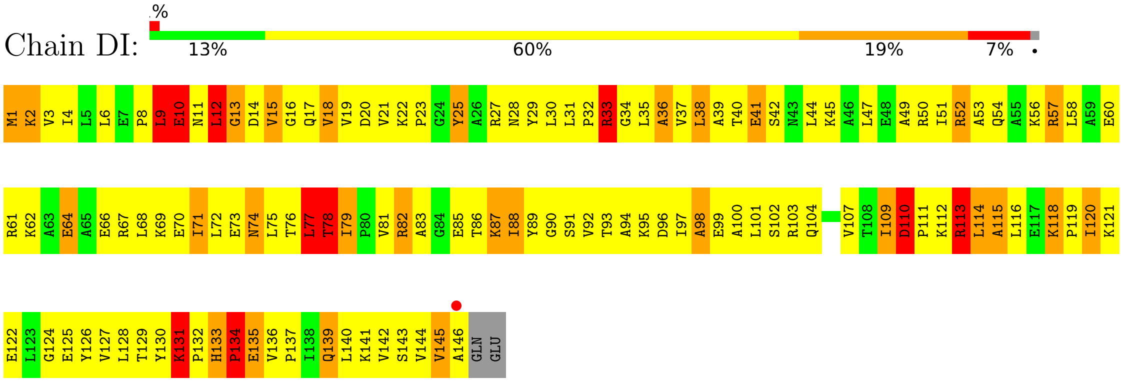
- Molecule 32: 50S RIBOSOMAL PROTEIN L6



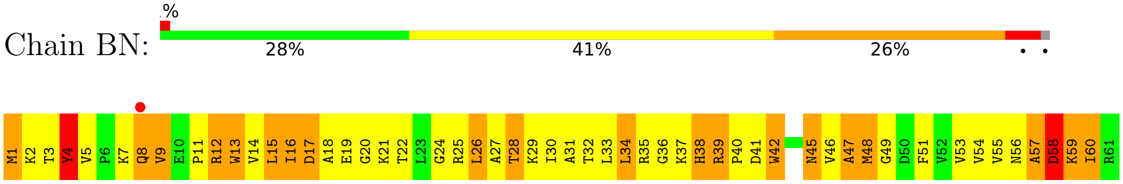
- Molecule 33: 50S RIBOSOMAL PROTEIN L9

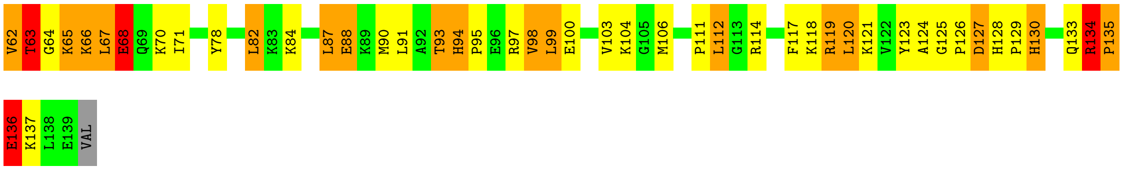


- Molecule 33: 50S RIBOSOMAL PROTEIN L9

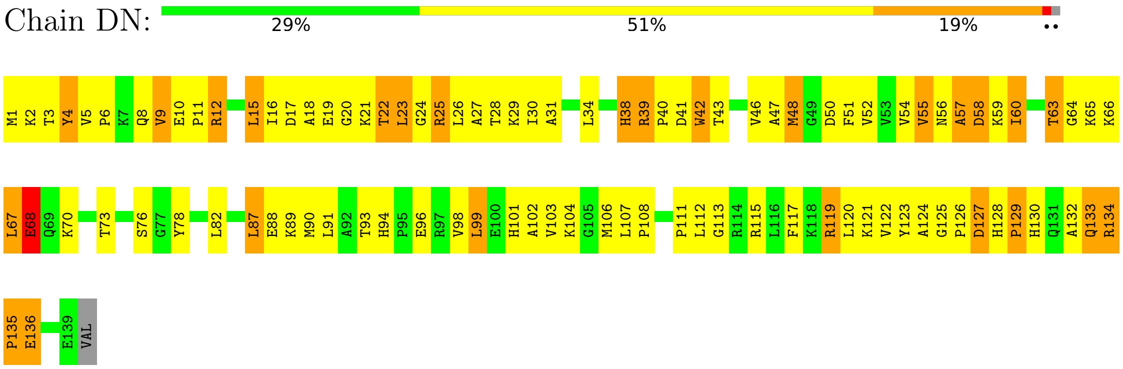


- Molecule 34: 50S RIBOSOMAL PROTEIN L13

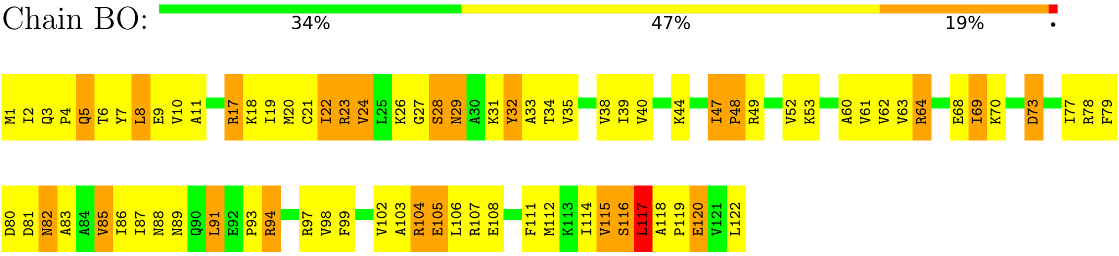




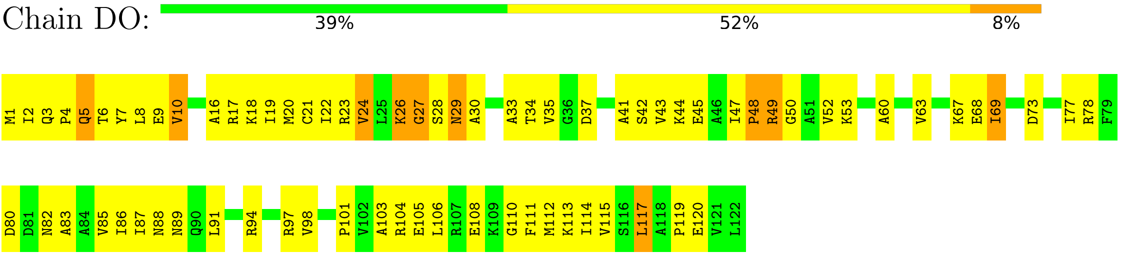
- Molecule 34: 50S RIBOSOMAL PROTEIN L13



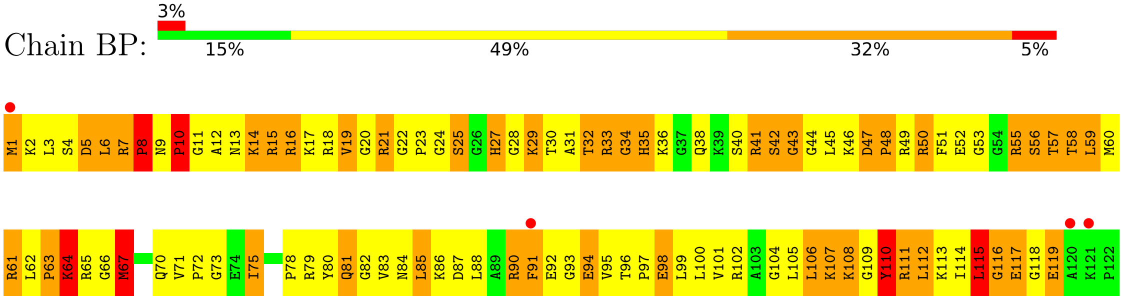
- Molecule 35: 50S RIBOSOMAL PROTEIN L14

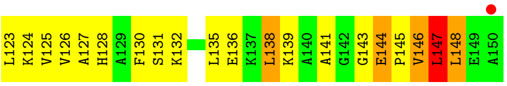


- Molecule 35: 50S RIBOSOMAL PROTEIN L14



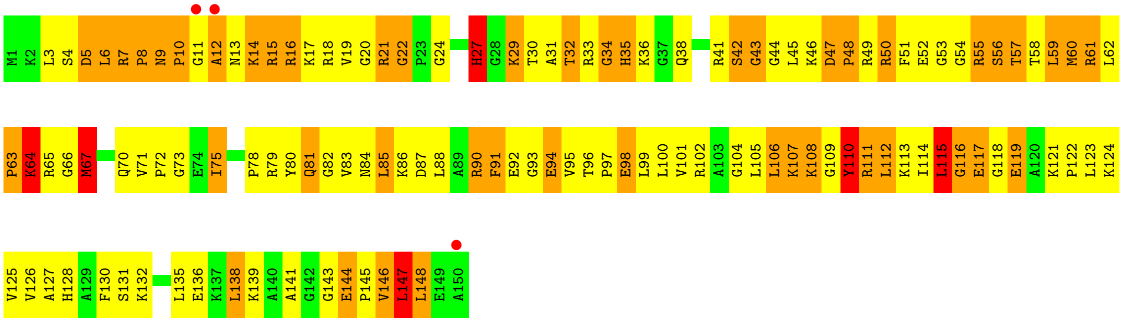
- Molecule 36: 50S RIBOSOMAL PROTEIN L15





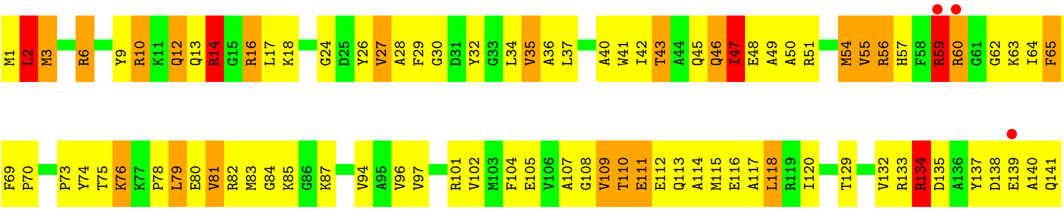
- Molecule 36: 50S RIBOSOMAL PROTEIN L15

Chain DP:



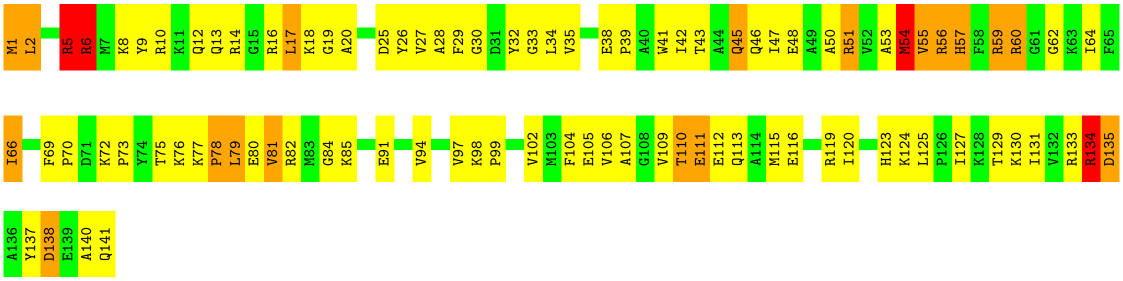
- Molecule 37: 50S RIBOSOMAL PROTEIN L16

Chain BQ:



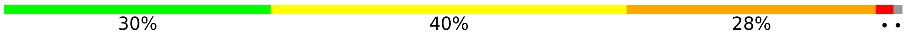
- Molecule 37: 50S RIBOSOMAL PROTEIN L16

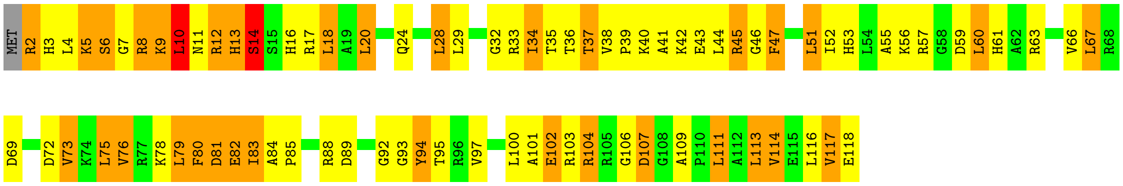
Chain DQ:



- Molecule 38: 50S RIBOSOMAL PROTEIN L17

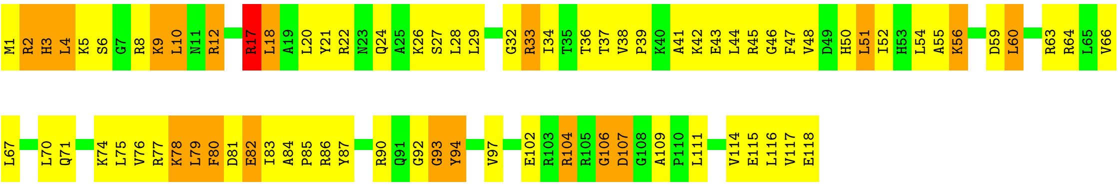
Chain BR:





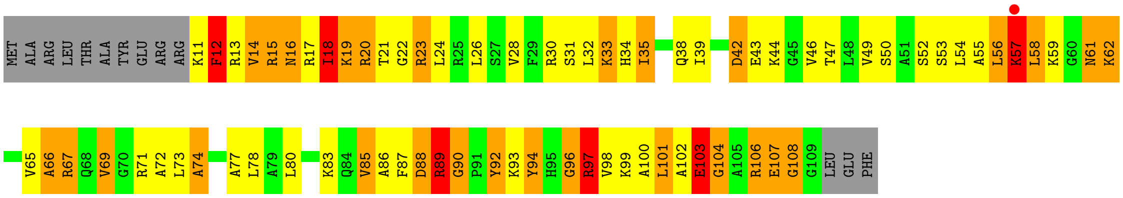
- Molecule 38: 50S RIBOSOMAL PROTEIN L17

Chain DR:



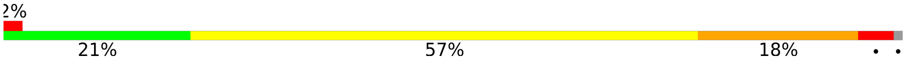
- Molecule 39: 50S RIBOSOMAL PROTEIN L18

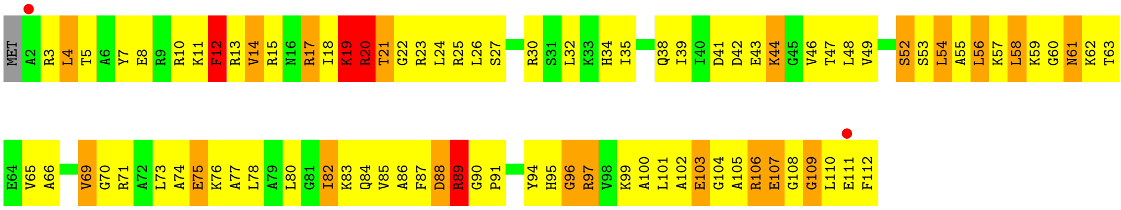
Chain BS:



- Molecule 39: 50S RIBOSOMAL PROTEIN L18

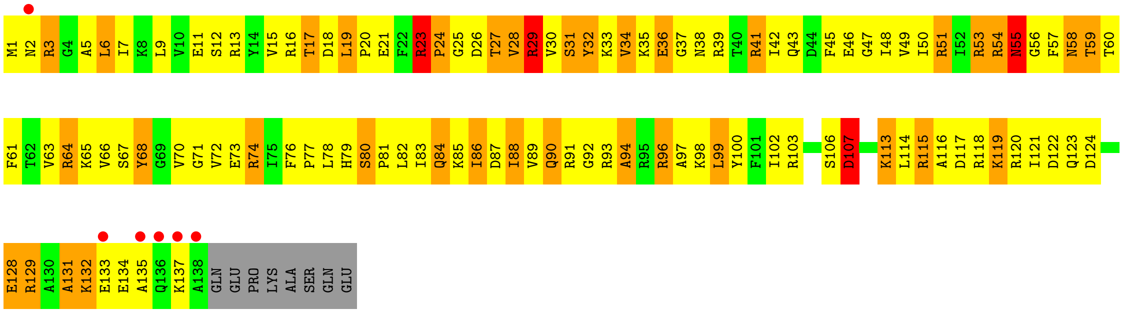
Chain DS:





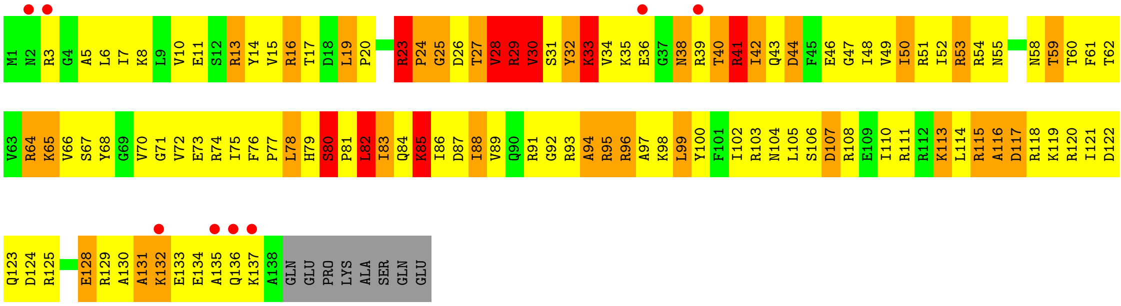
- Molecule 40: 50S RIBOSOMAL PROTEIN L19

Chain BT:



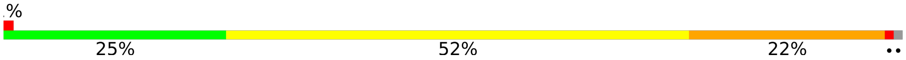
- Molecule 40: 50S RIBOSOMAL PROTEIN L19

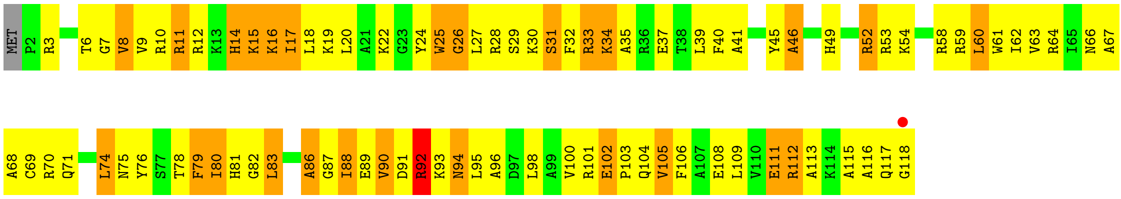
Chain DT:



- Molecule 41: 50S RIBOSOMAL PROTEIN L20

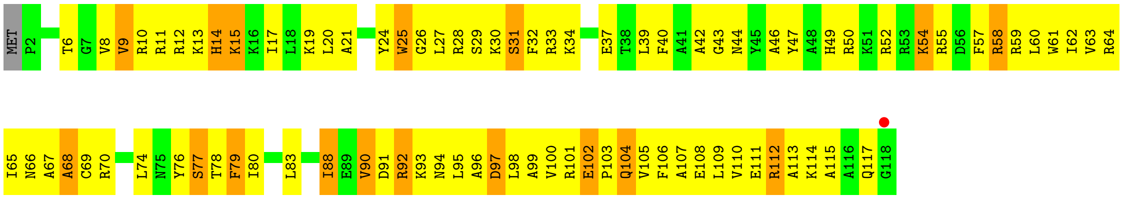
Chain BU:





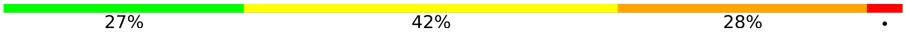
- Molecule 41: 50S RIBOSOMAL PROTEIN L20

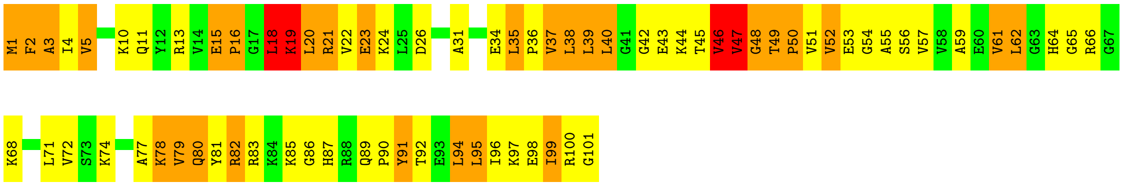
Chain DU:



- Molecule 42: 50S RIBOSOMAL PROTEIN L21

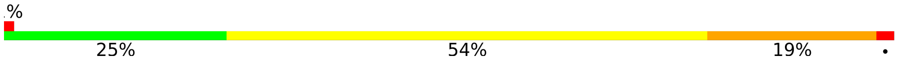
Chain BV:

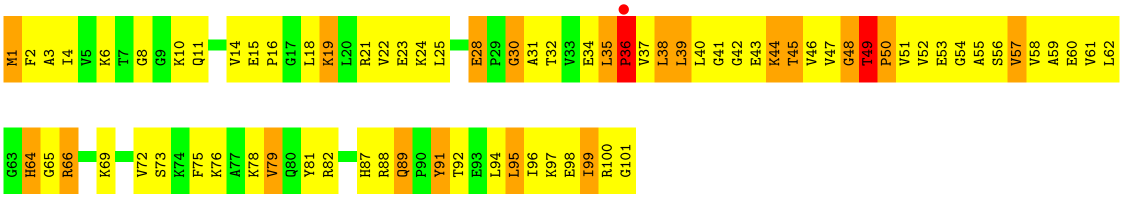




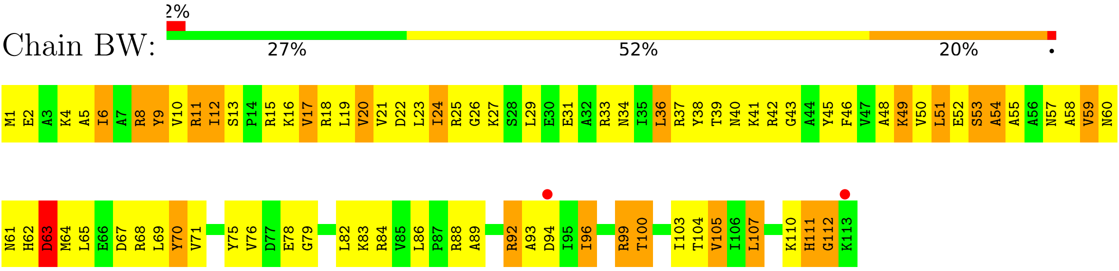
- Molecule 42: 50S RIBOSOMAL PROTEIN L21

Chain DV:

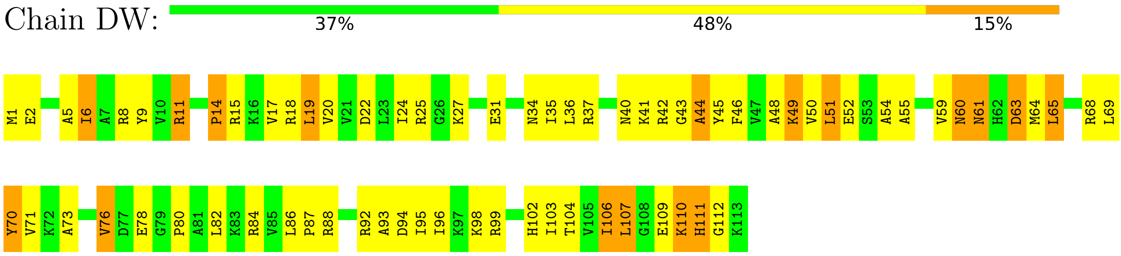




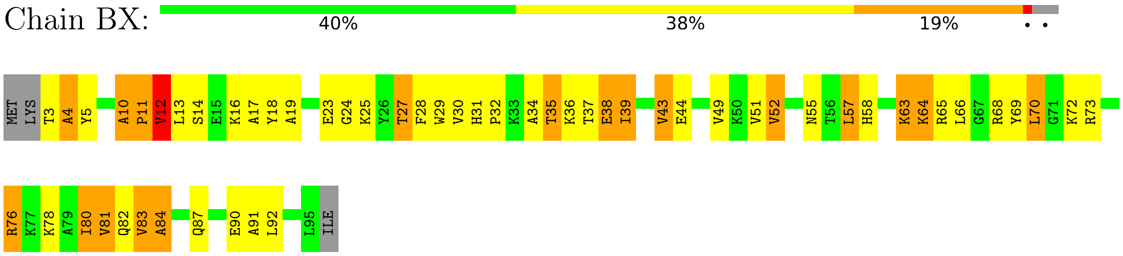
- Molecule 43: 50S RIBOSOMAL PROTEIN L22



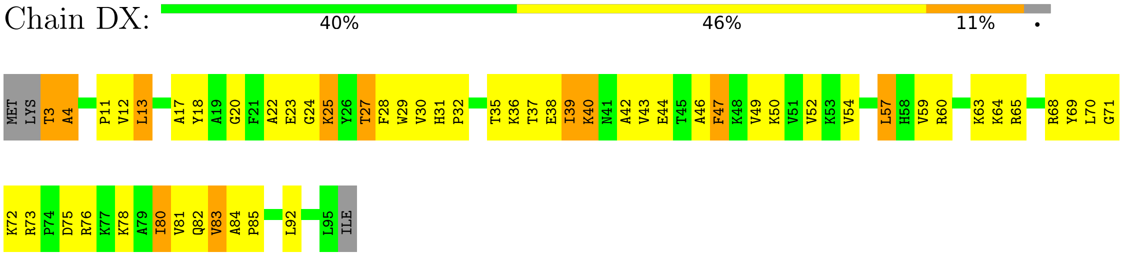
- Molecule 43: 50S RIBOSOMAL PROTEIN L22



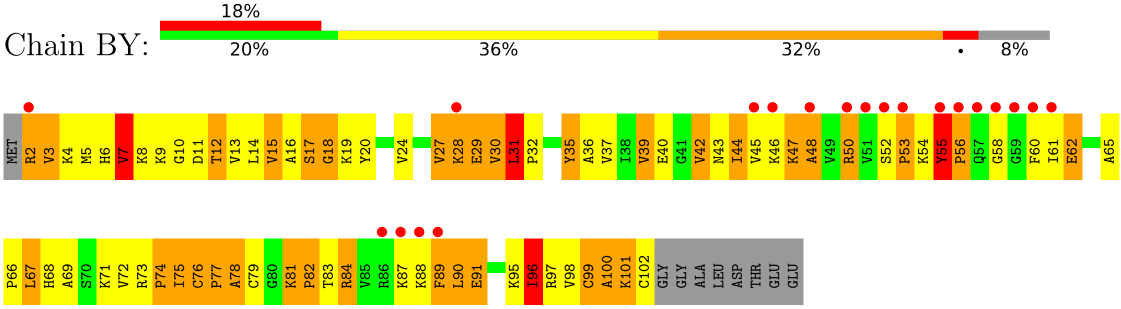
- Molecule 44: 50S RIBOSOMAL PROTEIN L23



- Molecule 44: 50S RIBOSOMAL PROTEIN L23

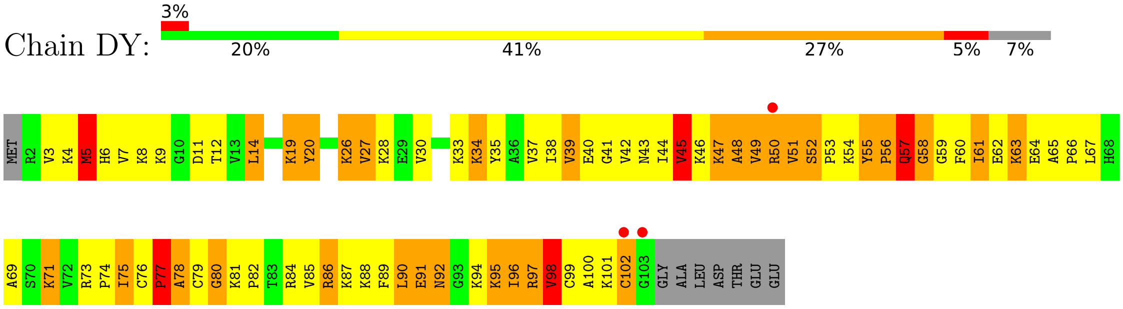


- Molecule 45: 50S RIBOSOMAL PROTEIN L24



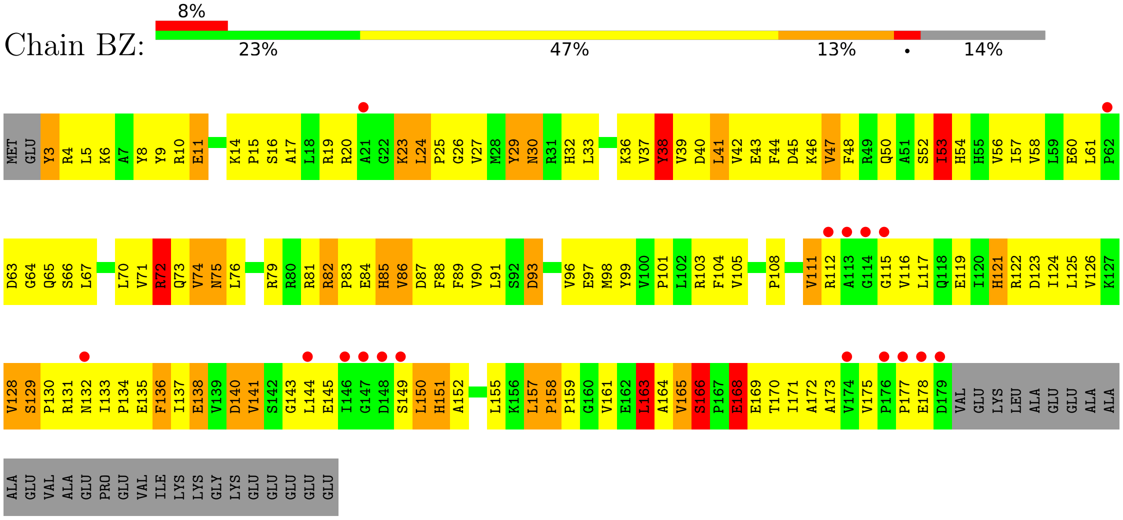
- Molecule 45: 50S RIBOSOMAL PROTEIN L24

Chain DY:



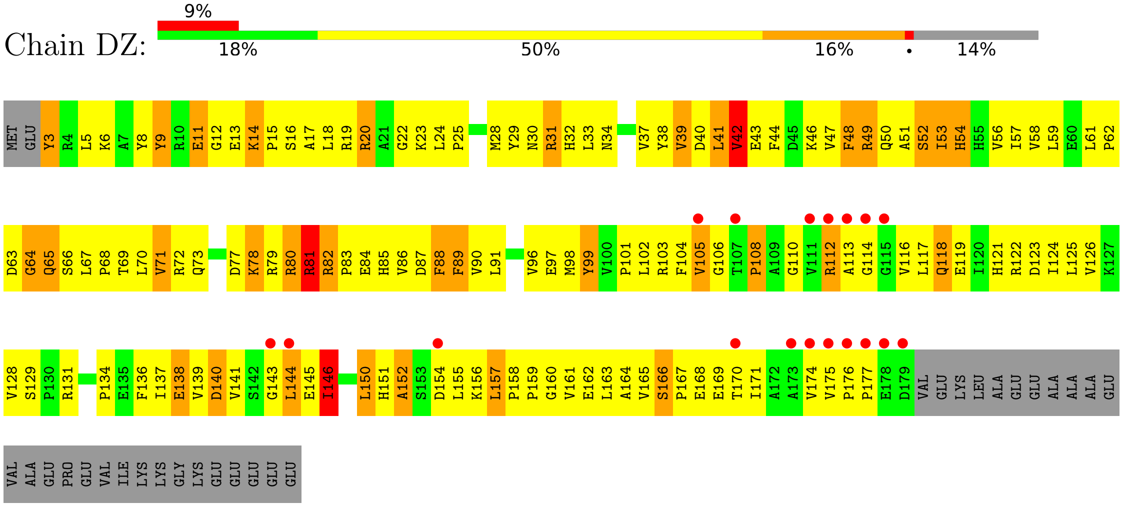
- Molecule 46: 50S RIBOSOMAL PROTEIN L25

Chain BZ:



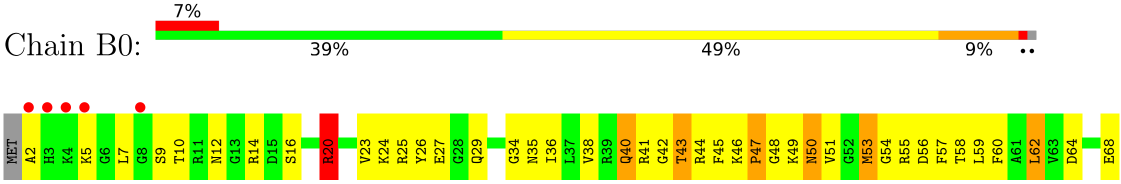
- Molecule 46: 50S RIBOSOMAL PROTEIN L25

Chain DZ:



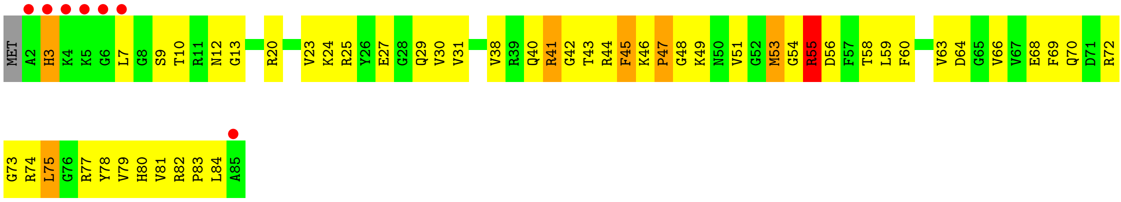
- Molecule 47: 50S RIBOSOMAL PROTEIN L27

Chain B0:



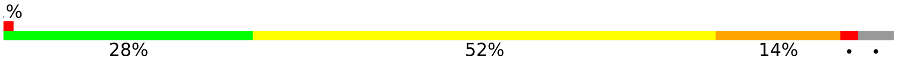
- Molecule 47: 50S RIBOSOMAL PROTEIN L27

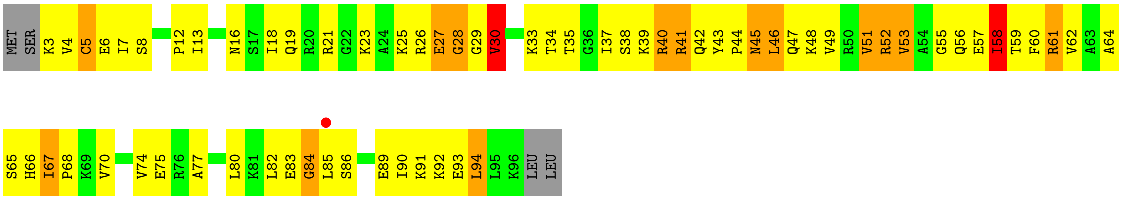
Chain D0:



- Molecule 48: 50S RIBOSOMAL PROTEIN L28

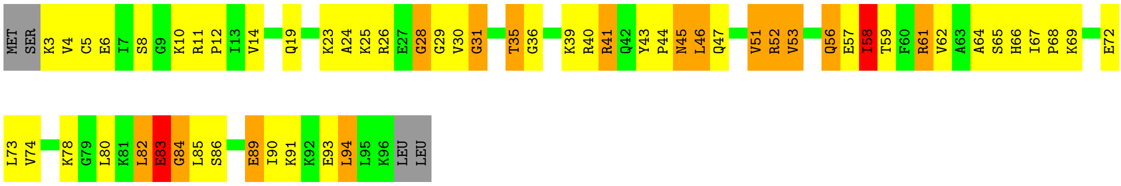
Chain B1:





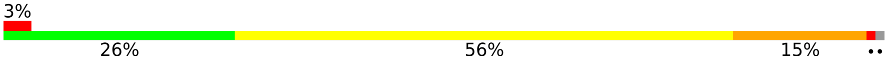
- Molecule 48: 50S RIBOSOMAL PROTEIN L28

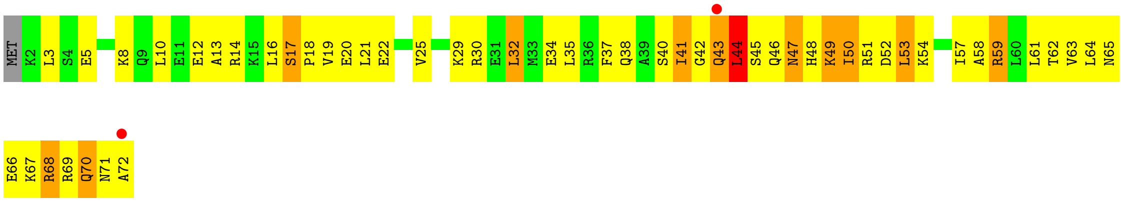
Chain D1:



- Molecule 49: 50S RIBOSOMAL PROTEIN L29

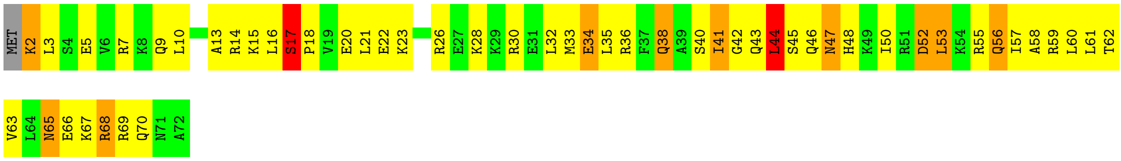
Chain B2:





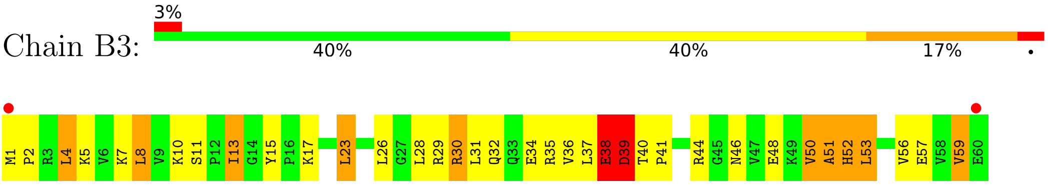
- Molecule 49: 50S RIBOSOMAL PROTEIN L29

Chain D2:



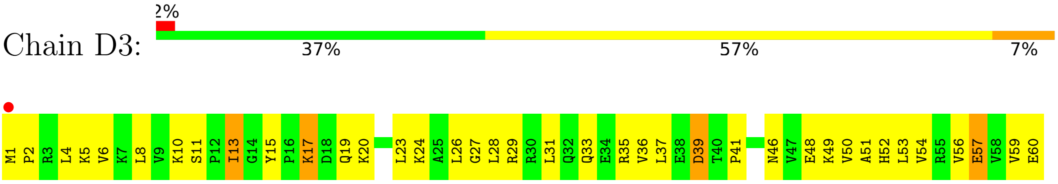
- Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain B3:



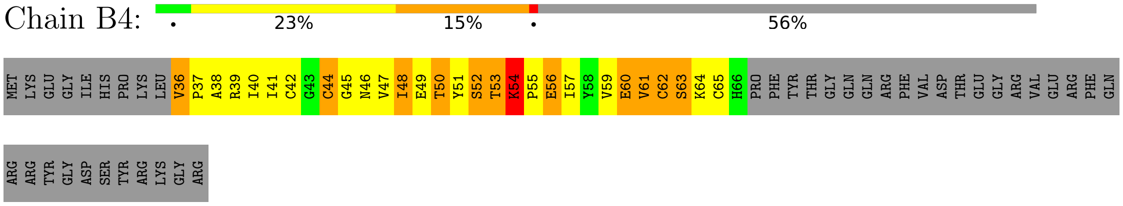
- Molecule 50: 50S RIBOSOMAL PROTEIN L30

Chain D3:



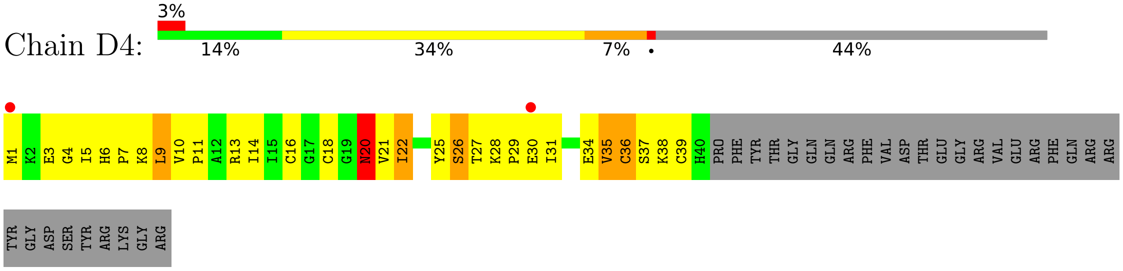
- Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain B4:



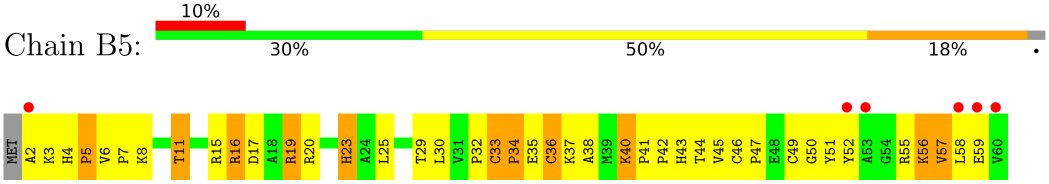
- Molecule 51: 50S RIBOSOMAL PROTEIN L31

Chain D4:



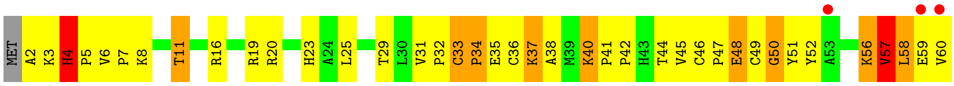
- Molecule 52: 50S RIBOSOMAL PROTEIN L32

Chain B5:

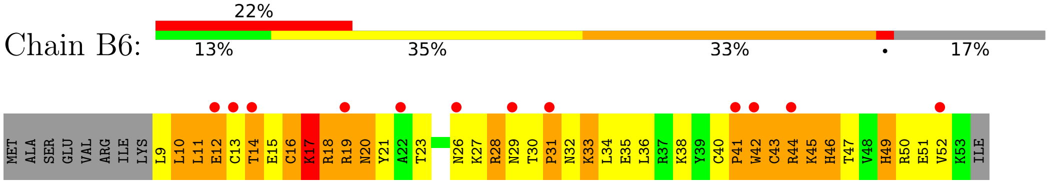


- Molecule 52: 50S RIBOSOMAL PROTEIN L32

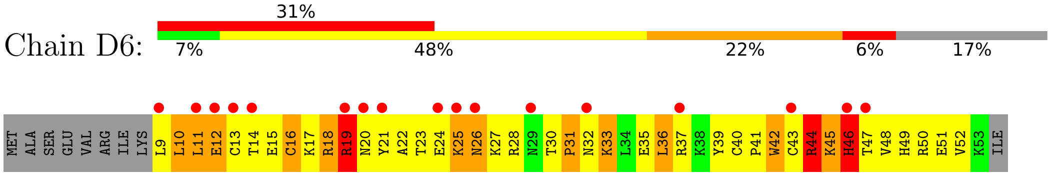
Chain D5:



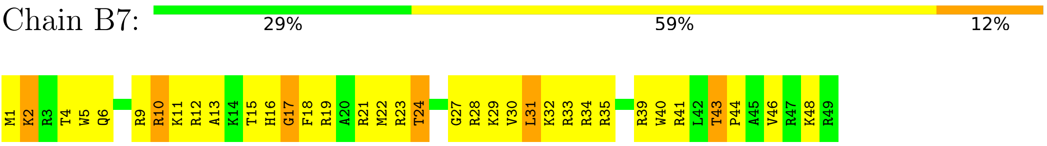
- Molecule 53: 50S RIBOSOMAL PROTEIN L33



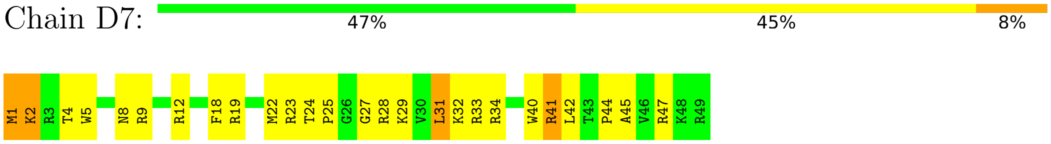
- Molecule 53: 50S RIBOSOMAL PROTEIN L33



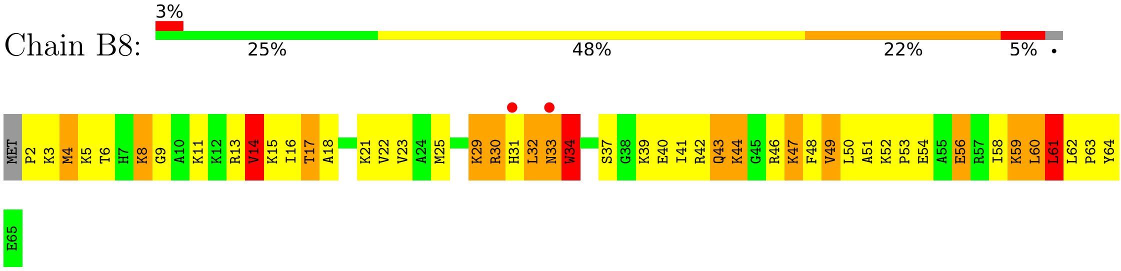
- Molecule 54: 50S RIBOSOMAL PROTEIN L34



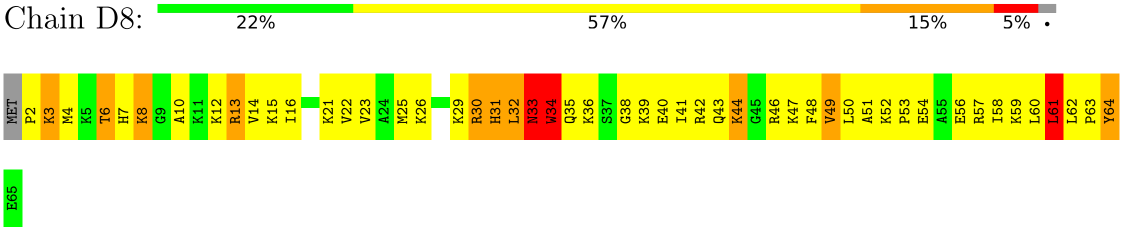
- Molecule 54: 50S RIBOSOMAL PROTEIN L34



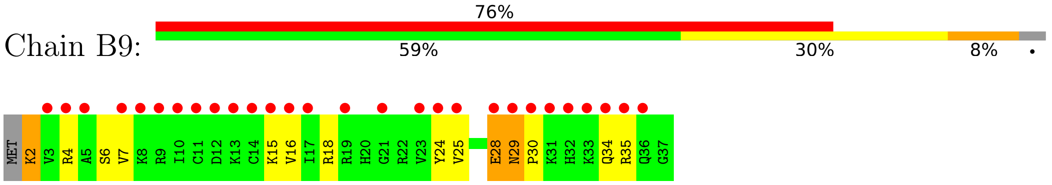
- Molecule 55: 50S RIBOSOMAL PROTEIN L35



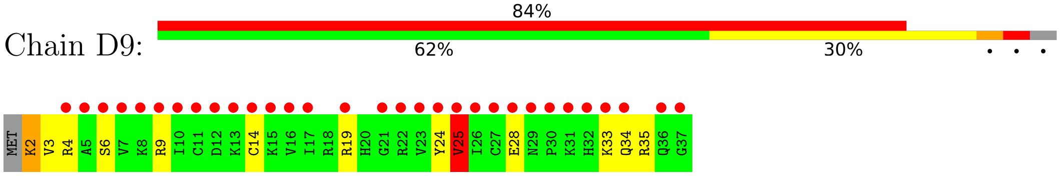
- Molecule 55: 50S RIBOSOMAL PROTEIN L35



- Molecule 56: 50S RIBOSOMAL PROTEIN L36



- Molecule 56: 50S RIBOSOMAL PROTEIN L36



4 Data and refinement statistics

Property	Value
Space group	P 21 21 21
Cell constants a, b, c, α, β, γ	210.46Å 447.34Å 622.30Å 90.00° 90.00° 90.00°
Resolution (Å)	35.07 – 3.52 35.07 – 3.52
% Data completeness (in resolution range)	99.9 (35.07-3.52) 99.9 (35.07-3.52)
R_{merge}	0.44
R_{sym}	0.46
$< I/\sigma(I) >$ [1]	1.81 (at 3.47Å)
Refinement program	PHENIX (phenix.refine: 1.7_641), PHENIX (phenix.refine: 1.8_1069)
R, R_{free}	0.210 , 0.249 0.214 , 0.254
R_{free} test set	32826 reflections (4.56%)
Wilson B-factor (Å^2)	91.1
Anisotropy	0.109
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 80.8
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$
Estimated twinning fraction	No twinning to report.
F_o,F_c correlation	0.91
Total number of atoms	293977
Average B, all atoms (Å^2)	79.0

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, PAR, ZN

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	0.28	0/36189	0.82	11/56484 (0.0%)
1	CA	0.29	0/36189	0.82	14/56484 (0.0%)
2	AB	0.59	0/1936	0.68	0/2611
2	CB	0.67	0/1936	0.77	0/2611
3	AC	0.70	0/1637	0.76	0/2207
3	CC	0.73	0/1637	0.82	0/2207
4	AD	0.69	0/1733	0.80	0/2318
4	CD	0.77	1/1733 (0.1%)	0.85	0/2318
5	AE	0.71	0/1163	0.88	0/1566
5	CE	0.74	0/1163	0.84	0/1566
6	AF	0.73	0/856	0.89	0/1154
6	CF	0.79	0/856	0.82	0/1154
7	AG	0.72	0/1276	0.79	0/1709
7	CG	0.71	0/1276	0.77	0/1709
8	AH	0.69	1/1136 (0.1%)	0.78	0/1527
8	CH	0.73	0/1136	0.80	1/1527 (0.1%)
9	AI	0.71	0/1029	0.80	0/1379
9	CI	0.70	0/1029	0.81	1/1379 (0.1%)
10	AJ	0.70	0/808	0.79	0/1087
10	CJ	0.65	0/808	0.77	0/1087
11	AK	0.67	0/900	0.81	0/1213
11	CK	0.70	0/900	0.82	0/1213
12	AL	0.86	0/987	0.95	0/1322
12	CL	0.92	1/987 (0.1%)	1.01	0/1322
13	AM	0.67	0/999	0.82	0/1338
13	CM	0.48	1/1008 (0.1%)	0.75	1/1347 (0.1%)
14	AN	0.73	0/501	0.83	1/664 (0.2%)
14	CN	0.77	0/501	0.95	0/664
15	AO	0.72	0/745	0.79	0/992
15	CO	0.71	0/745	0.81	0/992
16	AP	0.72	0/717	0.86	0/965
16	CP	0.79	0/717	0.84	0/965

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	AQ	0.69	0/837	0.79	0/1119
17	CQ	0.73	0/837	0.81	0/1119
18	AR	0.69	0/579	0.83	0/768
18	CR	0.76	0/579	0.98	0/768
19	AS	0.66	0/643	0.76	0/867
19	CS	0.80	1/643 (0.2%)	0.86	0/867
20	AT	0.73	0/765	0.77	0/1007
20	CT	0.61	0/765	0.63	0/1007
21	AU	0.73	0/213	0.83	0/279
21	CU	0.75	0/213	0.78	0/279
22	AV	1.13	5/1836 (0.3%)	1.33	13/2859 (0.5%)
22	CV	1.02	0/1835	1.20	13/2859 (0.5%)
23	AW	0.93	3/1809 (0.2%)	1.07	4/2819 (0.1%)
23	AY	1.07	1/408 (0.2%)	1.39	4/634 (0.6%)
23	CW	0.90	0/1809	1.01	0/2819
23	CY	1.15	0/408	1.42	4/634 (0.6%)
24	AX	1.10	1/285 (0.4%)	0.91	2/441 (0.5%)
24	CX	0.96	0/235	1.27	3/364 (0.8%)
25	BA	0.34	1/67788 (0.0%)	0.87	42/105819 (0.0%)
25	DA	0.35	0/68124	0.88	36/106343 (0.0%)
26	BB	0.26	0/2853	0.78	0/4451
26	DB	0.28	0/2853	0.80	0/4451
27	BC	0.65	1/1145 (0.1%)	0.67	0/1556
27	DC	0.24	0/1145	0.46	0/1556
28	BD	0.85	0/2155	0.95	1/2907 (0.0%)
28	DD	0.54	0/2155	0.74	0/2907
29	BE	0.75	0/1597	0.89	0/2155
29	DE	0.49	1/1597 (0.1%)	0.72	0/2155
30	BF	0.80	0/1659	0.87	1/2246 (0.0%)
30	DF	0.49	0/1620	0.76	1/2194 (0.0%)
31	BG	0.70	0/1499	0.78	1/2016 (0.0%)
31	DG	0.42	1/1499 (0.1%)	0.68	1/2016 (0.0%)
32	BH	0.63	0/1246	0.69	0/1684
32	DH	0.40	0/1315	0.79	1/1780 (0.1%)
33	BI	0.67	0/1146	0.81	0/1551
33	DI	0.36	0/1151	0.74	1/1558 (0.1%)
34	BN	0.76	0/1132	0.83	0/1527
34	DN	0.43	0/1132	0.69	0/1527
35	BO	0.76	0/943	0.87	0/1269
35	DO	0.46	0/943	0.68	0/1269
36	BP	0.40	1/1162 (0.1%)	0.78	2/1544 (0.1%)
36	DP	0.39	0/1162	0.76	1/1544 (0.1%)
37	BQ	0.75	0/1143	0.87	0/1527

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
37	DQ	0.48	0/1143	0.65	0/1527
38	BR	0.80	0/974	0.90	1/1302 (0.1%)
38	DR	0.57	1/982 (0.1%)	0.79	2/1312 (0.2%)
39	BS	0.77	0/779	0.90	0/1038
39	DS	0.40	0/892	0.81	1/1187 (0.1%)
40	BT	0.71	0/1156	0.90	1/1544 (0.1%)
40	DT	0.56	1/1156 (0.1%)	0.84	6/1544 (0.4%)
41	BU	0.81	0/982	0.91	1/1306 (0.1%)
41	DU	0.51	0/975	0.75	0/1297
42	BV	0.72	0/790	0.90	1/1057 (0.1%)
42	DV	0.53	1/790 (0.1%)	0.82	0/1057
43	BW	0.81	0/907	0.89	1/1216 (0.1%)
43	DW	0.48	0/907	0.69	1/1216 (0.1%)
44	BX	0.75	0/740	0.89	1/995 (0.1%)
44	DX	0.52	0/740	0.68	0/995
45	BY	0.74	0/789	0.95	2/1053 (0.2%)
45	DY	0.55	2/798 (0.3%)	0.78	0/1064
46	BZ	0.72	0/1436	0.74	1/1951 (0.1%)
46	DZ	0.35	0/1436	0.57	0/1951
47	B0	0.79	1/671 (0.1%)	0.84	0/892
47	D0	0.44	0/671	0.64	0/892
48	B1	0.87	0/739	0.94	0/983
48	D1	0.48	0/739	0.73	0/983
49	B2	0.72	0/600	0.83	0/793
49	D2	0.54	0/600	0.71	0/793
50	B3	0.73	0/473	0.83	0/636
50	D3	0.43	0/473	0.71	0/636
51	B4	0.72	0/229	0.76	0/311
51	D4	0.40	0/303	0.70	0/409
52	B5	0.82	1/473 (0.2%)	0.83	0/639
52	D5	0.44	0/473	0.65	0/639
53	B6	0.67	0/388	0.92	0/520
53	D6	0.30	0/388	0.58	0/520
54	B7	0.88	0/427	0.99	0/563
54	D7	0.54	0/427	0.75	1/563 (0.2%)
55	B8	0.76	0/516	0.91	0/681
55	D8	0.51	0/516	0.82	0/681
56	B9	0.64	0/302	0.59	0/397
56	D9	0.26	0/302	0.46	0/397
All	All	0.48	27/318178 (0.0%)	0.85	180/475682 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
28	BD	0	1

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1453	U	O3'-P	29.98	1.97	1.61
24	AX	14	A	O3'-P	-13.06	1.45	1.61
38	DR	12	ARG	C-N	11.33	1.60	1.34
40	DT	28	VAL	C-N	10.90	1.59	1.34
22	AV	1	C	OP3-P	-9.31	1.50	1.61

The worst 5 of 180 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	BA	1453	U	P-O3'-C3'	-10.66	106.91	119.70
38	DR	12	ARG	O-C-N	9.52	137.93	122.70
36	BP	1	MET	CG-SD-CE	9.44	115.30	100.20
40	DT	28	VAL	O-C-N	8.73	136.67	122.70
40	DT	28	VAL	CA-C-N	-7.49	100.72	117.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	BD	222	ARG	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	32328	0	16317	795	0
1	CA	32328	0	16317	871	1
2	AB	1901	0	1951	245	0
2	CB	1901	0	1951	232	0
3	AC	1613	0	1677	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CC	1613	0	1677	148	0
4	AD	1703	0	1765	191	0
4	CD	1703	0	1764	174	0
5	AE	1147	0	1207	148	0
5	CE	1147	0	1207	159	0
6	AF	843	0	857	87	0
6	CF	843	0	857	63	0
7	AG	1257	0	1296	123	0
7	CG	1257	0	1296	102	0
8	AH	1116	0	1177	111	0
8	CH	1116	0	1177	111	0
9	AI	1010	0	1037	133	0
9	CI	1010	0	1037	144	0
10	AJ	795	0	840	127	0
10	CJ	795	0	840	135	0
11	AK	885	0	904	97	0
11	CK	885	0	904	109	0
12	AL	971	0	1057	126	0
12	CL	971	0	1057	123	0
13	AM	988	0	1059	151	0
13	CM	997	0	1072	164	0
14	AN	492	0	529	87	0
14	CN	492	0	531	69	0
15	AO	734	0	771	61	0
15	CO	734	0	771	51	0
16	AP	701	0	720	62	0
16	CP	701	0	720	101	0
17	AQ	824	0	891	68	0
17	CQ	824	0	891	85	0
18	AR	574	0	644	62	0
18	CR	574	0	644	68	0
19	AS	630	0	652	117	0
19	CS	630	0	652	106	0
20	AT	763	0	861	132	0
20	CT	763	0	861	166	0
21	AU	209	0	221	12	0
21	CU	209	0	221	22	0
22	AV	1644	0	836	110	0
22	CV	1643	0	836	143	0
23	AW	1619	0	822	122	0
23	AY	365	0	185	29	0
23	CW	1619	0	822	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	CY	365	0	185	37	0
24	AX	255	0	129	49	0
24	CX	210	0	109	23	0
25	BA	60527	0	30515	1623	1
25	DA	60827	0	30663	1373	0
26	BB	2551	0	1295	57	1
26	DB	2551	0	1295	55	0
27	BC	1142	0	865	78	0
27	DC	1142	0	865	70	0
28	BD	2105	0	2182	310	0
28	DD	2105	0	2182	277	0
29	BE	1564	0	1629	216	0
29	DE	1564	0	1629	206	0
30	BF	1624	0	1677	246	0
30	DF	1585	0	1632	188	0
31	BG	1474	0	1535	264	0
31	DG	1474	0	1535	209	0
32	BH	1223	0	1282	136	1
32	DH	1290	0	1364	238	0
33	BI	1131	0	1218	152	0
33	DI	1136	0	1223	229	0
34	BN	1105	0	1180	188	0
34	DN	1105	0	1180	140	0
35	BO	933	0	996	117	0
35	DO	933	0	996	90	0
36	BP	1145	0	1228	279	0
36	DP	1145	0	1228	283	3
37	BQ	1122	0	1179	129	0
37	DQ	1122	0	1179	123	0
38	BR	960	0	1021	146	0
38	DR	968	0	1033	109	0
39	BS	771	0	832	127	0
39	DS	882	0	943	149	0
40	BT	1142	0	1202	240	0
40	DT	1142	0	1202	269	0
41	BU	964	0	1022	160	0
41	DU	958	0	1014	198	0
42	BV	779	0	852	135	0
42	DV	779	0	852	150	3
43	BW	896	0	953	104	0
43	DW	896	0	953	89	0
44	BX	726	0	778	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DX	726	0	778	67	0
45	BY	776	0	870	172	0
45	DY	785	0	878	176	0
46	BZ	1404	0	1432	148	0
46	DZ	1404	0	1432	214	0
47	B0	662	0	688	60	0
47	D0	662	0	688	60	0
48	B1	732	0	808	78	0
48	D1	732	0	808	66	0
49	B2	598	0	653	64	0
49	D2	598	0	653	53	0
50	B3	468	0	523	40	3
50	D3	468	0	523	50	0
51	B4	226	0	229	39	0
51	D4	298	0	312	43	0
52	B5	459	0	480	50	0
52	D5	459	0	480	53	3
53	B6	381	0	391	51	0
53	D6	381	0	391	99	0
54	B7	419	0	467	35	0
54	D7	419	0	467	33	0
55	B8	508	0	576	115	0
55	D8	508	0	576	85	0
56	B9	299	0	326	13	0
56	D9	299	0	326	14	0
57	AA	110	0	0	0	0
57	AE	1	0	0	0	0
57	AV	5	0	0	0	0
57	AX	1	0	0	0	0
57	B5	1	0	0	0	0
57	B7	1	0	0	0	0
57	BA	323	0	0	0	0
57	BB	5	0	0	0	0
57	BD	2	0	0	0	0
57	BE	3	0	0	0	0
57	BF	1	0	0	0	0
57	BN	1	0	0	0	0
57	BO	1	0	0	0	0
57	BP	1	0	0	0	0
57	BU	1	0	0	0	0
57	CA	141	0	0	0	0
57	CE	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	CV	5	0	0	0	0
57	CW	1	0	0	0	0
57	CX	1	0	0	0	0
57	CY	1	0	0	0	0
57	D0	2	0	0	0	0
57	D1	2	0	0	0	0
57	D2	1	0	0	0	0
57	D5	2	0	0	0	0
57	D8	1	0	0	0	0
57	DA	397	0	0	0	0
57	DB	5	0	0	0	0
57	DD	3	0	0	0	0
57	DE	2	0	0	0	0
57	DF	1	0	0	0	0
57	DP	3	0	0	0	0
57	DQ	1	0	0	0	0
57	DU	3	0	0	0	0
57	DW	1	0	0	0	0
57	DX	1	0	0	0	0
58	AA	42	0	45	3	0
58	CA	42	0	45	2	0
59	AD	1	0	0	0	0
59	AN	1	0	0	1	0
59	CD	1	0	0	0	0
59	CN	1	0	0	3	0
All	All	293977	0	199058	16442	8

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 34.

The worst 5 of 16442 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)
39:BS:34:HIS:CE1	39:BS:54:LEU:HB2	1.32	1.58
42:DV:1:MET:SD	42:DV:1:MET:CG	2.01	1.47
40:BT:28:VAL:CG1	40:BT:46:GLU:HA	1.42	1.44
1:CA:748:C:H1’	1:CA:749:C:C5	1.53	1.44
34:BN:62:VAL:HG22	34:BN:66:LYS:CD	1.49	1.42

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:B3:1:MET:N	36:DP:122:PRO:CG[3_455]	1.46	0.74
50:B3:1:MET:N	36:DP:122:PRO:CD[3_455]	1.64	0.56
42:DV:50:PRO:CG	52:D5:58:LEU:O[4_445]	1.80	0.40
42:DV:48:GLY:O	52:D5:58:LEU:CD1[4_445]	1.84	0.36
25:BA:1593:G:O2'	26:BB:54:G:OP1[1_655]	2.09	0.11

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AB	233/256 (91%)	159 (68%)	53 (23%)	21 (9%)	1	9
2	CB	233/256 (91%)	158 (68%)	45 (19%)	30 (13%)	0	4
3	AC	205/239 (86%)	129 (63%)	54 (26%)	22 (11%)	0	6
3	CC	205/239 (86%)	135 (66%)	52 (25%)	18 (9%)	1	9
4	AD	206/209 (99%)	142 (69%)	43 (21%)	21 (10%)	0	7
4	CD	206/209 (99%)	141 (68%)	47 (23%)	18 (9%)	1	9
5	AE	149/162 (92%)	117 (78%)	20 (13%)	12 (8%)	1	10
5	CE	149/162 (92%)	113 (76%)	22 (15%)	14 (9%)	0	8
6	AF	99/101 (98%)	63 (64%)	29 (29%)	7 (7%)	1	13
6	CF	99/101 (98%)	80 (81%)	14 (14%)	5 (5%)	2	20
7	AG	153/156 (98%)	116 (76%)	26 (17%)	11 (7%)	1	13
7	CG	153/156 (98%)	117 (76%)	29 (19%)	7 (5%)	2	22
8	AH	136/138 (99%)	96 (71%)	35 (26%)	5 (4%)	3	28
8	CH	136/138 (99%)	102 (75%)	28 (21%)	6 (4%)	2	23
9	AI	125/128 (98%)	84 (67%)	32 (26%)	9 (7%)	1	13
9	CI	125/128 (98%)	87 (70%)	23 (18%)	15 (12%)	0	5
10	AJ	97/105 (92%)	59 (61%)	31 (32%)	7 (7%)	1	13
10	CJ	97/105 (92%)	60 (62%)	25 (26%)	12 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	92 (79%)	19 (16%)	6 (5%)	2	20
11	CK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	9	44
12	AL	123/132 (93%)	78 (63%)	25 (20%)	20 (16%)	0	3
12	CL	123/132 (93%)	91 (74%)	20 (16%)	12 (10%)	0	8
13	AM	123/126 (98%)	82 (67%)	23 (19%)	18 (15%)	0	3
13	CM	123/126 (98%)	78 (63%)	22 (18%)	23 (19%)	0	1
14	AN	58/61 (95%)	40 (69%)	11 (19%)	7 (12%)	0	5
14	CN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	5
15	AO	86/89 (97%)	65 (76%)	20 (23%)	1 (1%)	13	51
15	CO	86/89 (97%)	55 (64%)	25 (29%)	6 (7%)	1	14
16	AP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	2	21
16	CP	82/88 (93%)	66 (80%)	13 (16%)	3 (4%)	3	28
17	AQ	98/105 (93%)	79 (81%)	13 (13%)	6 (6%)	1	16
17	CQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	1	16
18	AR	68/88 (77%)	49 (72%)	12 (18%)	7 (10%)	0	7
18	CR	68/88 (77%)	49 (72%)	11 (16%)	8 (12%)	0	5
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	11
19	CS	77/93 (83%)	47 (61%)	17 (22%)	13 (17%)	0	2
20	AT	97/106 (92%)	68 (70%)	22 (23%)	7 (7%)	1	13
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	0	5
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	1	9
27	BC	183/229 (80%)	85 (46%)	52 (28%)	46 (25%)	0	0
27	DC	183/229 (80%)	87 (48%)	45 (25%)	51 (28%)	0	0
28	BD	270/276 (98%)	200 (74%)	38 (14%)	32 (12%)	0	5
28	DD	270/276 (98%)	202 (75%)	44 (16%)	24 (9%)	1	9
29	BE	203/206 (98%)	145 (71%)	36 (18%)	22 (11%)	0	6
29	DE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	3
30	BF	206/210 (98%)	142 (69%)	44 (21%)	20 (10%)	0	8
30	DF	200/210 (95%)	160 (80%)	29 (14%)	11 (6%)	2	19
31	BG	179/182 (98%)	121 (68%)	36 (20%)	22 (12%)	0	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DG	179/182 (98%)	124 (69%)	30 (17%)	25 (14%)	0	4
32	BH	158/180 (88%)	96 (61%)	37 (23%)	25 (16%)	0	3
32	DH	166/180 (92%)	96 (58%)	42 (25%)	28 (17%)	0	2
33	BI	143/148 (97%)	101 (71%)	26 (18%)	16 (11%)	0	6
33	DI	144/148 (97%)	78 (54%)	39 (27%)	27 (19%)	0	1
34	BN	137/140 (98%)	91 (66%)	24 (18%)	22 (16%)	0	3
34	DN	137/140 (98%)	86 (63%)	39 (28%)	12 (9%)	1	9
35	BO	120/122 (98%)	95 (79%)	17 (14%)	8 (7%)	1	15
35	DO	120/122 (98%)	97 (81%)	18 (15%)	5 (4%)	3	24
36	BP	148/150 (99%)	86 (58%)	26 (18%)	36 (24%)	0	0
36	DP	148/150 (99%)	86 (58%)	23 (16%)	39 (26%)	0	0
37	BQ	139/141 (99%)	104 (75%)	24 (17%)	11 (8%)	1	11
37	DQ	139/141 (99%)	109 (78%)	18 (13%)	12 (9%)	1	9
38	BR	115/118 (98%)	78 (68%)	25 (22%)	12 (10%)	0	7
38	DR	116/118 (98%)	86 (74%)	20 (17%)	10 (9%)	1	9
39	BS	97/112 (87%)	53 (55%)	16 (16%)	28 (29%)	0	0
39	DS	109/112 (97%)	71 (65%)	21 (19%)	17 (16%)	0	3
40	BT	136/146 (93%)	90 (66%)	28 (21%)	18 (13%)	0	4
40	DT	136/146 (93%)	95 (70%)	19 (14%)	22 (16%)	0	3
41	BU	115/118 (98%)	73 (64%)	30 (26%)	12 (10%)	0	7
41	DU	115/118 (98%)	75 (65%)	30 (26%)	10 (9%)	1	9
42	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	3
42	DV	99/101 (98%)	80 (81%)	9 (9%)	10 (10%)	0	7
43	BW	111/113 (98%)	81 (73%)	22 (20%)	8 (7%)	1	13
43	DW	111/113 (98%)	82 (74%)	19 (17%)	10 (9%)	1	9
44	BX	91/96 (95%)	69 (76%)	16 (18%)	6 (7%)	1	15
44	DX	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	2	23
45	BY	99/110 (90%)	50 (50%)	22 (22%)	27 (27%)	0	0
45	DY	100/110 (91%)	64 (64%)	11 (11%)	25 (25%)	0	0
46	BZ	175/206 (85%)	114 (65%)	40 (23%)	21 (12%)	0	5
46	DZ	175/206 (85%)	101 (58%)	46 (26%)	28 (16%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B0	82/85 (96%)	64 (78%)	13 (16%)	5 (6%)	1	16
47	D0	82/85 (96%)	67 (82%)	8 (10%)	7 (8%)	1	10
48	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	0	5
48	D1	92/98 (94%)	69 (75%)	12 (13%)	11 (12%)	0	5
49	B2	69/72 (96%)	49 (71%)	15 (22%)	5 (7%)	1	13
49	D2	69/72 (96%)	57 (83%)	5 (7%)	7 (10%)	0	7
50	B3	58/60 (97%)	48 (83%)	3 (5%)	7 (12%)	0	5
50	D3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	1	9
51	B4	29/71 (41%)	17 (59%)	8 (28%)	4 (14%)	0	4
51	D4	38/71 (54%)	21 (55%)	12 (32%)	5 (13%)	0	4
52	B5	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	1	9
52	D5	57/60 (95%)	46 (81%)	5 (9%)	6 (10%)	0	7
53	B6	43/54 (80%)	17 (40%)	14 (33%)	12 (28%)	0	0
53	D6	43/54 (80%)	18 (42%)	15 (35%)	10 (23%)	0	0
54	B7	47/49 (96%)	38 (81%)	5 (11%)	4 (8%)	1	10
54	D7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	7	39
55	B8	62/65 (95%)	42 (68%)	14 (23%)	6 (10%)	0	8
55	D8	62/65 (95%)	41 (66%)	14 (23%)	7 (11%)	0	6
56	B9	34/37 (92%)	23 (68%)	10 (29%)	1 (3%)	4	33
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	4	33
All	All	11730/12586 (93%)	8097 (69%)	2283 (20%)	1350 (12%)	0	6

5 of 1350 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	195	ASP
2	AB	238	LEU
3	AC	18	TRP
3	AC	20	SER

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%)	161 (80%)	41 (20%)	1	7
2	CB	202/220 (92%)	155 (77%)	47 (23%)	1	4
3	AC	160/188 (85%)	127 (79%)	33 (21%)	1	7
3	CC	160/188 (85%)	130 (81%)	30 (19%)	1	8
4	AD	180/181 (99%)	149 (83%)	31 (17%)	2	12
4	CD	180/181 (99%)	151 (84%)	29 (16%)	2	15
5	AE	115/123 (94%)	97 (84%)	18 (16%)	2	16
5	CE	115/123 (94%)	87 (76%)	28 (24%)	0	4
6	AF	90/90 (100%)	76 (84%)	14 (16%)	2	17
6	CF	90/90 (100%)	79 (88%)	11 (12%)	5	24
7	AG	126/127 (99%)	103 (82%)	23 (18%)	1	9
7	CG	126/127 (99%)	106 (84%)	20 (16%)	2	15
8	AH	119/119 (100%)	101 (85%)	18 (15%)	3	18
8	CH	119/119 (100%)	87 (73%)	32 (27%)	0	3
9	AI	98/99 (99%)	77 (79%)	21 (21%)	1	6
9	CI	98/99 (99%)	72 (74%)	26 (26%)	0	3
10	AJ	88/92 (96%)	66 (75%)	22 (25%)	0	4
10	CJ	88/92 (96%)	66 (75%)	22 (25%)	0	4
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	10
11	CK	90/99 (91%)	72 (80%)	18 (20%)	1	7
12	AL	104/109 (95%)	85 (82%)	19 (18%)	1	9
12	CL	104/109 (95%)	84 (81%)	20 (19%)	1	8
13	AM	99/101 (98%)	82 (83%)	17 (17%)	2	12
13	CM	100/101 (99%)	83 (83%)	17 (17%)	2	12
14	AN	49/50 (98%)	37 (76%)	12 (24%)	0	4
14	CN	49/50 (98%)	38 (78%)	11 (22%)	1	5
15	AO	79/80 (99%)	64 (81%)	15 (19%)	1	8
15	CO	79/80 (99%)	66 (84%)	13 (16%)	2	14
16	AP	72/74 (97%)	58 (81%)	14 (19%)	1	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	58 (81%)	14 (19%)	1	8
17	AQ	94/97 (97%)	86 (92%)	8 (8%)	10	40
17	CQ	94/97 (97%)	82 (87%)	12 (13%)	4	23
18	AR	61/77 (79%)	51 (84%)	10 (16%)	2	14
18	CR	61/77 (79%)	50 (82%)	11 (18%)	1	10
19	AS	69/80 (86%)	51 (74%)	18 (26%)	0	3
19	CS	69/80 (86%)	49 (71%)	20 (29%)	0	3
20	AT	76/82 (93%)	56 (74%)	20 (26%)	0	3
20	CT	76/82 (93%)	53 (70%)	23 (30%)	0	2
21	AU	19/22 (86%)	18 (95%)	1 (5%)	22	56
21	CU	19/22 (86%)	14 (74%)	5 (26%)	0	3
27	BC	61/181 (34%)	49 (80%)	12 (20%)	1	8
27	DC	61/181 (34%)	53 (87%)	8 (13%)	4	22
28	BD	213/218 (98%)	164 (77%)	49 (23%)	1	5
28	DD	213/218 (98%)	178 (84%)	35 (16%)	2	14
29	BE	165/166 (99%)	125 (76%)	40 (24%)	0	4
29	DE	165/166 (99%)	141 (86%)	24 (14%)	3	19
30	BF	165/166 (99%)	127 (77%)	38 (23%)	1	5
30	DF	161/166 (97%)	136 (84%)	25 (16%)	2	17
31	BG	155/156 (99%)	118 (76%)	37 (24%)	0	4
31	DG	155/156 (99%)	135 (87%)	20 (13%)	4	22
32	BH	132/148 (89%)	114 (86%)	18 (14%)	3	21
32	DH	140/148 (95%)	114 (81%)	26 (19%)	1	9
33	BI	122/124 (98%)	95 (78%)	27 (22%)	1	5
33	DI	122/124 (98%)	92 (75%)	30 (25%)	0	4
34	BN	117/119 (98%)	88 (75%)	29 (25%)	0	4
34	DN	117/119 (98%)	96 (82%)	21 (18%)	2	10
35	BO	100/100 (100%)	77 (77%)	23 (23%)	1	5
35	DO	100/100 (100%)	90 (90%)	10 (10%)	7	33
36	BP	116/116 (100%)	86 (74%)	30 (26%)	0	3
36	DP	116/116 (100%)	89 (77%)	27 (23%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	3
37	DQ	111/111 (100%)	92 (83%)	19 (17%)	2	12
38	BR	100/101 (99%)	68 (68%)	32 (32%)	0	2
38	DR	101/101 (100%)	86 (85%)	15 (15%)	3	18
39	BS	77/88 (88%)	56 (73%)	21 (27%)	0	3
39	DS	87/88 (99%)	75 (86%)	12 (14%)	3	21
40	BT	120/127 (94%)	90 (75%)	30 (25%)	0	4
40	DT	120/127 (94%)	91 (76%)	29 (24%)	0	4
41	BU	93/94 (99%)	70 (75%)	23 (25%)	0	4
41	DU	92/94 (98%)	80 (87%)	12 (13%)	4	22
42	BV	82/82 (100%)	55 (67%)	27 (33%)	0	2
42	DV	82/82 (100%)	64 (78%)	18 (22%)	1	5
43	BW	91/92 (99%)	69 (76%)	22 (24%)	0	4
43	DW	91/92 (99%)	83 (91%)	8 (9%)	10	39
44	BX	74/78 (95%)	58 (78%)	16 (22%)	1	6
44	DX	74/78 (95%)	61 (82%)	13 (18%)	2	11
45	BY	84/91 (92%)	67 (80%)	17 (20%)	1	7
45	DY	85/91 (93%)	66 (78%)	19 (22%)	1	5
46	BZ	155/179 (87%)	124 (80%)	31 (20%)	1	7
46	DZ	155/179 (87%)	136 (88%)	19 (12%)	4	24
47	B0	66/67 (98%)	57 (86%)	9 (14%)	3	21
47	D0	66/67 (98%)	57 (86%)	9 (14%)	3	21
48	B1	78/83 (94%)	61 (78%)	17 (22%)	1	5
48	D1	78/83 (94%)	61 (78%)	17 (22%)	1	5
49	B2	66/67 (98%)	53 (80%)	13 (20%)	1	8
49	D2	66/67 (98%)	53 (80%)	13 (20%)	1	8
50	B3	51/52 (98%)	40 (78%)	11 (22%)	1	6
50	D3	51/52 (98%)	49 (96%)	2 (4%)	32	65
51	B4	27/63 (43%)	17 (63%)	10 (37%)	0	1
51	D4	35/63 (56%)	31 (89%)	4 (11%)	5	28
52	B5	51/52 (98%)	42 (82%)	9 (18%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	D5	51/52 (98%)	43 (84%)	8 (16%)	2	16
53	B6	43/52 (83%)	31 (72%)	12 (28%)	0	3
53	D6	43/52 (83%)	33 (77%)	10 (23%)	1	4
54	B7	41/42 (98%)	35 (85%)	6 (15%)	3	19
54	D7	41/42 (98%)	37 (90%)	4 (10%)	8	34
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	3
55	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
56	B9	33/34 (97%)	29 (88%)	4 (12%)	5	25
56	D9	33/34 (97%)	29 (88%)	4 (12%)	5	25
All	All	9688/10428 (93%)	7777 (80%)	1911 (20%)	1	8

5 of 1911 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
47	B0	43	THR
43	DW	70	TYR
5	CE	71	LEU
42	DV	32	THR
54	D7	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 115 such sidechains are listed below:

Mol	Chain	Res	Type
8	CH	82	HIS
50	D3	52	HIS
28	DD	201	HIS
50	D3	19	GLN
43	DW	61	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	366 (24%)	109 (7%)
1	CA	1503/1522 (98%)	359 (23%)	115 (7%)
22	AV	76/77 (98%)	26 (34%)	3 (3%)
22	CV	76/77 (98%)	30 (39%)	4 (5%)
23	AW	75/76 (98%)	22 (29%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
23	AY	16/76 (21%)	5 (31%)	0
23	CW	75/76 (98%)	26 (34%)	0
23	CY	16/76 (21%)	8 (50%)	0
24	AX	11/24 (45%)	4 (36%)	0
24	CX	9/24 (37%)	4 (44%)	1 (11%)
25	BA	2804/2915 (96%)	803 (28%)	260 (9%)
25	DA	2818/2915 (96%)	804 (28%)	264 (9%)
26	BB	118/122 (96%)	25 (21%)	5 (4%)
26	DB	118/122 (96%)	24 (20%)	7 (5%)
All	All	9218/9624 (95%)	2506 (27%)	768 (8%)

5 of 2506 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	6	G
1	AA	8	A
1	AA	9	G
1	AA	10	A
1	AA	13	U

5 of 768 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1101	A
25	DA	776	G
1	CA	1302	U
1	CA	1085	U
25	DA	241	A

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1039 ligands modelled in this entry, 1037 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	PAR	CA	1741	-	45,45,45	1.55	8 (17%)	64,67,67	1.18	5 (7%)
58	PAR	AA	7111	-	45,45,45	1.54	9 (20%)	64,67,67	1.18	4 (6%)

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
58	PAR	CA	1741	-	-	3/18/94/94	0/4/4/4
58	PAR	AA	7111	-	-	3/18/94/94	0/4/4/4

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	CA	1741	PAR	C64-C54	3.95	1.57	1.52
58	AA	7111	PAR	O54-C14	3.93	1.51	1.41
58	CA	1741	PAR	O54-C14	3.91	1.51	1.41
58	AA	7111	PAR	C64-C54	3.90	1.57	1.52
58	CA	1741	PAR	C31-C21	3.20	1.57	1.53

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	AA	7111	PAR	O33-C14-C24	3.35	113.99	108.22
58	CA	1741	PAR	O33-C14-C24	3.31	113.91	108.22
58	CA	1741	PAR	C14-O54-C54	3.22	120.01	113.69
58	AA	7111	PAR	C14-O54-C54	3.22	120.01	113.69
58	AA	7111	PAR	O54-C54-C64	3.22	112.00	106.01

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	AA	7111	PAR	C24-C14-O33-C33
58	CA	1741	PAR	C24-C14-O33-C33
58	AA	7111	PAR	C52-C42-O11-C11
58	CA	1741	PAR	C52-C42-O11-C11
58	AA	7111	PAR	C23-C13-O52-C52

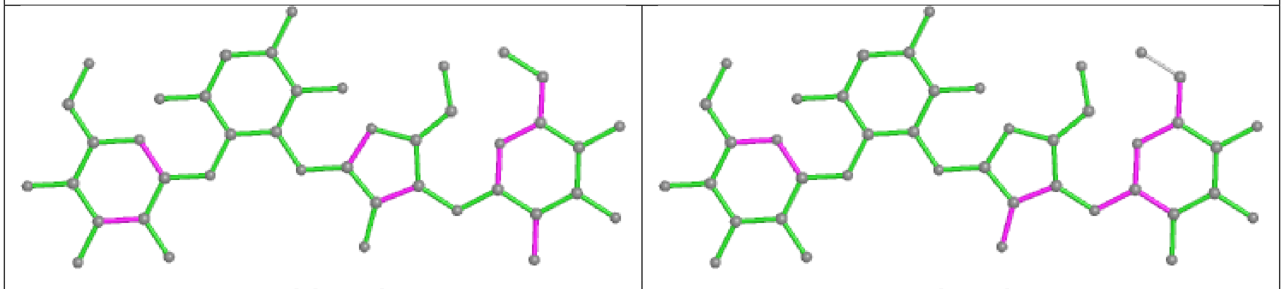
There are no ring outliers.

2 monomers are involved in 5 short contacts:

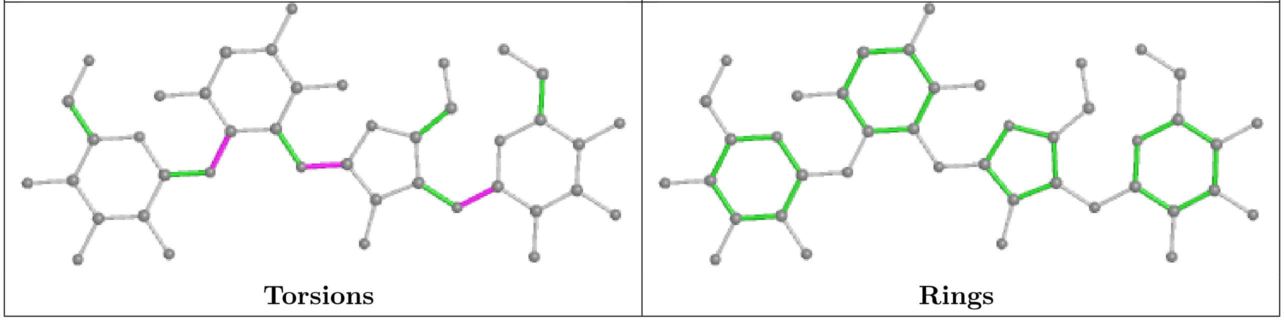
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	CA	1741	PAR	2	0
58	AA	7111	PAR	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PAR CA 1741

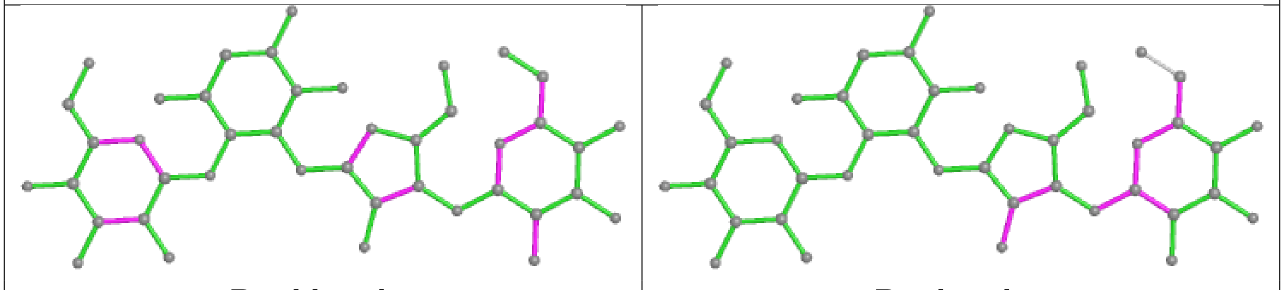


Bond lengths **Bond angles**



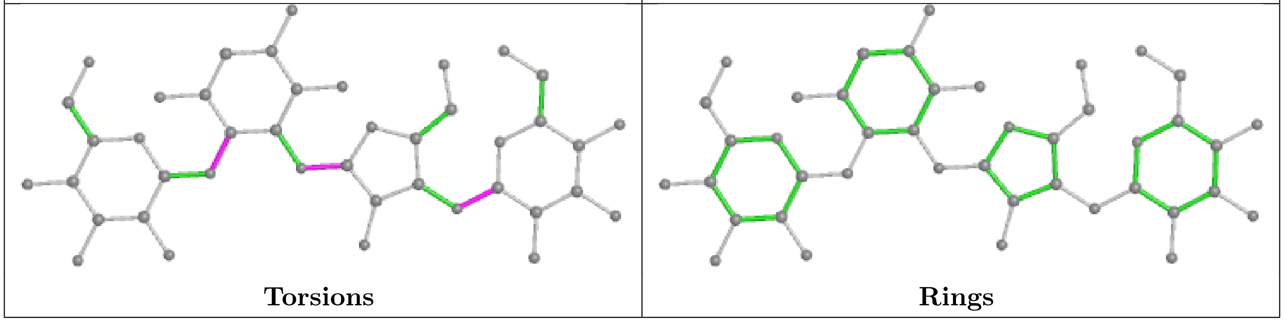
Torsions **Rings**

Ligand PAR AA 7111



Bond lengths

Bond angles



Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
25	BA	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	BA	1453:U	O3’	1455:G	P	1.97

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	AA	1504/1522 (98%)	0.18	46 (3%)	49	36	31, 78, 168, 331	0
1	CA	1504/1522 (98%)	0.21	58 (3%)	39	29	24, 68, 165, 363	0
2	AB	235/256 (91%)	-0.08	4 (1%)	70	57	67, 121, 201, 279	0
2	CB	235/256 (91%)	-0.10	9 (3%)	40	30	44, 109, 202, 287	0
3	AC	207/239 (86%)	-0.13	1 (0%)	91	84	44, 104, 173, 240	0
3	CC	207/239 (86%)	-0.21	1 (0%)	91	84	38, 90, 151, 227	0
4	AD	208/209 (99%)	-0.29	3 (1%)	75	62	37, 89, 153, 217	0
4	CD	208/209 (99%)	-0.31	1 (0%)	91	84	30, 77, 129, 209	0
5	AE	151/162 (93%)	-0.24	2 (1%)	77	65	44, 87, 151, 240	0
5	CE	151/162 (93%)	-0.24	2 (1%)	77	65	22, 71, 131, 266	0
6	AF	101/101 (100%)	-0.20	0	100	100	29, 74, 120, 178	0
6	CF	101/101 (100%)	-0.30	0	100	100	25, 68, 134, 192	0
7	AG	155/156 (99%)	-0.15	7 (4%)	33	24	50, 93, 149, 256	0
7	CG	155/156 (99%)	-0.14	5 (3%)	47	36	32, 87, 151, 269	0
8	AH	138/138 (100%)	-0.28	0	100	100	41, 85, 129, 183	0
8	CH	138/138 (100%)	-0.34	1 (0%)	87	79	38, 75, 123, 181	0
9	AI	127/128 (99%)	0.02	3 (2%)	59	45	55, 113, 161, 319	0
9	CI	127/128 (99%)	-0.06	3 (2%)	59	45	45, 97, 170, 245	0
10	AJ	99/105 (94%)	0.29	4 (4%)	38	28	58, 124, 197, 302	0
10	CJ	99/105 (94%)	0.26	5 (5%)	28	20	38, 115, 191, 204	0
11	AK	119/129 (92%)	-0.12	4 (3%)	45	34	41, 77, 147, 249	0
11	CK	119/129 (92%)	-0.06	3 (2%)	57	43	29, 73, 139, 188	0
12	AL	125/132 (94%)	-0.15	3 (2%)	59	45	31, 64, 129, 300	0
12	CL	125/132 (94%)	-0.29	3 (2%)	59	45	9, 47, 127, 252	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	AM	125/126 (99%)	0.03	4 (3%)	47	36	29, 94, 148, 314	0
13	CM	125/126 (99%)	0.08	6 (4%)	30	23	39, 87, 174, 274	0
14	AN	60/61 (98%)	-0.06	1 (1%)	70	57	53, 92, 138, 207	0
14	CN	60/61 (98%)	-0.12	0	100	100	34, 71, 111, 194	0
15	AO	88/89 (98%)	-0.28	0	100	100	35, 80, 132, 142	0
15	CO	88/89 (98%)	-0.33	0	100	100	23, 69, 122, 147	0
16	AP	84/88 (95%)	-0.43	0	100	100	48, 74, 122, 182	0
16	CP	84/88 (95%)	-0.30	0	100	100	44, 76, 139, 200	0
17	AQ	100/105 (95%)	-0.22	0	100	100	50, 91, 141, 174	0
17	CQ	100/105 (95%)	-0.18	1 (1%)	82	71	38, 87, 144, 192	0
18	AR	70/88 (79%)	-0.21	3 (4%)	35	26	35, 77, 126, 182	0
18	CR	70/88 (79%)	-0.35	1 (1%)	75	62	36, 70, 122, 205	0
19	AS	79/93 (84%)	0.13	1 (1%)	77	65	46, 104, 202, 268	0
19	CS	79/93 (84%)	0.08	0	100	100	27, 82, 153, 206	0
20	AT	99/106 (93%)	0.06	5 (5%)	28	20	42, 90, 173, 211	0
20	CT	99/106 (93%)	0.13	3 (3%)	50	37	40, 97, 192, 295	0
21	AU	25/27 (92%)	0.72	5 (20%)	1	1	36, 92, 165, 229	0
21	CU	25/27 (92%)	-0.03	0	100	100	50, 78, 107, 150	0
22	AV	77/77 (100%)	0.10	0	100	100	45, 82, 163, 276	0
22	CV	77/77 (100%)	0.19	3 (3%)	39	29	32, 72, 133, 253	0
23	AW	76/76 (100%)	1.27	17 (22%)	0	0	48, 175, 249, 317	0
23	AY	17/76 (22%)	0.41	0	100	100	64, 94, 167, 176	0
23	CW	76/76 (100%)	1.63	24 (31%)	0	0	34, 184, 271, 295	0
23	CY	17/76 (22%)	0.69	0	100	100	44, 75, 149, 186	0
24	AX	12/24 (50%)	0.73	2 (16%)	1	1	49, 74, 217, 234	0
24	CX	10/24 (41%)	0.55	1 (10%)	7	6	42, 58, 144, 213	0
25	BA	2810/2915 (96%)	0.18	115 (4%)	37	27	17, 58, 187, 375	0
25	DA	2824/2915 (96%)	0.11	106 (3%)	40	30	6, 42, 178, 370	0
26	BB	119/122 (97%)	0.17	1 (0%)	86	75	59, 94, 132, 182	0
26	DB	119/122 (97%)	0.12	2 (1%)	70	57	38, 68, 113, 174	0
27	BC	191/229 (83%)	1.88	74 (38%)	0	0	89, 200, 319, 378	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
27	DC	191/229 (83%)	2.28	93 (48%)	0	0	64, 208, 290, 334	0
28	BD	272/276 (98%)	-0.40	0	100	100	9, 45, 89, 166	0
28	DD	272/276 (98%)	-0.49	0	100	100	3, 33, 80, 197	0
29	BE	205/206 (99%)	-0.23	5 (2%)	59	45	17, 66, 128, 289	0
29	DE	205/206 (99%)	-0.23	4 (1%)	65	52	11, 55, 160, 338	0
30	BF	208/210 (99%)	-0.36	4 (1%)	66	53	14, 64, 164, 286	0
30	DF	202/210 (96%)	-0.32	2 (0%)	82	71	5, 51, 127, 208	0
31	BG	181/182 (99%)	-0.18	6 (3%)	46	35	40, 95, 175, 268	0
31	DG	181/182 (99%)	-0.18	4 (2%)	62	48	25, 76, 143, 219	0
32	BH	160/180 (88%)	0.89	31 (19%)	1	1	85, 179, 331, 429	0
32	DH	168/180 (93%)	0.02	1 (0%)	89	81	29, 81, 155, 234	0
33	BI	145/148 (97%)	-0.13	5 (3%)	45	34	33, 96, 156, 184	0
33	DI	146/148 (98%)	-0.07	1 (0%)	87	79	15, 104, 166, 207	0
34	BN	139/140 (99%)	-0.30	1 (0%)	87	79	36, 79, 147, 305	0
34	DN	139/140 (99%)	-0.34	0	100	100	7, 61, 137, 185	0
35	BO	122/122 (100%)	-0.50	0	100	100	32, 65, 97, 124	0
35	DO	122/122 (100%)	-0.61	0	100	100	10, 41, 84, 112	0
36	BP	150/150 (100%)	0.30	5 (3%)	46	35	27, 87, 179, 250	0
36	DP	150/150 (100%)	0.07	3 (2%)	65	52	23, 71, 151, 264	0
37	BQ	141/141 (100%)	-0.24	3 (2%)	63	50	36, 74, 126, 421	0
37	DQ	141/141 (100%)	-0.40	0	100	100	12, 52, 108, 281	0
38	BR	117/118 (99%)	-0.42	0	100	100	21, 57, 107, 148	0
38	DR	118/118 (100%)	-0.47	0	100	100	15, 50, 92, 126	0
39	BS	99/112 (88%)	-0.17	1 (1%)	82	71	38, 100, 171, 347	0
39	DS	111/112 (99%)	-0.13	2 (1%)	68	55	33, 73, 147, 197	0
40	BT	138/146 (94%)	-0.04	6 (4%)	35	26	29, 80, 225, 351	0
40	DT	138/146 (94%)	-0.05	8 (5%)	23	17	20, 71, 212, 304	0
41	BU	117/118 (99%)	-0.40	1 (0%)	84	73	29, 64, 131, 281	0
41	DU	117/118 (99%)	-0.51	1 (0%)	84	73	17, 52, 114, 180	0
42	BV	101/101 (100%)	-0.28	0	100	100	23, 90, 149, 344	0
42	DV	101/101 (100%)	-0.12	1 (0%)	82	71	9, 70, 131, 303	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
43	BW	113/113 (100%)	-0.23	2 (1%) 68 55	19, 49, 113, 319	0
43	DW	113/113 (100%)	-0.32	0 100 100	14, 42, 128, 204	0
44	BX	93/96 (96%)	-0.34	0 100 100	30, 63, 99, 149	0
44	DX	93/96 (96%)	-0.33	0 100 100	12, 42, 87, 144	0
45	BY	101/110 (91%)	0.88	20 (19%) 1 1	42, 92, 253, 363	0
45	DY	102/110 (92%)	0.06	3 (2%) 51 38	28, 82, 182, 226	0
46	BZ	177/206 (85%)	0.41	17 (9%) 8 6	45, 125, 202, 316	0
46	DZ	177/206 (85%)	0.54	18 (10%) 6 6	29, 116, 254, 322	0
47	B0	84/85 (98%)	-0.03	6 (7%) 16 13	31, 69, 170, 242	0
47	D0	84/85 (98%)	-0.08	7 (8%) 11 10	18, 52, 136, 286	0
48	B1	94/98 (95%)	-0.18	1 (1%) 80 69	17, 53, 113, 219	0
48	D1	94/98 (95%)	-0.31	0 100 100	7, 44, 122, 237	0
49	B2	71/72 (98%)	-0.24	2 (2%) 53 40	35, 77, 128, 195	0
49	D2	71/72 (98%)	-0.23	0 100 100	14, 54, 137, 267	0
50	B3	60/60 (100%)	-0.03	2 (3%) 46 35	35, 75, 125, 382	0
50	D3	60/60 (100%)	-0.25	1 (1%) 70 57	20, 65, 142, 236	0
51	B4	31/71 (43%)	-0.16	0 100 100	67, 121, 152, 204	0
51	D4	40/71 (56%)	0.07	2 (5%) 28 21	55, 116, 173, 266	0
52	B5	59/60 (98%)	0.15	6 (10%) 6 6	17, 72, 180, 340	0
52	D5	59/60 (98%)	0.16	3 (5%) 28 20	12, 63, 214, 299	0
53	B6	45/54 (83%)	1.21	12 (26%) 0 0	44, 138, 207, 343	0
53	D6	45/54 (83%)	1.82	17 (37%) 0 0	59, 139, 235, 285	0
54	B7	49/49 (100%)	-0.41	0 100 100	11, 41, 123, 149	0
54	D7	49/49 (100%)	-0.59	0 100 100	1, 23, 101, 204	0
55	B8	64/65 (98%)	-0.05	2 (3%) 49 36	20, 60, 129, 325	0
55	D8	64/65 (98%)	-0.38	0 100 100	12, 51, 115, 172	0
56	B9	36/37 (97%)	3.56	28 (77%) 0 0	120, 197, 269, 389	0
56	D9	36/37 (97%)	3.45	31 (86%) 0 0	115, 172, 217, 282	0
All	All	21184/22210 (95%)	0.06	911 (4%) 35 26	1, 71, 192, 429	0

The worst 5 of 911 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
25	DA	2802	G	15.7
25	BA	2802	G	13.6
1	AA	81	U	13.5
1	AA	89	C	12.6
23	CW	20	U	12.5

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
57	MG	BA	3315	1/1	0.16	0.44	84,84,84,84	0
57	MG	DA	9655	1/1	0.37	0.92	35,35,35,35	0
57	MG	DA	9350	1/1	0.44	0.18	48,48,48,48	1
57	MG	BA	3149	1/1	0.47	0.34	27,27,27,27	0
57	MG	BA	3036	1/1	0.47	0.19	78,78,78,78	1
57	MG	BA	3037	1/1	0.49	0.27	83,83,83,83	0
57	MG	BA	3126	1/1	0.49	0.61	44,44,44,44	0
57	MG	CA	1687	1/1	0.52	0.36	47,47,47,47	0
57	MG	BA	3122	1/1	0.55	0.30	13,13,13,13	0
57	MG	AA	7086	1/1	0.57	1.00	30,30,30,30	0
57	MG	DA	9626	1/1	0.57	0.19	8,8,8,8	1
57	MG	BA	3271	1/1	0.57	0.73	52,52,52,52	0
57	MG	DA	9661	1/1	0.57	0.38	57,57,57,57	0
57	MG	CA	1639	1/1	0.58	0.69	55,55,55,55	0
57	MG	BA	3227	1/1	0.58	0.72	40,40,40,40	0
57	MG	DA	9429	1/1	0.60	0.97	51,51,51,51	0
57	MG	CA	1702	1/1	0.61	0.14	49,49,49,49	0
57	MG	BB	205	1/1	0.61	0.11	19,19,19,19	1
57	MG	CA	1699	1/1	0.61	0.40	45,45,45,45	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3273	1/1	0.63	0.26	71,71,71,71	0
57	MG	BA	3248	1/1	0.63	0.70	49,49,49,49	0
57	MG	BA	3063	1/1	0.63	0.47	55,55,55,55	0
57	MG	CA	1651	1/1	0.64	0.44	39,39,39,39	0
57	MG	BA	3277	1/1	0.64	0.56	2,2,2,2	1
57	MG	AA	7002	1/1	0.64	0.48	35,35,35,35	0
57	MG	BA	3216	1/1	0.65	0.50	48,48,48,48	0
57	MG	CA	1683	1/1	0.65	0.26	29,29,29,29	0
57	MG	DA	9685	1/1	0.65	0.64	22,22,22,22	0
57	MG	BA	3306	1/1	0.66	0.47	48,48,48,48	0
57	MG	CA	1609	1/1	0.66	0.42	30,30,30,30	0
57	MG	CA	1621	1/1	0.66	0.38	52,52,52,52	0
57	MG	AA	7076	1/1	0.66	0.57	60,60,60,60	0
57	MG	BB	203	1/1	0.66	0.69	16,16,16,16	1
57	MG	D1	101	1/1	0.66	0.60	55,55,55,55	0
57	MG	DA	9440	1/1	0.67	0.49	25,25,25,25	0
57	MG	DA	9687	1/1	0.67	0.29	12,12,12,12	0
57	MG	CA	1704	1/1	0.67	0.99	28,28,28,28	0
57	MG	DA	9595	1/1	0.68	0.58	49,49,49,49	0
57	MG	AA	7055	1/1	0.68	0.46	29,29,29,29	0
57	MG	CA	1658	1/1	0.68	0.34	44,44,44,44	0
57	MG	CA	1723	1/1	0.68	0.34	15,15,15,15	0
57	MG	BA	3120	1/1	0.68	0.64	24,24,24,24	0
57	MG	BA	3203	1/1	0.68	0.45	37,37,37,37	0
57	MG	BA	3028	1/1	0.68	0.54	44,44,44,44	0
57	MG	BA	3313	1/1	0.69	0.26	42,42,42,42	0
57	MG	DA	9657	1/1	0.69	0.32	29,29,29,29	0
57	MG	BA	3039	1/1	0.69	0.39	30,30,30,30	0
57	MG	DA	9622	1/1	0.70	0.55	36,36,36,36	0
57	MG	DA	9624	1/1	0.70	0.23	18,18,18,18	1
57	MG	AA	7046	1/1	0.70	0.43	35,35,35,35	0
57	MG	CA	1731	1/1	0.70	0.15	30,30,30,30	0
57	MG	BA	3076	1/1	0.70	0.22	18,18,18,18	0
57	MG	AA	7071	1/1	0.70	0.52	38,38,38,38	0
57	MG	DA	9665	1/1	0.70	0.99	9,9,9,9	0
57	MG	DA	9434	1/1	0.70	0.45	4,4,4,4	0
57	MG	BA	3052	1/1	0.70	0.46	40,40,40,40	0
57	MG	CA	1708	1/1	0.70	0.67	34,34,34,34	0
57	MG	DA	9416	1/1	0.71	0.33	38,38,38,38	0
57	MG	CA	1691	1/1	0.71	0.69	91,91,91,91	0
57	MG	BA	3074	1/1	0.71	0.62	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	BA	3245	1/1	0.71	0.72	45,45,45,45	0
57	MG	DA	9559	1/1	0.71	0.55	58,58,58,58	0
57	MG	BA	3278	1/1	0.71	0.40	22,22,22,22	0
57	MG	DA	9395	1/1	0.71	0.24	29,29,29,29	0
57	MG	DA	9405	1/1	0.71	0.29	5,5,5,5	0
57	MG	CA	1716	1/1	0.72	0.46	26,26,26,26	0
57	MG	AA	7097	1/1	0.72	0.46	20,20,20,20	0
57	MG	AA	7080	1/1	0.72	0.43	8,8,8,8	1
57	MG	DA	9329	1/1	0.72	0.50	21,21,21,21	0
57	MG	CA	1674	1/1	0.72	0.40	89,89,89,89	0
57	MG	DA	9388	1/1	0.72	0.18	28,28,28,28	0
57	MG	CA	1637	1/1	0.72	0.34	57,57,57,57	0
57	MG	BA	3262	1/1	0.72	0.64	39,39,39,39	0
57	MG	BA	3173	1/1	0.73	0.62	27,27,27,27	0
57	MG	BA	3110	1/1	0.73	0.59	23,23,23,23	1
57	MG	BA	3119	1/1	0.73	0.32	42,42,42,42	0
57	MG	CA	1612	1/1	0.73	0.30	31,31,31,31	0
57	MG	DA	9550	1/1	0.73	0.44	55,55,55,55	0
57	MG	AA	7010	1/1	0.73	0.26	30,30,30,30	0
57	MG	DA	9674	1/1	0.73	0.81	17,17,17,17	0
57	MG	DA	9569	1/1	0.73	0.82	54,54,54,54	0
57	MG	CA	1713	1/1	0.73	0.54	31,31,31,31	0
57	MG	BA	3242	1/1	0.73	0.59	44,44,44,44	0
57	MG	DA	9467	1/1	0.74	0.39	53,53,53,53	1
57	MG	BA	3246	1/1	0.74	0.66	33,33,33,33	0
57	MG	DA	9432	1/1	0.74	0.63	38,38,38,38	0
57	MG	BA	3318	1/1	0.74	0.41	37,37,37,37	0
57	MG	CA	1714	1/1	0.74	0.45	53,53,53,53	0
57	MG	DA	9694	1/1	0.74	0.85	25,25,25,25	0
57	MG	DA	9658	1/1	0.74	0.19	36,36,36,36	0
57	MG	AA	7092	1/1	0.75	0.13	37,37,37,37	0
57	MG	DA	9412	1/1	0.75	0.34	27,27,27,27	0
57	MG	CA	1739	1/1	0.75	0.67	36,36,36,36	0
57	MG	BA	3196	1/1	0.75	0.76	30,30,30,30	0
57	MG	CA	1672	1/1	0.75	0.39	62,62,62,62	0
57	MG	BP	201	1/1	0.75	0.20	166,166,166,166	0
57	MG	AA	7074	1/1	0.75	0.76	26,26,26,26	0
57	MG	DA	9648	1/1	0.75	0.30	34,34,34,34	0
57	MG	DA	9399	1/1	0.75	0.78	52,52,52,52	0
57	MG	AA	7065	1/1	0.76	0.38	23,23,23,23	0
57	MG	CA	1682	1/1	0.76	0.27	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	9563	1/1	0.76	0.26	3,3,3,3	0
57	MG	DA	9628	1/1	0.76	0.28	35,35,35,35	1
57	MG	DA	9643	1/1	0.76	0.72	34,34,34,34	1
57	MG	BA	3155	1/1	0.76	0.56	33,33,33,33	0
57	MG	DA	9573	1/1	0.76	0.40	45,45,45,45	0
57	MG	BA	3290	1/1	0.76	0.76	19,19,19,19	1
57	MG	CA	1642	1/1	0.77	0.38	54,54,54,54	0
57	MG	DA	9645	1/1	0.77	0.72	4,4,4,4	0
57	MG	BA	3003	1/1	0.77	0.33	33,33,33,33	0
57	MG	BA	3095	1/1	0.77	1.02	35,35,35,35	0
57	MG	CA	1666	1/1	0.77	0.36	66,66,66,66	0
57	MG	CV	103	1/1	0.77	0.33	43,43,43,43	1
57	MG	BA	3257	1/1	0.77	0.31	21,21,21,21	0
57	MG	DA	9602	1/1	0.77	0.52	37,37,37,37	0
57	MG	DA	9671	1/1	0.77	0.19	45,45,45,45	0
57	MG	DA	9615	1/1	0.77	0.70	45,45,45,45	0
57	MG	DA	9677	1/1	0.77	0.50	27,27,27,27	0
57	MG	BA	3320	1/1	0.77	0.42	54,54,54,54	0
57	MG	DA	9438	1/1	0.77	0.38	21,21,21,21	0
57	MG	BA	3026	1/1	0.77	0.50	29,29,29,29	0
57	MG	AA	7069	1/1	0.77	0.76	11,11,11,11	1
57	MG	BA	3301	1/1	0.78	0.27	20,20,20,20	0
57	MG	CA	1722	1/1	0.78	0.34	27,27,27,27	0
57	MG	DA	9378	1/1	0.78	0.35	29,29,29,29	0
57	MG	BA	3082	1/1	0.78	0.32	23,23,23,23	0
57	MG	CA	1728	1/1	0.78	0.35	59,59,59,59	0
57	MG	BA	3164	1/1	0.78	0.43	39,39,39,39	0
57	MG	DA	9603	1/1	0.78	0.88	33,33,33,33	0
57	MG	BA	3286	1/1	0.78	0.25	22,22,22,22	0
57	MG	BA	3107	1/1	0.78	0.45	36,36,36,36	0
57	MG	DA	9441	1/1	0.79	0.58	31,31,31,31	1
57	MG	DA	9450	1/1	0.79	0.54	2,2,2,2	1
57	MG	DA	9458	1/1	0.79	0.41	22,22,22,22	0
57	MG	BA	3295	1/1	0.79	0.37	27,27,27,27	0
57	MG	BA	3317	1/1	0.79	0.73	21,21,21,21	0
57	MG	DA	9552	1/1	0.79	0.53	58,58,58,58	0
57	MG	CA	1694	1/1	0.79	0.72	51,51,51,51	0
57	MG	CA	1610	1/1	0.79	0.63	58,58,58,58	0
57	MG	BA	3297	1/1	0.79	0.93	46,46,46,46	0
57	MG	DA	9660	1/1	0.79	0.27	176,176,176,176	0
57	MG	DA	9570	1/1	0.79	0.31	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	7027	1/1	0.79	0.41	28,28,28,28	0
57	MG	CA	1706	1/1	0.79	0.36	32,32,32,32	0
57	MG	DA	9600	1/1	0.79	0.34	55,55,55,55	0
57	MG	DA	9676	1/1	0.79	0.23	13,13,13,13	0
57	MG	CA	1628	1/1	0.79	0.22	9,9,9,9	0
57	MG	DA	9336	1/1	0.79	0.33	52,52,52,52	0
57	MG	BA	3117	1/1	0.79	0.67	11,11,11,11	1
57	MG	DA	9620	1/1	0.79	0.41	26,26,26,26	0
57	MG	BA	3266	1/1	0.79	0.39	33,33,33,33	0
59	ZN	CN	101	1/1	0.79	0.19	171,171,171,171	0
57	MG	AA	7008	1/1	0.80	0.85	35,35,35,35	0
57	MG	BA	3108	1/1	0.80	0.25	27,27,27,27	0
57	MG	AX	101	1/1	0.80	0.28	43,43,43,43	0
57	MG	AA	7082	1/1	0.80	0.28	24,24,24,24	0
57	MG	BA	3274	1/1	0.80	0.26	8,8,8,8	1
57	MG	DA	9557	1/1	0.80	0.31	25,25,25,25	0
57	MG	DA	9419	1/1	0.80	0.95	10,10,10,10	1
57	MG	DA	9331	1/1	0.80	0.21	8,8,8,8	0
57	MG	DA	9681	1/1	0.80	0.35	13,13,13,13	0
57	MG	BA	3021	1/1	0.80	0.49	49,49,49,49	0
57	MG	CA	1692	1/1	0.80	0.37	28,28,28,28	0
57	MG	AA	7096	1/1	0.80	0.55	31,31,31,31	0
57	MG	DA	9379	1/1	0.80	0.31	41,41,41,41	0
57	MG	BA	3103	1/1	0.80	0.19	31,31,31,31	0
57	MG	DA	9383	1/1	0.81	0.41	18,18,18,18	0
57	MG	BA	3322	1/1	0.81	0.35	54,54,54,54	0
57	MG	BA	3162	1/1	0.81	0.73	4,4,4,4	0
57	MG	DA	9348	1/1	0.81	0.72	47,47,47,47	0
57	MG	DA	9578	1/1	0.81	0.43	44,44,44,44	0
57	MG	AV	104	1/1	0.81	0.41	16,16,16,16	0
57	MG	CA	1614	1/1	0.81	1.22	38,38,38,38	0
57	MG	DB	205	1/1	0.81	0.17	6,6,6,6	1
57	MG	DA	9635	1/1	0.81	0.59	24,24,24,24	0
57	MG	AA	7031	1/1	0.81	0.20	44,44,44,44	0
57	MG	AA	7011	1/1	0.82	0.40	43,43,43,43	0
57	MG	DA	9335	1/1	0.82	0.33	21,21,21,21	0
57	MG	AA	7075	1/1	0.82	0.49	53,53,53,53	0
57	MG	BA	3264	1/1	0.82	0.65	36,36,36,36	0
57	MG	AA	7049	1/1	0.82	0.25	41,41,41,41	0
57	MG	DA	9421	1/1	0.82	0.36	28,28,28,28	0
57	MG	DA	9374	1/1	0.82	0.40	28,28,28,28	0
57	MG	CA	1655	1/1	0.82	0.47	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CW	101	1/1	0.82	0.47	29,29,29,29	1
57	MG	CX	101	1/1	0.82	0.23	25,25,25,25	0
57	MG	DA	9439	1/1	0.82	0.23	32,32,32,32	0
57	MG	DA	9574	1/1	0.82	0.38	14,14,14,14	1
57	MG	DA	9325	1/1	0.82	0.48	32,32,32,32	0
57	MG	DA	9579	1/1	0.82	0.67	38,38,38,38	0
57	MG	BA	3231	1/1	0.82	0.38	90,90,90,90	0
57	MG	CA	1725	1/1	0.83	0.29	29,29,29,29	0
57	MG	DA	9461	1/1	0.83	0.34	13,13,13,13	0
57	MG	BA	3217	1/1	0.83	0.16	28,28,28,28	0
57	MG	DA	9385	1/1	0.83	0.24	5,5,5,5	0
57	MG	BA	3321	1/1	0.83	0.35	35,35,35,35	0
57	MG	CA	1638	1/1	0.83	0.42	24,24,24,24	0
57	MG	BA	3292	1/1	0.83	0.28	28,28,28,28	0
57	MG	BA	3033	1/1	0.83	0.19	6,6,6,6	0
57	MG	BA	3106	1/1	0.83	0.49	34,34,34,34	0
57	MG	DA	9659	1/1	0.83	0.26	52,52,52,52	0
57	MG	DA	9301	1/1	0.83	0.36	32,32,32,32	0
57	MG	DA	9572	1/1	0.83	0.42	4,4,4,4	0
57	MG	DA	9418	1/1	0.83	0.28	61,61,61,61	0
57	MG	BE	301	1/1	0.83	0.24	0,0,0,0	0
57	MG	AA	7034	1/1	0.83	0.74	43,43,43,43	0
57	MG	AA	7014	1/1	0.83	0.96	20,20,20,20	0
57	MG	DA	9431	1/1	0.83	0.30	12,12,12,12	0
57	MG	CA	1709	1/1	0.83	0.48	68,68,68,68	0
57	MG	BA	3070	1/1	0.83	0.43	34,34,34,34	0
57	MG	DA	9347	1/1	0.83	0.29	22,22,22,22	0
57	MG	DA	9688	1/1	0.83	0.40	78,78,78,78	0
57	MG	DA	9692	1/1	0.83	0.42	30,30,30,30	0
57	MG	DA	9693	1/1	0.83	0.97	47,47,47,47	0
57	MG	BA	3136	1/1	0.83	0.44	46,46,46,46	1
57	MG	DA	9695	1/1	0.83	0.39	63,63,63,63	0
57	MG	DB	202	1/1	0.83	0.23	28,28,28,28	0
57	MG	CA	1676	1/1	0.83	0.60	88,88,88,88	0
57	MG	BA	3249	1/1	0.83	0.41	25,25,25,25	0
57	MG	BA	3113	1/1	0.83	0.87	49,49,49,49	0
57	MG	DA	9614	1/1	0.84	0.25	12,12,12,12	0
57	MG	BA	3282	1/1	0.84	0.47	24,24,24,24	0
57	MG	AA	7105	1/1	0.84	0.74	42,42,42,42	0
57	MG	AE	201	1/1	0.84	0.39	45,45,45,45	0
57	MG	BA	3268	1/1	0.84	0.33	13,13,13,13	1
57	MG	AV	102	1/1	0.84	0.43	25,25,25,25	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	7100	1/1	0.84	0.81	21,21,21,21	0
57	MG	DA	9445	1/1	0.84	0.44	22,22,22,22	0
57	MG	BB	201	1/1	0.84	0.15	34,34,34,34	0
57	MG	BA	3254	1/1	0.84	0.91	54,54,54,54	0
57	MG	BA	3134	1/1	0.84	0.48	21,21,21,21	0
57	MG	BA	3310	1/1	0.84	0.40	35,35,35,35	0
57	MG	DA	9593	1/1	0.84	0.62	25,25,25,25	0
57	MG	DA	9504	1/1	0.84	0.15	27,27,27,27	0
57	MG	DA	9530	1/1	0.84	0.85	41,41,41,41	0
57	MG	DW	201	1/1	0.84	0.47	27,27,27,27	0
57	MG	DA	9544	1/1	0.84	0.41	10,10,10,10	0
57	MG	BA	3038	1/1	0.84	0.16	31,31,31,31	0
57	MG	DA	9667	1/1	0.85	0.36	10,10,10,10	0
57	MG	BA	3214	1/1	0.85	0.31	39,39,39,39	0
57	MG	BA	3116	1/1	0.85	0.27	38,38,38,38	0
57	MG	AA	7083	1/1	0.85	0.55	18,18,18,18	0
57	MG	BA	3221	1/1	0.85	0.69	17,17,17,17	0
57	MG	CA	1657	1/1	0.85	0.26	30,30,30,30	0
57	MG	BA	3137	1/1	0.85	0.61	1,1,1,1	1
57	MG	DA	9640	1/1	0.85	0.40	42,42,42,42	0
57	MG	CA	1660	1/1	0.85	0.37	9,9,9,9	0
57	MG	BA	3195	1/1	0.85	0.32	3,3,3,3	0
57	MG	DA	9462	1/1	0.85	0.40	30,30,30,30	0
57	MG	BA	3115	1/1	0.85	0.24	33,33,33,33	0
57	MG	DA	9352	1/1	0.85	0.22	89,89,89,89	0
57	MG	BA	3285	1/1	0.85	1.73	32,32,32,32	1
57	MG	DA	9377	1/1	0.85	0.19	19,19,19,19	0
57	MG	BA	3131	1/1	0.85	0.40	38,38,38,38	0
57	MG	CA	1681	1/1	0.85	0.86	18,18,18,18	1
57	MG	DA	9381	1/1	0.85	0.26	12,12,12,12	0
57	MG	AA	7047	1/1	0.86	0.36	41,41,41,41	0
57	MG	CA	1641	1/1	0.86	0.21	40,40,40,40	0
57	MG	BA	3130	1/1	0.86	0.19	3,3,3,3	0
57	MG	BA	3081	1/1	0.86	0.77	24,24,24,24	1
57	MG	BA	3251	1/1	0.86	0.22	34,34,34,34	0
57	MG	BF	301	1/1	0.86	0.22	39,39,39,39	0
57	MG	BA	3220	1/1	0.86	0.77	56,56,56,56	0
57	MG	DA	9327	1/1	0.86	0.17	20,20,20,20	0
57	MG	DA	9475	1/1	0.86	0.65	26,26,26,26	0
57	MG	AA	7067	1/1	0.86	0.45	28,28,28,28	0
57	MG	CA	1661	1/1	0.86	0.35	50,50,50,50	0
57	MG	BA	3284	1/1	0.86	0.33	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	BA	3193	1/1	0.86	0.44	12,12,12,12	0
57	MG	DA	9337	1/1	0.86	0.60	45,45,45,45	0
57	MG	CA	1673	1/1	0.86	0.25	18,18,18,18	0
57	MG	DA	9634	1/1	0.86	0.41	44,44,44,44	0
57	MG	BA	3059	1/1	0.86	0.16	0,0,0,0	0
57	MG	BA	3319	1/1	0.86	0.29	27,27,27,27	0
57	MG	DA	9565	1/1	0.86	0.38	11,11,11,11	0
57	MG	BA	3097	1/1	0.86	0.26	43,43,43,43	0
57	MG	DA	9361	1/1	0.86	0.34	5,5,5,5	0
57	MG	DX	101	1/1	0.86	0.36	6,6,6,6	0
57	MG	BA	3101	1/1	0.86	1.28	27,27,27,27	1
57	MG	BA	3294	1/1	0.86	0.50	15,15,15,15	1
57	MG	DA	9302	1/1	0.87	0.18	34,34,34,34	0
57	MG	CA	1675	1/1	0.87	0.42	55,55,55,55	0
57	MG	AA	7054	1/1	0.87	0.98	29,29,29,29	0
57	MG	BA	3077	1/1	0.87	0.43	21,21,21,21	0
57	MG	DA	9466	1/1	0.87	0.45	36,36,36,36	0
57	MG	BA	3258	1/1	0.87	1.06	19,19,19,19	0
57	MG	BA	3019	1/1	0.87	0.36	44,44,44,44	0
57	MG	DA	9673	1/1	0.87	0.42	8,8,8,8	0
57	MG	DA	9609	1/1	0.87	0.45	2,2,2,2	0
57	MG	DA	9502	1/1	0.87	0.42	3,3,3,3	0
57	MG	CA	1605	1/1	0.87	0.22	32,32,32,32	0
57	MG	DA	9616	1/1	0.87	0.54	54,54,54,54	0
57	MG	AA	7045	1/1	0.87	0.75	38,38,38,38	0
57	MG	BA	3093	1/1	0.87	0.29	49,49,49,49	0
57	MG	BA	3094	1/1	0.87	0.35	7,7,7,7	0
57	MG	CA	1735	1/1	0.87	0.47	29,29,29,29	0
57	MG	BA	3066	1/1	0.87	0.26	48,48,48,48	0
57	MG	CA	1740	1/1	0.87	0.60	48,48,48,48	0
57	MG	DA	9371	1/1	0.87	0.38	29,29,29,29	0
57	MG	CV	101	1/1	0.87	0.37	12,12,12,12	1
57	MG	AA	7107	1/1	0.87	0.45	24,24,24,24	0
57	MG	DF	301	1/1	0.87	0.14	20,20,20,20	0
57	MG	DP	202	1/1	0.87	0.25	173,173,173,173	0
57	MG	AA	7108	1/1	0.87	0.42	27,27,27,27	0
57	MG	BA	3298	1/1	0.87	0.80	18,18,18,18	0
57	MG	DA	9380	1/1	0.87	1.55	23,23,23,23	1
57	MG	BA	3102	1/1	0.87	0.49	1,1,1,1	0
57	MG	CA	1732	1/1	0.88	0.53	27,27,27,27	0
57	MG	AA	7036	1/1	0.88	0.38	42,42,42,42	0
57	MG	CA	1738	1/1	0.88	0.42	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	9422	1/1	0.88	0.96	56,56,56,56	0
57	MG	DA	9423	1/1	0.88	0.29	1,1,1,1	0
57	MG	BB	202	1/1	0.88	0.16	62,62,62,62	0
57	MG	BA	3031	1/1	0.88	0.23	44,44,44,44	0
57	MG	DA	9372	1/1	0.88	0.43	8,8,8,8	0
57	MG	DA	9373	1/1	0.88	0.16	0,0,0,0	0
57	MG	AA	7101	1/1	0.88	0.64	22,22,22,22	0
57	MG	CA	1633	1/1	0.88	0.27	9,9,9,9	0
57	MG	CA	1635	1/1	0.88	0.23	4,4,4,4	0
57	MG	DA	9670	1/1	0.88	0.48	11,11,11,11	0
57	MG	DA	9576	1/1	0.88	0.41	22,22,22,22	0
57	MG	BA	3276	1/1	0.88	0.56	31,31,31,31	0
57	MG	DA	9444	1/1	0.88	0.50	42,42,42,42	0
57	MG	DA	9589	1/1	0.88	0.18	32,32,32,32	0
57	MG	AA	7084	1/1	0.88	0.12	49,49,49,49	0
57	MG	CA	1710	1/1	0.88	0.50	19,19,19,19	0
57	MG	DA	9456	1/1	0.88	0.61	19,19,19,19	0
57	MG	DA	9686	1/1	0.88	0.20	11,11,11,11	0
57	MG	BO	201	1/1	0.88	0.42	45,45,45,45	0
57	MG	CA	1680	1/1	0.88	0.15	49,49,49,49	0
57	MG	DA	9690	1/1	0.88	0.11	5,5,5,5	0
57	MG	AV	103	1/1	0.88	0.26	7,7,7,7	1
57	MG	CA	1601	1/1	0.88	0.38	39,39,39,39	0
57	MG	AA	7004	1/1	0.88	0.29	30,30,30,30	0
57	MG	DA	9468	1/1	0.88	0.72	2,2,2,2	1
57	MG	DA	9402	1/1	0.88	0.38	25,25,25,25	0
57	MG	DA	9490	1/1	0.88	0.22	39,39,39,39	0
57	MG	CA	1684	1/1	0.88	0.21	41,41,41,41	0
57	MG	DA	9503	1/1	0.88	0.31	66,66,66,66	0
57	MG	BA	3267	1/1	0.88	0.39	41,41,41,41	0
57	MG	BA	3150	1/1	0.88	0.30	1,1,1,1	0
57	MG	DA	9535	1/1	0.88	0.42	14,14,14,14	0
57	MG	DA	9639	1/1	0.88	0.49	57,57,57,57	0
57	MG	DA	9443	1/1	0.89	0.24	37,37,37,37	0
57	MG	DA	9656	1/1	0.89	0.29	58,58,58,58	0
57	MG	BA	3104	1/1	0.89	0.24	16,16,16,16	0
57	MG	CA	1717	1/1	0.89	0.29	11,11,11,11	0
57	MG	DA	9328	1/1	0.89	0.33	1,1,1,1	0
57	MG	CA	1653	1/1	0.89	0.53	29,29,29,29	0
57	MG	BA	3177	1/1	0.89	0.20	0,0,0,0	0
57	MG	DA	9460	1/1	0.89	0.25	40,40,40,40	0
57	MG	AA	7090	1/1	0.89	1.01	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	1690	1/1	0.89	0.54	17,17,17,17	0
57	MG	DA	9465	1/1	0.89	0.39	34,34,34,34	0
57	MG	AA	7012	1/1	0.89	0.78	12,12,12,12	0
57	MG	BA	3144	1/1	0.89	0.71	41,41,41,41	0
57	MG	BA	3202	1/1	0.89	0.50	7,7,7,7	0
57	MG	CA	1737	1/1	0.89	0.63	28,28,28,28	0
57	MG	DA	9680	1/1	0.89	0.39	24,24,24,24	0
57	MG	DA	9351	1/1	0.89	0.45	2,2,2,2	0
57	MG	DA	9611	1/1	0.89	0.46	8,8,8,8	0
57	MG	BA	3022	1/1	0.89	0.23	40,40,40,40	0
57	MG	CA	1671	1/1	0.89	0.23	38,38,38,38	0
57	MG	DA	9367	1/1	0.89	0.41	35,35,35,35	0
57	MG	DA	9526	1/1	0.89	0.50	12,12,12,12	0
57	MG	DA	9370	1/1	0.89	0.39	0,0,0,0	0
57	MG	BA	3209	1/1	0.89	0.34	1,1,1,1	0
57	MG	DA	9541	1/1	0.89	0.39	2,2,2,2	0
57	MG	AA	7061	1/1	0.89	0.25	19,19,19,19	0
57	MG	BE	302	1/1	0.89	0.27	74,74,74,74	0
57	MG	DB	203	1/1	0.89	0.91	1,1,1,1	1
57	MG	BA	3111	1/1	0.89	0.33	35,35,35,35	0
57	MG	DA	9376	1/1	0.89	0.27	26,26,26,26	0
57	MG	BA	3157	1/1	0.89	0.22	6,6,6,6	0
57	MG	BA	3087	1/1	0.89	0.24	21,21,21,21	0
57	MG	BA	3053	1/1	0.89	0.28	17,17,17,17	0
57	MG	DA	9568	1/1	0.89	0.37	3,3,3,3	0
58	PAR	CA	1741	42/42	0.89	0.32	55,55,55,55	0
57	MG	DA	9651	1/1	0.89	0.13	81,81,81,81	0
57	MG	AA	7029	1/1	0.90	0.27	41,41,41,41	0
57	MG	DA	9339	1/1	0.90	0.20	13,13,13,13	0
57	MG	AA	7079	1/1	0.90	0.41	35,35,35,35	0
57	MG	CA	1646	1/1	0.90	0.42	7,7,7,7	0
57	MG	BA	3308	1/1	0.90	0.40	37,37,37,37	0
57	MG	DA	9551	1/1	0.90	0.21	48,48,48,48	0
57	MG	AA	7023	1/1	0.90	0.26	56,56,56,56	0
57	MG	DA	9425	1/1	0.90	0.41	37,37,37,37	0
57	MG	CA	1688	1/1	0.90	0.15	16,16,16,16	0
57	MG	CA	1689	1/1	0.90	0.25	15,15,15,15	0
57	MG	DA	9365	1/1	0.90	0.28	1,1,1,1	0
57	MG	CA	1654	1/1	0.90	0.35	31,31,31,31	0
57	MG	AA	7026	1/1	0.90	0.39	30,30,30,30	0
57	MG	AA	7073	1/1	0.90	0.23	29,29,29,29	0
57	MG	CE	202	1/1	0.90	0.38	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	BA	3281	1/1	0.90	0.62	53,53,53,53	0
57	MG	AV	105	1/1	0.90	0.34	54,54,54,54	0
57	MG	AA	7063	1/1	0.90	0.26	31,31,31,31	0
57	MG	DA	9577	1/1	0.90	0.90	102,102,102,102	0
57	MG	CA	1663	1/1	0.90	0.66	11,11,11,11	0
57	MG	DA	9679	1/1	0.90	0.31	16,16,16,16	0
57	MG	CY	101	1/1	0.90	0.57	33,33,33,33	0
57	MG	BA	3001	1/1	0.90	0.38	38,38,38,38	0
57	MG	BA	3158	1/1	0.90	0.37	29,29,29,29	0
57	MG	DA	9317	1/1	0.90	0.26	18,18,18,18	0
57	MG	DA	9382	1/1	0.90	0.45	0,0,0,0	0
57	MG	AA	7020	1/1	0.90	0.36	33,33,33,33	0
57	MG	BA	3012	1/1	0.90	0.60	29,29,29,29	0
57	MG	DA	9608	1/1	0.90	0.46	19,19,19,19	0
57	MG	AA	7088	1/1	0.90	0.13	60,60,60,60	0
57	MG	BA	3109	1/1	0.90	0.22	66,66,66,66	0
57	MG	DA	9396	1/1	0.90	0.23	26,26,26,26	0
57	MG	DA	9397	1/1	0.90	0.41	25,25,25,25	1
57	MG	DA	9477	1/1	0.90	0.56	36,36,36,36	0
57	MG	DA	9483	1/1	0.90	0.48	0,0,0,0	0
57	MG	DE	302	1/1	0.90	0.22	35,35,35,35	0
57	MG	BA	3269	1/1	0.90	0.50	20,20,20,20	0
57	MG	DA	9501	1/1	0.90	0.47	42,42,42,42	0
57	MG	DP	203	1/1	0.90	0.24	11,11,11,11	0
57	MG	DA	9333	1/1	0.90	0.11	31,31,31,31	0
57	MG	CA	1677	1/1	0.90	0.18	22,22,22,22	0
57	MG	DA	9409	1/1	0.90	0.31	4,4,4,4	0
57	MG	D2	101	1/1	0.90	0.25	34,34,34,34	0
57	MG	DA	9513	1/1	0.90	0.47	22,22,22,22	0
57	MG	BA	3187	1/1	0.90	0.61	24,24,24,24	0
57	MG	BA	3205	1/1	0.91	0.54	0,0,0,0	0
57	MG	DA	9407	1/1	0.91	0.22	2,2,2,2	0
57	MG	DA	9630	1/1	0.91	0.27	16,16,16,16	1
57	MG	DA	9633	1/1	0.91	0.73	30,30,30,30	0
57	MG	BA	3154	1/1	0.91	0.43	17,17,17,17	0
57	MG	BA	3058	1/1	0.91	0.33	1,1,1,1	0
57	MG	DA	9413	1/1	0.91	0.38	3,3,3,3	0
57	MG	CA	1608	1/1	0.91	0.39	16,16,16,16	0
57	MG	DA	9527	1/1	0.91	0.38	1,1,1,1	0
57	MG	DA	9338	1/1	0.91	0.55	58,58,58,58	0
57	MG	AA	7043	1/1	0.91	0.34	16,16,16,16	0
57	MG	DA	9539	1/1	0.91	0.25	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	DA	9420	1/1	0.91	0.52	6,6,6,6	0
57	MG	BA	3006	1/1	0.91	0.33	38,38,38,38	0
57	MG	AA	7009	1/1	0.91	0.27	18,18,18,18	0
57	MG	AA	7005	1/1	0.91	0.28	45,45,45,45	0
57	MG	CA	1616	1/1	0.91	0.41	44,44,44,44	0
57	MG	DA	9556	1/1	0.91	0.23	23,23,23,23	0
57	MG	BA	3226	1/1	0.91	0.65	36,36,36,36	0
57	MG	DA	9663	1/1	0.91	0.59	7,7,7,7	0
57	MG	BA	3171	1/1	0.91	0.45	7,7,7,7	0
57	MG	DA	9666	1/1	0.91	0.36	7,7,7,7	0
57	MG	CA	1630	1/1	0.91	0.23	34,34,34,34	0
57	MG	CA	1736	1/1	0.91	0.31	6,6,6,6	0
57	MG	BA	3112	1/1	0.91	0.57	14,14,14,14	0
57	MG	BA	3233	1/1	0.91	0.45	19,19,19,19	0
57	MG	BA	3236	1/1	0.91	0.56	17,17,17,17	0
57	MG	AA	7013	1/1	0.91	0.38	27,27,27,27	0
57	MG	BA	3183	1/1	0.91	0.64	56,56,56,56	0
57	MG	BA	3323	1/1	0.91	0.48	26,26,26,26	0
57	MG	AA	7048	1/1	0.91	0.27	27,27,27,27	0
57	MG	BA	3141	1/1	0.91	0.26	18,18,18,18	0
57	MG	DA	9453	1/1	0.91	0.44	4,4,4,4	1
57	MG	BA	3143	1/1	0.91	0.20	7,7,7,7	0
57	MG	DA	9585	1/1	0.91	0.18	18,18,18,18	0
57	MG	DA	9457	1/1	0.91	0.59	13,13,13,13	0
57	MG	BA	3287	1/1	0.91	0.36	30,30,30,30	0
57	MG	DA	9594	1/1	0.91	0.78	19,19,19,19	0
57	MG	CA	1697	1/1	0.91	0.18	49,49,49,49	0
57	MG	BA	3050	1/1	0.91	0.58	4,4,4,4	0
57	MG	CA	1700	1/1	0.91	0.28	20,20,20,20	0
57	MG	DA	9464	1/1	0.91	0.14	25,25,25,25	0
57	MG	DA	9604	1/1	0.91	0.33	21,21,21,21	0
57	MG	DB	204	1/1	0.91	0.70	0,0,0,0	1
57	MG	DA	9605	1/1	0.91	0.20	19,19,19,19	0
57	MG	DA	9607	1/1	0.91	0.34	49,49,49,49	0
57	MG	DA	9319	1/1	0.91	0.81	30,30,30,30	0
57	MG	BA	3201	1/1	0.91	0.32	6,6,6,6	0
57	MG	DA	9393	1/1	0.91	0.30	24,24,24,24	0
57	MG	CA	1656	1/1	0.91	0.21	22,22,22,22	0
57	MG	AA	7041	1/1	0.91	0.58	20,20,20,20	0
57	MG	BN	201	1/1	0.91	0.30	125,125,125,125	1
57	MG	DA	9480	1/1	0.91	0.27	30,30,30,30	0
57	MG	AA	7052	1/1	0.91	0.19	74,74,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	9332	1/1	0.91	0.37	34,34,34,34	0
57	MG	DA	9618	1/1	0.92	0.79	28,28,28,28	1
57	MG	CA	1634	1/1	0.92	0.31	43,43,43,43	0
57	MG	DA	9394	1/1	0.92	0.47	16,16,16,16	0
57	MG	DA	9484	1/1	0.92	0.40	5,5,5,5	0
57	MG	DA	9486	1/1	0.92	0.34	21,21,21,21	0
57	MG	DA	9489	1/1	0.92	0.41	37,37,37,37	0
57	MG	BA	3208	1/1	0.92	0.22	8,8,8,8	0
57	MG	DA	9631	1/1	0.92	0.32	21,21,21,21	0
57	MG	DA	9496	1/1	0.92	0.35	26,26,26,26	0
57	MG	AA	7022	1/1	0.92	0.25	32,32,32,32	0
57	MG	AA	7050	1/1	0.92	1.07	29,29,29,29	0
57	MG	DA	9636	1/1	0.92	0.28	16,16,16,16	0
57	MG	DA	9303	1/1	0.92	0.31	42,42,42,42	0
57	MG	BA	3123	1/1	0.92	0.20	14,14,14,14	0
57	MG	BA	3272	1/1	0.92	0.37	10,10,10,10	0
57	MG	AA	7018	1/1	0.92	0.56	27,27,27,27	0
57	MG	CA	1643	1/1	0.92	0.58	40,40,40,40	1
57	MG	AA	7053	1/1	0.92	0.49	32,32,32,32	0
57	MG	CA	1701	1/1	0.92	0.51	1,1,1,1	0
57	MG	BA	3002	1/1	0.92	0.27	53,53,53,53	0
57	MG	BA	3166	1/1	0.92	0.64	40,40,40,40	0
57	MG	BA	3168	1/1	0.92	0.71	36,36,36,36	0
57	MG	DA	9334	1/1	0.92	0.45	27,27,27,27	0
57	MG	BA	3132	1/1	0.92	0.32	51,51,51,51	0
57	MG	BA	3133	1/1	0.92	0.21	43,43,43,43	0
57	MG	BA	3283	1/1	0.92	0.20	22,22,22,22	0
57	MG	BA	3235	1/1	0.92	0.36	25,25,25,25	0
57	MG	BA	3088	1/1	0.92	0.39	43,43,43,43	0
57	MG	DA	9341	1/1	0.92	0.56	11,11,11,11	0
57	MG	BA	3061	1/1	0.92	0.25	32,32,32,32	0
57	MG	DA	9567	1/1	0.92	0.43	31,31,31,31	0
57	MG	DA	9433	1/1	0.92	0.22	13,13,13,13	0
57	MG	CA	1662	1/1	0.92	0.17	29,29,29,29	0
57	MG	DA	9435	1/1	0.92	0.97	30,30,30,30	0
57	MG	CA	1720	1/1	0.92	0.41	2,2,2,2	0
57	MG	BA	3184	1/1	0.92	0.95	22,22,22,22	0
57	MG	B5	101	1/1	0.92	0.30	2,2,2,2	0
57	MG	BA	3186	1/1	0.92	0.36	2,2,2,2	0
57	MG	DA	9683	1/1	0.92	0.52	19,19,19,19	0
57	MG	CA	1726	1/1	0.92	0.21	38,38,38,38	0
57	MG	CA	1727	1/1	0.92	0.34	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3062	1/1	0.92	0.15	27,27,27,27	0
57	MG	BA	3140	1/1	0.92	0.24	40,40,40,40	0
57	MG	DA	9588	1/1	0.92	0.14	16,16,16,16	0
57	MG	DA	9691	1/1	0.92	0.41	12,12,12,12	0
57	MG	DA	9451	1/1	0.92	0.56	35,35,35,35	0
57	MG	DA	9591	1/1	0.92	0.25	52,52,52,52	0
57	MG	BA	3024	1/1	0.92	0.61	22,22,22,22	0
57	MG	AA	7040	1/1	0.92	0.17	36,36,36,36	0
57	MG	BA	3256	1/1	0.92	0.15	13,13,13,13	0
57	MG	DA	9598	1/1	0.92	0.50	14,14,14,14	0
57	MG	BA	3199	1/1	0.92	0.48	1,1,1,1	0
57	MG	CA	1678	1/1	0.92	0.22	17,17,17,17	0
57	MG	BA	3067	1/1	0.92	0.79	2,2,2,2	0
57	MG	CA	1617	1/1	0.92	0.43	16,16,16,16	0
57	MG	BA	3145	1/1	0.92	0.28	22,22,22,22	0
57	MG	BA	3263	1/1	0.92	0.64	16,16,16,16	1
57	MG	DQ	201	1/1	0.92	0.31	36,36,36,36	0
57	MG	CV	102	1/1	0.92	0.21	1,1,1,1	0
57	MG	BA	3045	1/1	0.92	0.59	2,2,2,2	0
57	MG	CV	104	1/1	0.92	0.28	22,22,22,22	1
57	MG	DA	9469	1/1	0.92	0.58	17,17,17,17	0
58	PAR	AA	7111	42/42	0.92	0.26	58,58,58,58	0
57	MG	BA	3049	1/1	0.92	0.51	30,30,30,30	0
57	MG	DA	9389	1/1	0.92	0.14	11,11,11,11	0
57	MG	BA	3032	1/1	0.93	0.20	18,18,18,18	0
57	MG	DA	9625	1/1	0.93	0.36	26,26,26,26	0
57	MG	DA	9320	1/1	0.93	0.25	10,10,10,10	0
57	MG	AA	7039	1/1	0.93	0.34	11,11,11,11	0
57	MG	DA	9629	1/1	0.93	0.15	52,52,52,52	0
57	MG	AA	7066	1/1	0.93	0.54	36,36,36,36	0
57	MG	DA	9512	1/1	0.93	0.43	2,2,2,2	0
57	MG	DA	9415	1/1	0.93	0.49	0,0,0,0	0
57	MG	DA	9519	1/1	0.93	0.43	1,1,1,1	0
57	MG	DA	9525	1/1	0.93	0.30	4,4,4,4	0
57	MG	BA	3075	1/1	0.93	0.70	12,12,12,12	0
57	MG	DA	9417	1/1	0.93	0.29	20,20,20,20	0
57	MG	AA	7104	1/1	0.93	0.14	33,33,33,33	0
57	MG	DA	9533	1/1	0.93	0.30	0,0,0,0	0
57	MG	CA	1650	1/1	0.93	0.51	34,34,34,34	0
57	MG	CA	1705	1/1	0.93	0.27	15,15,15,15	0
57	MG	AA	7059	1/1	0.93	0.51	96,96,96,96	0
57	MG	BA	3153	1/1	0.93	0.55	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	7001	1/1	0.93	0.28	26,26,26,26	0
57	MG	BA	3044	1/1	0.93	0.58	18,18,18,18	0
57	MG	BA	3014	1/1	0.93	0.25	33,33,33,33	0
57	MG	DA	9555	1/1	0.93	0.32	39,39,39,39	0
57	MG	BA	3118	1/1	0.93	0.61	28,28,28,28	0
57	MG	BA	3160	1/1	0.93	0.39	22,22,22,22	0
57	MG	DA	9662	1/1	0.93	0.54	2,2,2,2	0
57	MG	BA	3017	1/1	0.93	0.55	22,22,22,22	0
57	MG	DA	9561	1/1	0.93	0.28	10,10,10,10	0
57	MG	BA	3163	1/1	0.93	0.32	28,28,28,28	0
57	MG	BA	3229	1/1	0.93	0.19	19,19,19,19	0
57	MG	BA	3230	1/1	0.93	0.61	22,22,22,22	0
57	MG	AA	7078	1/1	0.93	0.25	30,30,30,30	0
57	MG	BA	3232	1/1	0.93	0.18	44,44,44,44	0
57	MG	DA	9358	1/1	0.93	0.47	5,5,5,5	0
57	MG	AA	7070	1/1	0.93	0.15	61,61,61,61	0
57	MG	AA	7093	1/1	0.93	0.34	30,30,30,30	0
57	MG	CA	1730	1/1	0.93	0.15	49,49,49,49	0
57	MG	DA	9446	1/1	0.93	0.08	13,13,13,13	0
57	MG	CA	1607	1/1	0.93	0.49	32,32,32,32	0
57	MG	BA	3057	1/1	0.93	0.54	2,2,2,2	0
57	MG	CA	1734	1/1	0.93	0.24	22,22,22,22	0
57	MG	BA	3291	1/1	0.93	0.16	22,22,22,22	0
57	MG	BA	3098	1/1	0.93	0.29	36,36,36,36	0
57	MG	BA	3174	1/1	0.93	0.14	31,31,31,31	0
57	MG	DA	9689	1/1	0.93	0.80	25,25,25,25	0
57	MG	BA	3099	1/1	0.93	0.23	30,30,30,30	0
57	MG	AA	7094	1/1	0.93	0.54	8,8,8,8	0
57	MG	AA	7051	1/1	0.93	0.44	22,22,22,22	0
57	MG	BA	3300	1/1	0.93	0.45	1,1,1,1	0
57	MG	DA	9597	1/1	0.93	0.24	12,12,12,12	0
57	MG	AA	7072	1/1	0.93	0.15	23,23,23,23	0
57	MG	CA	1685	1/1	0.93	0.35	41,41,41,41	0
57	MG	CA	1686	1/1	0.93	0.21	77,77,77,77	0
57	MG	BA	3135	1/1	0.93	0.58	43,43,43,43	0
57	MG	CA	1632	1/1	0.93	0.15	18,18,18,18	0
57	MG	DA	9470	1/1	0.93	0.27	0,0,0,0	0
57	MG	DA	9606	1/1	0.93	0.94	4,4,4,4	0
57	MG	BA	3192	1/1	0.93	0.39	2,2,2,2	0
57	MG	BA	3029	1/1	0.93	0.15	24,24,24,24	0
57	MG	BA	3030	1/1	0.93	0.54	22,22,22,22	0
57	MG	DA	9482	1/1	0.93	0.21	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3314	1/1	0.93	0.05	42,42,42,42	0
57	MG	D0	102	1/1	0.93	0.54	15,15,15,15	0
57	MG	AA	7098	1/1	0.93	0.34	28,28,28,28	0
57	MG	DA	9306	1/1	0.93	0.35	4,4,4,4	0
57	MG	DA	9313	1/1	0.93	0.22	18,18,18,18	0
57	MG	DA	9314	1/1	0.93	0.32	1,1,1,1	0
59	ZN	AD	301	1/1	0.93	0.32	41,41,41,41	0
57	MG	CA	1695	1/1	0.93	0.36	15,15,15,15	0
57	MG	CA	1664	1/1	0.94	0.45	24,24,24,24	0
57	MG	DA	9511	1/1	0.94	0.80	7,7,7,7	0
57	MG	BA	3304	1/1	0.94	0.43	13,13,13,13	0
57	MG	CA	1668	1/1	0.94	0.34	56,56,56,56	0
57	MG	DA	9514	1/1	0.94	0.82	19,19,19,19	0
57	MG	CA	1721	1/1	0.94	0.20	1,1,1,1	0
57	MG	CA	1669	1/1	0.94	0.10	10,10,10,10	0
57	MG	DA	9632	1/1	0.94	0.48	12,12,12,12	1
57	MG	CA	1670	1/1	0.94	0.36	2,2,2,2	0
57	MG	BA	3225	1/1	0.94	0.28	2,2,2,2	0
57	MG	DA	9528	1/1	0.94	0.36	6,6,6,6	0
57	MG	DA	9340	1/1	0.94	0.33	1,1,1,1	0
57	MG	DA	9531	1/1	0.94	0.37	1,1,1,1	0
57	MG	DA	9532	1/1	0.94	0.44	9,9,9,9	0
57	MG	DA	9428	1/1	0.94	0.41	15,15,15,15	0
57	MG	BA	3090	1/1	0.94	0.41	2,2,2,2	0
57	MG	BA	3128	1/1	0.94	0.25	57,57,57,57	0
57	MG	BA	3185	1/1	0.94	0.26	14,14,14,14	0
57	MG	DA	9652	1/1	0.94	0.23	44,44,44,44	0
57	MG	DA	9653	1/1	0.94	0.41	5,5,5,5	0
57	MG	BA	3129	1/1	0.94	0.53	1,1,1,1	0
57	MG	DA	9549	1/1	0.94	0.74	44,44,44,44	0
57	MG	CA	1618	1/1	0.94	0.22	31,31,31,31	0
57	MG	AA	7032	1/1	0.94	0.47	24,24,24,24	0
57	MG	DA	9436	1/1	0.94	0.54	3,3,3,3	0
57	MG	CA	1625	1/1	0.94	0.43	26,26,26,26	0
57	MG	AA	7064	1/1	0.94	0.28	50,50,50,50	0
57	MG	AA	7102	1/1	0.94	0.49	38,38,38,38	0
57	MG	BA	3096	1/1	0.94	0.42	12,12,12,12	0
57	MG	DA	9442	1/1	0.94	0.54	36,36,36,36	0
57	MG	DA	9368	1/1	0.94	0.19	1,1,1,1	0
57	MG	BA	3159	1/1	0.94	0.53	9,9,9,9	0
57	MG	DA	9669	1/1	0.94	0.23	5,5,5,5	0
57	MG	BA	3241	1/1	0.94	0.45	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	7103	1/1	0.94	0.53	13,13,13,13	0
57	MG	CA	1636	1/1	0.94	0.32	19,19,19,19	0
57	MG	AA	7016	1/1	0.94	0.32	45,45,45,45	0
57	MG	AA	7085	1/1	0.94	0.17	15,15,15,15	0
57	MG	DA	9454	1/1	0.94	0.44	34,34,34,34	0
57	MG	BA	3023	1/1	0.94	0.28	4,4,4,4	0
57	MG	CA	1640	1/1	0.94	0.84	49,49,49,49	0
57	MG	CV	105	1/1	0.94	0.16	69,69,69,69	0
57	MG	BA	3079	1/1	0.94	0.33	29,29,29,29	1
57	MG	DA	9684	1/1	0.94	0.21	8,8,8,8	0
57	MG	AA	7062	1/1	0.94	0.11	31,31,31,31	0
57	MG	DA	9581	1/1	0.94	0.42	4,4,4,4	0
57	MG	DA	9582	1/1	0.94	0.88	21,21,21,21	0
57	MG	DA	9583	1/1	0.94	0.18	1,1,1,1	0
57	MG	BA	3253	1/1	0.94	0.60	34,34,34,34	0
57	MG	CA	1644	1/1	0.94	0.14	45,45,45,45	0
57	MG	BA	3169	1/1	0.94	0.51	3,3,3,3	0
57	MG	BA	3212	1/1	0.94	0.24	8,8,8,8	0
57	MG	DA	9304	1/1	0.94	0.44	27,27,27,27	0
57	MG	BA	3213	1/1	0.94	0.41	8,8,8,8	0
57	MG	BA	3170	1/1	0.94	0.79	1,1,1,1	0
57	MG	BA	3296	1/1	0.94	0.38	0,0,0,0	1
57	MG	DA	9471	1/1	0.94	0.55	50,50,50,50	1
57	MG	DA	9473	1/1	0.94	0.64	0,0,0,0	0
57	MG	CA	1703	1/1	0.94	0.45	9,9,9,9	0
57	MG	DD	7102	1/1	0.94	0.28	0,0,0,0	0
57	MG	DA	9476	1/1	0.94	0.47	2,2,2,2	0
57	MG	BU	201	1/1	0.94	0.30	170,170,170,170	1
57	MG	AA	7081	1/1	0.94	0.46	44,44,44,44	0
57	MG	DA	9321	1/1	0.94	0.50	35,35,35,35	0
57	MG	DA	9403	1/1	0.94	0.26	0,0,0,0	0
57	MG	DA	9323	1/1	0.94	0.56	33,33,33,33	0
57	MG	B7	101	1/1	0.94	0.39	13,13,13,13	0
57	MG	DA	9487	1/1	0.94	0.25	71,71,71,71	0
57	MG	BA	3042	1/1	0.94	0.67	8,8,8,8	0
57	MG	DA	9410	1/1	0.94	0.25	4,4,4,4	0
57	MG	AA	7089	1/1	0.94	0.24	21,21,21,21	0
57	MG	CA	1606	1/1	0.94	0.21	8,8,8,8	0
57	MG	BA	3148	1/1	0.94	0.38	16,16,16,16	0
57	MG	BA	3302	1/1	0.94	0.47	8,8,8,8	0
57	MG	DA	9505	1/1	0.95	0.29	0,0,0,0	0
57	MG	DA	9507	1/1	0.95	0.55	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	DA	9510	1/1	0.95	0.52	1,1,1,1	0
57	MG	CA	1626	1/1	0.95	0.55	28,28,28,28	0
57	MG	CA	1627	1/1	0.95	0.63	22,22,22,22	0
57	MG	DA	9424	1/1	0.95	0.51	5,5,5,5	0
57	MG	BA	3181	1/1	0.95	0.49	1,1,1,1	0
57	MG	DA	9426	1/1	0.95	0.43	9,9,9,9	1
57	MG	DA	9345	1/1	0.95	0.52	19,19,19,19	0
57	MG	BA	3228	1/1	0.95	0.61	13,13,13,13	0
57	MG	CA	1631	1/1	0.95	0.89	22,22,22,22	0
57	MG	AA	7044	1/1	0.95	0.35	21,21,21,21	0
57	MG	BA	3147	1/1	0.95	0.59	48,48,48,48	0
57	MG	DA	9638	1/1	0.95	0.27	8,8,8,8	1
57	MG	AA	7106	1/1	0.95	0.25	12,12,12,12	0
57	MG	DA	9356	1/1	0.95	0.32	1,1,1,1	0
57	MG	BA	3068	1/1	0.95	0.11	11,11,11,11	0
57	MG	BA	3069	1/1	0.95	0.32	5,5,5,5	0
57	MG	BA	3043	1/1	0.95	0.21	8,8,8,8	0
57	MG	DA	9540	1/1	0.95	0.34	0,0,0,0	0
57	MG	DA	9366	1/1	0.95	0.46	1,1,1,1	0
57	MG	AA	7015	1/1	0.95	0.29	4,4,4,4	0
57	MG	DA	9654	1/1	0.95	0.29	15,15,15,15	0
57	MG	DA	9548	1/1	0.95	0.72	26,26,26,26	0
57	MG	BA	3127	1/1	0.95	0.38	8,8,8,8	0
57	MG	CE	201	1/1	0.95	0.67	16,16,16,16	0
57	MG	AA	7058	1/1	0.95	0.27	13,13,13,13	0
57	MG	BB	204	1/1	0.95	0.31	23,23,23,23	0
57	MG	DA	9553	1/1	0.95	0.35	20,20,20,20	0
57	MG	BA	3005	1/1	0.95	0.26	22,22,22,22	0
57	MG	DA	9447	1/1	0.95	0.23	68,68,68,68	0
57	MG	DA	9448	1/1	0.95	0.37	18,18,18,18	0
57	MG	AA	7109	1/1	0.95	0.36	33,33,33,33	0
57	MG	DA	9375	1/1	0.95	0.54	0,0,0,0	0
57	MG	DA	9452	1/1	0.95	0.37	10,10,10,10	0
57	MG	BA	3289	1/1	0.95	0.51	21,21,21,21	0
57	MG	BA	3007	1/1	0.95	0.66	4,4,4,4	0
57	MG	DA	9455	1/1	0.95	0.46	0,0,0,0	0
57	MG	BA	3161	1/1	0.95	0.26	11,11,11,11	0
57	MG	CA	1696	1/1	0.95	0.34	49,49,49,49	0
57	MG	BA	3204	1/1	0.95	0.31	3,3,3,3	0
57	MG	DA	9459	1/1	0.95	0.52	3,3,3,3	0
57	MG	BA	3293	1/1	0.95	0.21	1,1,1,1	0
57	MG	AA	7021	1/1	0.95	0.31	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	AA	7060	1/1	0.95	0.13	8,8,8,8	0
57	MG	DA	9682	1/1	0.95	0.42	20,20,20,20	0
57	MG	DA	9463	1/1	0.95	0.26	12,12,12,12	0
57	MG	DA	9384	1/1	0.95	0.29	16,16,16,16	0
57	MG	DA	9580	1/1	0.95	0.46	0,0,0,0	0
57	MG	BA	3083	1/1	0.95	0.31	27,27,27,27	1
57	MG	AA	7024	1/1	0.95	0.50	27,27,27,27	0
57	MG	DA	9311	1/1	0.95	0.46	29,29,29,29	0
57	MG	BA	3035	1/1	0.95	0.39	0,0,0,0	0
57	MG	CA	1659	1/1	0.95	0.28	28,28,28,28	0
57	MG	BA	3018	1/1	0.95	0.17	37,37,37,37	0
57	MG	BA	3138	1/1	0.95	0.32	15,15,15,15	0
57	MG	BA	3114	1/1	0.95	0.32	41,41,41,41	0
57	MG	BA	3265	1/1	0.95	0.51	43,43,43,43	0
57	MG	CA	1711	1/1	0.95	0.12	26,26,26,26	0
57	MG	DA	9696	1/1	0.95	0.43	34,34,34,34	0
57	MG	DB	201	1/1	0.95	0.41	22,22,22,22	0
57	MG	DA	9596	1/1	0.95	0.14	27,27,27,27	0
57	MG	CA	1712	1/1	0.95	0.21	34,34,34,34	1
57	MG	DA	9326	1/1	0.95	0.24	1,1,1,1	0
57	MG	AA	7030	1/1	0.95	0.23	2,2,2,2	0
57	MG	CA	1665	1/1	0.95	0.40	16,16,16,16	0
57	MG	DE	301	1/1	0.95	0.32	1,1,1,1	0
57	MG	AA	7095	1/1	0.95	0.08	17,17,17,17	0
57	MG	DA	9485	1/1	0.95	0.41	15,15,15,15	0
57	MG	DA	9330	1/1	0.95	0.35	0,0,0,0	0
57	MG	BA	3309	1/1	0.95	0.79	25,25,25,25	0
57	MG	CA	1719	1/1	0.95	0.35	10,10,10,10	0
57	MG	DU	201	1/1	0.95	0.34	30,30,30,30	1
57	MG	BA	3223	1/1	0.95	0.19	9,9,9,9	0
57	MG	DA	9494	1/1	0.95	0.38	39,39,39,39	0
57	MG	D0	101	1/1	0.95	0.44	27,27,27,27	0
57	MG	DA	9610	1/1	0.95	0.63	19,19,19,19	0
57	MG	BA	3311	1/1	0.95	0.43	13,13,13,13	0
57	MG	D1	102	1/1	0.95	0.18	9,9,9,9	1
57	MG	DA	9497	1/1	0.95	0.36	29,29,29,29	0
57	MG	D5	102	1/1	0.95	0.33	32,32,32,32	1
57	MG	D8	101	1/1	0.95	0.23	3,3,3,3	0
57	MG	BA	3312	1/1	0.95	0.30	45,45,45,45	0
57	MG	BA	3064	1/1	0.95	0.26	29,29,29,29	1
57	MG	CA	1724	1/1	0.95	0.43	5,5,5,5	0
57	MG	BA	3178	1/1	0.95	0.23	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BA	3191	1/1	0.96	0.41	2,2,2,2	0
57	MG	BA	3016	1/1	0.96	0.35	8,8,8,8	0
57	MG	DA	9363	1/1	0.96	0.23	1,1,1,1	0
57	MG	DA	9529	1/1	0.96	0.29	0,0,0,0	0
57	MG	AA	7110	1/1	0.96	0.33	31,31,31,31	0
57	MG	BA	3194	1/1	0.96	0.28	1,1,1,1	0
57	MG	CA	1742	1/1	0.96	0.44	10,10,10,10	0
57	MG	AA	7091	1/1	0.96	0.23	22,22,22,22	0
57	MG	AV	101	1/1	0.96	0.14	2,2,2,2	0
57	MG	DA	9536	1/1	0.96	0.44	0,0,0,0	0
57	MG	DA	9538	1/1	0.96	0.46	1,1,1,1	0
57	MG	BA	3198	1/1	0.96	0.34	0,0,0,0	0
57	MG	DA	9642	1/1	0.96	0.30	1,1,1,1	0
57	MG	BA	3244	1/1	0.96	0.20	1,1,1,1	0
57	MG	BD	302	1/1	0.96	0.27	4,4,4,4	0
57	MG	DA	9646	1/1	0.96	0.22	31,31,31,31	0
57	MG	DA	9647	1/1	0.96	0.61	1,1,1,1	0
57	MG	DA	9543	1/1	0.96	0.30	5,5,5,5	0
57	MG	BA	3071	1/1	0.96	0.31	0,0,0,0	0
57	MG	DA	9545	1/1	0.96	0.43	1,1,1,1	0
57	MG	DA	9547	1/1	0.96	0.22	3,3,3,3	0
57	MG	CA	1693	1/1	0.96	0.39	24,24,24,24	0
57	MG	BA	3139	1/1	0.96	0.46	0,0,0,0	0
57	MG	BA	3004	1/1	0.96	0.59	1,1,1,1	0
57	MG	BA	3054	1/1	0.96	0.33	14,14,14,14	0
57	MG	CA	1648	1/1	0.96	0.42	23,23,23,23	0
57	MG	CA	1698	1/1	0.96	0.14	1,1,1,1	1
57	MG	CA	1649	1/1	0.96	0.10	33,33,33,33	0
57	MG	BA	3167	1/1	0.96	0.17	30,30,30,30	0
57	MG	DA	9305	1/1	0.96	0.46	0,0,0,0	0
57	MG	BA	3056	1/1	0.96	0.24	5,5,5,5	0
57	MG	DA	9664	1/1	0.96	0.54	1,1,1,1	0
57	MG	DA	9560	1/1	0.96	0.26	4,4,4,4	0
57	MG	AA	7017	1/1	0.96	0.08	29,29,29,29	0
57	MG	DA	9387	1/1	0.96	0.76	1,1,1,1	0
57	MG	AA	7087	1/1	0.96	0.13	24,24,24,24	0
57	MG	BA	3211	1/1	0.96	0.17	2,2,2,2	0
57	MG	DA	9391	1/1	0.96	0.17	1,1,1,1	0
57	MG	BA	3146	1/1	0.96	0.71	0,0,0,0	0
57	MG	DA	9318	1/1	0.96	0.40	2,2,2,2	0
57	MG	DA	9675	1/1	0.96	0.29	11,11,11,11	0
57	MG	CA	1602	1/1	0.96	0.16	14,14,14,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	CA	1707	1/1	0.96	0.83	1,1,1,1	1
57	MG	CA	1603	1/1	0.96	0.16	0,0,0,0	0
57	MG	DA	9575	1/1	0.96	0.12	35,35,35,35	0
57	MG	CA	1604	1/1	0.96	0.43	15,15,15,15	0
57	MG	DA	9401	1/1	0.96	0.55	21,21,21,21	1
57	MG	DA	9474	1/1	0.96	0.30	28,28,28,28	0
57	MG	BA	3261	1/1	0.96	0.31	10,10,10,10	0
57	MG	AA	7057	1/1	0.96	0.18	44,44,44,44	0
57	MG	BA	3303	1/1	0.96	0.29	19,19,19,19	0
57	MG	DA	9478	1/1	0.96	0.40	13,13,13,13	0
57	MG	BA	3025	1/1	0.96	0.16	37,37,37,37	0
57	MG	BA	3305	1/1	0.96	0.25	24,24,24,24	0
57	MG	CA	1715	1/1	0.96	0.51	12,12,12,12	0
57	MG	BA	3175	1/1	0.96	0.28	4,4,4,4	0
57	MG	BA	3307	1/1	0.96	0.54	25,25,25,25	0
57	MG	DA	9592	1/1	0.96	0.17	36,36,36,36	0
57	MG	CA	1667	1/1	0.96	0.29	12,12,12,12	0
57	MG	CA	1613	1/1	0.96	0.95	31,31,31,31	0
57	MG	BA	3041	1/1	0.96	0.51	7,7,7,7	0
57	MG	BA	3219	1/1	0.96	0.18	19,19,19,19	0
57	MG	DA	9491	1/1	0.96	0.45	11,11,11,11	0
57	MG	DA	9492	1/1	0.96	0.11	76,76,76,76	0
57	MG	DA	9599	1/1	0.96	0.34	20,20,20,20	0
57	MG	BA	3086	1/1	0.96	0.23	1,1,1,1	0
57	MG	BA	3152	1/1	0.96	0.32	18,18,18,18	0
57	MG	BA	3222	1/1	0.96	0.39	5,5,5,5	0
57	MG	DA	9498	1/1	0.96	0.50	2,2,2,2	0
57	MG	BA	3010	1/1	0.96	0.89	28,28,28,28	0
57	MG	DP	201	1/1	0.96	0.12	7,7,7,7	0
57	MG	AA	7028	1/1	0.96	0.85	30,30,30,30	0
57	MG	DA	9342	1/1	0.96	0.10	0,0,0,0	0
57	MG	AA	7038	1/1	0.96	0.63	10,10,10,10	0
57	MG	BA	3156	1/1	0.96	0.33	19,19,19,19	0
57	MG	DA	9506	1/1	0.96	0.23	0,0,0,0	0
57	MG	CA	1629	1/1	0.96	0.34	37,37,37,37	0
57	MG	DA	9612	1/1	0.96	0.70	1,1,1,1	1
57	MG	DA	9613	1/1	0.96	0.23	5,5,5,5	0
57	MG	DA	9508	1/1	0.96	0.25	0,0,0,0	0
57	MG	DA	9349	1/1	0.96	0.61	3,3,3,3	0
57	MG	CA	1679	1/1	0.96	0.28	9,9,9,9	0
57	MG	D5	101	1/1	0.96	0.36	7,7,7,7	0
57	MG	BA	3092	1/1	0.96	0.17	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	BA	3188	1/1	0.96	0.35	0,0,0,0	0
57	MG	DA	9353	1/1	0.96	0.55	24,24,24,24	0
57	MG	DA	9516	1/1	0.96	0.46	1,1,1,1	0
57	MG	BA	3189	1/1	0.96	0.46	1,1,1,1	0
57	MG	DA	9357	1/1	0.96	0.37	0,0,0,0	0
57	MG	BA	3200	1/1	0.97	0.51	5,5,5,5	0
57	MG	DA	9427	1/1	0.97	0.20	91,91,91,91	0
57	MG	DA	9644	1/1	0.97	0.16	25,25,25,25	0
57	MG	DA	9562	1/1	0.97	0.60	2,2,2,2	0
57	MG	BA	3275	1/1	0.97	0.27	1,1,1,1	1
57	MG	AA	7068	1/1	0.97	0.09	34,34,34,34	0
57	MG	DA	9566	1/1	0.97	0.30	18,18,18,18	0
57	MG	DA	9649	1/1	0.97	0.42	1,1,1,1	0
57	MG	DA	9650	1/1	0.97	0.26	7,7,7,7	0
57	MG	BA	3080	1/1	0.97	0.56	0,0,0,0	0
57	MG	DA	9307	1/1	0.97	0.38	12,12,12,12	0
57	MG	CA	1622	1/1	0.97	0.09	37,37,37,37	0
57	MG	DA	9495	1/1	0.97	0.74	3,3,3,3	0
57	MG	DA	9571	1/1	0.97	0.44	0,0,0,0	0
57	MG	CA	1623	1/1	0.97	0.27	19,19,19,19	0
57	MG	CA	1624	1/1	0.97	0.33	18,18,18,18	0
57	MG	DA	9315	1/1	0.97	0.10	26,26,26,26	0
57	MG	DA	9499	1/1	0.97	0.15	29,29,29,29	0
57	MG	DA	9500	1/1	0.97	0.22	1,1,1,1	0
57	MG	DA	9316	1/1	0.97	0.23	0,0,0,0	0
57	MG	BA	3240	1/1	0.97	0.13	21,21,21,21	0
57	MG	BA	3280	1/1	0.97	0.28	19,19,19,19	1
57	MG	BA	3172	1/1	0.97	0.28	58,58,58,58	0
57	MG	AA	7042	1/1	0.97	0.08	31,31,31,31	0
57	MG	BA	3243	1/1	0.97	0.45	5,5,5,5	0
57	MG	DA	9322	1/1	0.97	0.24	8,8,8,8	0
57	MG	DA	9668	1/1	0.97	0.50	4,4,4,4	0
57	MG	AA	7037	1/1	0.97	0.32	7,7,7,7	0
57	MG	DA	9586	1/1	0.97	0.20	3,3,3,3	0
57	MG	DA	9587	1/1	0.97	0.28	2,2,2,2	0
57	MG	DA	9509	1/1	0.97	0.44	17,17,17,17	0
57	MG	BA	3151	1/1	0.97	0.13	12,12,12,12	0
57	MG	DA	9590	1/1	0.97	0.49	1,1,1,1	0
57	MG	BA	3020	1/1	0.97	0.48	1,1,1,1	0
57	MG	BA	3247	1/1	0.97	0.81	55,55,55,55	0
57	MG	DA	9678	1/1	0.97	0.19	33,33,33,33	0
57	MG	BA	3085	1/1	0.97	0.26	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
57	MG	BD	301	1/1	0.97	0.57	7,7,7,7	0
57	MG	DA	9515	1/1	0.97	0.32	10,10,10,10	0
57	MG	BA	3180	1/1	0.97	0.60	2,2,2,2	0
57	MG	DA	9517	1/1	0.97	0.29	0,0,0,0	0
57	MG	BA	3250	1/1	0.97	0.32	18,18,18,18	0
57	MG	DA	9520	1/1	0.97	0.47	2,2,2,2	0
57	MG	DA	9521	1/1	0.97	0.57	2,2,2,2	0
57	MG	DA	9601	1/1	0.97	0.35	31,31,31,31	0
57	MG	DA	9522	1/1	0.97	0.47	2,2,2,2	0
57	MG	DA	9523	1/1	0.97	0.77	9,9,9,9	0
57	MG	BA	3047	1/1	0.97	0.29	0,0,0,0	0
57	MG	BA	3252	1/1	0.97	0.48	56,56,56,56	0
57	MG	BA	3065	1/1	0.97	0.65	2,2,2,2	0
57	MG	BA	3215	1/1	0.97	0.41	1,1,1,1	0
57	MG	BA	3255	1/1	0.97	0.44	45,45,45,45	0
57	MG	BA	3048	1/1	0.97	0.29	17,17,17,17	0
57	MG	BA	3089	1/1	0.97	0.23	18,18,18,18	0
57	MG	DA	9697	1/1	0.97	0.22	41,41,41,41	0
57	MG	AA	7056	1/1	0.97	0.34	12,12,12,12	0
57	MG	CA	1647	1/1	0.97	0.36	6,6,6,6	0
57	MG	DA	9534	1/1	0.97	0.51	1,1,1,1	0
57	MG	DA	9404	1/1	0.97	0.31	12,12,12,12	0
57	MG	AA	7003	1/1	0.97	0.10	27,27,27,27	0
57	MG	DD	7101	1/1	0.97	0.48	3,3,3,3	0
57	MG	AA	7033	1/1	0.97	0.18	35,35,35,35	0
57	MG	DD	7103	1/1	0.97	0.42	0,0,0,0	0
57	MG	DA	9617	1/1	0.97	0.29	11,11,11,11	0
57	MG	DA	9343	1/1	0.97	0.27	2,2,2,2	0
57	MG	DA	9344	1/1	0.97	0.44	33,33,33,33	0
57	MG	DA	9621	1/1	0.97	0.59	0,0,0,0	1
57	MG	DA	9411	1/1	0.97	0.27	2,2,2,2	0
57	MG	DA	9623	1/1	0.97	0.37	13,13,13,13	0
57	MG	BA	3011	1/1	0.97	0.52	36,36,36,36	0
57	MG	BA	3190	1/1	0.97	0.47	8,8,8,8	0
57	MG	DA	9414	1/1	0.97	0.81	16,16,16,16	0
57	MG	DA	9546	1/1	0.97	0.34	2,2,2,2	0
57	MG	CA	1652	1/1	0.97	0.60	6,6,6,6	0
57	MG	AA	7099	1/1	0.97	0.36	6,6,6,6	0
57	MG	BA	3055	1/1	0.97	0.20	11,11,11,11	0
57	MG	AA	7007	1/1	0.97	0.14	1,1,1,1	0
57	MG	BA	3165	1/1	0.97	0.57	0,0,0,0	0
57	MG	BA	3040	1/1	0.97	0.27	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
57	MG	BA	3270	1/1	0.97	0.51	0,0,0,0	1
57	MG	CA	1611	1/1	0.97	0.54	0,0,0,0	0
57	MG	DA	9637	1/1	0.97	0.37	18,18,18,18	0
57	MG	AA	7025	1/1	0.97	0.21	1,1,1,1	0
57	MG	BA	3121	1/1	0.97	0.60	1,1,1,1	0
59	ZN	AN	101	1/1	0.97	0.10	147,147,147,147	0
57	MG	BA	3100	1/1	0.97	0.15	21,21,21,21	0
57	MG	CA	1620	1/1	0.98	0.27	1,1,1,1	0
57	MG	BA	3124	1/1	0.98	0.20	17,17,17,17	0
57	MG	BA	3179	1/1	0.98	0.31	10,10,10,10	0
57	MG	BA	3260	1/1	0.98	0.57	8,8,8,8	0
57	MG	BA	3142	1/1	0.98	0.43	10,10,10,10	0
57	MG	DA	9386	1/1	0.98	0.46	2,2,2,2	0
57	MG	DA	9584	1/1	0.98	0.36	0,0,0,0	0
57	MG	BA	3125	1/1	0.98	0.29	20,20,20,20	0
57	MG	BA	3182	1/1	0.98	0.57	2,2,2,2	0
57	MG	DA	9449	1/1	0.98	0.43	0,0,0,0	0
57	MG	AA	7077	1/1	0.98	0.16	22,22,22,22	0
57	MG	DA	9390	1/1	0.98	0.28	0,0,0,0	0
57	MG	BA	3206	1/1	0.98	0.45	29,29,29,29	0
57	MG	DA	9392	1/1	0.98	0.70	12,12,12,12	0
57	MG	BA	3234	1/1	0.98	0.56	10,10,10,10	0
57	MG	BA	3207	1/1	0.98	0.38	1,1,1,1	0
57	MG	BA	3027	1/1	0.98	0.34	4,4,4,4	0
57	MG	BA	3237	1/1	0.98	0.24	43,43,43,43	0
57	MG	DA	9524	1/1	0.98	0.36	2,2,2,2	0
57	MG	DA	9672	1/1	0.98	0.37	5,5,5,5	0
57	MG	BA	3238	1/1	0.98	0.33	9,9,9,9	0
57	MG	BA	3034	1/1	0.98	0.22	7,7,7,7	0
57	MG	DA	9400	1/1	0.98	0.41	0,0,0,0	0
57	MG	BA	3210	1/1	0.98	0.74	11,11,11,11	0
57	MG	AA	7035	1/1	0.98	0.11	42,42,42,42	0
57	MG	BA	3060	1/1	0.98	0.57	1,1,1,1	0
57	MG	DA	9346	1/1	0.98	0.30	0,0,0,0	0
57	MG	BA	3051	1/1	0.98	0.40	6,6,6,6	0
57	MG	DA	9406	1/1	0.98	0.18	32,32,32,32	0
57	MG	BA	3072	1/1	0.98	0.17	25,25,25,25	0
57	MG	DA	9408	1/1	0.98	0.25	3,3,3,3	0
57	MG	BA	3073	1/1	0.98	0.67	8,8,8,8	0
57	MG	DA	9537	1/1	0.98	0.38	0,0,0,0	0
57	MG	BA	3008	1/1	0.98	0.46	2,2,2,2	0
57	MG	BA	3279	1/1	0.98	0.24	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	DA	9472	1/1	0.98	0.41	16,16,16,16	0
57	MG	BA	3009	1/1	0.98	0.15	2,2,2,2	0
57	MG	DA	9542	1/1	0.98	0.35	6,6,6,6	0
57	MG	CA	1718	1/1	0.98	0.27	27,27,27,27	0
57	MG	DA	9355	1/1	0.98	0.67	0,0,0,0	0
57	MG	DA	9308	1/1	0.98	0.44	2,2,2,2	0
57	MG	DA	9309	1/1	0.98	0.34	6,6,6,6	0
57	MG	DA	9619	1/1	0.98	0.15	0,0,0,0	0
57	MG	DA	9310	1/1	0.98	0.29	0,0,0,0	0
57	MG	DA	9479	1/1	0.98	0.63	0,0,0,0	0
57	MG	DA	9359	1/1	0.98	0.38	0,0,0,0	0
57	MG	DA	9481	1/1	0.98	0.09	0,0,0,0	0
57	MG	DA	9360	1/1	0.98	0.36	7,7,7,7	0
57	MG	BA	3218	1/1	0.98	0.30	24,24,24,24	0
57	MG	DA	9362	1/1	0.98	0.34	5,5,5,5	0
57	MG	DA	9627	1/1	0.98	0.29	0,0,0,0	1
57	MG	DA	9554	1/1	0.98	0.27	10,10,10,10	0
57	MG	DA	9312	1/1	0.98	0.67	4,4,4,4	0
57	MG	DA	9364	1/1	0.98	0.82	1,1,1,1	0
57	MG	CA	1645	1/1	0.98	0.35	20,20,20,20	0
57	MG	DA	9558	1/1	0.98	0.15	6,6,6,6	0
57	MG	DA	9488	1/1	0.98	0.56	0,0,0,0	0
57	MG	BA	3015	1/1	0.98	0.20	3,3,3,3	0
57	MG	BA	3316	1/1	0.98	0.42	7,7,7,7	0
57	MG	BA	3105	1/1	0.98	0.69	26,26,26,26	0
57	MG	BA	3091	1/1	0.98	0.19	0,0,0,0	0
57	MG	DU	202	1/1	0.98	0.15	6,6,6,6	0
57	MG	DA	9564	1/1	0.98	0.58	17,17,17,17	0
57	MG	DA	9493	1/1	0.98	0.26	1,1,1,1	0
57	MG	BA	3046	1/1	0.98	0.64	1,1,1,1	0
57	MG	DA	9641	1/1	0.98	0.07	11,11,11,11	0
57	MG	DA	9430	1/1	0.98	0.39	0,0,0,0	0
57	MG	BA	3197	1/1	0.98	0.22	1,1,1,1	0
57	MG	CA	1615	1/1	0.98	0.27	0,0,0,0	0
57	MG	BA	3176	1/1	0.98	0.33	0,0,0,0	0
57	MG	CA	1729	1/1	0.98	0.43	35,35,35,35	0
57	MG	BA	3288	1/1	0.98	0.14	18,18,18,18	0
57	MG	DA	9324	1/1	0.98	0.48	2,2,2,2	0
57	MG	DA	9437	1/1	0.98	0.19	14,14,14,14	0
57	MG	BA	3078	1/1	0.98	0.43	2,2,2,2	0
57	MG	CA	1619	1/1	0.98	0.52	11,11,11,11	0
59	ZN	CD	301	1/1	0.98	0.32	44,44,44,44	0

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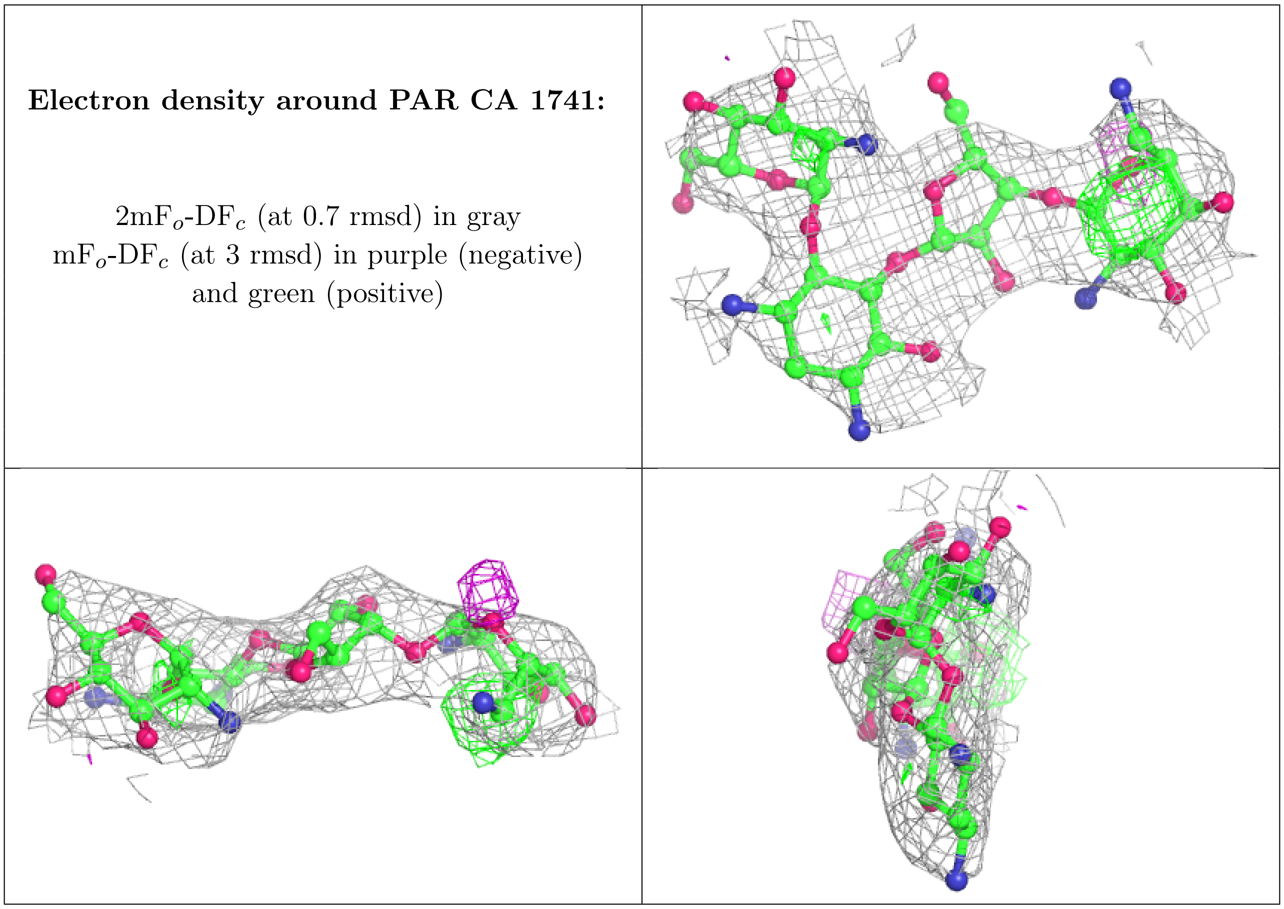
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
57	MG	CA	1733	1/1	0.98	0.46	11,11,11,11	0
57	MG	BA	3299	1/1	0.99	0.48	10,10,10,10	0
57	MG	BA	3239	1/1	0.99	0.35	1,1,1,1	0
57	MG	DA	9369	1/1	0.99	0.59	0,0,0,0	0
57	MG	BE	303	1/1	0.99	0.15	1,1,1,1	0
57	MG	BA	3224	1/1	0.99	0.17	5,5,5,5	0
57	MG	BA	3259	1/1	0.99	0.32	18,18,18,18	0
57	MG	BA	3084	1/1	0.99	0.50	1,1,1,1	0
57	MG	AA	7019	1/1	0.99	0.56	16,16,16,16	0
57	MG	DA	9354	1/1	0.99	0.49	2,2,2,2	0
57	MG	DA	9518	1/1	0.99	0.35	0,0,0,0	0
57	MG	DA	9398	1/1	0.99	0.44	0,0,0,0	0
57	MG	DU	203	1/1	0.99	0.14	0,0,0,0	1
57	MG	BA	3013	1/1	0.99	0.30	16,16,16,16	0
57	MG	AA	7006	1/1	0.99	0.37	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

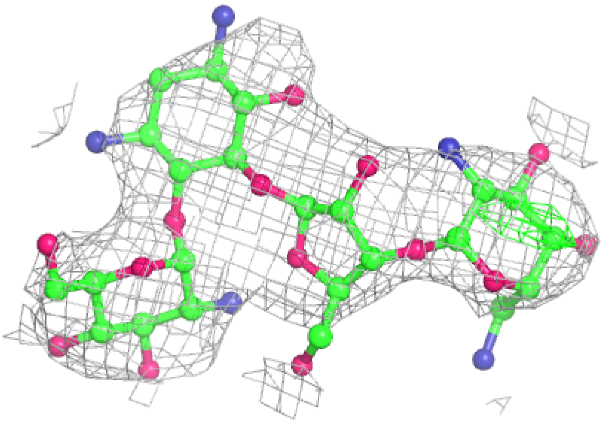


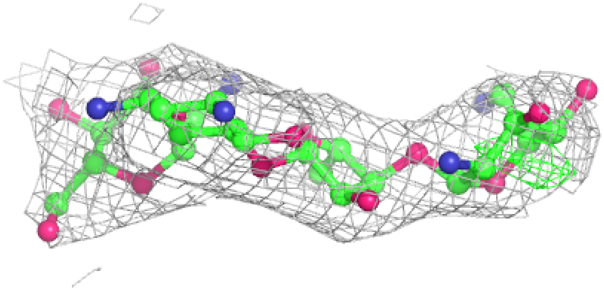
Electron density around PAR CA 1741:

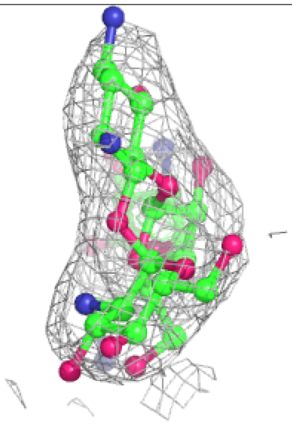
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around PAR AA 7111:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers

There are no such residues in this entry.