



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:37 AM UTC

PDB ID : 4V97 / pdb_00004v97
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

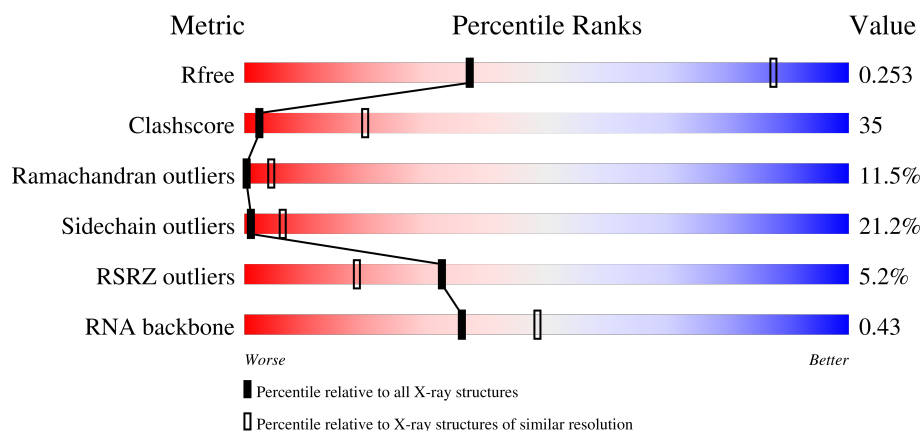
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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.



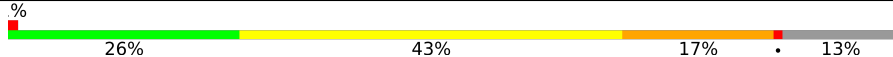
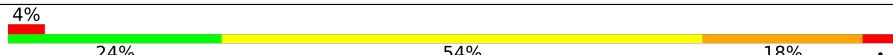
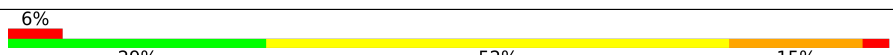
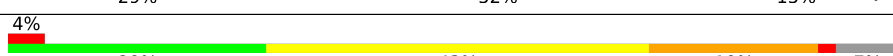
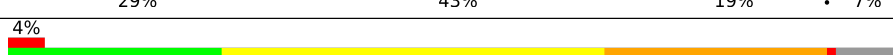
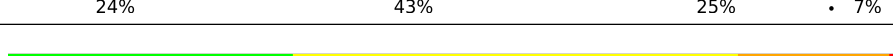
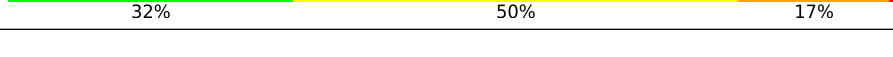
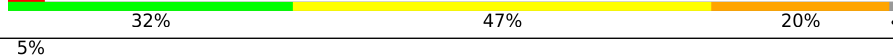
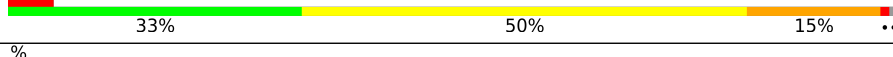
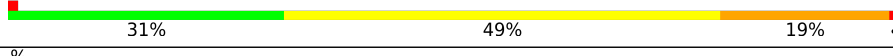
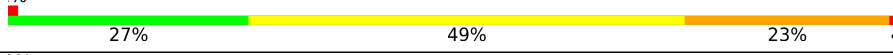
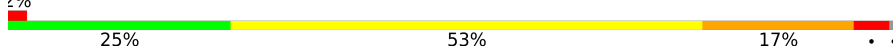
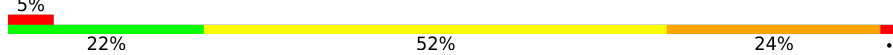
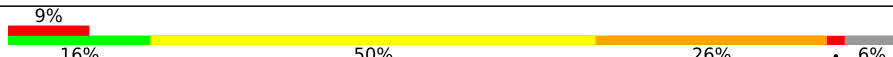
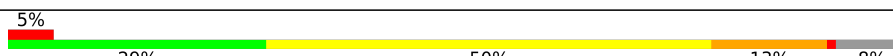
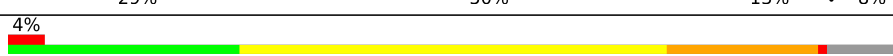
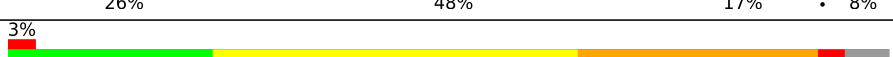
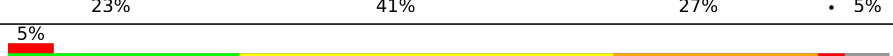
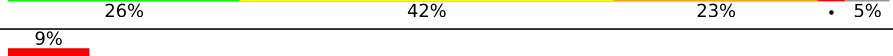
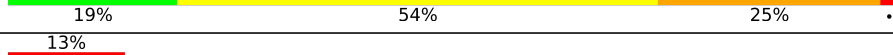
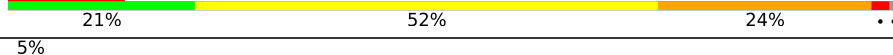
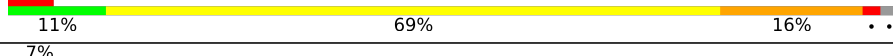
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)
RNA backbone	3983	1018 (4.00-3.04)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	5% 49% 35% 15%
1	CA	1522	5% 49% 34% 16%
2	AB	256	2% 20% 50% 20% 8%
2	CB	256	2% 16% 50% 23% 8%

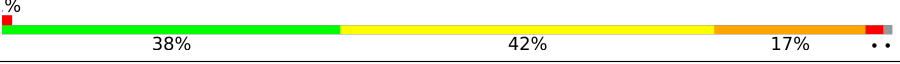
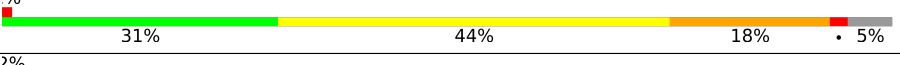
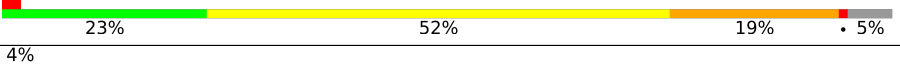
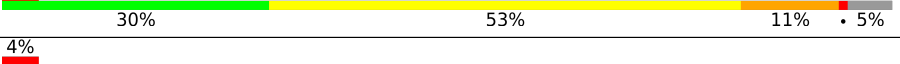
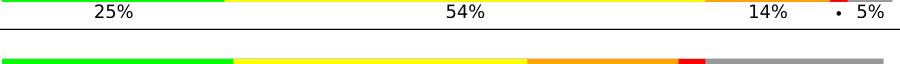
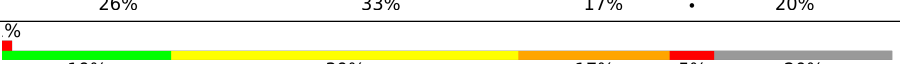
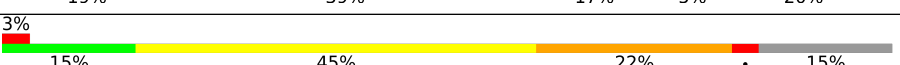
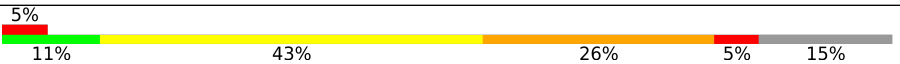
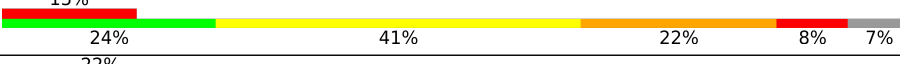
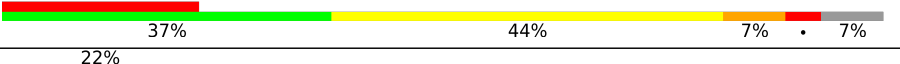
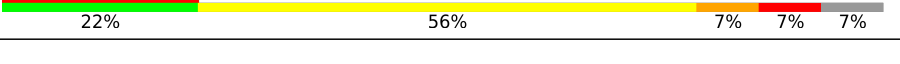
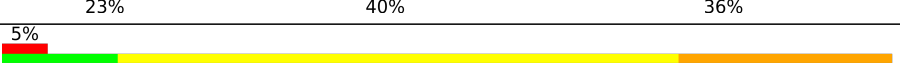
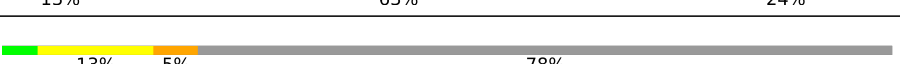
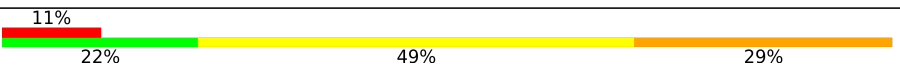
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
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	
40	BT	146	
40	DT	146	
41	BU	118	
41	DU	118	
42	BV	101	
42	DV	101	
43	BW	113	
43	DW	113	
44	BX	96	
44	DX	96	
45	BY	110	
45	DY	110	
46	BZ	206	
46	DZ	206	
47	B0	85	
47	D0	85	
48	B1	98	
48	D1	98	
49	B2	72	
49	D2	72	
50	B3	60	
50	D3	60	
51	B4	71	
51	D4	71	

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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	7008	-	-	-	X
57	MG	AA	7090	-	-	-	X
57	MG	BA	3101	-	-	-	X
57	MG	DA	9358	-	-	-	X
57	MG	DA	9399	-	-	-	X
57	MG	DB	204	-	-	-	X
59	ZN	CN	101	-	-	X	-

2 Entry composition

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
1	AA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32328	14390	5992	10443	1503			

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
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			
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
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			1619	723	290	531	75			
23	AY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			
23	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
23	CY	17	Total	C	N	O	P	0	0	0
			365	163	68	117	17			

- Molecule 24 is a RNA chain called mRNA.

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

- 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	0	0	0
			1145	712	232	198	3			
36	DP	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- 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	0	0	0
			1122	715	212	188	7			
37	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

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

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

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

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

- 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	0	0	1
			1142	710	235	196	1			
40	DT	138	Total	C	N	O	S	0	0	1
			1142	710	235	196	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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	0	0	0
			459	288	90	76	5			
52	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- 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	0	0	1
			381	235	78	64	4			
53	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- 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	0	0	1
			419	257	105	55	2			
54	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- 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	0	0	1
			508	326	102	78	2			
55	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- 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	0	0	0
			299	183	67	46	3			
56	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

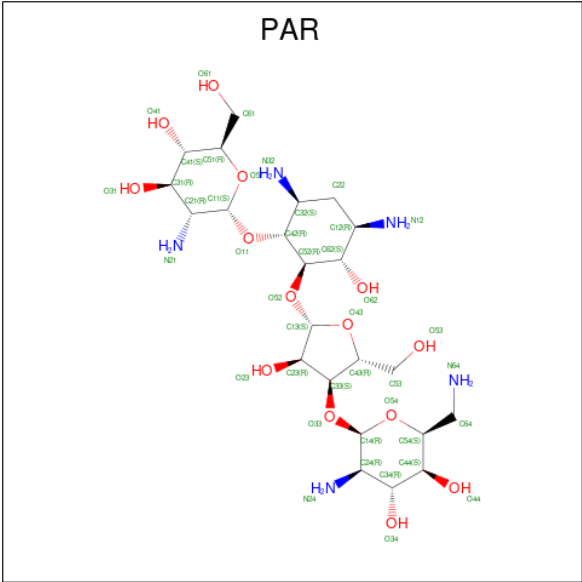
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
57	AA	110	Total Mg 110 110	0	0
57	AE	1	Total Mg 1 1	0	0
57	AV	5	Total Mg 5 5	0	0
57	AX	1	Total Mg 1 1	0	0
57	BA	323	Total Mg 323 323	0	0
57	BB	5	Total Mg 5 5	0	0
57	BD	2	Total Mg 2 2	0	0
57	BE	3	Total Mg 3 3	0	0
57	BF	1	Total Mg 1 1	0	0
57	BN	1	Total Mg 1 1	0	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 5	Mg 5	0	0
57	DD	3	Total 3	Mg 3	0	0
57	DE	2	Total 2	Mg 2	0	0
57	DF	1	Total 1	Mg 1	0	0
57	DP	3	Total 3	Mg 3	0	0
57	DQ	1	Total 1	Mg 1	0	0
57	DU	3	Total 3	Mg 3	0	0
57	DW	1	Total 1	Mg 1	0	0
57	DX	1	Total 1	Mg 1	0	0
57	D0	2	Total 2	Mg 2	0	0
57	D1	2	Total 2	Mg 2	0	0
57	D2	1	Total 1	Mg 1	0	0
57	D5	2	Total 2	Mg 2	0	0
57	D8	1	Total 1	Mg 1	0	0

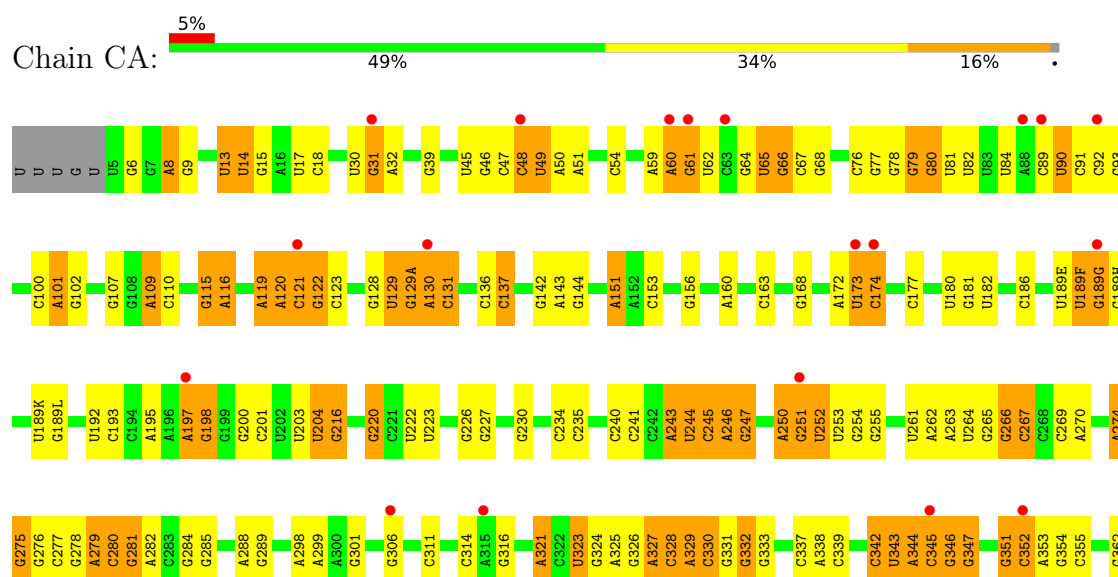
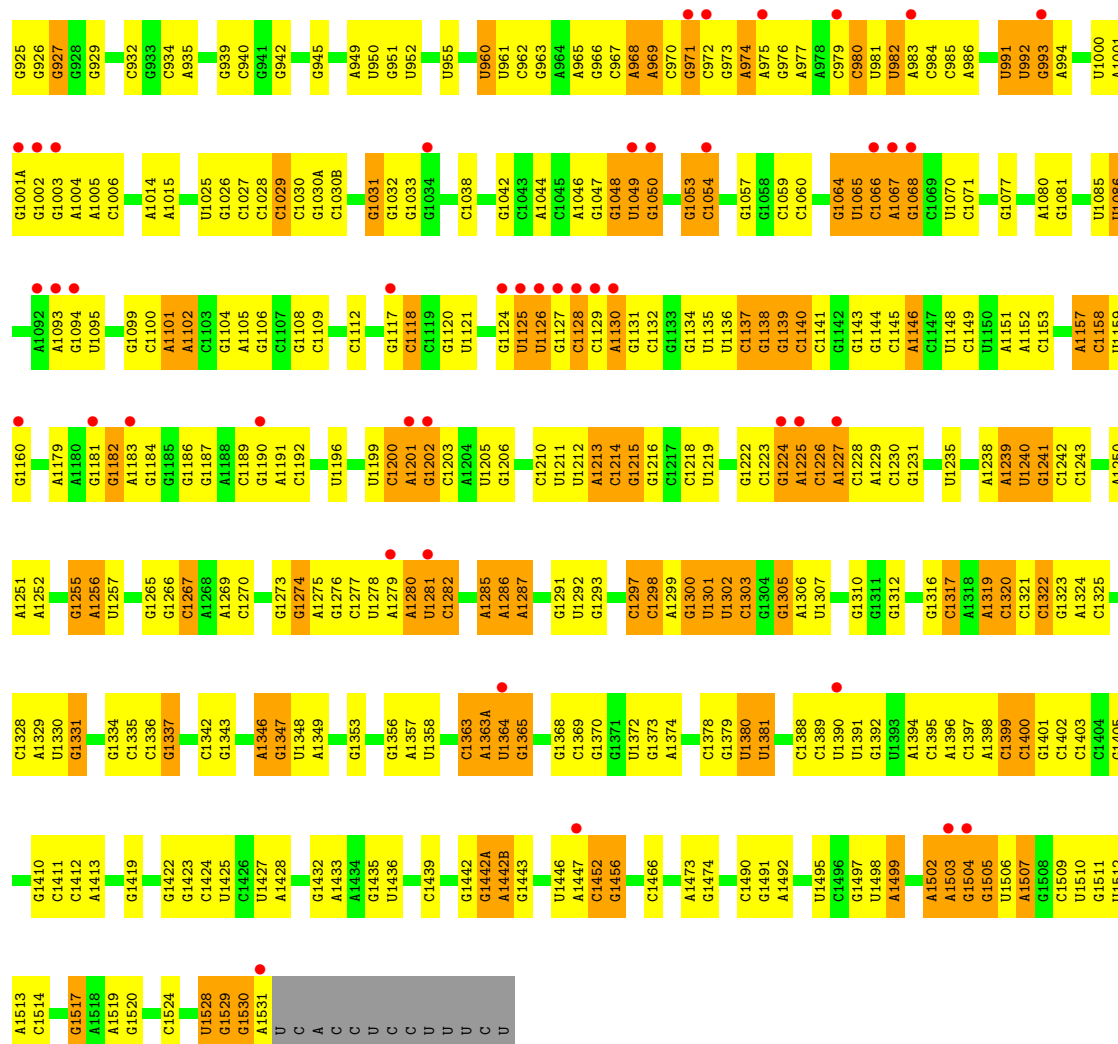
- Molecule 58 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



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

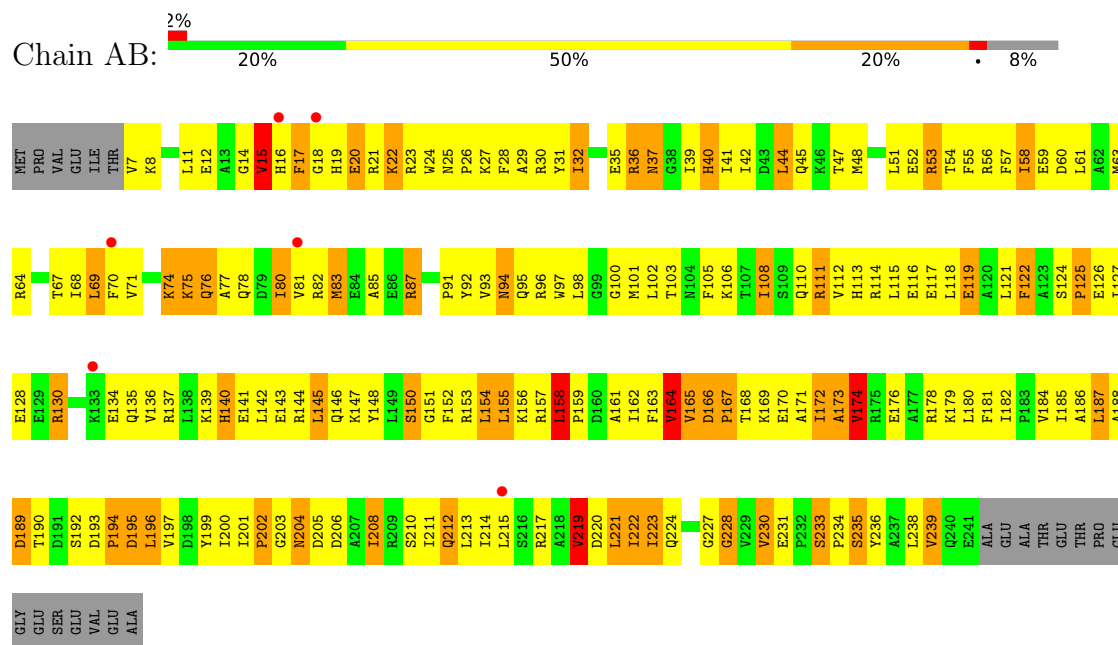
- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

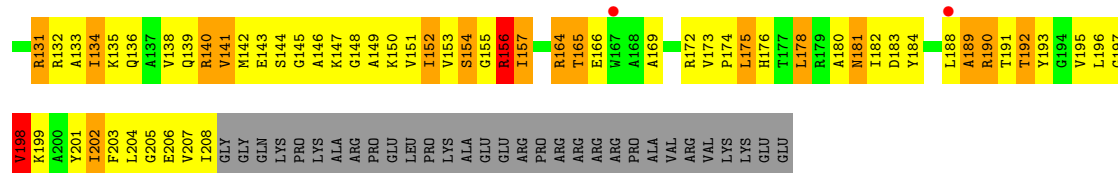
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AD	1	Total	Zn	0	0
			1	1		
59	AN	1	Total	Zn	0	0
			1	1		
59	CD	1	Total	Zn	0	0
			1	1		
59	CN	1	Total	Zn	0	0
			1	1		



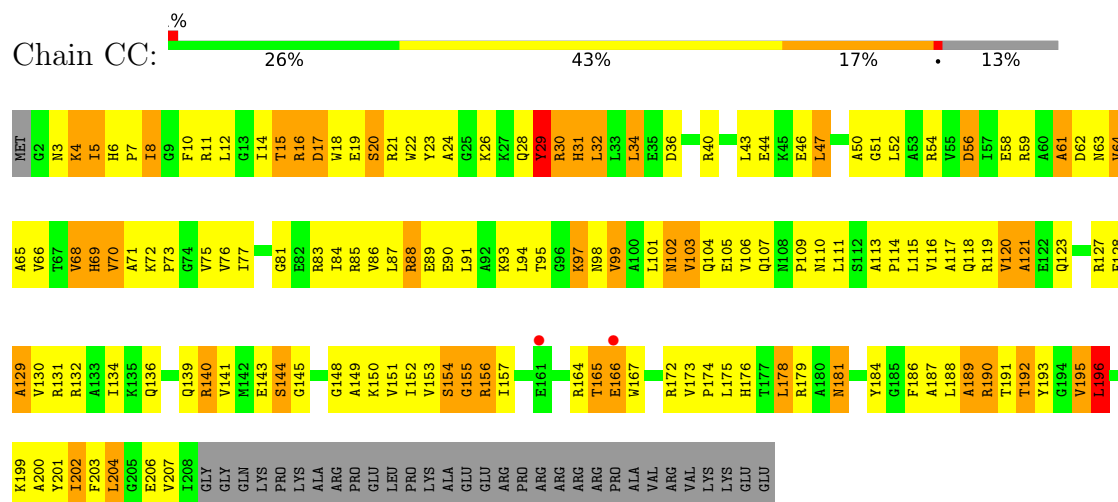
U1522	A1433	C1359	A1288	U211	A1130	A1046	A985	G858	C747	G657	G538	C442	A383
U1528	A1434	A1360	G1290	U1212	G1131	G1047	G966	A859	C748	G662	G542	C443	A364
G1529	G1435	C1363	G1291	A1213	G1132	U1048	C957	A860	C749	A663	G546	C444	U365
G1530	U1436	U1292	G1292	C1214	G1133	U1049	A968	G861	G748	A664	G547	C445	U367
	C1439	A1363A	G1293	G1215	G1134	G1050	A969	G869	U751	A665	G548	C446	
	G1440	G1365	G1294	U1216	U1135	U1051	G970	U870	G752	G666			G371
U	G1441	G1366	G1295	G1217	U1136	U1052	G971	U871	G753	G667			C372
C	G1442	C1367	C1296	C1218	C1137	G1053	G972	A872	G754	G668	A559	A452	C373
A	G1443	G1370	C1297	U1219	G1138	C1054	G973	A873	G755	G669	U560	A453	A374
C	G1442A	C1298	C1298	U1220	G1139	U1055	A974	G874	C756	G670	U561		U375
U	G1443	G1300	G1299	G1223	C1140	U1056	A975		U757	G671	C562	C460	G376
C	G1444	U1301	G1294	G1224	G1141	G1057	G976	C877	G758	G672	A563	C470	G377
C	G1445	U1302	G1295	A1225	G1142	G1058	G977	G878		G673	C564	C471	G378
U	G1446	G1143	C1226	G1143	G1144	C1059	A978		C764	G674	U565	A472	C379
U	A1447	C1144	A1227	G1144	C1145	U1060	C979	G881	G765	A675	C566	C473	G380
U	G1452	A1375	C1228	C1145	C1146	G1061	U981		G766	A676	C567	C474	C381
C	G1456	U1376	A1229	U1146	C1147	U1062	U982	G885	A777	U677			A382
U	G1457	A1377	G1230	U1148	C1148	G1063	A983	G886		U686	A572		A383
U	G1458	U1380	U1307	C1149	U1149	U1065	G984	G887	G786	A887	A573	U480	G384
G1459	A1460	U1381	U1308	U1150	U1150	U1066	C985	G888		A888	A574	C481	
		G1386	C1314	C1236	C1151	U1067	A986	A889	A790	C889	C575	C482	U387
A1468	A1469		G1315	A1237	A1152	A1067	U991	G890	G791	G690	C576	C483	G388
		C1389	G1316	U1238	A1153	C1069	U992	A901	A792	G691	C577	C484	A389
C1478		U1390		A1239	C1153		G993	G902	A793		C578	C485	G390
C1479		U1391	A1319	U1240		G1074	A994		A794	C701	C579	U486	G391
	G1487	U1392	G1320	G1241	A1157	G1077	C995	G906	C797	A702	U580	A487	
		U1393	C1321	C1244	C1158	G1077				G703	C581		G396
		A1394	C1322	A1245	U1159	A1080	U1000	A913	C812	A704	C595	C490	A397
		C1395	G1323	C1246	U1160	G1081	G1001	A914	U813	U705	C596	C491	C398
	G1491	A1396	A1323	U1247	C1162		G1001A	A915	A814	A706			C401
A1492		C1397	C1325	U1248	C1163	G1084	G1002		A815	C707	C599		C402
A1493		A1398	C1326	C1249	C1164	U1085	G1003	U921	A816	C708			U405
		C1400	C1327	A1250	C1171	U1086	A1004	G922	C817	G709	A607	U498	U406
	G1497	G1401	C1328	A1251	G1172	U1086	A1005	A923	G818	G710	A608	C500	G407
	U1498			A1252	G1178	G1094	G924	G925	A819	G713	A609		
A1499		C1402	G1331			U1095	A1014	G926	U820	G714	C508	C508	
A1500		C1403		G1255	G1181	U1096	A1015	G927	G821	A715	A509	A510	A411
A1502		G1404	G1334	U1257	G1182	C1097			G823	A716	C624	C511	A412
A1503		U1406	C1335	U1258	A1183	U1025	G1026	C934	G824	G721	U626	U512	A413
G1504		C1407	G1336	C1259	G1184	G1027	G1027	A935	G825	A722	G627		A414
G1505			G1337		C1189	A1101	G1028		C826	U723	G628		
U1506		C1412	A1339	G1266	G1190	G1108	C1029	G945	U827	G724	G629	U421	U421
A1507		A1413	A1340	C1267	A1191	C1109	C1030	A946	A828	G725	G630	C422	C422
G1508		U1414	C1341	A1268	C1192	G1120	G1030A	G947	C726	G726	G631	G423	G423
C1509		G1415	C1342	A1269	G1193	C1112	G1030B	C948	C834	G727	G633	G424	G424
U1510				C1270		C1118	G1030C	A949		A728	C534	G425	G425
G1511		A1346			U1196	C1119	A1030D	U950	G837	A729	G635	U427	U427
U1512		G1347		U1278	G1197	G1119	G1031	G951	G838	G730	U636	G428	G428
A1513		U1348		A1279	G1198	U1120	G1032	U952	U839	G731	U641	C528	C528
C1514		G1423		A1280	U1199	U1121	G1033	G953	C840	C732	A642	C529	A430
C1515				U1281	C1200	G1124	G1037	G954	U841	A733			
G1516		U1427	C1352	C1282	A1201	U1125	C1038	C848	C849	C736	C543	A532	C435
A1517		A1428	G1353		C1202	U1126	G1039	U960		A737		A533	C436
A1518		C1429		A1285	C1203	G1127	C1039	U961		C738	U652	U534	U437
A1519		C1430		A1286	U1204	G1128	A1044	G962	G854		A653	A535	G438
G1520		C1431		A1287	U1205	C1129	C1045	G963	G855		C536	C439	A439
		G1432		A1288				A964		G741	C556	U537	A441

- Molecule 2: 30S ribosomal protein S2

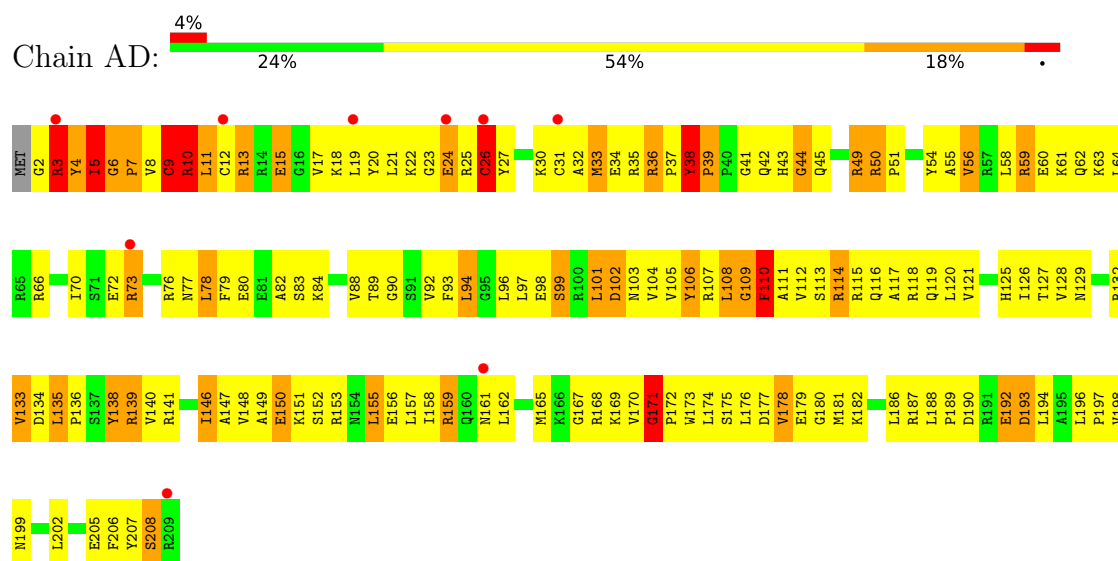




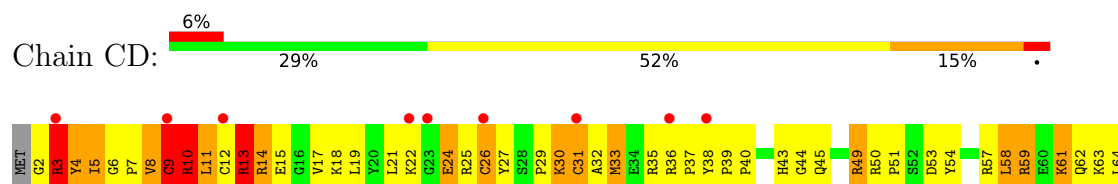
• Molecule 3: 30S ribosomal protein S3

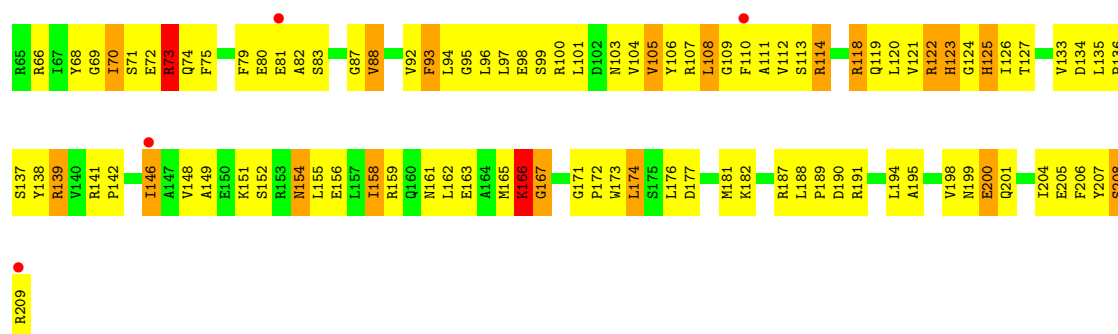


• Molecule 4: 30S ribosomal protein S4

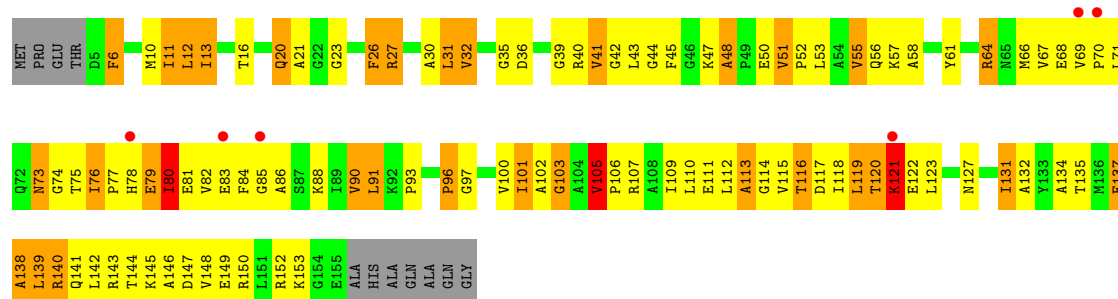


• Molecule 4: 30S ribosomal protein S4

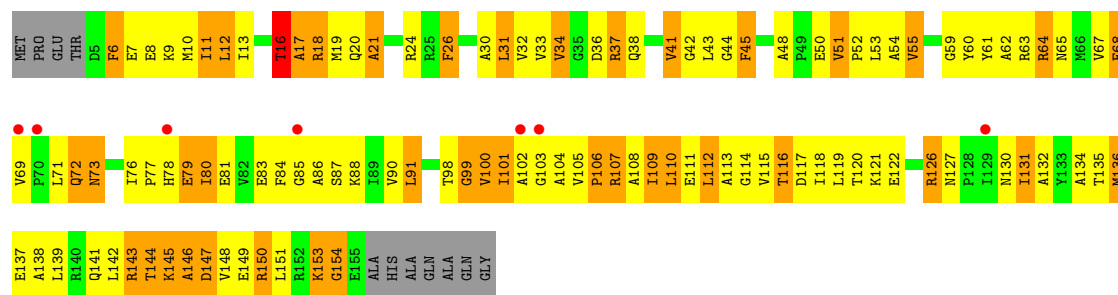




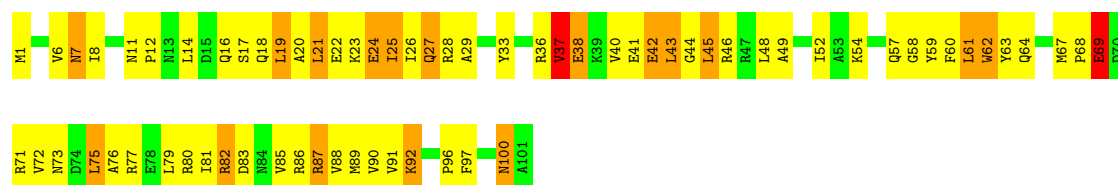
• Molecule 5: 30S ribosomal protein S5



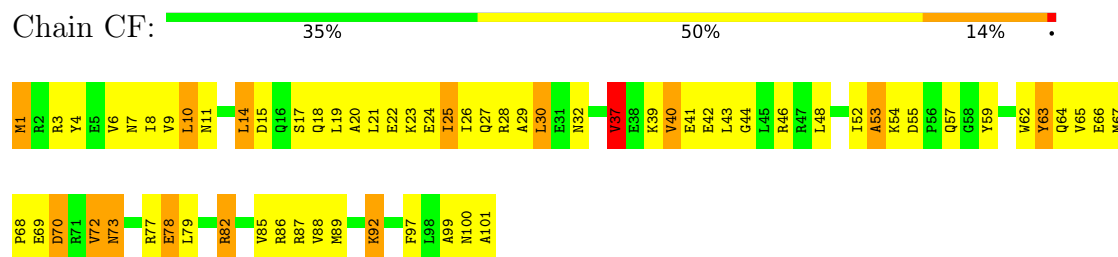
• Molecule 5: 30S ribosomal protein S5



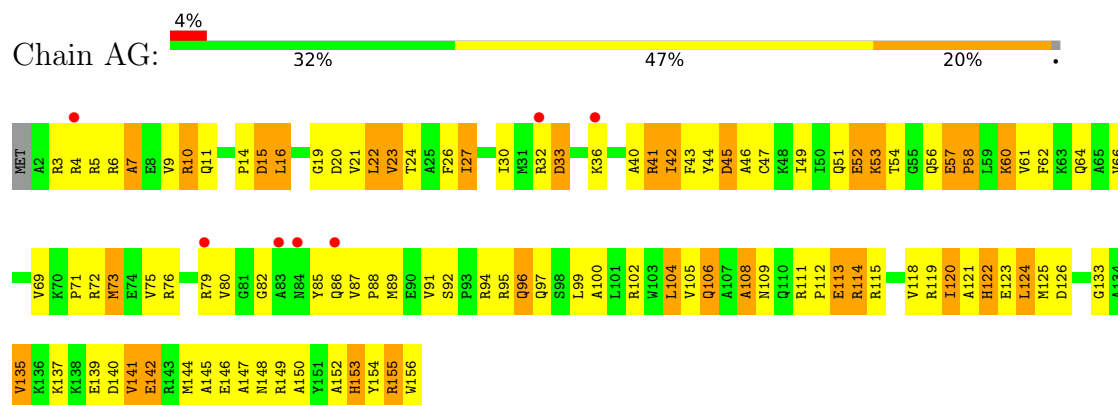
• Molecule 6: 30S ribosomal protein S6



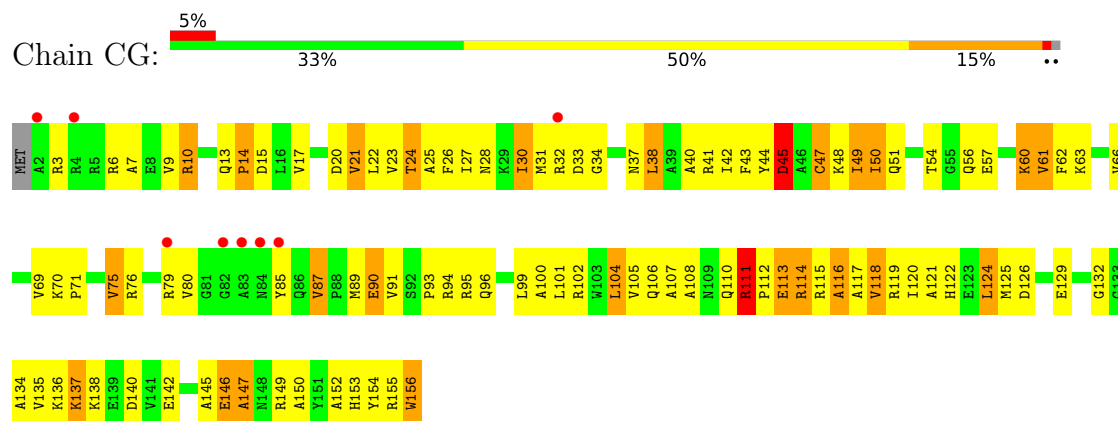
• Molecule 6: 30S ribosomal protein S6



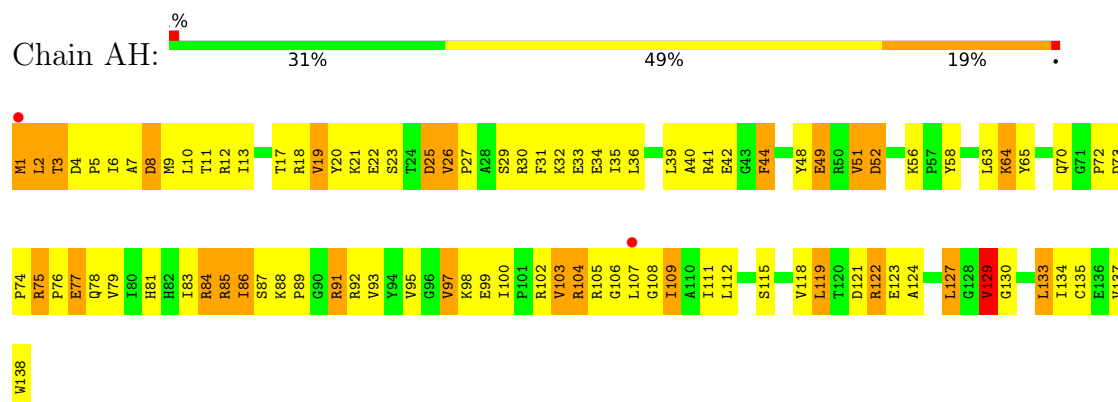
• Molecule 7: 30S ribosomal protein S7



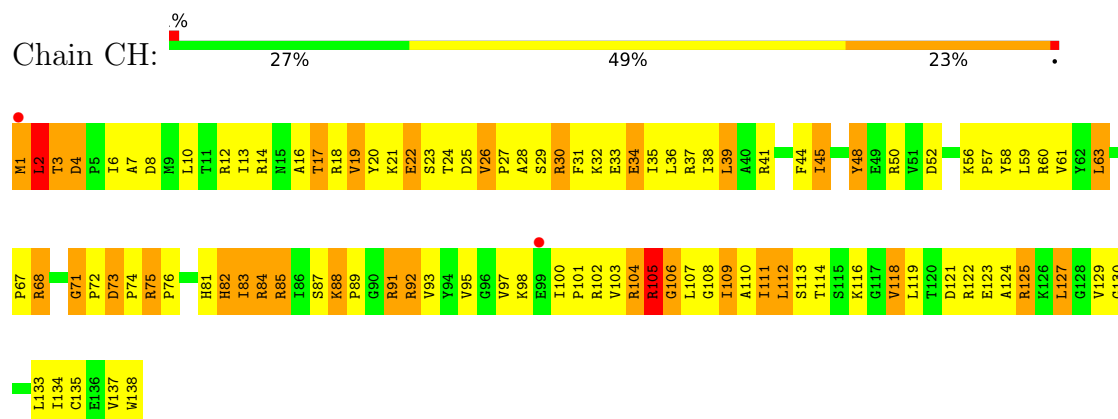
• Molecule 7: 30S ribosomal protein S7



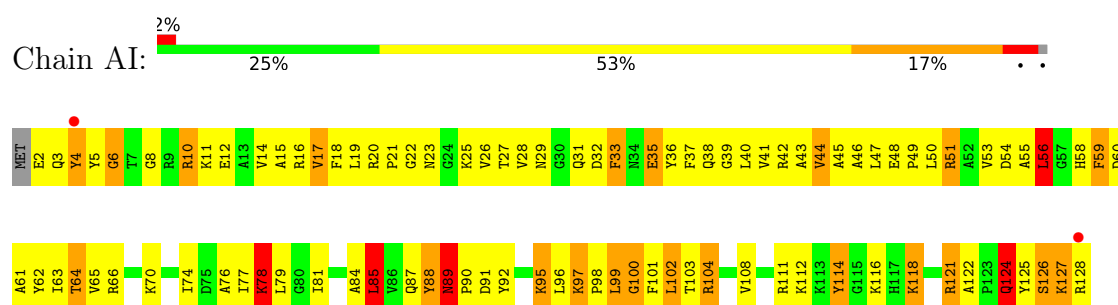
• Molecule 8: 30S ribosomal protein S8



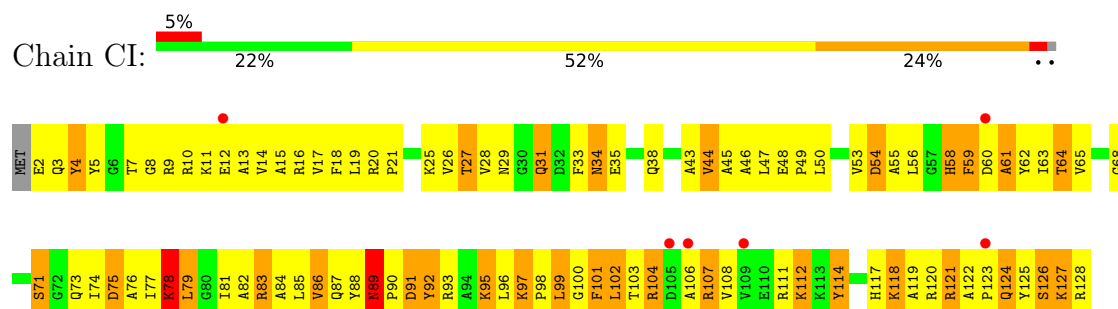
- Molecule 8: 30S ribosomal protein S8



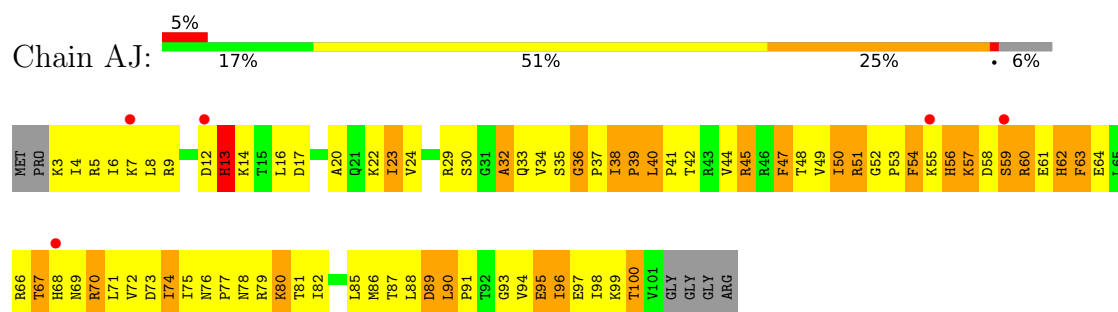
- Molecule 9: 30S ribosomal protein S9



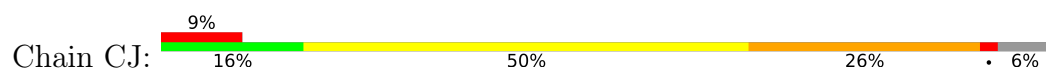
- Molecule 9: 30S ribosomal protein S9

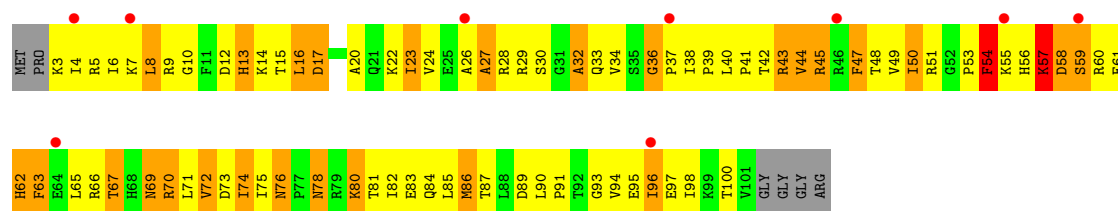


- Molecule 10: 30S ribosomal protein S10

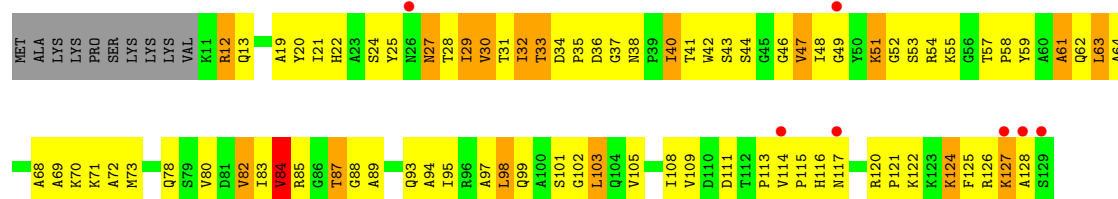


- Molecule 10: 30S ribosomal protein S10

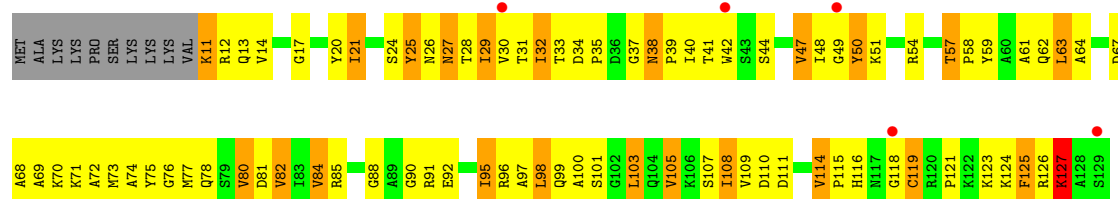




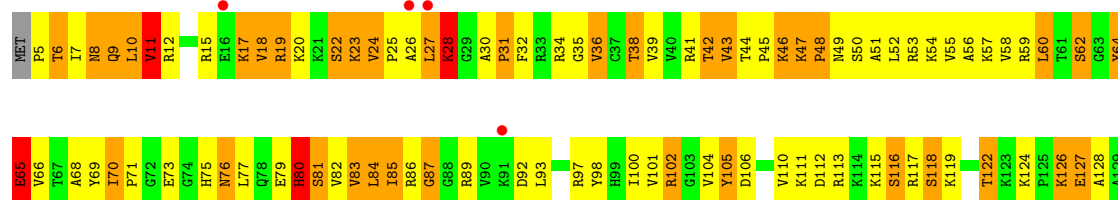
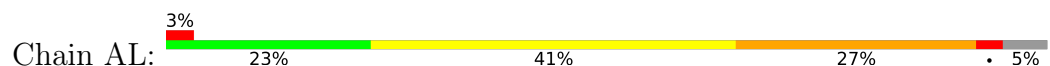
• Molecule 11: 30S ribosomal protein S11



• Molecule 11: 30S ribosomal protein S11



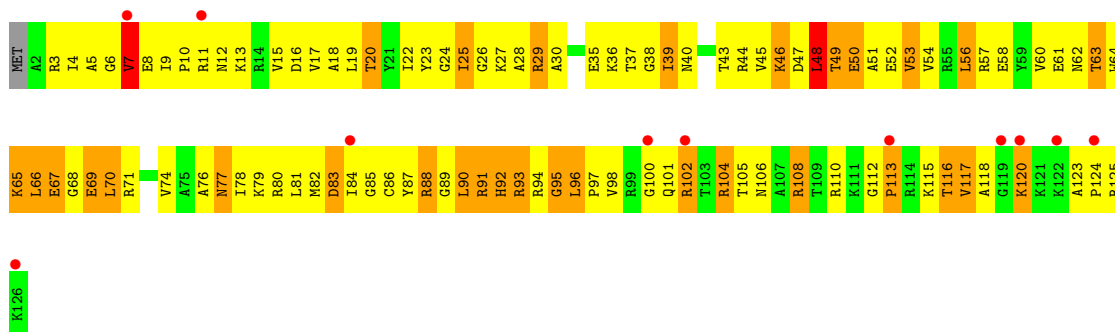
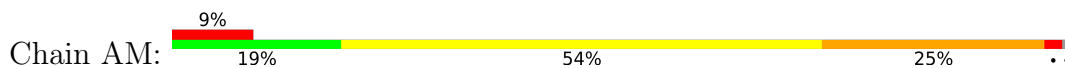
• Molecule 12: 30S ribosomal protein S12



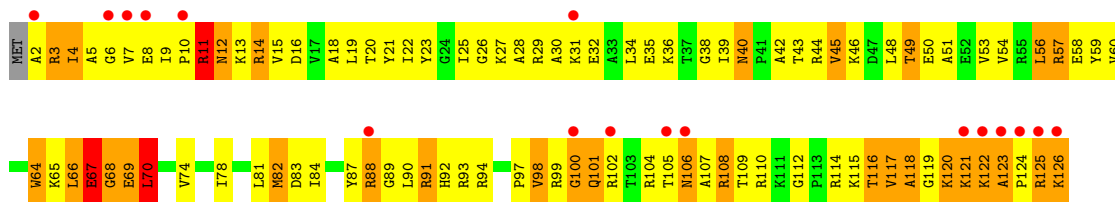
• Molecule 12: 30S ribosomal protein S12



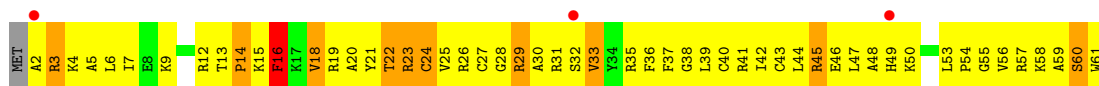
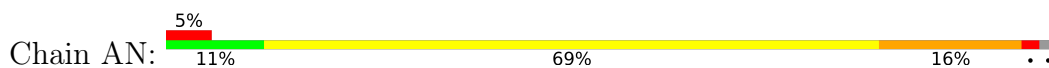
- Molecule 13: 30S ribosomal protein S13



- Molecule 13: 30S ribosomal protein S13



- Molecule 14: 30S ribosomal protein S14 type Z

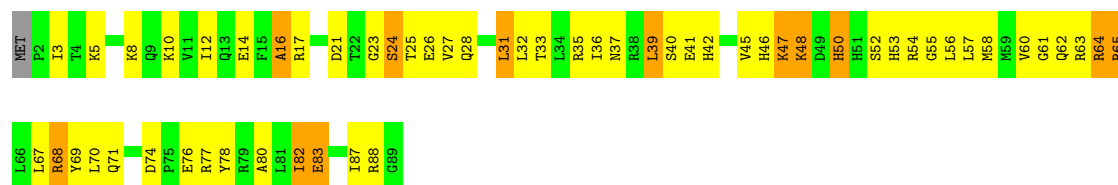


- Molecule 14: 30S ribosomal protein S14 type Z

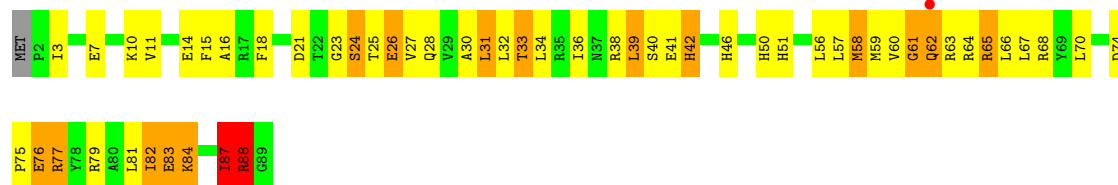
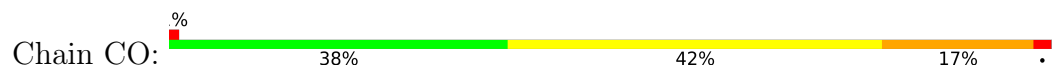


- Molecule 15: 30S ribosomal protein S15

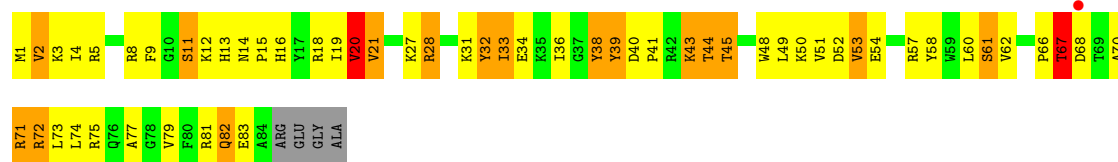




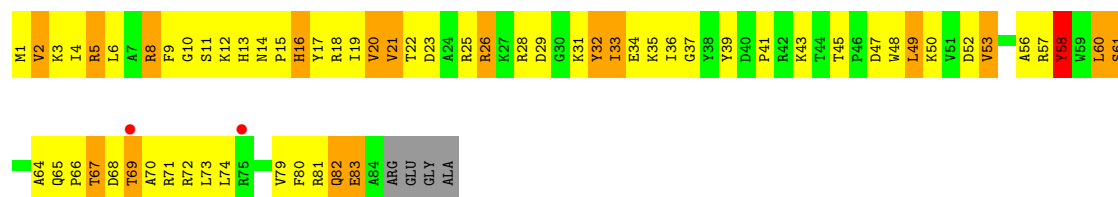
• Molecule 15: 30S ribosomal protein S15



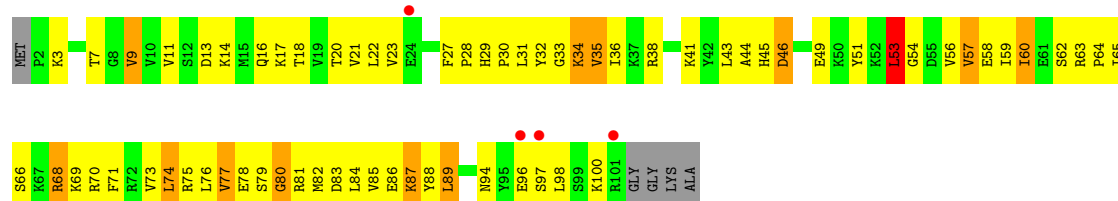
• Molecule 16: 30S ribosomal protein S16



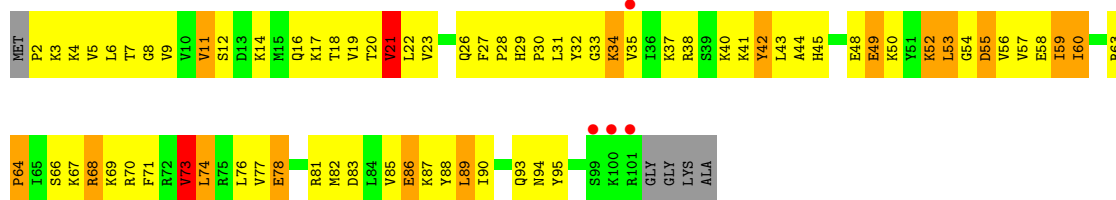
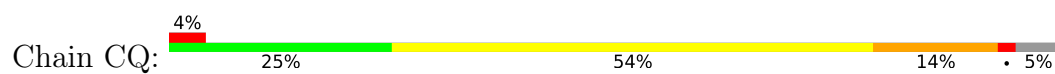
• Molecule 16: 30S ribosomal protein S16



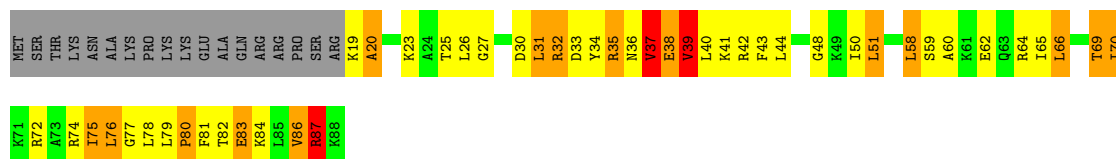
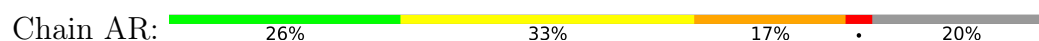
• Molecule 17: 30S ribosomal protein S17



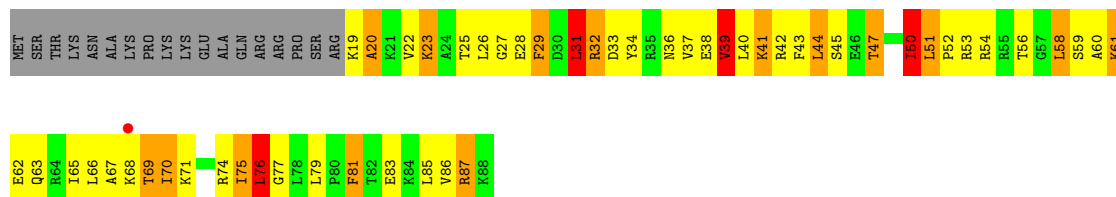
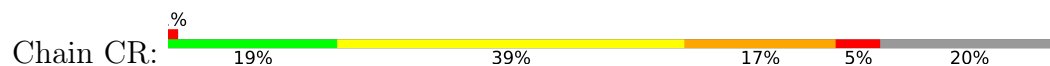
• Molecule 17: 30S ribosomal protein S17



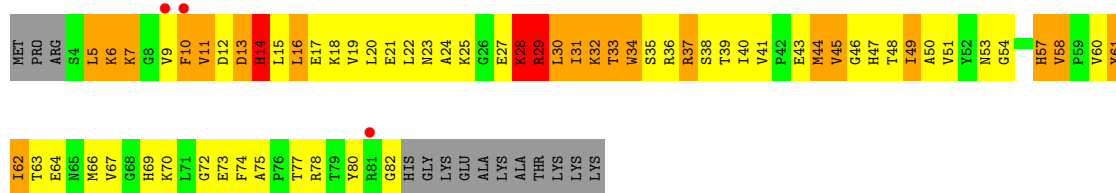
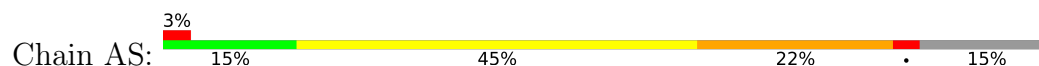
• Molecule 18: 30S ribosomal protein S18



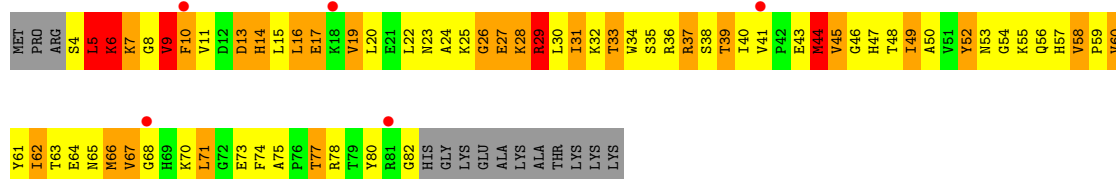
• Molecule 18: 30S ribosomal protein S18



• Molecule 19: 30S ribosomal protein S19

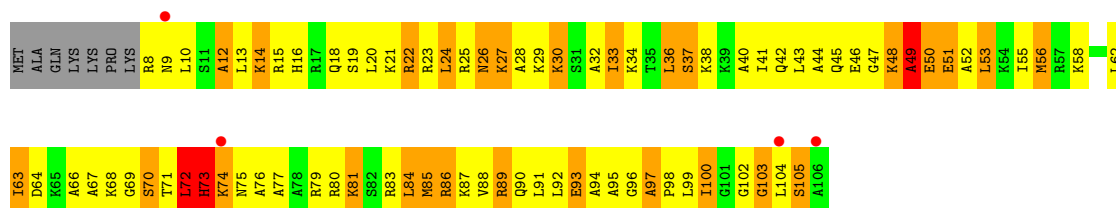


• Molecule 19: 30S ribosomal protein S19



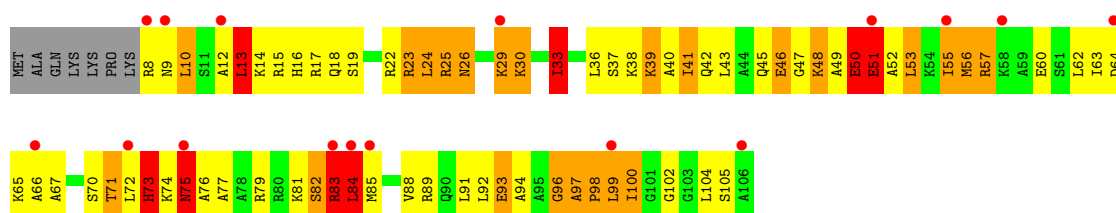
- Molecule 20: 30S ribosomal protein S20

Chain AT: 



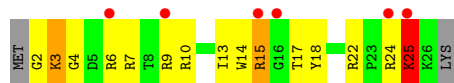
- Molecule 20: 30S ribosomal protein S20

Chain CT: 

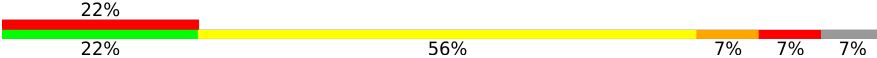


- Molecule 21: 30S ribosomal protein Thx

Chain AU: 



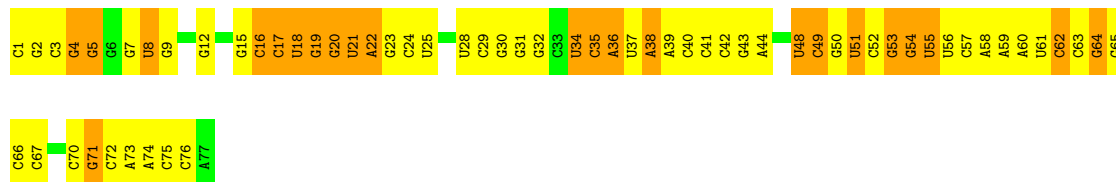
- Molecule 21: 30S ribosomal protein Thx

Chain CU: 



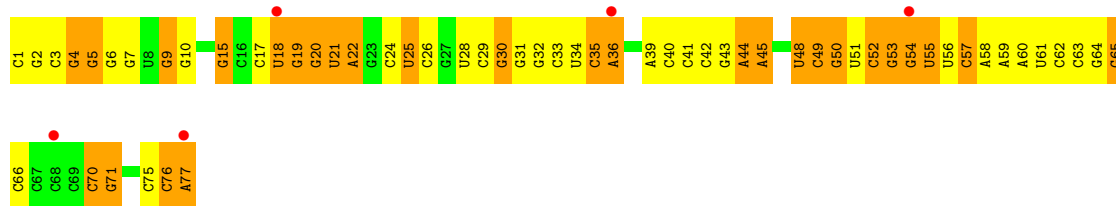
- Molecule 22: P-SITE tRNA fMet

Chain AV: 

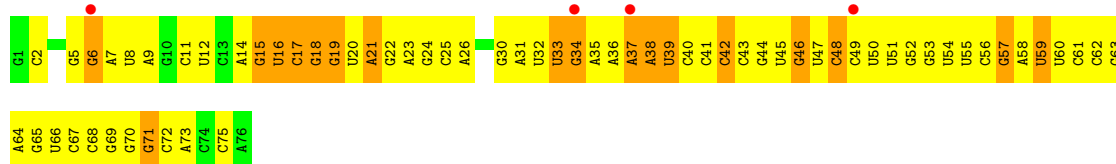
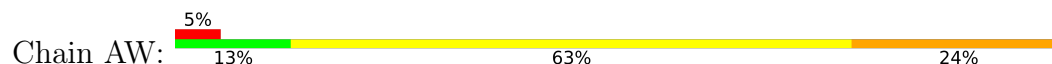


- Molecule 22: P-SITE tRNA fMet

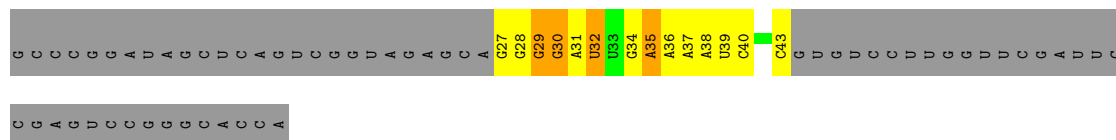
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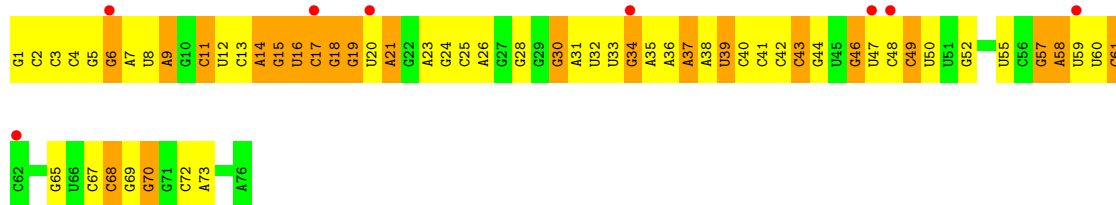
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



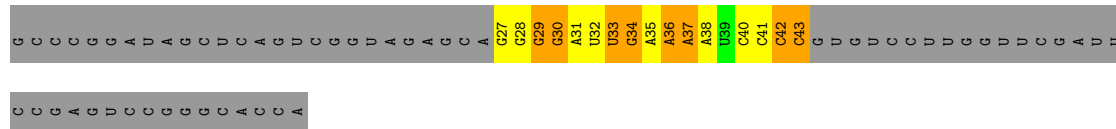
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe



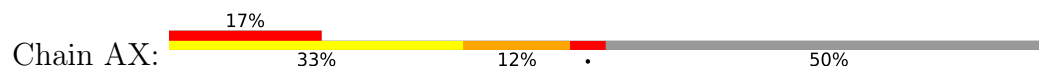
- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

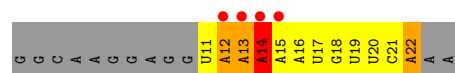


- Molecule 23: E-SITE TRNA PHE OR A-SITE tRNA Phe

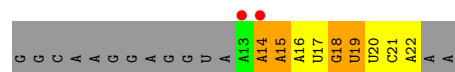


- Molecule 24: mRNA

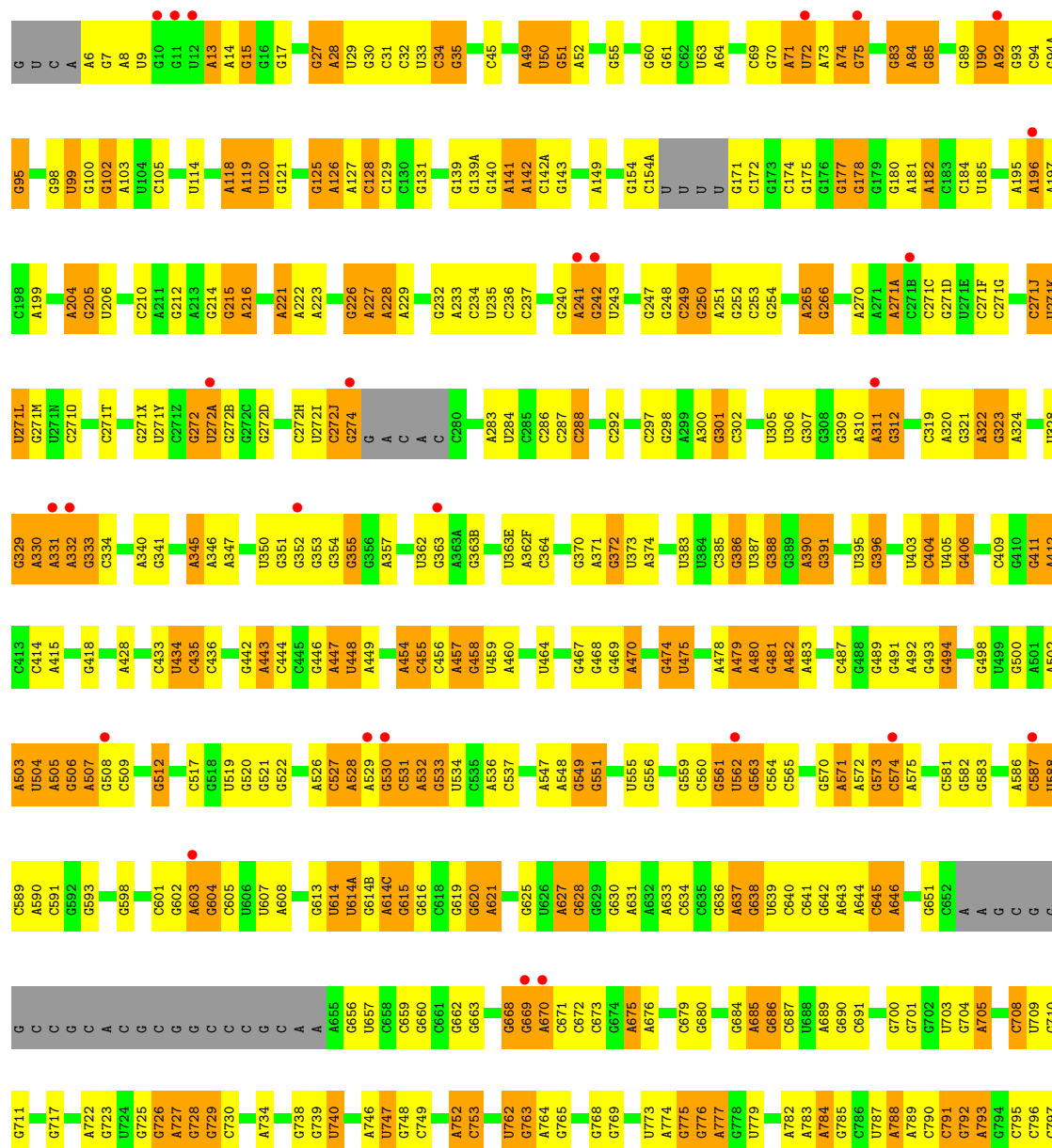




• Molecule 24: mRNA



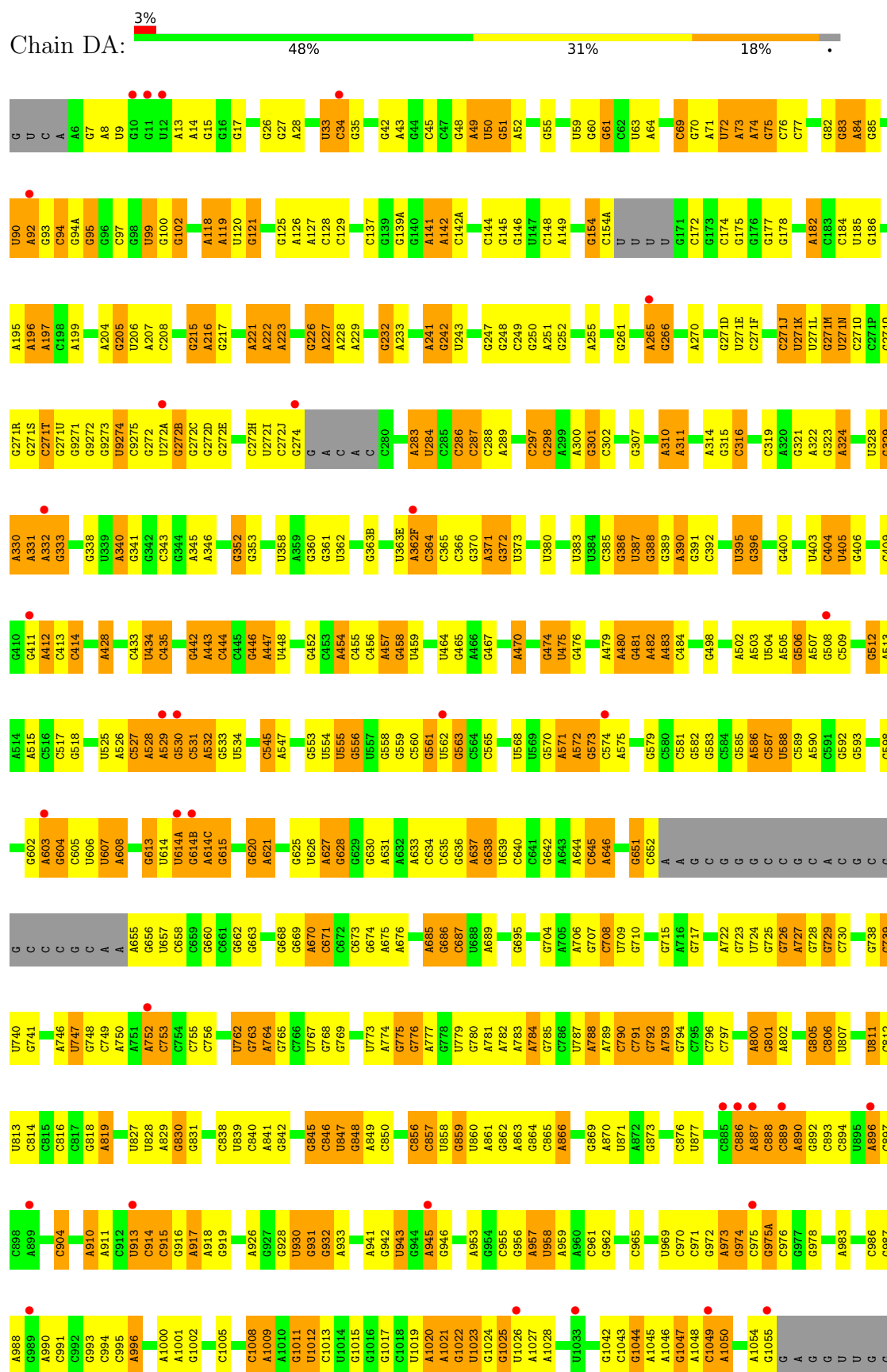
• Molecule 25: 23S rRNA



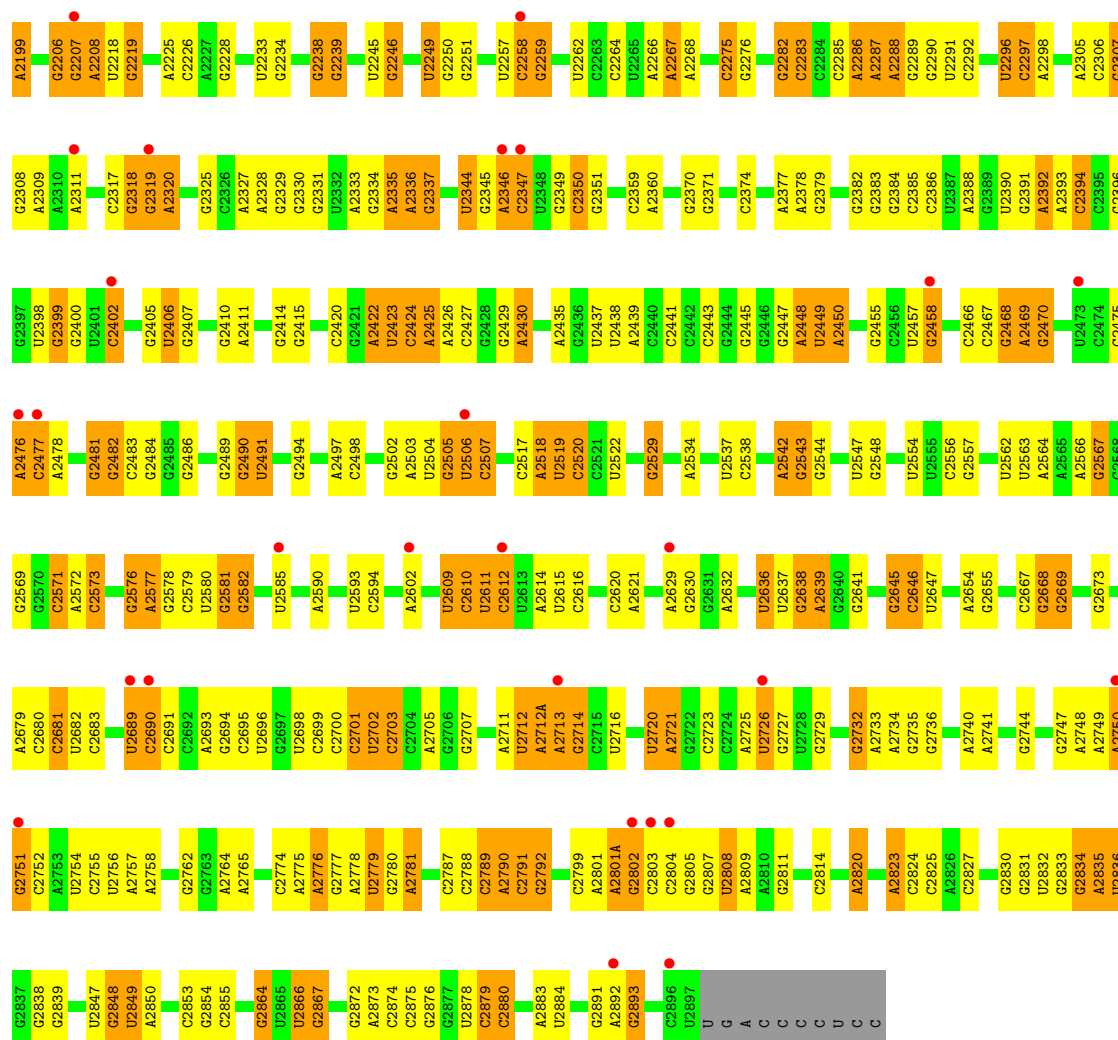
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• Molecule 25: 23S rRNA

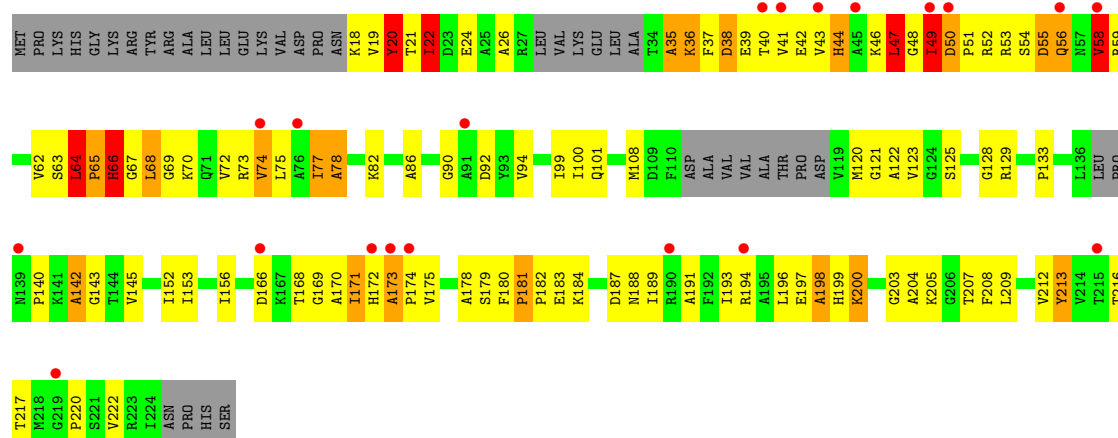


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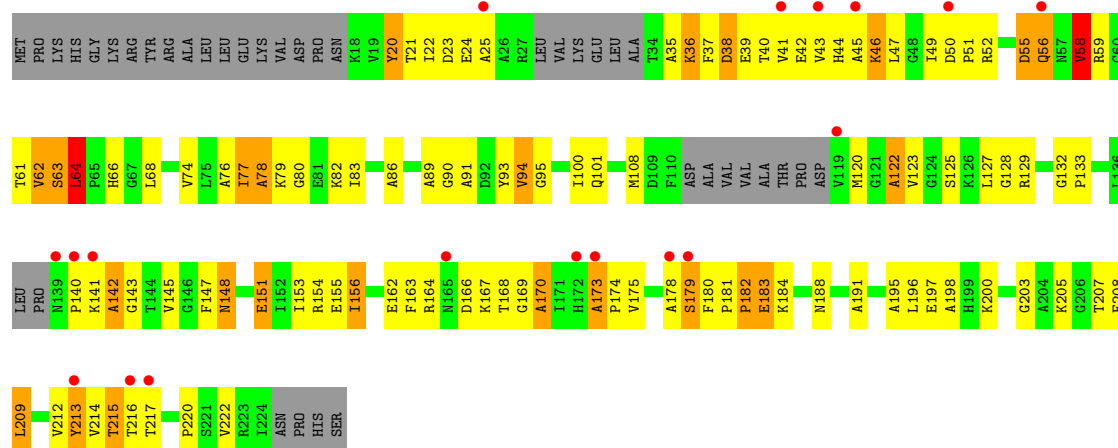




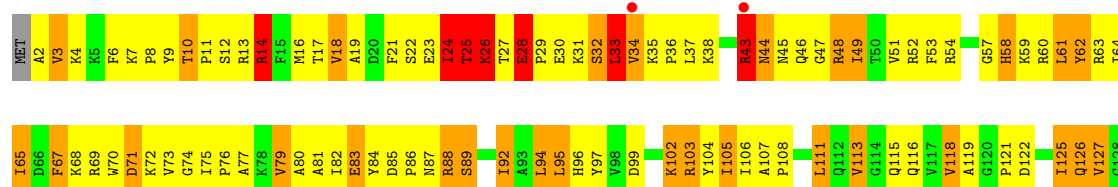
• Molecule 27: 50S RIBOSOMAL PROTEIN L1

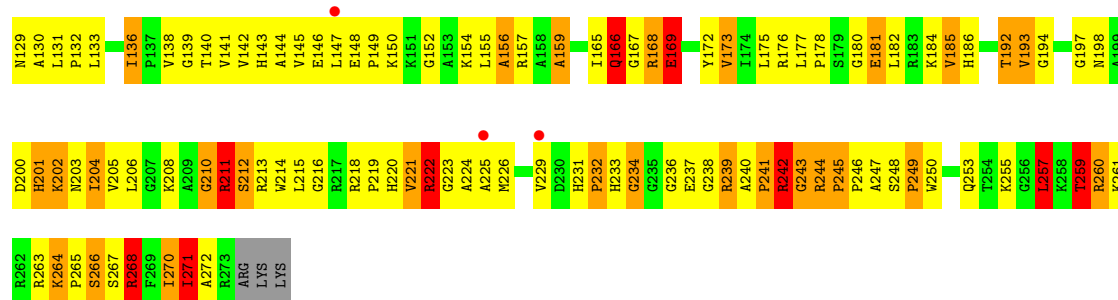


• Molecule 27: 50S RIBOSOMAL PROTEIN L1

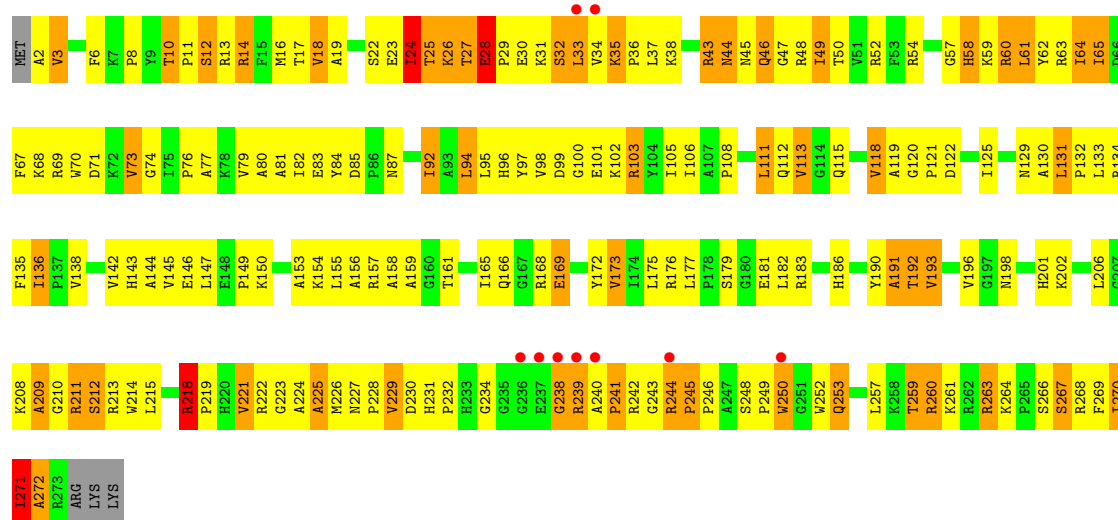


• Molecule 28: 50S RIBOSOMAL PROTEIN L2

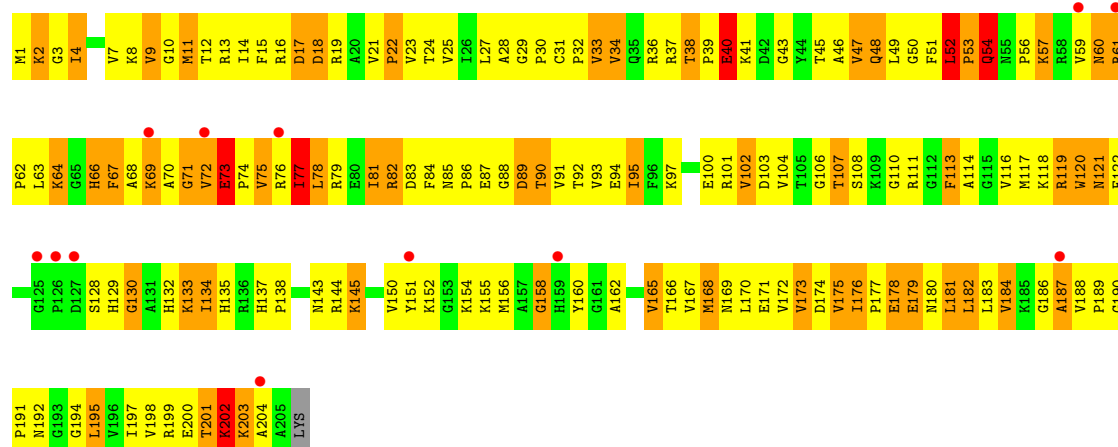




• Molecule 28: 50S RIBOSOMAL PROTEIN L2

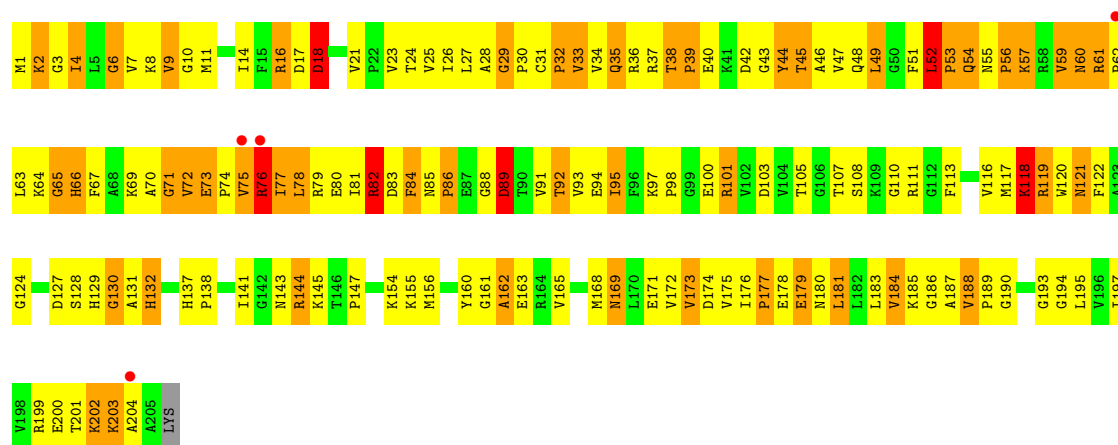


• Molecule 29: 50S RIBOSOMAL PROTEIN L3

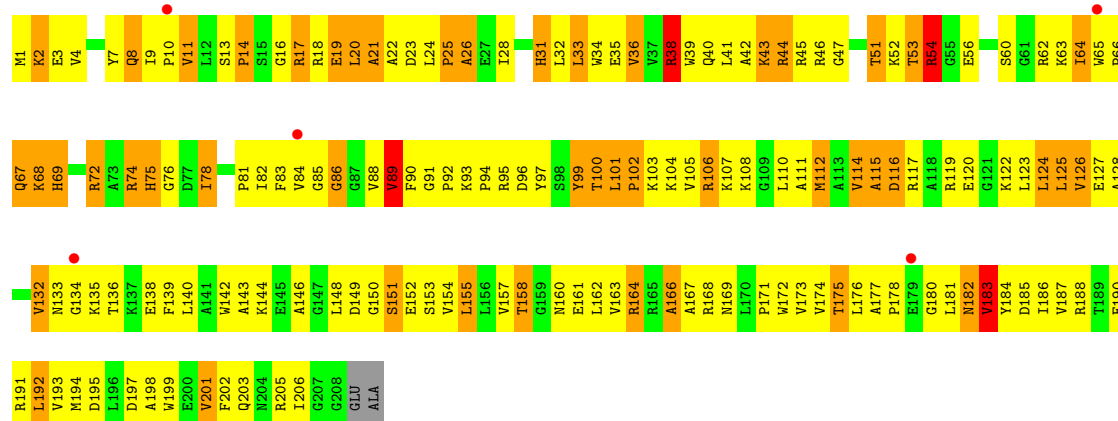


• Molecule 29: 50S RIBOSOMAL PROTEIN L3

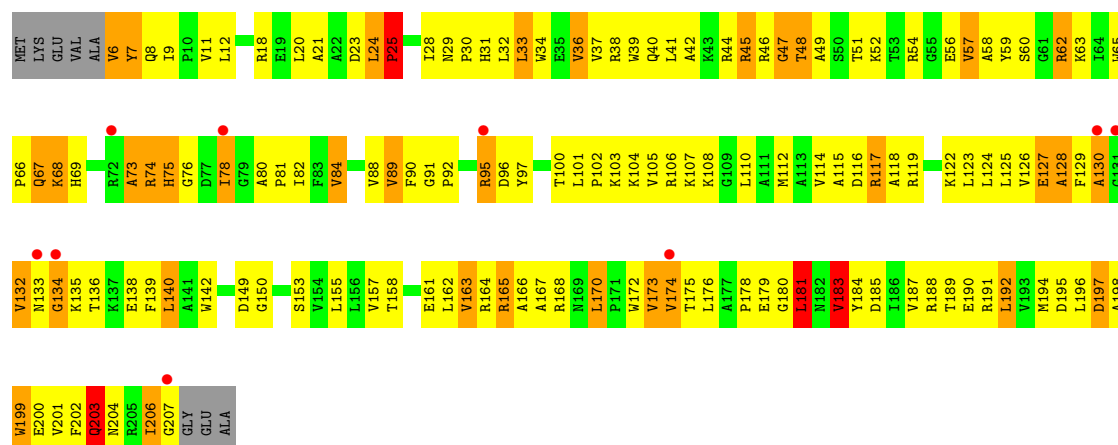




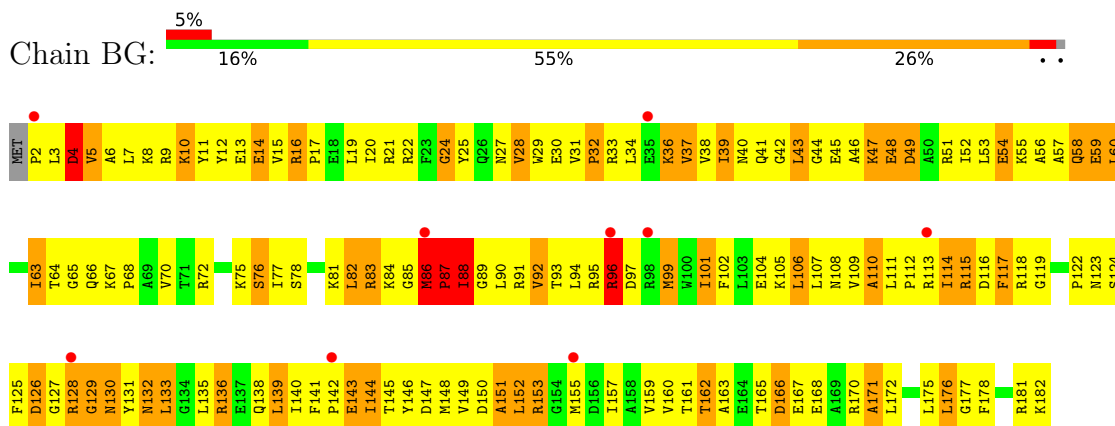
• Molecule 30: 50S RIBOSOMAL PROTEIN L4



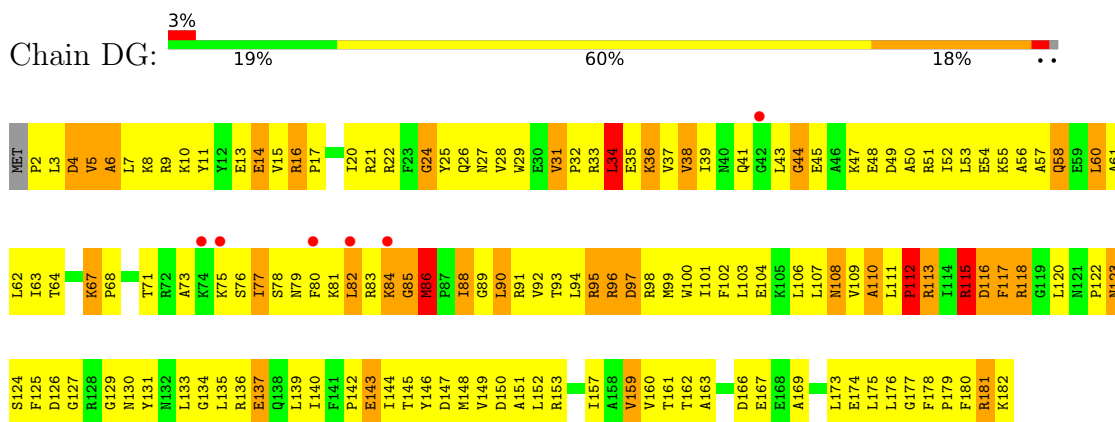
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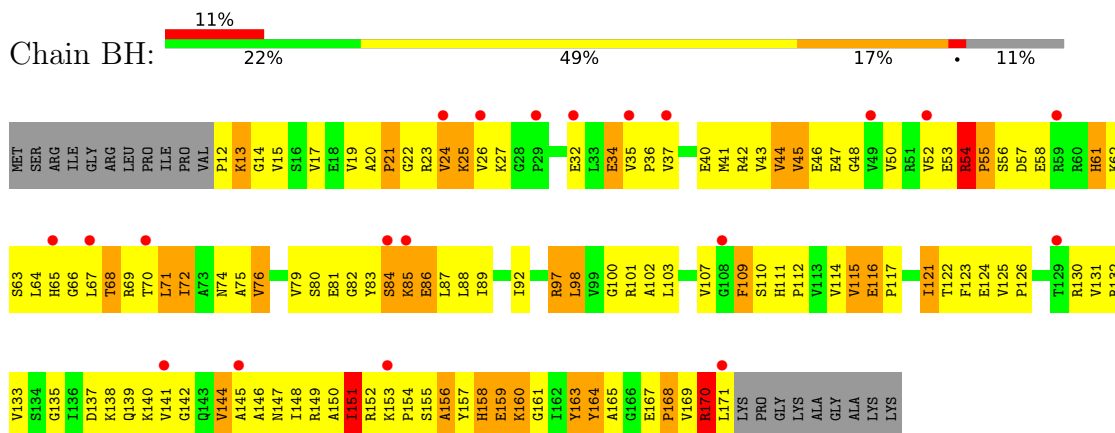
• Molecule 31: 50S RIBOSOMAL PROTEIN L5



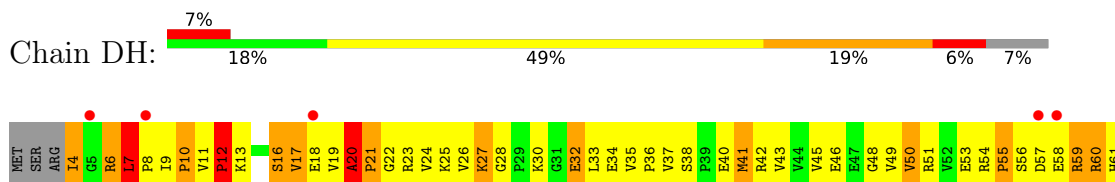
- Molecule 31: 50S RIBOSOMAL PROTEIN L5

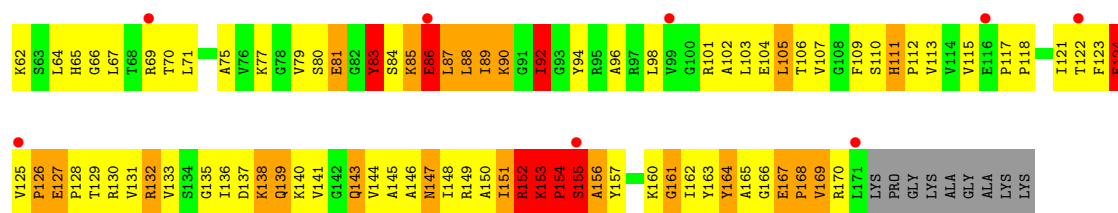


● Molecule 32: 50S RIBOSOMAL PROTEIN L6

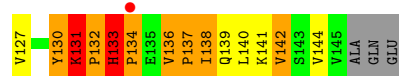
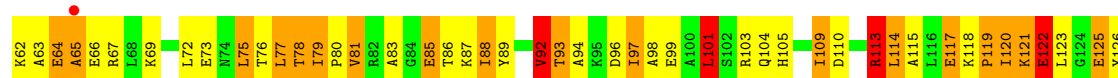
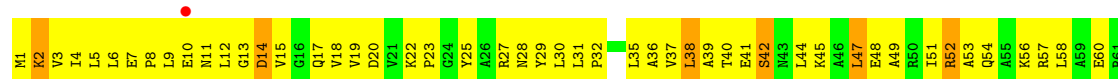


● Molecule 32: 50S RIBOSOMAL PROTEIN L6

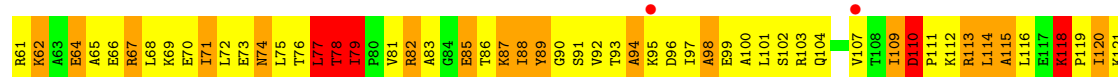
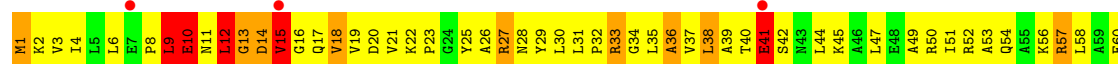
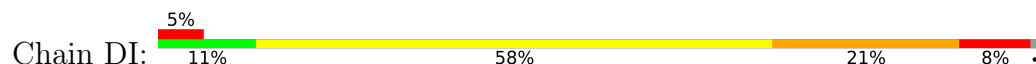




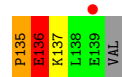
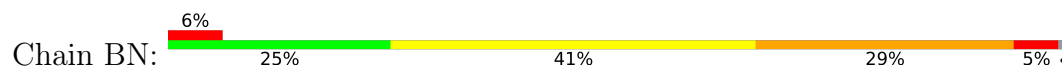
● Molecule 33: 50S RIBOSOMAL PROTEIN L9



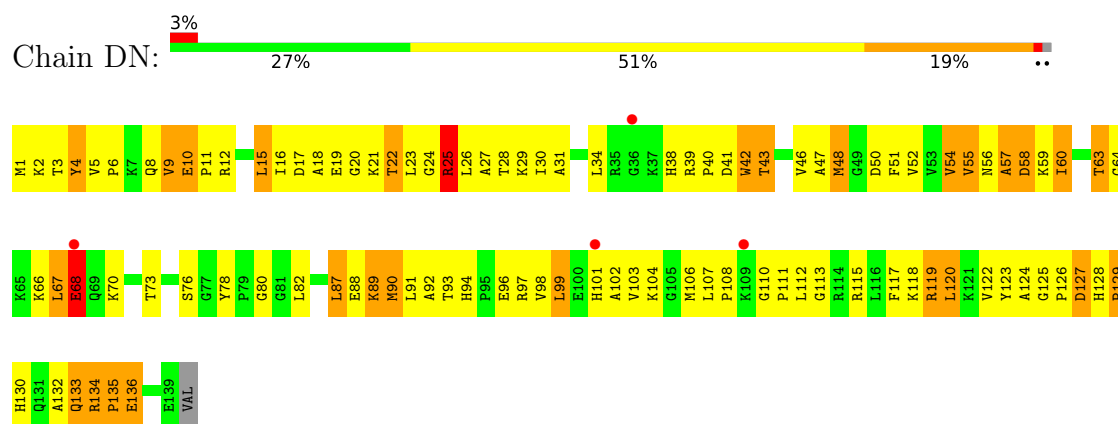
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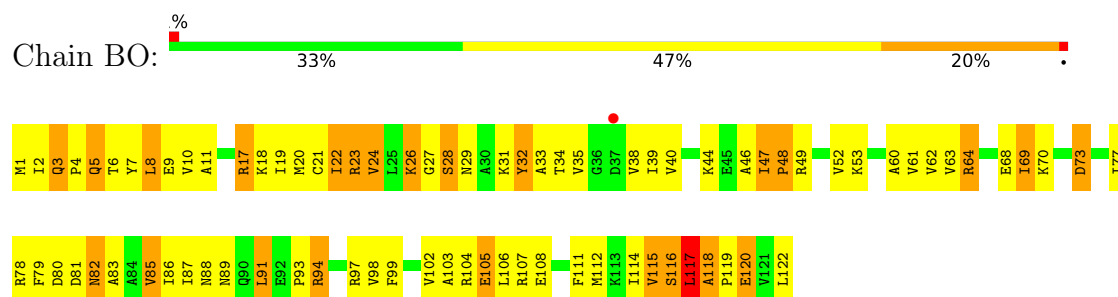
● Molecule 34: 50S RIBOSOMAL PROTEIN L13



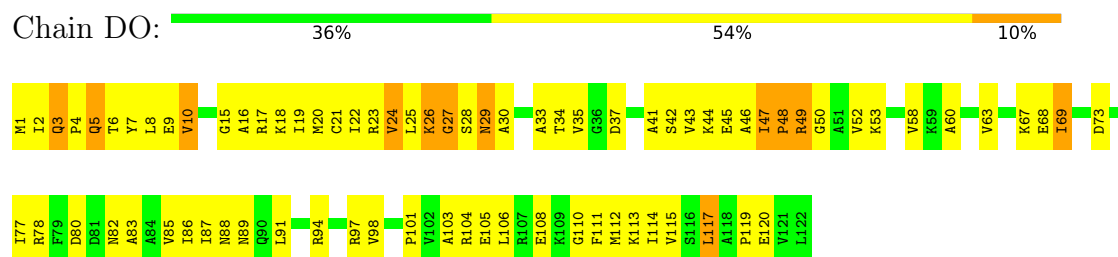
● Molecule 34: 50S RIBOSOMAL PROTEIN L13



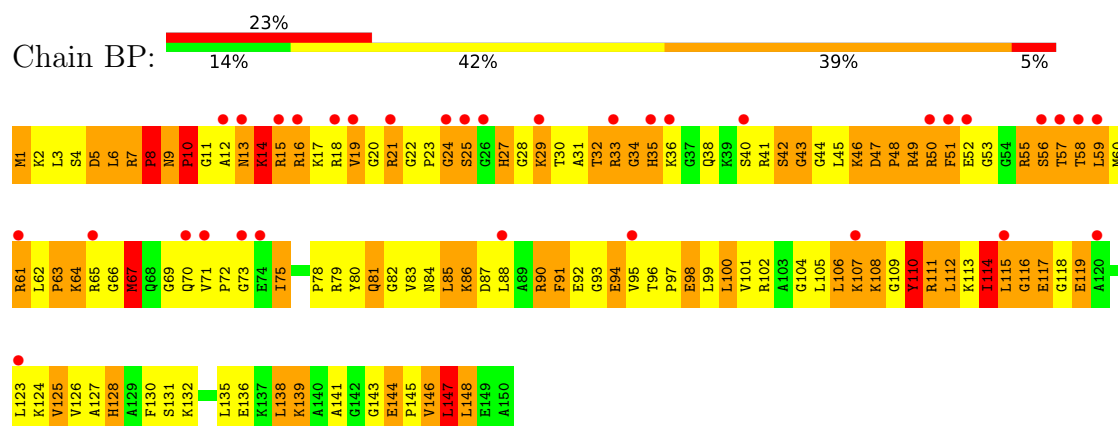
• Molecule 35: 50S RIBOSOMAL PROTEIN L14



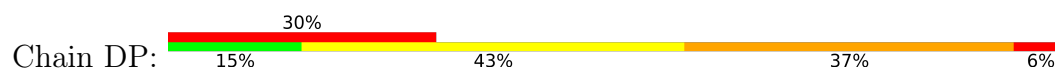
• Molecule 35: 50S RIBOSOMAL PROTEIN L14

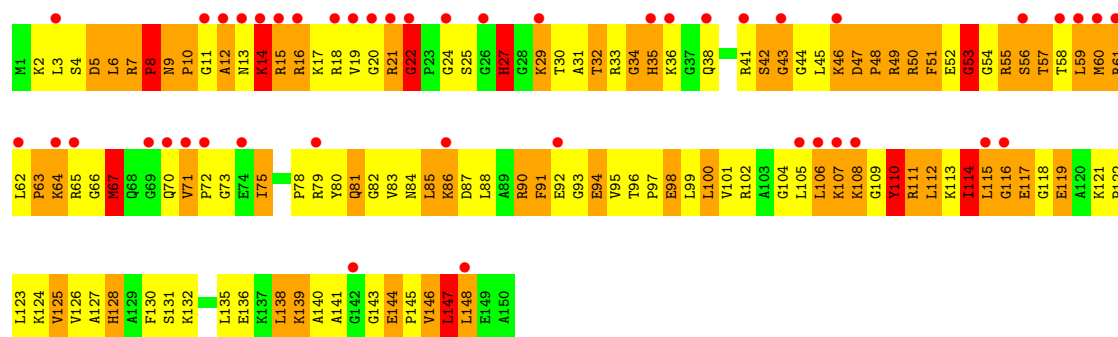


• Molecule 36: 50S RIBOSOMAL PROTEIN L15

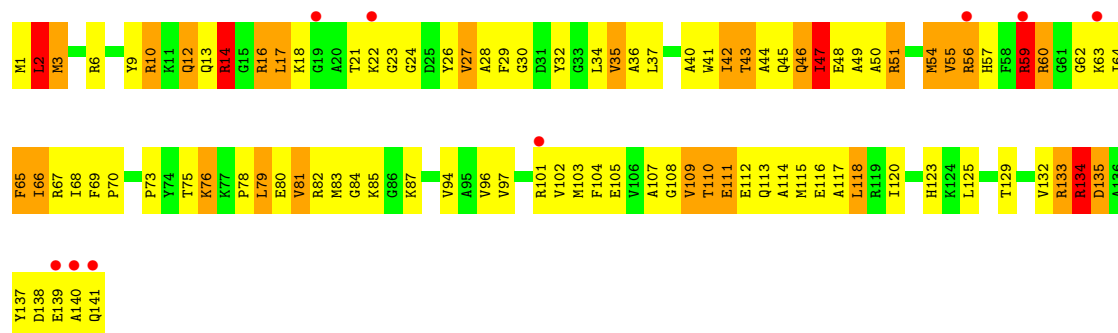


• Molecule 36: 50S RIBOSOMAL PROTEIN L15

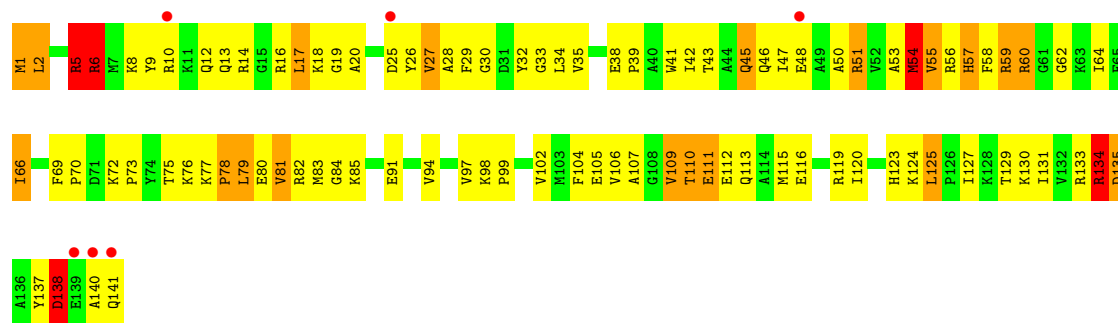




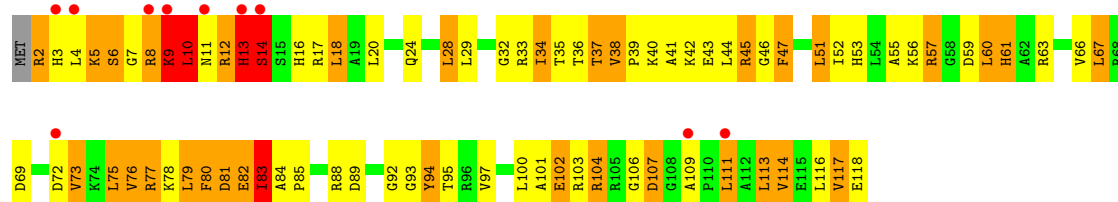
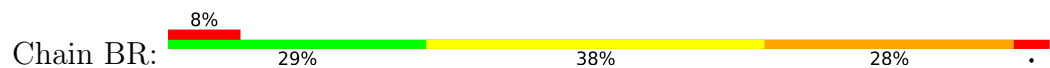
• Molecule 37: 50S RIBOSOMAL PROTEIN L16



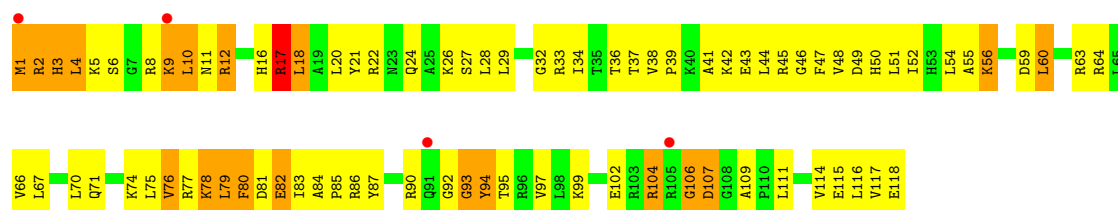
• Molecule 37: 50S RIBOSOMAL PROTEIN L16



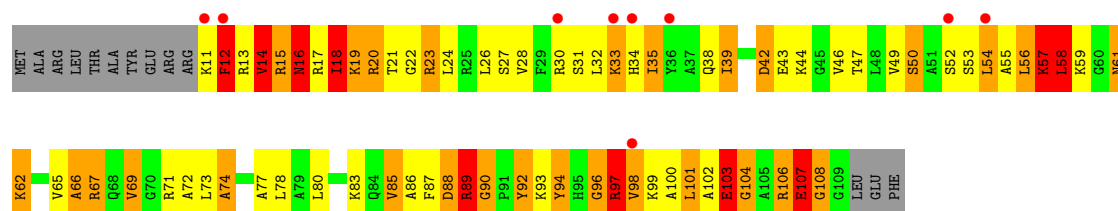
• Molecule 38: 50S RIBOSOMAL PROTEIN L17



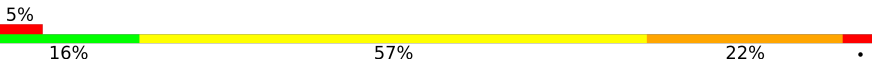
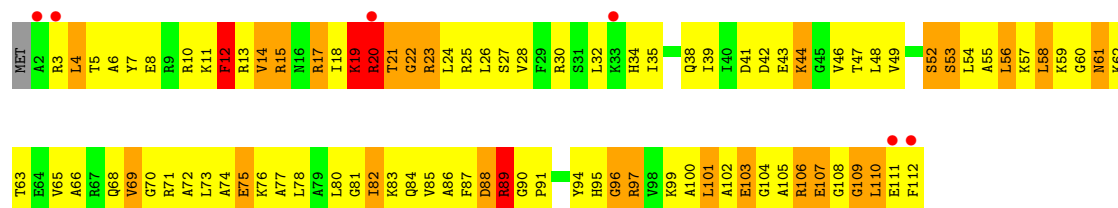
● Molecule 38: 50S RIBOSOMAL PROTEIN L17

Chain DR:  3% 29% 53% 17%

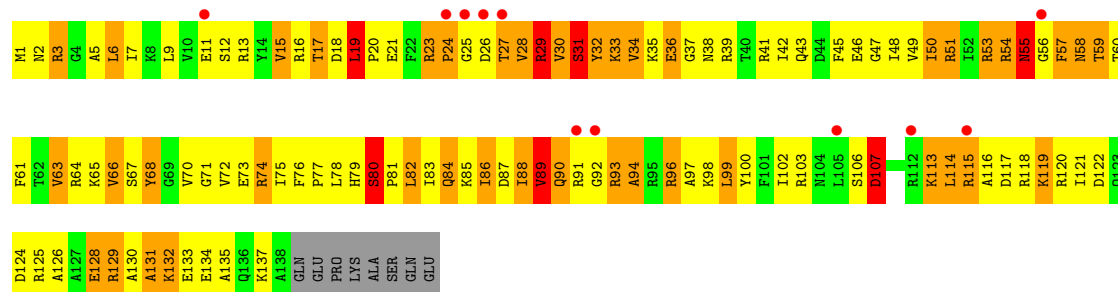
● Molecule 39: 50S RIBOSOMAL PROTEIN L18

Chain BS:  8% 21% 33% 25% 9% 12%

● Molecule 39: 50S RIBOSOMAL PROTEIN L18

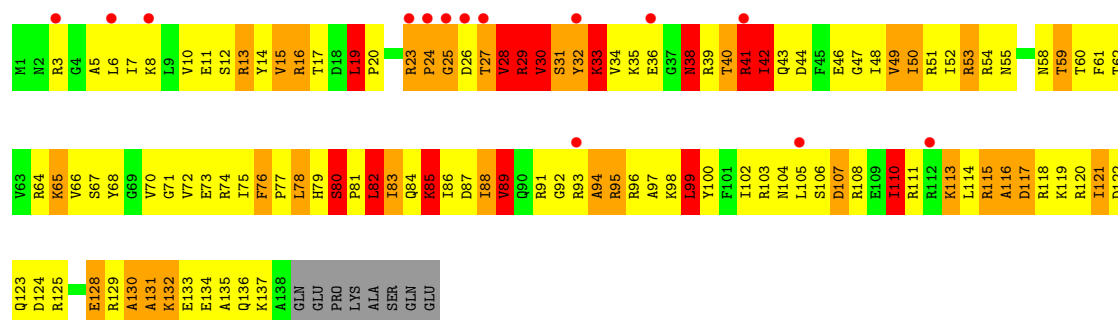
Chain DS:  5% 16% 57% 22%

● Molecule 40: 50S RIBOSOMAL PROTEIN L19

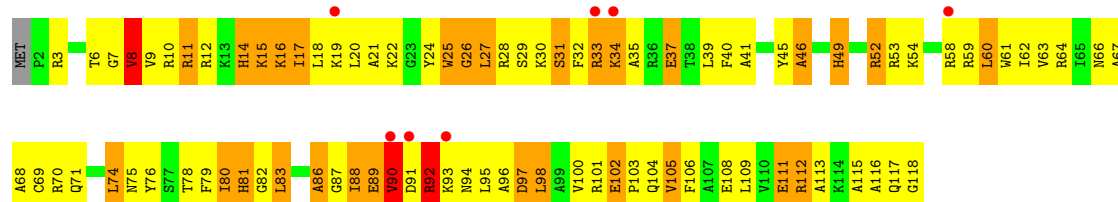
Chain BT:  8% 16% 46% 28% 5% 5%

● Molecule 40: 50S RIBOSOMAL PROTEIN L19

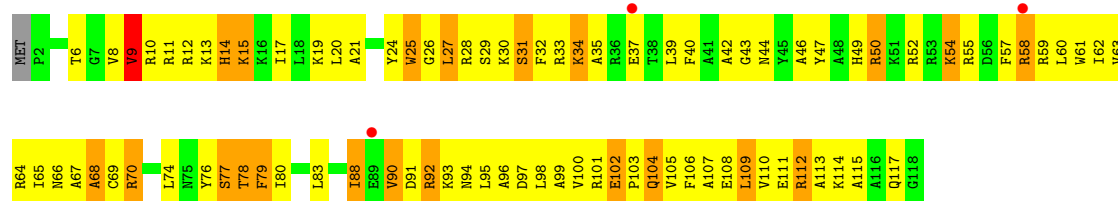
Chain DT:  10% 14% 50% 21% 10% 5%



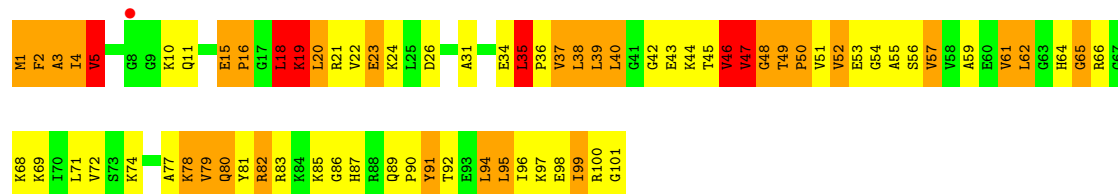
• Molecule 41: 50S RIBOSOMAL PROTEIN L20



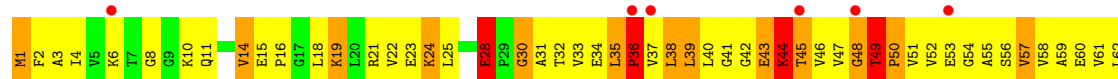
• Molecule 41: 50S RIBOSOMAL PROTEIN L20

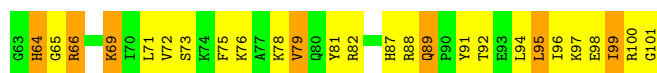


• Molecule 42: 50S RIBOSOMAL PROTEIN L21



• Molecule 42: 50S RIBOSOMAL PROTEIN L21

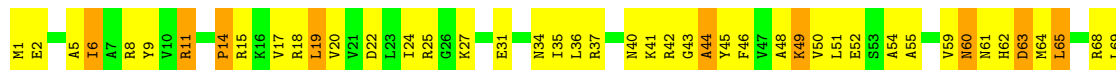




• Molecule 43: 50S RIBOSOMAL PROTEIN L22



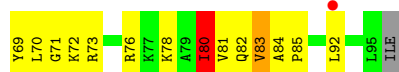
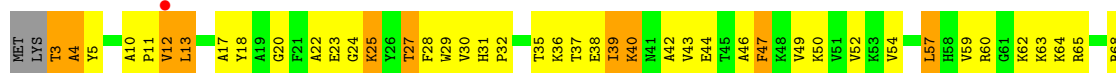
• Molecule 43: 50S RIBOSOMAL PROTEIN L22



• Molecule 44: 50S RIBOSOMAL PROTEIN L23

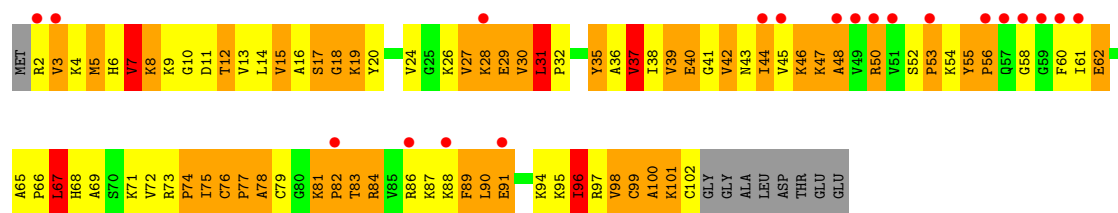


• Molecule 44: 50S RIBOSOMAL PROTEIN L23

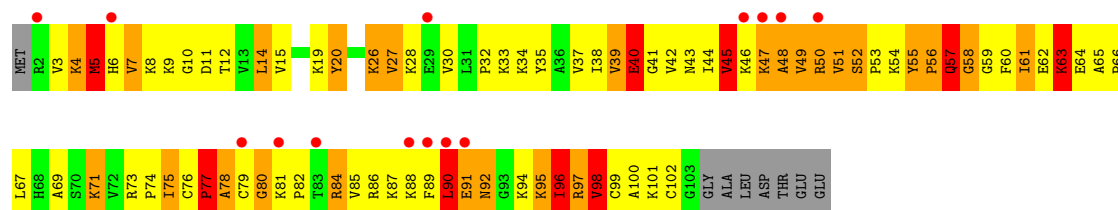
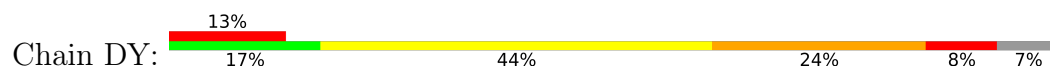


• Molecule 45: 50S RIBOSOMAL PROTEIN L24

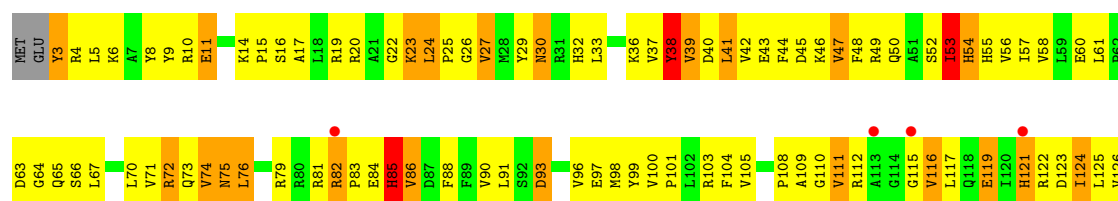
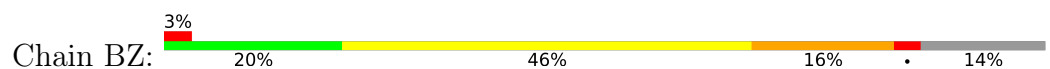




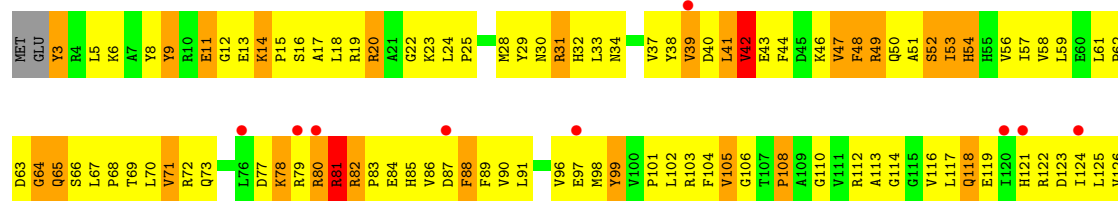
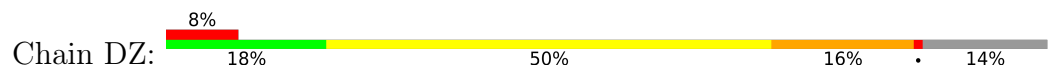
• Molecule 45: 50S RIBOSOMAL PROTEIN L24



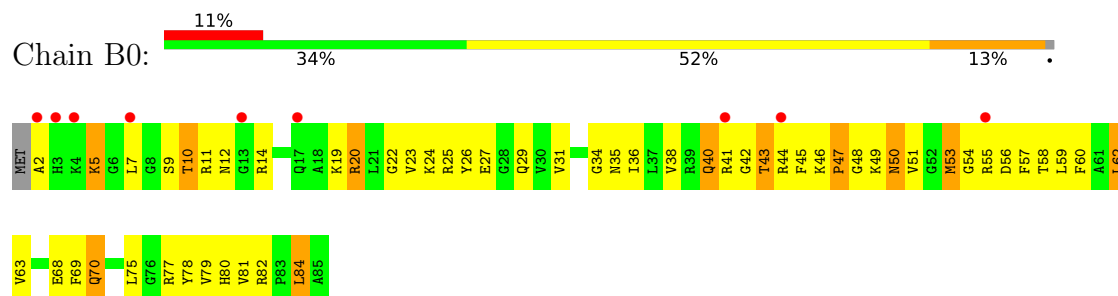
• Molecule 46: 50S RIBOSOMAL PROTEIN L25



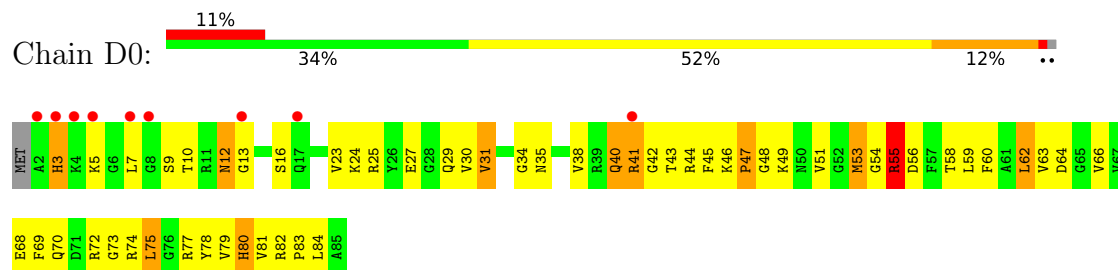
• Molecule 46: 50S RIBOSOMAL PROTEIN L25



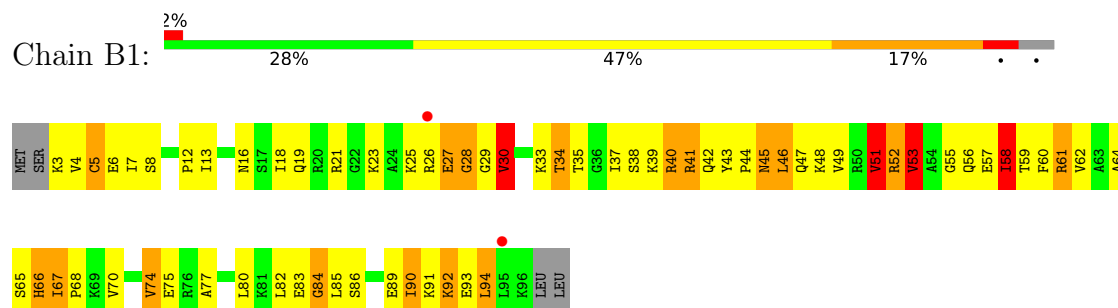
- Molecule 47: 50S RIBOSOMAL PROTEIN L27



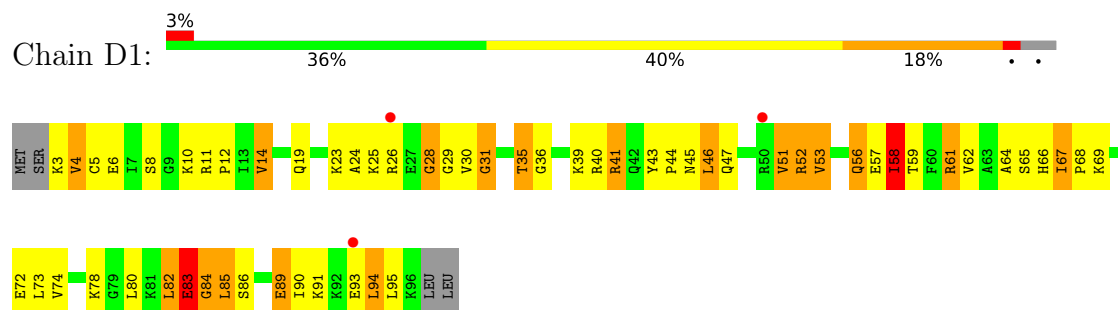
- Molecule 47: 50S RIBOSOMAL PROTEIN L27



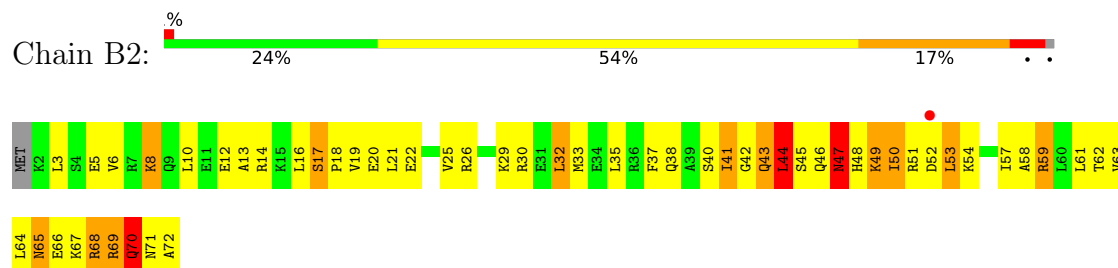
- Molecule 48: 50S RIBOSOMAL PROTEIN L28



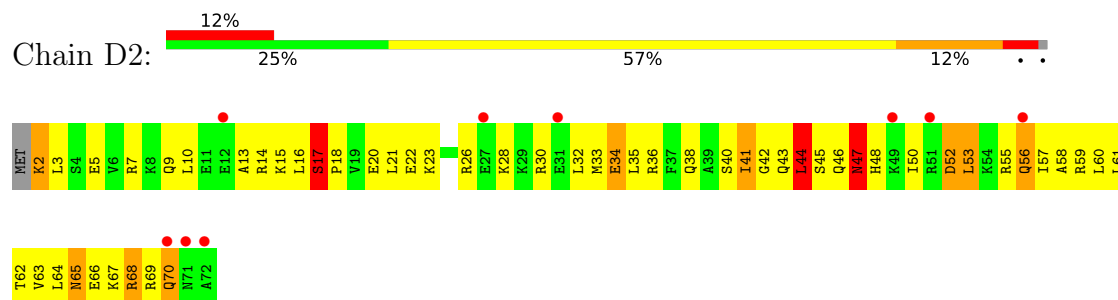
- Molecule 48: 50S RIBOSOMAL PROTEIN L28



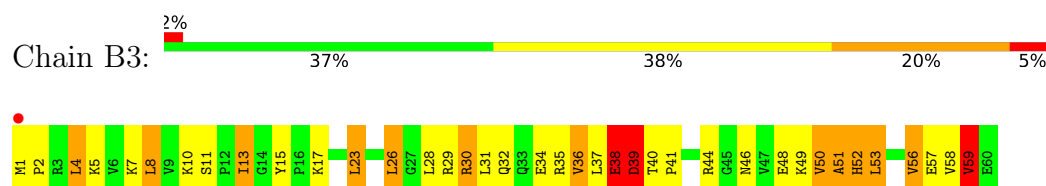
- Molecule 49: 50S RIBOSOMAL PROTEIN L29



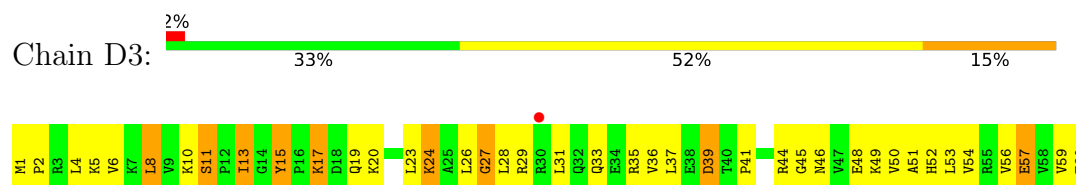
- Molecule 49: 50S RIBOSOMAL PROTEIN L29



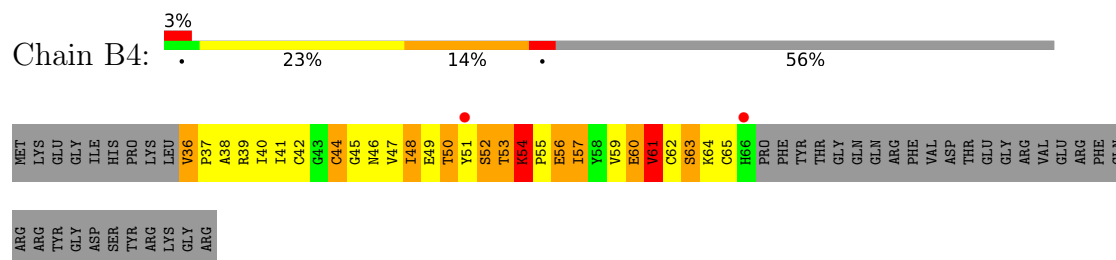
- Molecule 50: 50S RIBOSOMAL PROTEIN L30



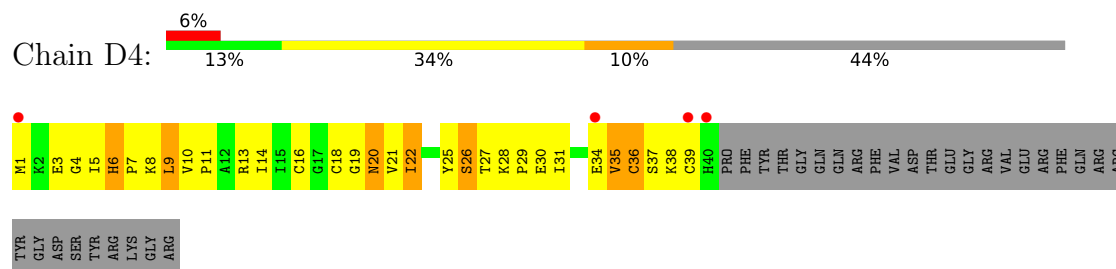
- Molecule 50: 50S RIBOSOMAL PROTEIN L30



- Molecule 51: 50S RIBOSOMAL PROTEIN L31

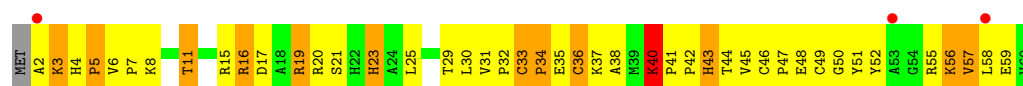


- Molecule 51: 50S RIBOSOMAL PROTEIN L31

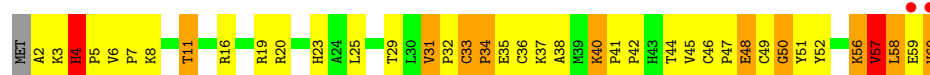


- Molecule 52: 50S RIBOSOMAL PROTEIN L32





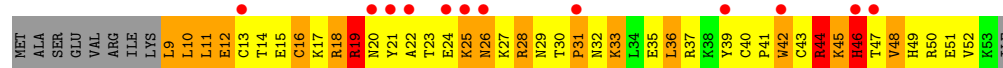
• Molecule 52: 50S RIBOSOMAL PROTEIN L32



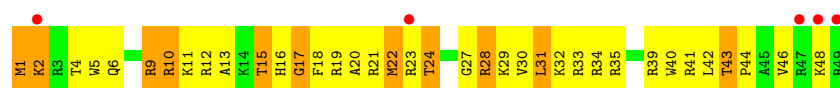
• Molecule 53: 50S RIBOSOMAL PROTEIN L33



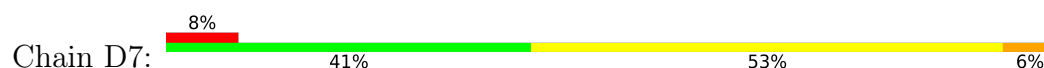
• Molecule 53: 50S RIBOSOMAL PROTEIN L33



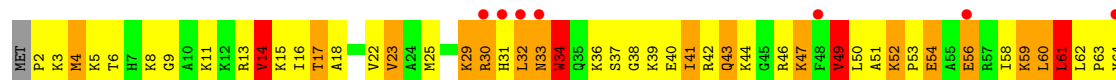
• Molecule 54: 50S RIBOSOMAL PROTEIN L34



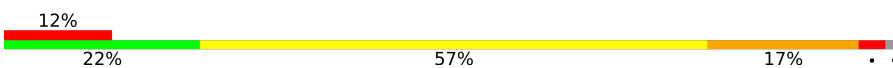
• Molecule 54: 50S RIBOSOMAL PROTEIN L34

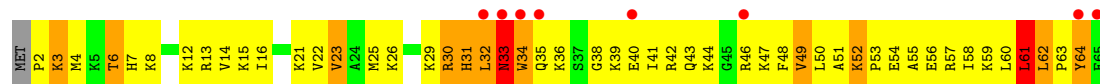


• Molecule 55: 50S RIBOSOMAL PROTEIN L35



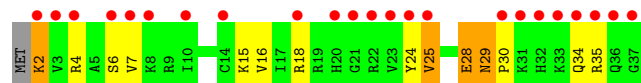
- Molecule 55: 50S RIBOSOMAL PROTEIN L35

Chain D8: 



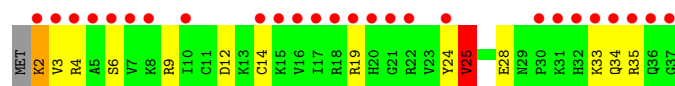
- Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain B9: 



- Molecule 56: 50S RIBOSOMAL PROTEIN L36

Chain D9: 



4 Data and refinement statistics

Property	Value
Space group	P 21 21 21
Cell constants a, b, c, α , β , γ	210.46 Å 447.34 Å 622.30 Å 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) 99.8 (35.07-3.52)
R_{merge}	0.44
R_{sym}	0.46
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.47 Å)
Refinement program	PHENIX (phenix.refine: 1.7_641), PHENIX (phenix.refine: 1.8_1069)
R, R_{free}	0.210 , 0.249 0.214 , 0.253
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)	0.28 , 81.4
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$
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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.19	0/36189	0.44	0/56484
1	CA	0.19	0/36189	0.43	0/56484
2	AB	0.81	2/1936 (0.1%)	1.03	6/2611 (0.2%)
2	CB	0.89	0/1936	1.06	3/2611 (0.1%)
3	AC	0.96	2/1637 (0.1%)	1.09	7/2207 (0.3%)
3	CC	1.05	3/1637 (0.2%)	1.18	6/2207 (0.3%)
4	AD	0.92	1/1733 (0.1%)	1.17	13/2318 (0.6%)
4	CD	1.02	2/1733 (0.1%)	1.18	13/2318 (0.6%)
5	AE	0.98	1/1163 (0.1%)	1.27	9/1566 (0.6%)
5	CE	0.96	0/1163	1.20	3/1566 (0.2%)
6	AF	0.97	0/856	1.17	6/1154 (0.5%)
6	CF	1.06	1/856 (0.1%)	1.17	4/1154 (0.3%)
7	AG	1.04	4/1276 (0.3%)	1.16	5/1709 (0.3%)
7	CG	0.95	0/1276	1.13	12/1709 (0.7%)
8	AH	0.98	3/1136 (0.3%)	1.13	2/1527 (0.1%)
8	CH	0.97	1/1136 (0.1%)	1.19	7/1527 (0.5%)
9	AI	0.94	0/1029	1.16	6/1379 (0.4%)
9	CI	0.95	0/1029	1.13	7/1379 (0.5%)
10	AJ	1.03	2/808 (0.2%)	1.16	3/1087 (0.3%)
10	CJ	0.89	0/808	1.08	5/1087 (0.5%)
11	AK	0.93	0/900	1.18	5/1213 (0.4%)
11	CK	0.95	0/900	1.25	8/1213 (0.7%)
12	AL	1.17	1/987 (0.1%)	1.30	5/1322 (0.4%)
12	CL	1.19	4/987 (0.4%)	1.39	8/1322 (0.6%)
13	AM	0.88	0/999	1.07	4/1338 (0.3%)
13	CM	0.55	1/1008 (0.1%)	1.08	7/1347 (0.5%)
14	AN	0.92	0/501	1.11	0/664
14	CN	1.01	0/501	1.25	2/664 (0.3%)
15	AO	1.08	2/745 (0.3%)	1.13	2/992 (0.2%)
15	CO	1.00	1/745 (0.1%)	1.09	2/992 (0.2%)
16	AP	0.94	0/717	1.15	4/965 (0.4%)
16	CP	0.99	0/717	1.23	5/965 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.95	0/837	1.18	6/1119 (0.5%)
17	CQ	1.01	0/837	1.13	4/1119 (0.4%)
18	AR	0.94	0/579	1.14	2/768 (0.3%)
18	CR	1.03	1/579 (0.2%)	1.24	6/768 (0.8%)
19	AS	1.02	3/643 (0.5%)	1.13	3/867 (0.3%)
19	CS	1.03	1/643 (0.2%)	1.17	2/867 (0.2%)
20	AT	1.04	3/765 (0.4%)	1.15	6/1007 (0.6%)
20	CT	0.87	0/765	1.02	4/1007 (0.4%)
21	AU	0.85	0/213	1.03	1/279 (0.4%)
21	CU	0.85	0/213	1.03	0/279
22	AV	0.64	0/1836	0.60	0/2859
22	CV	0.61	0/1835	0.62	0/2859
23	AW	0.52	0/1809	0.50	0/2819
23	AY	0.61	0/408	0.56	0/634
23	CW	0.53	0/1809	0.48	0/2819
23	CY	0.72	0/408	0.68	0/634
24	AX	0.82	1/285 (0.4%)	0.59	0/441
24	CX	0.59	0/235	0.66	0/364
25	BA	0.23	1/67788 (0.0%)	0.48	1/105819 (0.0%)
25	DA	0.22	0/68124	0.49	1/106343 (0.0%)
26	BB	0.16	0/2853	0.36	0/4451
26	DB	0.18	0/2853	0.40	0/4451
27	BC	0.98	2/1145 (0.2%)	1.13	6/1556 (0.4%)
27	DC	0.36	0/1145	0.80	0/1556
28	BD	1.14	3/2155 (0.1%)	1.35	16/2907 (0.6%)
28	DD	0.71	0/2155	1.13	14/2907 (0.5%)
29	BE	1.06	3/1597 (0.2%)	1.31	16/2155 (0.7%)
29	DE	0.68	1/1597 (0.1%)	1.12	12/2155 (0.6%)
30	BF	1.07	1/1659 (0.1%)	1.20	6/2246 (0.3%)
30	DF	0.61	0/1620	1.20	17/2194 (0.8%)
31	BG	0.92	0/1499	1.11	7/2016 (0.3%)
31	DG	0.51	1/1499 (0.1%)	0.98	10/2016 (0.5%)
32	BH	0.87	0/1246	1.11	5/1684 (0.3%)
32	DH	0.52	0/1315	1.15	9/1780 (0.5%)
33	BI	0.94	1/1146 (0.1%)	1.16	5/1551 (0.3%)
33	DI	0.49	1/1151 (0.1%)	1.08	10/1558 (0.6%)
34	BN	1.04	1/1132 (0.1%)	1.21	7/1527 (0.5%)
34	DN	0.57	0/1132	1.06	9/1527 (0.6%)
35	BO	1.00	0/943	1.26	3/1269 (0.2%)
35	DO	0.59	0/943	1.09	5/1269 (0.4%)
36	BP	0.51	2/1162 (0.2%)	1.20	12/1544 (0.8%)
36	DP	0.49	1/1162 (0.1%)	1.17	12/1544 (0.8%)
37	BQ	1.03	1/1143 (0.1%)	1.19	5/1527 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DQ	0.62	0/1143	0.99	3/1527 (0.2%)
38	BR	1.15	4/974 (0.4%)	1.24	6/1302 (0.5%)
38	DR	0.86	2/982 (0.2%)	1.07	3/1312 (0.2%)
39	BS	1.00	1/779 (0.1%)	1.21	6/1038 (0.6%)
39	DS	0.49	0/892	1.18	9/1187 (0.8%)
40	BT	0.93	0/1156	1.33	19/1544 (1.2%)
40	DT	0.80	1/1156 (0.1%)	1.27	20/1544 (1.3%)
41	BU	1.10	3/982 (0.3%)	1.26	6/1306 (0.5%)
41	DU	0.71	0/975	1.10	5/1297 (0.4%)
42	BV	0.99	0/790	1.20	3/1057 (0.3%)
42	DV	0.63	1/790 (0.1%)	1.12	5/1057 (0.5%)
43	BW	1.13	2/907 (0.2%)	1.25	7/1216 (0.6%)
43	DW	0.64	0/907	1.01	3/1216 (0.2%)
44	BX	1.02	3/740 (0.4%)	1.25	6/995 (0.6%)
44	DX	0.64	0/740	1.01	3/995 (0.3%)
45	BY	0.99	2/789 (0.3%)	1.40	12/1053 (1.1%)
45	DY	0.60	1/798 (0.1%)	1.17	5/1064 (0.5%)
46	BZ	1.00	4/1436 (0.3%)	1.11	9/1951 (0.5%)
46	DZ	0.47	0/1436	0.87	0/1951
47	B0	1.01	2/671 (0.3%)	1.17	3/892 (0.3%)
47	D0	0.59	0/671	1.00	3/892 (0.3%)
48	B1	1.22	4/739 (0.5%)	1.30	3/983 (0.3%)
48	D1	0.66	0/739	0.95	1/983 (0.1%)
49	B2	0.98	0/600	1.09	1/793 (0.1%)
49	D2	0.68	0/600	1.03	1/793 (0.1%)
50	B3	1.07	1/473 (0.2%)	1.17	0/636
50	D3	0.58	0/473	1.16	4/636 (0.6%)
51	B4	1.00	0/229	1.16	3/311 (1.0%)
51	D4	0.59	0/303	1.12	1/409 (0.2%)
52	B5	1.28	3/473 (0.6%)	1.29	5/639 (0.8%)
52	D5	0.59	0/473	1.06	2/639 (0.3%)
53	B6	1.02	1/388 (0.3%)	1.38	8/520 (1.5%)
53	D6	0.41	0/388	0.87	1/520 (0.2%)
54	B7	1.12	0/427	1.32	2/563 (0.4%)
54	D7	0.69	0/427	1.03	0/563
55	B8	0.97	0/516	1.22	6/681 (0.9%)
55	D8	0.65	0/516	1.21	5/681 (0.7%)
56	B9	0.87	0/302	0.90	0/397
56	D9	0.40	0/302	0.84	1/397 (0.3%)
All	All	0.53	94/318178 (0.0%)	0.72	571/475682 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

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

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	BA	1453	U	O3'-P	23.98	1.97	1.61
38	DR	12	ARG	C-N	18.60	1.60	1.33
40	DT	28	VAL	C-N	18.17	1.59	1.33
29	DE	127	ASP	C-N	12.25	1.50	1.33
24	AX	14	A	O3'-P	-10.45	1.45	1.61

The worst 5 of 571 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	DR	12	ARG	O-C-N	12.64	137.93	123.27
45	BY	38	ILE	N-CA-C	12.17	121.97	110.53
36	BP	14	LYS	N-CA-C	-11.61	98.36	111.71
40	DT	28	VAL	O-C-N	11.28	136.67	122.57
34	DN	25	ARG	N-CA-C	-10.76	99.55	111.28

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

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	801	0
1	CA	32328	0	16317	876	1
2	AB	1901	0	1951	255	0
2	CB	1901	0	1951	253	0
3	AC	1613	0	1677	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	CC	1613	0	1677	162	0
4	AD	1703	0	1765	199	0
4	CD	1703	0	1764	188	0
5	AE	1147	0	1207	152	0
5	CE	1147	0	1207	171	0
6	AF	843	0	857	92	0
6	CF	843	0	857	67	0
7	AG	1257	0	1296	125	0
7	CG	1257	0	1296	111	0
8	AH	1116	0	1177	117	0
8	CH	1116	0	1177	114	0
9	AI	1010	0	1037	138	0
9	CI	1010	0	1037	149	0
10	AJ	795	0	840	128	0
10	CJ	795	0	840	136	0
11	AK	885	0	904	103	0
11	CK	885	0	904	115	0
12	AL	971	0	1057	130	0
12	CL	971	0	1057	130	0
13	AM	988	0	1059	156	0
13	CM	997	0	1072	175	0
14	AN	492	0	529	96	0
14	CN	492	0	531	77	0
15	AO	734	0	771	64	0
15	CO	734	0	771	54	0
16	AP	701	0	720	64	0
16	CP	701	0	720	105	0
17	AQ	824	0	891	70	0
17	CQ	824	0	891	89	0
18	AR	574	0	644	67	0
18	CR	574	0	644	72	0
19	AS	630	0	652	123	0
19	CS	630	0	652	112	0
20	AT	763	0	861	137	0
20	CT	763	0	861	172	0
21	AU	209	0	221	13	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	108	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	1620	1
25	DA	60827	0	30663	1380	0
26	BB	2551	0	1295	56	1
26	DB	2551	0	1295	55	0
27	BC	1142	0	865	85	0
27	DC	1142	0	865	76	0
28	BD	2105	0	2182	326	0
28	DD	2105	0	2182	289	0
29	BE	1564	0	1629	226	0
29	DE	1564	0	1629	218	0
30	BF	1624	0	1677	258	0
30	DF	1585	0	1632	199	0
31	BG	1474	0	1535	272	0
31	DG	1474	0	1535	223	0
32	BH	1223	0	1282	138	1
32	DH	1290	0	1364	242	0
33	BI	1131	0	1218	159	0
33	DI	1136	0	1223	243	0
34	BN	1105	0	1180	191	0
34	DN	1105	0	1180	156	0
35	BO	933	0	996	119	0
35	DO	933	0	996	95	0
36	BP	1145	0	1228	285	0
36	DP	1145	0	1228	289	3
37	BQ	1122	0	1179	138	0
37	DQ	1122	0	1179	129	0
38	BR	960	0	1021	153	0
38	DR	968	0	1033	117	0
39	BS	771	0	832	129	0
39	DS	882	0	943	151	0
40	BT	1142	0	1202	245	0
40	DT	1142	0	1202	274	0
41	BU	964	0	1022	162	0
41	DU	958	0	1014	204	0
42	BV	779	0	852	138	0
42	DV	779	0	852	155	3
43	BW	896	0	953	110	0
43	DW	896	0	953	91	0
44	BX	726	0	778	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DX	726	0	778	69	0
45	BY	776	0	870	181	0
45	DY	785	0	878	182	0
46	BZ	1404	0	1432	154	0
46	DZ	1404	0	1432	223	0
47	B0	662	0	688	63	0
47	D0	662	0	688	63	0
48	B1	732	0	808	81	0
48	D1	732	0	808	70	0
49	B2	598	0	653	70	0
49	D2	598	0	653	56	0
50	B3	468	0	523	43	3
50	D3	468	0	523	55	0
51	B4	226	0	229	40	0
51	D4	298	0	312	45	0
52	B5	459	0	480	51	0
52	D5	459	0	480	53	3
53	B6	381	0	391	51	0
53	D6	381	0	391	104	0
54	B7	419	0	467	38	0
54	D7	419	0	467	35	0
55	B8	508	0	576	115	0
55	D8	508	0	576	89	0
56	B9	299	0	326	14	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	16999	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 35.

The worst 5 of 16999 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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	AK	117/129 (91%)	92 (79%)	19 (16%)	6 (5%)	1	15
11	CK	117/129 (91%)	92 (79%)	23 (20%)	2 (2%)	7	35
12	AL	123/132 (93%)	78 (63%)	25 (20%)	20 (16%)	0	2
12	CL	123/132 (93%)	91 (74%)	20 (16%)	12 (10%)	0	6
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	4
14	CN	58/61 (95%)	37 (64%)	14 (24%)	7 (12%)	0	4
15	AO	86/89 (97%)	65 (76%)	20 (23%)	1 (1%)	10	42
15	CO	86/89 (97%)	55 (64%)	25 (29%)	6 (7%)	1	10
16	AP	82/88 (93%)	53 (65%)	25 (30%)	4 (5%)	1	16
16	CP	82/88 (93%)	66 (80%)	13 (16%)	3 (4%)	2	21
17	AQ	98/105 (93%)	79 (81%)	13 (13%)	6 (6%)	1	12
17	CQ	98/105 (93%)	77 (79%)	15 (15%)	6 (6%)	1	12
18	AR	68/88 (77%)	49 (72%)	12 (18%)	7 (10%)	0	5
18	CR	68/88 (77%)	49 (72%)	11 (16%)	8 (12%)	0	4
19	AS	77/93 (83%)	56 (73%)	15 (20%)	6 (8%)	1	8
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	9
20	CT	97/106 (92%)	67 (69%)	18 (19%)	12 (12%)	0	4
21	AU	23/27 (85%)	15 (65%)	4 (17%)	4 (17%)	0	2
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	0	7
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	4
28	DD	270/276 (98%)	202 (75%)	44 (16%)	24 (9%)	0	7
29	BE	203/206 (98%)	145 (71%)	36 (18%)	22 (11%)	0	5
29	DE	203/206 (98%)	134 (66%)	36 (18%)	33 (16%)	0	2
30	BF	206/210 (98%)	142 (69%)	44 (21%)	20 (10%)	0	6
30	DF	200/210 (95%)	160 (80%)	29 (14%)	11 (6%)	1	13
31	BG	179/182 (98%)	121 (68%)	36 (20%)	22 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	DG	179/182 (98%)	124 (69%)	30 (17%)	25 (14%)	0	3
32	BH	158/180 (88%)	96 (61%)	37 (23%)	25 (16%)	0	2
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	4
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	2
34	DN	137/140 (98%)	86 (63%)	39 (28%)	12 (9%)	0	7
35	BO	120/122 (98%)	95 (79%)	17 (14%)	8 (7%)	1	11
35	DO	120/122 (98%)	97 (81%)	18 (15%)	5 (4%)	2	18
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	8
37	DQ	139/141 (99%)	109 (78%)	18 (13%)	12 (9%)	0	7
38	BR	115/118 (98%)	78 (68%)	25 (22%)	12 (10%)	0	5
38	DR	116/118 (98%)	86 (74%)	20 (17%)	10 (9%)	0	7
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	2
40	BT	136/146 (93%)	90 (66%)	28 (21%)	18 (13%)	0	3
40	DT	136/146 (93%)	95 (70%)	19 (14%)	22 (16%)	0	2
41	BU	115/118 (98%)	73 (64%)	30 (26%)	12 (10%)	0	5
41	DU	115/118 (98%)	75 (65%)	30 (26%)	10 (9%)	0	7
42	BV	99/101 (98%)	75 (76%)	9 (9%)	15 (15%)	0	2
42	DV	99/101 (98%)	80 (81%)	9 (9%)	10 (10%)	0	6
43	BW	111/113 (98%)	81 (73%)	22 (20%)	8 (7%)	1	9
43	DW	111/113 (98%)	82 (74%)	19 (17%)	10 (9%)	0	7
44	BX	91/96 (95%)	69 (76%)	16 (18%)	6 (7%)	1	11
44	DX	91/96 (95%)	76 (84%)	11 (12%)	4 (4%)	2	17
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	4
46	DZ	175/206 (85%)	101 (58%)	46 (26%)	28 (16%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	B0	82/85 (96%)	64 (78%)	13 (16%)	5 (6%)	1	12
47	D0	82/85 (96%)	67 (82%)	8 (10%)	7 (8%)	0	7
48	B1	92/98 (94%)	68 (74%)	13 (14%)	11 (12%)	0	4
48	D1	92/98 (94%)	69 (75%)	12 (13%)	11 (12%)	0	4
49	B2	69/72 (96%)	49 (71%)	15 (22%)	5 (7%)	1	9
49	D2	69/72 (96%)	57 (83%)	5 (7%)	7 (10%)	0	6
50	B3	58/60 (97%)	48 (83%)	3 (5%)	7 (12%)	0	4
50	D3	58/60 (97%)	46 (79%)	7 (12%)	5 (9%)	0	7
51	B4	29/71 (41%)	17 (59%)	8 (28%)	4 (14%)	0	3
51	D4	38/71 (54%)	21 (55%)	12 (32%)	5 (13%)	0	3
52	B5	57/60 (95%)	46 (81%)	6 (10%)	5 (9%)	0	7
52	D5	57/60 (95%)	46 (81%)	5 (9%)	6 (10%)	0	5
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%)	0	7
54	D7	47/49 (96%)	43 (92%)	3 (6%)	1 (2%)	5	31
55	B8	62/65 (95%)	42 (68%)	14 (23%)	6 (10%)	0	6
55	D8	62/65 (95%)	41 (66%)	14 (23%)	7 (11%)	0	4
56	B9	34/37 (92%)	23 (68%)	10 (29%)	1 (3%)	3	25
56	D9	34/37 (92%)	27 (79%)	6 (18%)	1 (3%)	3	25
All	All	11730/12586 (93%)	8097 (69%)	2283 (20%)	1350 (12%)	0	4

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%)	159 (79%)	43 (21%)	1	6
2	CB	202/220 (92%)	147 (73%)	55 (27%)	0	3
3	AC	160/188 (85%)	126 (79%)	34 (21%)	1	6
3	CC	160/188 (85%)	130 (81%)	30 (19%)	1	9
4	AD	180/181 (99%)	150 (83%)	30 (17%)	2	13
4	CD	180/181 (99%)	152 (84%)	28 (16%)	2	16
5	AE	115/123 (94%)	93 (81%)	22 (19%)	1	8
5	CE	115/123 (94%)	86 (75%)	29 (25%)	0	4
6	AF	90/90 (100%)	72 (80%)	18 (20%)	1	7
6	CF	90/90 (100%)	75 (83%)	15 (17%)	2	13
7	AG	126/127 (99%)	100 (79%)	26 (21%)	1	7
7	CG	126/127 (99%)	101 (80%)	25 (20%)	1	8
8	AH	119/119 (100%)	97 (82%)	22 (18%)	1	9
8	CH	119/119 (100%)	83 (70%)	36 (30%)	0	2
9	AI	98/99 (99%)	79 (81%)	19 (19%)	1	8
9	CI	98/99 (99%)	76 (78%)	22 (22%)	1	5
10	AJ	88/92 (96%)	65 (74%)	23 (26%)	0	3
10	CJ	88/92 (96%)	67 (76%)	21 (24%)	1	4
11	AK	90/99 (91%)	74 (82%)	16 (18%)	2	10
11	CK	90/99 (91%)	67 (74%)	23 (26%)	0	3
12	AL	104/109 (95%)	79 (76%)	25 (24%)	1	4
12	CL	104/109 (95%)	80 (77%)	24 (23%)	1	5
13	AM	99/101 (98%)	77 (78%)	22 (22%)	1	5
13	CM	100/101 (99%)	85 (85%)	15 (15%)	3	17
14	AN	49/50 (98%)	41 (84%)	8 (16%)	2	14
14	CN	49/50 (98%)	37 (76%)	12 (24%)	1	4
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%)	57 (79%)	15 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	CP	72/74 (97%)	56 (78%)	16 (22%)	1	5
17	AQ	94/97 (97%)	84 (89%)	10 (11%)	6	28
17	CQ	94/97 (97%)	77 (82%)	17 (18%)	2	10
18	AR	61/77 (79%)	47 (77%)	14 (23%)	1	5
18	CR	61/77 (79%)	49 (80%)	12 (20%)	1	8
19	AS	69/80 (86%)	49 (71%)	20 (29%)	0	2
19	CS	69/80 (86%)	46 (67%)	23 (33%)	0	2
20	AT	76/82 (93%)	52 (68%)	24 (32%)	0	2
20	CT	76/82 (93%)	50 (66%)	26 (34%)	0	2
21	AU	19/22 (86%)	17 (90%)	2 (10%)	6	28
21	CU	19/22 (86%)	12 (63%)	7 (37%)	0	1
27	BC	61/181 (34%)	49 (80%)	12 (20%)	1	8
27	DC	61/181 (34%)	54 (88%)	7 (12%)	5	25
28	BD	213/218 (98%)	157 (74%)	56 (26%)	0	3
28	DD	213/218 (98%)	178 (84%)	35 (16%)	2	14
29	BE	165/166 (99%)	124 (75%)	41 (25%)	1	4
29	DE	165/166 (99%)	137 (83%)	28 (17%)	2	12
30	BF	165/166 (99%)	124 (75%)	41 (25%)	1	4
30	DF	161/166 (97%)	133 (83%)	28 (17%)	2	11
31	BG	155/156 (99%)	116 (75%)	39 (25%)	0	4
31	DG	155/156 (99%)	137 (88%)	18 (12%)	5	25
32	BH	132/148 (89%)	110 (83%)	22 (17%)	2	13
32	DH	140/148 (95%)	113 (81%)	27 (19%)	1	8
33	BI	122/124 (98%)	95 (78%)	27 (22%)	1	6
33	DI	122/124 (98%)	96 (79%)	26 (21%)	1	6
34	BN	117/119 (98%)	87 (74%)	30 (26%)	0	3
34	DN	117/119 (98%)	99 (85%)	18 (15%)	2	16
35	BO	100/100 (100%)	77 (77%)	23 (23%)	1	5
35	DO	100/100 (100%)	88 (88%)	12 (12%)	5	23
36	BP	116/116 (100%)	85 (73%)	31 (27%)	0	3
36	DP	116/116 (100%)	86 (74%)	30 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	BQ	111/111 (100%)	79 (71%)	32 (29%)	0	2
37	DQ	111/111 (100%)	92 (83%)	19 (17%)	2	12
38	BR	100/101 (99%)	67 (67%)	33 (33%)	0	2
38	DR	101/101 (100%)	86 (85%)	15 (15%)	3	17
39	BS	77/88 (88%)	52 (68%)	25 (32%)	0	2
39	DS	87/88 (99%)	74 (85%)	13 (15%)	3	17
40	BT	120/127 (94%)	88 (73%)	32 (27%)	0	3
40	DT	120/127 (94%)	88 (73%)	32 (27%)	0	3
41	BU	93/94 (99%)	68 (73%)	25 (27%)	0	3
41	DU	92/94 (98%)	78 (85%)	14 (15%)	3	17
42	BV	82/82 (100%)	54 (66%)	28 (34%)	0	2
42	DV	82/82 (100%)	61 (74%)	21 (26%)	0	3
43	BW	91/92 (99%)	66 (72%)	25 (28%)	0	3
43	DW	91/92 (99%)	83 (91%)	8 (9%)	9	33
44	BX	74/78 (95%)	56 (76%)	18 (24%)	1	4
44	DX	74/78 (95%)	61 (82%)	13 (18%)	2	11
45	BY	84/91 (92%)	64 (76%)	20 (24%)	1	4
45	DY	85/91 (93%)	66 (78%)	19 (22%)	1	5
46	BZ	155/179 (87%)	122 (79%)	33 (21%)	1	6
46	DZ	155/179 (87%)	137 (88%)	18 (12%)	5	25
47	B0	66/67 (98%)	57 (86%)	9 (14%)	3	20
47	D0	66/67 (98%)	56 (85%)	10 (15%)	3	17
48	B1	78/83 (94%)	59 (76%)	19 (24%)	1	4
48	D1	78/83 (94%)	60 (77%)	18 (23%)	1	5
49	B2	66/67 (98%)	50 (76%)	16 (24%)	1	4
49	D2	66/67 (98%)	54 (82%)	12 (18%)	2	10
50	B3	51/52 (98%)	38 (74%)	13 (26%)	0	3
50	D3	51/52 (98%)	47 (92%)	4 (8%)	11	37
51	B4	27/63 (43%)	17 (63%)	10 (37%)	0	1
51	D4	35/63 (56%)	32 (91%)	3 (9%)	10	34
52	B5	51/52 (98%)	40 (78%)	11 (22%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	D5	51/52 (98%)	43 (84%)	8 (16%)	2	15
53	B6	43/52 (83%)	31 (72%)	12 (28%)	0	3
53	D6	43/52 (83%)	32 (74%)	11 (26%)	0	3
54	B7	41/42 (98%)	32 (78%)	9 (22%)	1	6
54	D7	41/42 (98%)	36 (88%)	5 (12%)	5	23
55	B8	53/55 (96%)	38 (72%)	15 (28%)	0	3
55	D8	53/55 (96%)	46 (87%)	7 (13%)	4	21
56	B9	33/34 (97%)	28 (85%)	5 (15%)	3	17
56	D9	33/34 (97%)	29 (88%)	4 (12%)	5	23
All	All	9688/10428 (93%)	7636 (79%)	2052 (21%)	1	6

5 of 2052 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	DT	30	VAL
42	DV	71	LEU
40	DT	27	THR
38	BR	51	LEU
37	BQ	110	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 163 such sidechains are listed below:

Mol	Chain	Res	Type
32	DH	158	HIS
43	DW	61	ASN
33	DI	139	GLN
40	DT	38	ASN
47	D0	70	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	369 (24%)	109 (7%)
1	CA	1503/1522 (98%)	363 (24%)	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%)	810 (28%)	260 (9%)
25	DA	2818/2915 (96%)	814 (28%)	264 (9%)
26	BB	118/122 (96%)	26 (22%)	5 (4%)
26	DB	118/122 (96%)	25 (21%)	7 (5%)
All	All	9218/9624 (95%)	2532 (27%)	768 (8%)

5 of 2532 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 oligosaccharides 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	AA	7111	-	44,45,45	1.44	7 (15%)	63,67,67	1.18	4 (6%)
58	PAR	CA	1741	-	44,45,45	1.44	7 (15%)	63,67,67	1.18	5 (7%)

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	AA	7111	-	-	2/18/94/94	0/4/4/4
58	PAR	CA	1741	-	-	2/18/94/94	0/4/4/4

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	AA	7111	PAR	O54-C14	3.89	1.51	1.41
58	CA	1741	PAR	O54-C14	3.87	1.51	1.41
58	CA	1741	PAR	C31-C21	3.20	1.57	1.53
58	AA	7111	PAR	C31-C21	3.15	1.57	1.53
58	AA	7111	PAR	C24-N24	2.87	1.51	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	AA	7111	PAR	O33-C14-C24	3.61	113.99	108.08
58	CA	1741	PAR	O33-C14-C24	3.57	113.91	108.08
58	CA	1741	PAR	C14-O54-C54	3.22	120.01	113.72
58	AA	7111	PAR	C14-O54-C54	3.22	120.01	113.72
58	AA	7111	PAR	O54-C54-C64	3.09	112.00	106.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

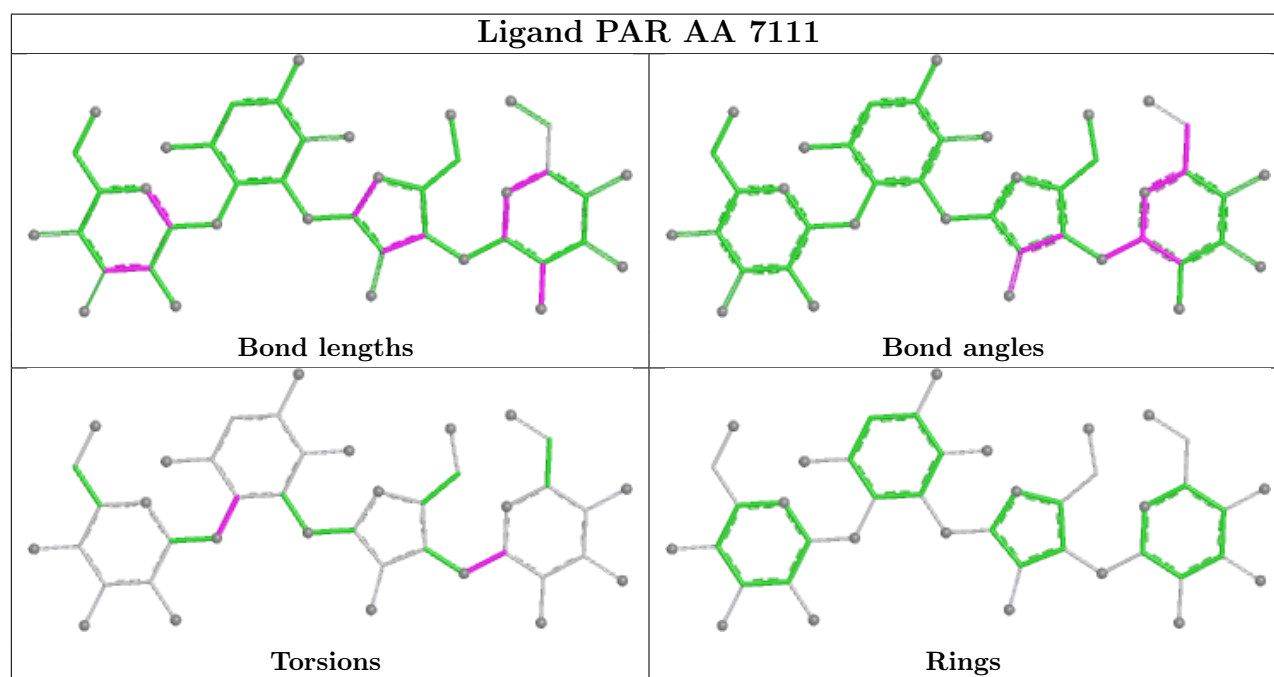
Mol	Chain	Res	Type	Atoms
58	AA	7111	PAR	C24-C14-O33-C33
58	CA	1741	PAR	C24-C14-O33-C33
58	AA	7111	PAR	C52-C42-O11-C11
58	CA	1741	PAR	C52-C42-O11-C11

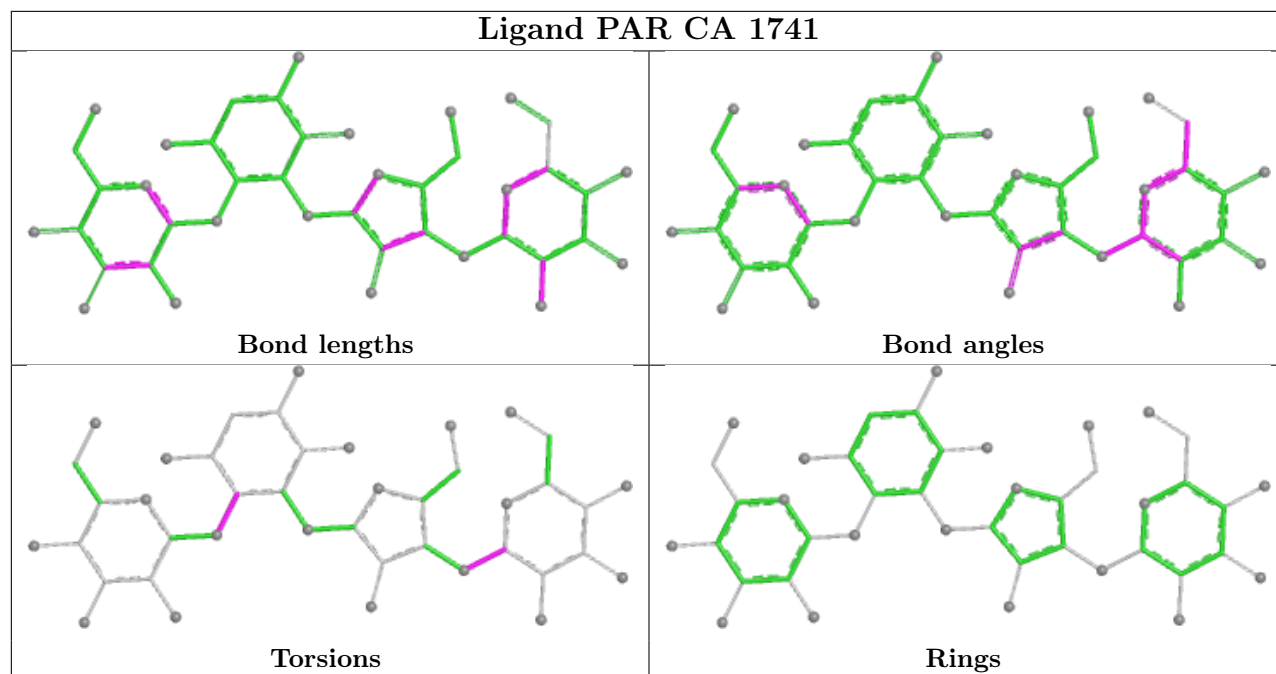
There are no ring outliers.

2 monomers are involved in 5 short contacts:

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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%)	0.29	72 (4%)	35	19	31, 78, 168, 331	0
1	CA	1504/1522 (98%)	0.30	69 (4%)	37	19	24, 68, 165, 363	0
2	AB	235/256 (91%)	0.24	6 (2%)	57	32	67, 121, 201, 279	0
2	CB	235/256 (91%)	0.22	5 (2%)	63	36	44, 109, 202, 287	0
3	AC	207/239 (86%)	0.05	2 (0%)	79	54	44, 104, 173, 240	0
3	CC	207/239 (86%)	-0.03	2 (0%)	79	54	38, 90, 151, 227	0
4	AD	208/209 (99%)	0.31	9 (4%)	40	21	37, 89, 153, 217	0
4	CD	208/209 (99%)	0.23	13 (6%)	26	16	30, 77, 129, 209	0
5	AE	151/162 (93%)	0.23	6 (3%)	42	23	44, 87, 151, 240	0
5	CE	151/162 (93%)	0.18	7 (4%)	37	19	22, 71, 131, 266	0
6	AF	101/101 (100%)	-0.12	0	100	100	29, 74, 120, 178	0
6	CF	101/101 (100%)	0.01	0	100	100	25, 68, 134, 192	0
7	AG	155/156 (99%)	0.12	7 (4%)	38	20	50, 93, 149, 256	0
7	CG	155/156 (99%)	0.14	8 (5%)	33	18	32, 87, 151, 269	0
8	AH	138/138 (100%)	-0.03	2 (1%)	73	46	41, 85, 129, 183	0
8	CH	138/138 (100%)	-0.02	2 (1%)	73	46	38, 75, 123, 181	0
9	AI	127/128 (99%)	0.31	2 (1%)	70	43	55, 113, 161, 319	0
9	CI	127/128 (99%)	0.46	6 (4%)	36	19	45, 97, 170, 245	0
10	AJ	99/105 (94%)	0.54	5 (5%)	33	19	58, 124, 197, 302	0
10	CJ	99/105 (94%)	0.71	9 (9%)	15	9	38, 115, 191, 204	0
11	AK	119/129 (92%)	0.25	7 (5%)	28	16	41, 77, 147, 249	0
11	CK	119/129 (92%)	0.11	5 (4%)	40	21	29, 73, 139, 188	0
12	AL	125/132 (94%)	0.25	4 (3%)	50	28	31, 64, 129, 300	0
12	CL	125/132 (94%)	0.16	6 (4%)	35	19	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%)	0.41	11 (8%) 15 10	29, 94, 148, 314	0
13	CM	125/126 (99%)	0.97	17 (13%) 7 5	39, 87, 174, 274	0
14	AN	60/61 (98%)	0.52	3 (5%) 34 19	53, 92, 138, 207	0
14	CN	60/61 (98%)	0.28	4 (6%) 24 15	34, 71, 111, 194	0
15	AO	88/89 (98%)	-0.02	0 100 100	35, 80, 132, 142	0
15	CO	88/89 (98%)	-0.02	1 (1%) 78 52	23, 69, 122, 147	0
16	AP	84/88 (95%)	0.04	1 (1%) 76 50	48, 74, 122, 182	0
16	CP	84/88 (95%)	0.35	2 (2%) 59 34	44, 76, 139, 200	0
17	AQ	100/105 (95%)	0.21	4 (4%) 42 23	50, 91, 141, 174	0
17	CQ	100/105 (95%)	0.30	4 (4%) 42 23	38, 87, 144, 192	0
18	AR	70/88 (79%)	-0.11	0 100 100	35, 77, 126, 182	0
18	CR	70/88 (79%)	-0.00	1 (1%) 73 46	36, 70, 122, 205	0
19	AS	79/93 (84%)	0.49	3 (3%) 44 24	46, 104, 202, 268	0
19	CS	79/93 (84%)	0.56	5 (6%) 26 16	27, 82, 153, 206	0
20	AT	99/106 (93%)	0.45	4 (4%) 42 23	42, 90, 173, 211	0
20	CT	99/106 (93%)	1.04	16 (16%) 4 4	40, 97, 192, 295	0
21	AU	25/27 (92%)	1.27	6 (24%) 2 2	36, 92, 165, 229	0
21	CU	25/27 (92%)	1.02	6 (24%) 2 2	50, 78, 107, 150	0
22	AV	77/77 (100%)	0.19	0 100 100	45, 82, 163, 276	0
22	CV	77/77 (100%)	0.35	5 (6%) 25 15	32, 72, 133, 253	0
23	AW	76/76 (100%)	0.68	4 (5%) 32 18	48, 175, 249, 317	0
23	AY	17/76 (22%)	0.28	0 100 100	64, 94, 167, 176	0
23	CW	76/76 (100%)	0.83	8 (10%) 11 7	34, 184, 271, 295	0
23	CY	17/76 (22%)	0.31	0 100 100	44, 75, 149, 186	0
24	AX	12/24 (50%)	1.16	4 (33%) 1 1	49, 74, 217, 234	0
24	CX	10/24 (41%)	1.53	2 (20%) 3 3	42, 58, 144, 213	0
25	BA	2810/2915 (96%)	0.25	103 (3%) 45 25	17, 58, 187, 375	0
25	DA	2824/2915 (96%)	0.12	100 (3%) 47 26	6, 42, 178, 370	0
26	BB	119/122 (97%)	0.36	3 (2%) 58 33	59, 94, 132, 182	0
26	DB	119/122 (97%)	0.29	3 (2%) 58 33	38, 68, 113, 174	0
27	BC	191/229 (83%)	0.87	20 (10%) 11 7	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%)	0.74	18 (9%) 14 9	64, 208, 290, 334	0
28	BD	272/276 (98%)	0.03	5 (1%) 67 40	9, 45, 89, 166	0
28	DD	272/276 (98%)	0.01	9 (3%) 49 27	3, 33, 80, 197	0
29	BE	205/206 (99%)	0.21	12 (5%) 28 16	17, 66, 128, 289	0
29	DE	205/206 (99%)	0.18	4 (1%) 65 37	11, 55, 160, 338	0
30	BF	208/210 (99%)	0.13	5 (2%) 59 34	14, 64, 164, 286	0
30	DF	202/210 (96%)	0.40	9 (4%) 38 20	5, 51, 127, 208	0
31	BG	181/182 (99%)	0.27	9 (4%) 34 19	40, 95, 175, 268	0
31	DG	181/182 (99%)	0.40	6 (3%) 49 27	25, 76, 143, 219	0
32	BH	160/180 (88%)	0.94	20 (12%) 8 6	85, 179, 331, 429	0
32	DH	168/180 (93%)	0.69	13 (7%) 19 13	29, 81, 155, 234	0
33	BI	145/148 (97%)	0.08	3 (2%) 63 36	33, 96, 156, 184	0
33	DI	146/148 (98%)	0.51	8 (5%) 30 17	15, 104, 166, 207	0
34	BN	139/140 (99%)	0.17	8 (5%) 29 17	36, 79, 147, 305	0
34	DN	139/140 (99%)	0.26	4 (2%) 53 30	7, 61, 137, 185	0
35	BO	122/122 (100%)	0.02	1 (0%) 82 58	32, 65, 97, 124	0
35	DO	122/122 (100%)	-0.29	0 100 100	10, 41, 84, 112	0
36	BP	150/150 (100%)	1.26	34 (22%) 2 2	27, 87, 179, 250	0
36	DP	150/150 (100%)	1.51	45 (30%) 1 2	23, 71, 151, 264	0
37	BQ	141/141 (100%)	0.20	9 (6%) 25 15	36, 74, 126, 421	0
37	DQ	141/141 (100%)	0.18	6 (4%) 40 21	12, 52, 108, 281	0
38	BR	117/118 (99%)	0.31	10 (8%) 16 11	21, 57, 107, 148	0
38	DR	118/118 (100%)	0.14	4 (3%) 48 27	15, 50, 92, 126	0
39	BS	99/112 (88%)	0.59	9 (9%) 15 9	38, 100, 171, 347	0
39	DS	111/112 (99%)	0.49	6 (5%) 31 18	33, 73, 147, 197	0
40	BT	138/146 (94%)	0.35	11 (7%) 18 12	29, 80, 225, 351	0
40	DT	138/146 (94%)	0.63	14 (10%) 12 8	20, 71, 212, 304	0
41	BU	117/118 (99%)	0.39	7 (5%) 27 16	29, 64, 131, 281	0
41	DU	117/118 (99%)	0.27	3 (2%) 57 32	17, 52, 114, 180	0
42	BV	101/101 (100%)	0.12	1 (0%) 79 54	23, 90, 149, 344	0
42	DV	101/101 (100%)	0.54	6 (5%) 28 16	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%)	-0.07	3 (2%) 56 32	19, 49, 113, 319	0
43	DW	113/113 (100%)	-0.04	0 100 100	14, 42, 128, 204	0
44	BX	93/96 (96%)	0.07	2 (2%) 62 35	30, 63, 99, 149	0
44	DX	93/96 (96%)	0.11	2 (2%) 62 35	12, 42, 87, 144	0
45	BY	101/110 (91%)	1.17	20 (19%) 3 3	42, 92, 253, 363	0
45	DY	102/110 (92%)	0.76	14 (13%) 6 5	28, 82, 182, 226	0
46	BZ	177/206 (85%)	0.40	7 (3%) 42 23	45, 125, 202, 316	0
46	DZ	177/206 (85%)	0.78	16 (9%) 15 9	29, 116, 254, 322	0
47	B0	84/85 (98%)	0.34	9 (10%) 11 7	31, 69, 170, 242	0
47	D0	84/85 (98%)	0.47	9 (10%) 11 7	18, 52, 136, 286	0
48	B1	94/98 (95%)	0.01	2 (2%) 63 36	17, 53, 113, 219	0
48	D1	94/98 (95%)	0.28	3 (3%) 50 28	7, 44, 122, 237	0
49	B2	71/72 (98%)	0.19	1 (1%) 73 46	35, 77, 128, 195	0
49	D2	71/72 (98%)	0.78	9 (12%) 8 6	14, 54, 137, 267	0
50	B3	60/60 (100%)	0.18	1 (1%) 69 41	35, 75, 125, 382	0
50	D3	60/60 (100%)	0.21	1 (1%) 69 41	20, 65, 142, 236	0
51	B4	31/71 (43%)	0.15	2 (6%) 25 15	67, 121, 152, 204	0
51	D4	40/71 (56%)	0.59	4 (10%) 12 8	55, 116, 173, 266	0
52	B5	59/60 (98%)	0.17	3 (5%) 33 19	17, 72, 180, 340	0
52	D5	59/60 (98%)	0.16	2 (3%) 48 27	12, 63, 214, 299	0
53	B6	45/54 (83%)	1.18	9 (20%) 3 3	44, 138, 207, 343	0
53	D6	45/54 (83%)	1.60	12 (26%) 1 2	59, 139, 235, 285	0
54	B7	49/49 (100%)	0.47	5 (10%) 12 8	11, 41, 123, 149	0
54	D7	49/49 (100%)	0.11	4 (8%) 17 12	1, 23, 101, 204	0
55	B8	64/65 (98%)	0.70	8 (12%) 8 6	20, 60, 129, 325	0
55	D8	64/65 (98%)	0.71	8 (12%) 8 6	12, 51, 115, 172	0
56	B9	36/37 (97%)	3.00	23 (63%) 0 0	120, 197, 269, 389	0
56	D9	36/37 (97%)	2.87	26 (72%) 0 0	115, 172, 217, 282	0
All	All	21184/22210 (95%)	0.30	1098 (5%) 33 18	1, 71, 192, 429	0

The worst 5 of 1098 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
53	D6	24	GLU	7.7
37	BQ	140	ALA	7.6
55	B8	31	HIS	7.4
56	B9	37	GLY	7.3
56	B9	23	VAL	7.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9660	1/1	0.30	0.27	176,176,176,176	0
57	MG	CA	1691	1/1	0.32	0.38	91,91,91,91	0
57	MG	BA	3315	1/1	0.34	0.15	84,84,84,84	0
57	MG	DA	9475	1/1	0.37	0.16	26,26,26,26	0
57	MG	BA	3086	1/1	0.38	0.17	1,1,1,1	0
57	MG	DB	204	1/1	0.38	0.52	0,0,0,0	1
57	MG	CA	1610	1/1	0.44	0.23	58,58,58,58	0
57	MG	BA	3082	1/1	0.48	0.27	23,23,23,23	0
57	MG	CA	1694	1/1	0.49	0.20	51,51,51,51	0
57	MG	BA	3322	1/1	0.51	0.24	54,54,54,54	0
57	MG	BA	3036	1/1	0.51	0.30	78,78,78,78	1
57	MG	DA	9441	1/1	0.51	0.24	31,31,31,31	1
57	MG	BA	3273	1/1	0.53	0.15	71,71,71,71	0
57	MG	BA	3033	1/1	0.55	0.11	6,6,6,6	0
57	MG	DA	9600	1/1	0.55	0.23	55,55,55,55	0
57	MG	DA	9380	1/1	0.56	0.40	23,23,23,23	1
57	MG	BB	205	1/1	0.56	0.28	19,19,19,19	1
57	MG	DA	9402	1/1	0.57	0.32	25,25,25,25	0
57	MG	AA	7071	1/1	0.58	0.16	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9352	1/1	0.58	0.09	89,89,89,89	0
57	MG	BA	3265	1/1	0.58	0.37	43,43,43,43	0
57	MG	BA	3286	1/1	0.59	0.15	22,22,22,22	0
57	MG	DA	9367	1/1	0.61	0.25	35,35,35,35	0
57	MG	CA	1716	1/1	0.62	0.15	26,26,26,26	0
57	MG	DA	9666	1/1	0.63	0.21	7,7,7,7	0
57	MG	BA	3037	1/1	0.64	0.23	83,83,83,83	0
57	MG	DA	9638	1/1	0.65	0.09	8,8,8,8	1
57	MG	DA	9685	1/1	0.65	0.26	22,22,22,22	0
57	MG	CA	1736	1/1	0.65	0.11	6,6,6,6	0
57	MG	D1	101	1/1	0.65	0.16	55,55,55,55	0
57	MG	AX	101	1/1	0.66	0.21	43,43,43,43	0
57	MG	BP	201	1/1	0.66	0.28	166,166,166,166	0
57	MG	BB	202	1/1	0.67	0.13	62,62,62,62	0
57	MG	CA	1719	1/1	0.67	0.19	10,10,10,10	0
57	MG	BA	3320	1/1	0.67	0.34	54,54,54,54	0
57	MG	AA	7076	1/1	0.67	0.27	60,60,60,60	0
57	MG	DA	9655	1/1	0.68	0.35	35,35,35,35	0
57	MG	BA	3063	1/1	0.68	0.21	55,55,55,55	0
57	MG	DA	9350	1/1	0.69	0.20	48,48,48,48	1
57	MG	DA	9661	1/1	0.69	0.29	57,57,57,57	0
57	MG	BA	3076	1/1	0.70	0.16	18,18,18,18	0
57	MG	DA	9425	1/1	0.70	0.31	37,37,37,37	0
57	MG	BA	3137	1/1	0.70	0.40	1,1,1,1	1
57	MG	DA	9658	1/1	0.70	0.13	36,36,36,36	0
57	MG	DB	205	1/1	0.70	0.14	6,6,6,6	1
57	MG	DW	201	1/1	0.70	0.23	27,27,27,27	0
57	MG	AA	7057	1/1	0.70	0.12	44,44,44,44	0
57	MG	CA	1739	1/1	0.71	0.23	36,36,36,36	0
57	MG	DA	9644	1/1	0.71	0.16	25,25,25,25	0
57	MG	BA	3196	1/1	0.71	0.39	30,30,30,30	0
57	MG	BA	3101	1/1	0.72	0.46	27,27,27,27	1
57	MG	DA	9674	1/1	0.72	0.25	17,17,17,17	0
57	MG	BA	3028	1/1	0.72	0.19	44,44,44,44	0
57	MG	DA	9429	1/1	0.72	0.32	51,51,51,51	0
57	MG	BA	3053	1/1	0.72	0.16	17,17,17,17	0
57	MG	BA	3242	1/1	0.72	0.26	44,44,44,44	0
57	MG	DA	9399	1/1	0.72	0.47	52,52,52,52	0
57	MG	DA	9630	1/1	0.73	0.18	16,16,16,16	1
57	MG	BA	3093	1/1	0.73	0.25	49,49,49,49	0
57	MG	CA	1672	1/1	0.73	0.26	62,62,62,62	0
57	MG	DA	9467	1/1	0.73	0.18	53,53,53,53	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1674	1/1	0.73	0.20	89,89,89,89	0
57	MG	DA	9494	1/1	0.73	0.27	39,39,39,39	0
57	MG	AV	105	1/1	0.73	0.25	54,54,54,54	0
57	MG	DA	9688	1/1	0.74	0.30	78,78,78,78	0
57	MG	CA	1609	1/1	0.74	0.16	30,30,30,30	0
57	MG	DA	9671	1/1	0.74	0.31	45,45,45,45	0
57	MG	BA	3149	1/1	0.74	0.11	27,27,27,27	0
57	MG	AA	7090	1/1	0.74	0.41	69,69,69,69	0
57	MG	CA	1708	1/1	0.75	0.16	34,34,34,34	0
57	MG	DB	202	1/1	0.75	0.10	28,28,28,28	0
57	MG	BA	3173	1/1	0.75	0.29	27,27,27,27	0
57	MG	BA	3313	1/1	0.75	0.12	42,42,42,42	0
57	MG	CA	1722	1/1	0.75	0.23	27,27,27,27	0
57	MG	DA	9634	1/1	0.75	0.20	44,44,44,44	0
57	MG	DA	9501	1/1	0.76	0.30	42,42,42,42	0
57	MG	DA	9567	1/1	0.76	0.16	31,31,31,31	0
57	MG	DA	9693	1/1	0.76	0.34	47,47,47,47	0
57	MG	AA	7088	1/1	0.76	0.14	60,60,60,60	0
57	MG	CA	1680	1/1	0.76	0.17	49,49,49,49	0
57	MG	CW	101	1/1	0.76	0.07	29,29,29,29	1
57	MG	BA	3248	1/1	0.76	0.22	49,49,49,49	0
57	MG	BA	3227	1/1	0.76	0.22	40,40,40,40	0
57	MG	AA	7059	1/1	0.77	0.29	96,96,96,96	0
57	MG	DA	9396	1/1	0.77	0.19	26,26,26,26	0
57	MG	DA	9503	1/1	0.77	0.20	66,66,66,66	0
57	MG	DA	9530	1/1	0.77	0.38	41,41,41,41	0
57	MG	AA	7083	1/1	0.77	0.22	18,18,18,18	0
57	MG	DA	9574	1/1	0.77	0.16	14,14,14,14	1
57	MG	BA	3133	1/1	0.77	0.14	43,43,43,43	0
57	MG	CA	1707	1/1	0.77	0.40	1,1,1,1	1
57	MG	DA	9695	1/1	0.77	0.34	63,63,63,63	0
57	MG	AA	7060	1/1	0.77	0.09	8,8,8,8	0
57	MG	AA	7008	1/1	0.77	0.40	35,35,35,35	0
57	MG	DA	9358	1/1	0.77	0.48	5,5,5,5	0
57	MG	AA	7074	1/1	0.77	0.32	26,26,26,26	0
57	MG	DA	9490	1/1	0.77	0.27	39,39,39,39	0
57	MG	CA	1614	1/1	0.78	0.28	38,38,38,38	0
57	MG	BA	3319	1/1	0.78	0.08	27,27,27,27	0
57	MG	BA	3262	1/1	0.78	0.22	39,39,39,39	0
57	MG	DA	9477	1/1	0.78	0.26	36,36,36,36	0
57	MG	AA	7023	1/1	0.79	0.10	56,56,56,56	0
57	MG	AA	7070	1/1	0.79	0.15	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3109	1/1	0.79	0.26	66,66,66,66	0
57	MG	DA	9453	1/1	0.79	0.39	4,4,4,4	1
57	MG	DA	9333	1/1	0.79	0.15	31,31,31,31	0
57	MG	DA	9347	1/1	0.79	0.18	22,22,22,22	0
57	MG	BA	3231	1/1	0.79	0.17	90,90,90,90	0
57	MG	BA	3236	1/1	0.79	0.23	17,17,17,17	0
57	MG	DA	9493	1/1	0.79	0.17	1,1,1,1	0
57	MG	BA	3126	1/1	0.79	0.25	44,44,44,44	0
57	MG	AA	7109	1/1	0.79	0.18	33,33,33,33	0
57	MG	BA	3252	1/1	0.79	0.30	56,56,56,56	0
57	MG	DA	9388	1/1	0.79	0.12	28,28,28,28	0
57	MG	BA	3030	1/1	0.79	0.28	22,22,22,22	0
57	MG	DA	9397	1/1	0.79	0.31	25,25,25,25	1
57	MG	BA	3088	1/1	0.79	0.20	43,43,43,43	0
57	MG	BA	3167	1/1	0.79	0.16	30,30,30,30	0
57	MG	DA	9419	1/1	0.79	0.19	10,10,10,10	1
57	MG	CA	1641	1/1	0.80	0.14	40,40,40,40	0
57	MG	CA	1697	1/1	0.80	0.13	49,49,49,49	0
57	MG	CA	1643	1/1	0.80	0.28	40,40,40,40	1
57	MG	BA	3128	1/1	0.80	0.14	57,57,57,57	0
57	MG	CA	1673	1/1	0.80	0.14	18,18,18,18	0
57	MG	AA	7029	1/1	0.80	0.22	41,41,41,41	0
57	MG	BA	3062	1/1	0.80	0.08	27,27,27,27	0
57	MG	CA	1687	1/1	0.80	0.21	47,47,47,47	0
57	MG	CA	1737	1/1	0.80	0.29	28,28,28,28	0
57	MG	BA	3095	1/1	0.80	0.31	35,35,35,35	0
57	MG	CA	1650	1/1	0.81	0.29	34,34,34,34	0
57	MG	AA	7002	1/1	0.81	0.15	35,35,35,35	0
57	MG	BA	3145	1/1	0.81	0.18	22,22,22,22	0
57	MG	CA	1728	1/1	0.81	0.11	59,59,59,59	0
57	MG	BB	203	1/1	0.81	0.31	16,16,16,16	1
57	MG	AA	7101	1/1	0.81	0.16	22,22,22,22	0
57	MG	BA	3312	1/1	0.81	0.19	45,45,45,45	0
57	MG	DA	9415	1/1	0.81	0.32	0,0,0,0	0
57	MG	BA	3001	1/1	0.81	0.23	38,38,38,38	0
57	MG	AA	7005	1/1	0.81	0.26	45,45,45,45	0
57	MG	BA	3318	1/1	0.81	0.27	37,37,37,37	0
57	MG	DA	9439	1/1	0.81	0.10	32,32,32,32	0
57	MG	CA	1704	1/1	0.81	0.31	28,28,28,28	0
57	MG	BA	3079	1/1	0.81	0.26	29,29,29,29	1
57	MG	BA	3216	1/1	0.81	0.24	48,48,48,48	0
57	MG	DA	9651	1/1	0.81	0.10	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	D5	102	1/1	0.81	0.14	32,32,32,32	1
57	MG	AA	7016	1/1	0.82	0.20	45,45,45,45	0
57	MG	AA	7069	1/1	0.82	0.13	11,11,11,11	1
57	MG	DA	9458	1/1	0.82	0.13	22,22,22,22	0
57	MG	BA	3077	1/1	0.82	0.15	21,21,21,21	0
57	MG	BA	3203	1/1	0.82	0.15	37,37,37,37	0
57	MG	BA	3115	1/1	0.82	0.19	33,33,33,33	0
57	MG	CA	1621	1/1	0.82	0.10	52,52,52,52	0
57	MG	BA	3147	1/1	0.82	0.28	48,48,48,48	0
57	MG	DA	9412	1/1	0.82	0.17	27,27,27,27	0
57	MG	CA	1702	1/1	0.82	0.08	49,49,49,49	0
57	MG	DA	9416	1/1	0.82	0.20	38,38,38,38	0
57	MG	DA	9523	1/1	0.82	0.33	9,9,9,9	0
57	MG	DA	9526	1/1	0.82	0.24	12,12,12,12	0
57	MG	BA	3228	1/1	0.82	0.24	13,13,13,13	0
57	MG	BA	3282	1/1	0.82	0.10	24,24,24,24	0
57	MG	DA	9569	1/1	0.82	0.17	54,54,54,54	0
57	MG	CA	1651	1/1	0.82	0.34	39,39,39,39	0
57	MG	DA	9431	1/1	0.82	0.29	12,12,12,12	0
57	MG	DA	9602	1/1	0.82	0.17	37,37,37,37	0
57	MG	DA	9603	1/1	0.82	0.21	33,33,33,33	0
57	MG	AA	7035	1/1	0.82	0.20	42,42,42,42	0
57	MG	CA	1675	1/1	0.83	0.12	55,55,55,55	0
57	MG	BA	3245	1/1	0.83	0.17	45,45,45,45	0
57	MG	CA	1684	1/1	0.83	0.17	41,41,41,41	0
57	MG	AA	7102	1/1	0.83	0.29	38,38,38,38	0
57	MG	CA	1637	1/1	0.83	0.27	57,57,57,57	0
57	MG	CE	202	1/1	0.83	0.08	34,34,34,34	0
57	MG	BA	3306	1/1	0.83	0.23	48,48,48,48	0
57	MG	AA	7084	1/1	0.83	0.14	49,49,49,49	0
57	MG	CA	1699	1/1	0.83	0.30	45,45,45,45	1
57	MG	BA	3255	1/1	0.83	0.23	45,45,45,45	0
57	MG	BD	301	1/1	0.83	0.32	7,7,7,7	0
57	MG	DA	9536	1/1	0.83	0.34	0,0,0,0	0
57	MG	DA	9677	1/1	0.83	0.25	27,27,27,27	0
57	MG	DA	9681	1/1	0.83	0.17	13,13,13,13	0
57	MG	DA	9543	1/1	0.83	0.21	5,5,5,5	0
57	MG	DA	9687	1/1	0.83	0.11	12,12,12,12	0
57	MG	DA	9545	1/1	0.83	0.21	1,1,1,1	0
57	MG	DA	9553	1/1	0.83	0.22	20,20,20,20	0
57	MG	DA	9434	1/1	0.83	0.21	4,4,4,4	0
57	MG	CA	1654	1/1	0.83	0.10	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9440	1/1	0.83	0.18	25,25,25,25	0
57	MG	BA	3087	1/1	0.83	0.15	21,21,21,21	0
57	MG	BA	3039	1/1	0.83	0.20	30,30,30,30	0
57	MG	BA	3154	1/1	0.83	0.25	17,17,17,17	0
57	MG	DA	9621	1/1	0.83	0.33	0,0,0,0	1
57	MG	BA	3121	1/1	0.84	0.27	1,1,1,1	0
57	MG	CA	1640	1/1	0.84	0.33	49,49,49,49	0
57	MG	DA	9337	1/1	0.84	0.39	45,45,45,45	0
57	MG	DA	9573	1/1	0.84	0.22	45,45,45,45	0
57	MG	BA	3058	1/1	0.84	0.23	1,1,1,1	0
57	MG	DA	9577	1/1	0.84	0.31	102,102,102,102	0
57	MG	BA	3106	1/1	0.84	0.23	34,34,34,34	0
57	MG	BA	3003	1/1	0.84	0.13	33,33,33,33	0
57	MG	BA	3136	1/1	0.84	0.17	46,46,46,46	1
57	MG	DA	9615	1/1	0.84	0.19	45,45,45,45	0
57	MG	BA	3195	1/1	0.84	0.19	3,3,3,3	0
57	MG	DA	9689	1/1	0.84	0.29	25,25,25,25	0
57	MG	DA	9692	1/1	0.84	0.25	30,30,30,30	0
57	MG	DA	9629	1/1	0.84	0.10	52,52,52,52	0
57	MG	DA	9377	1/1	0.84	0.17	19,19,19,19	0
57	MG	BA	3110	1/1	0.84	0.38	23,23,23,23	1
57	MG	AA	7036	1/1	0.84	0.18	42,42,42,42	0
57	MG	CA	1625	1/1	0.84	0.18	26,26,26,26	0
57	MG	DA	9645	1/1	0.84	0.23	4,4,4,4	0
57	MG	CV	103	1/1	0.84	0.16	43,43,43,43	1
57	MG	CV	105	1/1	0.84	0.11	69,69,69,69	0
57	MG	DA	9385	1/1	0.85	0.11	5,5,5,5	0
57	MG	CA	1676	1/1	0.85	0.52	88,88,88,88	0
57	MG	CA	1729	1/1	0.85	0.22	35,35,35,35	0
57	MG	BA	3111	1/1	0.85	0.23	35,35,35,35	0
57	MG	CA	1682	1/1	0.85	0.11	60,60,60,60	0
57	MG	BA	3278	1/1	0.85	0.27	22,22,22,22	0
57	MG	CA	1639	1/1	0.85	0.19	55,55,55,55	0
57	MG	BA	3130	1/1	0.85	0.12	3,3,3,3	0
57	MG	CV	104	1/1	0.85	0.21	22,22,22,22	1
57	MG	DA	9539	1/1	0.85	0.37	35,35,35,35	0
57	MG	BA	3160	1/1	0.85	0.26	22,22,22,22	0
57	MG	BA	3162	1/1	0.85	0.14	4,4,4,4	0
57	MG	BA	3222	1/1	0.85	0.23	5,5,5,5	0
57	MG	BA	3131	1/1	0.85	0.18	38,38,38,38	0
57	MG	CA	1605	1/1	0.85	0.17	32,32,32,32	0
57	MG	CA	1664	1/1	0.85	0.17	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3168	1/1	0.85	0.25	36,36,36,36	0
57	MG	BA	3316	1/1	0.85	0.29	7,7,7,7	0
57	MG	DA	9578	1/1	0.85	0.25	44,44,44,44	0
57	MG	DA	9448	1/1	0.85	0.18	18,18,18,18	0
57	MG	BA	3061	1/1	0.85	0.17	32,32,32,32	0
57	MG	DA	9371	1/1	0.85	0.20	29,29,29,29	0
57	MG	DA	9607	1/1	0.85	0.26	49,49,49,49	0
57	MG	BA	3267	1/1	0.85	0.18	41,41,41,41	0
57	MG	CA	1725	1/1	0.85	0.25	29,29,29,29	0
57	MG	D0	101	1/1	0.85	0.28	27,27,27,27	0
57	MG	DA	9383	1/1	0.85	0.29	18,18,18,18	0
57	MG	DA	9486	1/1	0.85	0.23	21,21,21,21	0
57	MG	DA	9487	1/1	0.86	0.29	71,71,71,71	0
57	MG	CA	1740	1/1	0.86	0.21	48,48,48,48	0
57	MG	BA	3113	1/1	0.86	0.17	49,49,49,49	0
57	MG	DA	9643	1/1	0.86	0.33	34,34,34,34	1
57	MG	CA	1696	1/1	0.86	0.20	49,49,49,49	0
57	MG	AA	7063	1/1	0.86	0.20	31,31,31,31	0
57	MG	DA	9405	1/1	0.86	0.11	5,5,5,5	0
57	MG	BU	201	1/1	0.86	0.28	170,170,170,170	1
57	MG	DA	9657	1/1	0.86	0.16	29,29,29,29	0
57	MG	CA	1659	1/1	0.86	0.25	28,28,28,28	0
57	MG	CY	101	1/1	0.86	0.30	33,33,33,33	0
57	MG	DA	9321	1/1	0.86	0.21	35,35,35,35	0
57	MG	DA	9421	1/1	0.86	0.21	28,28,28,28	0
57	MG	CA	1661	1/1	0.86	0.08	50,50,50,50	0
57	MG	BA	3181	1/1	0.86	0.20	1,1,1,1	0
57	MG	AA	7078	1/1	0.86	0.12	30,30,30,30	0
57	MG	BA	3122	1/1	0.86	0.11	13,13,13,13	0
57	MG	AA	7086	1/1	0.86	0.27	30,30,30,30	0
57	MG	DA	9570	1/1	0.86	0.12	61,61,61,61	0
57	MG	BA	3153	1/1	0.86	0.31	0,0,0,0	0
57	MG	CA	1723	1/1	0.86	0.15	15,15,15,15	0
57	MG	AA	7080	1/1	0.86	0.14	8,8,8,8	1
57	MG	AV	101	1/1	0.86	0.09	2,2,2,2	0
57	MG	DA	9579	1/1	0.86	0.32	38,38,38,38	0
57	MG	DA	9379	1/1	0.86	0.11	41,41,41,41	0
57	MG	DA	9460	1/1	0.86	0.06	40,40,40,40	0
57	MG	DA	9466	1/1	0.86	0.20	36,36,36,36	0
57	MG	BA	3066	1/1	0.86	0.49	48,48,48,48	0
57	MG	BA	3274	1/1	0.86	0.07	8,8,8,8	1
57	MG	BA	3067	1/1	0.86	0.19	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3233	1/1	0.86	0.19	19,19,19,19	0
58	PAR	CA	1741	42/42	0.86	0.18	55,55,55,55	0
57	MG	BA	3258	1/1	0.87	0.30	19,19,19,19	0
57	MG	AA	7027	1/1	0.87	0.15	28,28,28,28	0
57	MG	CA	1657	1/1	0.87	0.11	30,30,30,30	0
57	MG	BA	3031	1/1	0.87	0.29	44,44,44,44	0
57	MG	AA	7004	1/1	0.87	0.16	30,30,30,30	0
57	MG	BA	3268	1/1	0.87	0.24	13,13,13,13	1
57	MG	BA	3164	1/1	0.87	0.25	39,39,39,39	0
57	MG	AA	7020	1/1	0.87	0.20	33,33,33,33	0
57	MG	DA	9648	1/1	0.87	0.14	34,34,34,34	0
57	MG	DA	9650	1/1	0.87	0.21	7,7,7,7	0
57	MG	BA	3276	1/1	0.87	0.24	31,31,31,31	0
57	MG	DA	9404	1/1	0.87	0.20	12,12,12,12	0
57	MG	AA	7011	1/1	0.87	0.11	43,43,43,43	0
57	MG	CA	1607	1/1	0.87	0.26	32,32,32,32	0
57	MG	DA	9659	1/1	0.87	0.18	52,52,52,52	0
57	MG	BA	3117	1/1	0.87	0.29	11,11,11,11	1
57	MG	BA	3119	1/1	0.87	0.18	42,42,42,42	0
57	MG	BA	3299	1/1	0.87	0.26	10,10,10,10	0
57	MG	CA	1617	1/1	0.87	0.24	16,16,16,16	0
57	MG	BA	3102	1/1	0.87	0.28	1,1,1,1	0
57	MG	DA	9676	1/1	0.87	0.14	13,13,13,13	0
57	MG	DA	9550	1/1	0.87	0.21	55,55,55,55	0
57	MG	BA	3308	1/1	0.87	0.12	37,37,37,37	0
57	MG	DA	9555	1/1	0.87	0.32	39,39,39,39	0
57	MG	BA	3247	1/1	0.87	0.25	55,55,55,55	0
57	MG	DA	9433	1/1	0.87	0.11	13,13,13,13	0
57	MG	AA	7054	1/1	0.87	0.22	29,29,29,29	0
57	MG	DA	9436	1/1	0.87	0.27	3,3,3,3	0
57	MG	BA	3108	1/1	0.87	0.20	27,27,27,27	0
57	MG	CA	1700	1/1	0.87	0.15	20,20,20,20	0
57	MG	BA	3254	1/1	0.87	0.26	54,54,54,54	0
57	MG	DA	9445	1/1	0.87	0.18	22,22,22,22	0
57	MG	BA	3205	1/1	0.87	0.23	0,0,0,0	0
57	MG	DA	9601	1/1	0.87	0.22	31,31,31,31	0
57	MG	CA	1644	1/1	0.87	0.07	45,45,45,45	0
57	MG	BA	3257	1/1	0.87	0.08	21,21,21,21	0
57	MG	CA	1709	1/1	0.87	0.40	68,68,68,68	0
57	MG	CA	1711	1/1	0.87	0.16	26,26,26,26	0
59	ZN	AD	301	1/1	0.87	0.21	41,41,41,41	0
59	ZN	CN	101	1/1	0.87	0.10	171,171,171,171	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3253	1/1	0.88	0.18	34,34,34,34	0
57	MG	BA	3212	1/1	0.88	0.17	8,8,8,8	0
57	MG	AA	7081	1/1	0.88	0.21	44,44,44,44	0
57	MG	BA	3219	1/1	0.88	0.13	19,19,19,19	0
57	MG	BA	3114	1/1	0.88	0.17	41,41,41,41	0
57	MG	BA	3055	1/1	0.88	0.12	11,11,11,11	0
57	MG	DA	9443	1/1	0.88	0.28	37,37,37,37	0
57	MG	BA	3264	1/1	0.88	0.24	36,36,36,36	0
57	MG	CA	1681	1/1	0.88	0.28	18,18,18,18	1
57	MG	CA	1627	1/1	0.88	0.26	22,22,22,22	0
57	MG	CA	1683	1/1	0.88	0.32	29,29,29,29	0
57	MG	BA	3134	1/1	0.88	0.13	21,21,21,21	0
57	MG	DA	9462	1/1	0.88	0.14	30,30,30,30	0
57	MG	BA	3116	1/1	0.88	0.07	38,38,38,38	0
57	MG	CA	1690	1/1	0.88	0.30	17,17,17,17	0
57	MG	AA	7018	1/1	0.88	0.26	27,27,27,27	0
57	MG	DA	9476	1/1	0.88	0.28	2,2,2,2	0
57	MG	BA	3271	1/1	0.88	0.28	52,52,52,52	0
57	MG	BA	3323	1/1	0.88	0.21	26,26,26,26	0
57	MG	AA	7062	1/1	0.88	0.13	31,31,31,31	0
57	MG	DA	9610	1/1	0.88	0.22	19,19,19,19	0
57	MG	AA	7100	1/1	0.88	0.21	21,21,21,21	0
57	MG	BA	3025	1/1	0.88	0.09	37,37,37,37	0
57	MG	BA	3202	1/1	0.88	0.21	7,7,7,7	0
57	MG	DA	9329	1/1	0.88	0.26	21,21,21,21	0
57	MG	AV	103	1/1	0.88	0.18	7,7,7,7	1
57	MG	DA	9504	1/1	0.88	0.12	27,27,27,27	0
57	MG	BA	3044	1/1	0.88	0.17	18,18,18,18	0
57	MG	DA	9340	1/1	0.88	0.27	1,1,1,1	0
57	MG	DA	9528	1/1	0.88	0.24	6,6,6,6	0
57	MG	BA	3294	1/1	0.88	0.14	15,15,15,15	1
57	MG	CA	1653	1/1	0.89	0.15	29,29,29,29	0
57	MG	BA	3232	1/1	0.89	0.17	44,44,44,44	0
57	MG	BA	3184	1/1	0.89	0.30	22,22,22,22	0
57	MG	BA	3187	1/1	0.89	0.15	24,24,24,24	0
57	MG	DA	9376	1/1	0.89	0.10	26,26,26,26	0
57	MG	BA	3193	1/1	0.89	0.16	12,12,12,12	0
57	MG	BA	3052	1/1	0.89	0.12	40,40,40,40	0
57	MG	DA	9616	1/1	0.89	0.29	54,54,54,54	0
57	MG	BA	3284	1/1	0.89	0.07	21,21,21,21	0
57	MG	DA	9470	1/1	0.89	0.23	0,0,0,0	0
57	MG	DA	9471	1/1	0.89	0.15	50,50,50,50	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	7009	1/1	0.89	0.15	18,18,18,18	0
57	MG	BA	3103	1/1	0.89	0.14	31,31,31,31	0
57	MG	DA	9387	1/1	0.89	0.26	1,1,1,1	0
57	MG	CA	1608	1/1	0.89	0.18	16,16,16,16	0
57	MG	BA	3296	1/1	0.89	0.32	0,0,0,0	1
57	MG	CA	1731	1/1	0.89	0.10	30,30,30,30	0
57	MG	CA	1735	1/1	0.89	0.20	29,29,29,29	0
57	MG	BA	3297	1/1	0.89	0.54	46,46,46,46	0
57	MG	DA	9652	1/1	0.89	0.17	44,44,44,44	0
57	MG	AA	7046	1/1	0.89	0.28	35,35,35,35	0
57	MG	CA	1616	1/1	0.89	0.15	44,44,44,44	0
57	MG	AA	7073	1/1	0.89	0.08	29,29,29,29	0
57	MG	BA	3206	1/1	0.89	0.23	29,29,29,29	0
57	MG	BA	3085	1/1	0.89	0.19	29,29,29,29	0
57	MG	DA	9418	1/1	0.89	0.33	61,61,61,61	0
57	MG	CA	1688	1/1	0.89	0.13	16,16,16,16	0
57	MG	AA	7052	1/1	0.89	0.14	74,74,74,74	0
57	MG	DA	9422	1/1	0.89	0.14	56,56,56,56	0
57	MG	DA	9540	1/1	0.89	0.20	0,0,0,0	0
57	MG	AA	7031	1/1	0.89	0.25	44,44,44,44	0
57	MG	CA	1693	1/1	0.89	0.14	24,24,24,24	0
57	MG	BA	3220	1/1	0.89	0.45	56,56,56,56	0
57	MG	DA	9686	1/1	0.89	0.15	11,11,11,11	0
57	MG	DA	9432	1/1	0.89	0.22	38,38,38,38	0
57	MG	BA	3221	1/1	0.89	0.19	17,17,17,17	0
57	MG	DA	9559	1/1	0.89	0.22	58,58,58,58	0
57	MG	DA	9563	1/1	0.89	0.12	3,3,3,3	0
57	MG	DA	9565	1/1	0.89	0.22	11,11,11,11	0
57	MG	BA	3021	1/1	0.89	0.15	49,49,49,49	0
57	MG	BA	3022	1/1	0.89	0.17	40,40,40,40	0
57	MG	DA	9437	1/1	0.89	0.10	14,14,14,14	0
57	MG	BA	3321	1/1	0.89	0.25	35,35,35,35	0
57	MG	DD	7101	1/1	0.89	0.31	3,3,3,3	0
57	MG	AA	7010	1/1	0.89	0.10	30,30,30,30	0
57	MG	DA	9576	1/1	0.89	0.10	22,22,22,22	0
57	MG	DA	9348	1/1	0.89	0.38	47,47,47,47	0
57	MG	D1	102	1/1	0.89	0.09	9,9,9,9	1
57	MG	BA	3096	1/1	0.89	0.25	12,12,12,12	0
58	PAR	AA	7111	42/42	0.89	0.15	58,58,58,58	0
57	MG	DA	9444	1/1	0.89	0.16	42,42,42,42	0
57	MG	DA	9595	1/1	0.89	0.17	49,49,49,49	0
57	MG	DA	9596	1/1	0.89	0.10	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9633	1/1	0.90	0.48	30,30,30,30	0
57	MG	DA	9374	1/1	0.90	0.15	28,28,28,28	0
57	MG	BA	3159	1/1	0.90	0.20	9,9,9,9	0
57	MG	DA	9639	1/1	0.90	0.19	57,57,57,57	0
57	MG	CA	1734	1/1	0.90	0.12	22,22,22,22	0
57	MG	CA	1692	1/1	0.90	0.25	28,28,28,28	0
57	MG	BA	3198	1/1	0.90	0.24	0,0,0,0	0
57	MG	DA	9544	1/1	0.90	0.18	10,10,10,10	0
57	MG	BA	3050	1/1	0.90	0.16	4,4,4,4	0
57	MG	AA	7006	1/1	0.90	0.24	20,20,20,20	0
57	MG	BA	3204	1/1	0.90	0.21	3,3,3,3	0
57	MG	BA	3314	1/1	0.90	0.10	42,42,42,42	0
57	MG	DA	9656	1/1	0.90	0.15	58,58,58,58	0
57	MG	AA	7053	1/1	0.90	0.18	32,32,32,32	0
57	MG	DA	9561	1/1	0.90	0.10	10,10,10,10	0
57	MG	AA	7013	1/1	0.90	0.19	27,27,27,27	0
57	MG	AA	7050	1/1	0.90	0.28	29,29,29,29	0
57	MG	DA	9465	1/1	0.90	0.17	34,34,34,34	0
57	MG	BA	3141	1/1	0.90	0.22	18,18,18,18	0
57	MG	BA	3250	1/1	0.90	0.14	18,18,18,18	0
57	MG	CA	1626	1/1	0.90	0.23	28,28,28,28	0
57	MG	DA	9411	1/1	0.90	0.12	2,2,2,2	0
57	MG	DA	9325	1/1	0.90	0.15	32,32,32,32	0
57	MG	DA	9680	1/1	0.90	0.21	24,24,24,24	0
57	MG	DA	9327	1/1	0.90	0.17	20,20,20,20	0
57	MG	CA	1710	1/1	0.90	0.23	19,19,19,19	0
57	MG	DA	9479	1/1	0.90	0.33	0,0,0,0	0
57	MG	DA	9582	1/1	0.90	0.33	21,21,21,21	0
57	MG	DA	9586	1/1	0.90	0.24	3,3,3,3	0
57	MG	DA	9590	1/1	0.90	0.30	1,1,1,1	0
57	MG	DA	9591	1/1	0.90	0.10	52,52,52,52	0
57	MG	DA	9484	1/1	0.90	0.20	5,5,5,5	0
57	MG	BA	3217	1/1	0.90	0.10	28,28,28,28	0
57	MG	DA	9597	1/1	0.90	0.13	12,12,12,12	0
57	MG	CA	1713	1/1	0.90	0.26	31,31,31,31	0
57	MG	AA	7064	1/1	0.90	0.13	50,50,50,50	0
57	MG	AA	7108	1/1	0.90	0.10	27,27,27,27	0
57	MG	DQ	201	1/1	0.90	0.15	36,36,36,36	0
57	MG	BA	3290	1/1	0.90	0.29	19,19,19,19	1
57	MG	DX	101	1/1	0.90	0.08	6,6,6,6	0
57	MG	BA	3004	1/1	0.90	0.24	1,1,1,1	0
57	MG	AA	7065	1/1	0.90	0.17	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	7110	1/1	0.90	0.14	31,31,31,31	0
57	MG	DA	9515	1/1	0.90	0.20	10,10,10,10	0
57	MG	DA	9618	1/1	0.90	0.37	28,28,28,28	1
57	MG	DA	9361	1/1	0.90	0.20	5,5,5,5	0
57	MG	BA	3298	1/1	0.90	0.30	18,18,18,18	0
57	MG	CA	1730	1/1	0.90	0.10	49,49,49,49	0
57	MG	DA	9464	1/1	0.91	0.10	25,25,25,25	0
57	MG	DA	9366	1/1	0.91	0.27	1,1,1,1	0
57	MG	BA	3178	1/1	0.91	0.15	28,28,28,28	0
57	MG	BA	3135	1/1	0.91	0.28	43,43,43,43	0
57	MG	DA	9605	1/1	0.91	0.08	19,19,19,19	0
57	MG	CA	1655	1/1	0.91	0.18	24,24,24,24	0
57	MG	BA	3183	1/1	0.91	0.27	56,56,56,56	0
57	MG	AA	7066	1/1	0.91	0.25	36,36,36,36	0
57	MG	DA	9378	1/1	0.91	0.12	29,29,29,29	0
57	MG	BB	204	1/1	0.91	0.16	23,23,23,23	0
57	MG	BA	3185	1/1	0.91	0.17	14,14,14,14	0
57	MG	DA	9622	1/1	0.91	0.18	36,36,36,36	0
57	MG	DA	9628	1/1	0.91	0.19	35,35,35,35	1
57	MG	DA	9483	1/1	0.91	0.27	0,0,0,0	0
57	MG	CA	1724	1/1	0.91	0.07	5,5,5,5	0
57	MG	CA	1665	1/1	0.91	0.26	16,16,16,16	0
57	MG	CA	1727	1/1	0.91	0.15	27,27,27,27	0
57	MG	DA	9637	1/1	0.91	0.17	18,18,18,18	0
57	MG	CA	1666	1/1	0.91	0.09	66,66,66,66	0
57	MG	DA	9392	1/1	0.91	0.29	12,12,12,12	0
57	MG	DA	9394	1/1	0.91	0.19	16,16,16,16	0
57	MG	CA	1671	1/1	0.91	0.09	38,38,38,38	0
57	MG	AA	7055	1/1	0.91	0.15	29,29,29,29	0
57	MG	BO	201	1/1	0.91	0.22	45,45,45,45	0
57	MG	DA	9649	1/1	0.91	0.24	1,1,1,1	0
57	MG	BA	3241	1/1	0.91	0.19	4,4,4,4	0
57	MG	DA	9517	1/1	0.91	0.11	0,0,0,0	0
57	MG	BA	3189	1/1	0.91	0.12	1,1,1,1	0
57	MG	AA	7077	1/1	0.91	0.09	22,22,22,22	0
57	MG	CA	1606	1/1	0.91	0.11	8,8,8,8	0
57	MG	BA	3295	1/1	0.91	0.13	27,27,27,27	0
57	MG	BA	3143	1/1	0.91	0.18	7,7,7,7	0
57	MG	AV	102	1/1	0.91	0.20	25,25,25,25	1
57	MG	CV	101	1/1	0.91	0.15	12,12,12,12	1
57	MG	AA	7045	1/1	0.91	0.26	38,38,38,38	0
57	MG	DA	9420	1/1	0.91	0.28	6,6,6,6	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	7097	1/1	0.91	0.15	20,20,20,20	0
57	MG	DA	9549	1/1	0.91	0.26	44,44,44,44	0
57	MG	BA	3301	1/1	0.91	0.19	20,20,20,20	0
57	MG	BA	3302	1/1	0.91	0.17	8,8,8,8	0
57	MG	AA	7033	1/1	0.91	0.13	35,35,35,35	0
57	MG	DA	9557	1/1	0.91	0.13	25,25,25,25	0
57	MG	DA	9304	1/1	0.91	0.14	27,27,27,27	0
57	MG	DA	9313	1/1	0.91	0.15	18,18,18,18	0
57	MG	AA	7072	1/1	0.91	0.12	23,23,23,23	0
57	MG	BA	3310	1/1	0.91	0.11	35,35,35,35	0
57	MG	BA	3158	1/1	0.91	0.10	29,29,29,29	0
57	MG	CA	1628	1/1	0.91	0.08	9,9,9,9	0
57	MG	DA	9330	1/1	0.91	0.19	0,0,0,0	0
57	MG	BA	3072	1/1	0.91	0.15	25,25,25,25	0
57	MG	BA	3075	1/1	0.91	0.23	12,12,12,12	0
57	MG	BA	3105	1/1	0.91	0.18	26,26,26,26	0
57	MG	AA	7082	1/1	0.91	0.22	24,24,24,24	0
57	MG	CA	1703	1/1	0.91	0.28	9,9,9,9	0
57	MG	DF	301	1/1	0.91	0.08	20,20,20,20	0
57	MG	DP	203	1/1	0.91	0.16	11,11,11,11	0
57	MG	AA	7105	1/1	0.91	0.24	42,42,42,42	0
57	MG	DA	9581	1/1	0.91	0.12	4,4,4,4	0
57	MG	BA	3014	1/1	0.91	0.17	33,33,33,33	0
57	MG	DA	9454	1/1	0.91	0.31	34,34,34,34	0
57	MG	DA	9588	1/1	0.91	0.06	16,16,16,16	0
57	MG	AA	7034	1/1	0.91	0.22	43,43,43,43	0
57	MG	DA	9360	1/1	0.91	0.29	7,7,7,7	0
57	MG	DA	9592	1/1	0.91	0.18	36,36,36,36	0
57	MG	DA	9461	1/1	0.91	0.11	13,13,13,13	0
57	MG	BA	3177	1/1	0.91	0.17	0,0,0,0	0
57	MG	DA	9463	1/1	0.91	0.08	12,12,12,12	0
57	MG	BA	3038	1/1	0.92	0.07	31,31,31,31	0
57	MG	CA	1685	1/1	0.92	0.11	41,41,41,41	0
57	MG	CA	1686	1/1	0.92	0.17	77,77,77,77	0
57	MG	AA	7068	1/1	0.92	0.09	34,34,34,34	0
57	MG	BA	3190	1/1	0.92	0.17	8,8,8,8	0
57	MG	CA	1689	1/1	0.92	0.07	15,15,15,15	0
57	MG	DA	9619	1/1	0.92	0.06	0,0,0,0	0
57	MG	DA	9620	1/1	0.92	0.09	26,26,26,26	0
57	MG	DA	9499	1/1	0.92	0.12	29,29,29,29	0
57	MG	CA	1633	1/1	0.92	0.12	9,9,9,9	0
57	MG	DA	9502	1/1	0.92	0.23	3,3,3,3	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1634	1/1	0.92	0.14	43,43,43,43	0
57	MG	BA	3041	1/1	0.92	0.23	7,7,7,7	0
57	MG	DA	9510	1/1	0.92	0.23	1,1,1,1	0
57	MG	CA	1638	1/1	0.92	0.22	24,24,24,24	0
57	MG	DA	9636	1/1	0.92	0.16	16,16,16,16	0
57	MG	DA	9306	1/1	0.92	0.18	4,4,4,4	0
57	MG	DA	9519	1/1	0.92	0.23	1,1,1,1	0
57	MG	BA	3097	1/1	0.92	0.13	43,43,43,43	0
57	MG	DA	9315	1/1	0.92	0.11	26,26,26,26	0
57	MG	BA	3281	1/1	0.92	0.64	53,53,53,53	0
57	MG	BA	3070	1/1	0.92	0.32	34,34,34,34	0
57	MG	DA	9531	1/1	0.92	0.26	1,1,1,1	0
57	MG	BB	201	1/1	0.92	0.12	34,34,34,34	0
57	MG	AA	7037	1/1	0.92	0.18	7,7,7,7	0
57	MG	DA	9430	1/1	0.92	0.24	0,0,0,0	0
57	MG	DA	9542	1/1	0.92	0.20	6,6,6,6	0
57	MG	CA	1645	1/1	0.92	0.24	20,20,20,20	0
57	MG	BA	3073	1/1	0.92	0.17	8,8,8,8	0
57	MG	BA	3161	1/1	0.92	0.15	11,11,11,11	0
57	MG	CA	1706	1/1	0.92	0.17	32,32,32,32	0
57	MG	DA	9344	1/1	0.92	0.21	33,33,33,33	0
57	MG	DA	9551	1/1	0.92	0.13	48,48,48,48	0
57	MG	BA	3129	1/1	0.92	0.27	1,1,1,1	0
57	MG	DA	9663	1/1	0.92	0.25	7,7,7,7	0
57	MG	DA	9664	1/1	0.92	0.26	1,1,1,1	0
57	MG	DA	9665	1/1	0.92	0.31	9,9,9,9	0
57	MG	DA	9438	1/1	0.92	0.06	21,21,21,21	0
57	MG	DA	9667	1/1	0.92	0.23	10,10,10,10	0
57	MG	BA	3251	1/1	0.92	0.06	34,34,34,34	0
57	MG	BD	302	1/1	0.92	0.10	4,4,4,4	0
57	MG	CA	1656	1/1	0.92	0.16	22,22,22,22	0
57	MG	DA	9355	1/1	0.92	0.28	0,0,0,0	0
57	MG	DA	9564	1/1	0.92	0.20	17,17,17,17	0
57	MG	BF	301	1/1	0.92	0.10	39,39,39,39	0
57	MG	DA	9684	1/1	0.92	0.12	8,8,8,8	0
57	MG	CA	1658	1/1	0.92	0.09	44,44,44,44	0
57	MG	DA	9446	1/1	0.92	0.10	13,13,13,13	0
57	MG	BA	3045	1/1	0.92	0.36	2,2,2,2	0
57	MG	DA	9450	1/1	0.92	0.26	2,2,2,2	1
57	MG	DA	9362	1/1	0.92	0.21	5,5,5,5	0
57	MG	CA	1718	1/1	0.92	0.14	27,27,27,27	0
57	MG	AA	7091	1/1	0.92	0.12	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9369	1/1	0.92	0.23	0,0,0,0	0
57	MG	DB	201	1/1	0.92	0.25	22,22,22,22	0
57	MG	BA	3051	1/1	0.92	0.23	6,6,6,6	0
57	MG	CA	1604	1/1	0.92	0.22	15,15,15,15	0
57	MG	AA	7048	1/1	0.92	0.18	27,27,27,27	0
57	MG	BA	3300	1/1	0.92	0.21	1,1,1,1	0
57	MG	BA	3006	1/1	0.92	0.17	38,38,38,38	0
57	MG	BA	3032	1/1	0.92	0.12	18,18,18,18	0
57	MG	BA	3180	1/1	0.92	0.26	2,2,2,2	0
57	MG	BA	3263	1/1	0.92	0.17	16,16,16,16	1
57	MG	BA	3112	1/1	0.92	0.28	14,14,14,14	0
57	MG	DA	9474	1/1	0.92	0.15	28,28,28,28	0
57	MG	BA	3009	1/1	0.92	0.06	2,2,2,2	0
57	MG	DA	9598	1/1	0.92	0.22	14,14,14,14	0
57	MG	D2	101	1/1	0.92	0.17	34,34,34,34	0
57	MG	AV	104	1/1	0.92	0.19	16,16,16,16	0
57	MG	DA	9390	1/1	0.92	0.21	0,0,0,0	0
57	MG	AA	7017	1/1	0.92	0.17	29,29,29,29	0
57	MG	BA	3270	1/1	0.92	0.28	0,0,0,0	1
57	MG	DA	9604	1/1	0.92	0.13	21,21,21,21	0
57	MG	BA	3150	1/1	0.93	0.15	1,1,1,1	0
57	MG	DA	9640	1/1	0.93	0.20	42,42,42,42	0
57	MG	BA	3269	1/1	0.93	0.22	20,20,20,20	0
57	MG	DA	9316	1/1	0.93	0.24	0,0,0,0	0
57	MG	BA	3186	1/1	0.93	0.21	2,2,2,2	0
57	MG	AA	7098	1/1	0.93	0.20	28,28,28,28	0
57	MG	BA	3081	1/1	0.93	0.41	24,24,24,24	1
57	MG	DA	9468	1/1	0.93	0.43	2,2,2,2	1
57	MG	BA	3155	1/1	0.93	0.17	33,33,33,33	0
57	MG	AA	7003	1/1	0.93	0.14	27,27,27,27	0
57	MG	DA	9408	1/1	0.93	0.24	3,3,3,3	0
57	MG	DA	9332	1/1	0.93	0.14	34,34,34,34	0
57	MG	BA	3084	1/1	0.93	0.20	1,1,1,1	0
57	MG	DA	9334	1/1	0.93	0.20	27,27,27,27	0
57	MG	CA	1629	1/1	0.93	0.23	37,37,37,37	0
57	MG	DA	9339	1/1	0.93	0.25	13,13,13,13	0
57	MG	CA	1630	1/1	0.93	0.11	34,34,34,34	0
57	MG	BA	3243	1/1	0.93	0.26	5,5,5,5	0
57	MG	AA	7028	1/1	0.93	0.29	30,30,30,30	0
57	MG	DA	9489	1/1	0.93	0.28	37,37,37,37	0
57	MG	BA	3246	1/1	0.93	0.24	33,33,33,33	0
57	MG	DA	9589	1/1	0.93	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9669	1/1	0.93	0.13	5,5,5,5	0
57	MG	BA	3132	1/1	0.93	0.20	51,51,51,51	0
57	MG	DA	9427	1/1	0.93	0.16	91,91,91,91	0
57	MG	BA	3026	1/1	0.93	0.22	29,29,29,29	0
57	MG	BA	3042	1/1	0.93	0.20	8,8,8,8	0
57	MG	DA	9678	1/1	0.93	0.14	33,33,33,33	0
57	MG	AA	7061	1/1	0.93	0.07	19,19,19,19	0
57	MG	BA	3069	1/1	0.93	0.21	5,5,5,5	0
57	MG	BA	3171	1/1	0.93	0.12	7,7,7,7	0
57	MG	DA	9505	1/1	0.93	0.15	0,0,0,0	0
57	MG	BN	201	1/1	0.93	0.21	125,125,125,125	1
57	MG	DA	9365	1/1	0.93	0.16	1,1,1,1	0
57	MG	CA	1648	1/1	0.93	0.11	23,23,23,23	0
57	MG	BA	3029	1/1	0.93	0.15	24,24,24,24	0
57	MG	BA	3174	1/1	0.93	0.10	31,31,31,31	0
57	MG	DA	9525	1/1	0.93	0.19	4,4,4,4	0
57	MG	DA	9608	1/1	0.93	0.12	19,19,19,19	0
57	MG	DA	9370	1/1	0.93	0.33	0,0,0,0	0
57	MG	DA	9614	1/1	0.93	0.16	12,12,12,12	0
57	MG	BA	3138	1/1	0.93	0.26	15,15,15,15	0
57	MG	AA	7092	1/1	0.93	0.06	37,37,37,37	0
57	MG	BA	3259	1/1	0.93	0.12	18,18,18,18	0
57	MG	BA	3008	1/1	0.93	0.24	2,2,2,2	0
57	MG	DA	9538	1/1	0.93	0.22	1,1,1,1	0
57	MG	AA	7106	1/1	0.93	0.09	12,12,12,12	0
57	MG	BA	3012	1/1	0.93	0.24	29,29,29,29	0
57	MG	DA	9624	1/1	0.93	0.09	18,18,18,18	1
57	MG	DA	9626	1/1	0.93	0.09	8,8,8,8	1
57	MG	BA	3226	1/1	0.93	0.31	36,36,36,36	0
57	MG	DA	9302	1/1	0.93	0.17	34,34,34,34	0
57	MG	AA	7087	1/1	0.93	0.07	24,24,24,24	0
57	MG	DA	9455	1/1	0.93	0.23	0,0,0,0	0
57	MG	DA	9456	1/1	0.93	0.24	19,19,19,19	0
57	MG	CA	1612	1/1	0.93	0.17	31,31,31,31	0
57	MG	DA	9310	1/1	0.93	0.14	0,0,0,0	0
57	MG	DA	9312	1/1	0.93	0.19	4,4,4,4	0
57	MG	DA	9423	1/1	0.94	0.05	1,1,1,1	0
57	MG	BA	3277	1/1	0.94	0.32	2,2,2,2	1
57	MG	AA	7104	1/1	0.94	0.16	33,33,33,33	0
57	MG	DA	9512	1/1	0.94	0.24	2,2,2,2	0
57	MG	DA	9513	1/1	0.94	0.11	22,22,22,22	0
57	MG	DA	9428	1/1	0.94	0.12	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9346	1/1	0.94	0.19	0,0,0,0	0
57	MG	BA	3210	1/1	0.94	0.33	11,11,11,11	0
57	MG	DA	9520	1/1	0.94	0.22	2,2,2,2	0
57	MG	DA	9521	1/1	0.94	0.26	2,2,2,2	0
57	MG	CA	1726	1/1	0.94	0.10	38,38,38,38	0
57	MG	AA	7021	1/1	0.94	0.21	25,25,25,25	0
57	MG	DA	9351	1/1	0.94	0.15	2,2,2,2	0
57	MG	BA	3249	1/1	0.94	0.21	25,25,25,25	0
57	MG	CA	1632	1/1	0.94	0.13	18,18,18,18	0
57	MG	BA	3214	1/1	0.94	0.14	39,39,39,39	0
57	MG	BA	3120	1/1	0.94	0.29	24,24,24,24	0
57	MG	CA	1636	1/1	0.94	0.11	19,19,19,19	0
57	MG	BA	3292	1/1	0.94	0.11	28,28,28,28	0
57	MG	BA	3046	1/1	0.94	0.26	1,1,1,1	0
57	MG	DA	9442	1/1	0.94	0.20	36,36,36,36	0
57	MG	DA	9647	1/1	0.94	0.25	1,1,1,1	0
57	MG	BA	3218	1/1	0.94	0.18	24,24,24,24	0
57	MG	CA	1738	1/1	0.94	0.30	49,49,49,49	0
57	MG	AA	7051	1/1	0.94	0.23	22,22,22,22	0
57	MG	DA	9548	1/1	0.94	0.19	26,26,26,26	0
57	MG	BA	3123	1/1	0.94	0.08	14,14,14,14	0
57	MG	DA	9447	1/1	0.94	0.27	68,68,68,68	0
57	MG	CA	1642	1/1	0.94	0.09	54,54,54,54	0
57	MG	DA	9552	1/1	0.94	0.30	58,58,58,58	0
57	MG	DA	9372	1/1	0.94	0.17	8,8,8,8	0
57	MG	DA	9451	1/1	0.94	0.10	35,35,35,35	0
57	MG	AA	7043	1/1	0.94	0.11	16,16,16,16	0
57	MG	AA	7026	1/1	0.94	0.26	30,30,30,30	0
57	MG	BA	3225	1/1	0.94	0.20	2,2,2,2	0
57	MG	CA	1601	1/1	0.94	0.12	39,39,39,39	0
57	MG	DA	9457	1/1	0.94	0.18	13,13,13,13	0
57	MG	CA	1602	1/1	0.94	0.18	14,14,14,14	0
57	MG	DA	9459	1/1	0.94	0.16	3,3,3,3	0
57	MG	DA	9568	1/1	0.94	0.25	3,3,3,3	0
57	MG	CX	101	1/1	0.94	0.16	25,25,25,25	0
57	MG	DA	9382	1/1	0.94	0.28	0,0,0,0	0
57	MG	DA	9572	1/1	0.94	0.15	4,4,4,4	0
57	MG	AA	7030	1/1	0.94	0.17	2,2,2,2	0
57	MG	BA	3054	1/1	0.94	0.20	14,14,14,14	0
57	MG	DA	9575	1/1	0.94	0.08	35,35,35,35	0
57	MG	CA	1701	1/1	0.94	0.18	1,1,1,1	0
57	MG	AE	201	1/1	0.94	0.15	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	AA	7047	1/1	0.94	0.12	41,41,41,41	0
57	MG	BA	3083	1/1	0.94	0.20	27,27,27,27	1
57	MG	DA	9393	1/1	0.94	0.21	24,24,24,24	0
57	MG	CA	1705	1/1	0.94	0.05	15,15,15,15	0
57	MG	DA	9395	1/1	0.94	0.15	29,29,29,29	0
57	MG	DA	9314	1/1	0.94	0.17	1,1,1,1	0
57	MG	AA	7099	1/1	0.94	0.21	6,6,6,6	0
57	MG	DA	9694	1/1	0.94	0.19	25,25,25,25	0
57	MG	BA	3235	1/1	0.94	0.21	25,25,25,25	0
57	MG	DA	9696	1/1	0.94	0.31	34,34,34,34	0
57	MG	DA	9401	1/1	0.94	0.35	21,21,21,21	1
57	MG	DA	9478	1/1	0.94	0.24	13,13,13,13	0
57	MG	DA	9593	1/1	0.94	0.32	25,25,25,25	0
57	MG	BA	3017	1/1	0.94	0.16	22,22,22,22	0
57	MG	AA	7056	1/1	0.94	0.21	12,12,12,12	0
57	MG	DD	7102	1/1	0.94	0.13	0,0,0,0	0
57	MG	DA	9326	1/1	0.94	0.16	1,1,1,1	0
57	MG	DP	202	1/1	0.94	0.26	173,173,173,173	0
57	MG	CA	1662	1/1	0.94	0.10	29,29,29,29	0
57	MG	DA	9599	1/1	0.94	0.24	20,20,20,20	0
57	MG	DU	201	1/1	0.94	0.15	30,30,30,30	1
57	MG	BA	3064	1/1	0.94	0.19	29,29,29,29	1
57	MG	AA	7075	1/1	0.94	0.33	53,53,53,53	0
57	MG	DA	9331	1/1	0.94	0.06	8,8,8,8	0
57	MG	D0	102	1/1	0.94	0.18	15,15,15,15	0
57	MG	CA	1714	1/1	0.94	0.14	53,53,53,53	0
57	MG	BA	3275	1/1	0.94	0.07	1,1,1,1	1
57	MG	DA	9496	1/1	0.94	0.09	26,26,26,26	0
57	MG	DA	9497	1/1	0.94	0.22	29,29,29,29	0
57	MG	CA	1622	1/1	0.94	0.04	37,37,37,37	0
57	MG	CA	1624	1/1	0.94	0.22	18,18,18,18	0
57	MG	DA	9338	1/1	0.94	0.26	58,58,58,58	0
57	MG	AA	7022	1/1	0.94	0.13	32,32,32,32	0
57	MG	DA	9508	1/1	0.95	0.15	0,0,0,0	0
57	MG	DA	9342	1/1	0.95	0.08	0,0,0,0	0
57	MG	CA	1668	1/1	0.95	0.19	56,56,56,56	0
57	MG	BA	3307	1/1	0.95	0.17	25,25,25,25	0
57	MG	BA	3024	1/1	0.95	0.25	22,22,22,22	0
57	MG	DA	9516	1/1	0.95	0.28	1,1,1,1	0
57	MG	BA	3261	1/1	0.95	0.14	10,10,10,10	0
57	MG	BA	3311	1/1	0.95	0.16	13,13,13,13	0
57	MG	BA	3035	1/1	0.95	0.18	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3010	1/1	0.95	0.36	28,28,28,28	0
57	MG	DA	9522	1/1	0.95	0.25	2,2,2,2	0
57	MG	DA	9353	1/1	0.95	0.15	24,24,24,24	0
57	MG	DA	9524	1/1	0.95	0.22	2,2,2,2	0
57	MG	DA	9632	1/1	0.95	0.28	12,12,12,12	1
57	MG	DA	9435	1/1	0.95	0.43	30,30,30,30	0
57	MG	BA	3139	1/1	0.95	0.22	0,0,0,0	0
57	MG	DA	9356	1/1	0.95	0.17	1,1,1,1	0
57	MG	DA	9529	1/1	0.95	0.23	0,0,0,0	0
57	MG	BA	3078	1/1	0.95	0.14	2,2,2,2	0
57	MG	DA	9359	1/1	0.95	0.20	0,0,0,0	0
57	MG	BA	3118	1/1	0.95	0.25	28,28,28,28	0
57	MG	BA	3317	1/1	0.95	0.34	21,21,21,21	0
57	MG	BA	3182	1/1	0.95	0.21	2,2,2,2	0
57	MG	BA	3100	1/1	0.95	0.05	21,21,21,21	0
57	MG	AA	7049	1/1	0.95	0.15	41,41,41,41	0
57	MG	BA	3005	1/1	0.95	0.13	22,22,22,22	0
57	MG	CA	1742	1/1	0.95	0.22	10,10,10,10	0
57	MG	BA	3230	1/1	0.95	0.16	22,22,22,22	0
57	MG	DA	9546	1/1	0.95	0.24	2,2,2,2	0
57	MG	DA	9547	1/1	0.95	0.13	3,3,3,3	0
57	MG	DA	9653	1/1	0.95	0.19	5,5,5,5	0
57	MG	CA	1635	1/1	0.95	0.19	4,4,4,4	0
57	MG	DA	9449	1/1	0.95	0.23	0,0,0,0	0
57	MG	AA	7040	1/1	0.95	0.12	36,36,36,36	0
57	MG	BA	3151	1/1	0.95	0.07	12,12,12,12	0
57	MG	DA	9375	1/1	0.95	0.25	0,0,0,0	0
57	MG	BA	3188	1/1	0.95	0.10	0,0,0,0	0
57	MG	DA	9554	1/1	0.95	0.16	10,10,10,10	0
57	MG	DA	9662	1/1	0.95	0.29	2,2,2,2	0
57	MG	BA	3104	1/1	0.95	0.07	16,16,16,16	0
57	MG	BA	3125	1/1	0.95	0.22	20,20,20,20	0
57	MG	CA	1695	1/1	0.95	0.15	15,15,15,15	0
57	MG	BA	3068	1/1	0.95	0.06	11,11,11,11	0
57	MG	DA	9303	1/1	0.95	0.13	42,42,42,42	0
57	MG	BA	3194	1/1	0.95	0.18	1,1,1,1	0
57	MG	DA	9670	1/1	0.95	0.17	11,11,11,11	0
57	MG	DA	9384	1/1	0.95	0.23	16,16,16,16	0
57	MG	DA	9673	1/1	0.95	0.10	8,8,8,8	0
57	MG	DA	9305	1/1	0.95	0.25	0,0,0,0	0
57	MG	BA	3127	1/1	0.95	0.20	8,8,8,8	0
57	MG	DA	9308	1/1	0.95	0.24	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BE	302	1/1	0.95	0.17	74,74,74,74	0
57	MG	DA	9679	1/1	0.95	0.13	16,16,16,16	0
57	MG	BA	3019	1/1	0.95	0.17	44,44,44,44	0
57	MG	CA	1646	1/1	0.95	0.26	7,7,7,7	0
57	MG	DA	9682	1/1	0.95	0.14	20,20,20,20	0
57	MG	BA	3287	1/1	0.95	0.18	30,30,30,30	0
57	MG	CA	1649	1/1	0.95	0.08	33,33,33,33	0
57	MG	BA	3107	1/1	0.95	0.20	36,36,36,36	0
57	MG	DA	9472	1/1	0.95	0.20	16,16,16,16	0
57	MG	DA	9320	1/1	0.95	0.14	10,10,10,10	0
57	MG	BA	3291	1/1	0.95	0.08	22,22,22,22	0
57	MG	DA	9323	1/1	0.95	0.25	33,33,33,33	0
57	MG	AA	7014	1/1	0.95	0.26	20,20,20,20	0
57	MG	DA	9584	1/1	0.95	0.28	0,0,0,0	0
57	MG	DA	9403	1/1	0.95	0.16	0,0,0,0	0
57	MG	DA	9587	1/1	0.95	0.19	2,2,2,2	0
57	MG	BA	3057	1/1	0.95	0.18	2,2,2,2	0
57	MG	AA	7039	1/1	0.95	0.22	11,11,11,11	0
57	MG	DA	9407	1/1	0.95	0.09	2,2,2,2	0
57	MG	BA	3165	1/1	0.95	0.24	0,0,0,0	0
57	MG	DA	9409	1/1	0.95	0.23	4,4,4,4	0
57	MG	DA	9410	1/1	0.95	0.13	4,4,4,4	0
57	MG	DE	301	1/1	0.95	0.16	1,1,1,1	0
57	MG	BA	3074	1/1	0.95	0.34	34,34,34,34	0
57	MG	DA	9492	1/1	0.95	0.06	76,76,76,76	0
57	MG	BA	3089	1/1	0.95	0.23	18,18,18,18	0
57	MG	BA	3211	1/1	0.95	0.09	2,2,2,2	0
57	MG	BA	3169	1/1	0.95	0.26	3,3,3,3	0
57	MG	CA	1717	1/1	0.95	0.10	11,11,11,11	0
57	MG	DA	9498	1/1	0.95	0.22	2,2,2,2	0
57	MG	DA	9335	1/1	0.95	0.21	21,21,21,21	0
57	MG	BA	3213	1/1	0.95	0.22	8,8,8,8	0
57	MG	BA	3092	1/1	0.95	0.11	1,1,1,1	0
57	MG	BA	3172	1/1	0.95	0.24	58,58,58,58	0
57	MG	DA	9606	1/1	0.95	0.29	4,4,4,4	0
57	MG	D5	101	1/1	0.95	0.16	7,7,7,7	0
57	MG	CA	1613	1/1	0.95	0.23	31,31,31,31	0
57	MG	DA	9424	1/1	0.95	0.19	5,5,5,5	0
57	MG	DA	9507	1/1	0.95	0.26	2,2,2,2	0
57	MG	DA	9611	1/1	0.95	0.17	8,8,8,8	0
57	MG	DA	9612	1/1	0.95	0.17	1,1,1,1	1
57	MG	BA	3065	1/1	0.96	0.36	2,2,2,2	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1677	1/1	0.96	0.08	22,22,22,22	0
57	MG	CA	1678	1/1	0.96	0.11	17,17,17,17	0
57	MG	DA	9482	1/1	0.96	0.06	12,12,12,12	0
57	MG	CA	1732	1/1	0.96	0.27	27,27,27,27	0
57	MG	CA	1733	1/1	0.96	0.14	11,11,11,11	0
57	MG	DA	9485	1/1	0.96	0.17	15,15,15,15	0
57	MG	DA	9566	1/1	0.96	0.22	18,18,18,18	0
57	MG	AA	7096	1/1	0.96	0.23	31,31,31,31	0
57	MG	DA	9349	1/1	0.96	0.33	3,3,3,3	0
57	MG	AA	7032	1/1	0.96	0.15	24,24,24,24	0
57	MG	BA	3047	1/1	0.96	0.18	0,0,0,0	0
57	MG	DA	9571	1/1	0.96	0.23	0,0,0,0	0
57	MG	DA	9491	1/1	0.96	0.11	11,11,11,11	0
57	MG	BA	3229	1/1	0.96	0.12	19,19,19,19	0
57	MG	CA	1631	1/1	0.96	0.36	22,22,22,22	0
57	MG	DA	9354	1/1	0.96	0.25	2,2,2,2	0
57	MG	BA	3191	1/1	0.96	0.19	2,2,2,2	0
57	MG	BA	3192	1/1	0.96	0.22	2,2,2,2	0
57	MG	BA	3020	1/1	0.96	0.16	1,1,1,1	0
57	MG	CE	201	1/1	0.96	0.11	16,16,16,16	0
57	MG	BA	3163	1/1	0.96	0.16	28,28,28,28	0
57	MG	BA	3034	1/1	0.96	0.15	7,7,7,7	0
57	MG	DA	9583	1/1	0.96	0.15	1,1,1,1	0
57	MG	AA	7079	1/1	0.96	0.13	35,35,35,35	0
57	MG	DA	9585	1/1	0.96	0.11	18,18,18,18	0
57	MG	BA	3279	1/1	0.96	0.24	31,31,31,31	0
57	MG	BA	3280	1/1	0.96	0.24	19,19,19,19	1
57	MG	BA	3238	1/1	0.96	0.24	9,9,9,9	0
57	MG	BA	3166	1/1	0.96	0.27	40,40,40,40	0
57	MG	BA	3200	1/1	0.96	0.14	5,5,5,5	0
57	MG	DA	9511	1/1	0.96	0.30	7,7,7,7	0
57	MG	AA	7107	1/1	0.96	0.24	24,24,24,24	0
57	MG	AA	7019	1/1	0.96	0.14	16,16,16,16	0
57	MG	DA	9514	1/1	0.96	0.38	19,19,19,19	0
57	MG	BA	3289	1/1	0.96	0.20	21,21,21,21	0
57	MG	AA	7085	1/1	0.96	0.06	15,15,15,15	0
57	MG	CA	1647	1/1	0.96	0.15	6,6,6,6	0
57	MG	BA	3140	1/1	0.96	0.11	40,40,40,40	0
57	MG	DA	9309	1/1	0.96	0.16	6,6,6,6	0
57	MG	BA	3099	1/1	0.96	0.09	30,30,30,30	0
57	MG	BA	3209	1/1	0.96	0.13	1,1,1,1	0
57	MG	DA	9690	1/1	0.96	0.07	5,5,5,5	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3056	1/1	0.96	0.11	5,5,5,5	0
57	MG	BA	3144	1/1	0.96	0.40	41,41,41,41	0
57	MG	BA	3176	1/1	0.96	0.16	0,0,0,0	0
57	MG	AA	7058	1/1	0.96	0.10	13,13,13,13	0
57	MG	DA	9527	1/1	0.96	0.22	1,1,1,1	0
57	MG	DA	9317	1/1	0.96	0.07	18,18,18,18	0
57	MG	DA	9318	1/1	0.96	0.17	2,2,2,2	0
57	MG	DA	9389	1/1	0.96	0.06	11,11,11,11	0
57	MG	DA	9319	1/1	0.96	0.20	30,30,30,30	0
57	MG	DA	9533	1/1	0.96	0.19	0,0,0,0	0
57	MG	DA	9534	1/1	0.96	0.21	1,1,1,1	0
57	MG	DD	7103	1/1	0.96	0.15	0,0,0,0	0
57	MG	BA	3040	1/1	0.96	0.23	0,0,0,0	0
57	MG	DA	9537	1/1	0.96	0.25	0,0,0,0	0
57	MG	BA	3215	1/1	0.96	0.21	1,1,1,1	0
57	MG	BA	3059	1/1	0.96	0.07	0,0,0,0	0
57	MG	BA	3080	1/1	0.96	0.17	0,0,0,0	0
57	MG	BA	3304	1/1	0.96	0.18	13,13,13,13	0
57	MG	DU	202	1/1	0.96	0.06	6,6,6,6	0
57	MG	BA	3305	1/1	0.96	0.15	24,24,24,24	0
57	MG	DA	9328	1/1	0.96	0.17	1,1,1,1	0
57	MG	CA	1663	1/1	0.96	0.23	11,11,11,11	0
57	MG	BA	3013	1/1	0.96	0.13	16,16,16,16	0
57	MG	BA	3152	1/1	0.96	0.14	18,18,18,18	0
57	MG	DA	9631	1/1	0.96	0.19	21,21,21,21	0
57	MG	AA	7093	1/1	0.96	0.21	30,30,30,30	0
57	MG	BA	3309	1/1	0.96	0.34	25,25,25,25	0
57	MG	CA	1618	1/1	0.96	0.11	31,31,31,31	0
57	MG	BA	3043	1/1	0.96	0.11	8,8,8,8	0
57	MG	BA	3016	1/1	0.96	0.16	8,8,8,8	0
57	MG	BA	3223	1/1	0.96	0.09	9,9,9,9	0
57	MG	BA	3266	1/1	0.96	0.19	33,33,33,33	0
57	MG	DA	9336	1/1	0.97	0.16	52,52,52,52	0
57	MG	BA	3197	1/1	0.97	0.12	1,1,1,1	0
57	MG	BA	3244	1/1	0.97	0.05	1,1,1,1	0
57	MG	CA	1623	1/1	0.97	0.12	19,19,19,19	0
57	MG	DA	9654	1/1	0.97	0.14	15,15,15,15	0
57	MG	DA	9452	1/1	0.97	0.24	10,10,10,10	0
57	MG	CA	1660	1/1	0.97	0.13	9,9,9,9	0
57	MG	AA	7067	1/1	0.97	0.16	28,28,28,28	0
57	MG	DA	9398	1/1	0.97	0.19	0,0,0,0	0
57	MG	BA	3048	1/1	0.97	0.14	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	DA	9400	1/1	0.97	0.15	0,0,0,0	0
57	MG	BA	3094	1/1	0.97	0.19	7,7,7,7	0
57	MG	BA	3148	1/1	0.97	0.07	16,16,16,16	0
57	MG	BA	3002	1/1	0.97	0.21	53,53,53,53	0
57	MG	BA	3303	1/1	0.97	0.04	19,19,19,19	0
57	MG	BE	303	1/1	0.97	0.12	1,1,1,1	0
57	MG	DA	9301	1/1	0.97	0.18	32,32,32,32	0
57	MG	CA	1669	1/1	0.97	0.08	10,10,10,10	0
57	MG	DA	9668	1/1	0.97	0.30	4,4,4,4	0
57	MG	CA	1670	1/1	0.97	0.07	2,2,2,2	0
57	MG	AA	7042	1/1	0.97	0.05	31,31,31,31	0
57	MG	CA	1712	1/1	0.97	0.17	34,34,34,34	1
57	MG	AA	7095	1/1	0.97	0.08	17,17,17,17	0
57	MG	DA	9469	1/1	0.97	0.17	17,17,17,17	0
57	MG	DA	9413	1/1	0.97	0.21	3,3,3,3	0
57	MG	DA	9535	1/1	0.97	0.19	14,14,14,14	0
57	MG	DA	9307	1/1	0.97	0.16	12,12,12,12	0
57	MG	BA	3208	1/1	0.97	0.12	8,8,8,8	0
57	MG	BA	3023	1/1	0.97	0.10	4,4,4,4	0
57	MG	BA	3170	1/1	0.97	0.26	1,1,1,1	0
57	MG	DA	9311	1/1	0.97	0.25	29,29,29,29	0
57	MG	DA	9683	1/1	0.97	0.21	19,19,19,19	0
57	MG	DA	9541	1/1	0.97	0.25	2,2,2,2	0
57	MG	DA	9363	1/1	0.97	0.08	1,1,1,1	0
57	MG	DA	9609	1/1	0.97	0.14	2,2,2,2	0
57	MG	B5	101	1/1	0.97	0.11	2,2,2,2	0
57	MG	B7	101	1/1	0.97	0.18	13,13,13,13	0
57	MG	DA	9480	1/1	0.97	0.05	30,30,30,30	0
57	MG	DA	9613	1/1	0.97	0.08	5,5,5,5	0
57	MG	DA	9691	1/1	0.97	0.17	12,12,12,12	0
57	MG	CA	1720	1/1	0.97	0.19	2,2,2,2	0
57	MG	DA	9368	1/1	0.97	0.10	1,1,1,1	0
57	MG	CA	1721	1/1	0.97	0.12	1,1,1,1	0
57	MG	BA	3124	1/1	0.97	0.09	17,17,17,17	0
57	MG	BA	3256	1/1	0.97	0.03	13,13,13,13	0
57	MG	AA	7089	1/1	0.97	0.04	21,21,21,21	0
57	MG	BA	3283	1/1	0.97	0.13	22,22,22,22	0
57	MG	BA	3015	1/1	0.97	0.18	3,3,3,3	0
57	MG	BA	3285	1/1	0.97	0.40	32,32,32,32	1
57	MG	DA	9625	1/1	0.97	0.18	26,26,26,26	0
57	MG	BA	3234	1/1	0.97	0.35	10,10,10,10	0
57	MG	DA	9556	1/1	0.97	0.04	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3260	1/1	0.97	0.17	8,8,8,8	0
57	MG	AA	7001	1/1	0.97	0.17	26,26,26,26	0
57	MG	DA	9495	1/1	0.97	0.23	3,3,3,3	0
57	MG	DA	9562	1/1	0.97	0.38	2,2,2,2	0
57	MG	CA	1611	1/1	0.97	0.20	0,0,0,0	0
57	MG	DA	9381	1/1	0.97	0.08	12,12,12,12	0
57	MG	DA	9635	1/1	0.97	0.19	24,24,24,24	0
57	MG	BA	3175	1/1	0.97	0.12	4,4,4,4	0
57	MG	AA	7012	1/1	0.97	0.28	12,12,12,12	0
57	MG	DA	9500	1/1	0.97	0.11	1,1,1,1	0
57	MG	BA	3240	1/1	0.97	0.10	21,21,21,21	0
57	MG	CA	1615	1/1	0.97	0.17	0,0,0,0	0
57	MG	DA	9642	1/1	0.97	0.12	1,1,1,1	0
57	MG	DA	9386	1/1	0.97	0.19	2,2,2,2	0
57	MG	BA	3293	1/1	0.97	0.09	1,1,1,1	0
57	MG	BA	3142	1/1	0.97	0.18	10,10,10,10	0
57	MG	D8	101	1/1	0.97	0.04	3,3,3,3	0
57	MG	DA	9646	1/1	0.97	0.12	31,31,31,31	0
57	MG	BA	3090	1/1	0.97	0.19	2,2,2,2	0
57	MG	CA	1619	1/1	0.97	0.18	11,11,11,11	0
57	MG	DA	9509	1/1	0.97	0.10	17,17,17,17	0
57	MG	BA	3156	1/1	0.98	0.15	19,19,19,19	0
57	MG	DA	9345	1/1	0.98	0.23	19,19,19,19	0
57	MG	CA	1620	1/1	0.98	0.08	1,1,1,1	0
57	MG	BA	3288	1/1	0.98	0.10	18,18,18,18	0
57	MG	BA	3224	1/1	0.98	0.07	5,5,5,5	0
57	MG	BA	3018	1/1	0.98	0.13	37,37,37,37	0
57	MG	BA	3207	1/1	0.98	0.16	1,1,1,1	0
57	MG	BA	3027	1/1	0.98	0.18	4,4,4,4	0
57	MG	BA	3091	1/1	0.98	0.12	0,0,0,0	0
57	MG	DA	9426	1/1	0.98	0.21	9,9,9,9	1
57	MG	CA	1679	1/1	0.98	0.13	9,9,9,9	0
57	MG	CA	1652	1/1	0.98	0.24	6,6,6,6	0
57	MG	BA	3011	1/1	0.98	0.24	36,36,36,36	0
57	MG	DA	9391	1/1	0.98	0.12	1,1,1,1	0
57	MG	BA	3272	1/1	0.98	0.12	10,10,10,10	0
57	MG	DA	9357	1/1	0.98	0.12	0,0,0,0	0
57	MG	BA	3146	1/1	0.98	0.34	0,0,0,0	0
57	MG	AA	7038	1/1	0.98	0.25	10,10,10,10	0
57	MG	DA	9558	1/1	0.98	0.04	6,6,6,6	0
57	MG	DA	9473	1/1	0.98	0.34	0,0,0,0	0
57	MG	AA	7044	1/1	0.98	0.09	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	CA	1715	1/1	0.98	0.20	12,12,12,12	0
57	MG	DA	9518	1/1	0.98	0.14	0,0,0,0	0
57	MG	BA	3049	1/1	0.98	0.08	30,30,30,30	0
57	MG	BA	3071	1/1	0.98	0.19	0,0,0,0	0
57	MG	BA	3060	1/1	0.98	0.30	1,1,1,1	0
57	MG	DE	302	1/1	0.98	0.06	35,35,35,35	0
57	MG	BA	3199	1/1	0.98	0.08	1,1,1,1	0
57	MG	DP	201	1/1	0.98	0.05	7,7,7,7	0
57	MG	BA	3237	1/1	0.98	0.12	43,43,43,43	0
57	MG	DA	9481	1/1	0.98	0.07	0,0,0,0	0
57	MG	BA	3007	1/1	0.98	0.25	4,4,4,4	0
57	MG	BA	3239	1/1	0.98	0.16	1,1,1,1	0
57	MG	BA	3201	1/1	0.98	0.17	6,6,6,6	0
57	MG	DA	9406	1/1	0.98	0.20	32,32,32,32	0
57	MG	AA	7041	1/1	0.98	0.17	20,20,20,20	0
57	MG	CA	1667	1/1	0.98	0.13	12,12,12,12	0
57	MG	DA	9488	1/1	0.98	0.26	0,0,0,0	0
57	MG	DA	9623	1/1	0.98	0.15	13,13,13,13	0
57	MG	DA	9373	1/1	0.98	0.10	0,0,0,0	0
57	MG	BE	301	1/1	0.98	0.09	0,0,0,0	0
57	MG	DA	9672	1/1	0.98	0.12	5,5,5,5	0
57	MG	AA	7094	1/1	0.98	0.26	8,8,8,8	0
57	MG	CA	1698	1/1	0.98	0.15	1,1,1,1	1
57	MG	DA	9675	1/1	0.98	0.13	11,11,11,11	0
57	MG	DA	9341	1/1	0.98	0.25	11,11,11,11	0
57	MG	DA	9414	1/1	0.98	0.27	16,16,16,16	0
59	ZN	AN	101	1/1	0.98	0.04	147,147,147,147	0
59	ZN	CD	301	1/1	0.98	0.20	44,44,44,44	0
57	MG	AA	7015	1/1	0.98	0.14	4,4,4,4	0
57	MG	DA	9627	1/1	0.99	0.09	0,0,0,0	1
57	MG	DA	9364	1/1	0.99	0.36	1,1,1,1	0
57	MG	DA	9322	1/1	0.99	0.05	8,8,8,8	0
57	MG	DA	9594	1/1	0.99	0.31	19,19,19,19	0
57	MG	DA	9343	1/1	0.99	0.15	2,2,2,2	0
57	MG	DA	9506	1/1	0.99	0.09	0,0,0,0	0
57	MG	DU	203	1/1	0.99	0.07	0,0,0,0	1
57	MG	DA	9580	1/1	0.99	0.26	0,0,0,0	0
57	MG	BA	3179	1/1	0.99	0.10	10,10,10,10	0
57	MG	DA	9324	1/1	0.99	0.20	2,2,2,2	0
57	MG	DA	9617	1/1	0.99	0.10	11,11,11,11	0
57	MG	DA	9697	1/1	0.99	0.07	41,41,41,41	0
57	MG	DA	9417	1/1	0.99	0.16	20,20,20,20	0

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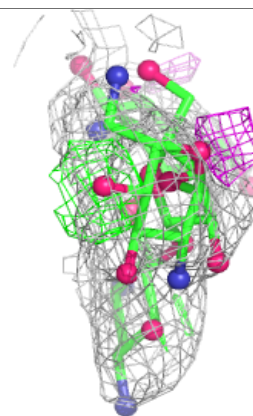
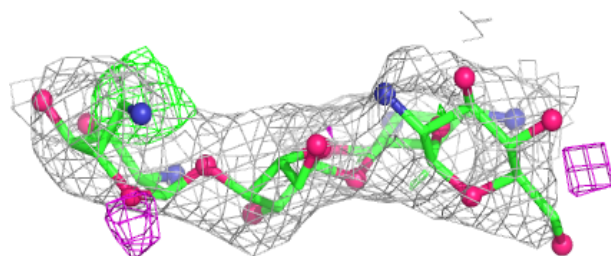
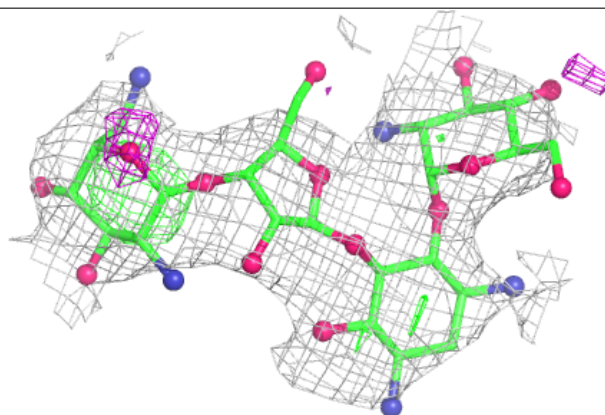
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
57	MG	BA	3098	1/1	0.99	0.22	36,36,36,36	0
57	MG	DB	203	1/1	0.99	0.48	1,1,1,1	1
57	MG	CA	1603	1/1	0.99	0.05	0,0,0,0	0
57	MG	AA	7025	1/1	0.99	0.09	1,1,1,1	0
57	MG	DA	9641	1/1	0.99	0.06	11,11,11,11	0
57	MG	CV	102	1/1	0.99	0.09	1,1,1,1	0
57	MG	AA	7024	1/1	0.99	0.19	27,27,27,27	0
57	MG	BA	3157	1/1	0.99	0.06	6,6,6,6	0
57	MG	AA	7103	1/1	0.99	0.17	13,13,13,13	0
57	MG	DA	9560	1/1	0.99	0.11	4,4,4,4	0
57	MG	DA	9532	1/1	1.00	0.19	9,9,9,9	0
57	MG	AA	7007	1/1	1.00	0.06	1,1,1,1	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.

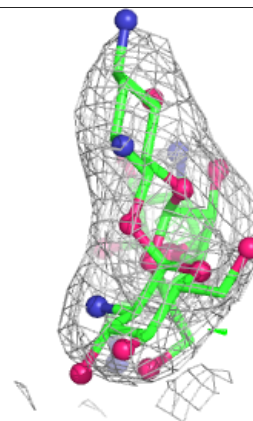
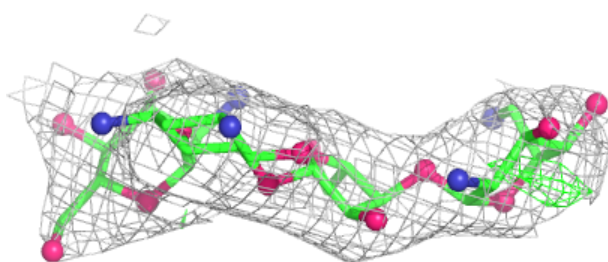
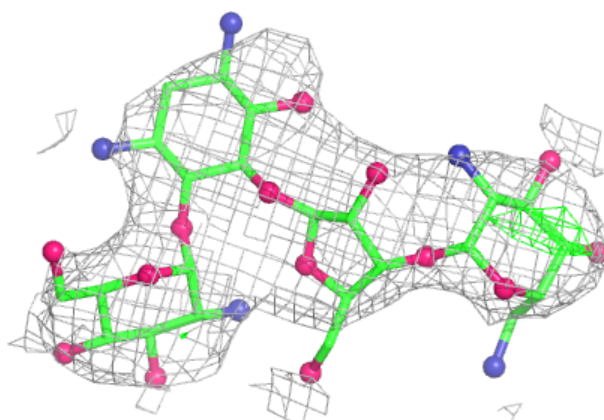
Electron density around PAR CA 1741:

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 [i](#)

There are no such residues in this entry.