



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:00 PM GMT

PDB ID : 4V9O
Title : Control of ribosomal subunit rotation by elongation factor G
Authors : Pulk, A.; Cate, J.H.D.
Deposited on : 2013-05-03
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

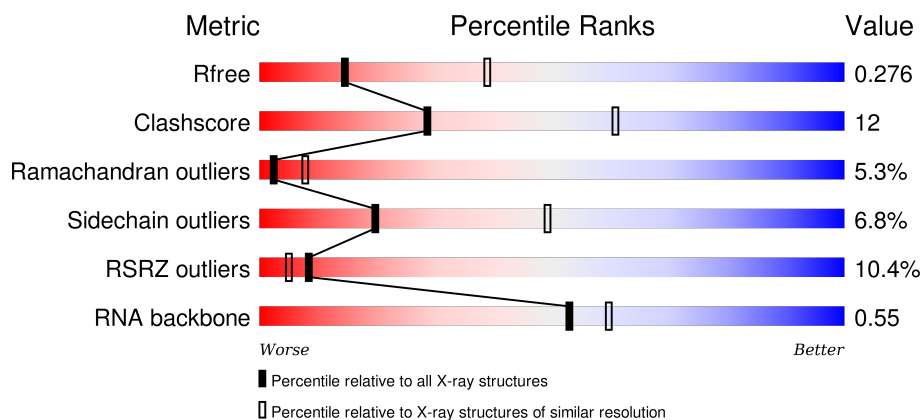
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.90 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.



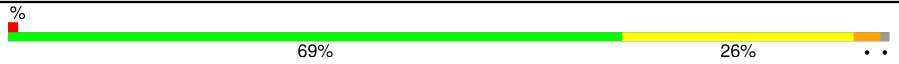

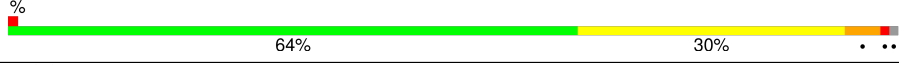

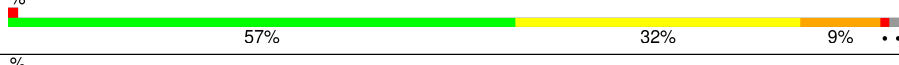
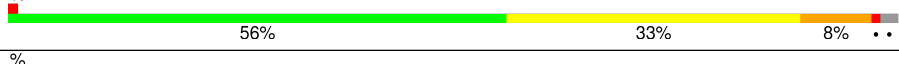
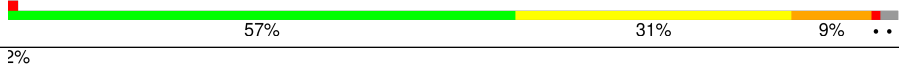
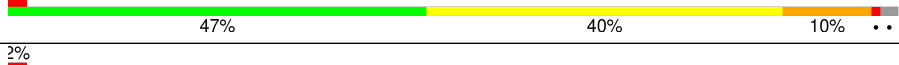
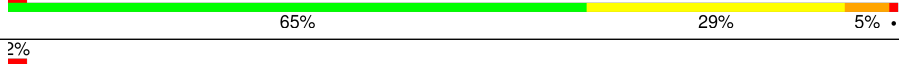


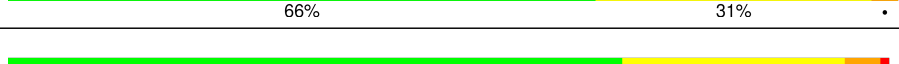
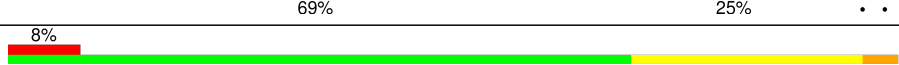
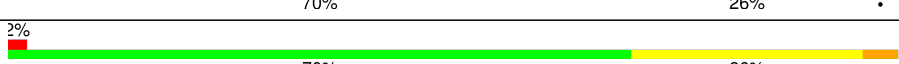

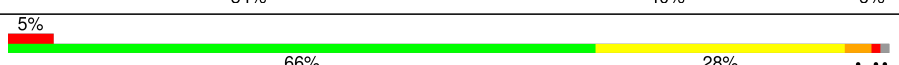
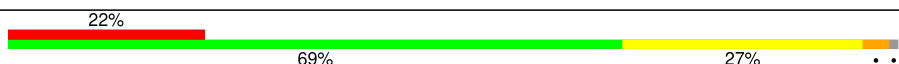
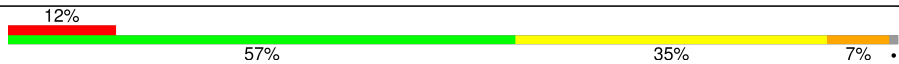



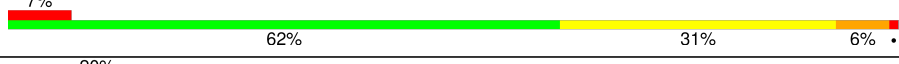
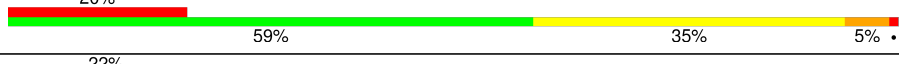


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)
RNA backbone	2183	1093 (3.30-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	AB	120	 66% 26% 7% .
1	CB	120	 60% 32% 7% .
1	EB	120	 63% 24% 9% . .
1	GB	120	 36% 51% 10% . .

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Mol	Chain	Length	Quality of chain
2	AC	273	
2	CC	273	
2	EC	273	
2	GC	273	
3	AA	2904	
3	CA	2904	
3	EA	2904	
3	GA	2904	
4	AD	209	
4	CD	209	
4	ED	209	
4	GD	209	
5	AE	201	
5	CE	201	
5	EE	201	
5	GE	201	
6	AF	179	
6	CF	179	
6	EF	179	
6	GF	179	
7	AG	177	
7	CG	177	
7	EG	177	
7	GG	177	
8	AH	50	

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Mol	Chain	Length	Quality of chain
8	CH	50	
8	EH	50	
8	GH	50	
9	AI	142	
9	CI	142	
9	EI	142	
9	GI	142	
10	AJ	142	
10	CJ	142	
10	EJ	142	
10	GJ	142	
11	AK	123	
11	CK	123	
11	EK	123	
11	GK	123	
12	AL	144	
12	CL	144	
12	EL	144	
12	GL	144	
13	AM	136	
13	CM	136	
13	EM	136	
13	GM	136	
14	AN	127	
14	CN	127	

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Mol	Chain	Length	Quality of chain
14	EN	127	
14	GN	127	
15	AO	117	
15	CO	117	
15	EO	117	
15	GO	117	
16	AP	115	
16	CP	115	
16	EP	115	
16	GP	115	
17	AQ	118	
17	CQ	118	
17	EQ	118	
17	GQ	118	
18	AR	103	
18	CR	103	
18	ER	103	
18	GR	103	
19	AS	110	
19	CS	110	
19	ES	110	
19	GS	110	
20	AT	100	
20	CT	100	
20	ET	100	

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Mol	Chain	Length	Quality of chain
20	GT	100	
21	AU	104	
21	CU	104	
21	EU	104	
21	GU	104	
22	AV	94	
22	CV	94	
22	EV	94	
22	GV	94	
23	AW	85	
23	CW	85	
23	EW	85	
23	GW	85	
24	AX	78	
24	CX	78	
24	EX	78	
24	GX	78	
25	AY	63	
25	CY	63	
25	EY	63	
25	GY	63	
26	AZ	59	
26	CZ	59	
26	EZ	59	
26	GZ	59	

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Mol	Chain	Length	Quality of chain
27	A0	57	
27	C0	57	
27	E0	57	
27	G0	57	
28	A1	55	
28	C1	55	
28	E1	55	
28	G1	55	
29	A2	46	
29	C2	46	
29	E2	46	
29	G2	46	
30	A3	65	
30	C3	65	
30	E3	65	
30	G3	65	
31	A4	38	
31	C4	38	
31	E4	38	
31	G4	38	
32	A5	165	
32	C5	165	
32	E5	165	
33	A6	121	
34	BB	241	

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Mol	Chain	Length	Quality of chain
34	DB	241	
34	FB	241	
34	HB	241	
35	BA	1542	
35	DA	1542	
35	FA	1542	
35	HA	1542	
36	BC	233	
36	DC	233	
36	FC	233	
36	HC	233	
37	BD	206	
37	DD	206	
37	FD	206	
37	HD	206	
38	BE	167	
38	DE	167	
38	FE	167	
38	HE	167	
39	BF	135	
39	DF	135	
39	FF	135	
39	HF	135	
40	BG	179	
40	DG	179	

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Mol	Chain	Length	Quality of chain
40	FG	179	
40	HG	179	
41	BH	130	
41	DH	130	
41	FH	130	
41	HH	130	
42	BI	130	
42	DI	130	
42	FI	130	
42	HI	130	
43	BJ	103	
43	DJ	103	
43	FJ	103	
43	HJ	103	
44	BK	129	
44	DK	129	
44	FK	129	
44	HK	129	
45	BL	124	
45	DL	124	
45	FL	124	
45	HL	124	
46	BM	118	
46	DM	118	
46	FM	118	

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Mol	Chain	Length	Quality of chain
46	HM	118	
47	BN	101	
47	DN	101	
47	FN	101	
47	HN	101	
48	BO	89	
48	DO	89	
48	FO	89	
48	HO	89	
49	BP	82	
49	DP	82	
49	FP	82	
49	HP	82	
50	BQ	84	
50	DQ	84	
50	FQ	84	
50	HQ	84	
51	BR	75	
51	DR	75	
51	FR	75	
51	HR	75	
52	BS	92	
52	DS	92	
52	FS	92	
52	HS	92	

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Mol	Chain	Length	Quality of chain
53	BT	87	
53	DT	87	
53	FT	87	
53	HT	87	
54	BU	71	
54	DU	71	
54	FU	71	
54	HU	71	
55	BV	704	
55	DV	704	
55	FV	704	
55	HV	704	
56	BW	6	
56	DW	6	
56	FW	6	
56	HW	6	

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	3026	-	-	-	X
57	MG	AA	3029	-	-	-	X
57	MG	AA	3037	-	-	-	X
57	MG	AA	3041	-	-	-	X
57	MG	AA	3047	-	-	-	X
57	MG	AA	3050	-	-	-	X
57	MG	AA	3068	-	-	-	X
57	MG	AA	3078	-	-	-	X
57	MG	AA	3090	-	-	-	X
57	MG	AA	3095	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	AA	3097	-	-	-	X
57	MG	AA	3100	-	-	-	X
57	MG	AA	3106	-	-	-	X
57	MG	AA	3107	-	-	-	X
57	MG	AA	3108	-	-	-	X
57	MG	AA	3111	-	-	-	X
57	MG	AA	3115	-	-	-	X
57	MG	AA	3129	-	-	-	X
57	MG	AA	3135	-	-	-	X
57	MG	BA	1607	-	-	-	X
57	MG	BA	1616	-	-	-	X
57	MG	BA	1627	-	-	-	X
57	MG	CA	3040	-	-	-	X
57	MG	CA	3046	-	-	-	X
57	MG	CA	3068	-	-	-	X
57	MG	CA	3105	-	-	-	X
57	MG	CA	3109	-	-	-	X
57	MG	CA	3112	-	-	-	X
57	MG	CA	3120	-	-	-	X
57	MG	CA	3131	-	-	-	X
57	MG	CA	3136	-	-	-	X
57	MG	DA	1628	-	-	-	X
57	MG	DA	1642	-	-	-	X
57	MG	DV	802	-	-	-	X
57	MG	EA	3005	-	-	-	X
57	MG	EA	3023	-	-	-	X
57	MG	EA	3025	-	-	-	X
57	MG	EA	3038	-	-	-	X
57	MG	EA	3040	-	-	-	X
57	MG	EA	3042	-	-	-	X
57	MG	EA	3046	-	-	-	X
57	MG	EA	3096	-	-	-	X
57	MG	EA	3100	-	-	-	X
57	MG	EA	3103	-	-	-	X
57	MG	EA	3104	-	-	-	X
57	MG	EA	3123	-	-	-	X
57	MG	FA	1609	-	-	-	X
57	MG	FA	1611	-	-	-	X
57	MG	FA	1613	-	-	-	X
57	MG	FA	1626	-	-	-	X
57	MG	FA	1635	-	-	-	X
57	MG	GA	3009	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
57	MG	GA	3021	-	-	-	X
57	MG	GA	3023	-	-	-	X
57	MG	GA	3030	-	-	-	X
57	MG	GA	3050	-	-	-	X
57	MG	GA	3055	-	-	-	X
57	MG	GA	3100	-	-	-	X
57	MG	GA	3104	-	-	-	X
57	MG	GA	3107	-	-	-	X
57	MG	GA	3115	-	-	-	X
57	MG	GA	3119	-	-	-	X
57	MG	GA	3131	-	-	-	X
57	MG	HA	1613	-	-	-	X
57	MG	HA	1628	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 592086 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 5S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
1	CB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
1	EB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			
1	GB	118	Total	C	N	O	P	0	0	0
			2529	1126	464	821	118			

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
2	CC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
2	EC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			
2	GC	271	Total	C	N	O	S	0	0	0
			2082	1288	423	364	7			

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
3	CA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
3	EA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			
3	GA	2854	Total	C	N	O	P	0	0	0
			61274	27334	11279	19807	2854			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	CD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	ED	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			
4	GD	209	Total	C	N	O	S	0	0	0
			1565	979	288	294	4			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	CE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	EE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			
5	GE	201	Total	C	N	O	S	0	0	0
			1552	974	283	290	5			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	CF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	EF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			
6	GF	177	Total	C	N	O	S	0	0	0
			1410	899	249	256	6			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	CG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			
7	EG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	GG	176	Total	C	N	O	S	0	0	0
			1323	832	243	246	2			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	CH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	EH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			
8	GH	50	Total	C	N	O	S	0	0	0
			384	247	68	68	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	CI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	EI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			
9	GI	141	Total	C	N	O	S	0	0	0
			1032	651	179	196	6			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	CJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	EJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			
10	GJ	142	Total	C	N	O	S	0	0	0
			1129	714	212	199	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	CK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	EK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			
11	GK	122	Total	C	N	O	S	0	0	0
			938	587	180	165	6			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	CL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	EL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			
12	GL	143	Total	C	N	O	S	0	0	0
			1045	649	206	189	1			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	CM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	EM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			
13	GM	136	Total	C	N	O	S	0	0	0
			1074	686	205	177	6			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	CN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			
14	EN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	GN	120	Total	C	N	O	S	0	0	0
			960	593	196	166	5			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	CO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	EO	116	Total	C	N	O		0	0	0
			892	552	178	162				
15	GO	116	Total	C	N	O		0	0	0
			892	552	178	162				

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	CP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	EP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			
16	GP	114	Total	C	N	O	S	0	0	0
			917	574	179	163	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	CQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	EQ	117	Total	C	N	O		0	0	0
			947	604	192	151				
17	GQ	117	Total	C	N	O		0	0	0
			947	604	192	151				

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	AR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	CR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	ER	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			
18	GR	103	Total	C	N	O	S	0	0	0
			816	516	153	145	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	CS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	ES	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			
19	GS	110	Total	C	N	O	S	0	0	0
			857	532	166	156	3			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	CT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	ET	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			
20	GT	93	Total	C	N	O	S	0	0	0
			738	466	139	131	2			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	CU	102	Total	C	N	O	0	0	0
			779	492	146	141			
21	EU	102	Total	C	N	O	0	0	0
			779	492	146	141			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	GU	102	Total	C	N	O	0	0	0
			779	492	146	141			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	CV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	EV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			
22	GV	94	Total	C	N	O	S	0	0	0
			753	479	137	134	3			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	CW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	EW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			
23	GW	79	Total	C	N	O	S	0	0	0
			596	367	120	108	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	CX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	EX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			
24	GX	77	Total	C	N	O	S	0	0	0
			625	388	129	106	2			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	CY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	EY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			
25	GY	63	Total	C	N	O	S	0	0	0
			509	313	99	95	2			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	AZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	CZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	EZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			
26	GZ	58	Total	C	N	O	S	0	0	0
			449	281	87	79	2			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	A0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	C0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	E0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			
27	G0	56	Total	C	N	O	S	0	0	0
			444	269	94	80	1			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	A1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	C1	50	Total	C	N	O	0	0	0
			409	263	75	71			
28	E1	50	Total	C	N	O	0	0	0
			409	263	75	71			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
28	G1	50	Total	C	N	O	0	0	0
			409	263	75	71			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	A2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	C2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	E2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			
29	G2	46	Total	C	N	O	S	0	0	0
			377	228	90	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	A3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	C3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	E3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			
30	G3	64	Total	C	N	O	S	0	0	0
			504	323	105	74	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	A4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	C4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	E4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			
31	G4	38	Total	C	N	O	S	0	0	0
			302	185	65	48	4			

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	A5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	C5	148	Total	C	N	O	S	0	0	0
			1117	705	196	209	7			
32	E5	145	Total	C	N	O	S	0	0	0
			1101	696	193	205	7			

- Molecule 33 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	A6	30	Total	C	N	O	S	0	0	0
			227	144	33	47	3			

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	DB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	FB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			
34	HB	218	Total	C	N	O	S	0	0	0
			1704	1081	305	311	7			

- Molecule 35 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
35	DA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
35	FA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			
35	HA	1533	Total	C	N	O	P	0	0	0
			32895	14671	6036	10655	1533			

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	DC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
36	FC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			
36	HC	206	Total	C	N	O	S	0	0	0
			1624	1028	305	288	3			

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
37	DD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
37	FD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			
37	HD	205	Total	C	N	O	S	0	0	0
			1643	1026	315	298	4			

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
38	DE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
38	FE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			
38	HE	150	Total	C	N	O	S	0	0	0
			1105	687	211	201	6			

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BF	102	Total	C	N	O	S	0	0	0
			832	525	150	150	7			
39	DF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
39	FF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			
39	HF	100	Total	C	N	O	S	0	0	0
			817	515	148	148	6			

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
40	DG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
40	FG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			
40	HG	151	Total	C	N	O	S	0	0	0
			1181	735	227	215	4			

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
41	DH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
41	FH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			
41	HH	129	Total	C	N	O	S	0	0	0
			979	616	173	184	6			

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
42	DI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
42	FI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			
42	HI	127	Total	C	N	O	S	0	0	0
			1022	634	206	179	3			

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	BJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
43	DJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			
43	FJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
43	HJ	98	Total	C	N	O	S	0	0	0
			786	493	150	142	1			

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
44	BK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
44	DK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
44	FK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			
44	HK	117	Total	C	N	O	S	0	0	0
			877	540	174	160	3			

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
45	DL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
45	FL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			
45	HL	123	Total	C	N	O	S	0	0	0
			955	590	196	165	4			

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
46	DM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
46	FM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			
46	HM	114	Total	C	N	O	S	0	0	0
			883	546	178	156	3			

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
47	DN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
47	FN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			
47	HN	96	Total	C	N	O	S	0	0	0
			774	483	160	128	3			

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
48	DO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
48	FO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			
48	HO	88	Total	C	N	O	S	0	0	0
			714	439	144	130	1			

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
49	DP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
49	FP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			
49	HP	82	Total	C	N	O	S	0	0	0
			649	406	128	114	1			

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	BQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
50	DQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			
50	FQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	HQ	80	Total	C	N	O	S	0	0	0
			648	411	121	113	3			

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	BR	55	Total	C	N	O		0	0	0
			455	288	86	81				
51	DR	55	Total	C	N	O		0	0	0
			455	288	86	81				
51	FR	55	Total	C	N	O		0	0	0
			455	288	86	81				
51	HR	55	Total	C	N	O		0	0	0
			455	288	86	81				

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	BS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
52	DS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
52	FS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			
52	HS	79	Total	C	N	O	S	0	0	0
			637	408	120	107	2			

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	BT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
53	DT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
53	FT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			
53	HT	85	Total	C	N	O	S	0	0	0
			665	411	137	114	3			

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	BU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
54	DU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
54	FU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			
54	HU	51	Total	C	N	O	S	0	0	0
			425	265	86	73	1			

- Molecule 55 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	BV	690	Total	C	N	O	S	0	0	0
			5345	3369	920	1031	25			
55	DV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			
55	FV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			
55	HV	689	Total	C	N	O	S	0	0	0
			5340	3366	919	1030	25			

- Molecule 56 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
56	BW	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	DW	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	FW	6	Total	C	N	O	0	0	0
			48	25	13	10			
56	HW	6	Total	C	N	O	0	0	0
			48	25	13	10			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	FA	39	Total	Mg	0	0
			39	39		
57	BA	40	Total	Mg	0	0
			40	40		
57	CA	136	Total	Mg	0	0
			136	136		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	HE	1	Total 1	Mg 1	0	0
57	AB	4	Total 4	Mg 4	0	0
57	BE	1	Total 1	Mg 1	0	0
57	GA	136	Total 136	Mg 136	0	0
57	HA	41	Total 41	Mg 41	0	0
57	EB	4	Total 4	Mg 4	0	0
57	FU	1	Total 1	Mg 1	0	0
57	FV	1	Total 1	Mg 1	0	0
57	C4	1	Total 1	Mg 1	0	0
57	AE	1	Total 1	Mg 1	0	0
57	AA	136	Total 136	Mg 136	0	0
57	FE	1	Total 1	Mg 1	0	0
57	DV	1	Total 1	Mg 1	0	0
57	EA	137	Total 137	Mg 137	0	0
57	BU	1	Total 1	Mg 1	0	0
57	HK	1	Total 1	Mg 1	0	0
57	CN	1	Total 1	Mg 1	0	0
57	BN	1	Total 1	Mg 1	0	0
57	EE	1	Total 1	Mg 1	0	0
57	GL	1	Total 1	Mg 1	0	0
57	A4	1	Total 1	Mg 1	0	0

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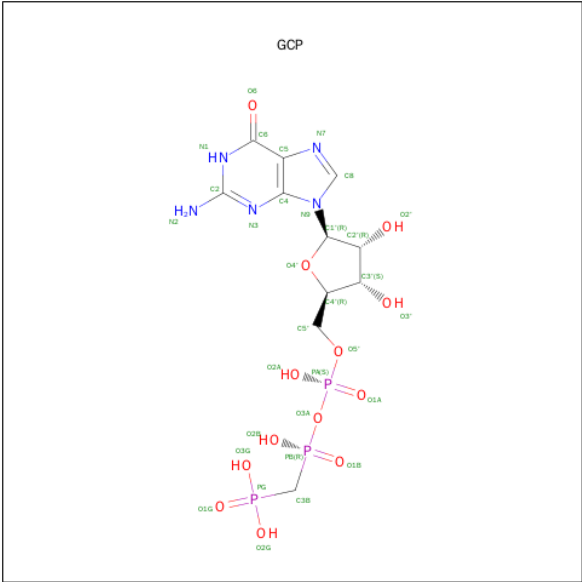
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
57	DA	43	Total 43	Mg 43	0	0
57	GC	2	Total 2	Mg 2	0	0
57	BV	1	Total 1	Mg 1	0	0
57	CB	4	Total 4	Mg 4	0	0
57	FN	2	Total 2	Mg 2	0	0
57	AC	1	Total 1	Mg 1	0	0
57	ED	1	Total 1	Mg 1	0	0
57	GB	4	Total 4	Mg 4	0	0
57	CE	1	Total 1	Mg 1	0	0
57	HV	1	Total 1	Mg 1	0	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
58	E4	1	Total 1	Zn 1	0	0
58	G4	1	Total 1	Zn 1	0	0
58	A4	1	Total 1	Zn 1	0	0
58	C4	1	Total 1	Zn 1	0	0

- Molecule 59 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
59	BV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
59	DV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
59	FV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		
59	HV	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

- Molecule 60 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AB	18	Total	O	0	0
			18	18		
60	AC	6	Total	O	0	0
			6	6		
60	AA	614	Total	O	0	0
			614	614		
60	AD	4	Total	O	0	0
			4	4		
60	AE	1	Total	O	0	0
			1	1		
60	AF	1	Total	O	0	0
			1	1		
60	AJ	1	Total	O	0	0
			1	1		
60	AL	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AN	2	Total 2	O 2	0	0
60	AP	1	Total 1	O 1	0	0
60	AQ	2	Total 2	O 2	0	0
60	AS	1	Total 1	O 1	0	0
60	A0	2	Total 2	O 2	0	0
60	A2	1	Total 1	O 1	0	0
60	A3	1	Total 1	O 1	0	0
60	A4	1	Total 1	O 1	0	0
60	BA	202	Total 202	O 202	0	0
60	BL	1	Total 1	O 1	0	0
60	BN	2	Total 2	O 2	0	0
60	BT	2	Total 2	O 2	0	0
60	BV	1	Total 1	O 1	0	0
60	CB	21	Total 21	O 21	0	0
60	CA	607	Total 607	O 607	0	0
60	CC	8	Total 8	O 8	0	0
60	CD	3	Total 3	O 3	0	0
60	CE	1	Total 1	O 1	0	0
60	CJ	2	Total 2	O 2	0	0
60	CL	5	Total 5	O 5	0	0
60	CN	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	CQ	1	Total 1	O 1	0	0
60	CS	2	Total 2	O 2	0	0
60	CT	2	Total 2	O 2	0	0
60	CU	1	Total 1	O 1	0	0
60	C0	1	Total 1	O 1	0	0
60	C2	1	Total 1	O 1	0	0
60	C3	1	Total 1	O 1	0	0
60	C4	2	Total 2	O 2	0	0
60	DA	186	Total 186	O 186	0	0
60	DC	2	Total 2	O 2	0	0
60	DD	1	Total 1	O 1	0	0
60	DE	1	Total 1	O 1	0	0
60	DG	1	Total 1	O 1	0	0
60	DK	1	Total 1	O 1	0	0
60	DL	2	Total 2	O 2	0	0
60	DN	8	Total 8	O 8	0	0
60	DQ	1	Total 1	O 1	0	0
60	DT	4	Total 4	O 4	0	0
60	DU	1	Total 1	O 1	0	0
60	DV	1	Total 1	O 1	0	0
60	EA	610	Total 610	O 610	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	EB	18	Total 18	O 18	0	0
60	EC	9	Total 9	O 9	0	0
60	ED	3	Total 3	O 3	0	0
60	EE	2	Total 2	O 2	0	0
60	EL	4	Total 4	O 4	0	0
60	EN	3	Total 3	O 3	0	0
60	ER	1	Total 1	O 1	0	0
60	ET	2	Total 2	O 2	0	0
60	EV	2	Total 2	O 2	0	0
60	E0	1	Total 1	O 1	0	0
60	E2	1	Total 1	O 1	0	0
60	E3	2	Total 2	O 2	0	0
60	E4	2	Total 2	O 2	0	0
60	FA	197	Total 197	O 197	0	0
60	FC	1	Total 1	O 1	0	0
60	FE	2	Total 2	O 2	0	0
60	FN	3	Total 3	O 3	0	0
60	FT	4	Total 4	O 4	0	0
60	FU	1	Total 1	O 1	0	0
60	FV	1	Total 1	O 1	0	0
60	GB	19	Total 19	O 19	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	GA	606	Total 606	O 606	0	0
60	GC	10	Total 10	O 10	0	0
60	GD	3	Total 3	O 3	0	0
60	GE	2	Total 2	O 2	0	0
60	GJ	1	Total 1	O 1	0	0
60	GL	4	Total 4	O 4	0	0
60	GN	4	Total 4	O 4	0	0
60	GQ	1	Total 1	O 1	0	0
60	GR	2	Total 2	O 2	0	0
60	GS	2	Total 2	O 2	0	0
60	GU	1	Total 1	O 1	0	0
60	GV	1	Total 1	O 1	0	0
60	G2	2	Total 2	O 2	0	0
60	G3	1	Total 1	O 1	0	0
60	G4	1	Total 1	O 1	0	0
60	HA	193	Total 193	O 193	0	0
60	HD	3	Total 3	O 3	0	0
60	HE	3	Total 3	O 3	0	0
60	HN	7	Total 7	O 7	0	0
60	HQ	1	Total 1	O 1	0	0
60	HT	1	Total 1	O 1	0	0

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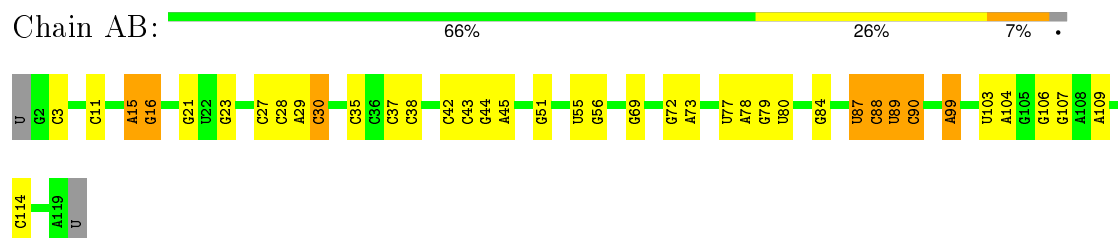
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	HV	1	Total	O	0	0
			1	1		

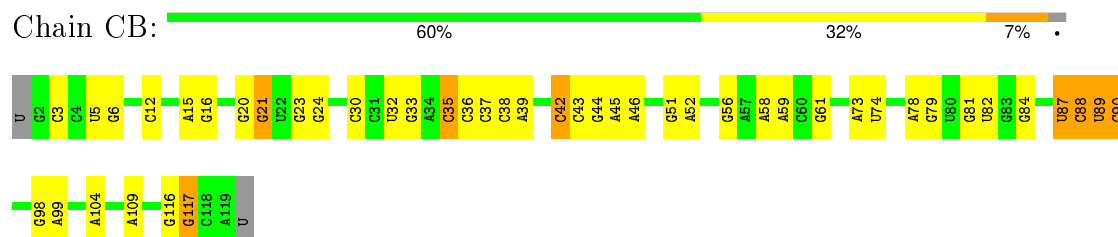
3 Residue-property plots

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

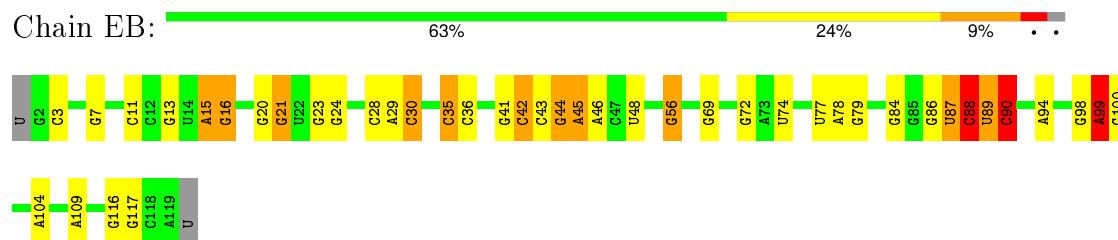
- Molecule 1: 5S rRNA



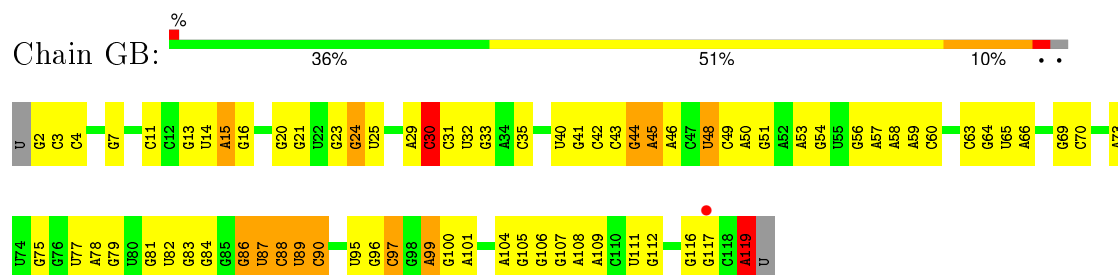
- Molecule 1: 5S rRNA



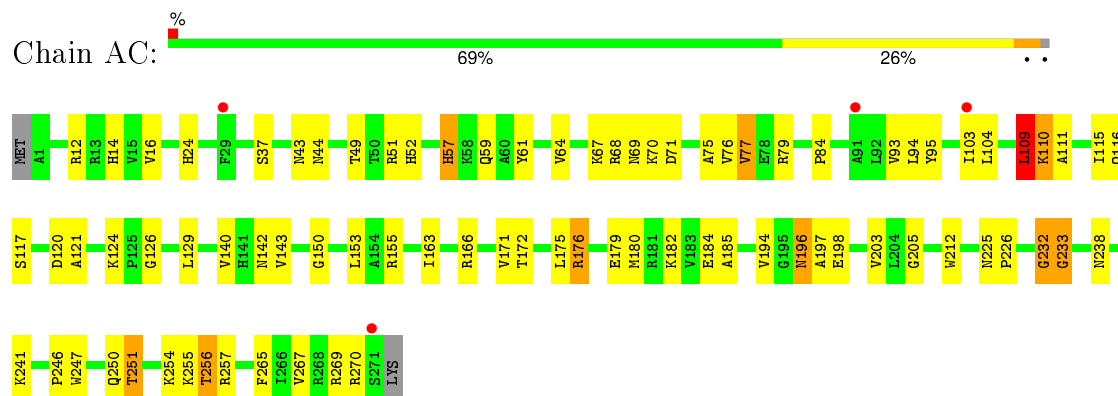
- Molecule 1: 5S rRNA



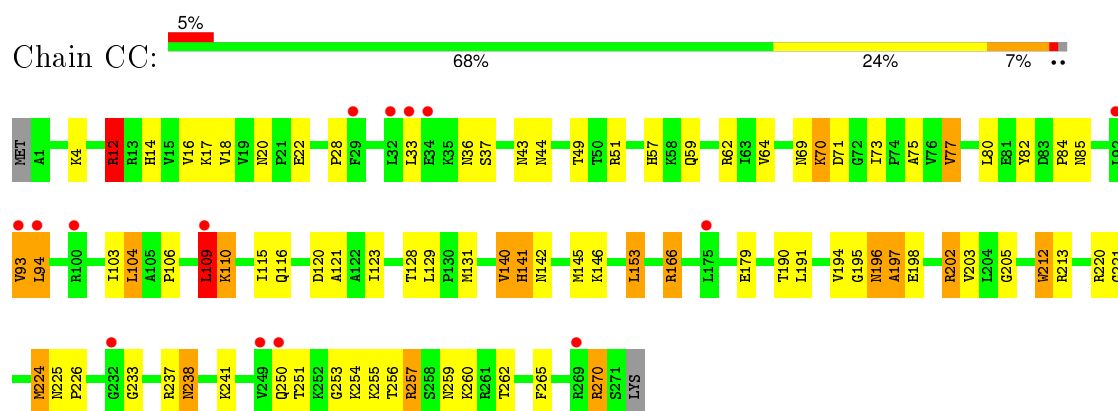
- Molecule 1: 5S rRNA



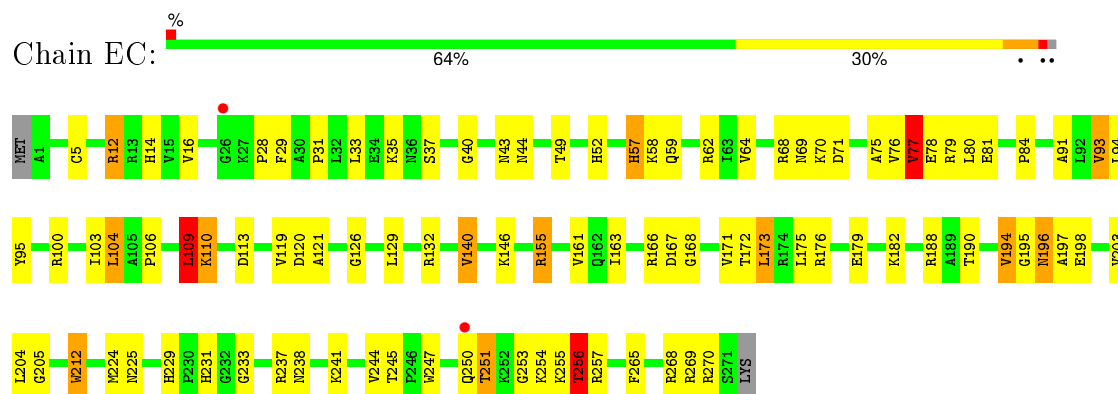
• Molecule 2: 50S ribosomal protein L2



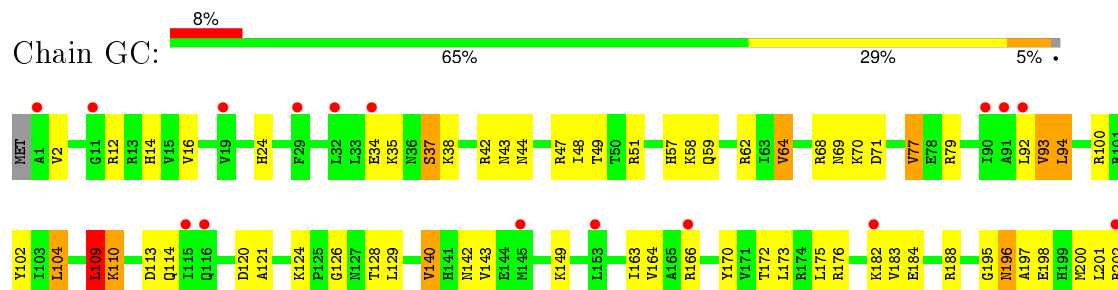
• Molecule 2: 50S ribosomal protein L2



• Molecule 2: 50S ribosomal protein L2

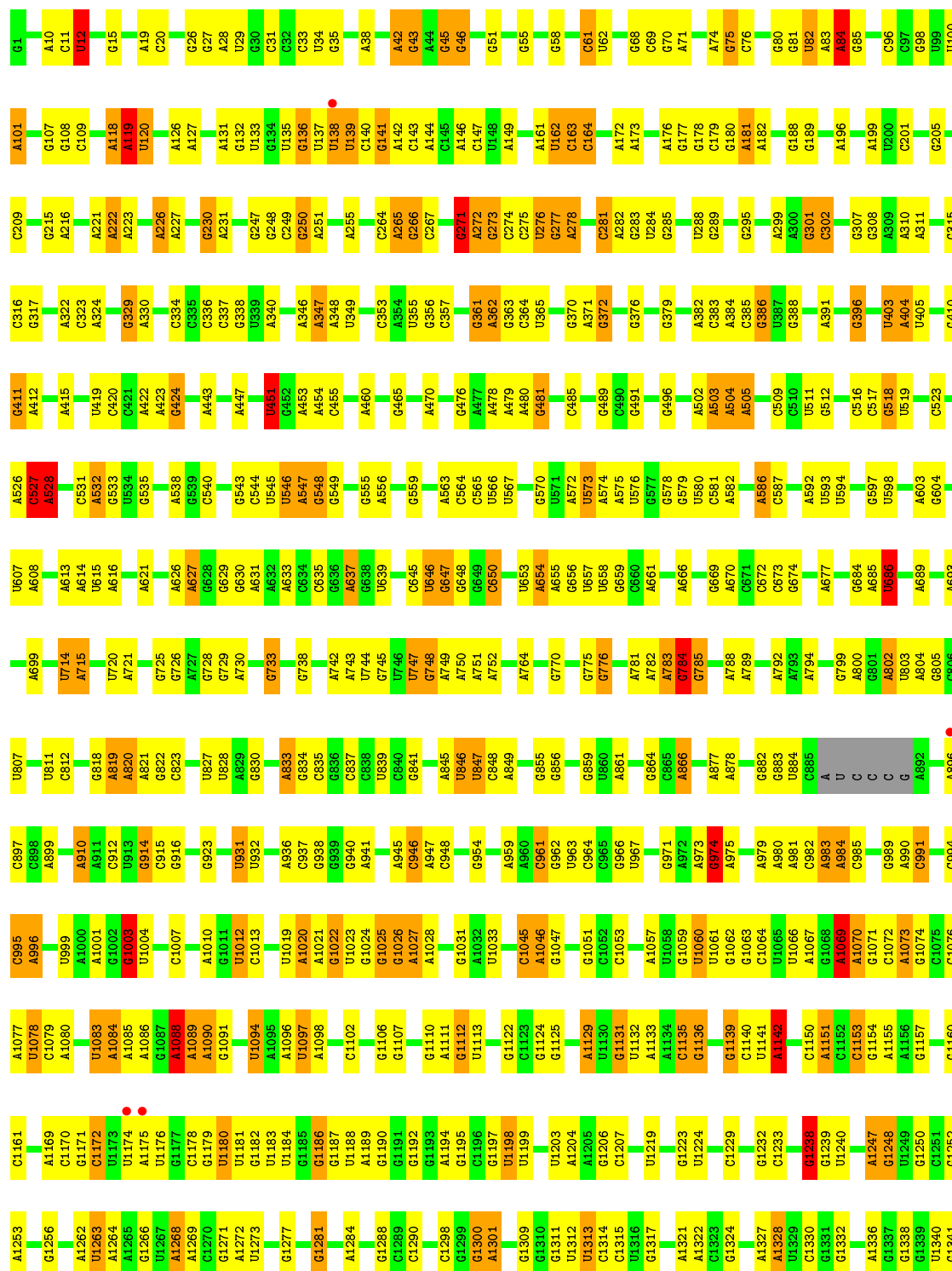


• Molecule 2: 50S ribosomal protein L2





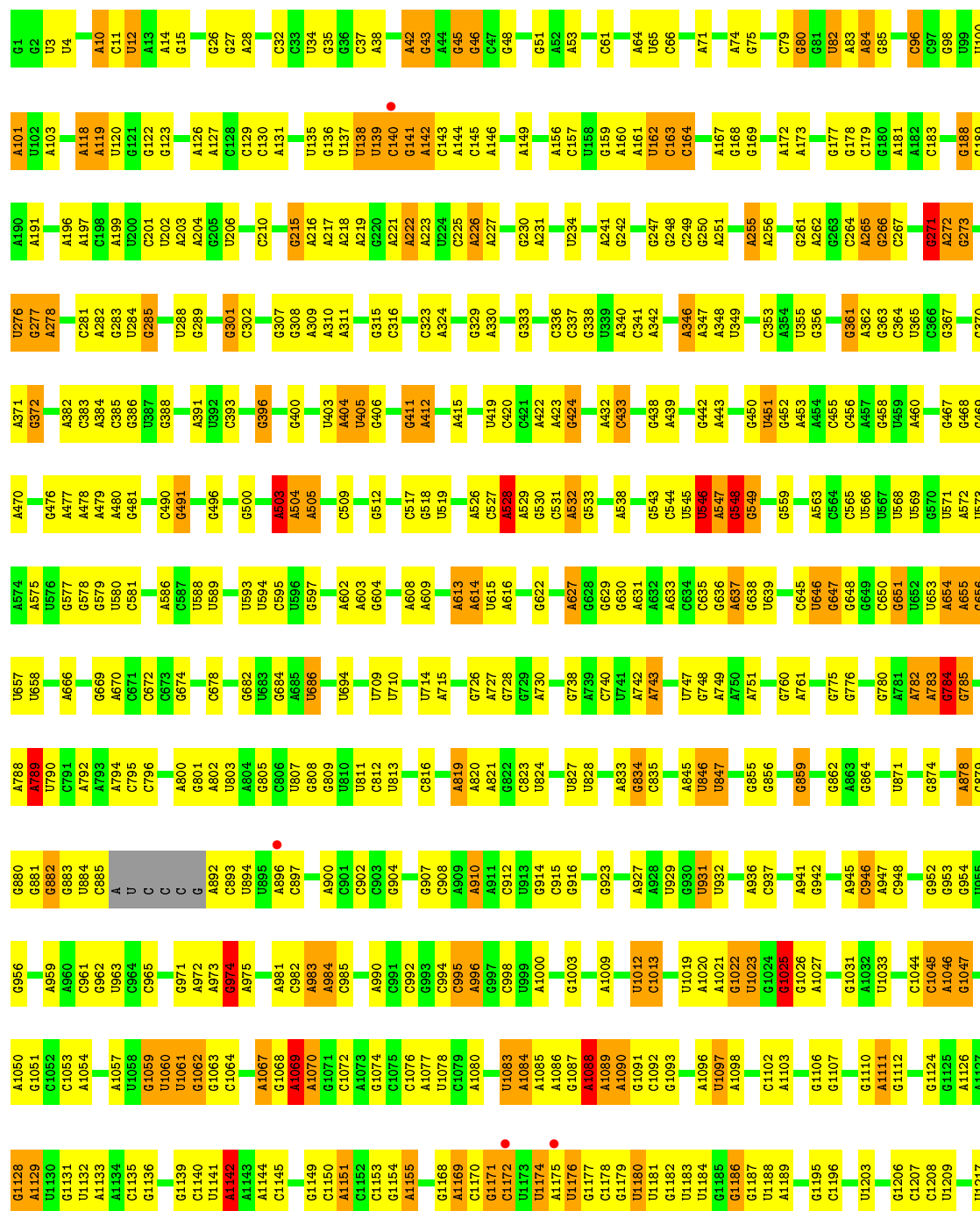
• Molecule 3: 23S rRNA



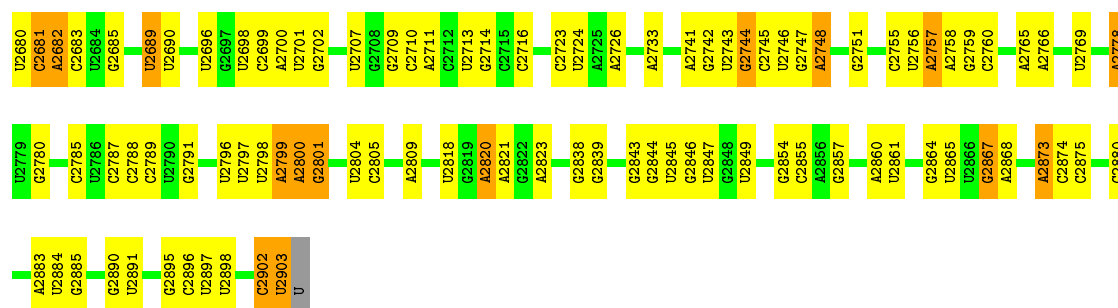




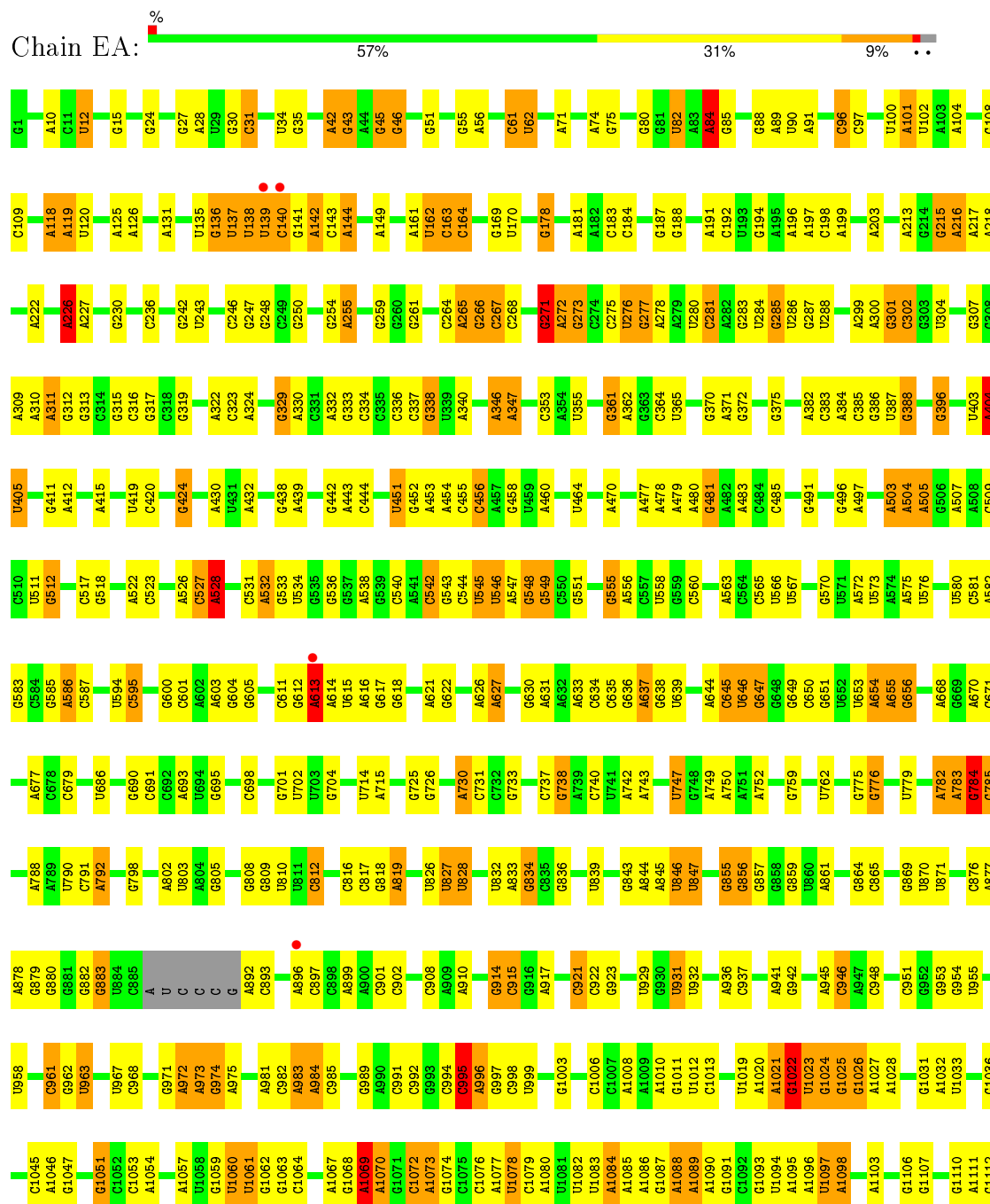
• Molecule 3: 23S rRNA



WORLDWIDE
PDB
PROTEIN DATA BANK



• Molecule 3: 23S rRNA

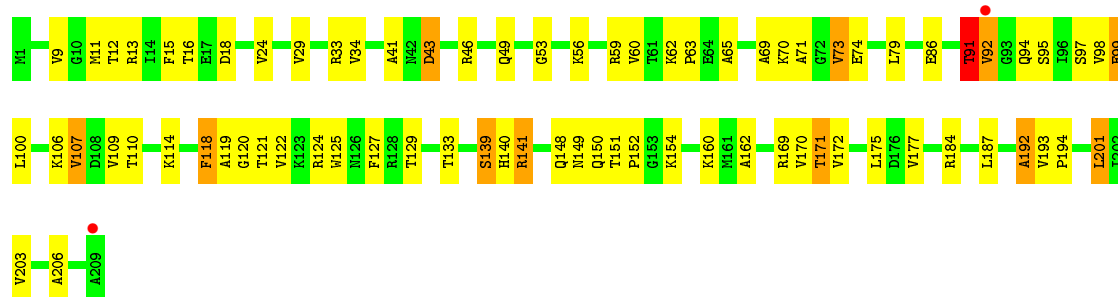


A2542	U2441	G2351	A2270	U	G	G2027	U1988	A1791	A1665	U1559	G1435	U1316	U1222	U119
G2543	G2446	A2352	G2271	A	U	A2030	G1906	A1794	G1666	G1569	G1436	G1317	G1223	G1125
G2544	G2447	G2353	C2275	C	A	G2031	G1907	C1795	G1667	C1564	C1437	U1325	U1224	
G2545	A2448	G2354	G2276	A	G	A2032	A1913	G1799	A1668	C1565	U1438	A1327	A1226	
A2547	U2449	U2355	G2277	C	A	G2033	C1914	C1800	A1669	A1566	G1326	U1249	A1229	A1129
U2548	A2450	G2361	A2278	U	U	A2034	A1927	C1801	U1671	C1567	A1327	U1249	C1229	U1130
	A2451	G2362	G2279	A	A	A2035	A1928	A1802	G1674	G1568	G1332	G1238	G1238	G1132
C2551	G2455	A2366	U2280	U	G	G2036	A1929	C1806	C1675	A1569	U1340	A1247	U1238	U1133
U2554	A2459	G2367	G2281	U	U	G2037	G1930	G1807	C1676	U1578	G1341	A1247	A1247	A1133
G2557	U2460	A2368	A2183	U	G	G2038	G1931	A1808	A1677	A1579	G1341	U1249	U1249	G1135
C2558		G2369	G2284	G	G	U2040	C1934	U1808	A1678	G1451	G1350	U1249	U1249	G1136
U2561	G2470	G2373	G2285	G	G	A2042	G1935	U1811	U1688	C1582	C1351	G1250	G1250	
G2471	A2471	G2374	G2286	A	A	C2043	A1936	G1812	U1688	G1456	U1352	A1253	A1253	G1139
G2472	G2472	G2375	A2187	G	G	C2044	A1937	G1813	U1688	U1457	A1353	A1253	A1253	G1140
U2473	U2473	G2376	U2187	G	G	G2045	A1938	G1814	C1694	U1458	A1354	G1257	G1257	U1141
U2474		G2377	G2190	C	C	G2046	U1939	G1814	C1694	G1459	A1355	G1257	G1257	A1142
U2475	U2474	A2378	G2191	U	U	G2047	U1940	A1815	A1700	U1468	G1356	A1144	A1144	A1143
G2476	G2475	U2379	U2194	U	U	A2048	U1941	C1816	U1712	U1468	C1357	A1260	A1260	A1144
A2477	C2195	G2381	U2195	U	U	G2049	U1942	G1817	U1712	U1474	G1360	A1261	A1261	G1149
A2478	U2196	G2382	C2054	U	A	C2050	U1943	U1818	A1714	G1475	G1360	A1262	A1262	G1150
	U2197	G2383	C2055	U	A	G2051	U1944	U1818	A1714	G1475	G1360	A1263	A1263	G1150
G2481	A2198	G2384	G2056	U	A	G2052	G1959	G1823	G1715	A1603	G1364	U1263	U1263	A1151
A2482	A2199	G2385	G2057	U	A	G2053	G1960	G1824	G1715	C1604	G1364	U1263	U1263	A1151
G2483	C2200	G2386	G2058	U	U	G2054	G1961	G1824	G1715	C1604	G1364	U1263	U1263	A1151
G2484	G2204	G2387	A2060	U	U	G2055	G1962	U1827	G1723	C1606	G1364	U1263	U1263	A1151
U2491	U2210	G2388	G2061	U	U	G2056	G1963	G1828	C1727	C1607	G1364	U1263	U1263	A1151
G2499	A2211	G2389	C2062	U	U	G2057	A1964	G1829	C1727	U1485	G1364	U1263	U1263	A1151
U2500	A2212	G2390	C2063	U	U	G2058	A1965	U1830	C1728	U1486	G1364	U1263	U1263	A1151
C2501	G2213	G2391	C2064	U	U	G2059	G1966	G1831	C1729	U1487	G1364	U1263	U1263	A1151
G2502	C2214	G2392	G2065	U	U	G2060	G1967	G1832	C1730	C1493	G1376	C1270	C1270	G1157
A2503	G2215	G2393	A2071	U	U	G2061	G1968	G1833	C1731	A1494	C1377	C1271	C1271	C1158
U2504	C2216	G2394	G2072	U	U	G2062	A1969	G1834	C1732	A1495	C1377	C1271	C1271	C1158
G2505	A2225	G2395	G2073	U	U	G2063	U1971	G1835	C1733	G1613	C1377	C1271	C1271	C1158
U2506	C2226	G2396	G2074	U	U	G2064	G1972	C1843	C1733	A1504	C1377	C1271	C1271	C1158
C2507	G2227	G2397	U2075	U	U	G2065	G1973	A1847	C1733	A1504	C1377	C1271	C1271	C1158
U2511	G2228	G2398	U2076	U	U	G2066	G1974	A1848	C1733	A1504	C1377	C1271	C1271	C1158
U2512	G2229	G2399	U2077	U	U	G2067	G1975	A1849	C1733	A1504	C1377	C1271	C1271	C1158
U2513	G2230	G2400	A2077	U	U	G2068	G1976	A1853	C1733	A1504	C1377	C1271	C1271	C1158
U2514	G2231	G2401	G2078	U	U	G2069	G1977	A1854	C1733	A1504	C1377	C1271	C1271	C1158
U2515	G2232	G2402	G2079	U	U	G2070	G1978	A1855	C1733	A1504	C1377	C1271	C1271	C1158
U2516	G2233	G2403	U2080	U	U	G2071	G1979	A1856	C1733	A1504	C1377	C1271	C1271	C1158
U2517	G2234	G2404	U2081	U	U	G2072	G1980	A1857	C1733	A1504	C1377	C1271	C1271	C1158
U2518	G2235	G2405	U2082	U	U	G2073	G1981	A1858	C1733	A1504	C1377	C1271	C1271	C1158
U2519	G2236	G2406	U2083	U	U	G2074	G1982	A1859	C1733	A1504	C1377	C1271	C1271	C1158
U2520	G2237	G2407	U2084	U	U	G2075	G1983	A1860	C1733	A1504	C1377	C1271	C1271	C1158
U2521	G2238	G2408	U2085	U	U	G2076	G1984	A1861	C1733	A1504	C1377	C1271	C1271	C1158
U2522	G2239	G2409	U2086	U	U	G2077	G1985	A1862	C1733	A1504	C1377	C1271	C1271	C1158
U2523	G2240	G2410	U2087	U	U	G2078	G1986	A1863	C1733	A1504	C1377	C1271	C1271	C1158
U2524	G2241	G2411	U2088	U	U	G2079	G1987	A1864	C1733	A1504	C1377	C1271	C1271	C1158
U2525	G2242	G2412	U2089	U	U	G2080	G1988	A1865	C1733	A1504	C1377	C1271	C1271	C1158
U2526	G2243	G2413	U2090	U	U	G2081	G1989	A1866	C1733	A1504	C1377	C1271	C1271	C1158
U2527	G2244	G2414	U2091	U	U	G2082	G1990	A1867	C1733	A1504	C1377	C1271	C1271	C1158
U2528	G2245	G2415	U2092	U	U	G2083	G1991	A1868	C1733	A1504	C1377	C1271	C1271	C1158
U2529	G2246	G2416	U2093	U	U	G2084	G1992	A1869	C1733	A1504	C1377	C1271	C1271	C1158
U2530	G2247	G2417	U2094	U	U	G2085	G1993	A1870	C1733	A1504	C1377	C1271	C1271	C1158
U2531	G2248	G2418	U2095	U	U	G2086	G1994	A1871	C1733	A1504	C1377	C1271	C1271	C1158
U2532	G2249	G2419	U2096	U	U	G2087	G1995	A1872	C1733	A1504	C1377	C1271	C1271	C1158
U2533	G2250	G2420	U2097	U	U	G2088	G1996	A1873	C1733	A1504	C1377	C1271	C1271	C1158
U2534	G2251	G2421	U2098	U	U	G2089	G1997	A1874	C1733	A1504	C1377	C1271	C1271	C1158
U2535	G2252	G2422	U2099	U	U	G2090	G1998	A1875	C1733	A1504	C1377	C1271	C1271	C1158
U2536	G2253	G2423	U2100	U	U	G2091	G1999	A1876	C1733	A1504	C1377	C1271	C1271	C1158
U2537	G2254	G2424	U2101	U	U	G2092	G2005	A1877	C1733	A1504	C1377	C1271	C1271	C1158
U2538	G2255	G2425	U2102	U	U	G2093	A2013	A1878	C1733	A1504	C1377	C1271	C1271	C1158
U2539	G2256	G2426	U2103	U	U	G2094	U2016	G1879	C1733	A1504	C1377	C1271	C1271	C1158
U2540	G2257	G2427	U2104	U	U	G2095	U2017	A1880	C1733	A1504	C1377	C1271	C1271	C1158
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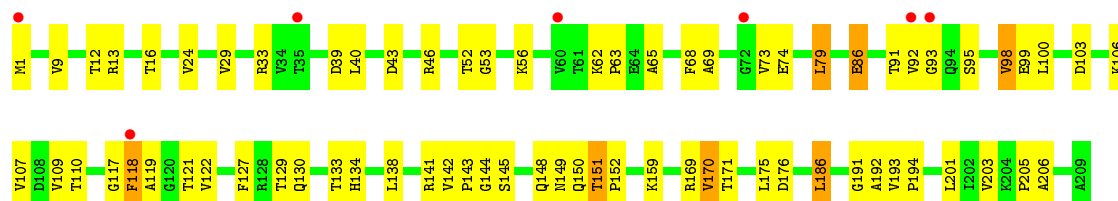


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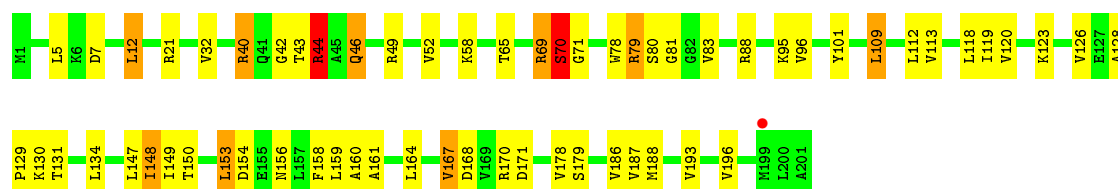




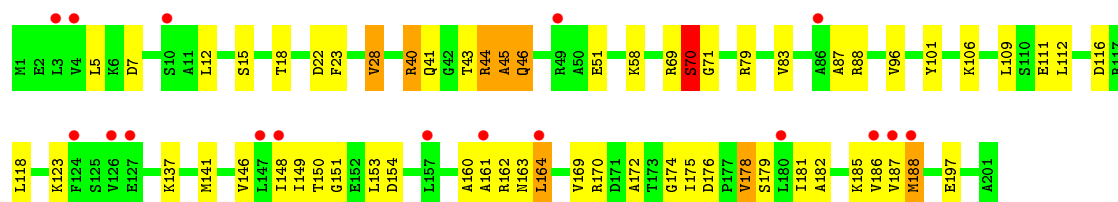
- Molecule 4: 50S ribosomal protein L3



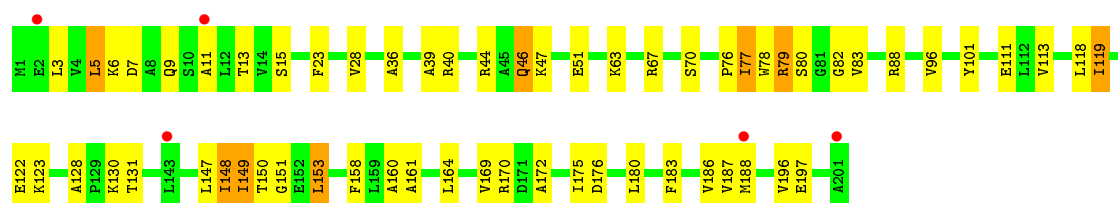
- Molecule 5: 50S ribosomal protein L4



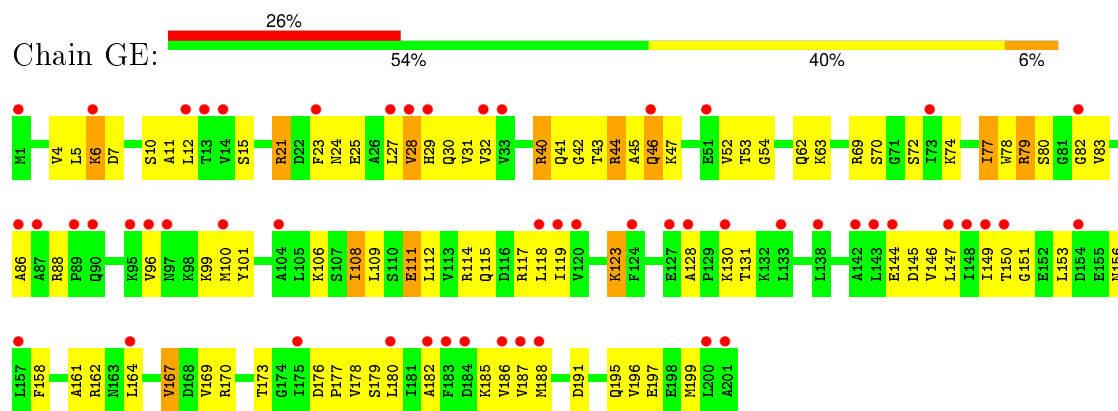
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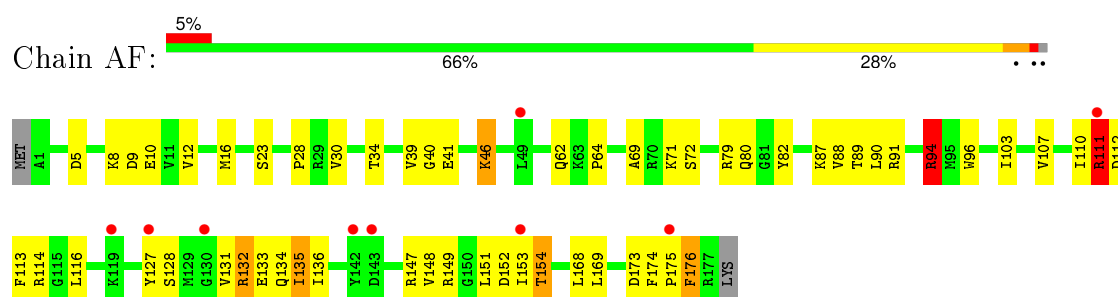
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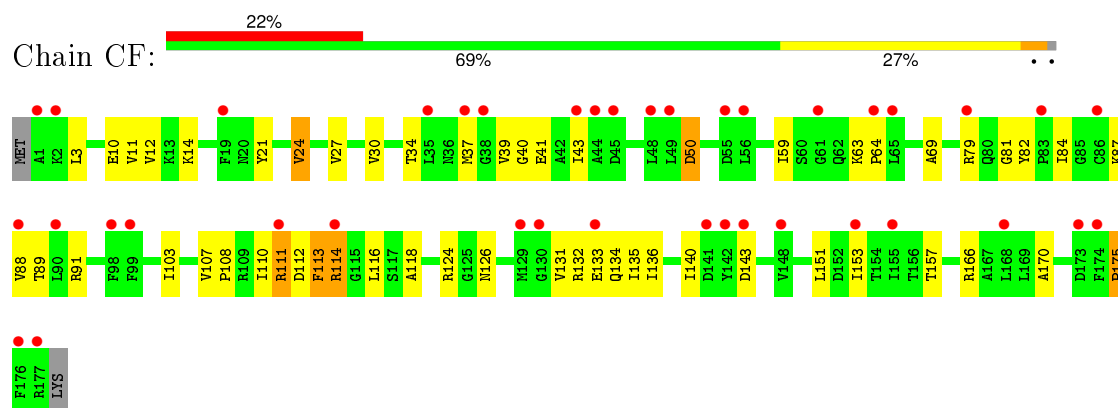
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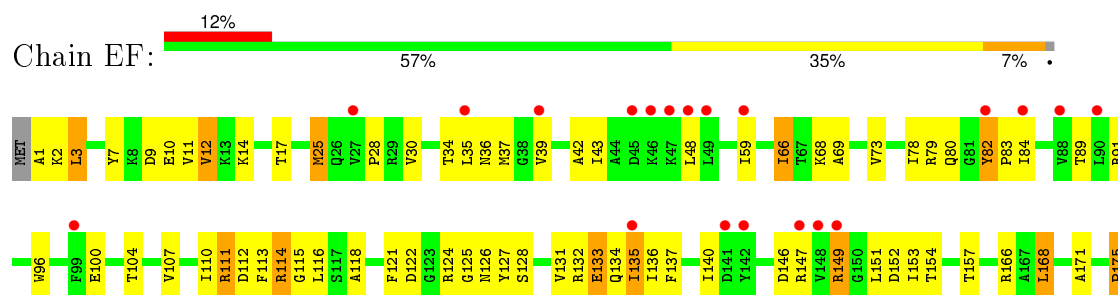
- Molecule 6: 50S ribosomal protein L5



- Molecule 6: 50S ribosomal protein L5

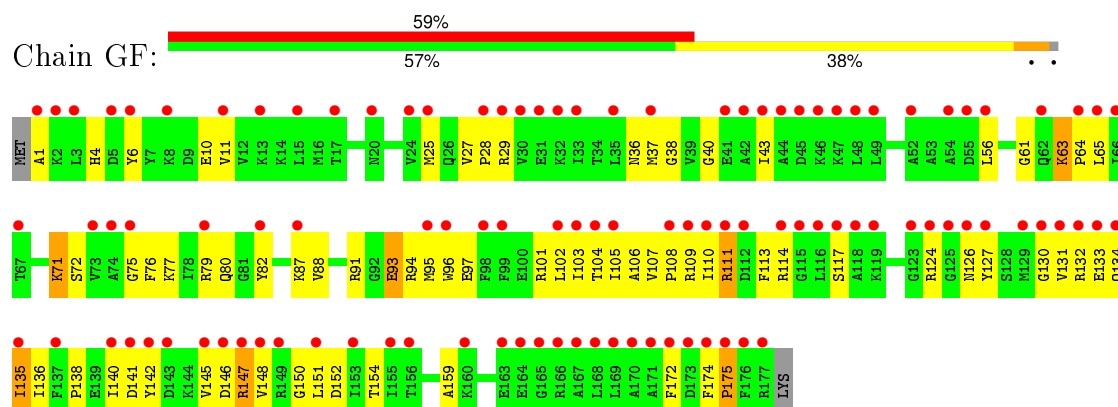


- Molecule 6: 50S ribosomal protein L5

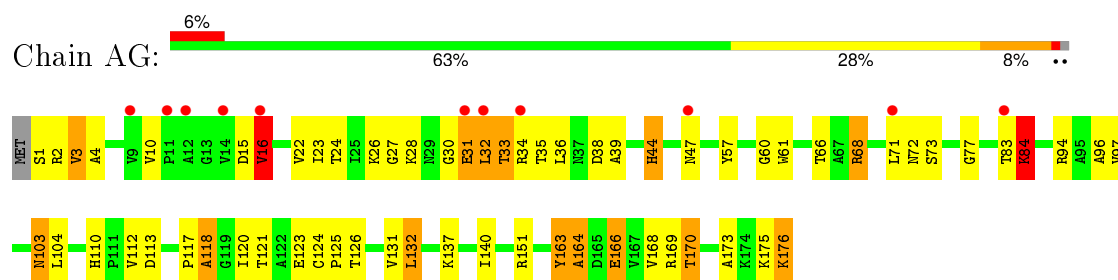




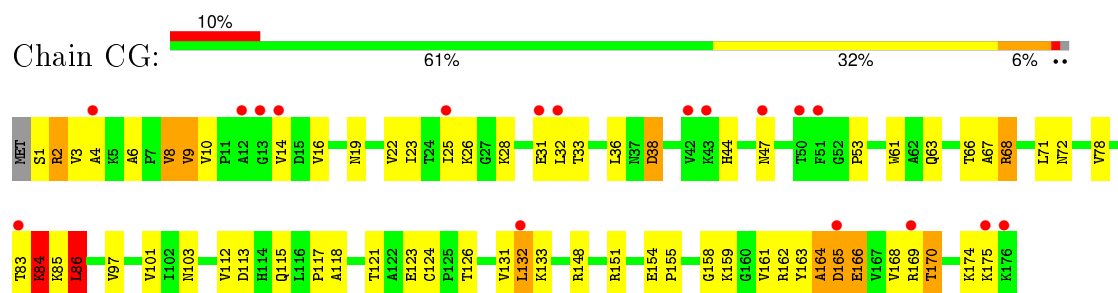
- Molecule 6: 50S ribosomal protein L5



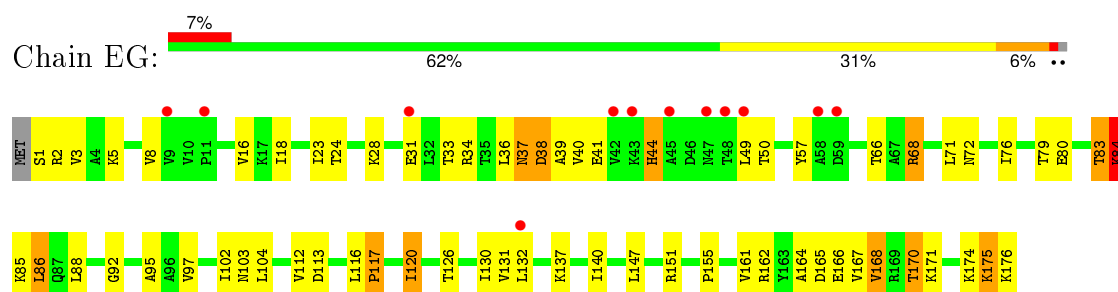
- Molecule 7: 50S ribosomal protein L6



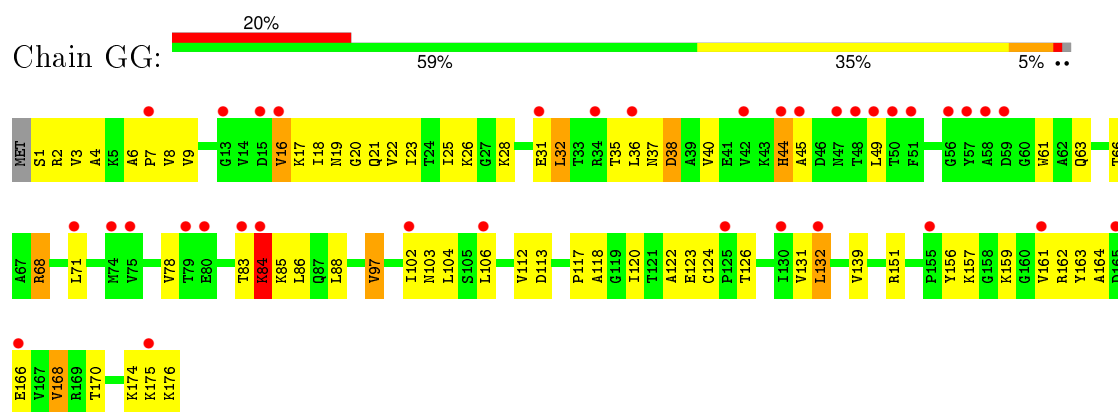
- Molecule 7: 50S ribosomal protein L6



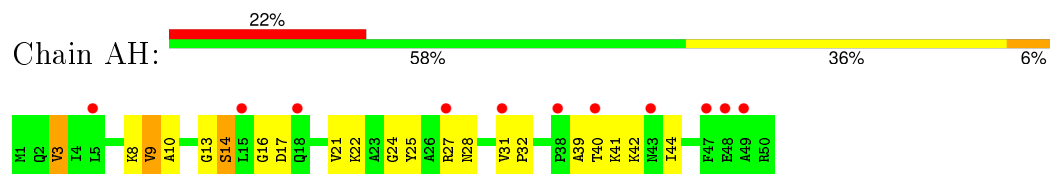
- Molecule 7: 50S ribosomal protein L6



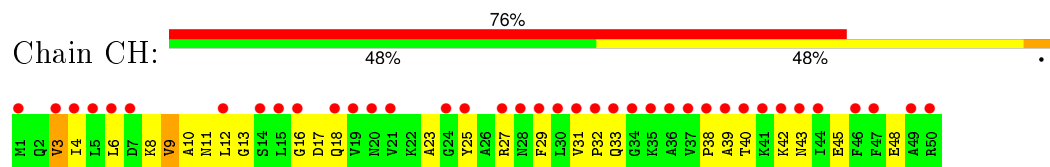
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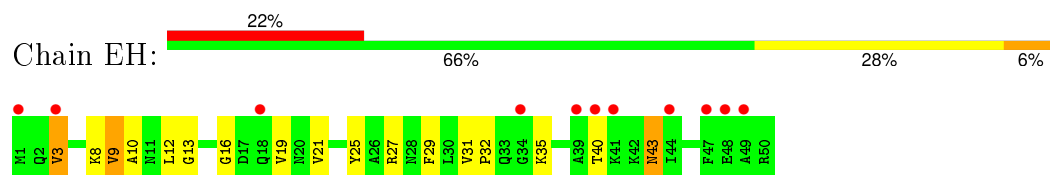
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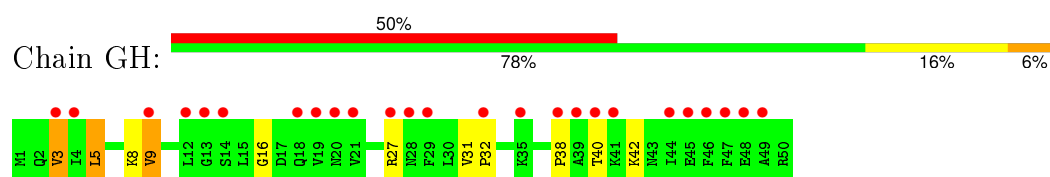
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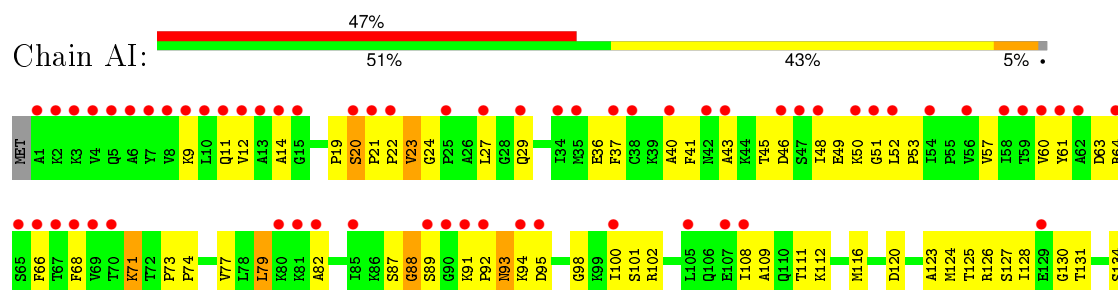
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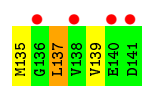


- Molecule 8: 50S ribosomal protein L9

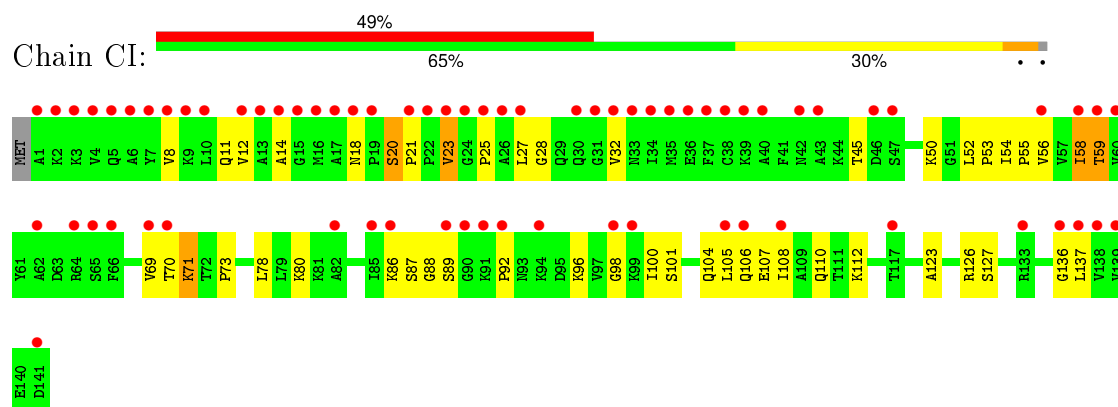


- Molecule 9: 50S ribosomal protein L11

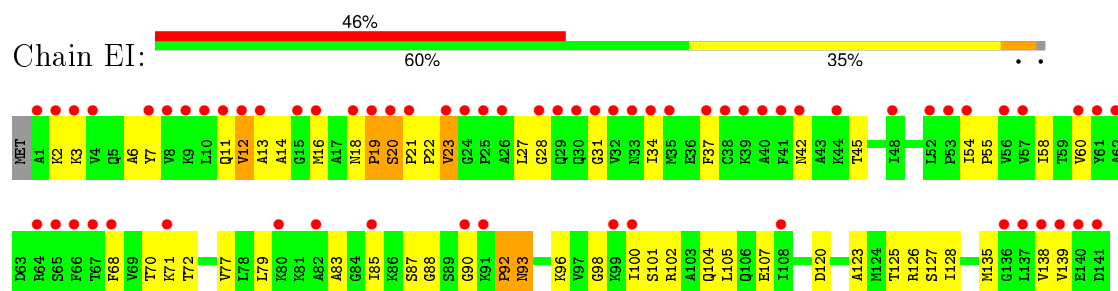




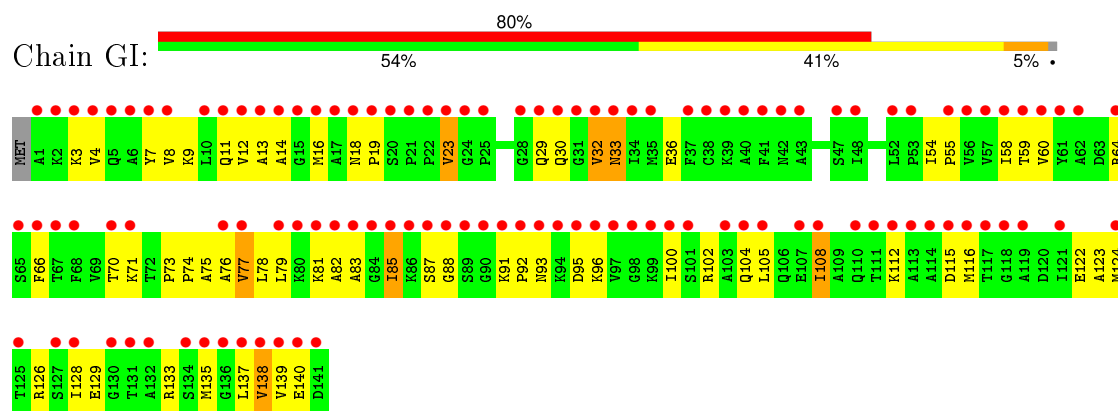
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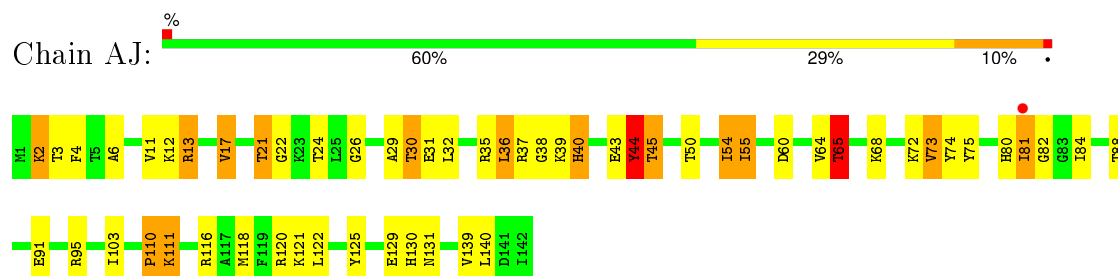
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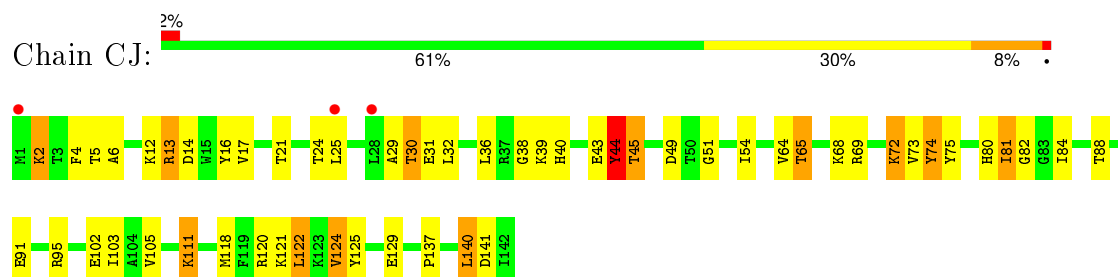
• Molecule 9: 50S ribosomal protein L11



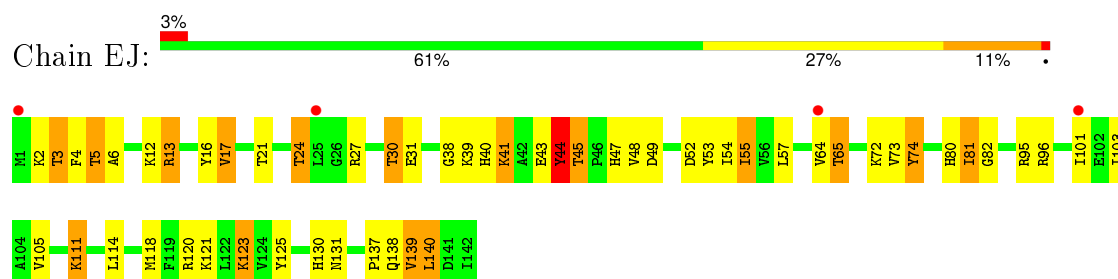
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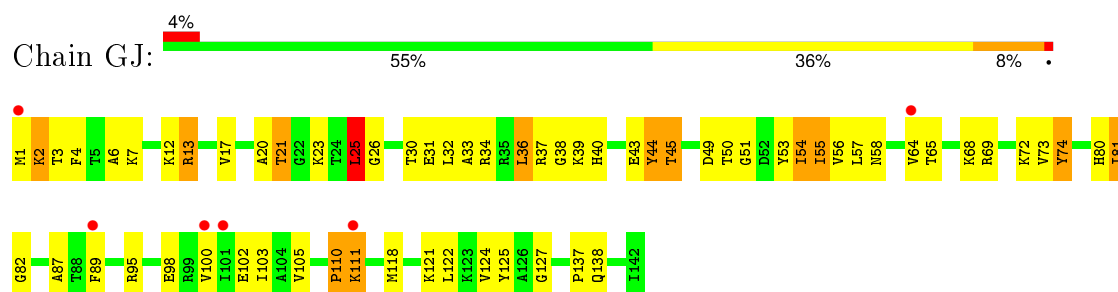
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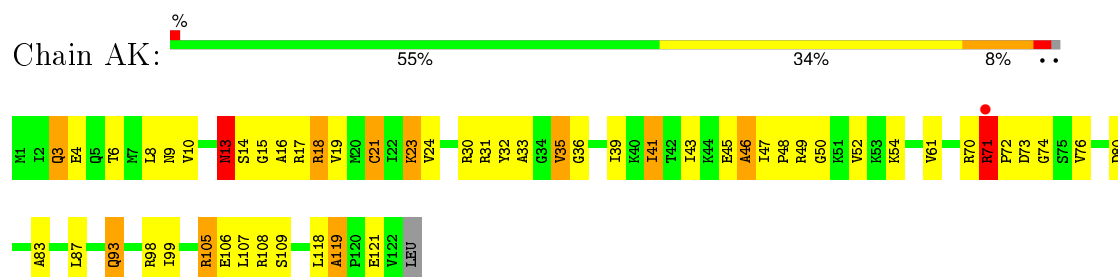
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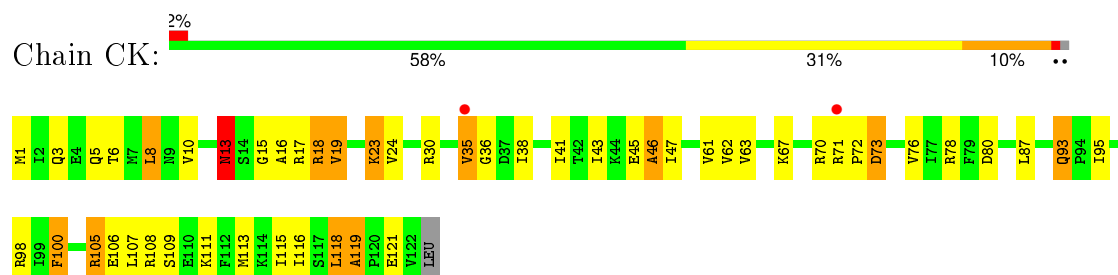
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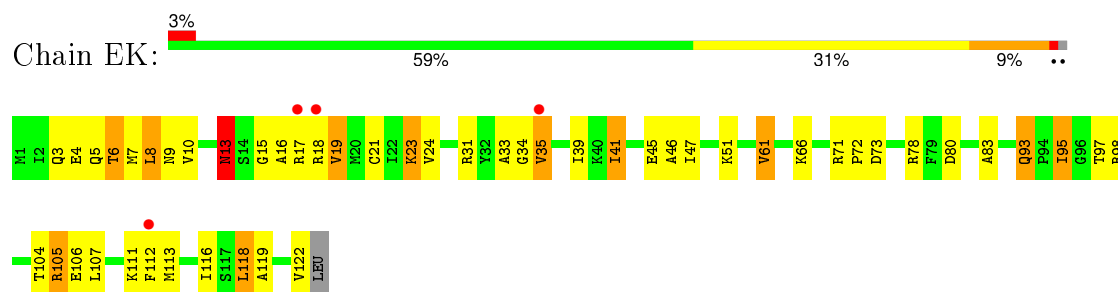
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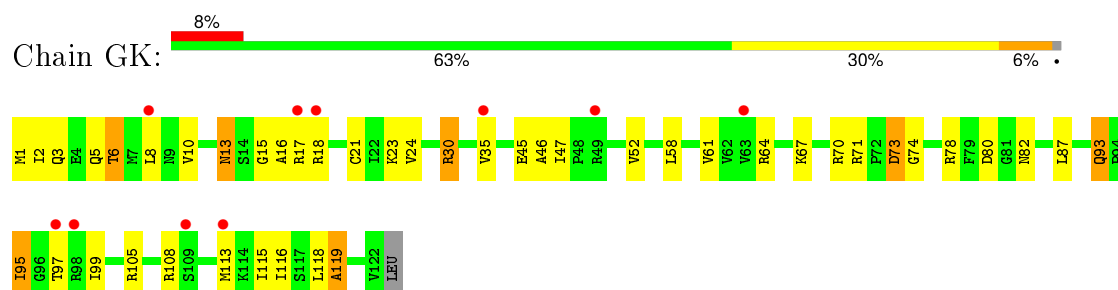
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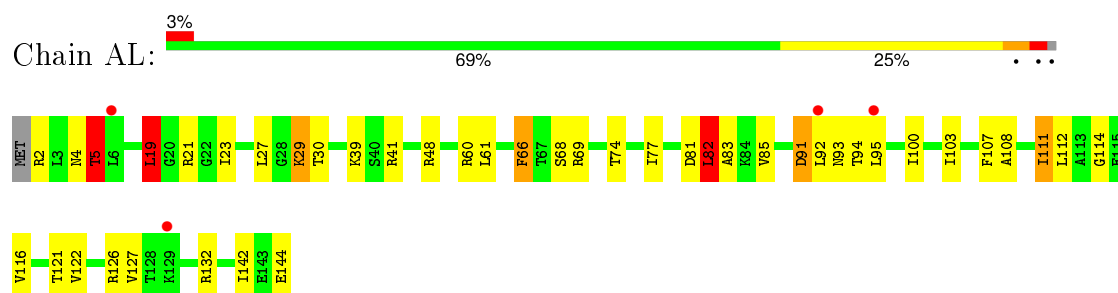
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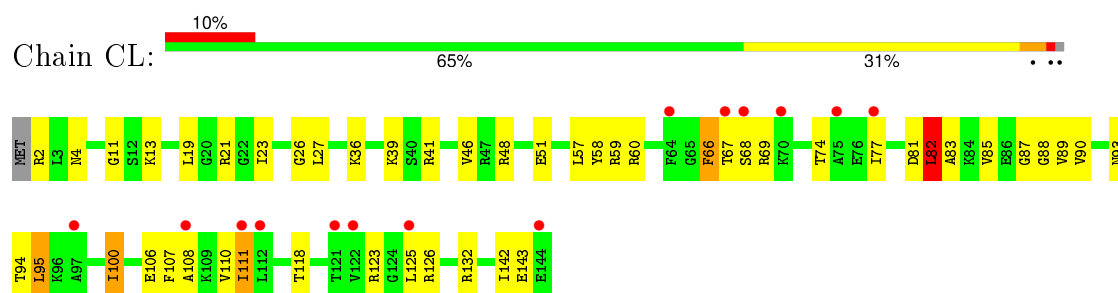
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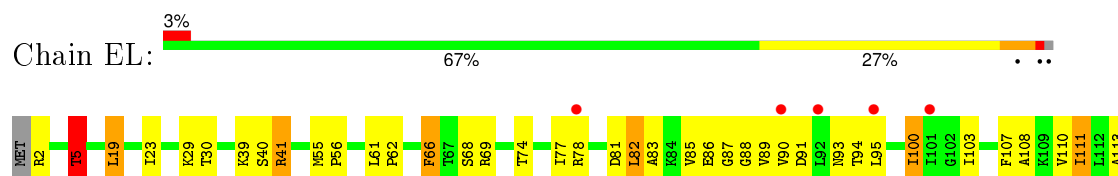
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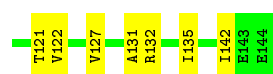


- Molecule 12: 50S ribosomal protein L15

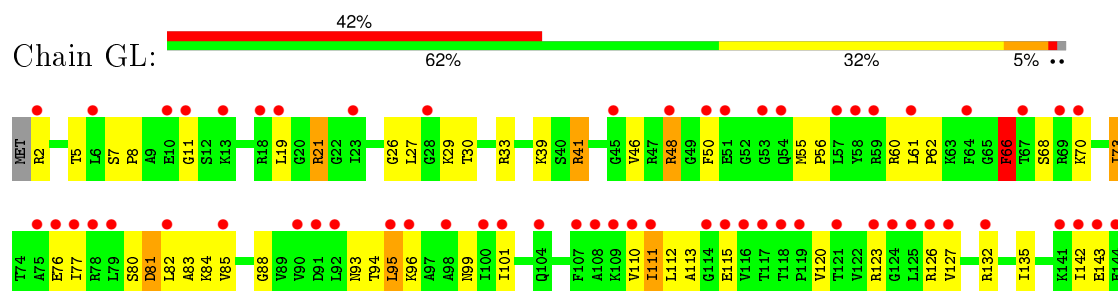


- Molecule 12: 50S ribosomal protein L15

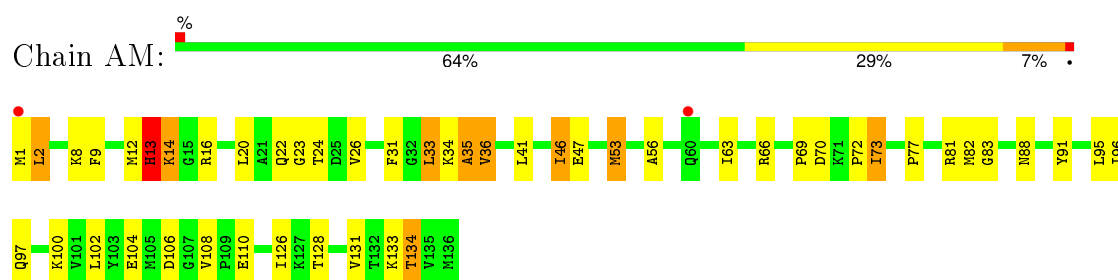




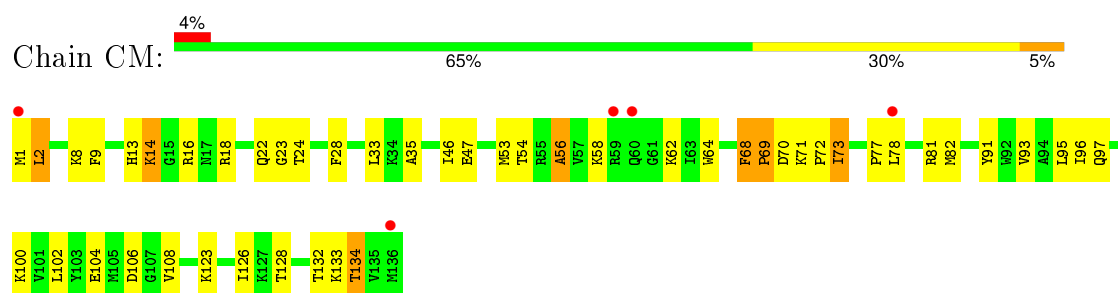
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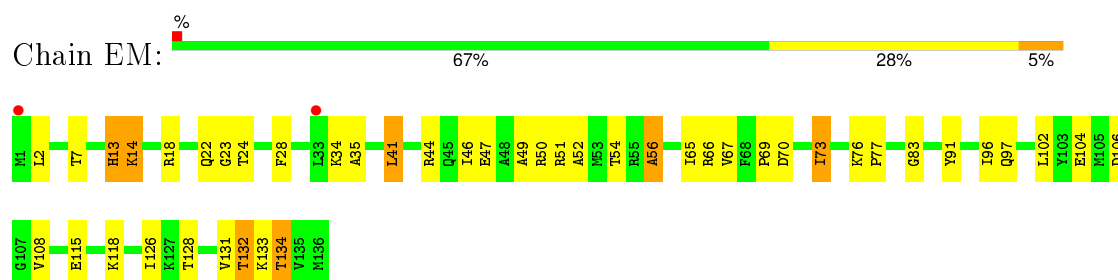
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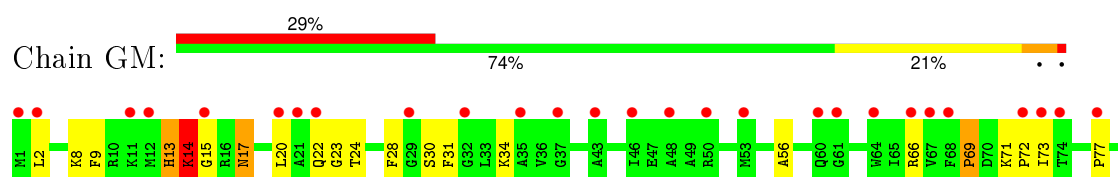
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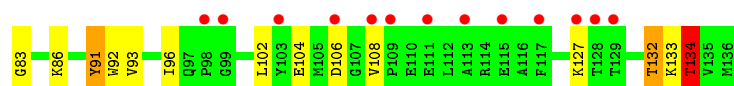


• Molecule 13: 50S ribosomal protein L16

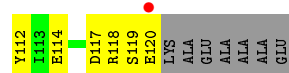
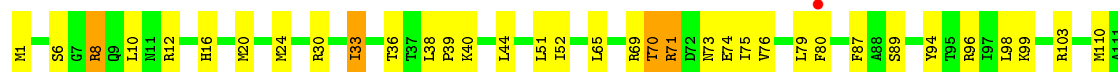


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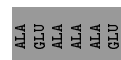
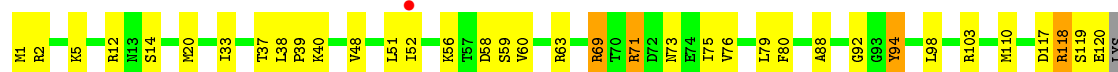




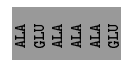
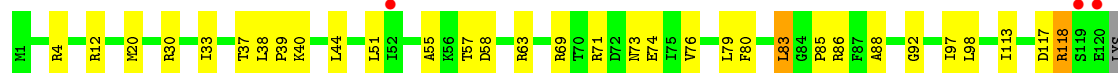
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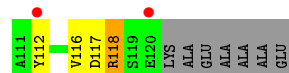
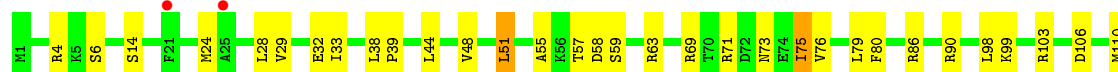
- Molecule 14: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L17

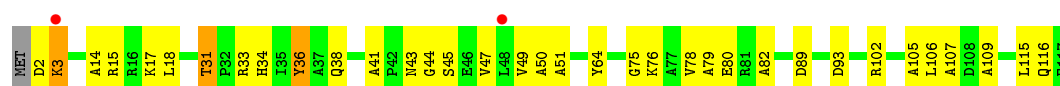


- Molecule 14: 50S ribosomal protein L17

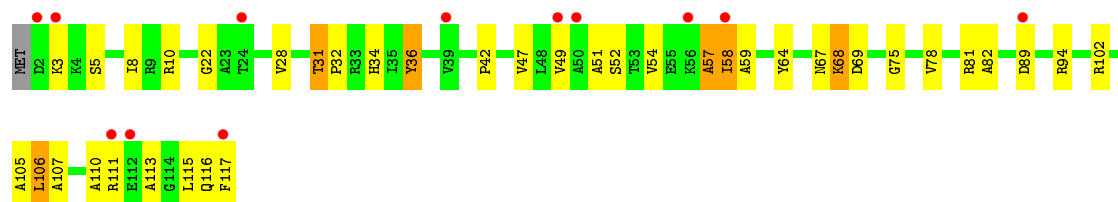


- Molecule 15: 50S ribosomal protein L18

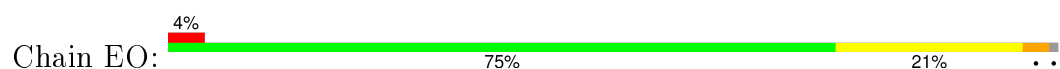




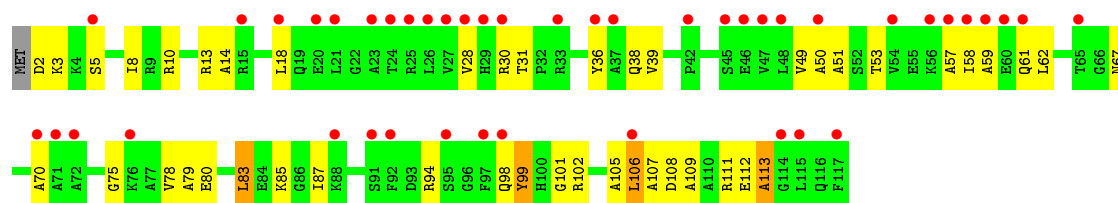
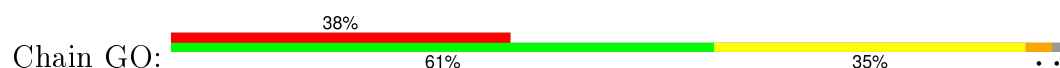
- Molecule 15: 50S ribosomal protein L18



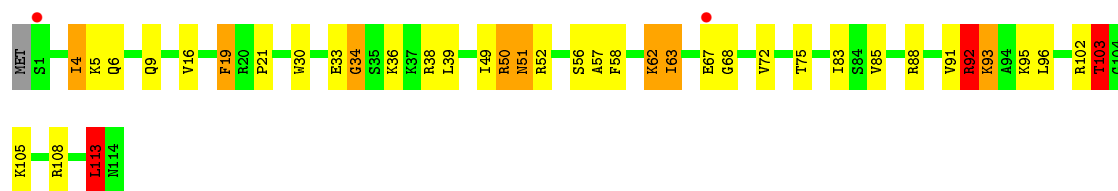
- Molecule 15: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19

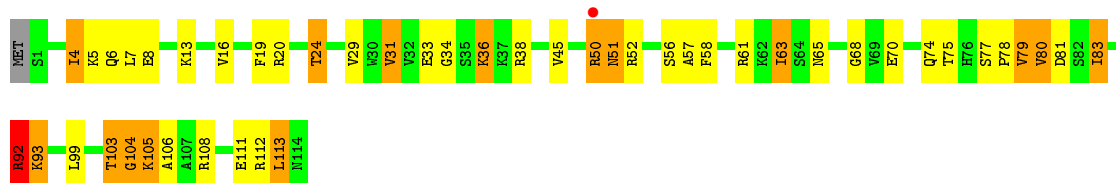


- Molecule 16: 50S ribosomal protein L19

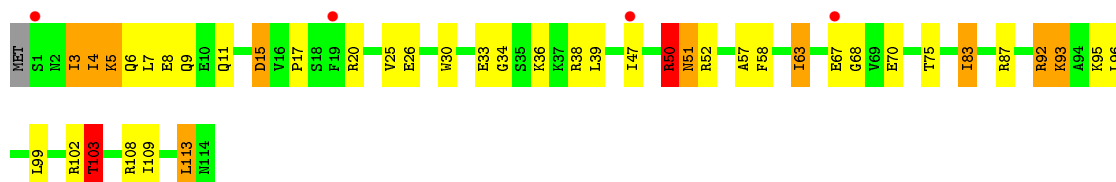




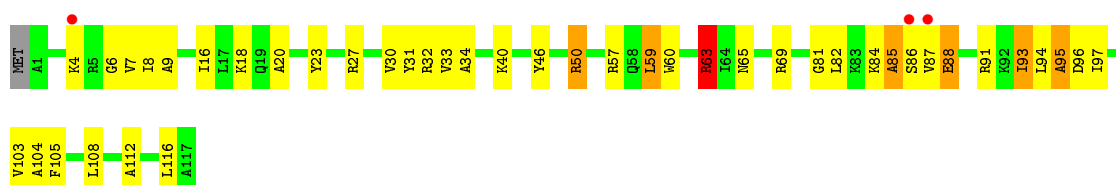
- Molecule 16: 50S ribosomal protein L19



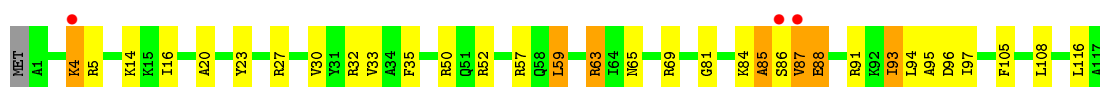
- Molecule 16: 50S ribosomal protein L19



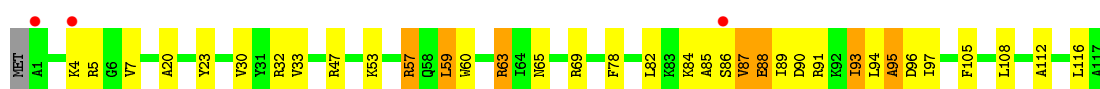
- Molecule 17: 50S ribosomal protein L20



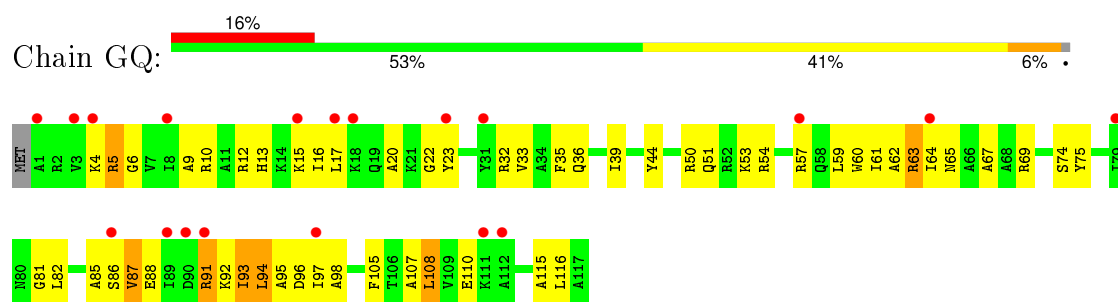
- Molecule 17: 50S ribosomal protein L20



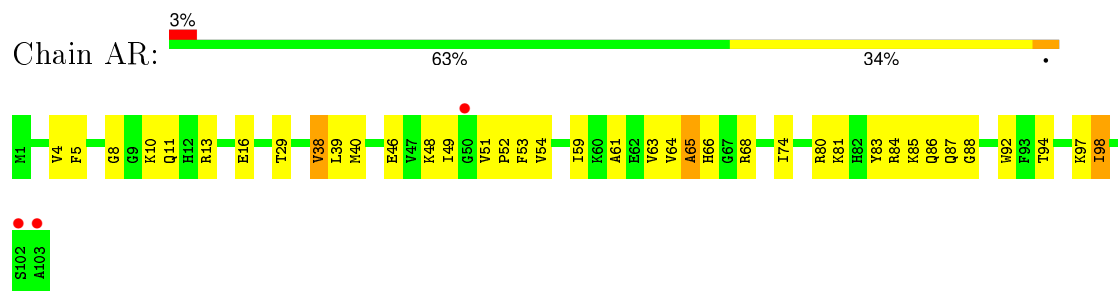
- Molecule 17: 50S ribosomal protein L20



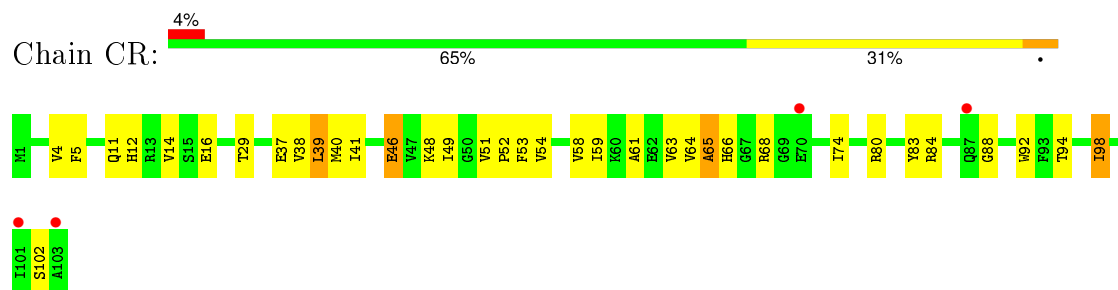
- Molecule 17: 50S ribosomal protein L20



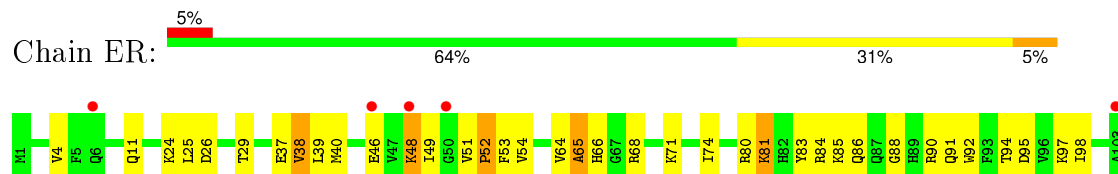
- Molecule 18: 50S ribosomal protein L21



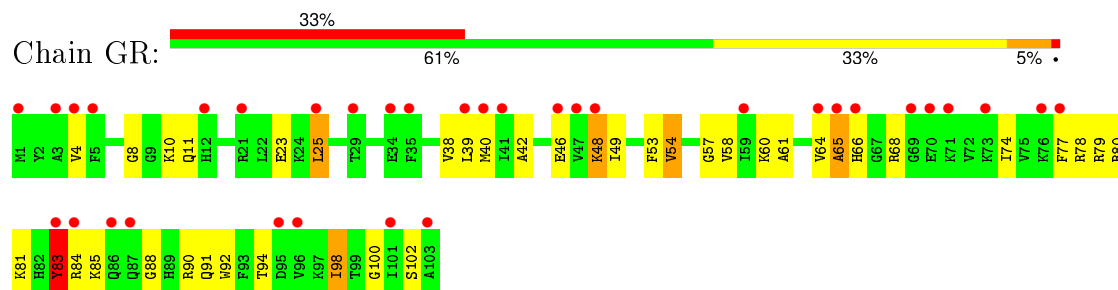
- Molecule 18: 50S ribosomal protein L21



- Molecule 18: 50S ribosomal protein L21

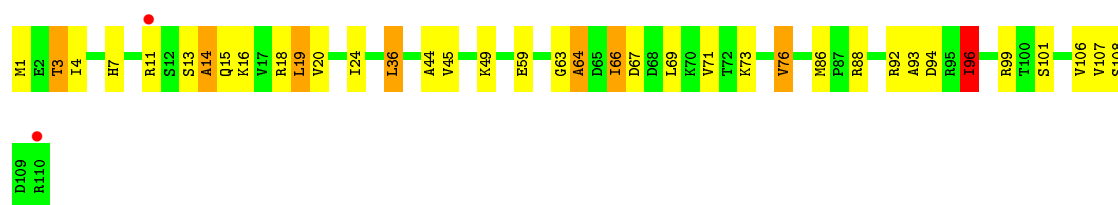


- Molecule 18: 50S ribosomal protein L21

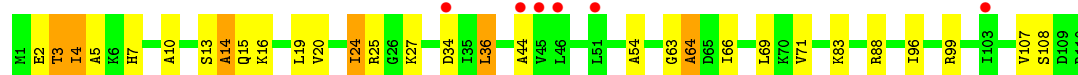
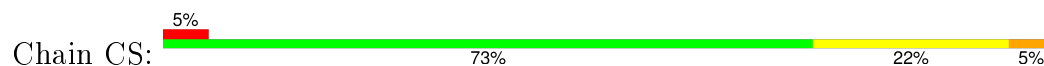


- Molecule 19: 50S ribosomal protein L22

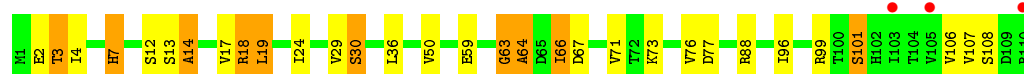
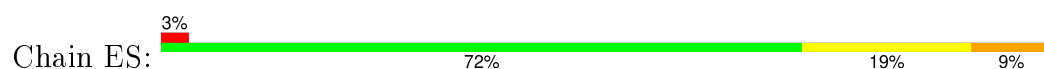




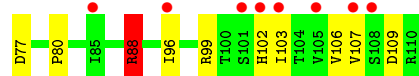
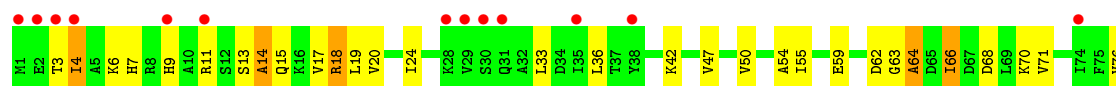
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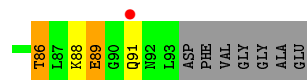
- Molecule 19: 50S ribosomal protein L22



- Molecule 19: 50S ribosomal protein L22

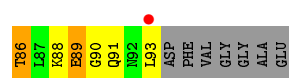


- Molecule 20: 50S ribosomal protein L23

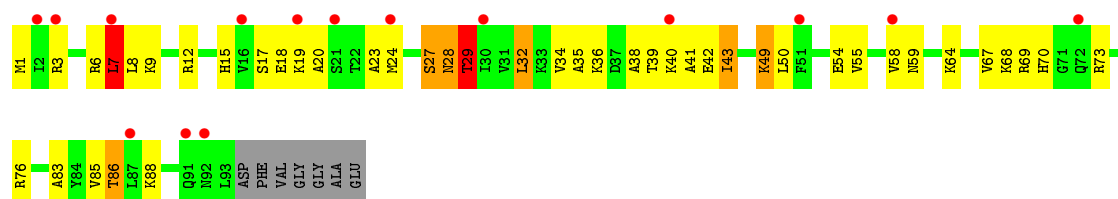


- Molecule 20: 50S ribosomal protein L23

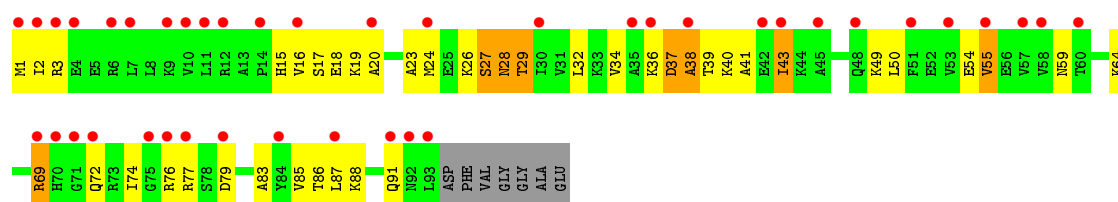
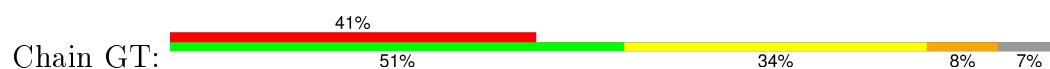




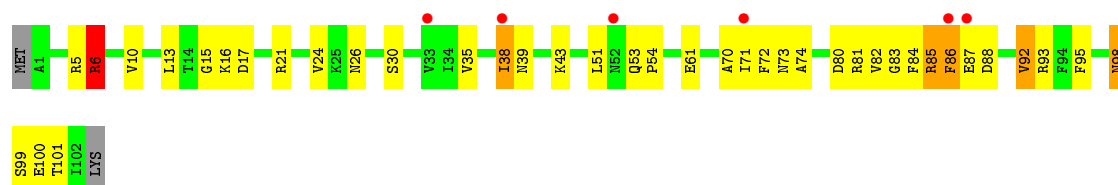
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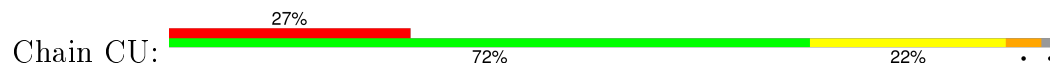
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- Molecule 21: 50S ribosomal protein L24

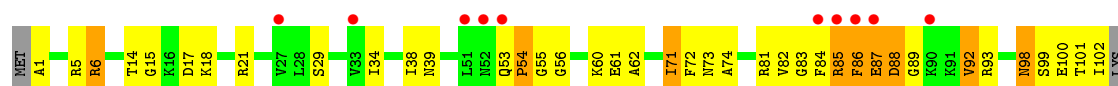


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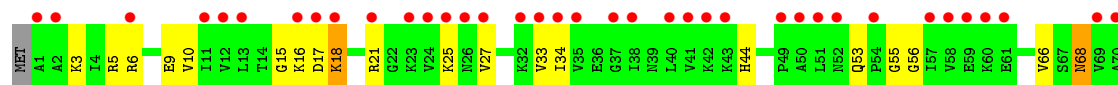


- Molecule 21: 50S ribosomal protein L24

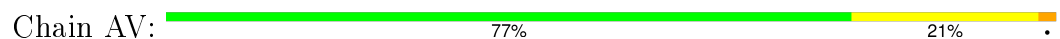




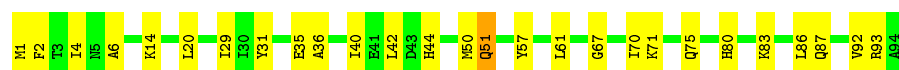
- Molecule 21: 50S ribosomal protein L24



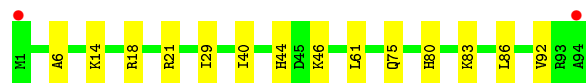
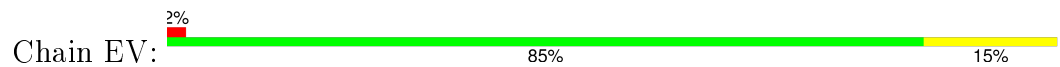
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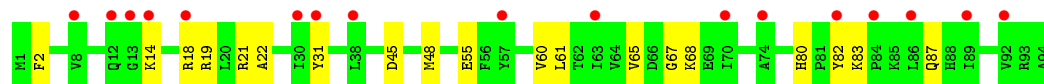
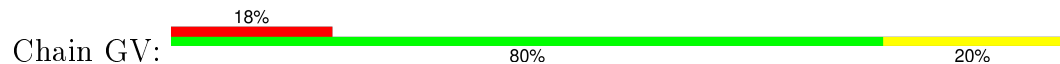
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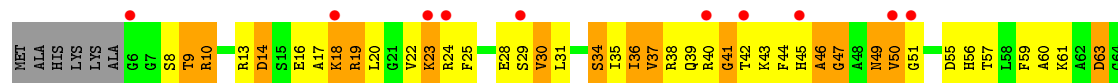
- Molecule 22: 50S ribosomal protein L25



- Molecule 22: 50S ribosomal protein L25

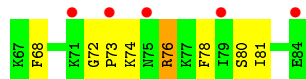
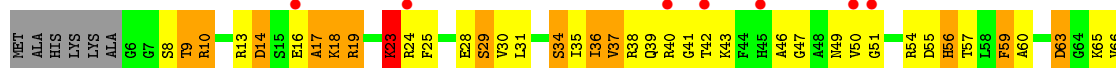


- Molecule 23: 50S ribosomal protein L27

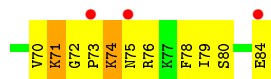
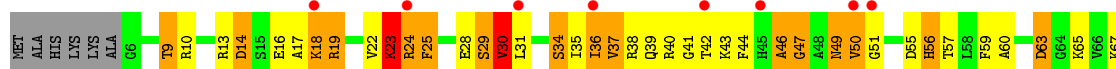




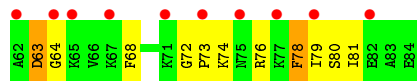
- Molecule 23: 50S ribosomal protein L27



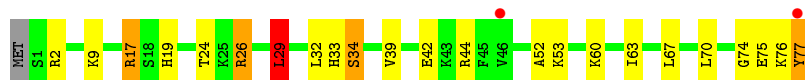
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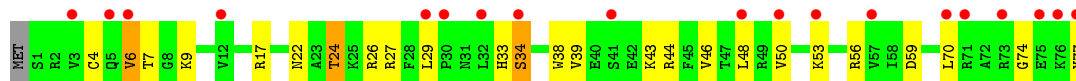
- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28

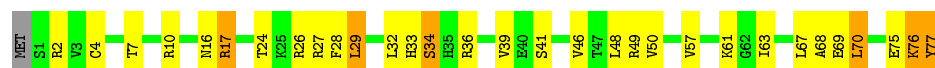


- Molecule 24: 50S ribosomal protein L28



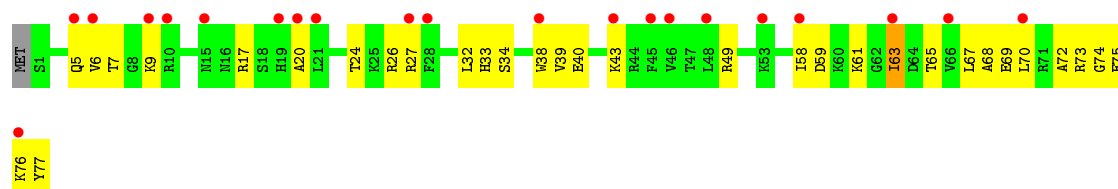
- Molecule 24: 50S ribosomal protein L28

Chain EX: 



- Molecule 24: 50S ribosomal protein L28

Chain GX: 




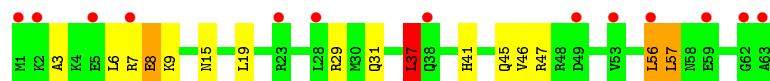
- Molecule 25: 50S ribosomal protein L29

Chain AY: 



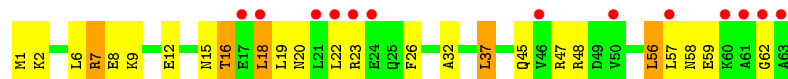
- Molecule 25: 50S ribosomal protein L29

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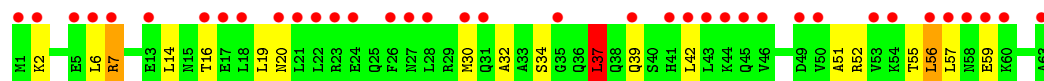
- Molecule 25: 50S ribosomal protein L29

Chain EY: 



- Molecule 25: 50S ribosomal protein L29

Chain GY: 

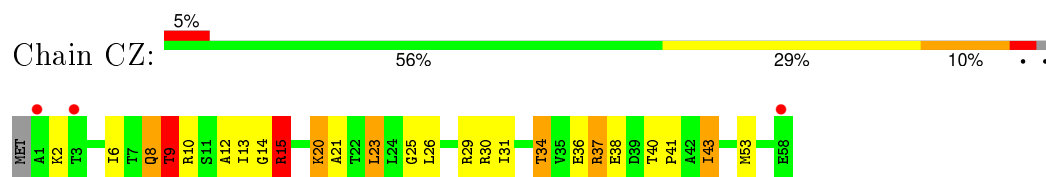


- Molecule 26: 50S ribosomal protein L30

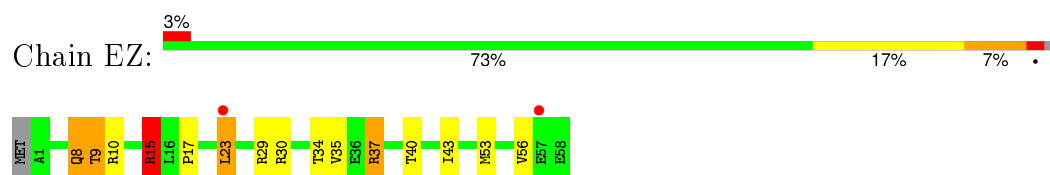
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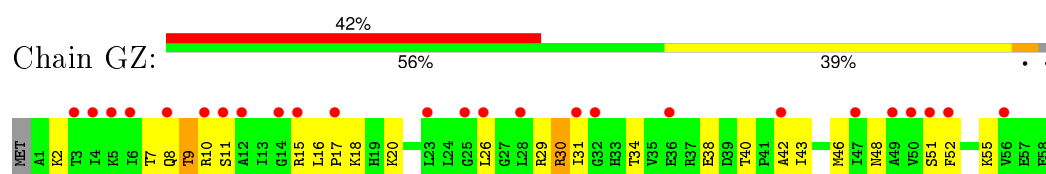
- Molecule 26: 50S ribosomal protein L30



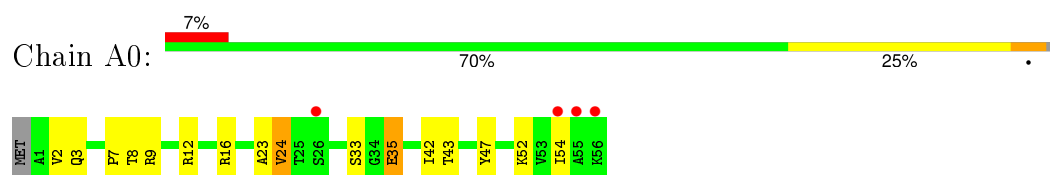
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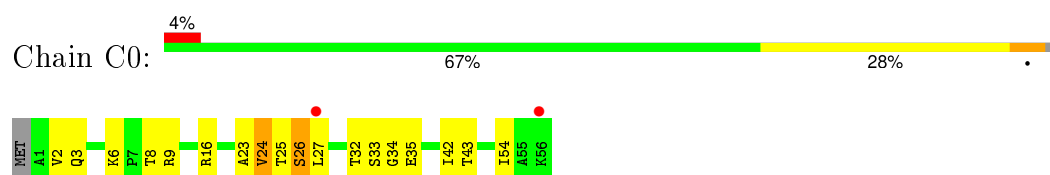
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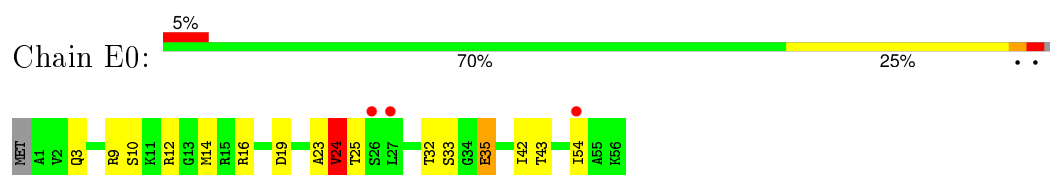
- Molecule 27: 50S ribosomal protein L32



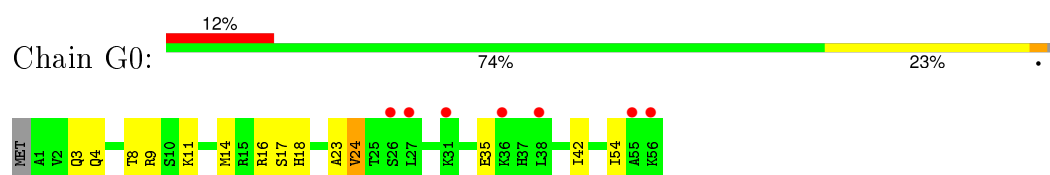
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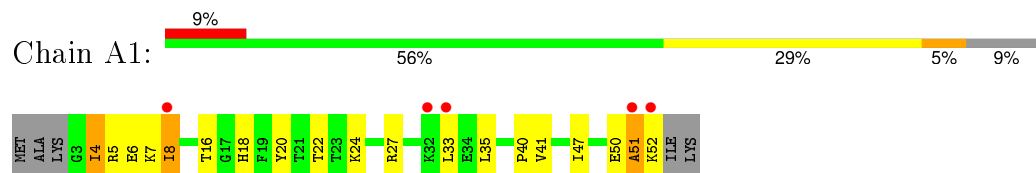
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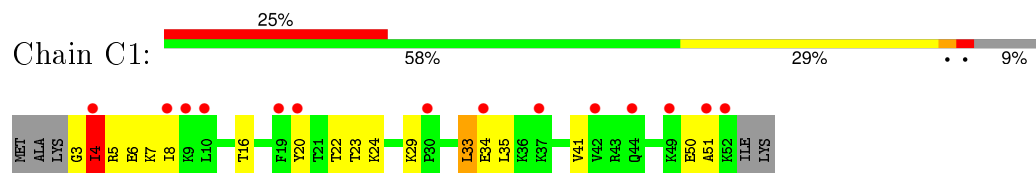
- Molecule 27: 50S ribosomal protein L32



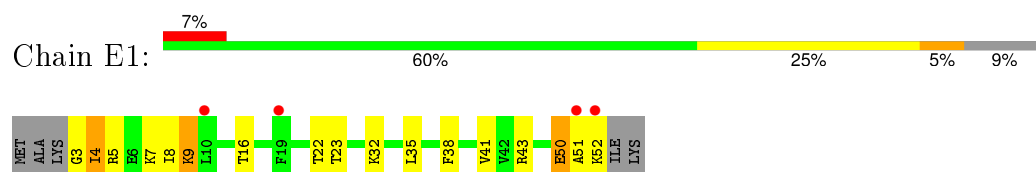
- Molecule 28: 50S ribosomal protein L33



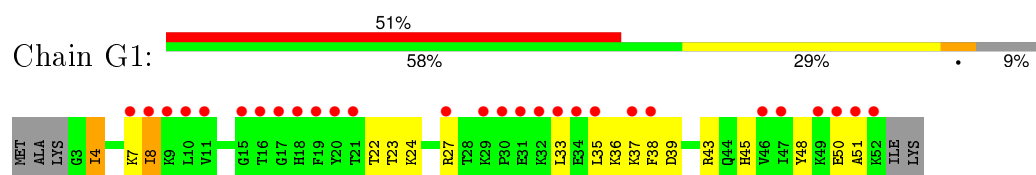
- Molecule 28: 50S ribosomal protein L33



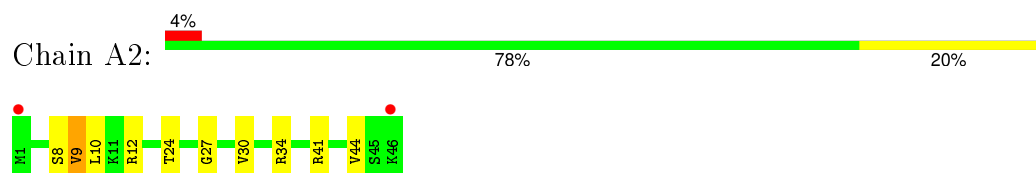
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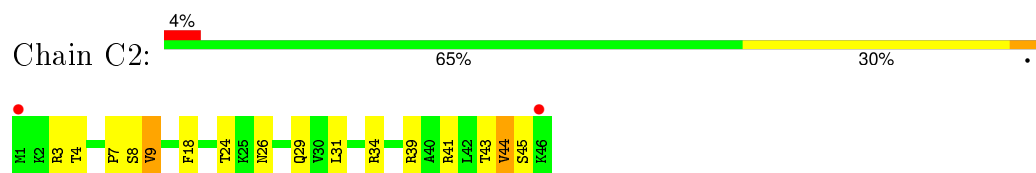
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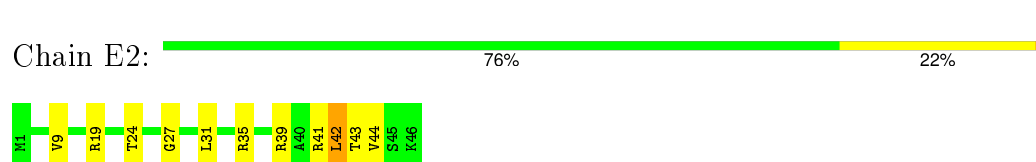
- Molecule 29: 50S ribosomal protein L34



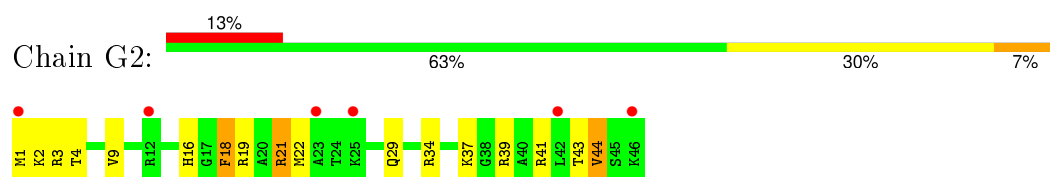
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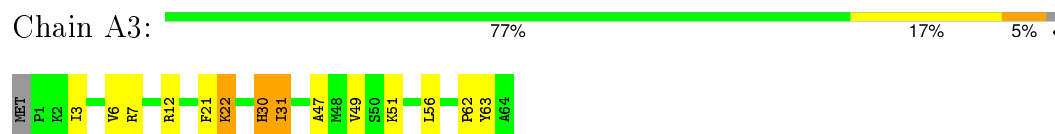
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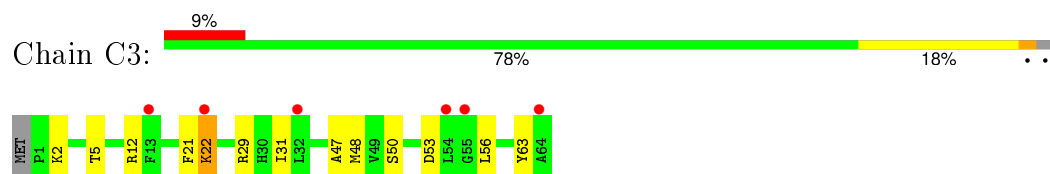
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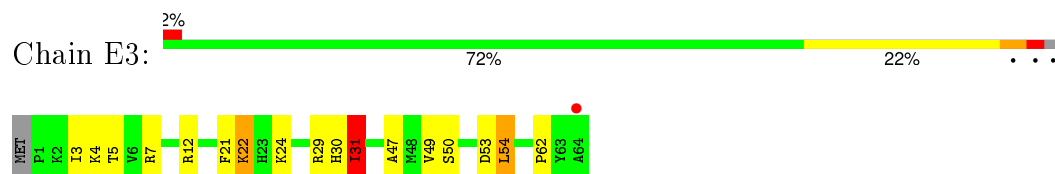
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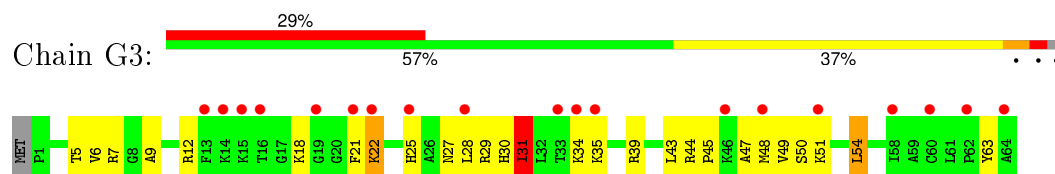
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



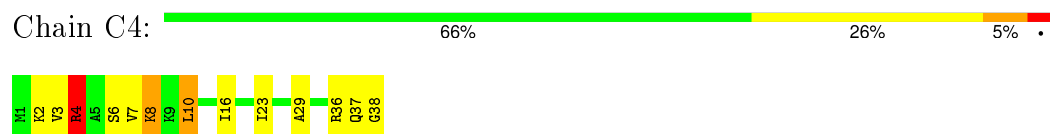
- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 50S ribosomal protein L36

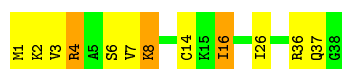


- Molecule 31: 50S ribosomal protein L36

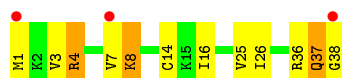


- Molecule 31: 50S ribosomal protein L36

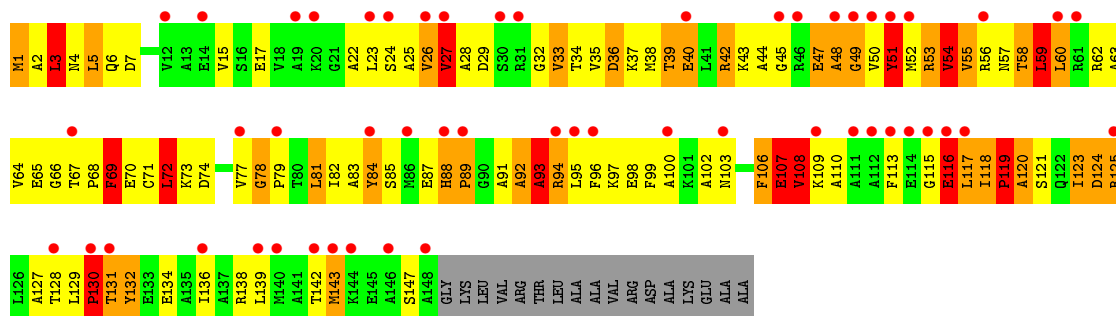
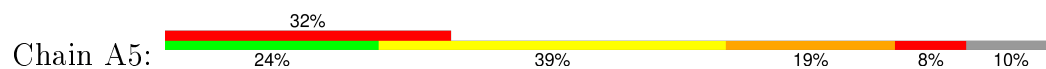




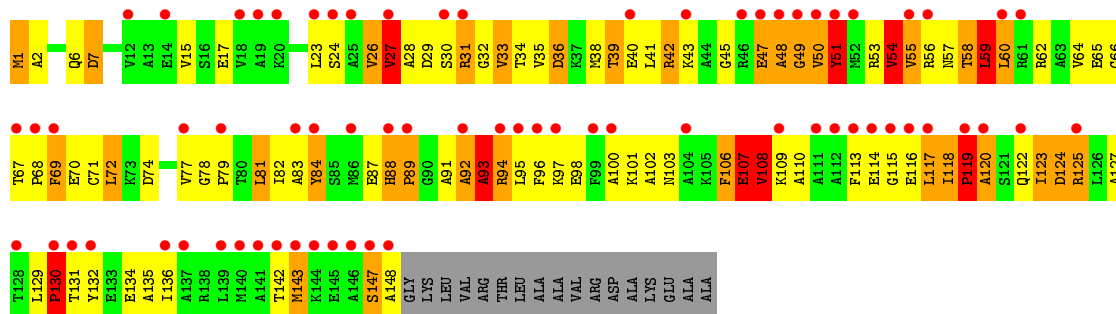
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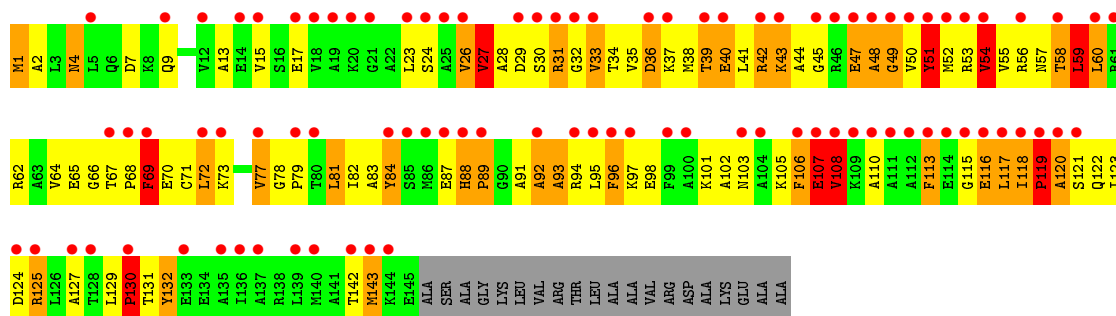
- Molecule 32: 50S ribosomal protein L10



- Molecule 32: 50S ribosomal protein L10



- Molecule 32: 50S ribosomal protein L10

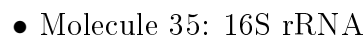
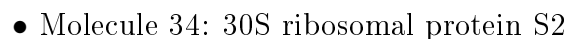


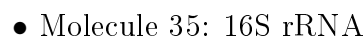
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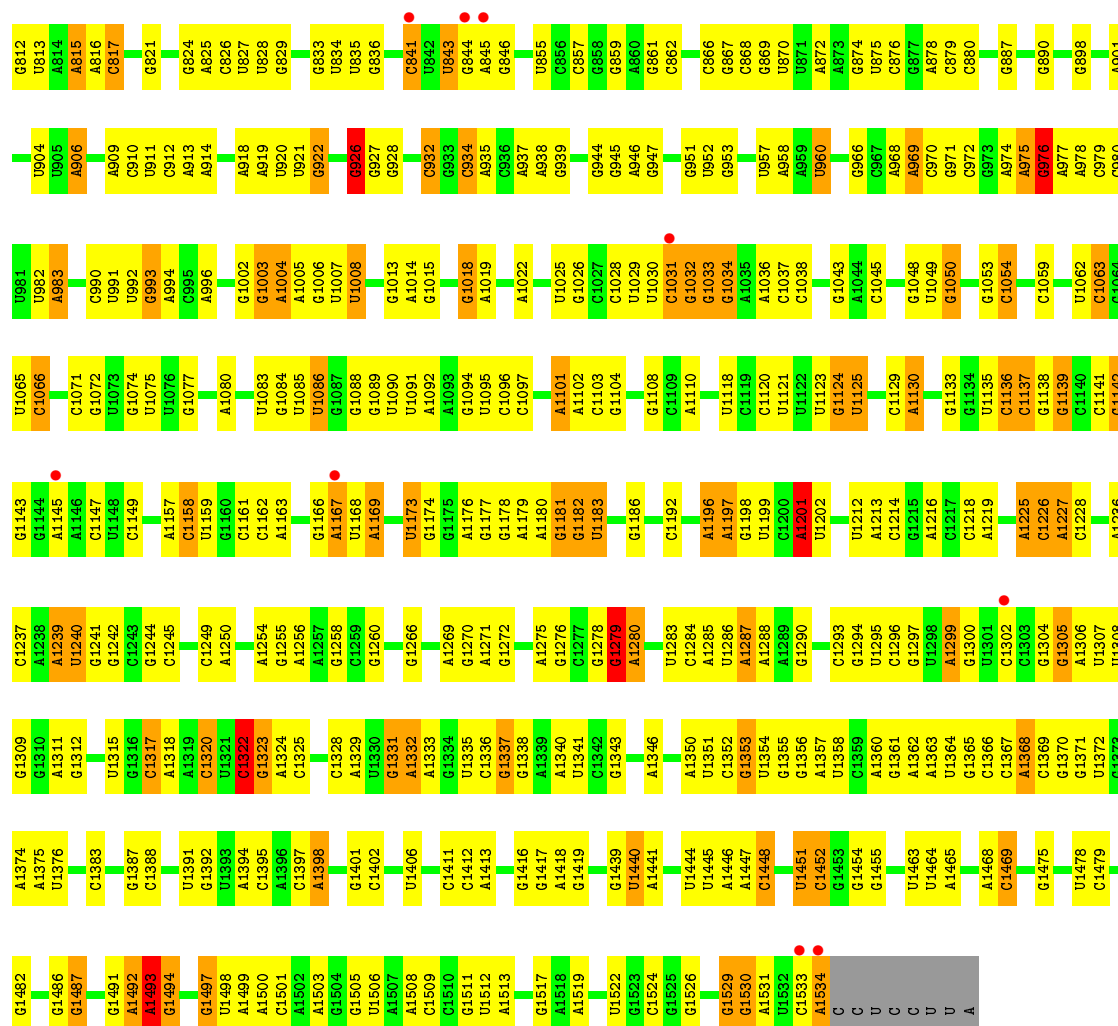
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- Chain FB:
-
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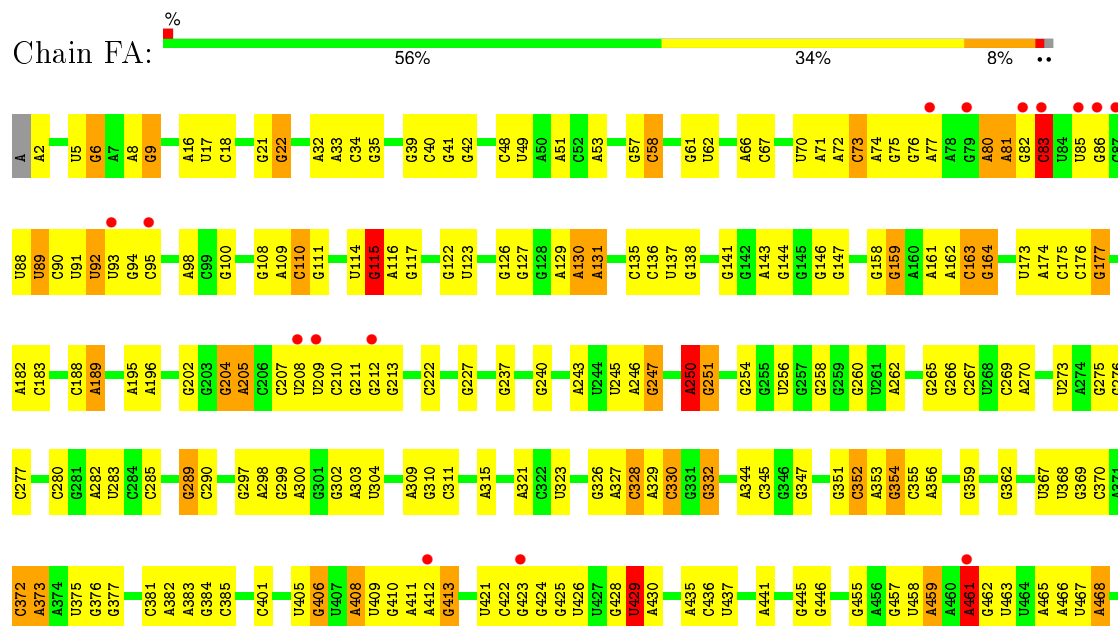




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A729	U619	U508	G399	C277	A196	A98	U5
G730	U625	A510	C400	C285	A197	C99	A8
G732	G626	C511	C401	C286	G198	G108	G9
G733	G627	C518	G404	G289	G201	G110	A10
G734	U632	C525	U405	G292	G202	G111	U12
G735	G633	C526	G406	G293	G204	U114	A16
G737	G633	G527	U407	G294	A205	G115	U17
G739	U636	G530	A408	U294	C206	A116	C18
U740	G637	G531	U409	A313	C207	G117	G21
G741	U641	U531	A411	A321	U209	G122	G22
G745	A642	A532	A412	C322	C210	G126	G31
A746	G643	A533	G413	U323	G213	G127	A32
A747	U649	G537	U420	G324	C214	A128	A33
G748	G650	A538	U421	A325	A129	A130	G34
A749	G651	A539	C422	G326	G220	A131	G35
C750	G651	C561	G423	A327	C221	C132	G39
U751	U652	A546	G424	C328	C222	G141	G42
G752	U653	A547	A429	A329	A223	A143	A44
A753	G664	G548	U429	C330	U224	G142	C47
C754	A665	C549	A430	A331	C225	A146	U49
G755	G668	C556	A431	G332	G240	U154	A50
U756	U672	A559	A435	C341	G243	G158	A51
U757	A673	U562	A441	C342	U244	G159	C58
G760	G674	A563	A451	U343	A245	A160	U62
C764	A675	C564	A452	A344	A246	A161	G70
G765	U676	C564	A452	A345	A247	A162	A71
G769	U683	U571	G457	G346	C248	G164	C73
C770	G683	A572	U458	G347	U249	U166	A74
G776	U684	A574	A460	A353	A250	A167	G75
A777	A687	G576	G462	G354	G251	G168	G76
G778	G690	C576	U463	A362	G254	U173	A77
C779	A696	G577	U464	G362	C257	A174	G79
A780	U697	C578	A465	U367	G259	G176	A80
G781	G698	C580	A466	U368	G260	G177	A81
A782	U701	G581	U467	G369	U861	A181	G82
G783	G702	G587	A468	C372	A262	A182	C83
U784	A702	G588	C470	A373	G385	U85	U85
G791	U707	A595	U480	C381	C384	G183	G86
A792	C708	U598	A481	A382	A383	A184	C87
U793	G714	C599	A482	G384	G385	A185	U87
A794	G721	A601	G483	C386	A388	G186	C88
G802	U722	A602	U485	G388	G389	A187	U88
U803	U723	U603	U486	G390	C391	G188	C89
A811	C724	C604	C487	A392	C392	A189	U89

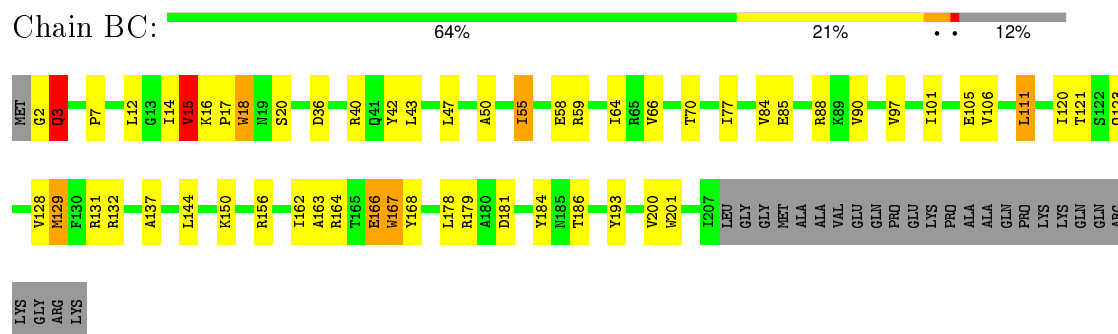


• Molecule 35: 16S rRNA

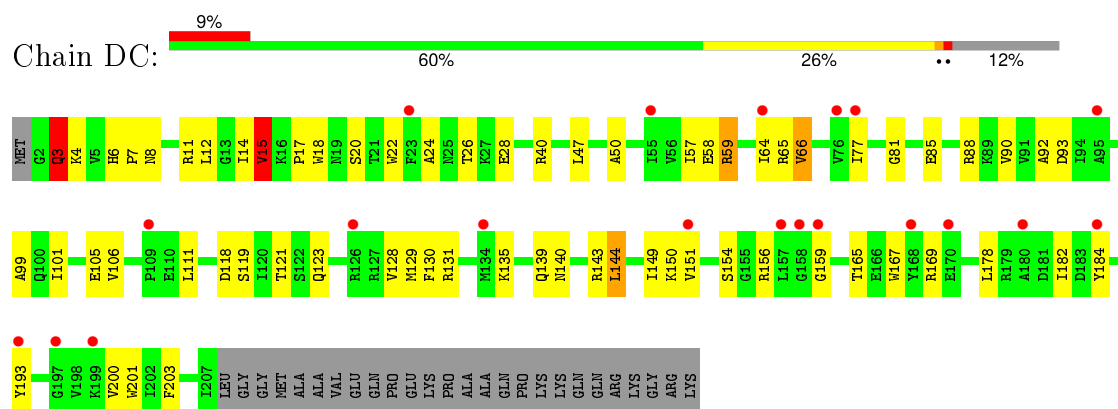


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U1495	G1392	U1321	G1258	G1190	G1106	A1036	C970	G895	A815	G742	A559	C469	G384
G1496	C1322	C1322	G1259	A1191	G1107	C1037	G971	G896	A816	A665	C470	C385	C386
G1497	G1323	G1324	A1261	C1192	G1108	C1038	C972	G897	C817	G743	U562	U387	U387
A1503	A1398	A1325	C1262	G1193	A1109	G1039	G973	G898	G818	G744	C564	U480	C392
G1504	G1401	U1326	G1263	C1195	A1110	G1040	A974	G899	A819	G745	U565	U481	A397
U1505	C1402	C1327	U1264	C1196	C1113	A1042	A975	A901	U820	A746	G566	A482	U398
U1506	C1403	C1328	C1265	A1197	C1114	A1043	G976	G902	G821	A747	G567	C483	G399
C1509	C1404	G1329	G1266	G1198	U1115	C1046	A978	G903	U822	A748	G568	C484	C400
G1510	G1405	U1330	G1267	C1200	U1118	G1047	C980	G904	C823	C750	A572	U485	C401
G1511	U1406	G1331	A1268	A1201	U1119	G1048	C981	U905	U827	U751	A573	U486	G402
U1512	A1332	A1332	A1269	U1202	G1124	U1049	U982	A913	G829	G752	A574	G491	C403
A1513	A1333	A1333	G1270	C1203	U1125	G1050	U983	A914	G832	G753	C575	G404	U405
G1517	C1412	U1334	A1271	U1204	C1128	C1051	C984	A915	G833	G755	G577	A498	U406
A1518	A1413	U1335	G1272	U1205	G1129	U1052	C985	A916	G834	A759	C578	G501	U407
U1519	G1414	G1336	C1273	G1206	U1130	G1053	U986	G917	U834	G760	C579	A502	A408
A1520	G1415	G1337	A1274	G1207	A1131	C1054	G987	A918	U835	G761	C580	A503	U409
G1521	G1416	G1338	A1275	C1208	G1132	A1055	G988	A919	G836	G762	C581	C504	A411
U1522	G1417	A1339	G1276	C1209	C1133	G1057	A994	U921	G837	G763	C582	C505	G412
G1523	G1418	A1340	C1277	C1210	G1134	G1058	G995	G922	C838	C764	C583	G506	G413
C1524	G1419	G1341	G1278	U1211	G1135	C1059	A1000	G926	C841	G765	C584	C507	A414
G1525	G1423	U1344	A1280	U1212	U1136	U1060	G1001	G927	U842	A766	G587	U508	A415
G1526	U1424	U1345	C1281	A1213	C1137	G1061	G1002	G928	U843	G769	G588	A509	G416
U1527	A1430	G1347	U1283	G1215	G1138	U1062	C1003	G929	G844	C770	A510	A511	C419
U1528	G1435	U1348	C1284	C1217	C1140	G1064	G1004	C931	A845	G771	A596	C511	U420
G1529	A1436	A1350	U1285	G1218	G1143	U1065	A1004	C932	G846	G772	C597	U512	G421
U1530	U1436	U1351	A1287	A1219	G1144	C1066	G1005	G933	G847	G773	U598	C513	C422
A1531	U1440	C1352	A1288	G1220	A1145	A1067	G1006	G934	C848	G774	G604	C517	G423
U1532	A1441	G1353	G1292	G1222	A1146	C1071	U1007	A935	G849	G775	C615	C518	G424
C1533	A1446	U1354	C1293	C1223	C1147	G1072	U1008	C936	U850	G776	G615	U519	U428
C	A1458	G1355	G1294	U1224	U1148	U1073	U1010	G939	G852	C779	U619	G527	U429
U	U1451	U1358	U1295	A1225	G1149	U1075	A1011	C940	G858	A780	C620	U530	A430
C	C1462	G1359	C1296	C1226	A1150	U1076	A1012	G941	G859	A781	A621	A532	A435
U	G1463	A1360	G1297	A1227	C1158	G1077	G1013	G942	A864	A784	C623	A533	U439
C	G1454	G1361	U1298	A1228	U1159	U1078	G1015	U943	A865	G785	U534	A534	C440
U	G1458	A1362	A1299	C1230	G1166	G1079	A1016	G944	G866	G791	A640	C536	A441
A	U1464	U1364	C1302	G1233	U1167	A1080	U1017	G945	C867	A792	G626	A535	A451
		G1365	C1303	G1236	U1168	G1084	G1018	A946	G868	G793	G627	A536	A452
		C1366	G1304	A1237	A1169	U1085	A1019	G947	G869	A794	U641	G537	A453
		G1367	G1305	C1238	A1170	U1086	G1020	C948			G721	A538	U457
		A1368	A1306	A1239	A1171	G1087	A1021				G722	A539	U458
		C1369	U1307	U1240	C1172	G1088	A1022	U952	A872	C796	G723	G540	U459
		G1370	U1308	U1241	G1177	G1089	U1023	A958	G874	C797	G724	A547	A460
		G1373	G1309	G1242	G1178		U1024	U959		U798	G725	U463	G462
		A1374	A1311	G1243	U1179	G1094	U1025	U960	G877	G799	G726	U464	U467
		U1375	A1312	C1244	A1180	U1095	G1026	U961	A878	A728	G727	U543	U468
		G1376	U1313	C1245	C1181	C1096	C1027	U962	C879	A729	G728	G544	U469
		A1377	G1314	C1246	G1182	C1097	C1028	G963		U801	G729	C545	A461
		G1378	U1315	U1250	U1183	C1098	U1029	G964	G885	A802	G730	A546	A462
		G1379	G1316	A1251	U1187	A1101	U1030	U965	G886	U804	G731	U653	U463
		U1380	C1317	A1256	G1187	A1102	C1031	G966	G887	C811	G732	G654	U464
		A1493	A1318	A1257	A1188	G1104	G1033	C967	G888	G734	G735	A655	A465
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												C557	U467

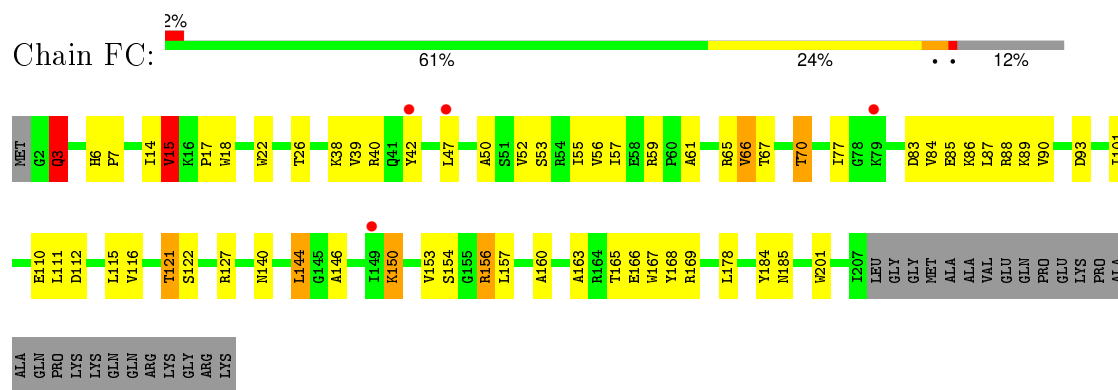
- Molecule 36: 30S ribosomal protein S3



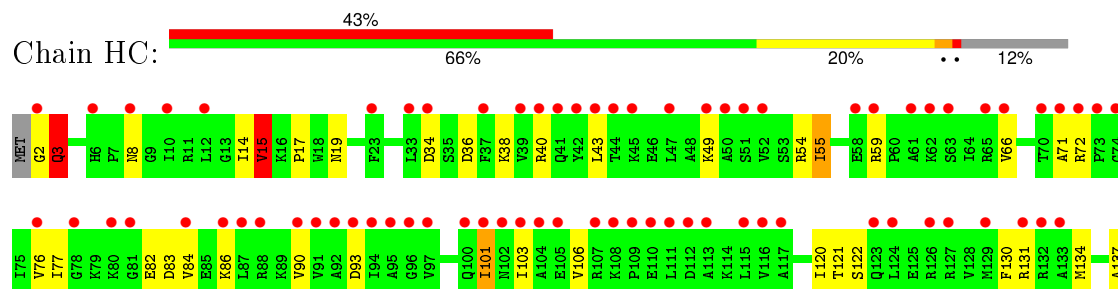
- Molecule 36: 30S ribosomal protein S3

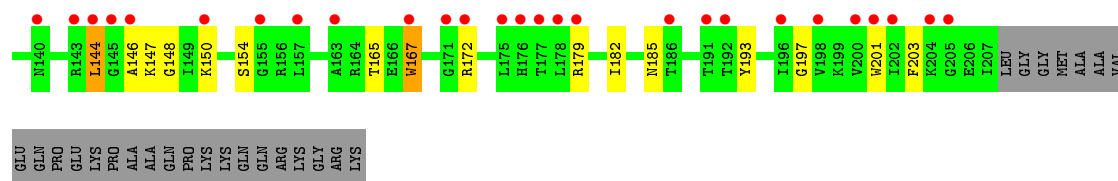


- Molecule 36: 30S ribosomal protein S3

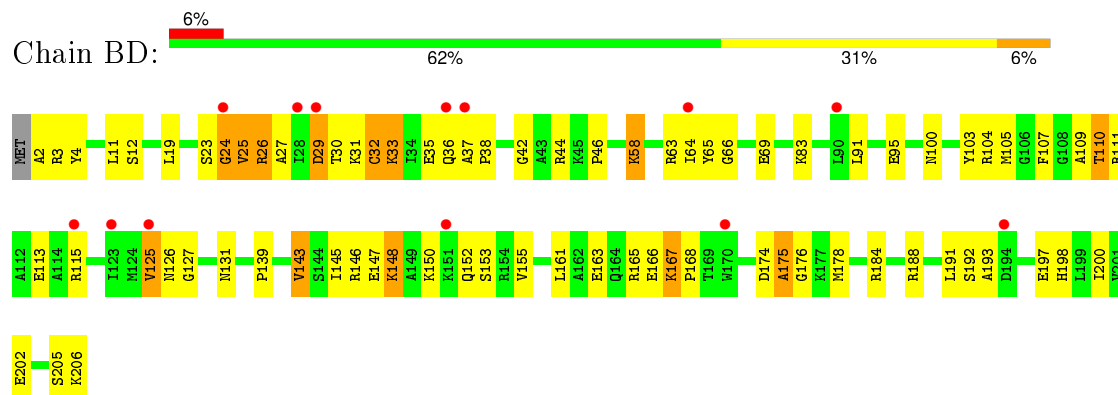


- Molecule 36: 30S ribosomal protein S3

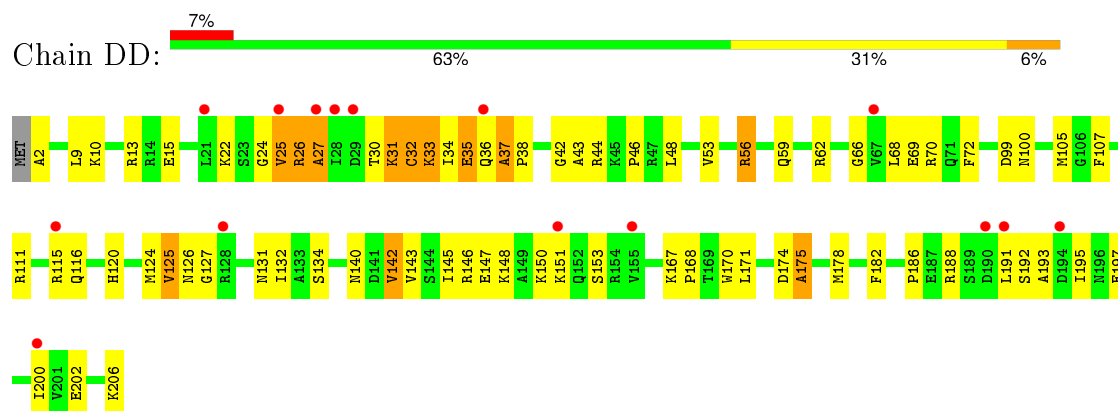




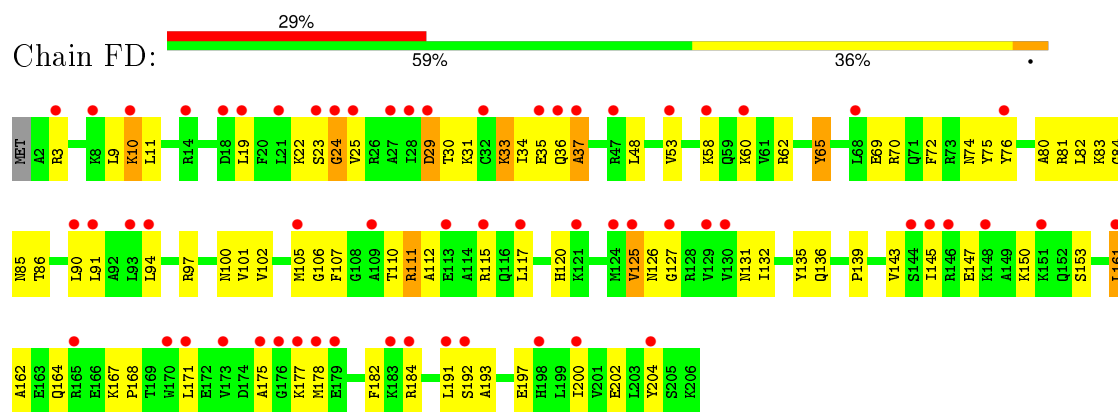
- Molecule 37: 30S ribosomal protein S4



- Molecule 37: 30S ribosomal protein S4

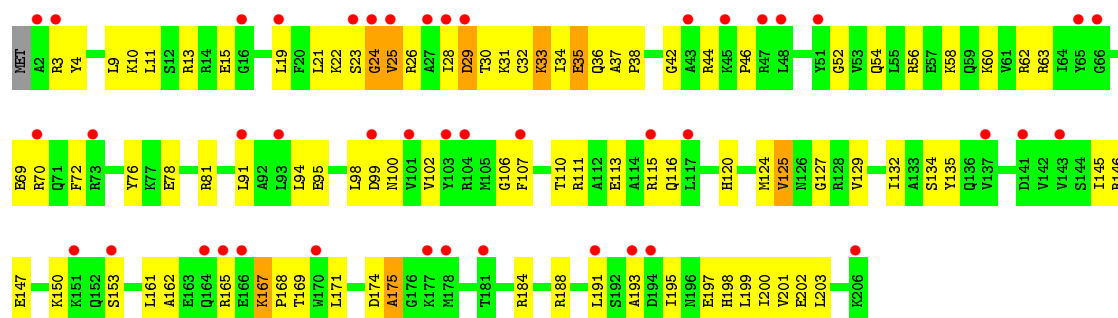


- Molecule 37: 30S ribosomal protein S4

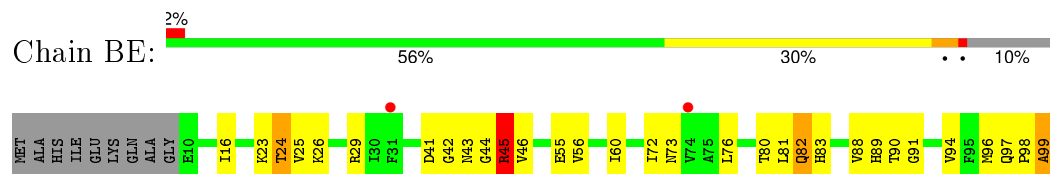


- Molecule 37: 30S ribosomal protein S4

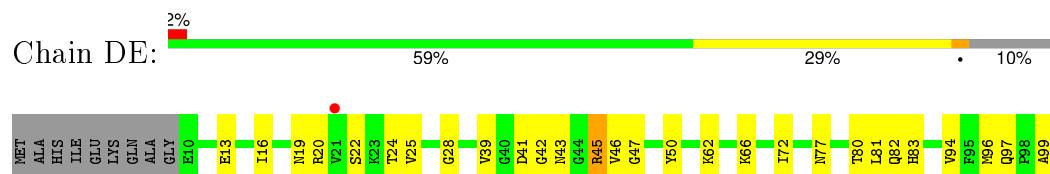




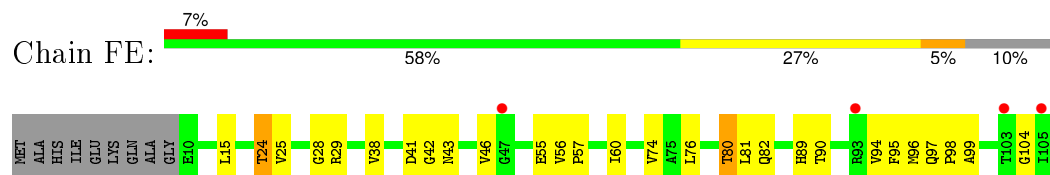
- Molecule 38: 30S ribosomal protein S5



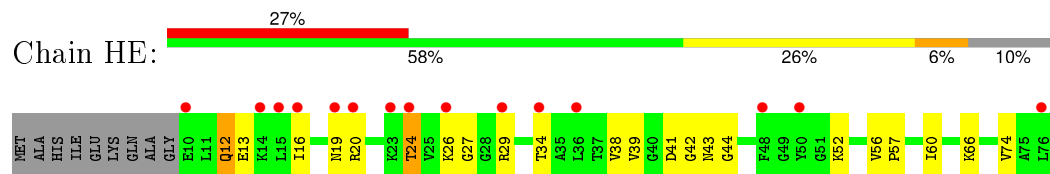
- Molecule 38: 30S ribosomal protein S5

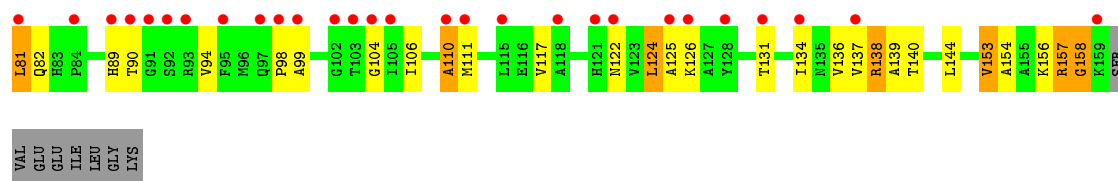


- Molecule 38: 30S ribosomal protein S5



- Molecule 38: 30S ribosomal protein S5





- Molecule 39: 30S ribosomal protein S6



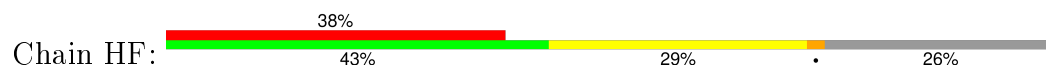
- Molecule 39: 30S ribosomal protein S6



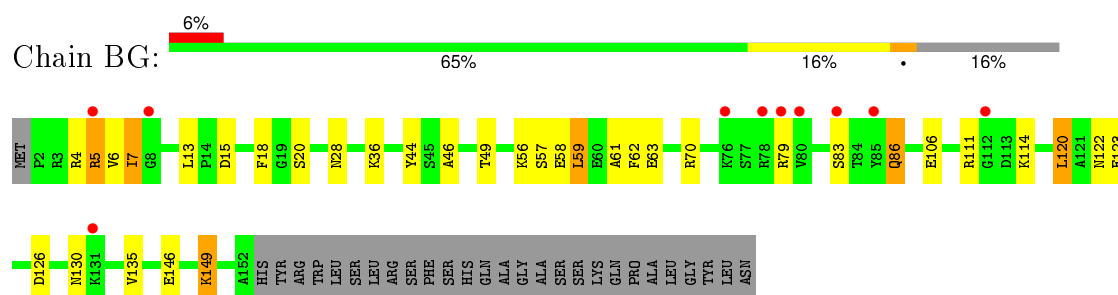
- Molecule 39: 30S ribosomal protein S6



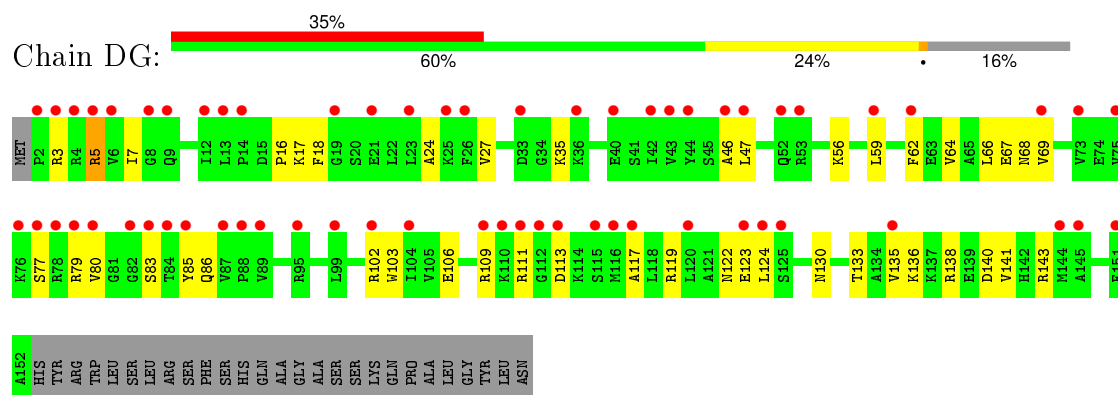
- Molecule 39: 30S ribosomal protein S6



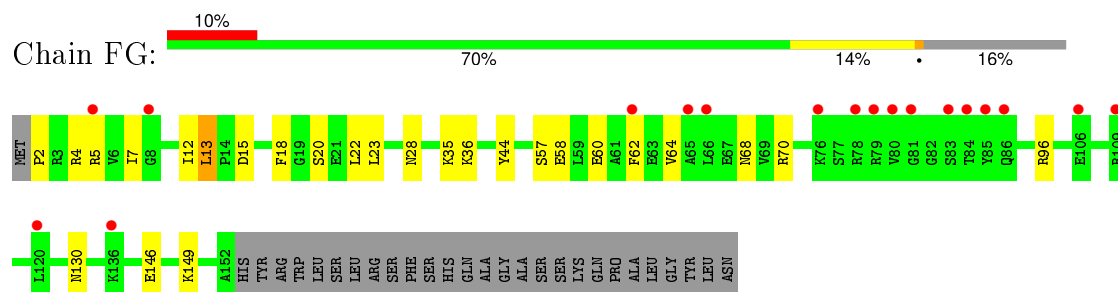
- Molecule 40: 30S ribosomal protein S7



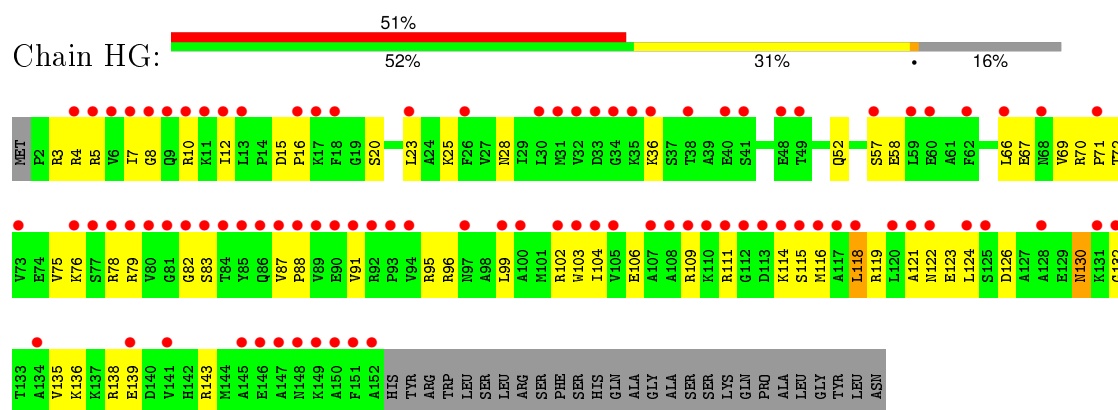
- Molecule 40: 30S ribosomal protein S7



- Molecule 40: 30S ribosomal protein S7

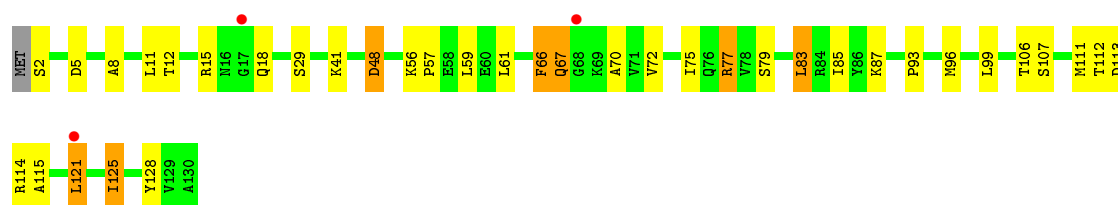


- Molecule 40: 30S ribosomal protein S7

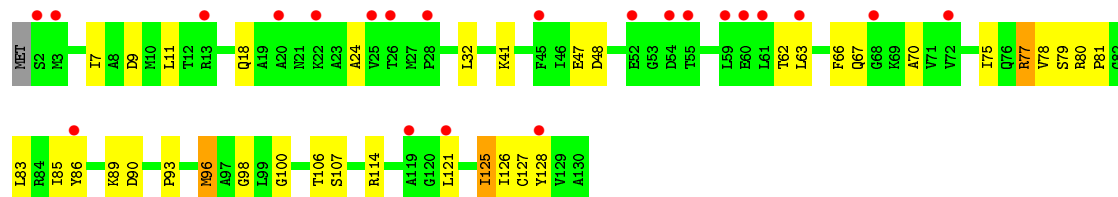
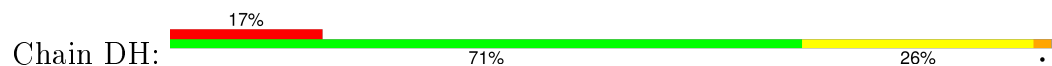


- Molecule 41: 30S ribosomal protein S8

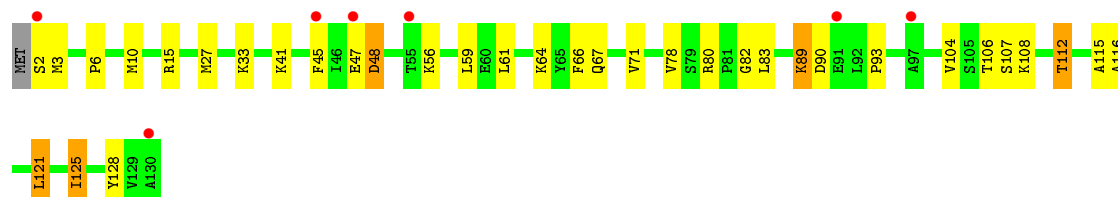
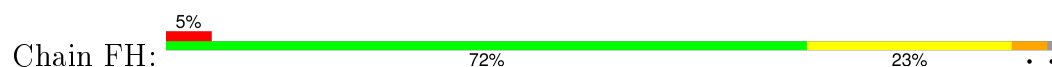




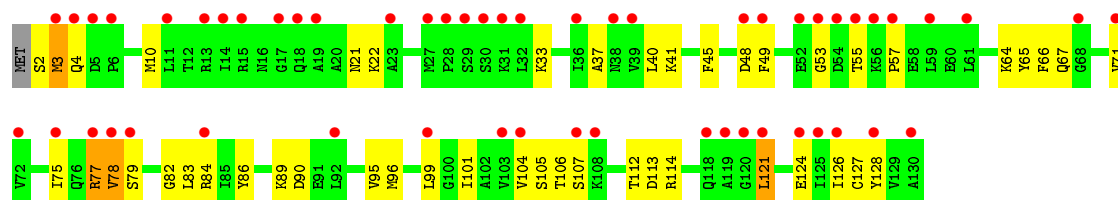
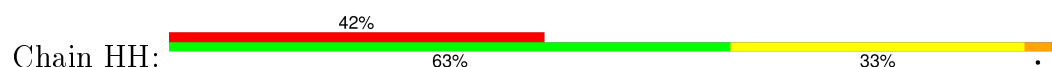
- Molecule 41: 30S ribosomal protein S8



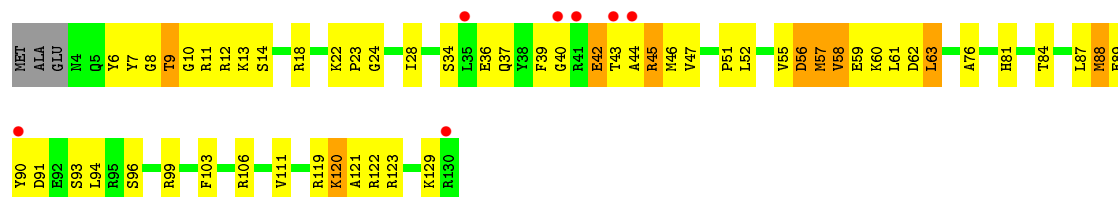
- Molecule 41: 30S ribosomal protein S8



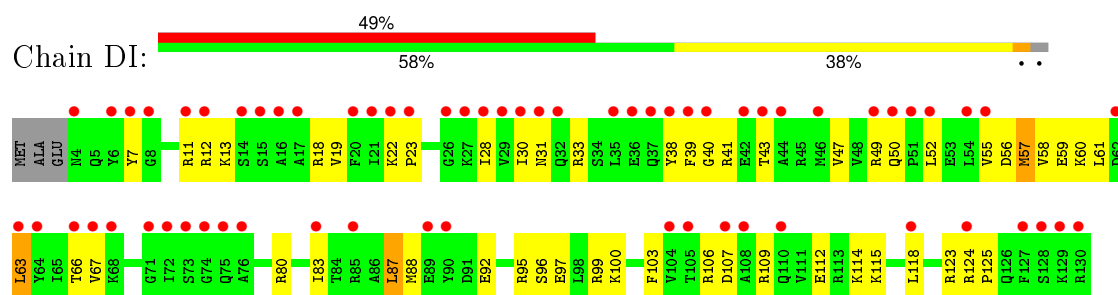
- Molecule 41: 30S ribosomal protein S8



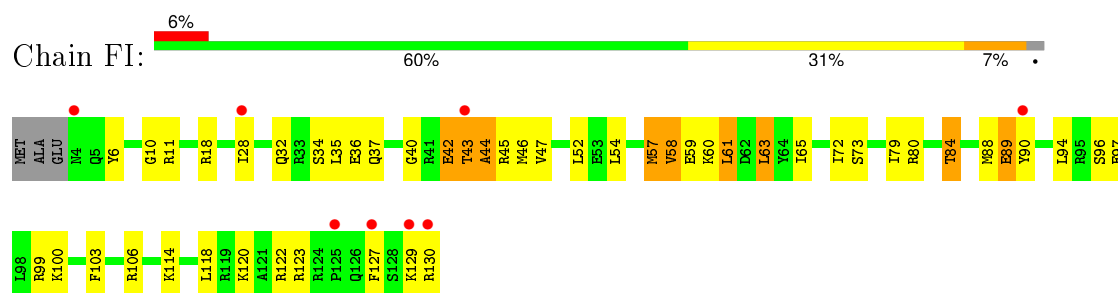
- Molecule 42: 30S ribosomal protein S9



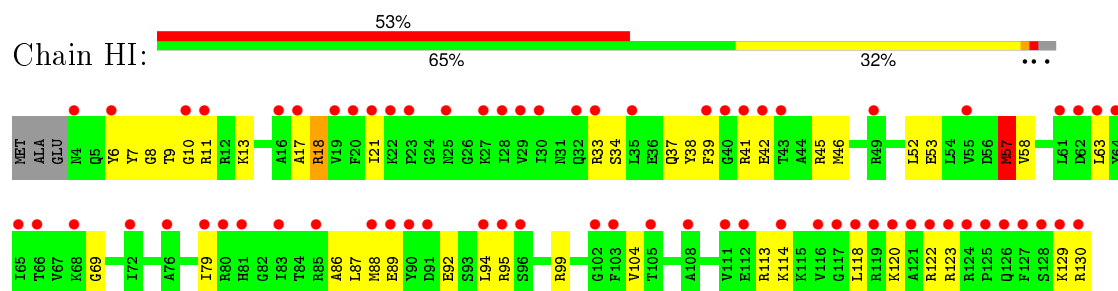
- Molecule 42: 30S ribosomal protein S9



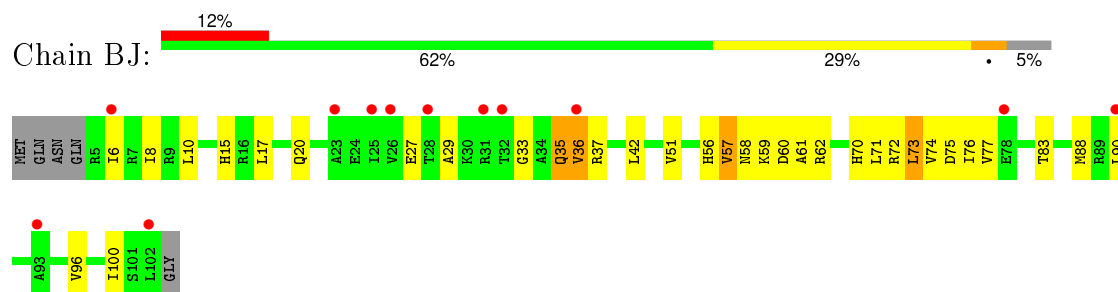
- Molecule 42: 30S ribosomal protein S9



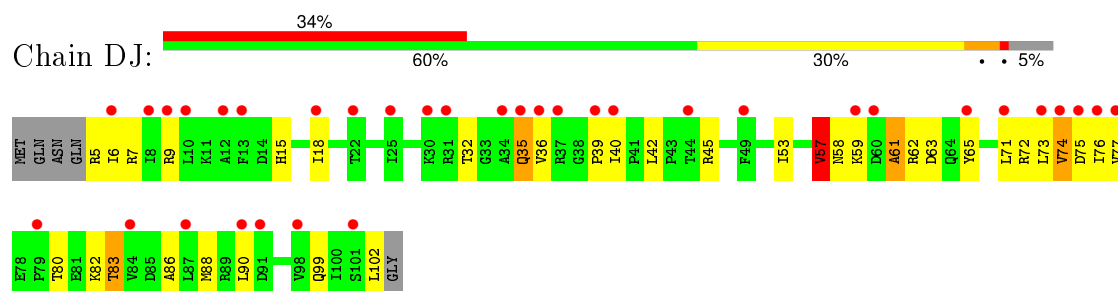
- Molecule 42: 30S ribosomal protein S9



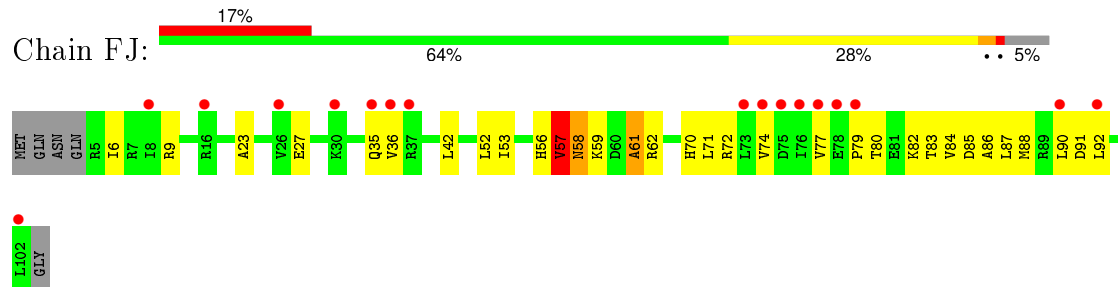
- Molecule 43: 30S ribosomal protein S10



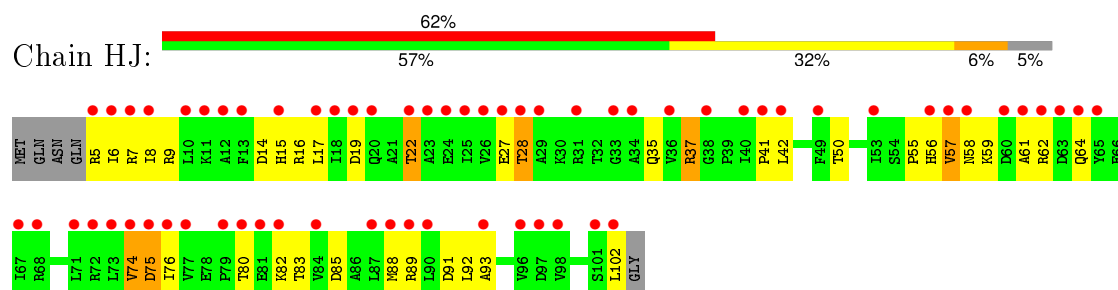
- Molecule 43: 30S ribosomal protein S10



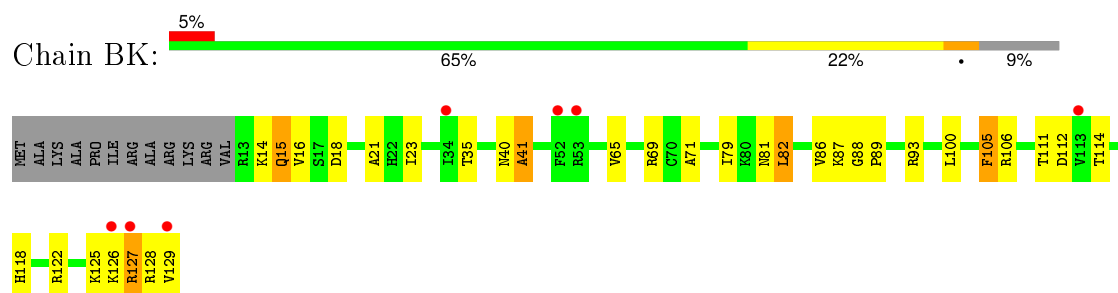
- Molecule 43: 30S ribosomal protein S10



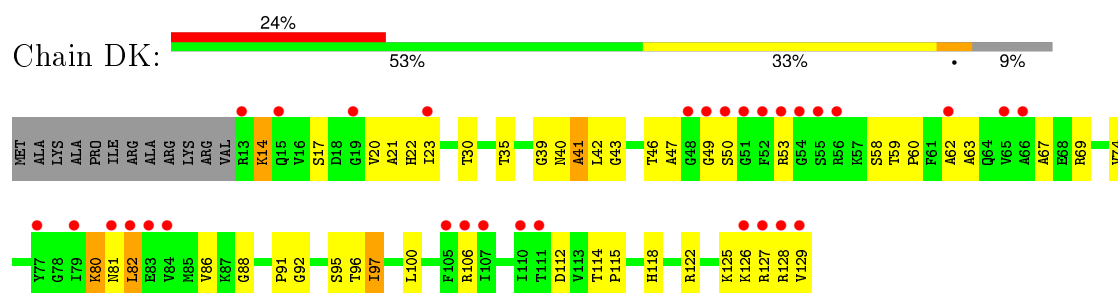
- Molecule 43: 30S ribosomal protein S10



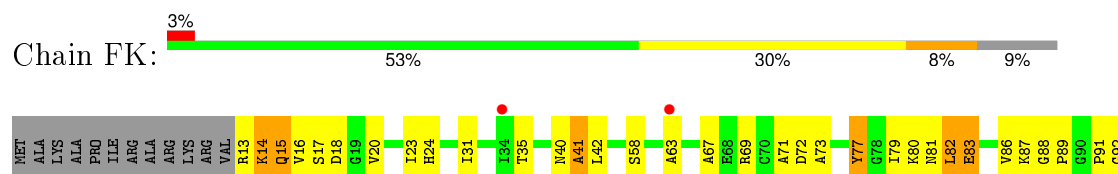
- Molecule 44: 30S ribosomal protein S11



- Molecule 44: 30S ribosomal protein S11

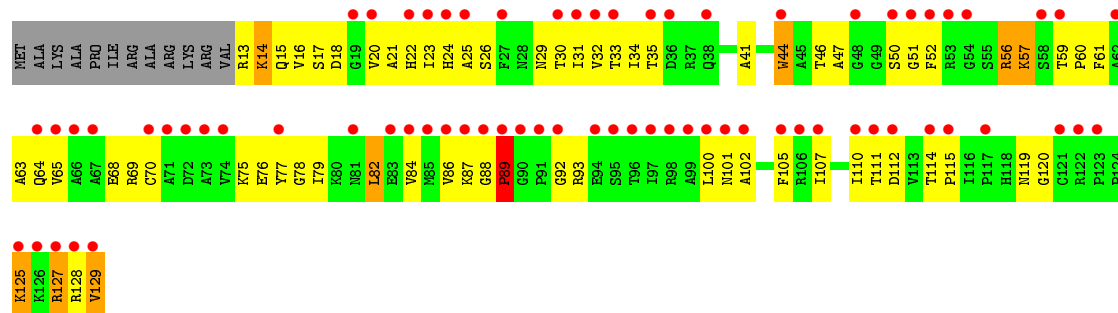


- Molecule 44: 30S ribosomal protein S11

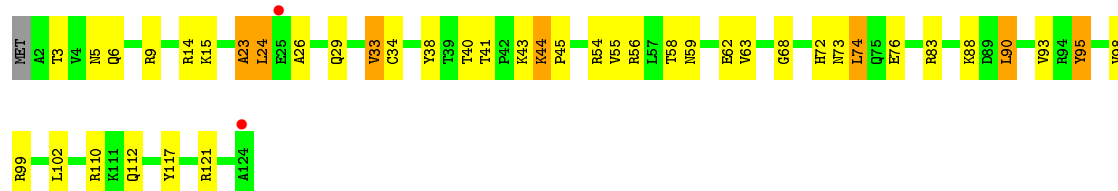




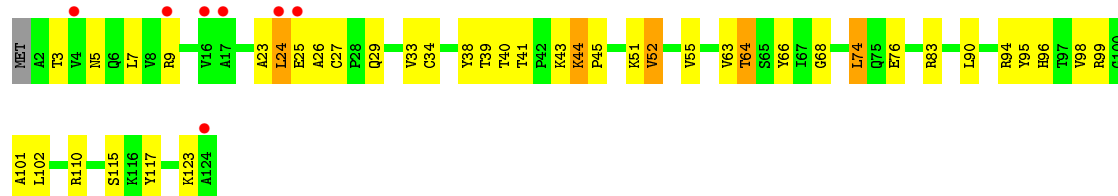
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12



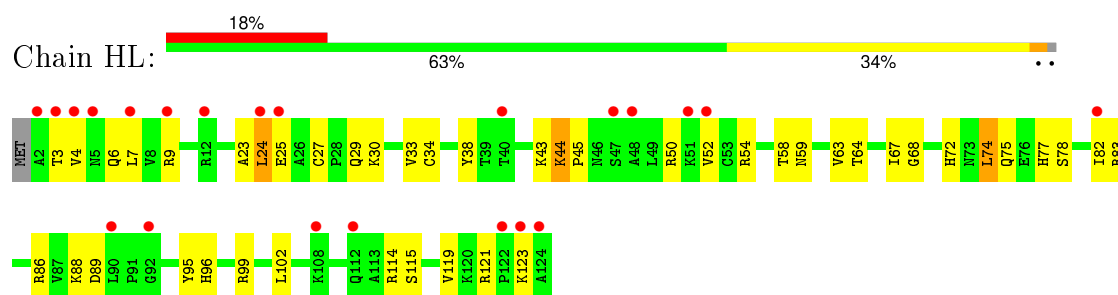
- Molecule 45: 30S ribosomal protein S12



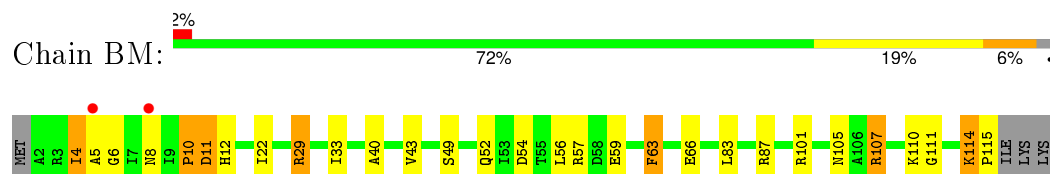
- Molecule 45: 30S ribosomal protein S12



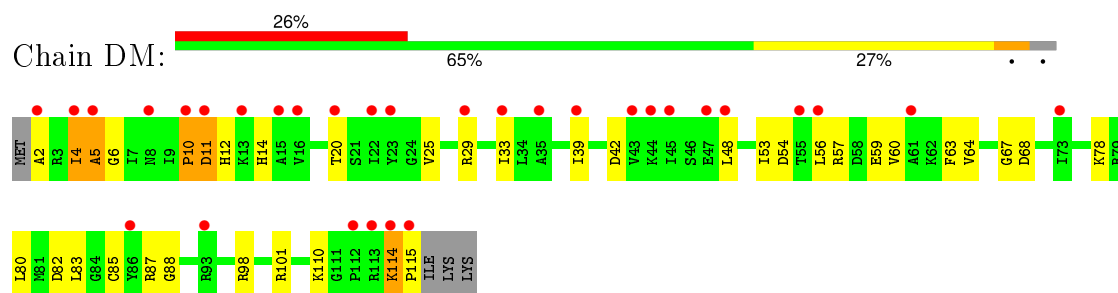
- Molecule 45: 30S ribosomal protein S12



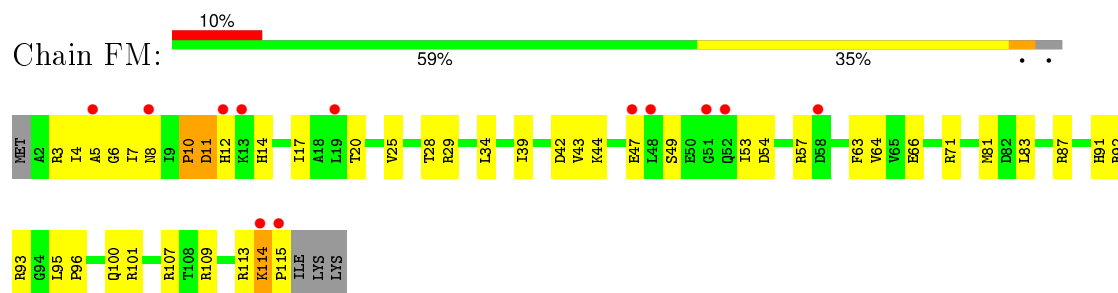
- Molecule 46: 30S ribosomal protein S13



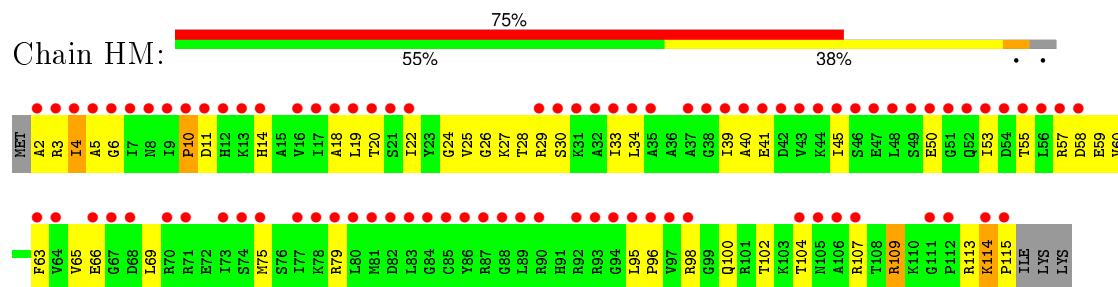
- Molecule 46: 30S ribosomal protein S13



- Molecule 46: 30S ribosomal protein S13

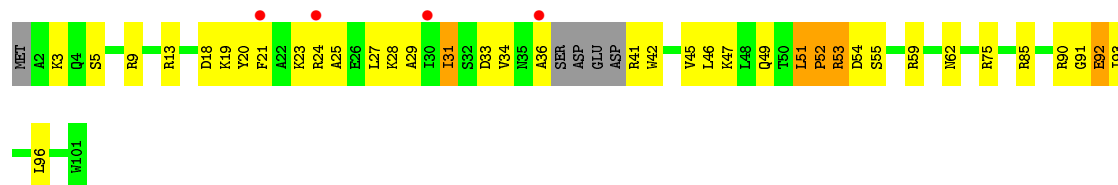


- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14





- Molecule 47: 30S ribosomal protein S14



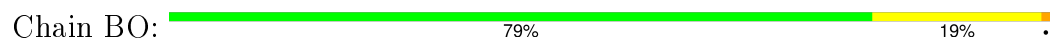
- Molecule 47: 30S ribosomal protein S14



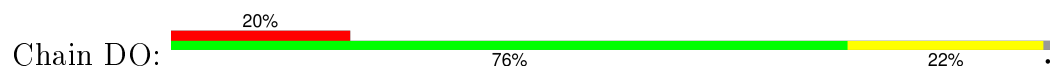
- Molecule 47: 30S ribosomal protein S14



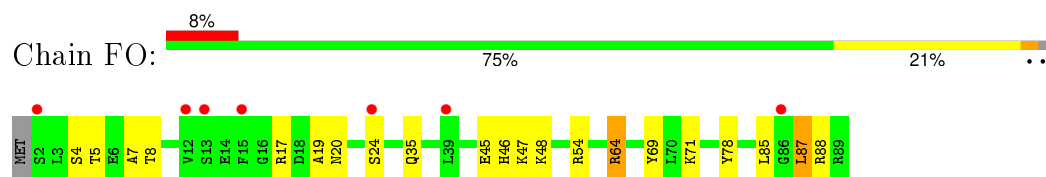
- Molecule 48: 30S ribosomal protein S15



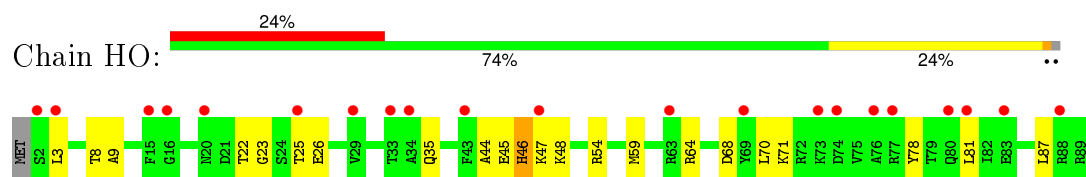
- Molecule 48: 30S ribosomal protein S15



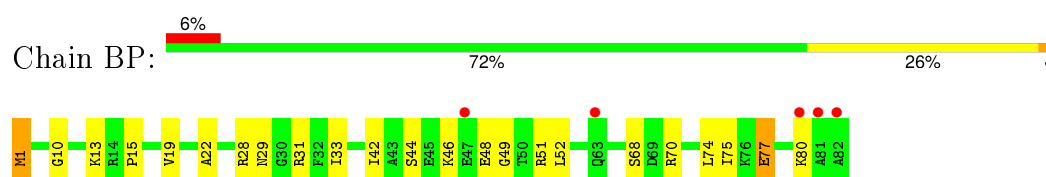
- Molecule 48: 30S ribosomal protein S15



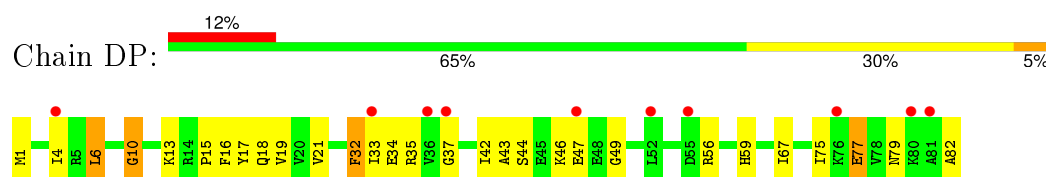
- Molecule 48: 30S ribosomal protein S15



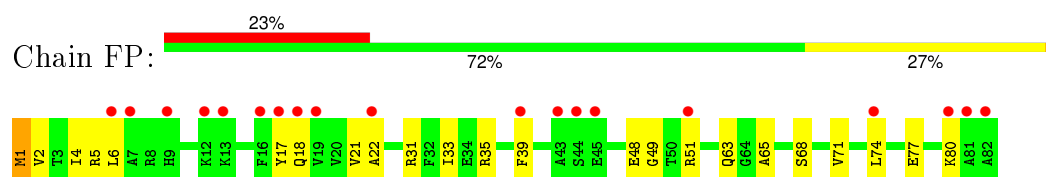
- Molecule 49: 30S ribosomal protein S16



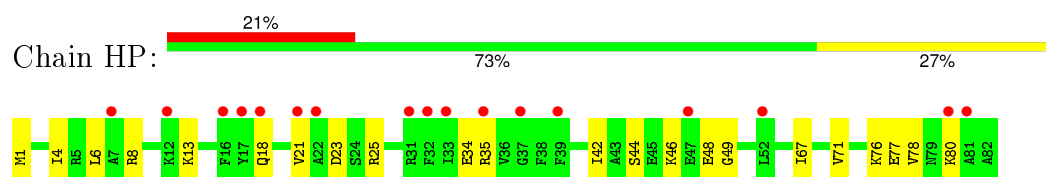
- Molecule 49: 30S ribosomal protein S16



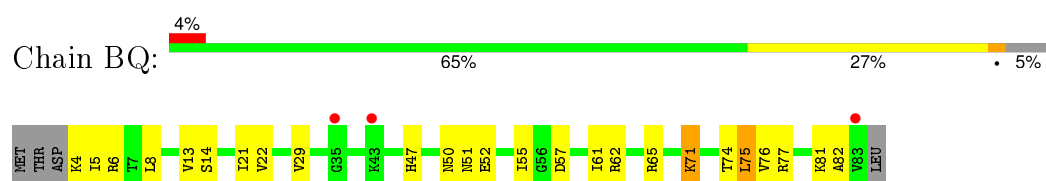
- Molecule 49: 30S ribosomal protein S16



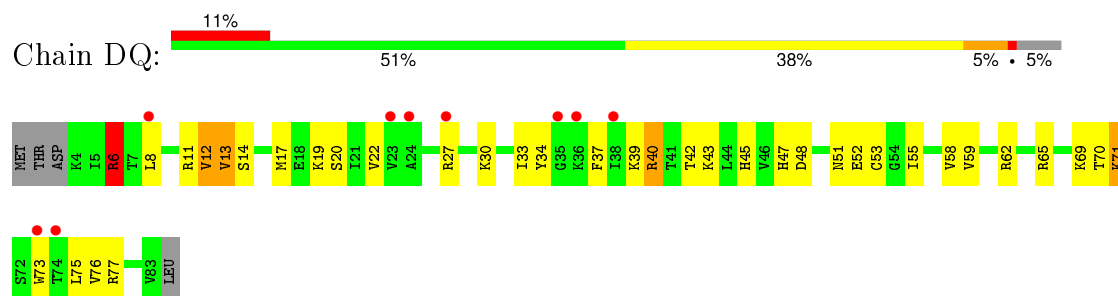
- Molecule 49: 30S ribosomal protein S16



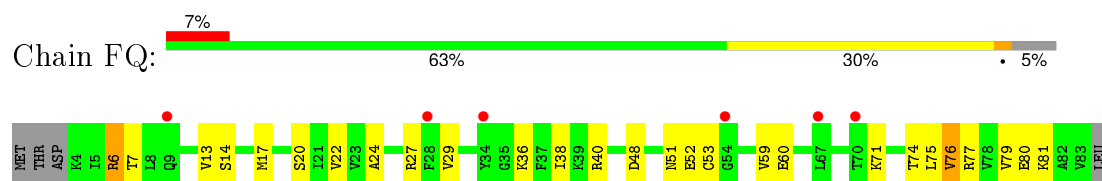
- Molecule 50: 30S ribosomal protein S17



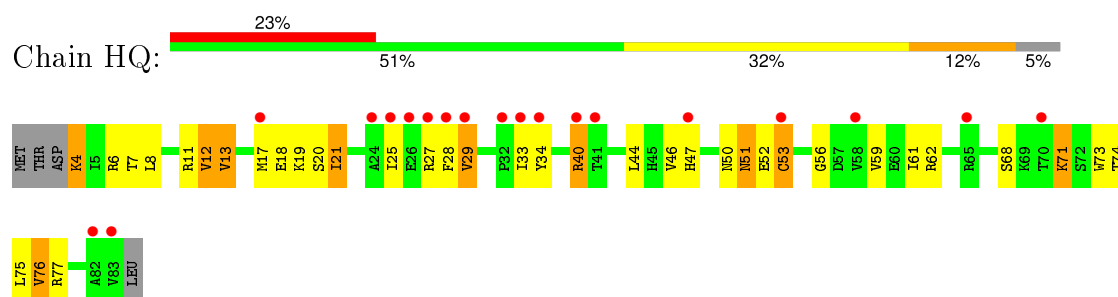
- Molecule 50: 30S ribosomal protein S17



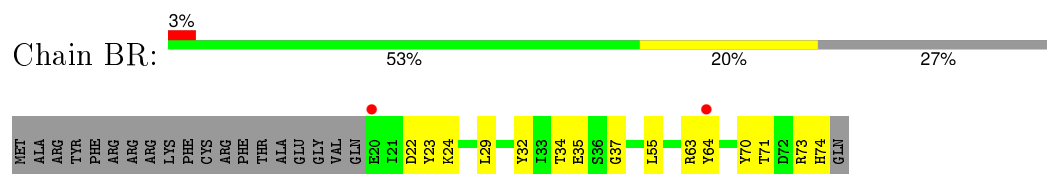
- Molecule 50: 30S ribosomal protein S17



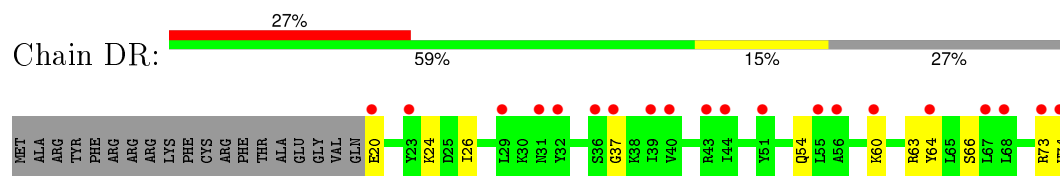
- Molecule 50: 30S ribosomal protein S17



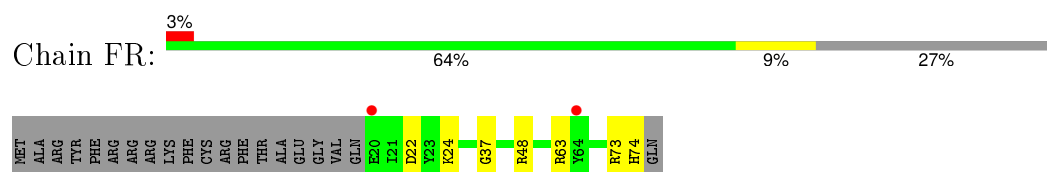
- Molecule 51: 30S ribosomal protein S18



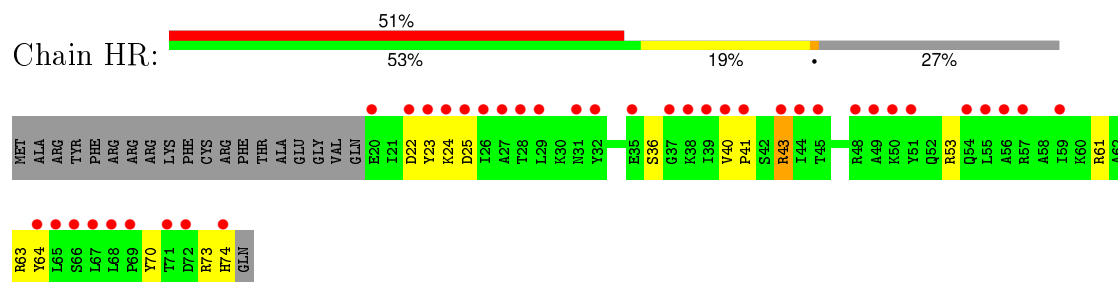
- Molecule 51: 30S ribosomal protein S18



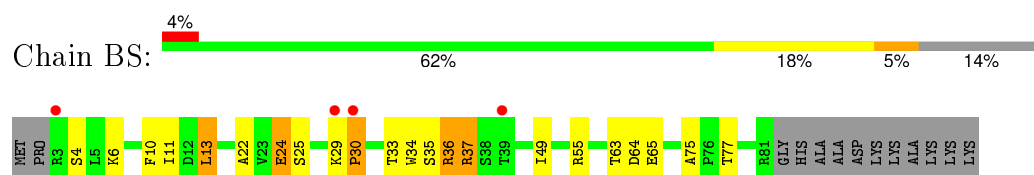
- Molecule 51: 30S ribosomal protein S18



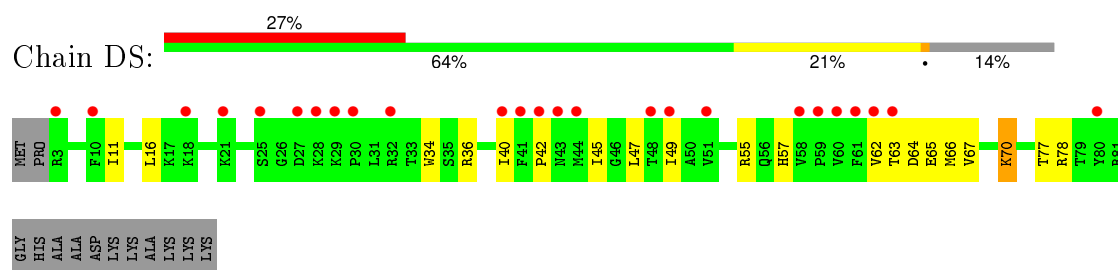
- Molecule 51: 30S ribosomal protein S18



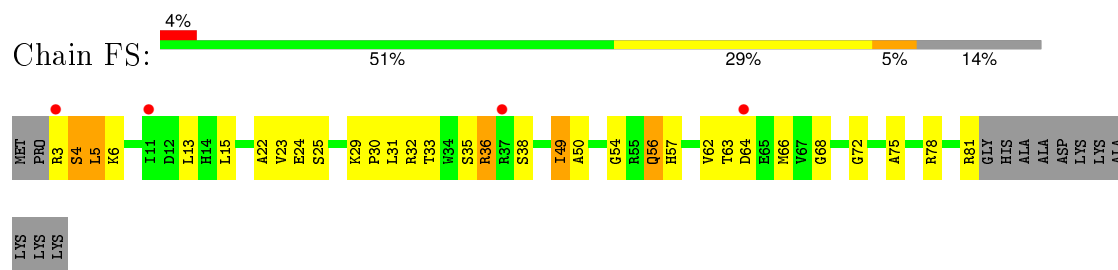
- Molecule 52: 30S ribosomal protein S19



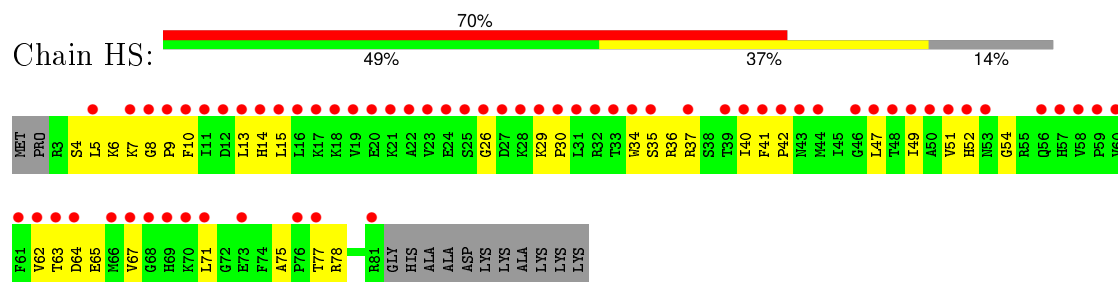
- Molecule 52: 30S ribosomal protein S19



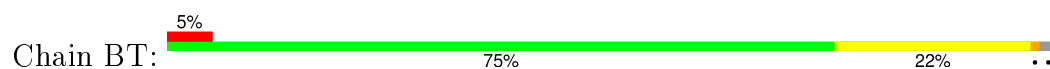
- Molecule 52: 30S ribosomal protein S19

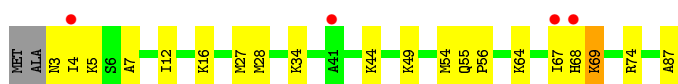


- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20

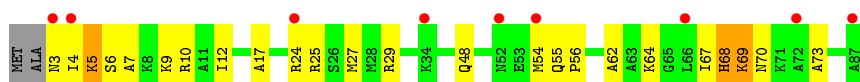
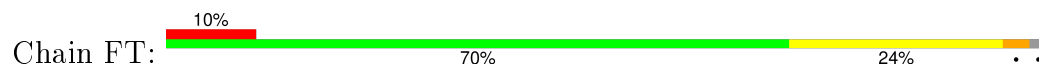




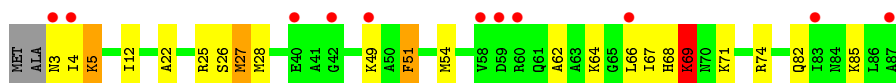
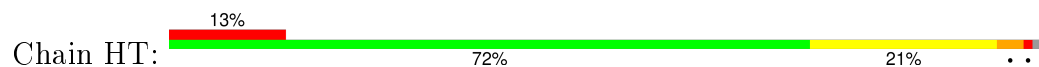
- Molecule 53: 30S ribosomal protein S20



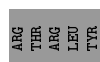
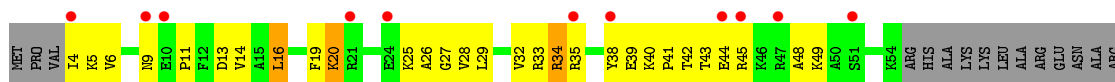
- Molecule 53: 30S ribosomal protein S20



- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S21

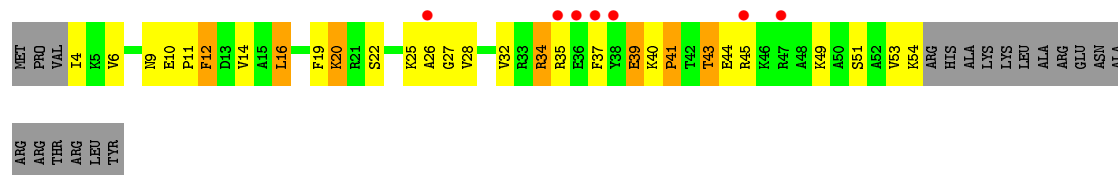


- Molecule 54: 30S ribosomal protein S21

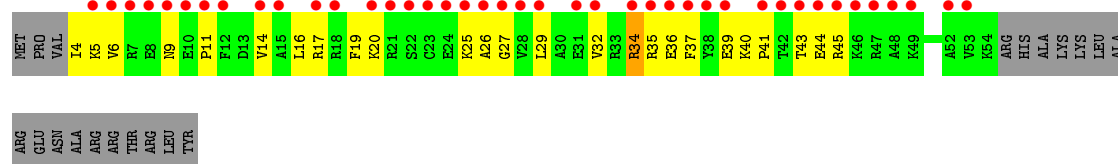
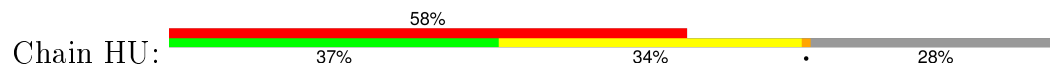


- Molecule 54: 30S ribosomal protein S21

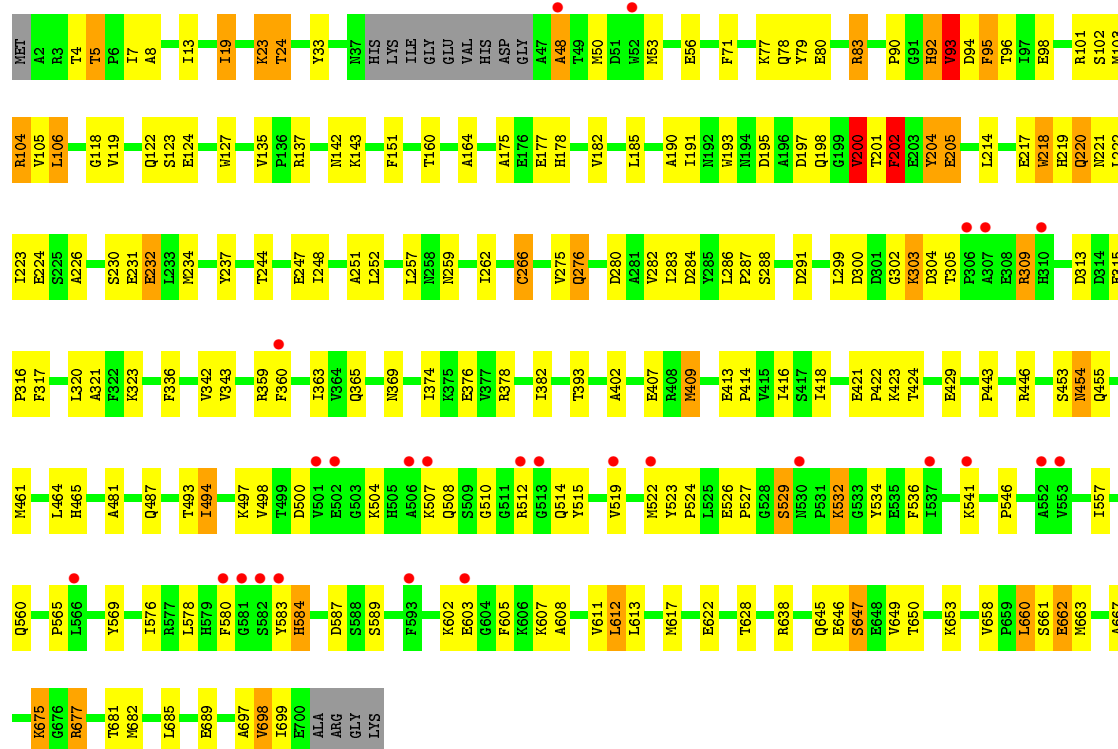




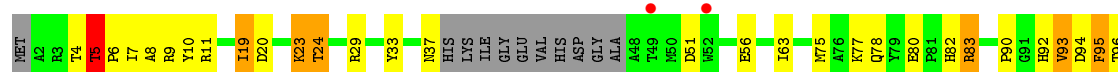
- Molecule 54: 30S ribosomal protein S21

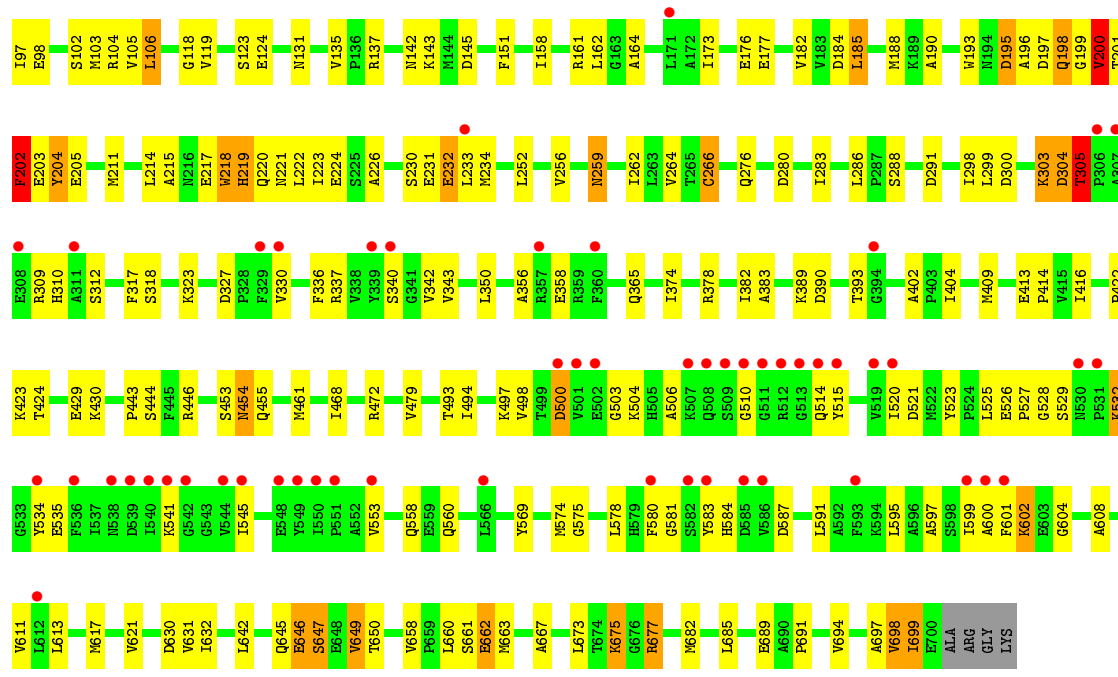


- Molecule 55: Elongation factor G

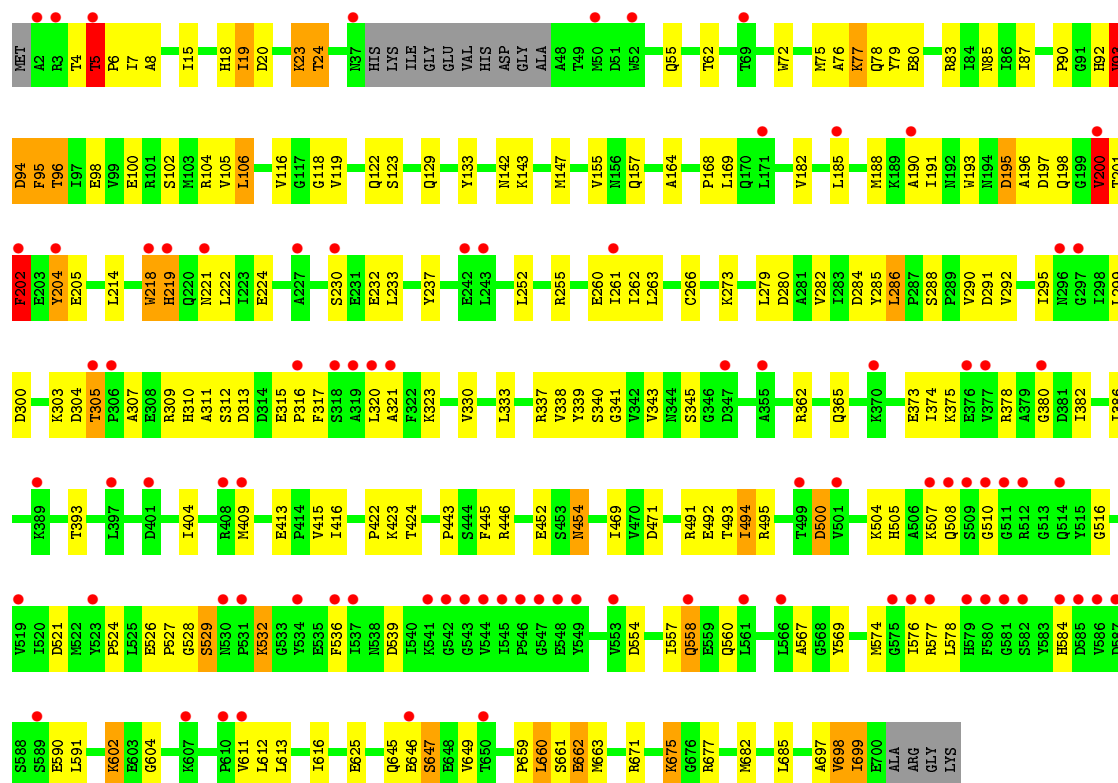


- Molecule 55: Elongation factor G



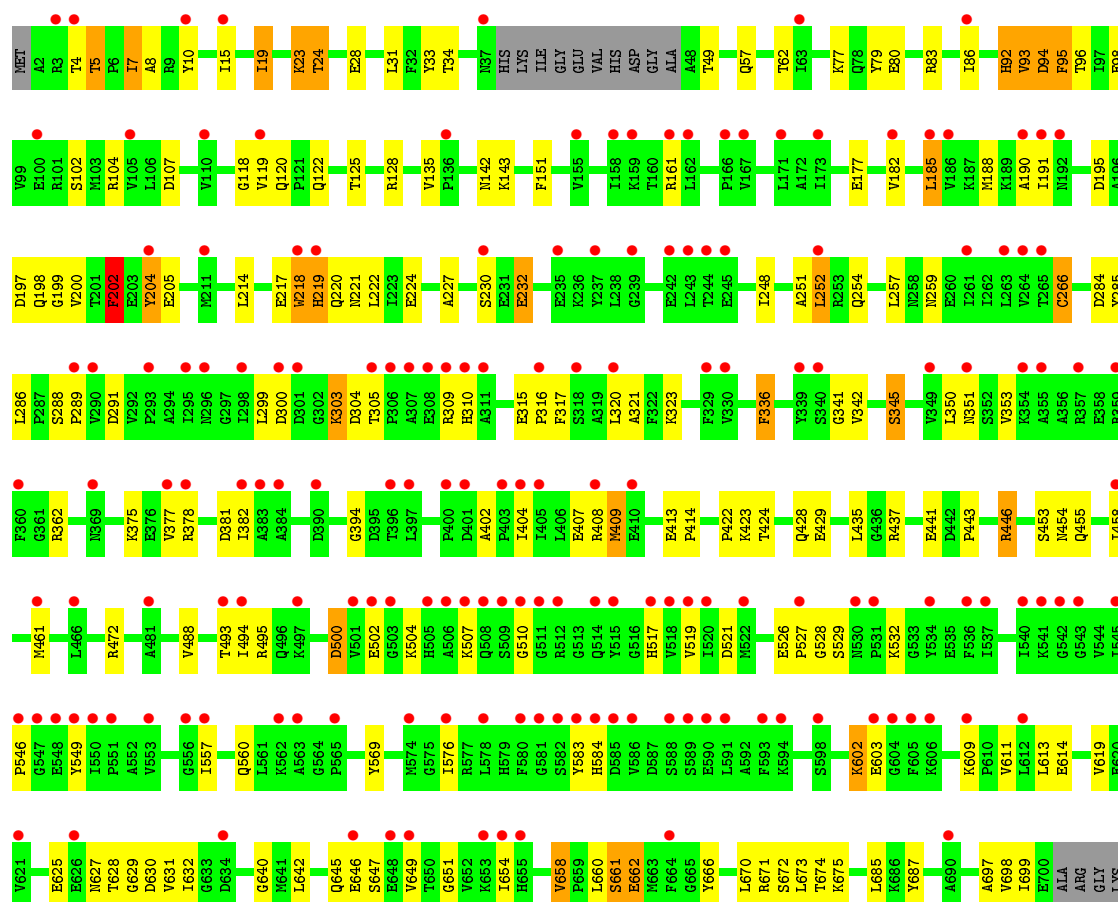


• Molecule 55: Elongation factor G

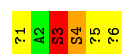
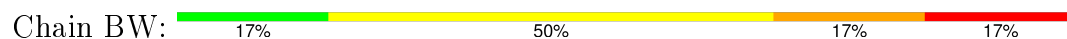


• Molecule 55: Elongation factor G

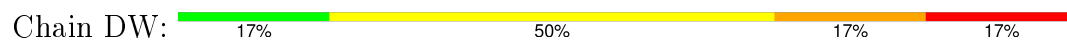




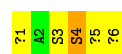
- Molecule 56: Viomycin



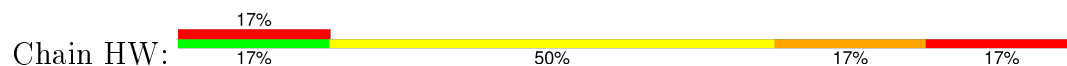
- Molecule 56: Viomycin



- Molecule 56: Viomycin



- Molecule 56: Viomycin



?	A2	S3	S4	?	?
1				5	6

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	361.60Å 361.77Å 433.20Å 90.00° 103.57° 90.00°	Depositor
Resolution (Å)	70.00 – 2.90 69.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (70.00-2.90) 78.9 (69.05-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.223 , 0.272 0.230 , 0.276	Depositor DCC
R_{free} test set	8388 reflections (0.45%)	DCC
Wilson B-factor (Å ²)	73.3	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 28.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 1874570 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	592086	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.65 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4952e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, DPP, MG, KBE, GCP, UAL, 5OH

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	AB	0.66	0/2828	1.10	2/4410 (0.0%)
1	CB	0.53	0/2828	1.02	1/4410 (0.0%)
1	EB	0.63	0/2828	1.15	8/4410 (0.2%)
1	GB	0.75	0/2828	1.13	10/4410 (0.2%)
2	AC	0.54	0/2121	0.79	2/2852 (0.1%)
2	CC	0.46	0/2121	0.72	2/2852 (0.1%)
2	EC	0.52	0/2121	0.76	2/2852 (0.1%)
2	GC	0.46	0/2121	0.74	1/2852 (0.0%)
3	AA	0.81	17/68626 (0.0%)	1.22	304/107056 (0.3%)
3	CA	0.62	4/68626 (0.0%)	1.08	117/107056 (0.1%)
3	EA	0.76	17/68626 (0.0%)	1.22	292/107056 (0.3%)
3	GA	0.64	0/68626	1.14	193/107056 (0.2%)
4	AD	0.57	0/1586	0.77	1/2134 (0.0%)
4	CD	0.51	0/1586	0.75	1/2134 (0.0%)
4	ED	0.55	0/1586	0.74	0/2134
4	GD	0.48	0/1586	0.72	1/2134 (0.0%)
5	AE	0.53	0/1571	0.76	2/2113 (0.1%)
5	CE	0.43	0/1571	0.66	0/2113
5	EE	0.51	0/1571	0.72	0/2113
5	GE	0.54	0/1571	0.75	2/2113 (0.1%)
6	AF	0.49	0/1434	0.71	1/1926 (0.1%)
6	CF	0.48	0/1434	0.70	0/1926
6	EF	0.50	0/1434	0.73	0/1926
6	GF	0.60	0/1434	0.75	0/1926
7	AG	0.55	0/1343	0.73	0/1816
7	CG	0.49	0/1343	0.73	1/1816 (0.1%)
7	EG	0.50	0/1343	0.75	0/1816
7	GG	0.51	0/1343	0.68	0/1816
8	AH	0.53	0/389	0.73	0/523
8	CH	0.61	0/389	0.74	0/523
8	EH	0.50	0/389	0.73	0/523
8	GH	0.55	0/389	0.69	0/523

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	AI	0.62	0/1046	0.84	1/1410 (0.1%)
9	CI	0.57	0/1046	0.72	0/1410
9	EI	0.53	0/1046	0.72	0/1410
9	GI	0.71	0/1046	0.80	0/1410
10	AJ	0.63	1/1152 (0.1%)	0.78	0/1551
10	CJ	0.52	1/1152 (0.1%)	0.72	0/1551
10	EJ	0.63	1/1152 (0.1%)	0.78	0/1551
10	GJ	0.48	0/1152	0.71	1/1551 (0.1%)
11	AK	0.65	1/947 (0.1%)	0.77	0/1268
11	CK	0.55	0/947	0.78	0/1268
11	EK	0.53	0/947	0.74	0/1268
11	GK	0.49	0/947	0.77	0/1268
12	AL	0.56	0/1054	0.79	2/1403 (0.1%)
12	CL	0.44	0/1054	0.74	1/1403 (0.1%)
12	EL	0.55	0/1054	0.77	1/1403 (0.1%)
12	GL	0.53	0/1054	0.73	0/1403
13	AM	0.61	0/1093	0.77	0/1460
13	CM	0.47	0/1093	0.67	0/1460
13	EM	0.55	0/1093	0.72	0/1460
13	GM	0.48	0/1093	0.68	0/1460
14	AN	0.51	0/973	0.68	0/1301
14	CN	0.45	0/973	0.64	0/1301
14	EN	0.48	0/973	0.65	0/1301
14	GN	0.45	0/973	0.65	0/1301
15	AO	0.46	0/902	0.70	0/1209
15	CO	0.42	0/902	0.70	0/1209
15	EO	0.44	0/902	0.74	0/1209
15	GO	0.55	0/902	0.82	1/1209 (0.1%)
16	AP	0.52	0/929	0.78	1/1242 (0.1%)
16	CP	0.51	0/929	0.80	0/1242
16	EP	0.55	0/929	0.80	0/1242
16	GP	0.51	0/929	0.81	2/1242 (0.2%)
17	AQ	0.62	0/960	0.71	1/1278 (0.1%)
17	CQ	0.50	0/960	0.67	0/1278
17	EQ	0.58	0/960	0.68	0/1278
17	GQ	0.49	0/960	0.69	1/1278 (0.1%)
18	AR	0.61	1/829 (0.1%)	0.76	0/1107
18	CR	0.50	0/829	0.70	0/1107
18	ER	0.57	1/829 (0.1%)	0.77	0/1107
18	GR	0.55	0/829	0.78	1/1107 (0.1%)
19	AS	0.54	0/864	0.73	0/1156
19	CS	0.46	0/864	0.66	0/1156
19	ES	0.52	0/864	0.75	0/1156

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	GS	0.45	0/864	0.75	2/1156 (0.2%)
20	AT	0.54	0/744	0.85	1/994 (0.1%)
20	CT	0.49	0/744	0.74	0/994
20	ET	0.59	0/744	0.87	3/994 (0.3%)
20	GT	0.54	0/744	0.76	0/994
21	AU	0.56	0/787	0.78	0/1051
21	CU	0.47	0/787	0.69	0/1051
21	EU	0.48	0/787	0.79	0/1051
21	GU	0.56	0/787	0.73	0/1051
22	AV	0.48	0/766	0.67	1/1025 (0.1%)
22	CV	0.44	0/766	0.62	0/1025
22	EV	0.49	0/766	0.67	0/1025
22	GV	0.55	0/766	0.70	0/1025
23	AW	0.69	0/603	1.00	1/797 (0.1%)
23	CW	0.63	0/603	0.88	0/797
23	EW	0.69	0/603	0.97	0/797
23	GW	0.63	0/603	0.87	0/797
24	AX	0.50	0/635	0.79	1/848 (0.1%)
24	CX	0.41	0/635	0.71	0/848
24	EX	0.51	0/635	0.78	0/848
24	GX	0.45	0/635	0.68	0/848
25	AY	0.46	0/510	0.75	0/677
25	CY	0.47	0/510	0.74	0/677
25	EY	0.49	0/510	0.81	0/677
25	GY	0.55	0/510	0.75	0/677
26	AZ	0.54	0/453	0.84	1/605 (0.2%)
26	CZ	0.48	0/453	0.80	1/605 (0.2%)
26	EZ	0.50	0/453	0.75	2/605 (0.3%)
26	GZ	0.57	0/453	0.83	0/605
27	A0	0.54	0/450	0.70	0/599
27	C0	0.48	0/450	0.69	0/599
27	E0	0.49	0/450	0.71	1/599 (0.2%)
27	G0	0.43	0/450	0.64	0/599
28	A1	0.53	0/416	0.74	0/554
28	C1	0.49	0/416	0.73	0/554
28	E1	0.49	0/416	0.70	0/554
28	G1	0.54	0/416	0.78	0/554
29	A2	0.53	0/380	0.70	0/498
29	C2	0.46	0/380	0.77	0/498
29	E2	0.51	0/380	0.69	0/498
29	G2	0.48	0/380	0.65	0/498
30	A3	0.53	0/513	0.75	0/676
30	C3	0.41	0/513	0.63	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	E3	0.54	0/513	0.74	0/676
30	G3	0.49	0/513	0.65	0/676
31	A4	0.59	0/303	0.84	0/397
31	C4	0.48	0/303	0.70	0/397
31	E4	0.56	0/303	0.78	1/397 (0.3%)
31	G4	0.50	0/303	0.78	0/397
32	A5	0.74	0/1131	1.32	26/1524 (1.7%)
32	C5	0.70	0/1131	1.31	26/1524 (1.7%)
32	E5	0.69	0/1115	1.33	24/1502 (1.6%)
33	A6	0.59	0/227	0.65	0/304
34	BB	0.49	0/1735	0.71	0/2338
34	DB	0.51	0/1735	0.72	0/2338
34	FB	0.50	0/1735	0.76	0/2338
34	HB	0.56	0/1735	0.73	0/2338
35	BA	0.65	3/36834 (0.0%)	1.14	96/57462 (0.2%)
35	DA	0.60	0/36834	1.06	47/57462 (0.1%)
35	FA	0.62	1/36834 (0.0%)	1.11	98/57462 (0.2%)
35	HA	0.72	2/36834 (0.0%)	1.11	74/57462 (0.1%)
36	BC	0.45	0/1651	0.69	0/2225
36	DC	0.43	0/1651	0.66	0/2225
36	FC	0.46	0/1651	0.70	0/2225
36	HC	0.57	0/1651	0.73	1/2225 (0.0%)
37	BD	0.53	0/1665	0.79	0/2227
37	DD	0.51	0/1665	0.73	0/2227
37	FD	0.52	0/1665	0.69	0/2227
37	HD	0.52	0/1665	0.73	0/2227
38	BE	0.49	0/1118	0.76	0/1504
38	DE	0.46	0/1118	0.71	0/1504
38	FE	0.47	0/1118	0.69	0/1504
38	HE	0.48	0/1118	0.68	0/1504
39	BF	0.50	0/851	0.70	0/1150
39	DF	0.54	0/835	0.75	0/1128
39	FF	0.47	0/835	0.72	0/1128
39	HF	0.56	0/835	0.73	0/1128
40	BG	0.49	0/1195	0.67	0/1602
40	DG	0.52	0/1195	0.69	0/1602
40	FG	0.48	0/1195	0.69	0/1602
40	HG	0.60	0/1195	0.74	1/1602 (0.1%)
41	BH	0.48	0/989	0.65	0/1326
41	DH	0.48	0/989	0.63	0/1326
41	FH	0.44	0/989	0.62	0/1326
41	HH	0.54	0/989	0.77	1/1326 (0.1%)
42	BI	0.54	0/1034	0.81	0/1375

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
42	DI	0.52	0/1034	0.70	0/1375
42	FI	0.54	0/1034	0.77	0/1375
42	HI	0.57	0/1034	0.79	2/1375 (0.1%)
43	BJ	0.54	0/796	0.80	0/1077
43	DJ	0.55	0/796	0.73	0/1077
43	FJ	0.51	0/796	0.74	0/1077
43	HJ	0.59	0/796	0.80	0/1077
44	BK	0.50	0/893	0.74	0/1205
44	DK	0.51	0/893	0.67	0/1205
44	FK	0.50	0/893	0.75	1/1205 (0.1%)
44	HK	0.63	0/893	0.79	0/1205
45	BL	0.54	0/969	0.82	0/1300
45	DL	0.51	0/969	0.79	0/1300
45	FL	0.47	0/969	0.78	0/1300
45	HL	0.47	0/969	0.77	0/1300
46	BM	0.48	0/892	0.70	0/1193
46	DM	0.51	0/892	0.71	0/1193
46	FM	0.42	0/892	0.71	0/1193
46	HM	0.66	0/892	0.80	0/1193
47	BN	0.48	0/785	0.78	0/1043
47	DN	0.47	0/785	0.72	0/1043
47	FN	0.50	0/785	0.80	0/1043
47	HN	0.53	0/785	0.73	0/1043
48	BO	0.44	0/722	0.66	0/964
48	DO	0.44	0/722	0.67	0/964
48	FO	0.42	0/722	0.63	0/964
48	HO	0.56	0/722	0.69	0/964
49	BP	0.48	0/659	0.74	0/884
49	DP	0.45	0/659	0.69	0/884
49	FP	0.48	0/659	0.68	0/884
49	HP	0.46	0/659	0.65	0/884
50	BQ	0.46	0/657	0.73	0/881
50	DQ	0.49	0/657	0.82	2/881 (0.2%)
50	FQ	0.47	0/657	0.68	0/881
50	HQ	0.53	0/657	0.78	0/881
51	BR	0.45	0/462	0.62	0/621
51	DR	0.50	0/462	0.67	0/621
51	FR	0.46	0/462	0.62	0/621
51	HR	0.58	0/462	0.74	1/621 (0.2%)
52	BS	0.47	0/652	0.81	0/877
52	DS	0.50	0/652	0.72	0/877
52	FS	0.46	0/652	0.71	0/877
52	HS	0.67	0/652	0.85	1/877 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
53	BT	0.47	0/671	0.60	0/888
53	DT	0.49	0/671	0.64	0/888
53	FT	0.45	0/671	0.64	0/888
53	HT	0.43	0/671	0.66	0/888
54	BU	0.66	0/430	0.84	0/570
54	DU	0.73	0/430	0.83	0/570
54	FU	0.73	1/430 (0.2%)	0.88	0/570
54	HU	0.68	0/430	0.73	0/570
55	BV	0.46	0/5444	0.67	2/7367 (0.0%)
55	DV	0.45	0/5439	0.65	0/7360
55	FV	0.46	0/5439	0.65	1/7360 (0.0%)
55	HV	0.48	0/5439	0.65	0/7360
56	BW	2.29	1/11 (9.1%)	1.55	0/13
56	DW	2.28	1/11 (9.1%)	1.54	0/13
56	FW	2.37	1/11 (9.1%)	1.57	0/13
56	HW	2.38	1/11 (9.1%)	1.80	0/13
All	All	0.64	55/636829 (0.0%)	1.05	1375/948879 (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
2	AC	0	1
2	GC	0	1
4	AD	0	1
4	CD	0	2
4	ED	0	1
4	GD	0	1
10	AJ	0	1
10	GJ	0	1
11	AK	0	1
32	A5	0	1
39	BF	0	1
39	FF	0	1
42	DI	0	1
45	BL	0	1
45	DL	0	1
45	HL	0	1
53	DT	0	1
55	BV	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
55	DV	0	1
55	FV	0	1
55	HV	0	1
All	All	0	22

The worst 5 of 55 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	HA	753	A	N7-C5	8.68	1.44	1.39
3	EA	528	A	N9-C4	-8.47	1.32	1.37
3	AA	984	A	N9-C4	-8.47	1.32	1.37
35	BA	1362	A	N7-C5	7.96	1.44	1.39
3	AA	528	A	N9-C4	-6.66	1.33	1.37

The worst 5 of 1375 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AA	1073	A	N1-C6-N6	-20.05	106.57	118.60
3	EA	1936	A	N1-C6-N6	15.79	128.07	118.60
3	AA	1073	A	C5-C6-N6	14.08	134.96	123.70
3	AA	2053	G	N1-C6-O6	13.88	128.23	119.90
3	EA	1936	A	C5-C6-N6	-13.76	112.69	123.70

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	A5	130	PRO	Peptide
2	AC	233	GLY	Peptide
4	AD	9	VAL	Peptide
10	AJ	110	PRO	Peptide
11	AK	71	ARG	Peptide

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	AB	2529	0	1281	20	0
1	CB	2529	0	1281	30	0
1	EB	2529	0	1281	33	0
1	GB	2529	0	1281	59	0
2	AC	2082	0	2157	52	0
2	CC	2082	0	2157	66	0
2	EC	2082	0	2157	65	0
2	GC	2082	0	2157	68	0
3	AA	61274	0	30819	778	0
3	CA	61274	0	30819	819	0
3	EA	61274	0	30819	734	0
3	GA	61274	0	30817	1239	2
4	AD	1565	0	1616	53	0
4	CD	1565	0	1616	49	0
4	ED	1565	0	1616	49	0
4	GD	1565	0	1616	48	0
5	AE	1552	0	1619	36	0
5	CE	1552	0	1619	44	0
5	EE	1552	0	1619	34	0
5	GE	1552	0	1619	72	0
6	AF	1410	0	1447	41	0
6	CF	1410	0	1447	39	0
6	EF	1410	0	1447	48	0
6	GF	1410	0	1447	57	0
7	AG	1323	0	1374	39	0
7	CG	1323	0	1374	50	0
7	EG	1323	0	1374	43	0
7	GG	1323	0	1374	56	0
8	AH	384	0	405	14	0
8	CH	384	0	405	20	0
8	EH	384	0	405	9	0
8	GH	384	0	405	7	0
9	AI	1032	0	1088	52	0
9	CI	1032	0	1088	38	0
9	EI	1032	0	1088	45	0
9	GI	1032	0	1088	64	0
10	AJ	1129	0	1162	53	0
10	CJ	1129	0	1162	54	0
10	EJ	1129	0	1162	49	0
10	GJ	1129	0	1162	53	0
11	AK	938	0	1012	40	0
11	CK	938	0	1012	38	0
11	EK	938	0	1012	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	GK	938	0	1012	24	0
12	AL	1045	0	1117	35	0
12	CL	1045	0	1116	36	0
12	EL	1045	0	1117	34	0
12	GL	1045	0	1117	52	0
13	AM	1074	0	1157	26	0
13	CM	1074	0	1157	32	0
13	EM	1074	0	1157	23	0
13	GM	1074	0	1157	26	0
14	AN	960	0	1000	30	0
14	CN	960	0	1000	34	0
14	EN	960	0	1000	24	0
14	GN	960	0	1000	23	0
15	AO	892	0	923	18	0
15	CO	892	0	923	27	0
15	EO	892	0	923	18	0
15	GO	892	0	923	32	0
16	AP	917	0	965	44	0
16	CP	917	0	965	41	0
16	EP	917	0	965	44	0
16	GP	917	0	965	36	0
17	AQ	947	0	1022	52	0
17	CQ	947	0	1022	50	0
17	EQ	947	0	1022	44	0
17	GQ	947	0	1022	56	0
18	AR	816	0	839	35	0
18	CR	816	0	839	36	0
18	ER	816	0	839	34	0
18	GR	816	0	839	46	0
19	AS	857	0	922	29	0
19	CS	857	0	922	18	0
19	ES	857	0	922	20	0
19	GS	857	0	922	29	0
20	AT	738	0	807	35	0
20	CT	738	0	807	26	0
20	ET	738	0	807	33	0
20	GT	738	0	807	29	0
21	AU	779	0	834	27	0
21	CU	779	0	834	12	0
21	EU	779	0	834	23	0
21	GU	779	0	834	29	0
22	AV	753	0	780	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	CV	753	0	780	17	0
22	EV	753	0	780	10	0
22	GV	753	0	780	13	0
23	AW	596	0	610	77	0
23	CW	596	0	610	62	0
23	EW	596	0	610	74	0
23	GW	596	0	610	60	0
24	AX	625	0	655	17	0
24	CX	625	0	655	14	0
24	EX	625	0	655	21	0
24	GX	625	0	655	18	0
25	AY	509	0	543	13	0
25	CY	509	0	543	9	0
25	EY	509	0	543	16	0
25	GY	509	0	543	11	0
26	AZ	449	0	491	16	0
26	CZ	449	0	491	21	0
26	EZ	449	0	491	10	0
26	GZ	449	0	491	27	0
27	A0	444	0	461	19	0
27	C0	444	0	461	17	0
27	E0	444	0	461	12	0
27	G0	444	0	461	8	0
28	A1	409	0	440	15	0
28	C1	409	0	440	11	0
28	E1	409	0	440	15	0
28	G1	409	0	440	17	0
29	A2	377	0	418	5	0
29	C2	377	0	418	11	0
29	E2	377	0	418	9	0
29	G2	377	0	418	17	0
30	A3	504	0	574	10	0
30	C3	504	0	574	7	0
30	E3	504	0	574	15	0
30	G3	504	0	574	27	0
31	A4	302	0	340	15	0
31	C4	302	0	340	12	0
31	E4	302	0	340	8	0
31	G4	302	0	340	12	0
32	A5	1117	0	1155	122	0
32	C5	1117	0	1155	136	0
32	E5	1101	0	1140	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	A6	227	0	237	7	0
34	BB	1704	0	1732	54	0
34	DB	1704	0	1732	62	0
34	FB	1704	0	1732	74	0
34	HB	1704	0	1732	58	0
35	BA	32895	0	16553	336	0
35	DA	32895	0	16553	472	0
35	FA	32895	0	16553	401	1
35	HA	32895	0	16552	581	0
36	BC	1624	0	1696	33	0
36	DC	1624	0	1696	41	0
36	FC	1624	0	1696	44	0
36	HC	1624	0	1696	35	0
37	BD	1643	0	1707	69	0
37	DD	1643	0	1707	63	0
37	FD	1643	0	1707	63	0
37	HD	1643	0	1707	73	0
38	BE	1105	0	1148	45	0
38	DE	1105	0	1148	35	0
38	FE	1105	0	1148	36	0
38	HE	1105	0	1148	36	0
39	BF	832	0	824	23	0
39	DF	817	0	808	36	0
39	FF	817	0	808	21	0
39	HF	817	0	808	36	0
40	BG	1181	0	1238	22	0
40	DG	1181	0	1238	30	0
40	FG	1181	0	1238	18	0
40	HG	1181	0	1238	50	0
41	BH	979	0	1031	28	0
41	DH	979	0	1031	25	0
41	FH	979	0	1031	28	0
41	HH	979	0	1031	33	0
42	BI	1022	0	1070	46	0
42	DI	1022	0	1070	39	0
42	FI	1022	0	1070	43	0
42	HI	1022	0	1070	38	0
43	BJ	786	0	828	23	0
43	DJ	786	0	828	28	0
43	FJ	786	0	828	18	1
43	HJ	786	0	828	29	0
44	BK	877	0	887	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	DK	877	0	887	40	0
44	FK	877	0	887	40	0
44	HK	877	0	887	57	0
45	BL	955	0	1016	36	0
45	DL	955	0	1016	37	0
45	FL	955	0	1016	33	0
45	HL	955	0	1016	41	0
46	BM	883	0	941	20	0
46	DM	883	0	941	33	0
46	FM	883	0	941	33	0
46	HM	883	0	941	39	0
47	BN	774	0	824	25	0
47	DN	774	0	824	31	0
47	FN	774	0	824	27	0
47	HN	774	0	824	28	0
48	BO	714	0	734	8	0
48	DO	714	0	734	13	0
48	FO	714	0	734	12	0
48	HO	714	0	734	18	0
49	BP	649	0	666	13	0
49	DP	649	0	666	17	0
49	FP	649	0	666	15	0
49	HP	649	0	666	12	0
50	BQ	648	0	691	11	0
50	DQ	648	0	691	33	0
50	FQ	648	0	691	23	0
50	HQ	648	0	691	28	0
51	BR	455	0	478	10	0
51	DR	455	0	478	9	0
51	FR	455	0	478	4	0
51	HR	455	0	478	24	0
52	BS	637	0	665	18	0
52	DS	637	0	665	14	0
52	FS	637	0	665	29	0
52	HS	637	0	665	32	0
53	BT	665	0	714	11	0
53	DT	665	0	714	23	0
53	FT	665	0	714	15	0
53	HT	665	0	714	13	0
54	BU	425	0	449	30	0
54	DU	425	0	449	17	0
54	FU	425	0	449	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	HU	425	0	449	27	0
55	BV	5345	0	5311	117	0
55	DV	5340	0	5306	132	0
55	FV	5340	0	5306	103	0
55	HV	5340	0	5307	116	0
56	BW	48	0	41	5	0
56	DW	48	0	41	5	0
56	FW	48	0	41	3	0
56	HW	48	0	40	6	0
57	A4	1	0	0	0	0
57	AA	136	0	0	0	0
57	AB	4	0	0	0	0
57	AC	1	0	0	0	0
57	AE	1	0	0	0	0
57	BA	40	0	0	0	0
57	BE	1	0	0	0	0
57	BN	1	0	0	0	0
57	BU	1	0	0	0	0
57	BV	1	0	0	0	0
57	C4	1	0	0	0	0
57	CA	136	0	0	0	0
57	CB	4	0	0	0	0
57	CE	1	0	0	0	0
57	CN	1	0	0	0	0
57	DA	43	0	0	0	0
57	DV	1	0	0	0	0
57	EA	137	0	0	0	0
57	EB	4	0	0	0	0
57	ED	1	0	0	0	0
57	EE	1	0	0	0	0
57	FA	39	0	0	0	0
57	FE	1	0	0	0	0
57	FN	2	0	0	0	0
57	FU	1	0	0	0	0
57	FV	1	0	0	0	0
57	GA	136	0	0	0	0
57	GB	4	0	0	0	0
57	GC	2	0	0	0	0
57	GL	1	0	0	0	0
57	HA	41	0	0	0	0
57	HE	1	0	0	0	0
57	HK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	HV	1	0	0	0	0
58	A4	1	0	0	0	0
58	C4	1	0	0	0	0
58	E4	1	0	0	0	0
58	G4	1	0	0	0	0
59	BV	32	0	14	1	0
59	DV	32	0	14	2	0
59	FV	32	0	14	2	0
59	HV	32	0	14	1	0
60	A0	2	0	0	0	0
60	A2	1	0	0	0	0
60	A3	1	0	0	0	0
60	A4	1	0	0	0	0
60	AA	614	0	0	102	0
60	AB	18	0	0	1	0
60	AC	6	0	0	1	0
60	AD	4	0	0	0	0
60	AE	1	0	0	0	0
60	AF	1	0	0	0	0
60	AJ	1	0	0	0	0
60	AL	5	0	0	1	0
60	AN	2	0	0	0	0
60	AP	1	0	0	0	0
60	AQ	2	0	0	0	0
60	AS	1	0	0	0	0
60	BA	202	0	0	31	0
60	BL	1	0	0	0	0
60	BN	2	0	0	0	0
60	BT	2	0	0	0	0
60	BV	1	0	0	1	0
60	C0	1	0	0	0	0
60	C2	1	0	0	0	0
60	C3	1	0	0	0	0
60	C4	2	0	0	0	0
60	CA	607	0	0	84	0
60	CB	21	0	0	2	0
60	CC	8	0	0	0	0
60	CD	3	0	0	0	0
60	CE	1	0	0	0	0
60	CJ	2	0	0	1	0
60	CL	5	0	0	0	0
60	CN	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	CQ	1	0	0	1	0
60	CS	2	0	0	1	0
60	CT	2	0	0	1	0
60	CU	1	0	0	0	0
60	DA	186	0	0	27	0
60	DC	2	0	0	0	0
60	DD	1	0	0	0	0
60	DE	1	0	0	0	0
60	DG	1	0	0	0	0
60	DK	1	0	0	0	0
60	DL	2	0	0	0	0
60	DN	8	0	0	3	0
60	DQ	1	0	0	0	0
60	DT	4	0	0	1	0
60	DU	1	0	0	0	0
60	DV	1	0	0	0	0
60	E0	1	0	0	0	0
60	E2	1	0	0	0	0
60	E3	2	0	0	0	0
60	E4	2	0	0	0	0
60	EA	610	0	0	105	0
60	EB	18	0	0	3	0
60	EC	9	0	0	1	0
60	ED	3	0	0	0	0
60	EE	2	0	0	1	0
60	EL	4	0	0	0	0
60	EN	3	0	0	0	0
60	ER	1	0	0	0	0
60	ET	2	0	0	0	0
60	EV	2	0	0	0	0
60	FA	197	0	0	24	0
60	FC	1	0	0	0	0
60	FE	2	0	0	0	0
60	FN	3	0	0	0	0
60	FT	4	0	0	0	0
60	FU	1	0	0	0	0
60	FV	1	0	0	0	0
60	G2	2	0	0	0	0
60	G3	1	0	0	0	0
60	G4	1	0	0	0	0
60	GA	606	0	0	136	0
60	GB	19	0	0	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	GC	10	0	0	0	0
60	GD	3	0	0	0	0
60	GE	2	0	0	1	0
60	GJ	1	0	0	0	0
60	GL	4	0	0	1	0
60	GN	4	0	0	0	0
60	GQ	1	0	0	0	0
60	GR	2	0	0	1	0
60	GS	2	0	0	0	0
60	GU	1	0	0	0	0
60	GV	1	0	0	0	0
60	HA	193	0	0	31	0
60	HD	3	0	0	2	0
60	HE	3	0	0	0	0
60	HN	7	0	0	3	0
60	HQ	1	0	0	0	0
60	HT	1	0	0	0	0
60	HV	1	0	0	0	0
All	All	592086	0	404164	11056	2

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 12.

The worst 5 of 11056 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)
32:C5:24:SER:CB	32:C5:116:GLU:HG2	1.46	1.44
32:C5:24:SER:O	32:C5:116:GLU:HB3	1.41	1.16
32:C5:24:SER:HB2	32:C5:116:GLU:CG	1.76	1.14
32:E5:24:SER:HB2	32:E5:116:GLU:HG2	1.27	1.14
3:AA:912:C:OP1	13:AM:8:LYS:NZ	1.79	1.12

All (2) 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)
35:FA:1029:U:O3'	3:GA:1508:A:N6[1_565]	2.04	0.16
43:FJ:85:ASP:OD1	3:GA:1722:A:O2'[1_565]	2.16	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	AC	269/273 (98%)	211 (78%)	43 (16%)	15 (6%)	2	7
2	CC	269/273 (98%)	211 (78%)	42 (16%)	16 (6%)	2	6
2	EC	269/273 (98%)	212 (79%)	44 (16%)	13 (5%)	3	10
2	GC	269/273 (98%)	210 (78%)	42 (16%)	17 (6%)	2	5
4	AD	207/209 (99%)	163 (79%)	30 (14%)	14 (7%)	1	4
4	CD	207/209 (99%)	166 (80%)	27 (13%)	14 (7%)	1	4
4	ED	207/209 (99%)	165 (80%)	29 (14%)	13 (6%)	2	5
4	GD	207/209 (99%)	161 (78%)	32 (16%)	14 (7%)	1	4
5	AE	199/201 (99%)	162 (81%)	27 (14%)	10 (5%)	3	9
5	CE	199/201 (99%)	159 (80%)	27 (14%)	13 (6%)	1	4
5	EE	199/201 (99%)	164 (82%)	24 (12%)	11 (6%)	2	7
5	GE	199/201 (99%)	159 (80%)	30 (15%)	10 (5%)	3	9
6	AF	175/179 (98%)	141 (81%)	30 (17%)	4 (2%)	8	30
6	CF	175/179 (98%)	145 (83%)	25 (14%)	5 (3%)	6	23
6	EF	175/179 (98%)	140 (80%)	26 (15%)	9 (5%)	2	9
6	GF	175/179 (98%)	140 (80%)	26 (15%)	9 (5%)	2	9
7	AG	174/177 (98%)	127 (73%)	30 (17%)	17 (10%)	1	2
7	CG	174/177 (98%)	131 (75%)	28 (16%)	15 (9%)	1	2
7	EG	174/177 (98%)	125 (72%)	35 (20%)	14 (8%)	1	3
7	GG	174/177 (98%)	126 (72%)	30 (17%)	18 (10%)	1	1
8	AH	48/50 (96%)	29 (60%)	14 (29%)	5 (10%)	1	1
8	CH	48/50 (96%)	31 (65%)	12 (25%)	5 (10%)	1	1
8	EH	48/50 (96%)	31 (65%)	12 (25%)	5 (10%)	1	1
8	GH	48/50 (96%)	30 (62%)	15 (31%)	3 (6%)	2	5
9	AI	139/142 (98%)	97 (70%)	33 (24%)	9 (6%)	1	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	CI	139/142 (98%)	95 (68%)	38 (27%)	6 (4%)	3	13
9	EI	139/142 (98%)	97 (70%)	38 (27%)	4 (3%)	6	23
9	GI	139/142 (98%)	95 (68%)	34 (24%)	10 (7%)	1	3
10	AJ	140/142 (99%)	113 (81%)	18 (13%)	9 (6%)	2	5
10	CJ	140/142 (99%)	112 (80%)	20 (14%)	8 (6%)	2	6
10	EJ	140/142 (99%)	114 (81%)	17 (12%)	9 (6%)	2	5
10	GJ	140/142 (99%)	113 (81%)	19 (14%)	8 (6%)	2	6
11	AK	120/123 (98%)	96 (80%)	14 (12%)	10 (8%)	1	2
11	CK	120/123 (98%)	93 (78%)	21 (18%)	6 (5%)	3	9
11	EK	120/123 (98%)	92 (77%)	21 (18%)	7 (6%)	2	6
11	GK	120/123 (98%)	92 (77%)	20 (17%)	8 (7%)	1	4
12	AL	141/144 (98%)	104 (74%)	32 (23%)	5 (4%)	4	18
12	CL	141/144 (98%)	103 (73%)	33 (23%)	5 (4%)	4	18
12	EL	141/144 (98%)	108 (77%)	26 (18%)	7 (5%)	3	9
12	GL	141/144 (98%)	103 (73%)	32 (23%)	6 (4%)	3	13
13	AM	134/136 (98%)	107 (80%)	16 (12%)	11 (8%)	1	2
13	CM	134/136 (98%)	110 (82%)	16 (12%)	8 (6%)	2	6
13	EM	134/136 (98%)	106 (79%)	18 (13%)	10 (8%)	1	3
13	GM	134/136 (98%)	109 (81%)	17 (13%)	8 (6%)	2	6
14	AN	118/127 (93%)	101 (86%)	16 (14%)	1 (1%)	24	60
14	CN	118/127 (93%)	103 (87%)	14 (12%)	1 (1%)	24	60
14	EN	118/127 (93%)	100 (85%)	17 (14%)	1 (1%)	24	60
14	GN	118/127 (93%)	98 (83%)	19 (16%)	1 (1%)	24	60
15	AO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	21	57
15	CO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	4	18
15	EO	114/117 (97%)	95 (83%)	18 (16%)	1 (1%)	21	57
15	GO	114/117 (97%)	95 (83%)	15 (13%)	4 (4%)	4	18
16	AP	112/115 (97%)	86 (77%)	17 (15%)	9 (8%)	1	3
16	CP	112/115 (97%)	87 (78%)	16 (14%)	9 (8%)	1	3
16	EP	112/115 (97%)	84 (75%)	16 (14%)	12 (11%)	0	1
16	GP	112/115 (97%)	85 (76%)	19 (17%)	8 (7%)	1	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	18
17	CQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	18
17	EQ	115/118 (98%)	99 (86%)	12 (10%)	4 (4%)	4	18
17	GQ	115/118 (98%)	99 (86%)	14 (12%)	2 (2%)	11	38
18	AR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	22
18	CR	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	22
18	ER	101/103 (98%)	83 (82%)	15 (15%)	3 (3%)	5	22
18	GR	101/103 (98%)	83 (82%)	13 (13%)	5 (5%)	3	9
19	AS	108/110 (98%)	94 (87%)	9 (8%)	5 (5%)	3	11
19	CS	108/110 (98%)	95 (88%)	9 (8%)	4 (4%)	4	17
19	ES	108/110 (98%)	92 (85%)	10 (9%)	6 (6%)	2	7
19	GS	108/110 (98%)	91 (84%)	11 (10%)	6 (6%)	2	7
20	AT	91/100 (91%)	57 (63%)	24 (26%)	10 (11%)	0	1
20	CT	91/100 (91%)	55 (60%)	25 (28%)	11 (12%)	0	1
20	ET	91/100 (91%)	56 (62%)	26 (29%)	9 (10%)	1	2
20	GT	91/100 (91%)	58 (64%)	23 (25%)	10 (11%)	0	1
21	AU	100/104 (96%)	74 (74%)	16 (16%)	10 (10%)	1	2
21	CU	100/104 (96%)	75 (75%)	17 (17%)	8 (8%)	1	3
21	EU	100/104 (96%)	74 (74%)	15 (15%)	11 (11%)	0	1
21	GU	100/104 (96%)	76 (76%)	14 (14%)	10 (10%)	1	2
22	AV	92/94 (98%)	81 (88%)	11 (12%)	0	100	100
22	CV	92/94 (98%)	80 (87%)	11 (12%)	1 (1%)	17	51
22	EV	92/94 (98%)	80 (87%)	12 (13%)	0	100	100
22	GV	92/94 (98%)	78 (85%)	13 (14%)	1 (1%)	17	51
23	AW	77/85 (91%)	39 (51%)	22 (29%)	16 (21%)	0	0
23	CW	77/85 (91%)	41 (53%)	17 (22%)	19 (25%)	0	0
23	EW	77/85 (91%)	41 (53%)	21 (27%)	15 (20%)	0	0
23	GW	77/85 (91%)	40 (52%)	21 (27%)	16 (21%)	0	0
24	AX	75/78 (96%)	64 (85%)	8 (11%)	3 (4%)	4	15
24	CX	75/78 (96%)	63 (84%)	10 (13%)	2 (3%)	6	25
24	EX	75/78 (96%)	63 (84%)	9 (12%)	3 (4%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	GX	75/78 (96%)	63 (84%)	9 (12%)	3 (4%)	4	15
25	AY	61/63 (97%)	39 (64%)	18 (30%)	4 (7%)	1	4
25	CY	61/63 (97%)	42 (69%)	15 (25%)	4 (7%)	1	4
25	EY	61/63 (97%)	40 (66%)	17 (28%)	4 (7%)	1	4
25	GY	61/63 (97%)	39 (64%)	20 (33%)	2 (3%)	5	20
26	AZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	18
26	CZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	18
26	EZ	56/59 (95%)	46 (82%)	8 (14%)	2 (4%)	4	18
26	GZ	56/59 (95%)	44 (79%)	10 (18%)	2 (4%)	4	18
27	A0	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1	3
27	C0	54/57 (95%)	45 (83%)	3 (6%)	6 (11%)	0	1
27	E0	54/57 (95%)	44 (82%)	6 (11%)	4 (7%)	1	3
27	G0	54/57 (95%)	46 (85%)	4 (7%)	4 (7%)	1	3
28	A1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	2	5
28	C1	48/55 (87%)	42 (88%)	4 (8%)	2 (4%)	3	13
28	E1	48/55 (87%)	42 (88%)	4 (8%)	2 (4%)	3	13
28	G1	48/55 (87%)	42 (88%)	3 (6%)	3 (6%)	2	5
29	A2	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
29	C2	44/46 (96%)	41 (93%)	2 (4%)	1 (2%)	8	30
29	E2	44/46 (96%)	40 (91%)	4 (9%)	0	100	100
29	G2	44/46 (96%)	40 (91%)	3 (7%)	1 (2%)	8	30
30	A3	62/65 (95%)	53 (86%)	7 (11%)	2 (3%)	5	20
30	C3	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	5	20
30	E3	62/65 (95%)	56 (90%)	4 (6%)	2 (3%)	5	20
30	G3	62/65 (95%)	54 (87%)	6 (10%)	2 (3%)	5	20
31	A4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	2
31	C4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	2
31	E4	36/38 (95%)	29 (81%)	4 (11%)	3 (8%)	1	2
31	G4	36/38 (95%)	30 (83%)	2 (6%)	4 (11%)	0	1
32	A5	146/165 (88%)	77 (53%)	40 (27%)	29 (20%)	0	0
32	C5	146/165 (88%)	78 (53%)	45 (31%)	23 (16%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	E5	143/165 (87%)	79 (55%)	41 (29%)	23 (16%)	0	0
33	A6	28/121 (23%)	20 (71%)	7 (25%)	1 (4%)	4	18
34	BB	216/241 (90%)	151 (70%)	51 (24%)	14 (6%)	1	4
34	DB	216/241 (90%)	157 (73%)	47 (22%)	12 (6%)	2	7
34	FB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	2	7
34	HB	216/241 (90%)	153 (71%)	51 (24%)	12 (6%)	2	7
36	BC	204/233 (88%)	181 (89%)	18 (9%)	5 (2%)	7	27
36	DC	204/233 (88%)	179 (88%)	20 (10%)	5 (2%)	7	27
36	FC	204/233 (88%)	180 (88%)	18 (9%)	6 (3%)	6	23
36	HC	204/233 (88%)	181 (89%)	17 (8%)	6 (3%)	6	23
37	BD	203/206 (98%)	162 (80%)	30 (15%)	11 (5%)	2	7
37	DD	203/206 (98%)	162 (80%)	29 (14%)	12 (6%)	2	6
37	FD	203/206 (98%)	163 (80%)	29 (14%)	11 (5%)	2	7
37	HD	203/206 (98%)	165 (81%)	26 (13%)	12 (6%)	2	6
38	BE	148/167 (89%)	123 (83%)	18 (12%)	7 (5%)	3	11
38	DE	148/167 (89%)	125 (84%)	18 (12%)	5 (3%)	5	19
38	FE	148/167 (89%)	122 (82%)	20 (14%)	6 (4%)	3	14
38	HE	148/167 (89%)	121 (82%)	20 (14%)	7 (5%)	3	11
39	BF	100/135 (74%)	79 (79%)	15 (15%)	6 (6%)	2	6
39	DF	98/135 (73%)	80 (82%)	13 (13%)	5 (5%)	2	9
39	FF	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	2	5
39	HF	98/135 (73%)	76 (78%)	18 (18%)	4 (4%)	3	14
40	BG	149/179 (83%)	128 (86%)	20 (13%)	1 (1%)	26	63
40	DG	149/179 (83%)	125 (84%)	22 (15%)	2 (1%)	15	46
40	FG	149/179 (83%)	127 (85%)	21 (14%)	1 (1%)	26	63
40	HG	149/179 (83%)	127 (85%)	20 (13%)	2 (1%)	15	46
41	BH	127/130 (98%)	114 (90%)	12 (9%)	1 (1%)	24	60
41	DH	127/130 (98%)	113 (89%)	12 (9%)	2 (2%)	12	40
41	FH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	12	40
41	HH	127/130 (98%)	112 (88%)	13 (10%)	2 (2%)	12	40
42	BI	125/130 (96%)	105 (84%)	14 (11%)	6 (5%)	3	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	DI	125/130 (96%)	102 (82%)	22 (18%)	1 (1%)	24	60
42	FI	125/130 (96%)	106 (85%)	13 (10%)	6 (5%)	3	10
42	HI	125/130 (96%)	103 (82%)	19 (15%)	3 (2%)	7	29
43	BJ	96/103 (93%)	69 (72%)	20 (21%)	7 (7%)	1	3
43	DJ	96/103 (93%)	71 (74%)	19 (20%)	6 (6%)	2	5
43	FJ	96/103 (93%)	69 (72%)	21 (22%)	6 (6%)	2	5
43	HJ	96/103 (93%)	68 (71%)	19 (20%)	9 (9%)	1	2
44	BK	115/129 (89%)	97 (84%)	12 (10%)	6 (5%)	2	8
44	DK	115/129 (89%)	92 (80%)	19 (16%)	4 (4%)	4	18
44	FK	115/129 (89%)	96 (84%)	13 (11%)	6 (5%)	2	8
44	HK	115/129 (89%)	91 (79%)	15 (13%)	9 (8%)	1	3
45	BL	121/124 (98%)	101 (84%)	16 (13%)	4 (3%)	5	20
45	DL	121/124 (98%)	98 (81%)	20 (16%)	3 (2%)	7	27
45	FL	121/124 (98%)	100 (83%)	14 (12%)	7 (6%)	2	6
45	HL	121/124 (98%)	101 (84%)	15 (12%)	5 (4%)	3	14
46	BM	112/118 (95%)	98 (88%)	8 (7%)	6 (5%)	2	7
46	DM	112/118 (95%)	96 (86%)	11 (10%)	5 (4%)	3	12
46	FM	112/118 (95%)	99 (88%)	7 (6%)	6 (5%)	2	7
46	HM	112/118 (95%)	92 (82%)	12 (11%)	8 (7%)	1	3
47	BN	92/101 (91%)	73 (79%)	13 (14%)	6 (6%)	1	4
47	DN	92/101 (91%)	71 (77%)	19 (21%)	2 (2%)	8	31
47	FN	92/101 (91%)	71 (77%)	17 (18%)	4 (4%)	3	13
47	HN	92/101 (91%)	70 (76%)	18 (20%)	4 (4%)	3	13
48	BO	86/89 (97%)	75 (87%)	9 (10%)	2 (2%)	8	30
48	DO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
48	FO	86/89 (97%)	75 (87%)	11 (13%)	0	100	100
48	HO	86/89 (97%)	72 (84%)	11 (13%)	3 (4%)	4	18
49	BP	80/82 (98%)	60 (75%)	17 (21%)	3 (4%)	4	16
49	DP	80/82 (98%)	60 (75%)	15 (19%)	5 (6%)	2	5
49	FP	80/82 (98%)	62 (78%)	15 (19%)	3 (4%)	4	16
49	HP	80/82 (98%)	56 (70%)	21 (26%)	3 (4%)	4	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	BQ	78/84 (93%)	59 (76%)	15 (19%)	4 (5%)	2	9
50	DQ	78/84 (93%)	58 (74%)	14 (18%)	6 (8%)	1	3
50	FQ	78/84 (93%)	58 (74%)	17 (22%)	3 (4%)	4	16
50	HQ	78/84 (93%)	58 (74%)	13 (17%)	7 (9%)	1	2
51	BR	53/75 (71%)	47 (89%)	6 (11%)	0	100	100
51	DR	53/75 (71%)	46 (87%)	7 (13%)	0	100	100
51	FR	53/75 (71%)	48 (91%)	5 (9%)	0	100	100
51	HR	53/75 (71%)	49 (92%)	4 (8%)	0	100	100
52	BS	77/92 (84%)	65 (84%)	11 (14%)	1 (1%)	15	46
52	DS	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
52	FS	77/92 (84%)	64 (83%)	11 (14%)	2 (3%)	7	26
52	HS	77/92 (84%)	66 (86%)	9 (12%)	2 (3%)	7	26
53	BT	83/87 (95%)	74 (89%)	7 (8%)	2 (2%)	7	29
53	DT	83/87 (95%)	74 (89%)	6 (7%)	3 (4%)	4	18
53	FT	83/87 (95%)	75 (90%)	6 (7%)	2 (2%)	7	29
53	HT	83/87 (95%)	73 (88%)	8 (10%)	2 (2%)	7	29
54	BU	49/71 (69%)	26 (53%)	20 (41%)	3 (6%)	2	5
54	DU	49/71 (69%)	25 (51%)	20 (41%)	4 (8%)	1	2
54	FU	49/71 (69%)	24 (49%)	21 (43%)	4 (8%)	1	2
54	HU	49/71 (69%)	29 (59%)	18 (37%)	2 (4%)	3	14
55	BV	686/704 (97%)	559 (82%)	92 (13%)	35 (5%)	2	9
55	DV	685/704 (97%)	559 (82%)	93 (14%)	33 (5%)	3	10
55	FV	685/704 (97%)	564 (82%)	89 (13%)	32 (5%)	3	11
55	HV	685/704 (97%)	562 (82%)	88 (13%)	35 (5%)	2	9
56	BW	2/6 (33%)	0	0	2 (100%)	0	0
56	DW	2/6 (33%)	0	1 (50%)	1 (50%)	0	0
56	FW	2/6 (33%)	2 (100%)	0	0	100	100
56	HW	2/6 (33%)	1 (50%)	0	1 (50%)	0	0
All	All	25302/27000 (94%)	20075 (79%)	3885 (15%)	1342 (5%)	2	8

5 of 1342 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AC	70	LYS
2	AC	104	LEU
2	AC	121	ALA
2	AC	140	VAL
4	AD	43	ASP

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	AC	216/218 (99%)	202 (94%)	14 (6%)	21	52
2	CC	216/218 (99%)	197 (91%)	19 (9%)	12	35
2	EC	216/218 (99%)	194 (90%)	22 (10%)	9	27
2	GC	216/218 (99%)	203 (94%)	13 (6%)	24	57
4	AD	164/164 (100%)	151 (92%)	13 (8%)	15	41
4	CD	164/164 (100%)	152 (93%)	12 (7%)	17	45
4	ED	164/164 (100%)	152 (93%)	12 (7%)	17	45
4	GD	164/164 (100%)	151 (92%)	13 (8%)	15	41
5	AE	165/165 (100%)	146 (88%)	19 (12%)	7	21
5	CE	165/165 (100%)	157 (95%)	8 (5%)	31	67
5	EE	165/165 (100%)	153 (93%)	12 (7%)	17	45
5	GE	165/165 (100%)	152 (92%)	13 (8%)	15	41
6	AF	148/150 (99%)	138 (93%)	10 (7%)	20	49
6	CF	148/150 (99%)	140 (95%)	8 (5%)	27	62
6	EF	148/150 (99%)	133 (90%)	15 (10%)	9	28
6	GF	148/150 (99%)	146 (99%)	2 (1%)	74	93
7	AG	137/138 (99%)	122 (89%)	15 (11%)	8	23
7	CG	137/138 (99%)	125 (91%)	12 (9%)	12	35
7	EG	137/138 (99%)	119 (87%)	18 (13%)	5	15
7	GG	137/138 (99%)	128 (93%)	9 (7%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	AH	40/40 (100%)	39 (98%)	1 (2%)	55	85
8	CH	40/40 (100%)	38 (95%)	2 (5%)	30	65
8	EH	40/40 (100%)	37 (92%)	3 (8%)	17	44
8	GH	40/40 (100%)	39 (98%)	1 (2%)	55	85
9	AI	109/110 (99%)	105 (96%)	4 (4%)	41	77
9	CI	109/110 (99%)	106 (97%)	3 (3%)	51	84
9	EI	109/110 (99%)	106 (97%)	3 (3%)	51	84
9	GI	109/110 (99%)	107 (98%)	2 (2%)	66	90
10	AJ	116/116 (100%)	100 (86%)	16 (14%)	4	13
10	CJ	116/116 (100%)	101 (87%)	15 (13%)	5	16
10	EJ	116/116 (100%)	97 (84%)	19 (16%)	3	8
10	GJ	116/116 (100%)	104 (90%)	12 (10%)	9	26
11	AK	103/104 (99%)	92 (89%)	11 (11%)	8	24
11	CK	103/104 (99%)	87 (84%)	16 (16%)	3	10
11	EK	103/104 (99%)	87 (84%)	16 (16%)	3	10
11	GK	103/104 (99%)	90 (87%)	13 (13%)	5	16
12	AL	102/103 (99%)	95 (93%)	7 (7%)	19	48
12	CL	102/103 (99%)	94 (92%)	8 (8%)	16	41
12	EL	102/103 (99%)	96 (94%)	6 (6%)	24	58
12	GL	102/103 (99%)	96 (94%)	6 (6%)	24	58
13	AM	109/109 (100%)	93 (85%)	16 (15%)	4	11
13	CM	109/109 (100%)	98 (90%)	11 (10%)	9	28
13	EM	109/109 (100%)	100 (92%)	9 (8%)	14	38
13	GM	109/109 (100%)	103 (94%)	6 (6%)	27	61
14	AN	100/103 (97%)	93 (93%)	7 (7%)	19	47
14	CN	100/103 (97%)	96 (96%)	4 (4%)	38	74
14	EN	100/103 (97%)	96 (96%)	4 (4%)	38	74
14	GN	100/103 (97%)	93 (93%)	7 (7%)	19	47
15	AO	86/87 (99%)	78 (91%)	8 (9%)	11	32
15	CO	86/87 (99%)	80 (93%)	6 (7%)	19	47
15	EO	86/87 (99%)	81 (94%)	5 (6%)	25	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	GO	86/87 (99%)	81 (94%)	5 (6%)	25	58
16	AP	99/100 (99%)	91 (92%)	8 (8%)	15	39
16	CP	99/100 (99%)	90 (91%)	9 (9%)	12	34
16	EP	99/100 (99%)	88 (89%)	11 (11%)	8	22
16	GP	99/100 (99%)	90 (91%)	9 (9%)	12	34
17	AQ	89/90 (99%)	81 (91%)	8 (9%)	12	34
17	CQ	89/90 (99%)	84 (94%)	5 (6%)	26	60
17	EQ	89/90 (99%)	83 (93%)	6 (7%)	20	50
17	GQ	89/90 (99%)	83 (93%)	6 (7%)	20	50
18	AR	84/84 (100%)	78 (93%)	6 (7%)	18	47
18	CR	84/84 (100%)	79 (94%)	5 (6%)	24	57
18	ER	84/84 (100%)	76 (90%)	8 (10%)	11	31
18	GR	84/84 (100%)	79 (94%)	5 (6%)	24	57
19	AS	93/93 (100%)	84 (90%)	9 (10%)	10	30
19	CS	93/93 (100%)	86 (92%)	7 (8%)	17	44
19	ES	93/93 (100%)	84 (90%)	9 (10%)	10	30
19	GS	93/93 (100%)	88 (95%)	5 (5%)	27	62
20	AT	80/84 (95%)	77 (96%)	3 (4%)	40	76
20	CT	80/84 (95%)	75 (94%)	5 (6%)	22	54
20	ET	80/84 (95%)	74 (92%)	6 (8%)	17	44
20	GT	80/84 (95%)	77 (96%)	3 (4%)	40	76
21	AU	83/85 (98%)	76 (92%)	7 (8%)	14	37
21	CU	83/85 (98%)	80 (96%)	3 (4%)	42	78
21	EU	83/85 (98%)	78 (94%)	5 (6%)	24	57
21	GU	83/85 (98%)	79 (95%)	4 (5%)	31	67
22	AV	78/78 (100%)	75 (96%)	3 (4%)	40	76
22	CV	78/78 (100%)	73 (94%)	5 (6%)	22	53
22	EV	78/78 (100%)	75 (96%)	3 (4%)	40	76
22	GV	78/78 (100%)	77 (99%)	1 (1%)	76	94
23	AW	59/63 (94%)	53 (90%)	6 (10%)	9	27
23	CW	59/63 (94%)	55 (93%)	4 (7%)	20	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	EW	59/63 (94%)	49 (83%)	10 (17%)	2	8
23	GW	59/63 (94%)	57 (97%)	2 (3%)	44	79
24	AX	67/68 (98%)	61 (91%)	6 (9%)	12	34
24	CX	67/68 (98%)	60 (90%)	7 (10%)	9	26
24	EX	67/68 (98%)	57 (85%)	10 (15%)	4	11
24	GX	67/68 (98%)	63 (94%)	4 (6%)	24	57
25	AY	55/55 (100%)	52 (94%)	3 (6%)	27	61
25	CY	55/55 (100%)	51 (93%)	4 (7%)	17	45
25	EY	55/55 (100%)	50 (91%)	5 (9%)	12	34
25	GY	55/55 (100%)	52 (94%)	3 (6%)	27	61
26	AZ	48/49 (98%)	40 (83%)	8 (17%)	3	8
26	CZ	48/49 (98%)	39 (81%)	9 (19%)	2	6
26	EZ	48/49 (98%)	41 (85%)	7 (15%)	4	12
26	GZ	48/49 (98%)	46 (96%)	2 (4%)	36	73
27	A0	47/48 (98%)	46 (98%)	1 (2%)	61	88
27	C0	47/48 (98%)	47 (100%)	0	100	100
27	E0	47/48 (98%)	46 (98%)	1 (2%)	61	88
27	G0	47/48 (98%)	45 (96%)	2 (4%)	35	71
28	A1	45/49 (92%)	42 (93%)	3 (7%)	20	50
28	C1	45/49 (92%)	42 (93%)	3 (7%)	20	50
28	E1	45/49 (92%)	42 (93%)	3 (7%)	20	50
28	G1	45/49 (92%)	43 (96%)	2 (4%)	35	70
29	A2	38/38 (100%)	35 (92%)	3 (8%)	15	41
29	C2	38/38 (100%)	34 (90%)	4 (10%)	8	25
29	E2	38/38 (100%)	36 (95%)	2 (5%)	28	63
29	G2	38/38 (100%)	35 (92%)	3 (8%)	15	41
30	A3	51/52 (98%)	46 (90%)	5 (10%)	10	30
30	C3	51/52 (98%)	49 (96%)	2 (4%)	39	75
30	E3	51/52 (98%)	47 (92%)	4 (8%)	16	41
30	G3	51/52 (98%)	48 (94%)	3 (6%)	24	58
31	A4	34/34 (100%)	31 (91%)	3 (9%)	12	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	C4	34/34 (100%)	32 (94%)	2 (6%)	24	58
31	E4	34/34 (100%)	32 (94%)	2 (6%)	24	58
31	G4	34/34 (100%)	33 (97%)	1 (3%)	50	83
32	A5	112/123 (91%)	93 (83%)	19 (17%)	2	7
32	C5	112/123 (91%)	95 (85%)	17 (15%)	3	10
32	E5	111/123 (90%)	93 (84%)	18 (16%)	3	9
33	A6	26/85 (31%)	22 (85%)	4 (15%)	3	10
34	BB	180/199 (90%)	170 (94%)	10 (6%)	26	60
34	DB	180/199 (90%)	170 (94%)	10 (6%)	26	60
34	FB	180/199 (90%)	171 (95%)	9 (5%)	30	65
34	HB	180/199 (90%)	174 (97%)	6 (3%)	45	80
36	BC	170/190 (90%)	156 (92%)	14 (8%)	14	39
36	DC	170/190 (90%)	162 (95%)	8 (5%)	32	68
36	FC	170/190 (90%)	158 (93%)	12 (7%)	18	47
36	HC	170/190 (90%)	163 (96%)	7 (4%)	37	73
37	BD	172/173 (99%)	165 (96%)	7 (4%)	37	73
37	DD	172/173 (99%)	163 (95%)	9 (5%)	29	64
37	FD	172/173 (99%)	165 (96%)	7 (4%)	37	73
37	HD	172/173 (99%)	167 (97%)	5 (3%)	50	83
38	BE	113/126 (90%)	108 (96%)	5 (4%)	35	70
38	DE	113/126 (90%)	109 (96%)	4 (4%)	43	78
38	FE	113/126 (90%)	107 (95%)	6 (5%)	28	63
38	HE	113/126 (90%)	105 (93%)	8 (7%)	18	47
39	BF	89/116 (77%)	82 (92%)	7 (8%)	15	41
39	DF	87/116 (75%)	86 (99%)	1 (1%)	80	95
39	FF	87/116 (75%)	82 (94%)	5 (6%)	25	59
39	HF	87/116 (75%)	85 (98%)	2 (2%)	58	87
40	BG	124/147 (84%)	115 (93%)	9 (7%)	17	45
40	DG	124/147 (84%)	123 (99%)	1 (1%)	86	96
40	FG	124/147 (84%)	122 (98%)	2 (2%)	70	91
40	HG	124/147 (84%)	124 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	BH	104/105 (99%)	96 (92%)	8 (8%)	16	42
41	DH	104/105 (99%)	97 (93%)	7 (7%)	20	50
41	FH	104/105 (99%)	99 (95%)	5 (5%)	31	67
41	HH	104/105 (99%)	97 (93%)	7 (7%)	20	50
42	BI	105/107 (98%)	96 (91%)	9 (9%)	13	36
42	DI	105/107 (98%)	101 (96%)	4 (4%)	40	76
42	FI	105/107 (98%)	96 (91%)	9 (9%)	13	36
42	HI	105/107 (98%)	102 (97%)	3 (3%)	50	83
43	BJ	86/90 (96%)	83 (96%)	3 (4%)	43	78
43	DJ	86/90 (96%)	82 (95%)	4 (5%)	32	68
43	FJ	86/90 (96%)	83 (96%)	3 (4%)	43	78
43	HJ	86/90 (96%)	81 (94%)	5 (6%)	25	58
44	BK	90/99 (91%)	85 (94%)	5 (6%)	26	60
44	DK	90/99 (91%)	87 (97%)	3 (3%)	45	80
44	FK	90/99 (91%)	81 (90%)	9 (10%)	9	28
44	HK	90/99 (91%)	83 (92%)	7 (8%)	16	41
45	BL	103/104 (99%)	96 (93%)	7 (7%)	20	49
45	DL	103/104 (99%)	96 (93%)	7 (7%)	20	49
45	FL	103/104 (99%)	96 (93%)	7 (7%)	20	49
45	HL	103/104 (99%)	99 (96%)	4 (4%)	39	75
46	BM	92/96 (96%)	88 (96%)	4 (4%)	35	71
46	DM	92/96 (96%)	92 (100%)	0	100	100
46	FM	92/96 (96%)	91 (99%)	1 (1%)	80	95
46	HM	92/96 (96%)	91 (99%)	1 (1%)	80	95
47	BN	79/84 (94%)	75 (95%)	4 (5%)	29	65
47	DN	79/84 (94%)	78 (99%)	1 (1%)	76	94
47	FN	79/84 (94%)	76 (96%)	3 (4%)	40	76
47	HN	79/84 (94%)	79 (100%)	0	100	100
48	BO	76/77 (99%)	72 (95%)	4 (5%)	28	63
48	DO	76/77 (99%)	74 (97%)	2 (3%)	54	85
48	FO	76/77 (99%)	71 (93%)	5 (7%)	21	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	HO	76/77 (99%)	74 (97%)	2 (3%)	54	85
49	BP	65/65 (100%)	61 (94%)	4 (6%)	23	55
49	DP	65/65 (100%)	62 (95%)	3 (5%)	33	69
49	FP	65/65 (100%)	64 (98%)	1 (2%)	72	92
49	HP	65/65 (100%)	63 (97%)	2 (3%)	47	82
50	BQ	74/78 (95%)	66 (89%)	8 (11%)	8	24
50	DQ	74/78 (95%)	71 (96%)	3 (4%)	37	73
50	FQ	74/78 (95%)	72 (97%)	2 (3%)	52	84
50	HQ	74/78 (95%)	68 (92%)	6 (8%)	15	39
51	BR	48/65 (74%)	47 (98%)	1 (2%)	61	88
51	DR	48/65 (74%)	48 (100%)	0	100	100
51	FR	48/65 (74%)	48 (100%)	0	100	100
51	HR	48/65 (74%)	48 (100%)	0	100	100
52	BS	70/79 (89%)	64 (91%)	6 (9%)	13	36
52	DS	70/79 (89%)	67 (96%)	3 (4%)	35	71
52	FS	70/79 (89%)	67 (96%)	3 (4%)	35	71
52	HS	70/79 (89%)	69 (99%)	1 (1%)	74	93
53	BT	65/66 (98%)	60 (92%)	5 (8%)	16	42
53	DT	65/66 (98%)	58 (89%)	7 (11%)	8	24
53	FT	65/66 (98%)	58 (89%)	7 (11%)	8	24
53	HT	65/66 (98%)	57 (88%)	8 (12%)	6	17
54	BU	44/61 (72%)	36 (82%)	8 (18%)	2	6
54	DU	44/61 (72%)	42 (96%)	2 (4%)	34	70
54	FU	44/61 (72%)	39 (89%)	5 (11%)	7	21
54	HU	44/61 (72%)	43 (98%)	1 (2%)	58	87
55	BV	568/578 (98%)	521 (92%)	47 (8%)	14	38
55	DV	568/578 (98%)	527 (93%)	41 (7%)	18	46
55	FV	568/578 (98%)	528 (93%)	40 (7%)	19	47
55	HV	568/578 (98%)	535 (94%)	33 (6%)	25	58
56	BW	2/2 (100%)	1 (50%)	1 (50%)	0	0
56	DW	2/2 (100%)	1 (50%)	1 (50%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
56	FW	2/2 (100%)	1 (50%)	1 (50%)	0 0
56	HW	2/2 (100%)	0	2 (100%)	0 0
All	All	21011/21990 (96%)	19590 (93%)	1421 (7%)	20 49

5 of 1421 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
34	DB	71	THR
5	EE	44	ARG
34	HB	90	PHE
37	DD	171	LEU
55	DV	77	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
55	DV	465	HIS
38	FE	82	GLN
43	HJ	56	HIS
4	ED	49	GLN
18	ER	66	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AB	117/120 (97%)	17 (14%)	0
1	CB	117/120 (97%)	19 (16%)	0
1	EB	117/120 (97%)	18 (15%)	0
1	GB	117/120 (97%)	20 (17%)	0
3	AA	2850/2904 (98%)	455 (15%)	40 (1%)
3	CA	2850/2904 (98%)	457 (16%)	39 (1%)
3	EA	2850/2904 (98%)	452 (15%)	36 (1%)
3	GA	2850/2904 (98%)	459 (16%)	38 (1%)
35	BA	1532/1542 (99%)	264 (17%)	17 (1%)
35	DA	1532/1542 (99%)	264 (17%)	14 (0%)
35	FA	1532/1542 (99%)	263 (17%)	16 (1%)
35	HA	1532/1542 (99%)	268 (17%)	15 (0%)
All	All	17996/18264 (98%)	2956 (16%)	215 (1%)

5 of 2956 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AB	3	C
1	AB	15	A
1	AB	16	G
1	AB	21	G
1	AB	30	C

5 of 215 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	DA	209	U
3	EA	827	U
3	GA	2873	A
35	DA	481	G
35	DA	1451	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
56	KBE	BW	1	56	8,8,9	1.29	1 (12%)	7,8,10	1.43	1 (14%)
56	DPP	BW	2	56	3,5,6	0.95	0	1,5,7	3.25	1 (100%)
56	UAL	BW	5	56	7,8,9	2.58	4 (57%)	4,9,11	3.84	1 (25%)
56	5OH	BW	6	56	7,12,13	1.60	2 (28%)	7,16,18	2.35	4 (57%)
56	KBE	DW	1	56	8,8,9	1.04	1 (12%)	7,8,10	2.35	3 (42%)
56	DPP	DW	2	56	3,5,6	0.88	0	1,5,7	2.34	1 (100%)
56	UAL	DW	5	56	7,8,9	2.55	4 (57%)	4,9,11	3.78	2 (50%)
56	5OH	DW	6	56	7,12,13	1.62	2 (28%)	7,16,18	1.67	3 (42%)
56	KBE	FW	1	56	8,8,9	1.02	1 (12%)	7,8,10	1.27	1 (14%)
56	DPP	FW	2	56	3,5,6	0.98	0	1,5,7	2.84	1 (100%)
56	UAL	FW	5	56	7,8,9	2.48	4 (57%)	4,9,11	4.43	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
56	5OH	FW	6	56	7,12,13	1.83	2 (28%)	7,16,18	1.69	2 (28%)
56	KBE	HW	1	56	8,8,9	1.03	1 (12%)	7,8,10	0.99	1 (14%)
56	DPP	HW	2	56	3,5,6	0.94	0	1,5,7	2.96	1 (100%)
56	UAL	HW	5	56	7,8,9	3.08	4 (57%)	4,9,11	4.06	3 (75%)
56	5OH	HW	6	56	7,12,13	1.58	2 (28%)	7,16,18	1.54	2 (28%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	KBE	BW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	BW	2	56	-	0/1/4/6	0/0/0/0
56	UAL	BW	5	56	-	0/3/7/9	0/0/0/0
56	5OH	BW	6	56	-	0/1/18/20	0/1/1/1
56	KBE	DW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	DW	2	56	-	0/1/4/6	0/0/0/0
56	UAL	DW	5	56	-	1/3/7/9	0/0/0/0
56	5OH	DW	6	56	-	0/1/18/20	0/1/1/1
56	KBE	FW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	FW	2	56	-	0/1/4/6	0/0/0/0
56	UAL	FW	5	56	-	0/3/7/9	0/0/0/0
56	5OH	FW	6	56	-	0/1/18/20	0/1/1/1
56	KBE	HW	1	56	-	0/7/7/8	0/0/0/0
56	DPP	HW	2	56	-	0/1/4/6	0/0/0/0
56	UAL	HW	5	56	-	0/3/7/9	0/0/0/0
56	5OH	HW	6	56	-	0/1/18/20	0/1/1/1

The worst 5 of 28 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	FW	6	5OH	CR-CB	-3.07	1.47	1.53
56	BW	1	KBE	CB-N	-2.66	1.39	1.47
56	BW	6	5OH	CR-CB	-2.45	1.48	1.53
56	HW	1	KBE	CB-N	-2.42	1.40	1.47
56	FW	1	KBE	CB-N	-2.25	1.40	1.47

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	FW	5	UAL	O-C-CA	-8.62	112.69	125.40
56	BW	5	UAL	O-C-CA	-7.50	114.35	125.40
56	HW	5	UAL	O-C-CA	-7.43	114.45	125.40
56	DW	5	UAL	O-C-CA	-7.01	115.06	125.40
56	BW	6	5OH	O-C-CA	-3.85	115.26	125.44

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	DW	5	UAL	CA-CB-N1-C1

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
56	BW	1	KBE	2	0
56	BW	5	UAL	2	0
56	BW	6	5OH	1	0
56	DW	1	KBE	2	0
56	DW	5	UAL	2	0
56	DW	6	5OH	1	0
56	FW	1	KBE	1	0
56	FW	5	UAL	1	0
56	FW	6	5OH	1	0
56	HW	1	KBE	3	0
56	HW	2	DPP	1	0
56	HW	6	5OH	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 756 ligands modelled in this entry, 752 are monoatomic - leaving 4 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$
59	GCP	BV	801	57	26,34,34	2.11	6 (23%)	34,54,54	2.37	9 (26%)
59	GCP	DV	801	57	26,34,34	2.04	6 (23%)	34,54,54	2.45	10 (29%)
59	GCP	FV	801	57	26,34,34	2.14	5 (19%)	34,54,54	2.11	11 (32%)
59	GCP	HV	801	57	26,34,34	2.06	5 (19%)	34,54,54	2.38	13 (38%)

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
59	GCP	BV	801	57	-	0/15/38/38	0/3/3/3
59	GCP	DV	801	57	-	0/15/38/38	0/3/3/3
59	GCP	FV	801	57	-	0/15/38/38	0/3/3/3
59	GCP	HV	801	57	-	0/15/38/38	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	FV	801	GCP	C2'-C3'	-4.17	1.42	1.53
59	DV	801	GCP	C2'-C3'	-4.15	1.42	1.53
59	HV	801	GCP	C2'-C3'	-3.93	1.42	1.53
59	BV	801	GCP	C2'-C3'	-3.91	1.42	1.53
59	BV	801	GCP	PB-O3A	-3.64	1.54	1.58

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	DV	801	GCP	C4'-O4'-C1'	-8.16	100.76	109.72
59	HV	801	GCP	C4'-O4'-C1'	-7.81	101.14	109.72
59	BV	801	GCP	C4'-O4'-C1'	-7.56	101.41	109.72
59	BV	801	GCP	PA-O3A-PB	-6.89	113.39	132.73
59	DV	801	GCP	PA-O3A-PB	-6.19	115.35	132.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	BV	801	GCP	1	0
59	DV	801	GCP	2	0
59	FV	801	GCP	2	0
59	HV	801	GCP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AB	118/120 (98%)	-0.45	0 100 100	7, 25, 37, 49	0
1	CB	118/120 (98%)	-0.62	0 100 100	19, 41, 55, 61	0
1	EB	118/120 (98%)	-0.37	0 100 100	6, 27, 41, 51	0
1	GB	118/120 (98%)	0.04	1 (0%) 87 86	34, 57, 66, 70	0
2	AC	271/273 (99%)	-0.00	4 (1%) 76 74	2, 14, 26, 50	0
2	CC	271/273 (99%)	0.33	14 (5%) 31 24	14, 33, 45, 54	0
2	EC	271/273 (99%)	0.04	2 (0%) 89 88	3, 17, 30, 42	0
2	GC	271/273 (99%)	0.36	21 (7%) 16 11	12, 29, 43, 52	0
3	AA	2854/2904 (98%)	-0.05	41 (1%) 78 76	2, 14, 50, 79	0
3	CA	2854/2904 (98%)	-0.21	35 (1%) 81 78	8, 29, 57, 78	0
3	EA	2854/2904 (98%)	-0.06	42 (1%) 76 74	2, 16, 52, 83	0
3	GA	2854/2904 (98%)	-0.06	52 (1%) 71 68	10, 42, 64, 76	0
4	AD	209/209 (100%)	0.03	4 (1%) 70 66	2, 15, 35, 57	0
4	CD	209/209 (100%)	0.19	5 (2%) 62 57	5, 23, 42, 56	0
4	ED	209/209 (100%)	0.03	2 (0%) 84 82	2, 20, 40, 52	0
4	GD	209/209 (100%)	0.21	7 (3%) 50 42	10, 30, 46, 55	0
5	AE	201/201 (100%)	0.06	1 (0%) 91 90	3, 19, 40, 51	0
5	CE	201/201 (100%)	0.39	17 (8%) 13 8	9, 34, 47, 57	0
5	EE	201/201 (100%)	0.11	5 (2%) 61 55	2, 21, 43, 57	0
5	GE	201/201 (100%)	1.30	53 (26%) 1 0	25, 51, 61, 68	0
6	AF	177/179 (98%)	0.41	9 (5%) 32 25	19, 33, 50, 60	0
6	CF	177/179 (98%)	1.01	39 (22%) 1 0	31, 47, 56, 62	0
6	EF	177/179 (98%)	0.61	21 (11%) 6 3	16, 34, 49, 58	0
6	GF	177/179 (98%)	3.14	106 (59%) 0 0	47, 59, 67, 72	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
7	AG	176/177 (99%)	0.31	11 (6%) 23 17	9, 25, 46, 59	0
7	CG	176/177 (99%)	0.52	18 (10%) 9 5	18, 36, 51, 61	0
7	EG	176/177 (99%)	0.31	12 (6%) 20 14	16, 31, 44, 55	0
7	GG	176/177 (99%)	1.05	36 (20%) 1 1	26, 43, 54, 65	0
8	AH	50/50 (100%)	0.90	11 (22%) 1 0	16, 41, 55, 57	0
8	CH	50/50 (100%)	3.76	38 (76%) 0 0	46, 57, 64, 68	0
8	EH	50/50 (100%)	1.19	11 (22%) 1 0	14, 38, 56, 62	0
8	GH	50/50 (100%)	2.32	25 (50%) 0 0	39, 52, 61, 64	0
9	AI	141/142 (99%)	2.53	67 (47%) 0 0	31, 53, 66, 78	0
9	CI	141/142 (99%)	2.20	70 (49%) 0 0	36, 54, 63, 72	0
9	EI	141/142 (99%)	2.27	65 (46%) 0 0	32, 54, 66, 76	0
9	GI	141/142 (99%)	4.04	114 (80%) 0 0	42, 59, 69, 80	0
10	AJ	142/142 (100%)	0.04	1 (0%) 89 88	4, 11, 29, 39	0
10	CJ	142/142 (100%)	0.23	3 (2%) 67 62	8, 24, 37, 54	0
10	EJ	142/142 (100%)	0.20	4 (2%) 56 50	5, 14, 28, 43	0
10	GJ	142/142 (100%)	0.37	6 (4%) 40 33	21, 36, 47, 55	0
11	AK	122/123 (99%)	0.12	1 (0%) 87 86	4, 10, 25, 50	0
11	CK	122/123 (99%)	0.07	2 (1%) 74 72	9, 18, 35, 42	0
11	EK	122/123 (99%)	0.19	4 (3%) 50 42	7, 18, 34, 47	0
11	GK	122/123 (99%)	0.66	10 (8%) 14 9	12, 24, 39, 53	0
12	AL	143/144 (99%)	0.17	4 (2%) 56 50	2, 18, 34, 39	0
12	CL	143/144 (99%)	0.53	14 (9%) 10 6	11, 31, 46, 54	0
12	EL	143/144 (99%)	0.26	5 (3%) 48 40	2, 18, 37, 49	0
12	GL	143/144 (99%)	1.79	61 (42%) 0 0	29, 46, 59, 65	0
13	AM	136/136 (100%)	0.17	2 (1%) 76 74	2, 9, 25, 48	0
13	CM	136/136 (100%)	0.35	5 (3%) 45 38	10, 21, 36, 52	0
13	EM	136/136 (100%)	0.15	2 (1%) 76 74	4, 13, 29, 43	0
13	GM	136/136 (100%)	1.47	40 (29%) 1 0	28, 44, 56, 60	0
14	AN	120/127 (94%)	0.18	2 (1%) 73 70	5, 13, 25, 56	0
14	CN	120/127 (94%)	0.22	1 (0%) 87 86	13, 24, 35, 56	0
14	EN	120/127 (94%)	0.21	3 (2%) 61 55	9, 19, 31, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
14	GN	120/127 (94%)	0.25	4 (3%) 50 42	16, 28, 37, 58	0
15	AO	116/117 (99%)	0.05	2 (1%) 73 70	12, 24, 37, 46	0
15	CO	116/117 (99%)	0.58	12 (10%) 9 5	29, 40, 53, 59	0
15	EO	116/117 (99%)	0.34	5 (4%) 39 32	14, 27, 40, 44	0
15	GO	116/117 (99%)	1.77	44 (37%) 0 0	39, 52, 58, 65	0
16	AP	114/115 (99%)	0.05	2 (1%) 71 68	5, 19, 36, 44	0
16	CP	114/115 (99%)	0.18	3 (2%) 59 54	11, 25, 41, 54	0
16	EP	114/115 (99%)	0.02	1 (0%) 85 84	14, 26, 41, 60	0
16	GP	114/115 (99%)	0.14	4 (3%) 48 40	13, 27, 42, 51	0
17	AQ	117/118 (99%)	0.11	3 (2%) 59 54	3, 10, 26, 53	0
17	CQ	117/118 (99%)	0.17	3 (2%) 59 54	9, 23, 35, 54	0
17	EQ	117/118 (99%)	0.16	3 (2%) 59 54	2, 12, 27, 52	0
17	GQ	117/118 (99%)	0.94	19 (16%) 3 1	24, 41, 53, 58	0
18	AR	103/103 (100%)	0.02	3 (2%) 55 49	2, 18, 34, 47	0
18	CR	103/103 (100%)	0.30	4 (3%) 43 36	12, 31, 45, 55	0
18	ER	103/103 (100%)	0.28	5 (4%) 33 27	3, 23, 42, 49	0
18	GR	103/103 (100%)	1.53	34 (33%) 0 0	30, 47, 56, 64	0
19	AS	110/110 (100%)	0.19	2 (1%) 71 68	3, 12, 32, 54	0
19	CS	110/110 (100%)	0.42	6 (5%) 29 22	13, 22, 40, 47	0
19	ES	110/110 (100%)	0.31	3 (2%) 58 52	5, 14, 36, 51	0
19	GS	110/110 (100%)	1.01	21 (19%) 2 1	20, 39, 50, 55	0
20	AT	93/100 (93%)	0.64	10 (10%) 8 4	7, 24, 51, 55	0
20	CT	93/100 (93%)	1.00	16 (17%) 2 1	22, 36, 52, 56	0
20	ET	93/100 (93%)	0.88	15 (16%) 3 1	13, 26, 50, 58	0
20	GT	93/100 (93%)	1.80	41 (44%) 0 0	26, 45, 57, 64	0
21	AU	102/104 (98%)	0.57	6 (5%) 26 19	9, 22, 41, 62	0
21	CU	102/104 (98%)	1.35	28 (27%) 1 0	25, 36, 52, 65	0
21	EU	102/104 (98%)	0.60	10 (9%) 10 6	14, 30, 44, 59	0
21	GU	102/104 (98%)	2.73	63 (61%) 0 0	35, 53, 61, 68	0
22	AV	94/94 (100%)	-0.23	0 100 100	8, 23, 40, 46	0
22	CV	94/94 (100%)	-0.14	0 100 100	22, 31, 44, 52	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
22	EV	94/94 (100%)	-0.08	2 (2%) 67 62	12, 23, 40, 48	0
22	GV	94/94 (100%)	0.89	17 (18%) 2 1	36, 49, 59, 61	0
23	AW	79/85 (92%)	0.76	13 (16%) 2 1	8, 19, 41, 49	0
23	CW	79/85 (92%)	0.89	12 (15%) 3 1	18, 32, 48, 60	0
23	EW	79/85 (92%)	0.75	11 (13%) 4 2	6, 20, 38, 51	0
23	GW	79/85 (92%)	2.42	41 (51%) 0 0	35, 49, 59, 71	0
24	AX	77/78 (98%)	0.36	2 (2%) 59 54	7, 17, 37, 41	0
24	CX	77/78 (98%)	1.22	19 (24%) 1 0	22, 37, 49, 54	0
24	EX	77/78 (98%)	0.45	0 100 100	5, 15, 36, 37	0
24	GX	77/78 (98%)	1.28	21 (27%) 1 0	26, 44, 53, 58	0
25	AY	63/63 (100%)	0.54	7 (11%) 7 4	16, 34, 48, 52	0
25	CY	63/63 (100%)	1.08	13 (20%) 1 1	30, 43, 55, 62	0
25	EY	63/63 (100%)	0.90	13 (20%) 1 1	18, 33, 45, 56	0
25	GY	63/63 (100%)	2.55	37 (58%) 0 0	44, 51, 58, 60	0
26	AZ	58/59 (98%)	0.57	1 (1%) 73 70	4, 13, 39, 51	0
26	CZ	58/59 (98%)	0.68	3 (5%) 31 24	11, 26, 46, 59	0
26	EZ	58/59 (98%)	0.31	2 (3%) 49 41	3, 15, 37, 47	0
26	GZ	58/59 (98%)	1.87	25 (43%) 0 0	25, 48, 58, 63	0
27	A0	56/57 (98%)	0.45	4 (7%) 19 13	3, 19, 42, 51	0
27	C0	56/57 (98%)	0.29	2 (3%) 46 38	10, 27, 44, 55	0
27	E0	56/57 (98%)	0.33	3 (5%) 29 23	3, 22, 40, 47	0
27	G0	56/57 (98%)	0.63	7 (12%) 5 3	18, 35, 49, 57	0
28	A1	50/55 (90%)	0.68	5 (10%) 9 5	13, 24, 37, 43	0
28	C1	50/55 (90%)	1.64	14 (28%) 1 0	25, 39, 50, 51	0
28	E1	50/55 (90%)	0.70	4 (8%) 15 10	12, 22, 36, 43	0
28	G1	50/55 (90%)	2.74	28 (56%) 0 0	38, 50, 60, 65	0
29	A2	46/46 (100%)	0.10	2 (4%) 39 32	4, 8, 18, 44	0
29	C2	46/46 (100%)	0.48	2 (4%) 39 32	17, 24, 34, 43	0
29	E2	46/46 (100%)	0.07	0 100 100	5, 11, 21, 36	0
29	G2	46/46 (100%)	1.03	6 (13%) 5 3	20, 36, 43, 54	0
30	A3	64/65 (98%)	0.18	0 100 100	3, 10, 18, 30	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
30	C3	64/65 (98%)	0.67	6 (9%) 11 6	15, 28, 36, 39	0
30	E3	64/65 (98%)	0.32	1 (1%) 74 72	4, 9, 19, 31	0
30	G3	64/65 (98%)	1.66	19 (29%) 1 0	32, 43, 52, 60	0
31	A4	38/38 (100%)	0.18	0 100 100	5, 11, 25, 27	0
31	C4	38/38 (100%)	0.32	0 100 100	14, 23, 37, 39	0
31	E4	38/38 (100%)	0.11	0 100 100	7, 16, 27, 30	0
31	G4	38/38 (100%)	0.72	3 (7%) 15 10	24, 37, 50, 53	0
32	A5	148/165 (89%)	1.84	53 (35%) 0 0	30, 49, 61, 72	0
32	C5	148/165 (89%)	2.52	70 (47%) 0 0	37, 54, 64, 72	0
32	E5	145/165 (87%)	3.19	92 (63%) 0 0	36, 53, 62, 67	0
33	A6	30/121 (24%)	3.18	15 (50%) 0 0	47, 53, 62, 65	0
34	BB	218/241 (90%)	0.77	31 (14%) 4 2	24, 41, 56, 66	0
34	DB	218/241 (90%)	1.79	87 (39%) 0 0	35, 52, 61, 69	0
34	FB	218/241 (90%)	0.74	34 (15%) 3 1	25, 43, 56, 66	0
34	HB	218/241 (90%)	2.19	103 (47%) 0 0	42, 56, 66, 71	0
35	BA	1533/1542 (99%)	-0.20	13 (0%) 87 86	7, 21, 52, 78	0
35	DA	1533/1542 (99%)	-0.20	19 (1%) 81 78	13, 42, 64, 78	0
35	FA	1533/1542 (99%)	-0.15	22 (1%) 78 76	9, 31, 57, 75	0
35	HA	1533/1542 (99%)	0.36	129 (8%) 14 9	20, 52, 71, 78	0
36	BC	206/233 (88%)	-0.06	0 100 100	8, 26, 39, 57	0
36	DC	206/233 (88%)	0.61	20 (9%) 10 6	30, 45, 52, 59	0
36	FC	206/233 (88%)	0.26	4 (1%) 70 66	15, 30, 44, 57	0
36	HC	206/233 (88%)	2.18	100 (48%) 0 0	36, 52, 61, 67	0
37	BD	205/206 (99%)	0.35	13 (6%) 23 17	12, 28, 44, 51	0
37	DD	205/206 (99%)	0.39	15 (7%) 18 12	14, 30, 47, 55	0
37	FD	205/206 (99%)	1.50	60 (29%) 1 0	29, 45, 56, 68	0
37	HD	205/206 (99%)	1.01	44 (21%) 1 0	32, 45, 56, 65	0
38	BE	150/167 (89%)	0.06	4 (2%) 58 52	11, 26, 45, 63	0
38	DE	150/167 (89%)	0.10	3 (2%) 68 64	24, 38, 51, 60	0
38	FE	150/167 (89%)	0.28	11 (7%) 18 12	16, 35, 49, 64	0
38	HE	150/167 (89%)	1.24	45 (30%) 1 0	34, 49, 56, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
39	BF	102/135 (75%)	-0.00	1 (0%) 84 82	15, 30, 42, 51	0
39	DF	100/135 (74%)	1.58	32 (32%) 1 0	42, 52, 59, 63	0
39	FF	100/135 (74%)	0.24	4 (4%) 42 35	13, 32, 44, 49	0
39	HF	100/135 (74%)	2.43	51 (51%) 0 0	46, 56, 65, 69	0
40	BG	151/179 (84%)	0.30	10 (6%) 22 16	10, 27, 46, 60	0
40	DG	151/179 (84%)	1.86	62 (41%) 0 0	41, 54, 61, 67	0
40	FG	151/179 (84%)	0.73	18 (11%) 6 3	15, 32, 50, 59	0
40	HG	151/179 (84%)	3.35	92 (60%) 0 0	46, 58, 66, 69	0
41	BH	129/130 (99%)	0.17	3 (2%) 64 59	15, 26, 40, 58	0
41	DH	129/130 (99%)	0.80	22 (17%) 2 1	27, 43, 55, 61	0
41	FH	129/130 (99%)	0.30	7 (5%) 29 23	19, 35, 47, 55	0
41	HH	129/130 (99%)	1.88	54 (41%) 0 0	36, 50, 58, 64	0
42	BI	127/130 (97%)	0.45	7 (5%) 29 22	8, 25, 47, 58	0
42	DI	127/130 (97%)	2.33	64 (50%) 0 0	41, 55, 62, 68	0
42	FI	127/130 (97%)	0.36	8 (6%) 23 17	9, 27, 50, 56	0
42	HI	127/130 (97%)	2.48	69 (54%) 0 0	46, 57, 65, 68	0
43	BJ	98/103 (95%)	0.74	12 (12%) 5 3	9, 35, 56, 61	0
43	DJ	98/103 (95%)	1.65	35 (35%) 0 0	38, 52, 60, 68	0
43	FJ	98/103 (95%)	0.92	17 (17%) 2 1	16, 31, 53, 59	0
43	HJ	98/103 (95%)	2.71	64 (65%) 0 0	40, 54, 63, 66	0
44	BK	117/129 (90%)	0.21	7 (5%) 25 18	14, 26, 40, 52	0
44	DK	117/129 (90%)	1.31	31 (26%) 1 0	38, 52, 60, 62	0
44	FK	117/129 (90%)	-0.04	4 (3%) 49 41	13, 24, 36, 41	0
44	HK	117/129 (90%)	2.85	71 (60%) 0 0	45, 58, 68, 73	0
45	BL	123/124 (99%)	0.07	2 (1%) 74 72	5, 12, 29, 52	0
45	DL	123/124 (99%)	0.22	7 (5%) 27 21	12, 24, 40, 49	0
45	FL	123/124 (99%)	0.19	3 (2%) 62 57	11, 26, 43, 51	0
45	HL	123/124 (99%)	0.98	22 (17%) 2 1	24, 41, 53, 63	0
46	BM	114/118 (96%)	-0.01	2 (1%) 71 68	11, 30, 51, 54	0
46	DM	114/118 (96%)	1.37	31 (27%) 1 0	39, 53, 62, 66	0
46	FM	114/118 (96%)	0.35	12 (10%) 8 5	17, 36, 52, 59	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
46	HM	114/118 (96%)	4.36	88 (77%) 0 0	48, 60, 68, 77	0
47	BN	96/101 (95%)	0.31	4 (4%) 40 33	10, 22, 46, 57	0
47	DN	96/101 (95%)	0.70	12 (12%) 5 3	31, 45, 55, 62	0
47	FN	96/101 (95%)	0.51	7 (7%) 18 12	19, 29, 50, 64	0
47	HN	96/101 (95%)	2.34	46 (47%) 0 0	41, 56, 66, 71	0
48	BO	88/89 (98%)	0.04	0 100 100	12, 27, 40, 42	0
48	DO	88/89 (98%)	0.98	18 (20%) 1 1	36, 46, 55, 59	0
48	FO	88/89 (98%)	0.48	7 (7%) 15 10	16, 31, 44, 51	0
48	HO	88/89 (98%)	1.17	21 (23%) 1 0	37, 49, 58, 63	0
49	BP	82/82 (100%)	0.57	5 (6%) 25 18	13, 21, 46, 63	0
49	DP	82/82 (100%)	0.86	10 (12%) 5 3	16, 27, 48, 59	0
49	FP	82/82 (100%)	1.27	19 (23%) 1 0	24, 35, 54, 70	0
49	HP	82/82 (100%)	0.98	17 (20%) 1 1	25, 37, 49, 59	0
50	BQ	80/84 (95%)	0.35	3 (3%) 44 37	14, 26, 39, 48	0
50	DQ	80/84 (95%)	0.64	9 (11%) 7 4	26, 37, 45, 48	0
50	FQ	80/84 (95%)	0.60	6 (7%) 17 11	18, 36, 50, 55	0
50	HQ	80/84 (95%)	1.21	19 (23%) 1 0	35, 44, 55, 62	0
51	BR	55/75 (73%)	0.33	2 (3%) 46 38	16, 26, 39, 48	0
51	DR	55/75 (73%)	2.06	20 (36%) 0 0	43, 52, 60, 62	0
51	FR	55/75 (73%)	0.31	2 (3%) 46 38	18, 26, 37, 45	0
51	HR	55/75 (73%)	3.37	38 (69%) 0 0	43, 54, 61, 63	0
52	BS	79/92 (85%)	0.25	4 (5%) 32 25	14, 23, 39, 65	0
52	DS	79/92 (85%)	1.46	25 (31%) 1 0	31, 49, 58, 61	0
52	FS	79/92 (85%)	0.27	4 (5%) 32 25	22, 34, 48, 52	0
52	HS	79/92 (85%)	4.48	64 (81%) 0 0	50, 60, 70, 73	0
53	BT	85/87 (97%)	0.48	4 (4%) 35 29	12, 23, 42, 47	0
53	DT	85/87 (97%)	0.53	7 (8%) 14 9	17, 28, 44, 53	0
53	FT	85/87 (97%)	0.76	9 (10%) 8 5	25, 38, 47, 63	0
53	HT	85/87 (97%)	0.94	11 (12%) 5 3	22, 33, 46, 52	0
54	BU	51/71 (71%)	1.01	11 (21%) 1 0	22, 37, 52, 61	0
54	DU	51/71 (71%)	2.22	25 (49%) 0 0	36, 54, 60, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
54	FU	51/71 (71%)	0.80	7 (13%) 4 2	25, 35, 54, 61	0
54	HU	51/71 (71%)	4.17	41 (80%) 0 0	40, 54, 65, 71	0
55	BV	690/704 (98%)	0.03	26 (3%) 44 37	10, 30, 48, 66	0
55	DV	689/704 (97%)	0.27	56 (8%) 15 9	16, 37, 53, 63	0
55	FV	689/704 (97%)	0.59	87 (12%) 5 3	16, 41, 54, 63	0
55	HV	689/704 (97%)	1.17	171 (24%) 1 0	25, 51, 62, 73	0
56	BW	2/6 (33%)	0.16	0 100 100	16, 16, 16, 20	0
56	DW	2/6 (33%)	-0.22	0 100 100	32, 32, 32, 34	0
56	FW	2/6 (33%)	0.79	0 100 100	23, 23, 23, 29	0
56	HW	2/6 (33%)	0.89	1 (50%) 0 0	51, 51, 51, 58	0
All	All	43746/45264 (96%)	0.45	4563 (10%) 8 5	2, 33, 60, 83	0

The worst 5 of 4563 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
46	HM	84	GLY	19.9
26	CZ	1	ALA	18.5
26	AZ	1	ALA	16.2
6	GF	169	LEU	15.8
28	C1	52	LYS	15.5

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
56	KBE	DW	1	9/10	0.83	0.27	-	33,35,41,48	0
56	5OH	BW	6	12/13	0.94	0.14	-	11,17,21,21	0
56	5OH	DW	6	12/13	0.95	0.13	-	22,29,35,37	0
56	5OH	FW	6	12/13	0.96	0.16	-	10,24,29,30	0
56	KBE	FW	1	9/10	0.89	0.42	-	17,21,37,51	0
56	KBE	HW	1	9/10	0.84	0.31	-	27,45,52,55	0
56	KBE	BW	1	9/10	0.93	0.19	-	4,9,22,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
56	UAL	BW	5	9/10	0.92	0.21	-	16,20,27,32	0
56	DPP	HW	2	6/7	0.82	0.15	-	30,41,49,53	0
56	DPP	BW	2	6/7	0.96	0.18	-	6,12,15,22	0
56	UAL	HW	5	9/10	0.87	0.25	-	36,48,56,60	0
56	DPP	FW	2	6/7	0.98	0.20	-	18,22,27,32	0
56	5OH	HW	6	12/13	0.80	0.27	-	48,54,58,60	0
56	UAL	DW	5	9/10	0.93	0.12	-	17,27,36,48	0
56	UAL	FW	5	9/10	0.93	0.15	-	15,18,29,38	0
56	DPP	DW	2	6/7	0.96	0.12	-	25,37,38,39	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	GA	3131	1/1	0.83	1.13	47.87	43,43,43,43	0
57	MG	AA	3097	1/1	0.70	0.56	28.93	34,34,34,34	0
57	MG	GA	3055	1/1	0.91	0.64	22.04	21,21,21,21	0
57	MG	GA	3021	1/1	0.97	0.67	19.81	20,20,20,20	0
57	MG	EA	3040	1/1	0.97	0.28	16.70	11,11,11,11	0
57	MG	CA	3112	1/1	0.99	0.30	16.06	10,10,10,10	0
57	MG	AA	3078	1/1	0.99	0.34	10.55	13,13,13,13	0
57	MG	AA	3129	1/1	0.98	0.24	10.06	9,9,9,9	0
57	MG	HA	1628	1/1	0.98	0.26	9.28	29,29,29,29	0
57	MG	AA	3111	1/1	0.99	0.25	7.12	3,3,3,3	0
57	MG	GA	3050	1/1	0.96	0.28	6.75	26,26,26,26	0
57	MG	AA	3037	1/1	0.96	0.43	6.71	30,30,30,30	0
57	MG	AA	3100	1/1	0.95	0.29	6.37	1,1,1,1	0
57	MG	GA	3107	1/1	0.99	0.26	5.98	13,13,13,13	0
57	MG	AA	3041	1/1	0.99	0.24	5.97	7,7,7,7	0
57	MG	AA	3135	1/1	0.97	0.37	5.96	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3047	1/1	0.95	0.21	5.89	12,12,12,12	0
57	MG	EA	3005	1/1	0.99	0.20	5.78	16,16,16,16	0
57	MG	DA	1628	1/1	0.97	0.32	5.64	44,44,44,44	0
57	MG	BA	1616	1/1	0.99	0.27	5.59	3,3,3,3	0
57	MG	AA	3107	1/1	1.00	0.24	5.54	4,4,4,4	0
57	MG	EA	3042	1/1	0.99	0.23	5.39	13,13,13,13	0
57	MG	AA	3095	1/1	0.98	0.26	5.21	4,4,4,4	0
57	MG	CA	3046	1/1	0.99	0.22	5.21	21,21,21,21	0
57	MG	AA	3068	1/1	0.99	0.23	4.84	2,2,2,2	0
57	MG	GA	3100	1/1	0.98	0.29	4.79	12,12,12,12	0
57	MG	AA	3115	1/1	0.99	0.24	4.71	1,1,1,1	0
57	MG	AA	3090	1/1	0.94	0.24	4.62	32,32,32,32	0
57	MG	BA	1627	1/1	0.98	0.22	4.35	19,19,19,19	0
57	MG	GA	3009	1/1	0.95	0.22	4.22	35,35,35,35	0
57	MG	FA	1635	1/1	0.85	0.34	4.11	41,41,41,41	0
57	MG	EA	3123	1/1	0.99	0.23	4.07	3,3,3,3	0
57	MG	HA	1613	1/1	0.97	0.27	4.04	32,32,32,32	0
57	MG	FA	1609	1/1	0.99	0.25	4.00	7,7,7,7	0
57	MG	EA	3046	1/1	0.97	0.23	3.90	9,9,9,9	0
57	MG	CA	3131	1/1	0.99	0.27	3.87	11,11,11,11	0
57	MG	EA	3038	1/1	0.98	0.22	3.85	2,2,2,2	0
57	MG	AA	3026	1/1	0.99	0.22	3.76	4,4,4,4	0
57	MG	CA	3068	1/1	0.98	0.19	3.69	9,9,9,9	0
57	MG	GA	3104	1/1	0.99	0.29	3.62	12,12,12,12	0
57	MG	CA	3040	1/1	0.99	0.21	3.52	11,11,11,11	0
57	MG	FA	1626	1/1	0.98	0.23	3.24	22,22,22,22	0
57	MG	AA	3050	1/1	1.00	0.20	3.21	2,2,2,2	0
57	MG	BA	1607	1/1	0.88	0.27	3.19	34,34,34,34	0
57	MG	AA	3108	1/1	0.99	0.26	3.18	1,1,1,1	0
57	MG	GA	3023	1/1	0.99	0.33	3.17	27,27,27,27	0
57	MG	EA	3103	1/1	0.99	0.26	3.10	0,0,0,0	0
57	MG	AA	3029	1/1	0.99	0.24	3.02	0,0,0,0	0
57	MG	GA	3030	1/1	0.98	0.26	2.96	15,15,15,15	0
57	MG	CA	3109	1/1	0.98	0.24	2.93	7,7,7,7	0
57	MG	AA	3106	1/1	0.99	0.21	2.85	4,4,4,4	0
57	MG	GA	3115	1/1	0.98	0.23	2.80	20,20,20,20	0
57	MG	DA	1642	1/1	1.00	0.21	2.71	4,4,4,4	0
57	MG	CA	3105	1/1	0.99	0.23	2.65	14,14,14,14	0
57	MG	GA	3119	1/1	0.97	0.21	2.60	18,18,18,18	0
57	MG	EA	3025	1/1	0.98	0.23	2.57	1,1,1,1	0
57	MG	EA	3096	1/1	0.99	0.22	2.50	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	FA	1611	1/1	0.98	0.21	2.50	7,7,7,7	0
57	MG	CA	3136	1/1	0.85	0.28	2.42	22,22,22,22	0
57	MG	FA	1613	1/1	1.00	0.20	2.35	6,6,6,6	0
57	MG	EA	3104	1/1	0.99	0.23	2.34	0,0,0,0	0
57	MG	EA	3023	1/1	0.99	0.22	2.33	9,9,9,9	0
57	MG	DV	802	1/1	0.99	0.20	2.27	14,14,14,14	0
57	MG	EA	3100	1/1	0.98	0.22	2.23	1,1,1,1	0
57	MG	CA	3120	1/1	0.99	0.21	2.08	11,11,11,11	0
57	MG	CA	3023	1/1	0.98	0.26	1.81	5,5,5,5	0
57	MG	AA	3060	1/1	0.89	0.27	1.68	34,34,34,34	0
57	MG	FA	1622	1/1	0.98	0.20	1.63	9,9,9,9	0
57	MG	HA	1623	1/1	0.98	0.20	1.58	36,36,36,36	0
57	MG	GA	3049	1/1	1.00	0.22	1.55	12,12,12,12	0
57	MG	EA	3037	1/1	0.99	0.19	1.51	2,2,2,2	0
57	MG	CN	201	1/1	0.97	0.21	1.44	20,20,20,20	0
57	MG	DA	1616	1/1	0.98	0.34	1.42	28,28,28,28	0
57	MG	CA	3110	1/1	0.96	0.18	1.42	23,23,23,23	0
57	MG	CA	3009	1/1	0.99	0.18	1.37	10,10,10,10	0
57	MG	DA	1639	1/1	0.98	0.16	1.36	30,30,30,30	0
57	MG	CA	3024	1/1	0.98	0.20	1.32	6,6,6,6	0
57	MG	AA	3035	1/1	0.98	0.20	1.31	5,5,5,5	0
57	MG	CB	1202	1/1	0.92	0.16	1.29	44,44,44,44	0
57	MG	BA	1638	1/1	1.00	0.18	1.29	13,13,13,13	0
57	MG	CA	3005	1/1	0.99	0.15	1.24	35,35,35,35	0
57	MG	CA	3079	1/1	0.99	0.20	1.24	27,27,27,27	0
57	MG	AA	3094	1/1	1.00	0.19	1.19	16,16,16,16	0
57	MG	BA	1626	1/1	0.98	0.21	1.06	5,5,5,5	0
57	MG	CA	3121	1/1	1.00	0.22	1.05	8,8,8,8	0
57	MG	EA	3053	1/1	0.99	0.20	1.02	1,1,1,1	0
57	MG	EA	3084	1/1	0.99	0.22	1.00	7,7,7,7	0
57	MG	CA	3066	1/1	0.98	0.17	0.97	4,4,4,4	0
57	MG	BA	1605	1/1	0.98	0.16	0.91	28,28,28,28	0
57	MG	BV	802	1/1	0.98	0.20	0.83	22,22,22,22	0
57	MG	DA	1610	1/1	0.98	0.10	0.81	28,28,28,28	0
57	MG	EA	3130	1/1	0.98	0.20	0.63	0,0,0,0	0
57	MG	BA	1640	1/1	0.99	0.22	0.61	11,11,11,11	0
57	MG	BA	1632	1/1	0.99	0.16	0.51	14,14,14,14	0
57	MG	BA	1628	1/1	1.00	0.19	0.50	18,18,18,18	0
57	MG	GA	3109	1/1	0.87	0.16	0.44	35,35,35,35	0
57	MG	EA	3120	1/1	0.99	0.20	0.37	5,5,5,5	0
57	MG	CA	3113	1/1	0.95	0.20	0.33	10,10,10,10	0
57	MG	GA	3022	1/1	0.99	0.17	0.31	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	GA	3040	1/1	0.97	0.16	0.21	15,15,15,15	0
57	MG	CA	3133	1/1	0.99	0.21	0.17	13,13,13,13	0
57	MG	AA	3009	1/1	1.00	0.19	0.15	2,2,2,2	0
57	MG	FV	802	1/1	0.99	0.18	0.15	24,24,24,24	0
57	MG	AA	3130	1/1	0.98	0.20	0.13	3,3,3,3	0
57	MG	DA	1606	1/1	0.98	0.20	0.13	15,15,15,15	0
57	MG	CA	3107	1/1	0.98	0.17	0.13	14,14,14,14	0
57	MG	GA	3108	1/1	0.97	0.18	0.09	38,38,38,38	0
57	MG	GA	3099	1/1	0.97	0.14	0.06	33,33,33,33	0
57	MG	BA	1636	1/1	0.95	0.15	0.03	24,24,24,24	0
57	MG	AA	3114	1/1	0.95	0.20	-0.03	10,10,10,10	0
57	MG	HV	802	1/1	0.99	0.17	-0.04	38,38,38,38	0
57	MG	GA	3024	1/1	0.96	0.19	-0.10	14,14,14,14	0
57	MG	CA	3116	1/1	0.98	0.16	-0.10	7,7,7,7	0
57	MG	GA	3047	1/1	0.99	0.12	-0.12	38,38,38,38	0
57	MG	EA	3133	1/1	1.00	0.21	-0.14	0,0,0,0	0
57	MG	AA	3065	1/1	1.00	0.18	-0.15	11,11,11,11	0
57	MG	HA	1611	1/1	0.88	0.20	-0.15	26,26,26,26	0
57	MG	BA	1613	1/1	0.96	0.17	-0.17	8,8,8,8	0
57	MG	GA	3053	1/1	0.99	0.17	-0.20	6,6,6,6	0
57	MG	FA	1628	1/1	0.99	0.16	-0.22	27,27,27,27	0
59	GCP	FV	801	32/32	0.95	0.16	-0.23	16,28,45,57	0
57	MG	EA	3014	1/1	0.97	0.21	-0.28	1,1,1,1	0
57	MG	GL	201	1/1	0.85	0.30	-0.31	47,47,47,47	0
57	MG	CA	3049	1/1	0.98	0.17	-0.31	7,7,7,7	0
57	MG	GA	3008	1/1	0.93	0.17	-0.32	24,24,24,24	0
57	MG	BA	1619	1/1	0.99	0.17	-0.34	13,13,13,13	0
57	MG	HA	1606	1/1	0.98	0.17	-0.35	29,29,29,29	0
57	MG	HA	1633	1/1	0.99	0.17	-0.38	46,46,46,46	0
59	GCP	DV	801	32/32	0.96	0.14	-0.39	17,28,38,41	0
57	MG	AA	3104	1/1	0.98	0.20	-0.41	2,2,2,2	0
57	MG	HA	1627	1/1	0.96	0.20	-0.42	41,41,41,41	0
57	MG	CA	3069	1/1	0.84	0.12	-0.42	61,61,61,61	0
57	MG	EA	3024	1/1	0.99	0.19	-0.43	2,2,2,2	0
57	MG	EA	3115	1/1	0.98	0.17	-0.43	6,6,6,6	0
57	MG	EA	3112	1/1	0.99	0.17	-0.43	2,2,2,2	0
57	MG	EA	3008	1/1	1.00	0.18	-0.48	1,1,1,1	0
57	MG	EA	3113	1/1	0.99	0.14	-0.49	7,7,7,7	0
57	MG	CA	3028	1/1	1.00	0.18	-0.52	9,9,9,9	0
57	MG	AA	3103	1/1	0.98	0.18	-0.55	0,0,0,0	0
57	MG	HA	1637	1/1	0.92	0.14	-0.56	51,51,51,51	0
57	MG	EA	3034	1/1	0.98	0.17	-0.57	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	EB	1202	1/1	0.98	0.13	-0.60	17,17,17,17	0
57	MG	GA	3078	1/1	0.98	0.12	-0.61	35,35,35,35	0
59	GCP	BV	801	32/32	0.98	0.14	-0.62	9,25,32,35	0
57	MG	GA	3032	1/1	0.94	0.16	-0.65	22,22,22,22	0
57	MG	EA	3108	1/1	0.98	0.20	-0.66	15,15,15,15	0
57	MG	FN	202	1/1	1.00	0.15	-0.80	26,26,26,26	0
57	MG	GA	3113	1/1	0.97	0.13	-0.80	32,32,32,32	0
57	MG	HA	1640	1/1	1.00	0.15	-0.81	18,18,18,18	0
57	MG	HA	1620	1/1	0.94	0.17	-0.83	32,32,32,32	0
57	MG	GA	3012	1/1	0.99	0.16	-0.85	22,22,22,22	0
57	MG	GA	3062	1/1	0.98	0.17	-0.86	19,19,19,19	0
57	MG	EA	3079	1/1	0.99	0.15	-0.88	8,8,8,8	0
57	MG	AA	3073	1/1	0.99	0.18	-0.89	2,2,2,2	0
58	ZN	C4	102	1/1	0.99	0.14	-0.90	41,41,41,41	0
57	MG	GA	3122	1/1	0.99	0.17	-0.93	16,16,16,16	0
57	MG	CA	3008	1/1	0.99	0.16	-0.95	14,14,14,14	0
57	MG	AA	3109	1/1	0.99	0.08	-0.96	20,20,20,20	0
57	MG	AA	3039	1/1	0.99	0.18	-0.97	3,3,3,3	0
57	MG	CA	3003	1/1	0.98	0.13	-0.98	10,10,10,10	0
57	MG	GA	3069	1/1	0.83	0.11	-0.99	70,70,70,70	0
57	MG	GA	3132	1/1	0.98	0.15	-1.00	28,28,28,28	0
57	MG	AA	3002	1/1	0.98	0.15	-1.00	25,25,25,25	0
57	MG	AA	3062	1/1	0.99	0.18	-1.01	4,4,4,4	0
57	MG	DA	1609	1/1	0.98	0.15	-1.01	13,13,13,13	0
57	MG	GA	3036	1/1	0.98	0.15	-1.04	38,38,38,38	0
57	MG	GA	3106	1/1	0.98	0.15	-1.04	7,7,7,7	0
59	GCP	HV	801	32/32	0.96	0.12	-1.04	18,36,48,55	0
57	MG	AA	3132	1/1	0.99	0.17	-1.07	0,0,0,0	0
57	MG	EA	3035	1/1	0.98	0.18	-1.07	12,12,12,12	0
57	MG	CA	3104	1/1	0.99	0.16	-1.10	8,8,8,8	0
57	MG	CA	3071	1/1	0.99	0.17	-1.14	10,10,10,10	0
57	MG	GA	3111	1/1	0.98	0.14	-1.15	35,35,35,35	0
57	MG	DA	1621	1/1	0.98	0.12	-1.16	44,44,44,44	0
58	ZN	A4	102	1/1	0.99	0.13	-1.17	42,42,42,42	0
57	MG	CA	3114	1/1	0.99	0.12	-1.17	26,26,26,26	0
57	MG	CA	3053	1/1	0.98	0.15	-1.18	20,20,20,20	0
57	MG	CE	301	1/1	0.98	0.07	-1.20	19,19,19,19	0
57	MG	ED	301	1/1	0.99	0.16	-1.21	7,7,7,7	0
57	MG	CA	3027	1/1	0.99	0.10	-1.23	10,10,10,10	0
57	MG	DA	1613	1/1	0.99	0.13	-1.24	23,23,23,23	0
57	MG	GA	3064	1/1	0.99	0.12	-1.25	11,11,11,11	0
57	MG	GA	3130	1/1	1.00	0.11	-1.32	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	BU	101	1/1	0.98	0.14	-1.36	19,19,19,19	0
57	MG	EA	3022	1/1	0.99	0.17	-1.36	2,2,2,2	0
57	MG	FA	1630	1/1	0.98	0.08	-1.38	44,44,44,44	0
57	MG	HA	1629	1/1	0.91	0.12	-1.38	45,45,45,45	0
58	ZN	G4	101	1/1	0.98	0.07	-1.47	66,66,66,66	0
57	MG	EA	3131	1/1	0.98	0.11	-1.47	3,3,3,3	0
57	MG	GA	3017	1/1	0.96	0.12	-1.48	10,10,10,10	0
57	MG	BA	1604	1/1	0.99	0.07	-1.50	17,17,17,17	0
57	MG	EA	3049	1/1	0.98	0.17	-1.51	8,8,8,8	0
57	MG	BA	1610	1/1	0.98	0.09	-1.52	41,41,41,41	0
57	MG	DA	1607	1/1	0.98	0.14	-1.54	16,16,16,16	0
57	MG	CA	3095	1/1	0.98	0.15	-1.55	14,14,14,14	0
57	MG	EA	3114	1/1	0.96	0.17	-1.55	17,17,17,17	0
57	MG	EA	3002	1/1	0.99	0.14	-1.61	7,7,7,7	0
57	MG	AA	3113	1/1	0.97	0.12	-1.63	8,8,8,8	0
57	MG	GA	3007	1/1	0.92	0.07	-1.65	39,39,39,39	0
57	MG	DA	1633	1/1	0.99	0.08	-1.87	29,29,29,29	0
57	MG	GA	3134	1/1	0.98	0.08	-1.88	28,28,28,28	0
57	MG	FA	1604	1/1	0.96	0.08	-2.06	34,34,34,34	0
57	MG	EA	3095	1/1	0.94	0.13	-2.07	6,6,6,6	0
57	MG	FA	1620	1/1	0.97	0.09	-2.08	41,41,41,41	0
57	MG	FA	1607	1/1	0.99	0.10	-2.09	21,21,21,21	0
57	MG	FA	1631	1/1	0.99	0.10	-2.13	24,24,24,24	0
57	MG	EA	3105	1/1	0.99	0.14	-2.14	5,5,5,5	0
57	MG	CA	3118	1/1	0.98	0.12	-2.14	31,31,31,31	0
57	MG	EA	3110	1/1	0.91	0.14	-2.15	12,12,12,12	0
57	MG	CA	3073	1/1	0.98	0.13	-2.17	4,4,4,4	0
57	MG	AA	3018	1/1	1.00	0.16	-2.19	2,2,2,2	0
57	MG	GA	3096	1/1	0.99	0.15	-2.23	15,15,15,15	0
57	MG	EA	3107	1/1	1.00	0.15	-2.23	5,5,5,5	0
57	MG	AA	3025	1/1	0.97	0.15	-2.25	0,0,0,0	0
57	MG	EA	3065	1/1	0.99	0.14	-2.30	5,5,5,5	0
57	MG	FA	1616	1/1	0.99	0.12	-2.50	18,18,18,18	0
57	MG	DA	1604	1/1	0.96	0.07	-2.51	18,18,18,18	0
57	MG	FA	1638	1/1	0.98	0.12	-2.51	16,16,16,16	0
57	MG	DA	1634	1/1	0.93	0.08	-2.58	34,34,34,34	0
57	MG	AA	3003	1/1	0.99	0.13	-2.59	11,11,11,11	0
57	MG	GA	3128	1/1	0.92	0.10	-2.61	18,18,18,18	0
57	MG	CA	3124	1/1	0.99	0.13	-2.63	26,26,26,26	0
57	MG	AA	3004	1/1	0.99	0.12	-2.72	20,20,20,20	0
57	MG	DA	1630	1/1	0.96	0.11	-2.72	25,25,25,25	0
57	MG	HA	1604	1/1	0.96	0.04	-2.74	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3012	1/1	0.97	0.21	-2.77	32,32,32,32	0
57	MG	DA	1624	1/1	0.96	0.14	-2.77	18,18,18,18	0
57	MG	CA	3063	1/1	0.99	0.14	-2.85	4,4,4,4	0
57	MG	EA	3106	1/1	0.99	0.13	-2.86	9,9,9,9	0
57	MG	DA	1611	1/1	0.99	0.11	-2.88	35,35,35,35	0
57	MG	AA	3054	1/1	1.00	0.14	-3.01	3,3,3,3	0
57	MG	AA	3024	1/1	0.99	0.15	-3.15	5,5,5,5	0
57	MG	AA	3119	1/1	0.98	0.15	-3.20	0,0,0,0	0
57	MG	EA	3109	1/1	0.96	0.11	-3.22	19,19,19,19	0
57	MG	AA	3082	1/1	0.99	0.07	-3.26	22,22,22,22	0
58	ZN	E4	101	1/1	0.99	0.09	-3.28	59,59,59,59	0
57	MG	EA	3064	1/1	0.99	0.14	-3.32	2,2,2,2	0
57	MG	AB	1202	1/1	0.99	0.08	-3.35	25,25,25,25	0
57	MG	AA	3014	1/1	0.99	0.14	-3.43	2,2,2,2	0
57	MG	GA	3002	1/1	0.98	0.07	-3.61	31,31,31,31	0
57	MG	CA	3012	1/1	0.94	0.13	-3.63	6,6,6,6	0
57	MG	GA	3118	1/1	0.99	0.11	-3.72	39,39,39,39	0
57	MG	GA	3074	1/1	0.99	0.14	-3.75	10,10,10,10	0
57	MG	EA	3111	1/1	0.98	0.13	-3.92	5,5,5,5	0
57	MG	DA	1617	1/1	0.97	0.08	-4.07	39,39,39,39	0
57	MG	CA	3070	1/1	0.99	0.10	-4.10	8,8,8,8	0
57	MG	CA	3058	1/1	1.00	0.14	-4.21	18,18,18,18	0
57	MG	CA	3050	1/1	0.99	0.08	-4.25	14,14,14,14	0
57	MG	AA	3123	1/1	0.99	0.11	-4.26	5,5,5,5	0
57	MG	AA	3131	1/1	0.99	0.10	-4.43	3,3,3,3	0
57	MG	EA	3066	1/1	0.99	0.12	-4.82	1,1,1,1	0
57	MG	AA	3071	1/1	1.00	0.12	-5.33	4,4,4,4	0
57	MG	EA	3128	1/1	0.98	0.18	-5.44	0,0,0,0	0
57	MG	BA	1631	1/1	0.99	0.07	-5.93	16,16,16,16	0
57	MG	GA	3027	1/1	0.99	0.09	-5.97	17,17,17,17	0
57	MG	AA	3128	1/1	1.00	0.15	-6.05	0,0,0,0	0
57	MG	CA	3119	1/1	0.94	0.08	-6.25	34,34,34,34	0
57	MG	AA	3028	1/1	0.99	0.12	-7.11	4,4,4,4	0
57	MG	CA	3013	1/1	0.99	0.07	-7.12	9,9,9,9	0
57	MG	GA	3065	1/1	0.98	0.12	-	20,20,20,20	0
57	MG	FA	1621	1/1	0.97	0.14	-	13,13,13,13	0
57	MG	FA	1614	1/1	0.98	0.20	-	13,13,13,13	0
57	MG	DA	1631	1/1	0.99	0.06	-	13,13,13,13	0
57	MG	GA	3121	1/1	0.96	0.15	-	16,16,16,16	0
57	MG	EA	3006	1/1	0.99	0.11	-	9,9,9,9	0
57	MG	EA	3134	1/1	0.99	0.24	-	7,7,7,7	0
57	MG	FA	1601	1/1	0.98	0.08	-	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	AA	3008	1/1	0.99	0.06	-	19,19,19,19	0
57	MG	GA	3054	1/1	0.98	0.14	-	12,12,12,12	0
57	MG	EA	3082	1/1	0.99	0.12	-	6,6,6,6	0
57	MG	EA	3124	1/1	0.99	0.43	-	4,4,4,4	0
57	MG	CA	3020	1/1	0.99	0.11	-	6,6,6,6	0
57	MG	GA	3083	1/1	0.91	0.12	-	26,26,26,26	0
57	MG	EA	3126	1/1	0.99	0.13	-	6,6,6,6	0
57	MG	GA	3052	1/1	0.98	0.18	-	4,4,4,4	0
57	MG	AA	3093	1/1	0.91	0.31	-	34,34,34,34	0
57	MG	EA	3045	1/1	0.98	0.17	-	9,9,9,9	0
57	MG	GA	3135	1/1	0.84	0.41	-	28,28,28,28	0
57	MG	AA	3101	1/1	0.99	0.16	-	8,8,8,8	0
57	MG	EA	3125	1/1	0.95	0.24	-	18,18,18,18	0
57	MG	AA	3059	1/1	0.99	0.24	-	1,1,1,1	0
57	MG	CA	3123	1/1	0.99	0.24	-	26,26,26,26	0
57	MG	FU	101	1/1	0.95	0.17	-	21,21,21,21	0
57	MG	EA	3102	1/1	0.98	0.08	-	23,23,23,23	0
57	MG	AA	3084	1/1	0.96	0.19	-	2,2,2,2	0
57	MG	BA	1603	1/1	0.97	0.15	-	18,18,18,18	0
57	MG	GA	3127	1/1	0.98	0.13	-	18,18,18,18	0
57	MG	GA	3105	1/1	0.98	0.17	-	16,16,16,16	0
57	MG	AA	3030	1/1	0.99	0.09	-	1,1,1,1	0
57	MG	GB	1203	1/1	0.98	0.07	-	23,23,23,23	0
57	MG	GA	3014	1/1	0.99	0.07	-	15,15,15,15	0
57	MG	GA	3043	1/1	0.99	0.09	-	20,20,20,20	0
57	MG	GA	3026	1/1	0.98	0.16	-	31,31,31,31	0
57	MG	FA	1625	1/1	0.98	0.15	-	21,21,21,21	0
57	MG	FA	1605	1/1	0.99	0.09	-	30,30,30,30	0
57	MG	AA	3074	1/1	0.99	0.18	-	5,5,5,5	0
57	MG	GA	3094	1/1	0.99	0.06	-	14,14,14,14	0
57	MG	GA	3077	1/1	0.97	0.12	-	55,55,55,55	0
57	MG	HA	1609	1/1	0.91	0.20	-	23,23,23,23	0
57	MG	A4	101	1/1	0.98	0.12	-	20,20,20,20	0
57	MG	BA	1612	1/1	0.99	0.18	-	3,3,3,3	0
57	MG	CA	3117	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	CA	3075	1/1	0.99	0.25	-	11,11,11,11	0
57	MG	AA	3064	1/1	0.99	0.12	-	3,3,3,3	0
57	MG	HA	1608	1/1	0.94	0.43	-	47,47,47,47	0
57	MG	CA	3128	1/1	1.00	0.16	-	17,17,17,17	0
57	MG	CA	3088	1/1	0.96	0.28	-	23,23,23,23	0
57	MG	CA	3134	1/1	0.98	0.20	-	21,21,21,21	0
57	MG	AA	3089	1/1	0.99	0.09	-	4,4,4,4	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	GA	3010	1/1	0.98	0.32	-	16,16,16,16	0
57	MG	CA	3025	1/1	0.94	0.14	-	24,24,24,24	0
57	MG	EA	3020	1/1	1.00	0.15	-	7,7,7,7	0
57	MG	BA	1602	1/1	0.88	0.23	-	38,38,38,38	0
57	MG	EA	3121	1/1	0.97	0.30	-	5,5,5,5	0
57	MG	GA	3124	1/1	0.94	0.20	-	36,36,36,36	0
57	MG	EA	3122	1/1	0.97	0.28	-	4,4,4,4	0
57	MG	CA	3044	1/1	0.95	0.08	-	28,28,28,28	0
57	MG	GA	3045	1/1	0.99	0.20	-	17,17,17,17	0
57	MG	FA	1637	1/1	0.97	0.09	-	29,29,29,29	0
57	MG	GA	3004	1/1	0.95	0.39	-	25,25,25,25	0
57	MG	CB	1203	1/1	0.99	0.10	-	12,12,12,12	0
57	MG	GA	3082	1/1	0.98	0.09	-	38,38,38,38	0
57	MG	CA	3122	1/1	1.00	0.20	-	5,5,5,5	0
57	MG	AA	3022	1/1	1.00	0.11	-	2,2,2,2	0
57	MG	EA	3099	1/1	0.99	0.16	-	3,3,3,3	0
57	MG	EA	3068	1/1	1.00	0.20	-	2,2,2,2	0
57	MG	BA	1615	1/1	0.91	0.30	-	25,25,25,25	0
57	MG	HA	1607	1/1	0.98	0.07	-	33,33,33,33	0
57	MG	CA	3026	1/1	0.98	0.15	-	14,14,14,14	0
57	MG	FA	1606	1/1	0.95	0.16	-	15,15,15,15	0
57	MG	EA	3091	1/1	0.95	0.27	-	40,40,40,40	0
57	MG	FA	1629	1/1	0.99	0.12	-	30,30,30,30	0
57	MG	GA	3011	1/1	0.88	0.11	-	46,46,46,46	0
57	MG	EA	3041	1/1	0.98	0.18	-	3,3,3,3	0
57	MG	CA	3074	1/1	0.98	0.16	-	13,13,13,13	0
57	MG	GA	3029	1/1	0.99	0.08	-	16,16,16,16	0
57	MG	BA	1601	1/1	0.98	0.10	-	23,23,23,23	0
57	MG	EA	3058	1/1	0.99	0.14	-	5,5,5,5	0
57	MG	CA	3065	1/1	0.99	0.17	-	11,11,11,11	0
57	MG	EA	3118	1/1	0.93	0.13	-	17,17,17,17	0
57	MG	HA	1624	1/1	0.88	0.11	-	38,38,38,38	0
57	MG	CA	3089	1/1	0.99	0.19	-	14,14,14,14	0
57	MG	DA	1623	1/1	0.97	0.17	-	42,42,42,42	0
57	MG	GA	3016	1/1	0.98	0.12	-	12,12,12,12	0
57	MG	CA	3041	1/1	0.99	0.08	-	12,12,12,12	0
57	MG	EA	3007	1/1	0.98	0.08	-	12,12,12,12	0
57	MG	GA	3028	1/1	0.96	0.17	-	12,12,12,12	0
57	MG	BA	1621	1/1	1.00	0.09	-	11,11,11,11	0
57	MG	EA	3012	1/1	1.00	0.20	-	2,2,2,2	0
57	MG	EA	3059	1/1	1.00	0.17	-	10,10,10,10	0
57	MG	FA	1619	1/1	0.99	0.12	-	7,7,7,7	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	EA	3132	1/1	0.96	0.14	-	21,21,21,21	0
57	MG	BA	1609	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	HA	1632	1/1	0.97	0.10	-	31,31,31,31	0
57	MG	EA	3013	1/1	1.00	0.13	-	1,1,1,1	0
57	MG	EA	3019	1/1	0.96	0.13	-	10,10,10,10	0
57	MG	HA	1631	1/1	0.96	0.17	-	31,31,31,31	0
57	MG	EA	3021	1/1	0.99	0.16	-	11,11,11,11	0
57	MG	CA	3032	1/1	0.99	0.17	-	8,8,8,8	0
57	MG	DA	1619	1/1	0.99	0.18	-	34,34,34,34	0
57	MG	AB	1201	1/1	0.99	0.08	-	34,34,34,34	0
57	MG	AA	3083	1/1	0.94	0.26	-	18,18,18,18	0
57	MG	GA	3080	1/1	0.90	0.21	-	36,36,36,36	0
57	MG	FN	201	1/1	0.96	0.24	-	14,14,14,14	0
57	MG	CA	3087	1/1	0.99	0.14	-	23,23,23,23	0
57	MG	AA	3105	1/1	0.99	0.15	-	2,2,2,2	0
57	MG	AA	3045	1/1	0.97	0.21	-	8,8,8,8	0
57	MG	EB	1203	1/1	0.99	0.17	-	0,0,0,0	0
57	MG	CA	3093	1/1	0.97	0.11	-	40,40,40,40	0
57	MG	AA	3118	1/1	0.97	0.07	-	14,14,14,14	0
57	MG	EA	3061	1/1	0.99	0.17	-	5,5,5,5	0
57	MG	CA	3061	1/1	0.98	0.10	-	4,4,4,4	0
57	MG	CA	3057	1/1	1.00	0.11	-	7,7,7,7	0
57	MG	DA	1622	1/1	0.99	0.14	-	13,13,13,13	0
57	MG	GA	3037	1/1	0.99	0.32	-	18,18,18,18	0
57	MG	CA	3001	1/1	1.00	0.09	-	16,16,16,16	0
57	MG	AA	3086	1/1	0.99	0.08	-	14,14,14,14	0
57	MG	CA	3084	1/1	0.99	0.22	-	20,20,20,20	0
57	MG	EA	3016	1/1	0.99	0.23	-	0,0,0,0	0
57	MG	CA	3031	1/1	0.99	0.15	-	7,7,7,7	0
57	MG	CA	3022	1/1	0.99	0.12	-	17,17,17,17	0
57	MG	AA	3136	1/1	0.97	0.34	-	11,11,11,11	0
57	MG	GA	3116	1/1	0.92	0.31	-	22,22,22,22	0
57	MG	GA	3042	1/1	1.00	0.14	-	20,20,20,20	0
57	MG	GA	3097	1/1	0.99	0.28	-	10,10,10,10	0
57	MG	EA	3076	1/1	0.97	0.13	-	6,6,6,6	0
57	MG	EA	3003	1/1	0.99	0.19	-	9,9,9,9	0
57	MG	CA	3126	1/1	0.99	0.14	-	22,22,22,22	0
57	MG	FE	201	1/1	0.98	0.12	-	35,35,35,35	0
57	MG	HA	1612	1/1	0.97	0.28	-	20,20,20,20	0
57	MG	EA	3043	1/1	1.00	0.17	-	8,8,8,8	0
57	MG	EA	3031	1/1	1.00	0.16	-	1,1,1,1	0
57	MG	GA	3087	1/1	0.98	0.12	-	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	EA	3036	1/1	0.98	0.13	-	12,12,12,12	0
57	MG	HA	1616	1/1	0.96	0.38	-	40,40,40,40	0
57	MG	AA	3031	1/1	0.99	0.20	-	5,5,5,5	0
57	MG	BA	1639	1/1	0.98	0.26	-	12,12,12,12	0
57	MG	AA	3076	1/1	0.98	0.14	-	13,13,13,13	0
57	MG	FA	1634	1/1	0.99	0.18	-	13,13,13,13	0
57	MG	AA	3121	1/1	0.99	0.22	-	3,3,3,3	0
57	MG	HA	1625	1/1	0.94	0.32	-	44,44,44,44	0
57	MG	CA	3052	1/1	1.00	0.14	-	4,4,4,4	0
57	MG	AA	3006	1/1	0.88	0.15	-	32,32,32,32	0
57	MG	AA	3056	1/1	1.00	0.13	-	11,11,11,11	0
57	MG	GA	3041	1/1	0.99	0.12	-	10,10,10,10	0
57	MG	GA	3051	1/1	0.96	0.25	-	20,20,20,20	0
57	MG	CA	3125	1/1	1.00	0.23	-	11,11,11,11	0
57	MG	GA	3092	1/1	0.98	0.17	-	16,16,16,16	0
57	MG	CA	3132	1/1	0.98	0.10	-	9,9,9,9	0
57	MG	EA	3069	1/1	0.95	0.09	-	25,25,25,25	0
57	MG	AE	301	1/1	0.95	0.30	-	21,21,21,21	0
57	MG	HA	1615	1/1	0.89	0.17	-	36,36,36,36	0
57	MG	AA	3046	1/1	0.98	0.29	-	13,13,13,13	0
57	MG	BA	1611	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	CA	3115	1/1	0.87	0.23	-	51,51,51,51	0
57	MG	AA	3077	1/1	0.99	0.11	-	16,16,16,16	0
57	MG	BA	1630	1/1	0.99	0.16	-	26,26,26,26	0
57	MG	EA	3070	1/1	0.93	0.60	-	23,23,23,23	0
57	MG	CA	3056	1/1	0.88	0.72	-	27,27,27,27	0
57	MG	EA	3050	1/1	0.91	0.19	-	23,23,23,23	0
57	MG	BA	1633	1/1	0.98	0.10	-	20,20,20,20	0
57	MG	FA	1632	1/1	0.99	0.13	-	24,24,24,24	0
57	MG	GA	3076	1/1	0.91	0.27	-	34,34,34,34	0
57	MG	EA	3052	1/1	0.97	0.17	-	12,12,12,12	0
57	MG	GA	3114	1/1	0.92	0.31	-	27,27,27,27	0
57	MG	DA	1635	1/1	0.94	0.08	-	37,37,37,37	0
57	MG	EA	3073	1/1	0.99	0.15	-	0,0,0,0	0
57	MG	GA	3071	1/1	0.99	0.16	-	16,16,16,16	0
57	MG	HA	1617	1/1	0.89	0.14	-	49,49,49,49	0
57	MG	AA	3102	1/1	0.99	0.11	-	10,10,10,10	0
57	MG	FA	1608	1/1	0.99	0.23	-	13,13,13,13	0
57	MG	EA	3030	1/1	0.99	0.28	-	7,7,7,7	0
57	MG	HA	1602	1/1	0.95	0.16	-	26,26,26,26	0
57	MG	AA	3088	1/1	0.98	0.18	-	4,4,4,4	0
57	MG	EA	3081	1/1	0.99	0.20	-	0,0,0,0	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	FA	1610	1/1	0.97	0.25	-	33,33,33,33	0
57	MG	CA	3037	1/1	0.99	0.27	-	6,6,6,6	0
57	MG	AA	3017	1/1	1.00	0.11	-	0,0,0,0	0
57	MG	DA	1638	1/1	0.98	0.09	-	25,25,25,25	0
57	MG	GA	3058	1/1	0.99	0.13	-	24,24,24,24	0
57	MG	EA	3028	1/1	0.98	0.17	-	7,7,7,7	0
57	MG	CA	3098	1/1	0.97	0.15	-	29,29,29,29	0
57	MG	FA	1617	1/1	0.97	0.12	-	40,40,40,40	0
57	MG	HA	1621	1/1	0.99	0.14	-	7,7,7,7	0
57	MG	GA	3075	1/1	0.98	0.18	-	16,16,16,16	0
57	MG	AA	3079	1/1	0.99	0.11	-	4,4,4,4	0
57	MG	AA	3011	1/1	1.00	0.25	-	6,6,6,6	0
57	MG	BA	1620	1/1	0.93	0.12	-	15,15,15,15	0
57	MG	AA	3066	1/1	1.00	0.21	-	0,0,0,0	0
57	MG	BN	201	1/1	0.98	0.20	-	13,13,13,13	0
57	MG	AA	3058	1/1	0.99	0.14	-	9,9,9,9	0
57	MG	CA	3007	1/1	0.98	0.15	-	35,35,35,35	0
57	MG	EA	3117	1/1	0.97	0.09	-	15,15,15,15	0
57	MG	EA	3071	1/1	0.99	0.17	-	0,0,0,0	0
57	MG	BA	1618	1/1	0.99	0.17	-	1,1,1,1	0
57	MG	GC	301	1/1	0.98	0.24	-	26,26,26,26	0
57	MG	CA	3082	1/1	0.98	0.16	-	14,14,14,14	0
57	MG	EA	3063	1/1	0.99	0.14	-	2,2,2,2	0
57	MG	DA	1629	1/1	0.90	0.53	-	43,43,43,43	0
57	MG	CA	3019	1/1	0.98	0.14	-	27,27,27,27	0
57	MG	GA	3006	1/1	0.94	0.12	-	29,29,29,29	0
57	MG	HA	1626	1/1	0.74	0.27	-	32,32,32,32	0
57	MG	EA	3055	1/1	0.89	0.56	-	30,30,30,30	0
57	MG	EA	3078	1/1	0.98	0.10	-	20,20,20,20	0
57	MG	CA	3060	1/1	0.99	0.12	-	7,7,7,7	0
57	MG	EA	3129	1/1	0.99	0.21	-	2,2,2,2	0
57	MG	GA	3066	1/1	0.99	0.16	-	12,12,12,12	0
57	MG	EA	3075	1/1	1.00	0.21	-	11,11,11,11	0
57	MG	CA	3083	1/1	0.99	0.04	-	32,32,32,32	0
57	MG	AA	3040	1/1	1.00	0.25	-	1,1,1,1	0
57	MG	EA	3090	1/1	0.99	0.07	-	11,11,11,11	0
57	MG	CA	3072	1/1	0.99	0.14	-	14,14,14,14	0
57	MG	HK	201	1/1	0.81	0.24	-	28,28,28,28	0
57	MG	EA	3116	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	EB	1201	1/1	0.97	0.10	-	30,30,30,30	0
57	MG	CA	3043	1/1	0.99	0.16	-	4,4,4,4	0
57	MG	HA	1639	1/1	0.96	0.14	-	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	EA	3093	1/1	0.98	0.13	-	11,11,11,11	0
57	MG	GA	3112	1/1	0.99	0.20	-	13,13,13,13	0
57	MG	GA	3085	1/1	0.99	0.17	-	10,10,10,10	0
57	MG	GA	3073	1/1	0.99	0.17	-	10,10,10,10	0
57	MG	AA	3049	1/1	0.99	0.19	-	17,17,17,17	0
57	MG	BA	1637	1/1	0.94	0.34	-	15,15,15,15	0
57	MG	CA	3011	1/1	0.90	0.22	-	31,31,31,31	0
57	MG	CA	3051	1/1	0.99	0.32	-	6,6,6,6	0
57	MG	EA	3086	1/1	1.00	0.19	-	8,8,8,8	0
57	MG	CA	3034	1/1	0.98	0.14	-	13,13,13,13	0
57	MG	FA	1623	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	AA	3033	1/1	0.99	0.19	-	1,1,1,1	0
57	MG	EA	3032	1/1	1.00	0.17	-	1,1,1,1	0
57	MG	HA	1601	1/1	0.94	0.06	-	27,27,27,27	0
57	MG	GA	3056	1/1	1.00	0.06	-	13,13,13,13	0
57	MG	GA	3091	1/1	0.98	0.06	-	28,28,28,28	0
57	MG	GA	3003	1/1	0.98	0.10	-	26,26,26,26	0
57	MG	HA	1634	1/1	0.96	0.10	-	35,35,35,35	0
57	MG	AA	3126	1/1	0.99	0.13	-	2,2,2,2	0
57	MG	EA	3127	1/1	0.99	0.15	-	11,11,11,11	0
57	MG	AA	3133	1/1	0.99	0.18	-	10,10,10,10	0
57	MG	AA	3007	1/1	0.97	0.10	-	19,19,19,19	0
57	MG	AA	3099	1/1	0.99	0.14	-	13,13,13,13	0
57	MG	DA	1615	1/1	0.99	0.20	-	45,45,45,45	0
57	MG	EA	3027	1/1	1.00	0.17	-	4,4,4,4	0
57	MG	BE	201	1/1	0.81	0.15	-	31,31,31,31	0
57	MG	AA	3001	1/1	0.95	0.72	-	20,20,20,20	0
57	MG	EA	3060	1/1	0.99	0.20	-	2,2,2,2	0
57	MG	DA	1602	1/1	0.97	0.08	-	28,28,28,28	0
57	MG	AA	3052	1/1	0.98	0.16	-	3,3,3,3	0
57	MG	AA	3019	1/1	0.98	0.14	-	15,15,15,15	0
57	MG	AA	3127	1/1	0.99	0.13	-	10,10,10,10	0
57	MG	GA	3067	1/1	0.99	0.27	-	29,29,29,29	0
57	MG	GA	3103	1/1	0.99	0.22	-	12,12,12,12	0
57	MG	DA	1612	1/1	0.97	0.14	-	33,33,33,33	0
57	MG	EA	3051	1/1	0.98	0.27	-	6,6,6,6	0
57	MG	FA	1633	1/1	0.98	0.15	-	24,24,24,24	0
57	MG	EA	3101	1/1	0.98	0.14	-	7,7,7,7	0
57	MG	EA	3067	1/1	0.99	0.21	-	3,3,3,3	0
57	MG	GA	3133	1/1	0.91	0.42	-	15,15,15,15	0
57	MG	CA	3106	1/1	0.99	0.26	-	12,12,12,12	0
57	MG	AA	3069	1/1	0.86	0.13	-	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	EA	3039	1/1	0.93	0.19	-	15,15,15,15	0
57	MG	AA	3016	1/1	0.95	0.17	-	11,11,11,11	0
57	MG	DA	1608	1/1	0.96	0.22	-	30,30,30,30	0
57	MG	CA	3077	1/1	0.90	0.63	-	37,37,37,37	0
57	MG	DA	1625	1/1	0.98	0.14	-	29,29,29,29	0
57	MG	EA	3083	1/1	0.59	0.43	-	35,35,35,35	0
57	MG	CA	3091	1/1	0.94	0.43	-	38,38,38,38	0
57	MG	BA	1625	1/1	0.96	0.17	-	23,23,23,23	0
57	MG	FA	1624	1/1	0.98	0.20	-	27,27,27,27	0
57	MG	CA	3067	1/1	1.00	0.20	-	6,6,6,6	0
57	MG	CA	3054	1/1	0.99	0.09	-	14,14,14,14	0
57	MG	BA	1608	1/1	0.99	0.23	-	11,11,11,11	0
57	MG	EA	3089	1/1	0.99	0.14	-	6,6,6,6	0
57	MG	HA	1622	1/1	0.97	0.21	-	30,30,30,30	0
57	MG	GA	3129	1/1	0.94	0.28	-	29,29,29,29	0
57	MG	GA	3120	1/1	0.97	0.20	-	19,19,19,19	0
57	MG	CA	3035	1/1	1.00	0.13	-	7,7,7,7	0
57	MG	EA	3062	1/1	0.99	0.16	-	4,4,4,4	0
57	MG	AA	3112	1/1	0.98	0.25	-	0,0,0,0	0
57	MG	EA	3085	1/1	0.99	0.26	-	11,11,11,11	0
57	MG	GA	3015	1/1	0.95	0.22	-	27,27,27,27	0
57	MG	AA	3032	1/1	0.99	0.17	-	0,0,0,0	0
57	MG	CA	3004	1/1	0.99	0.09	-	24,24,24,24	0
57	MG	CA	3103	1/1	0.98	0.11	-	17,17,17,17	0
57	MG	GA	3095	1/1	0.85	0.42	-	43,43,43,43	0
57	MG	AA	3042	1/1	0.98	0.20	-	8,8,8,8	0
57	MG	CA	3101	1/1	1.00	0.18	-	5,5,5,5	0
57	MG	AA	3027	1/1	0.99	0.17	-	15,15,15,15	0
57	MG	GA	3072	1/1	0.99	0.08	-	24,24,24,24	0
57	MG	AA	3124	1/1	0.97	0.25	-	4,4,4,4	0
57	MG	EA	3080	1/1	0.98	0.20	-	15,15,15,15	0
57	MG	GB	1201	1/1	0.82	0.26	-	62,62,62,62	0
57	MG	DA	1626	1/1	0.92	0.15	-	44,44,44,44	0
57	MG	GA	3098	1/1	1.00	0.15	-	15,15,15,15	0
57	MG	BA	1614	1/1	0.99	0.11	-	7,7,7,7	0
57	MG	CA	3097	1/1	0.99	0.13	-	3,3,3,3	0
57	MG	GA	3019	1/1	1.00	0.15	-	6,6,6,6	0
57	MG	FA	1636	1/1	0.71	0.24	-	35,35,35,35	0
57	MG	DA	1620	1/1	1.00	0.04	-	12,12,12,12	0
57	MG	AA	3070	1/1	0.98	0.27	-	6,6,6,6	0
57	MG	BA	1617	1/1	0.99	0.06	-	21,21,21,21	0
57	MG	CA	3100	1/1	0.99	0.07	-	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	GA	3070	1/1	0.94	0.14	-	22,22,22,22	0
57	MG	GA	3048	1/1	0.99	0.16	-	15,15,15,15	0
57	MG	EA	3056	1/1	0.98	0.13	-	13,13,13,13	0
57	MG	GA	3001	1/1	0.99	0.06	-	31,31,31,31	0
57	MG	CA	3036	1/1	0.98	0.12	-	28,28,28,28	0
57	MG	GA	3126	1/1	0.98	0.07	-	35,35,35,35	0
57	MG	GA	3039	1/1	0.98	0.25	-	28,28,28,28	0
57	MG	CA	3078	1/1	0.96	0.08	-	34,34,34,34	0
57	MG	AA	3075	1/1	0.98	0.11	-	15,15,15,15	0
57	MG	AA	3134	1/1	0.96	0.23	-	21,21,21,21	0
57	MG	FA	1603	1/1	0.92	0.14	-	20,20,20,20	0
57	MG	AA	3043	1/1	0.99	0.15	-	5,5,5,5	0
57	MG	CA	3059	1/1	0.98	0.18	-	10,10,10,10	0
57	MG	AA	3072	1/1	0.99	0.17	-	5,5,5,5	0
57	MG	CB	1204	1/1	0.97	0.05	-	15,15,15,15	0
57	MG	GA	3018	1/1	0.96	0.05	-	21,21,21,21	0
57	MG	FA	1639	1/1	0.99	0.16	-	20,20,20,20	0
57	MG	GA	3034	1/1	0.99	0.09	-	36,36,36,36	0
57	MG	GA	3123	1/1	0.98	0.20	-	44,44,44,44	0
57	MG	HA	1618	1/1	0.92	0.16	-	35,35,35,35	0
57	MG	CA	3029	1/1	0.99	0.15	-	19,19,19,19	0
57	MG	CA	3081	1/1	0.99	0.24	-	6,6,6,6	0
57	MG	GA	3136	1/1	0.95	0.22	-	27,27,27,27	0
57	MG	CA	3135	1/1	0.94	0.36	-	8,8,8,8	0
57	MG	CA	3085	1/1	0.95	0.16	-	5,5,5,5	0
57	MG	GA	3093	1/1	0.99	0.11	-	21,21,21,21	0
57	MG	CA	3039	1/1	0.99	0.25	-	4,4,4,4	0
57	MG	GA	3033	1/1	0.97	0.28	-	30,30,30,30	0
57	MG	EA	3017	1/1	0.99	0.15	-	8,8,8,8	0
57	MG	AA	3005	1/1	0.97	0.13	-	16,16,16,16	0
57	MG	GA	3063	1/1	0.98	0.14	-	27,27,27,27	0
57	MG	EB	1204	1/1	0.99	0.12	-	8,8,8,8	0
57	MG	DA	1640	1/1	0.98	0.06	-	24,24,24,24	0
57	MG	AA	3092	1/1	0.94	0.10	-	14,14,14,14	0
57	MG	DA	1643	1/1	0.94	0.22	-	32,32,32,32	0
57	MG	EA	3015	1/1	0.87	0.55	-	2,2,2,2	0
57	MG	AA	3038	1/1	0.98	0.26	-	3,3,3,3	0
57	MG	GA	3057	1/1	0.92	0.14	-	28,28,28,28	0
57	MG	HA	1603	1/1	0.99	0.08	-	25,25,25,25	0
57	MG	EA	3077	1/1	0.99	0.09	-	18,18,18,18	0
57	MG	EA	3029	1/1	1.00	0.25	-	2,2,2,2	0
57	MG	DA	1603	1/1	0.95	0.13	-	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	FA	1618	1/1	0.96	0.27	-	21,21,21,21	0
57	MG	AA	3080	1/1	0.99	0.22	-	0,0,0,0	0
57	MG	GA	3090	1/1	0.94	0.10	-	27,27,27,27	0
57	MG	CA	3062	1/1	0.99	0.16	-	15,15,15,15	0
57	MG	GA	3060	1/1	0.98	0.15	-	18,18,18,18	0
57	MG	DA	1637	1/1	0.98	0.12	-	25,25,25,25	0
57	MG	HA	1605	1/1	0.98	0.15	-	40,40,40,40	0
57	MG	BA	1624	1/1	0.99	0.21	-	9,9,9,9	0
57	MG	EA	3057	1/1	0.97	0.07	-	18,18,18,18	0
57	MG	HA	1619	1/1	0.91	0.10	-	19,19,19,19	0
57	MG	CA	3092	1/1	0.93	0.27	-	58,58,58,58	0
57	MG	AA	3021	1/1	0.99	0.20	-	6,6,6,6	0
57	MG	AB	1204	1/1	0.99	0.06	-	18,18,18,18	0
57	MG	EA	3088	1/1	0.96	0.35	-	19,19,19,19	0
57	MG	CA	3108	1/1	1.00	0.21	-	11,11,11,11	0
57	MG	DA	1632	1/1	0.98	0.09	-	22,22,22,22	0
57	MG	CA	3010	1/1	0.96	0.28	-	8,8,8,8	0
57	MG	HA	1641	1/1	0.93	0.19	-	30,30,30,30	0
57	MG	CA	3094	1/1	0.92	0.43	-	37,37,37,37	0
57	MG	AA	3048	1/1	0.99	0.08	-	16,16,16,16	0
57	MG	EA	3033	1/1	0.97	0.26	-	0,0,0,0	0
57	MG	EA	3010	1/1	1.00	0.16	-	6,6,6,6	0
57	MG	CA	3017	1/1	1.00	0.18	-	7,7,7,7	0
57	MG	GA	3086	1/1	0.95	0.13	-	24,24,24,24	0
57	MG	GA	3046	1/1	0.99	0.12	-	35,35,35,35	0
57	MG	CA	3002	1/1	0.97	0.16	-	38,38,38,38	0
57	MG	AA	3051	1/1	0.99	0.10	-	9,9,9,9	0
57	MG	GA	3110	1/1	0.92	0.21	-	11,11,11,11	0
57	MG	CA	3064	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	GA	3079	1/1	0.72	0.80	-	52,52,52,52	0
57	MG	EA	3092	1/1	0.97	0.13	-	22,22,22,22	0
57	MG	AA	3013	1/1	0.99	0.18	-	0,0,0,0	0
57	MG	EA	3011	1/1	0.91	0.88	-	24,24,24,24	0
57	MG	AA	3110	1/1	0.98	0.20	-	9,9,9,9	0
57	MG	CA	3111	1/1	0.96	0.15	-	18,18,18,18	0
57	MG	CA	3047	1/1	0.99	0.10	-	23,23,23,23	0
57	MG	EA	3074	1/1	0.98	0.20	-	11,11,11,11	0
57	MG	AA	3036	1/1	1.00	0.18	-	2,2,2,2	0
57	MG	BA	1622	1/1	0.99	0.16	-	17,17,17,17	0
57	MG	AA	3015	1/1	0.99	0.27	-	0,0,0,0	0
57	MG	CA	3076	1/1	0.98	0.13	-	16,16,16,16	0
57	MG	AA	3010	1/1	0.99	0.18	-	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	HA	1610	1/1	0.98	0.07	-	31,31,31,31	0
57	MG	AA	3081	1/1	0.99	0.11	-	1,1,1,1	0
57	MG	DA	1627	1/1	0.99	0.14	-	23,23,23,23	0
57	MG	CA	3006	1/1	0.94	0.08	-	30,30,30,30	0
57	MG	GA	3025	1/1	0.94	0.17	-	25,25,25,25	0
57	MG	CA	3048	1/1	0.99	0.17	-	17,17,17,17	0
57	MG	AA	3087	1/1	0.97	0.15	-	19,19,19,19	0
57	MG	EA	3047	1/1	0.99	0.08	-	25,25,25,25	0
57	MG	CA	3127	1/1	0.99	0.17	-	3,3,3,3	0
57	MG	CA	3090	1/1	0.97	0.21	-	19,19,19,19	0
57	MG	CA	3102	1/1	0.99	0.24	-	9,9,9,9	0
57	MG	EE	301	1/1	0.98	0.09	-	19,19,19,19	0
57	MG	GA	3125	1/1	1.00	0.12	-	10,10,10,10	0
57	MG	AC	301	1/1	0.99	0.14	-	3,3,3,3	0
57	MG	AA	3091	1/1	0.99	0.08	-	33,33,33,33	0
57	MG	CA	3055	1/1	0.96	0.19	-	19,19,19,19	0
57	MG	C4	101	1/1	0.97	0.09	-	17,17,17,17	0
57	MG	GA	3068	1/1	0.94	0.40	-	30,30,30,30	0
57	MG	GA	3061	1/1	0.98	0.11	-	20,20,20,20	0
57	MG	EA	3009	1/1	0.98	0.25	-	2,2,2,2	0
57	MG	DA	1618	1/1	0.97	0.04	-	37,37,37,37	0
57	MG	EA	3135	1/1	0.98	0.14	-	25,25,25,25	0
57	MG	HA	1614	1/1	0.94	0.17	-	49,49,49,49	0
57	MG	CA	3086	1/1	0.99	0.17	-	15,15,15,15	0
57	MG	GA	3038	1/1	0.98	0.17	-	21,21,21,21	0
57	MG	AA	3096	1/1	1.00	0.15	-	0,0,0,0	0
57	MG	GA	3013	1/1	0.98	0.08	-	18,18,18,18	0
57	MG	CA	3129	1/1	0.99	0.12	-	9,9,9,9	0
57	MG	CA	3080	1/1	0.97	0.17	-	20,20,20,20	0
57	MG	CA	3015	1/1	0.94	0.12	-	25,25,25,25	0
57	MG	AA	3098	1/1	0.99	0.21	-	0,0,0,0	0
57	MG	GA	3020	1/1	0.99	0.19	-	3,3,3,3	0
57	MG	AA	3034	1/1	0.99	0.21	-	4,4,4,4	0
57	MG	EA	3044	1/1	0.99	0.10	-	15,15,15,15	0
57	MG	AB	1203	1/1	0.98	0.16	-	0,0,0,0	0
57	MG	CA	3042	1/1	0.98	0.08	-	16,16,16,16	0
57	MG	FA	1615	1/1	0.99	0.12	-	16,16,16,16	0
57	MG	AA	3057	1/1	0.99	0.09	-	25,25,25,25	0
57	MG	CA	3038	1/1	0.99	0.20	-	9,9,9,9	0
57	MG	GA	3081	1/1	0.99	0.19	-	14,14,14,14	0
57	MG	GA	3089	1/1	0.99	0.20	-	8,8,8,8	0
57	MG	FA	1602	1/1	0.98	0.12	-	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	EA	3098	1/1	0.99	0.17	-	4,4,4,4	0
57	MG	HE	201	1/1	0.90	0.34	-	55,55,55,55	0
57	MG	GA	3117	1/1	0.97	0.13	-	10,10,10,10	0
57	MG	AA	3116	1/1	0.99	0.14	-	0,0,0,0	0
57	MG	GA	3044	1/1	0.98	0.06	-	21,21,21,21	0
57	MG	HA	1635	1/1	0.98	0.11	-	28,28,28,28	0
57	MG	DA	1641	1/1	0.99	0.11	-	28,28,28,28	0
57	MG	AA	3044	1/1	0.98	0.10	-	4,4,4,4	0
57	MG	HA	1636	1/1	0.99	0.13	-	28,28,28,28	0
57	MG	HA	1630	1/1	0.99	0.23	-	32,32,32,32	0
57	MG	AA	3053	1/1	1.00	0.17	-	4,4,4,4	0
57	MG	BA	1634	1/1	0.99	0.10	-	13,13,13,13	0
57	MG	CA	3030	1/1	0.99	0.16	-	39,39,39,39	0
57	MG	GA	3031	1/1	0.98	0.10	-	15,15,15,15	0
57	MG	AA	3122	1/1	0.99	0.16	-	6,6,6,6	0
57	MG	DA	1601	1/1	0.97	0.12	-	26,26,26,26	0
57	MG	CA	3096	1/1	0.98	0.21	-	16,16,16,16	0
57	MG	CA	3033	1/1	0.99	0.17	-	6,6,6,6	0
57	MG	AA	3063	1/1	1.00	0.19	-	0,0,0,0	0
57	MG	AA	3085	1/1	1.00	0.14	-	7,7,7,7	0
57	MG	AA	3125	1/1	0.99	0.22	-	8,8,8,8	0
57	MG	GB	1202	1/1	0.93	0.14	-	64,64,64,64	0
57	MG	CA	3021	1/1	0.98	0.11	-	5,5,5,5	0
57	MG	EA	3072	1/1	1.00	0.15	-	2,2,2,2	0
57	MG	DA	1636	1/1	0.95	0.77	-	34,34,34,34	0
57	MG	GA	3101	1/1	0.96	0.14	-	13,13,13,13	0
57	MG	GA	3059	1/1	0.96	0.12	-	25,25,25,25	0
57	MG	FA	1627	1/1	0.49	0.53	-	53,53,53,53	0
57	MG	GA	3005	1/1	0.83	0.11	-	42,42,42,42	0
57	MG	GB	1204	1/1	0.97	0.04	-	37,37,37,37	0
57	MG	BA	1629	1/1	0.98	0.15	-	15,15,15,15	0
57	MG	AA	3120	1/1	0.98	0.24	-	9,9,9,9	0
57	MG	GA	3088	1/1	0.90	0.67	-	37,37,37,37	0
57	MG	GA	3035	1/1	0.92	0.14	-	24,24,24,24	0
57	MG	EA	3136	1/1	0.86	0.37	-	15,15,15,15	0
57	MG	AA	3117	1/1	0.99	0.10	-	11,11,11,11	0
57	MG	EA	3048	1/1	0.99	0.22	-	25,25,25,25	0
57	MG	GA	3084	1/1	0.97	0.40	-	30,30,30,30	0
57	MG	DA	1605	1/1	0.99	0.15	-	18,18,18,18	0
57	MG	BA	1606	1/1	0.99	0.18	-	14,14,14,14	0
57	MG	DA	1614	1/1	0.85	0.25	-	46,46,46,46	0
57	MG	BA	1623	1/1	0.99	0.10	-	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
57	MG	EA	3119	1/1	0.98	0.23	-	1,1,1,1	0
57	MG	EA	3097	1/1	0.94	0.21	-	19,19,19,19	0
57	MG	CA	3014	1/1	1.00	0.27	-	13,13,13,13	0
57	MG	EA	3137	1/1	0.98	0.32	-	11,11,11,11	0
57	MG	EA	3094	1/1	0.93	0.12	-	33,33,33,33	0
57	MG	AA	3023	1/1	1.00	0.08	-	0,0,0,0	0
57	MG	CB	1201	1/1	0.93	0.19	-	28,28,28,28	0
57	MG	GA	3102	1/1	0.99	0.14	-	19,19,19,19	0
57	MG	AA	3061	1/1	0.98	0.28	-	5,5,5,5	0
57	MG	EA	3001	1/1	0.97	0.18	-	11,11,11,11	0
57	MG	CA	3099	1/1	0.99	0.18	-	5,5,5,5	0
57	MG	EA	3018	1/1	0.99	0.19	-	9,9,9,9	0
57	MG	EA	3026	1/1	0.99	0.18	-	0,0,0,0	0
57	MG	EA	3054	1/1	0.99	0.12	-	2,2,2,2	0
57	MG	AA	3067	1/1	0.99	0.17	-	2,2,2,2	0
57	MG	GC	302	1/1	0.98	0.07	-	22,22,22,22	0
57	MG	CA	3045	1/1	0.98	0.20	-	5,5,5,5	0
57	MG	EA	3004	1/1	0.98	0.13	-	12,12,12,12	0
57	MG	CA	3016	1/1	0.97	0.18	-	11,11,11,11	0
57	MG	AA	3055	1/1	0.99	0.16	-	0,0,0,0	0
57	MG	BA	1635	1/1	0.98	0.14	-	29,29,29,29	0
57	MG	CA	3018	1/1	0.99	0.08	-	30,30,30,30	0
57	MG	AA	3020	1/1	0.99	0.09	-	9,9,9,9	0
57	MG	CA	3130	1/1	0.99	0.16	-	21,21,21,21	0
57	MG	EA	3087	1/1	0.98	0.10	-	21,21,21,21	0
57	MG	HA	1638	1/1	0.99	0.04	-	28,28,28,28	0
57	MG	FA	1612	1/1	0.99	0.30	-	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.