wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 9, 2024 – 09:46 pm BST

PDB ID : 8CQW
Title : Crystal structure of the Candida albicans 80S ribosome in complex with Hygromycin B
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on : 2023-03-07
Resolution : 3.05 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

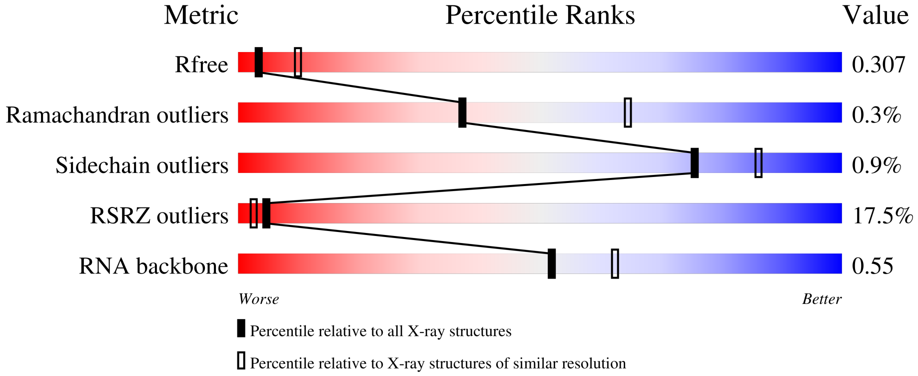
MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.002 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.38.2

1 Overall quality at a glance ⓘ

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

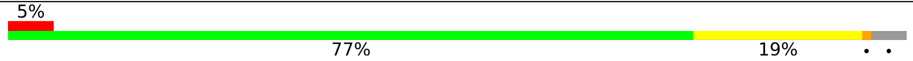
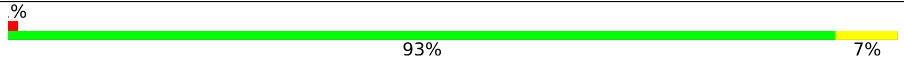
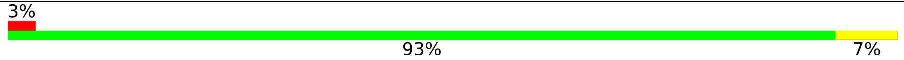
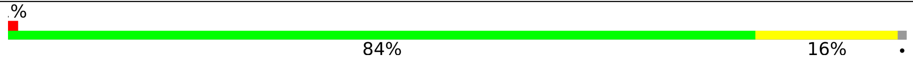
The reported resolution of this entry is 3.05 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	2258 (3.10-3.02)
Ramachandran outliers	177936	2269 (3.10-3.02)
Sidechain outliers	177891	2268 (3.10-3.02)
RSRZ outliers	164620	2258 (3.10-3.02)
RNA backbone	3690	1166 (3.32-2.80)

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

Mol	Chain	Length	Quality of chain
1	1	3359	
1	AS	3359	
2	3	121	
2	AT	121	
3	4	158	

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Mol	Chain	Length	Quality of chain
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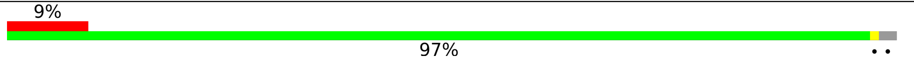
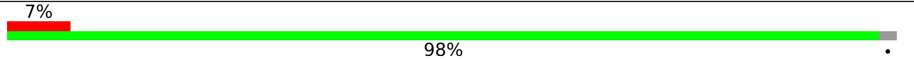
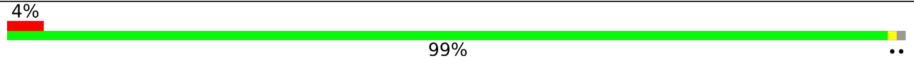
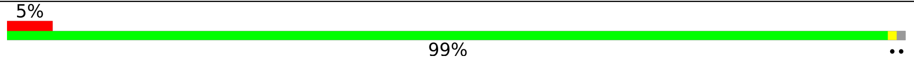
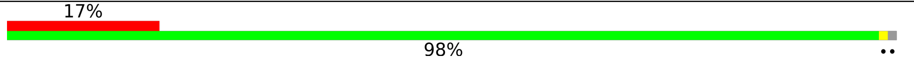
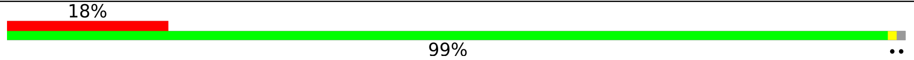
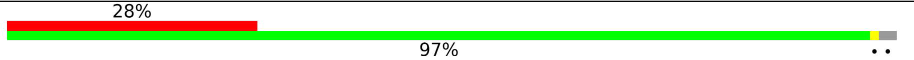
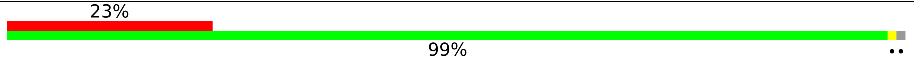
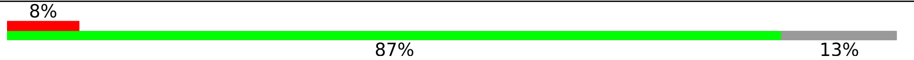
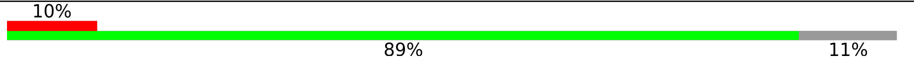
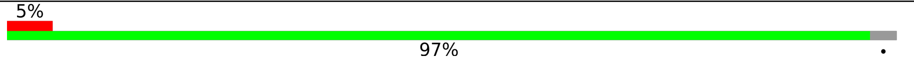
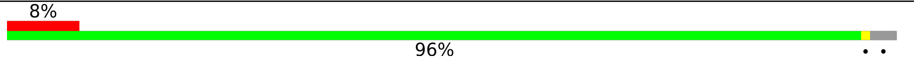
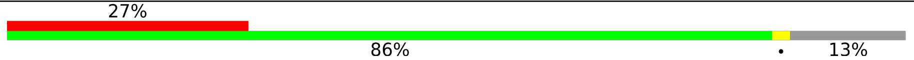
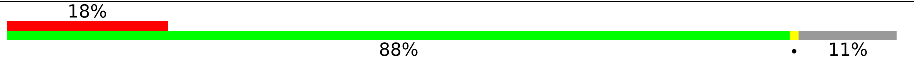
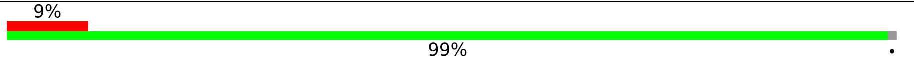
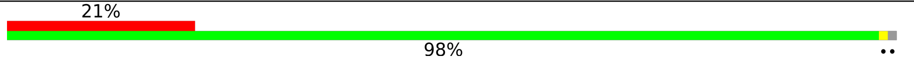
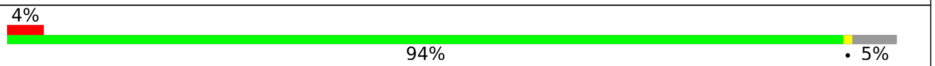
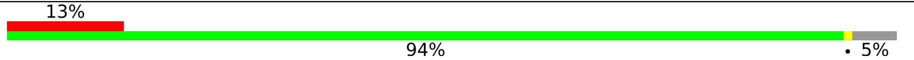
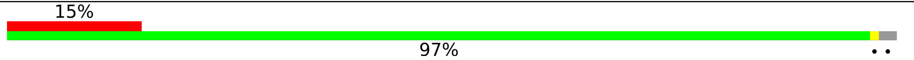
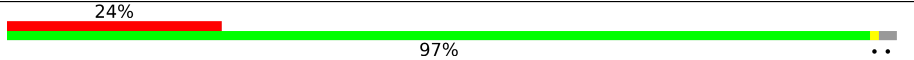
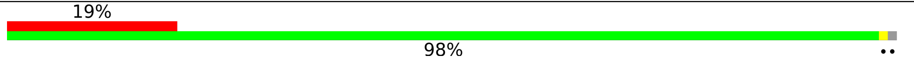
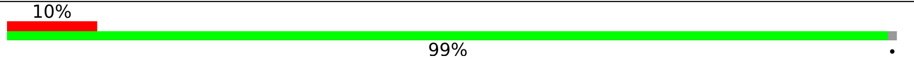
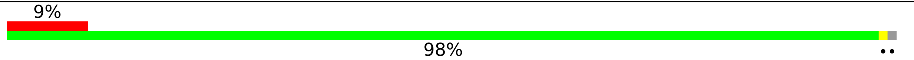
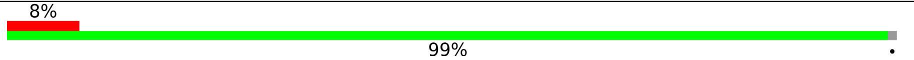
4	AW	254	
4	j	254	
5	AX	389	
5	k	389	
6	AY	363	
6	l	363	
7	AZ	298	
7	m	298	
8	BA	176	
8	n	176	
9	BB	241	
9	o	241	
10	BC	262	
10	p	262	
11	BD	191	
11	q	191	
12	BE	220	
12	r	220	
13	BF	174	
13	s	174	
14	BG	202	
14	t	202	
15	BH	131	
15	u	131	

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Mol	Chain	Length	Quality of chain
16	BI	204	25% 99%
16	v	204	11% 99%
17	BJ	200	4% 100%
17	w	200	8% 100%
18	BK	185	12% 94% • 5%
18	x	185	11% 94% 6%
19	BL	186	8% 99% •
19	y	186	27% 99% •
20	BM	190	13% 92% • 6%
20	z	190	7% 94% 6%
21	0	172	12% 98% ••
21	BN	172	5% 99% •
22	2	160	15% 99% ••
22	BO	160	15% 99% ••
23	5	124	12% 81% • 18%
23	BP	124	19% 78% • 18%
24	6	137	6% 96% •
24	BQ	137	8% 96% •
25	7	155	14% 75% • 24%
25	BR	155	12% 63% • 37%
26	8	142	8% 83% • 15%
26	BS	142	22% 84% 16%
27	9	127	28% 98% ••
27	BT	127	17% 98% ••
28	AA	136	21% 99% •

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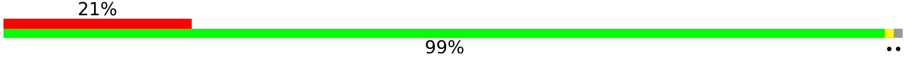
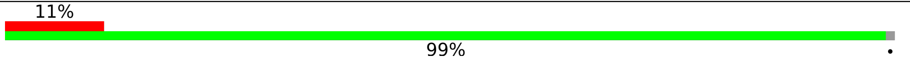
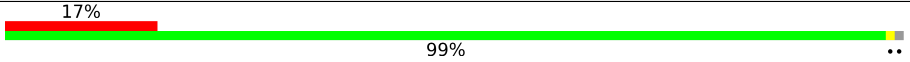
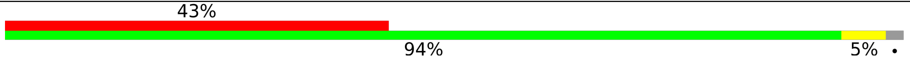
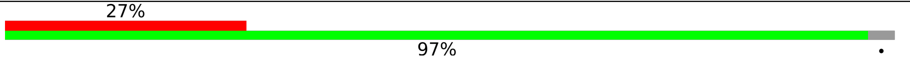
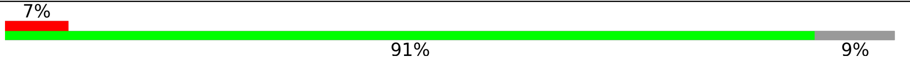
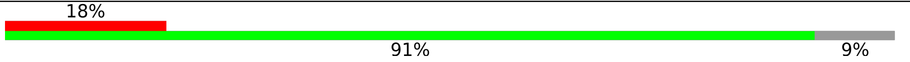
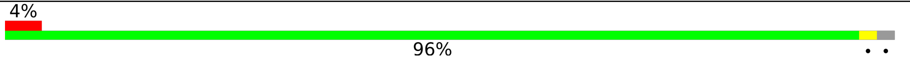
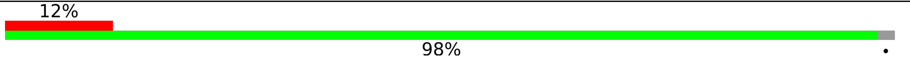
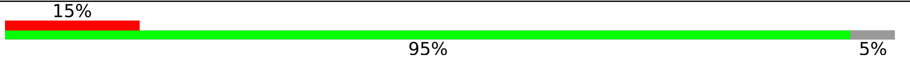
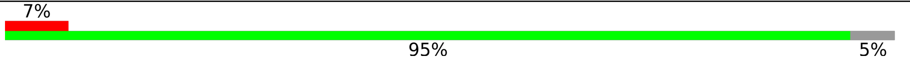
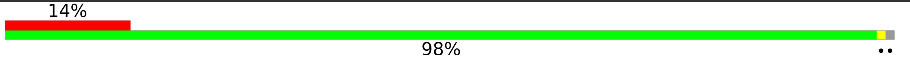
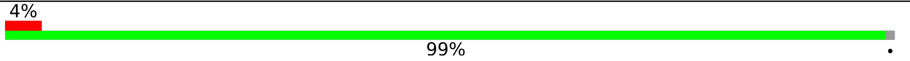
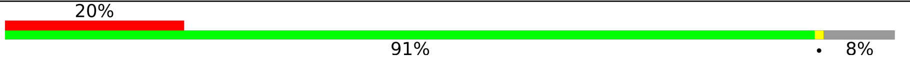
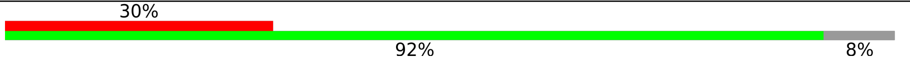
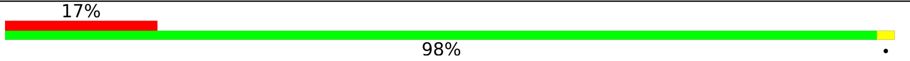
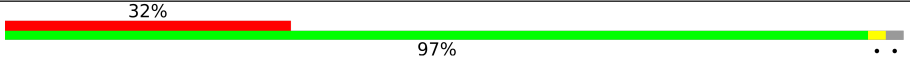
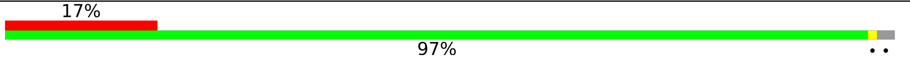
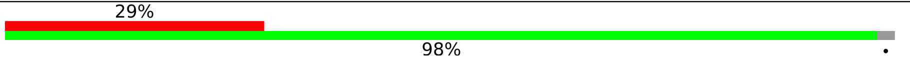
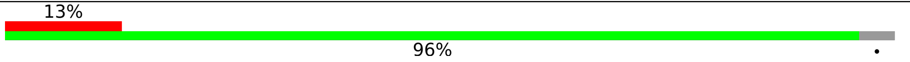
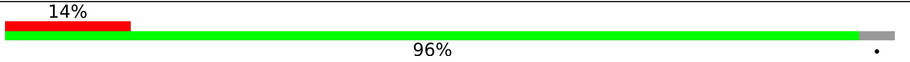
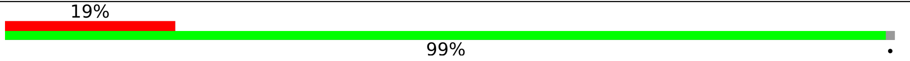
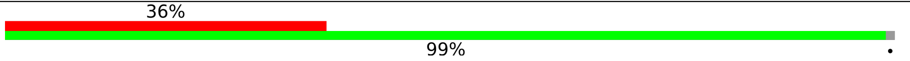
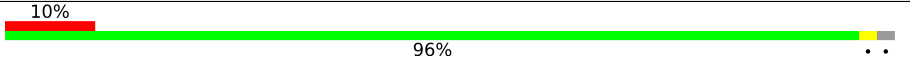
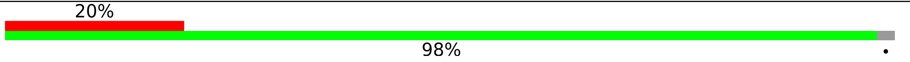
Mol	Chain	Length	Quality of chain
28	BU	136	
29	AB	149	
29	BV	149	
30	AC	63	
30	BW	63	
31	AD	106	
31	BX	106	
32	AE	112	
32	BY	112	
33	AF	131	
33	BZ	131	
34	AG	107	
34	CA	107	
35	AH	122	
35	CB	122	
36	AI	120	
36	CC	120	
37	AJ	99	
37	CD	99	
38	AK	90	
38	CE	90	
39	AL	78	
39	CF	78	
40	AM	51	
40	CG	51	

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Mol	Chain	Length	Quality of chain
41	AN	52	58% 100%
41	CH	52	63% 92% 6% •
42	AO	25	40% 92% 8%
42	CI	25	28% 96% •
43	AP	106	14% 97% •
43	CJ	106	14% 97% •
44	AQ	92	4% 99% •
44	CK	92	9% 99% •
45	CL	267	15% 43% • 55%
45	i	267	19% 44% • 55%
46	B	1787	10% 71% 25% • •
46	CM	1787	7% 71% 27% ••
47	C	261	18% 79% 20%
47	CN	261	12% 79% • 20%
48	CO	256	23% 83% 16%
48	D	256	13% 83% 16%
49	CP	249	11% 86% • 13%
49	E	249	24% 87% 13%
50	CQ	251	18% 86% • 11%
50	F	251	39% 88% • 11%
51	CR	262	33% 99% •
51	G	262	38% 99% •
52	CS	225	34% 91% • 8%
52	H	225	40% 90% • 8%
53	CT	236	24% 99% •

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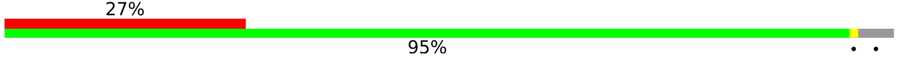
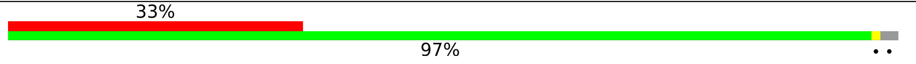
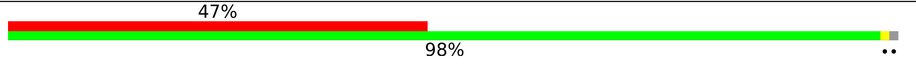
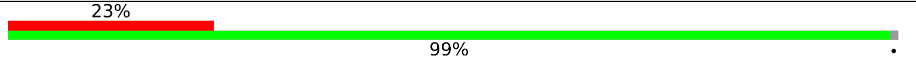
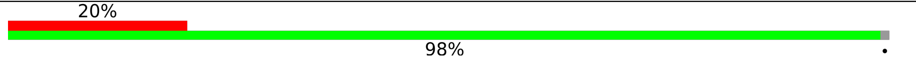
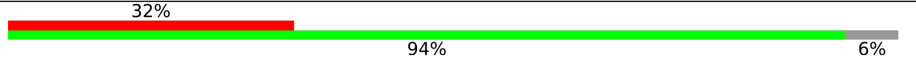
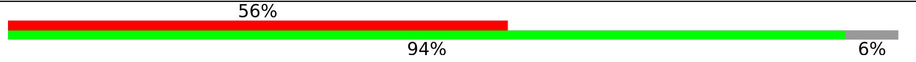
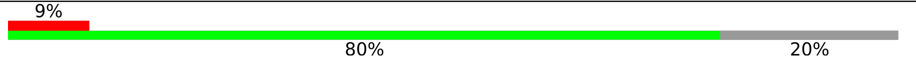
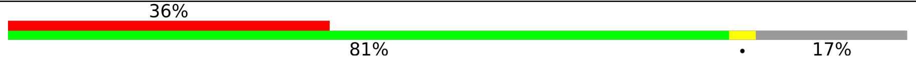
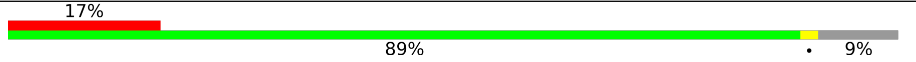
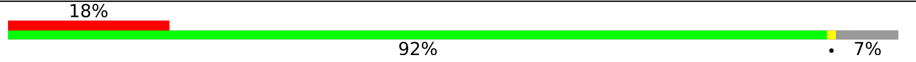
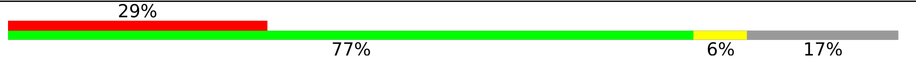
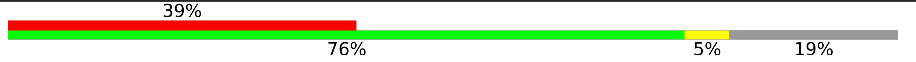
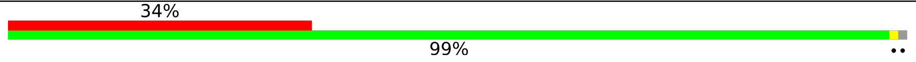
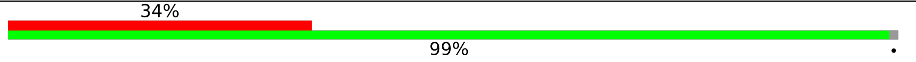
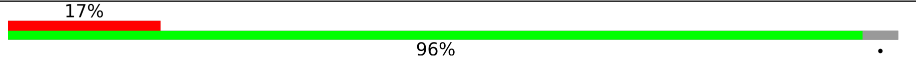
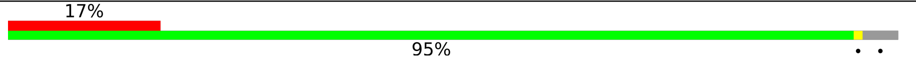
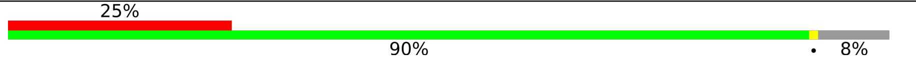
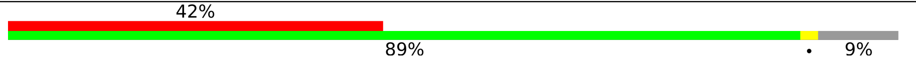
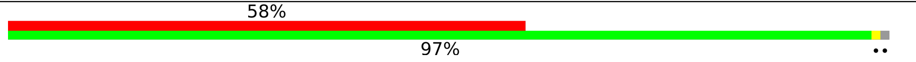
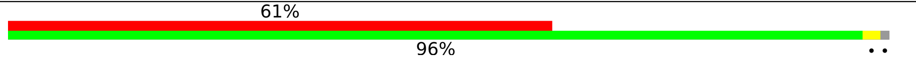
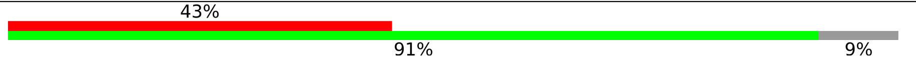
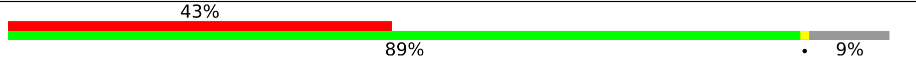
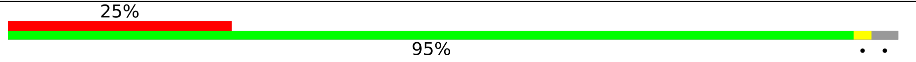
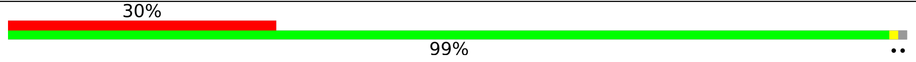
Mol	Chain	Length	Quality of chain
53	I	236	
54	CU	186	
54	J	186	
55	CV	206	
55	K	206	
56	CW	189	
56	L	189	
57	CX	118	
57	M	118	
58	CY	155	
58	N	155	
59	CZ	143	
59	O	143	
60	DA	151	
60	P	151	
61	DB	132	
61	Q	132	
62	DC	142	
62	R	142	
63	DD	142	
63	S	142	
64	DE	137	
64	T	137	
65	DF	145	
65	U	145	

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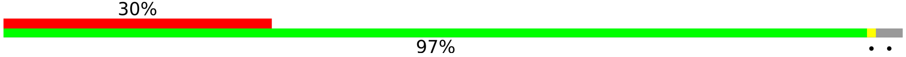
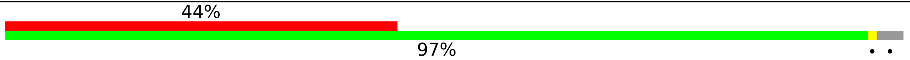
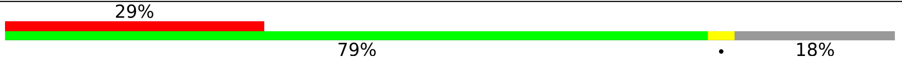
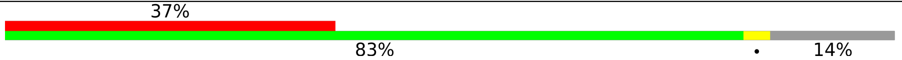
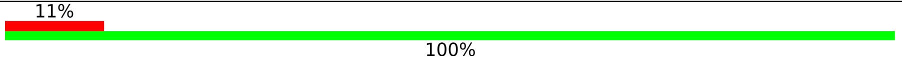
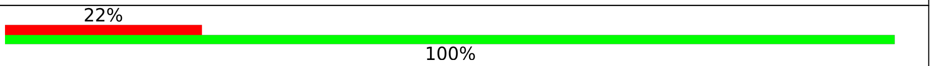
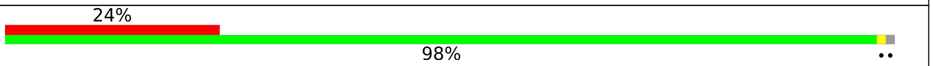
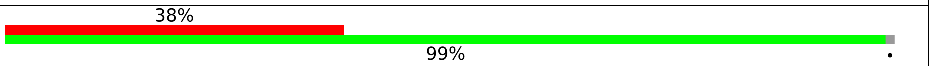
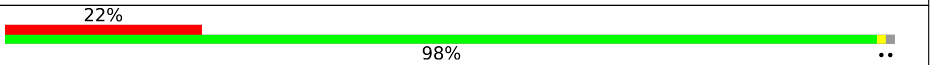
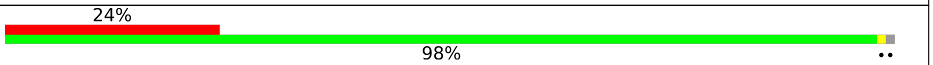
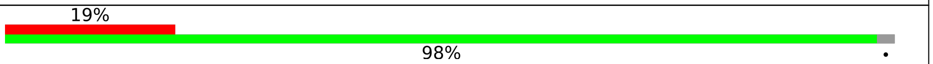
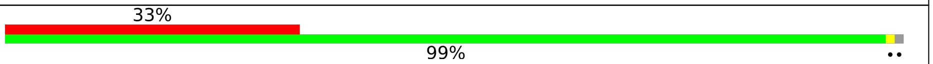
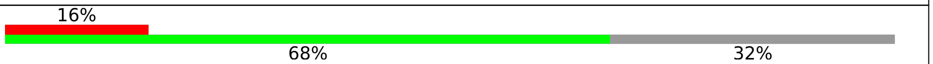
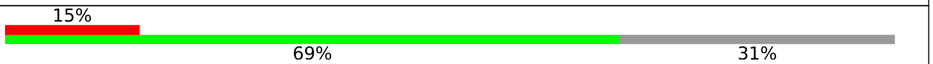
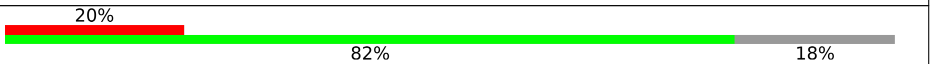
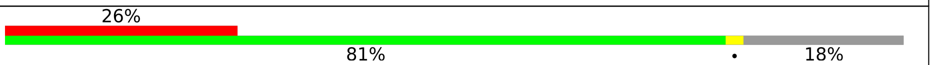
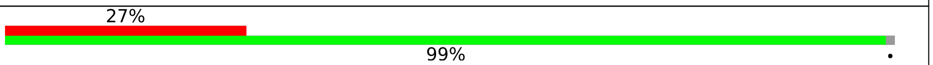
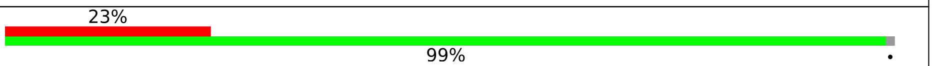
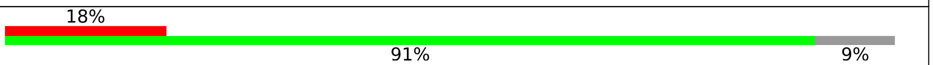
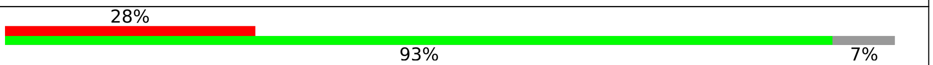
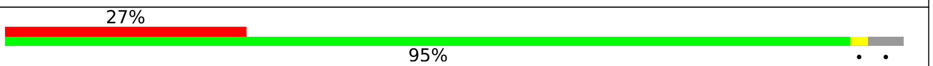
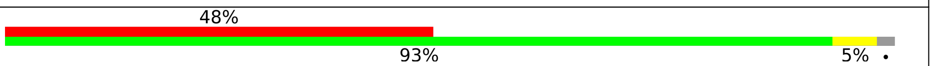
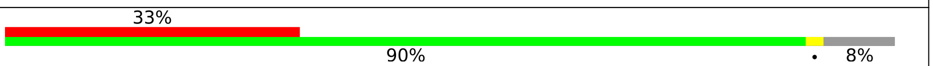
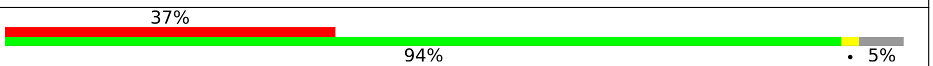
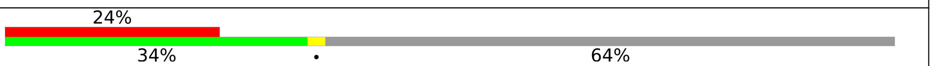
Mol	Chain	Length	Quality of chain
66	DG	145	
66	V	145	
67	DH	119	
67	W	119	
68	DI	87	
68	X	87	
69	DJ	130	
69	Y	130	
70	DK	145	
70	Z	145	
71	DL	135	
71	a	135	
72	DM	105	
72	b	105	
73	DN	119	
73	c	119	
74	DO	82	
74	d	82	
75	DP	67	
75	e	67	
76	DQ	56	
76	f	56	
77	DR	63	
77	g	63	
78	DS	193	

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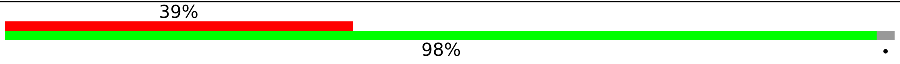
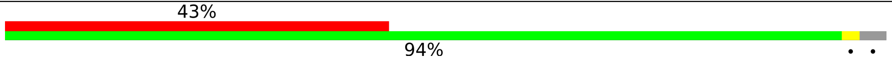
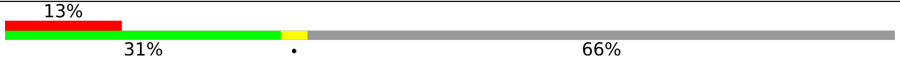
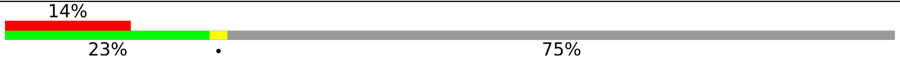
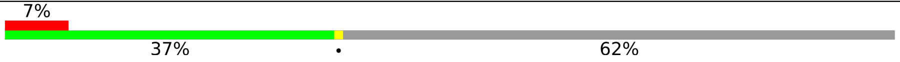
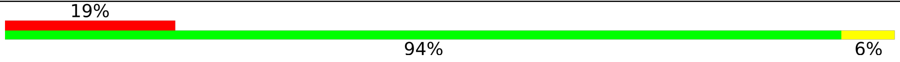
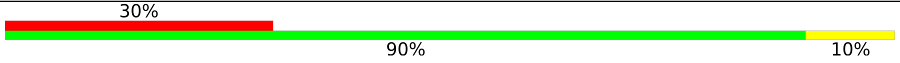
Mol	Chain	Length	Quality of chain
78	h	193	18% 35% 64%
79	AR	317	39% 98%
79	DT	317	43% 94%
80	P0	312	13% 31% 66%
80	p0	312	14% 23% 75%
81	12	165	7% 37% 62%
82	L1	217	19% 94% 6%
82	l1	217	30% 90% 10%

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
83	MG	1	3630	-	-	-	X
83	MG	1	3651	-	-	-	X
83	MG	1	3688	-	-	-	X
83	MG	1	3715	-	-	-	X
83	MG	1	3776	-	-	-	X
83	MG	8	202	-	-	-	X
83	MG	9	201	-	-	-	X
83	MG	CL	302	-	-	-	X

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 408804 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 25S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	3208	68581	30637	12330	22406	3208	0	0	0
1	AS	3227	68985	30817	12402	22539	3227	0	0	0

- Molecule 2 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	3	121	2579	1153	463	842	121	0	0	0
2	AT	121	2579	1153	463	842	121	0	0	0

- Molecule 3 is a RNA chain called 5.8S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	157	3333	1491	583	1102	157	0	0	0
3	AU	157	3333	1491	583	1102	157	0	0	0

- Molecule 4 is a protein called 60S ribosomal protein L2-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	j	249	1888	1180	376	330	2	0	0	0
4	AW	249	1888	1180	376	330	2	0	0	0

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	k	386	Total C N O S 3077 1950 582 538 7	0	0	0
5	AX	386	Total C N O S 3077 1950 582 538 7	0	0	0

- Molecule 6 is a protein called 60S ribosomal protein L4-B.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	l	361	Total C N O S 2751 1729 529 490 3	0	0	0
6	AY	361	Total C N O S 2751 1729 529 490 3	0	0	0

- Molecule 7 is a protein called Uncharacterized protein CaJ7.0206.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
7	m	296	Total C N O S 2426 1544 422 458 2	0	0	0
7	AZ	292	Total C N O S 2394 1526 416 450 2	0	0	0

- Molecule 8 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
8	n	157	Total C N O S 1242 796 226 219 1	0	0	0
8	BA	153	Total C N O 1210 777 221 212	0	0	0

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
9	o	233	Total C N O S 1876 1203 344 328 1	0	0	0
9	BB	234	Total C N O S 1885 1208 345 331 1	0	0	0

- Molecule 10 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
10	p	233	Total C N O S 1805 1156 321 325 3	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	BC	229	1778	1140	316	319	3	0	0	0

- Molecule 11 is a protein called 60S ribosomal protein L9-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	q	189	1510	953	275	278	4	0	0	0
11	BD	190	1519	958	276	281	4	0	0	0

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	r	208	1689	1069	322	291	7	0	0	0
12	BE	208	1689	1069	322	291	7	0	0	0

- Molecule 13 is a protein called 60S ribosomal protein L11-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	s	171	1371	857	260	250	4	0	0	0
13	BF	171	1371	857	260	250	4	0	0	0

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
14	t	200	1610	1009	318	283	0	0	0
14	BG	200	1610	1009	318	283	0	0	0

- Molecule 15 is a protein called 60S ribosomal protein L14-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
15	u	130	1029	660	193	175	1	0	0	0
15	BH	130	1029	660	193	175	1	0	0	0

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
16	v	203	Total C N O S 1713 1075 356 280 2	0	0	0
16	BI	203	Total C N O S 1713 1075 356 280 2	0	0	0

- Molecule 17 is a protein called Ribosomal protein L13.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
17	w	199	Total C N O S 1590 1025 294 269 2	0	0	0
17	BJ	199	Total C N O S 1590 1025 294 269 2	0	0	0

- Molecule 18 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
18	x	173	Total C N O 1387 856 280 251	0	0	0
18	BK	176	Total C N O 1406 868 284 254	0	0	0

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
19	y	185	Total C N O 1458 916 297 245	0	0	0
19	BL	185	Total C N O 1458 916 297 245	0	0	0

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
20	z	179	Total C N O S 1457 901 310 243 3	0	0	0
20	BM	179	Total C N O S 1457 901 310 243 3	0	0	0

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
21	0	170	Total C N O S 1423 921 258 241 3	0	0	0
21	BN	170	Total C N O S 1423 921 258 241 3	0	0	0

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
22	2	159	Total C N O S 1262 798 241 221 2	0	0	0
22	BO	159	Total C N O S 1262 798 241 221 2	0	0	0

- Molecule 23 is a protein called 60S ribosomal protein L22-B.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
23	5	102	Total C N O 826 536 137 153	0	0	0
23	BP	102	Total C N O 826 536 137 153	0	0	0

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
24	6	131	Total C N O S 977 615 183 171 8	0	0	0
24	BQ	131	Total C N O S 977 615 183 171 8	0	0	0

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
25	7	118	Total C N O S 945 591 192 161 1	0	0	0
25	BR	98	Total C N O S 801 501 162 137 1	0	0	0

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	8	120	Total C N O S 965 616 173 175 1	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
26	BS	119	Total C N O S 960 613 172 174 1	0	0	0

- Molecule 27 is a protein called Ribosomal protein L24.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
27	9	126	Total C N O 989 618 190 181	0	0	0
27	BT	126	Total C N O 989 618 190 181	0	0	0

- Molecule 28 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
28	AA	135	Total C N O S 1087 705 197 183 2	0	0	0
28	BU	135	Total C N O S 1087 705 197 183 2	0	0	0

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
29	AB	148	Total C N O S 1170 741 231 197 1	0	0	0
29	BV	148	Total C N O S 1170 741 231 197 1	0	0	0

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
30	AC	62	Total C N O 493 307 105 81	0	0	0
30	BW	61	Total C N O 488 304 104 80	0	0	0

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
31	AD	96	Total C N O S 729 469 121 137 2	0	0	0
31	BX	96	Total C N O S 729 469 121 137 2	0	0	0

- Molecule 32 is a protein called 60S ribosomal protein L31-B.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
32	AE	110	Total C N O S 894 565 168 159 2	0	0	0
32	BY	110	Total C N O S 894 565 168 159 2	0	0	0

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
33	AF	124	Total C N O S 1000 638 194 167 1	0	0	0
33	BZ	124	Total C N O S 1004 641 195 167 1	0	0	0

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
34	AG	106	Total C N O S 847 543 161 142 1	0	0	0
34	CA	106	Total C N O S 847 543 161 142 1	0	0	0

- Molecule 35 is a protein called 60S ribosomal protein L34-B.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
35	AH	112	Total C N O S 887 547 182 154 4	0	0	0
35	CB	112	Total C N O S 887 547 182 154 4	0	0	0

- Molecule 36 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
36	AI	120	Total C N O S 992 629 195 167 1	0	0	0
36	CC	118	Total C N O 979 621 193 165	0	0	0

- Molecule 37 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	AJ	97	Total	C	N	O	S	0	0	0
			758	471	156	130	1			
37	CD	97	Total	C	N	O	S	0	0	0
			758	471	156	130	1			

- Molecule 38 is a protein called 60S ribosomal protein L37-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	AK	86	Total	C	N	O	S	0	0	0
			677	413	148	110	6			
38	CE	86	Total	C	N	O	S	0	0	0
			677	413	148	110	6			

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
39	AL	77	Total	C	N	O	0	0	0
			617	393	115	109			
39	CF	77	Total	C	N	O	0	0	0
			617	393	115	109			

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	AM	50	Total	C	N	O	0	0	0
			438	275	97	66			
40	CG	50	Total	C	N	O	0	0	0
			438	275	97	66			

- Molecule 41 is a protein called 60S ribosomal protein L40-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AN	52	Total	C	N	O	S	0	0	0
			419	260	86	67	6			
41	CH	51	Total	C	N	O	S	0	0	0
			411	255	85	66	5			

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	AO	25	Total	C	N	O	S	0	0	0
			236	144	63	28	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
42	CI	24	227	138	61	27	1	0	0	0

- Molecule 43 is a protein called 60S ribosomal protein L42-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
43	AP	103	828	521	165	137	5	0	0	0
			Total	C	N	O	S			
43	CJ	103	828	521	165	137	5	0	0	0

- Molecule 44 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
44	AQ	91	698	430	140	124	4	0	0	0
			Total	C	N	O	S			
44	CK	91	698	430	140	124	4	0	0	0

- Molecule 45 is a protein called 60S ribosomal protein CAALFM_C304810CA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
45	i	120	922	558	165	199	0	0	0
			Total	C	N	O			
45	CL	121	931	563	166	202	0	0	0

- Molecule 46 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
46	B	1741	37113	16590	6583	12199	1741	0	0	0
			Total	C	N	O	P			
46	CM	1765	37621	16818	6670	12368	1765	0	0	0

- Molecule 47 is a protein called 40S ribosomal protein S0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
47	C	208	1627	1041	284	297	5	0	0	0
			Total	C	N	O	S			
47	CN	208	1627	1041	284	297	5	0	0	0

- Molecule 48 is a protein called 40S ribosomal protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
48	D	214	1724	1094	313	313	4	0	0	0
48	CO	214	1724	1094	313	313	4	0	0	0

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
49	E	217	1629	1039	289	296	5	0	0	0
49	CP	217	1629	1039	289	296	5	0	0	0

- Molecule 50 is a protein called Ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
50	F	223	1707	1087	311	305	4	0	0	0
50	CQ	223	1707	1087	311	305	4	0	0	0

- Molecule 51 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
51	G	259	2051	1304	385	357	5	0	0	0
51	CR	260	2055	1306	386	358	5	0	0	0

- Molecule 52 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
52	H	206	1614	1008	301	301	4	0	0	0
52	CS	206	1614	1008	301	301	4	0	0	0

- Molecule 53 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	I	226	Total	C	N	O	S	0	0	0
			1820	1133	351	330	6			
53	CT	236	Total	C	N	O	S	0	0	0
			1904	1184	369	345	6			

- Molecule 54 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
54	J	184	Total	C	N	O	0	0	0
			1485	950	268	267			
54	CU	183	Total	C	N	O	0	0	0
			1475	944	265	266			

- Molecule 55 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	K	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			
55	CV	203	Total	C	N	O	S	0	0	0
			1579	973	322	283	1			

- Molecule 56 is a protein called Ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	L	178	Total	C	N	O	S	0	0	0
			1453	918	286	248	1			
56	CW	178	Total	C	N	O	S	0	0	0
			1453	918	286	248	1			

- Molecule 57 is a protein called 40S ribosomal protein S10-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	M	98	Total	C	N	O	S	0	0	0
			817	531	135	150	1			
57	CX	94	Total	C	N	O	S	0	0	0
			791	515	131	144	1			

- Molecule 58 is a protein called 40S ribosomal protein S11A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	N	144	Total	C	N	O	S	0	0	0
			1150	734	215	198	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
58	CY	141	1129	722	212	192	3	0	0	0

- Molecule 59 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
59	O	116	885	550	158	172	5	0	0	0
			Total	C	N	O	S			
59	CZ	119	913	566	163	179	5	0	0	0

- Molecule 60 is a protein called 40S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
60	P	150	1187	757	219	210	1	0	0	0
			Total	C	N	O	S			
60	DA	150	1187	757	219	210	1	0	0	0

- Molecule 61 is a protein called 40S ribosomal protein S14-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
61	Q	127	942	579	186	174	3	0	0	0
			Total	C	N	O	S			
61	DB	127	942	579	186	174	3	0	0	0

- Molecule 62 is a protein called 40S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
62	R	129	1018	649	185	177	7	0	0	0
			Total	C	N	O	S			
62	DC	130	1029	655	189	178	7	0	0	0

- Molecule 63 is a protein called 40S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
63	S	140	1091	700	198	192	1	0	0	0
			Total	C	N	O	S			
63	DD	140	1091	700	198	192	1	0	0	0

- Molecule 64 is a protein called 40S ribosomal protein S17-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
64	T	124	997	628	183	185	1	0	0	0
64	DE	124	997	628	183	185	1	0	0	0

- Molecule 65 is a protein called 40S ribosomal protein S18-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
65	U	144	1187	744	233	207	3	0	0	0
65	DF	141	1161	727	227	204	3	0	0	0

- Molecule 66 is a protein called 40S ribosomal protein S19-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
66	V	141	1100	689	210	200	1	0	0	0
66	DG	141	1100	689	210	200	1	0	0	0

- Molecule 67 is a protein called Ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
67	W	102	808	509	150	147	2	0	0	0
67	DH	97	763	481	140	140	2	0	0	0

- Molecule 68 is a protein called 40S ribosomal protein S21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
68	X	87	676	415	126	133	2	0	0	0
68	DI	87	676	415	126	133	2	0	0	0

- Molecule 69 is a protein called 40S ribosomal protein S22-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
69	Y	129	Total 1032	C 655	N 191	O 183	S 3	0	0	0
69	DJ	129	Total 1032	C 655	N 191	O 183	S 3	0	0	0

- Molecule 70 is a protein called Ribosomal protein S23 (S12).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
70	Z	143	Total 1110	C 701	N 219	O 188	S 2	0	0	0
70	DK	143	Total 1110	C 701	N 219	O 188	S 2	0	0	0

- Molecule 71 is a protein called 40S ribosomal protein S24.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
71	a	134	Total 1086	C 677	N 218	O 191	0	0	0
71	DL	132	Total 1072	C 670	N 216	O 186	0	0	0

- Molecule 72 is a protein called 40S ribosomal protein S25.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
72	b	72	Total 578	C 369	N 103	O 106	0	0	0
72	DM	71	Total 570	C 365	N 102	O 103	0	0	0

- Molecule 73 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
73	c	98	Total 779	C 482	N 163	O 128	S 6	0	0	0
73	DN	97	Total 770	C 477	N 161	O 126	S 6	0	0	0

- Molecule 74 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	d	81	Total 614	C 383	N 110	O 114	S 7	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
74	DO	81	614	383	110	114	7	0	0	0

- Molecule 75 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
75	e	62	487	299	98	88	2	0	0	0
75	DP	61	476	293	94	87	2	0	0	0

- Molecule 76 is a protein called 40S ribosomal protein S29A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
76	f	55	454	281	94	75	4	0	0	0
76	DQ	54	449	278	93	74	4	0	0	0

- Molecule 77 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
77	g	60	474	297	96	79	2	0	0	0
77	DR	58	461	289	93	77	2	0	0	0

- Molecule 78 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
78	h	70	574	362	113	93	6	0	0	0
78	DS	70	574	362	113	93	6	0	0	0

- Molecule 79 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
79	AR	311	2398	1519	412	462	5	0	0	0
79	DT	306	2357	1494	402	456	5	0	0	0

- Molecule 80 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	P0	107	Total 845	C 542	N 150	O 150	S 3	0	0	0
80	p0	79	Total 635	C 404	N 114	O 115	S 2	0	0	0

- Molecule 81 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	12	63	Total 480	C 297	N 85	O 96	S 2	0	0	0

- Molecule 82 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	L1	217	Total 1711	C 1096	N 294	O 312	S 9	0	0	0
82	l1	217	Total 1711	C 1096	N 294	O 312	S 9	0	0	0

- Molecule 83 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	1	530	Total 530	Mg 530	0	0
83	3	14	Total 14	Mg 14	0	0
83	4	12	Total 12	Mg 12	0	0
83	j	3	Total 3	Mg 3	0	0
83	k	4	Total 4	Mg 4	0	0
83	o	3	Total 3	Mg 3	0	0
83	r	2	Total 2	Mg 2	0	0
83	s	1	Total 1	Mg 1	0	0
83	u	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	v	3	Total Mg 3 3	0	0
83	w	3	Total Mg 3 3	0	0
83	x	3	Total Mg 3 3	0	0
83	y	1	Total Mg 1 1	0	0
83	0	5	Total Mg 5 5	0	0
83	2	3	Total Mg 3 3	0	0
83	5	1	Total Mg 1 1	0	0
83	6	3	Total Mg 3 3	0	0
83	8	2	Total Mg 2 2	0	0
83	9	2	Total Mg 2 2	0	0
83	AB	2	Total Mg 2 2	0	0
83	AC	1	Total Mg 1 1	0	0
83	AD	1	Total Mg 1 1	0	0
83	AE	2	Total Mg 2 2	0	0
83	AF	1	Total Mg 1 1	0	0
83	AG	2	Total Mg 2 2	0	0
83	AH	2	Total Mg 2 2	0	0
83	AJ	1	Total Mg 1 1	0	0
83	AK	1	Total Mg 1 1	0	0
83	AM	1	Total Mg 1 1	0	0
83	AP	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	B	152	Total Mg 152 152	0	0
83	D	1	Total Mg 1 1	0	0
83	G	2	Total Mg 2 2	0	0
83	I	2	Total Mg 2 2	0	0
83	J	1	Total Mg 1 1	0	0
83	K	1	Total Mg 1 1	0	0
83	L	1	Total Mg 1 1	0	0
83	Q	1	Total Mg 1 1	0	0
83	R	1	Total Mg 1 1	0	0
83	V	1	Total Mg 1 1	0	0
83	Y	3	Total Mg 3 3	0	0
83	Z	2	Total Mg 2 2	0	0
83	a	1	Total Mg 1 1	0	0
83	f	1	Total Mg 1 1	0	0
83	AR	1	Total Mg 1 1	0	0
83	AS	278	Total Mg 278 278	0	0
83	AT	9	Total Mg 9 9	0	0
83	AU	2	Total Mg 2 2	0	0
83	AW	4	Total Mg 4 4	0	0
83	BB	2	Total Mg 2 2	0	0
83	BE	2	Total Mg 2 2	0	0

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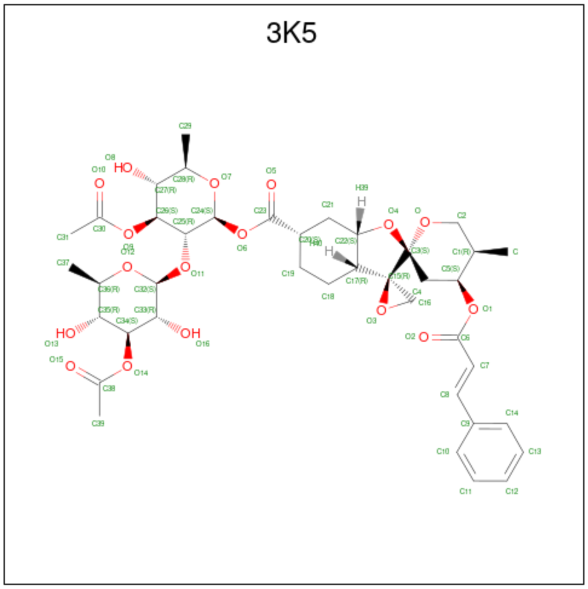
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	BF	1	Total Mg 1 1	0	0
83	BH	1	Total Mg 1 1	0	0
83	BJ	3	Total Mg 3 3	0	0
83	BK	1	Total Mg 1 1	0	0
83	BN	1	Total Mg 1 1	0	0
83	BQ	1	Total Mg 1 1	0	0
83	BV	1	Total Mg 1 1	0	0
83	BZ	2	Total Mg 2 2	0	0
83	CA	1	Total Mg 1 1	0	0
83	CJ	1	Total Mg 1 1	0	0
83	CK	1	Total Mg 1 1	0	0
83	CL	3	Total Mg 3 3	0	0
83	CM	102	Total Mg 102 102	0	0
83	CO	1	Total Mg 1 1	0	0
83	CP	1	Total Mg 1 1	0	0
83	CQ	1	Total Mg 1 1	0	0
83	DA	1	Total Mg 1 1	0	0
83	DB	3	Total Mg 3 3	0	0
83	DG	2	Total Mg 2 2	0	0
83	DQ	1	Total Mg 1 1	0	0

- Molecule 84 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose (three-letter code: 3K5) (formula: $C_{40}H_{52}O_{17}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	1	1	Total C O 57 40 17	0	0
84	AS	1	Total C O 57 40 17	0	0

- Molecule 85 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	AH	1	Total Zn 1 1	0	0
85	AK	1	Total Zn 1 1	0	0
85	AN	1	Total Zn 1 1	0	0
85	AP	1	Total Zn 1 1	0	0
85	AQ	1	Total Zn 1 1	0	0
85	c	1	Total Zn 1 1	0	0
85	d	1	Total Zn 1 1	0	0
85	f	1	Total Zn 1 1	0	0
85	h	1	Total Zn 1 1	0	0

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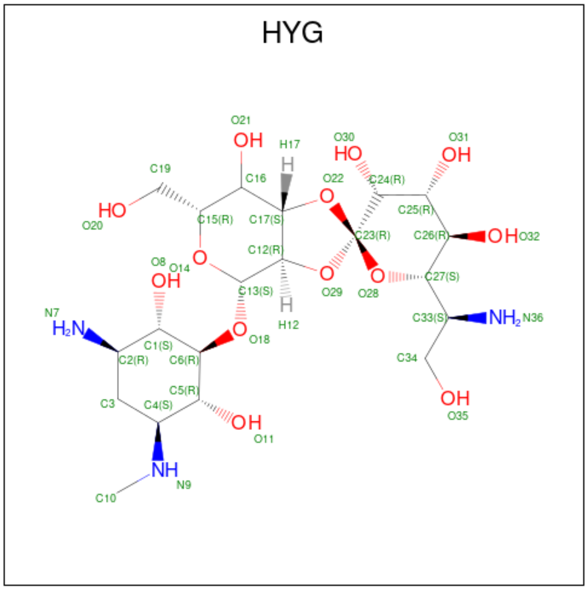
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	CB	1	Total Zn 1 1	0	0
85	CE	1	Total Zn 1 1	0	0
85	CH	1	Total Zn 1 1	0	0
85	CJ	1	Total Zn 1 1	0	0
85	CK	1	Total Zn 1 1	0	0
85	DN	1	Total Zn 1 1	0	0
85	DQ	1	Total Zn 1 1	0	0
85	DS	1	Total Zn 1 1	0	0

- Molecule 86 is HYGROMYCIN B (three-letter code: HYG) (formula: $C_{20}H_{37}N_3O_{13}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
86	B	1	Total C N O 36 20 3 13	0	0
86	CM	1	Total C N O 36 20 3 13	0	0

- Molecule 87 is water.

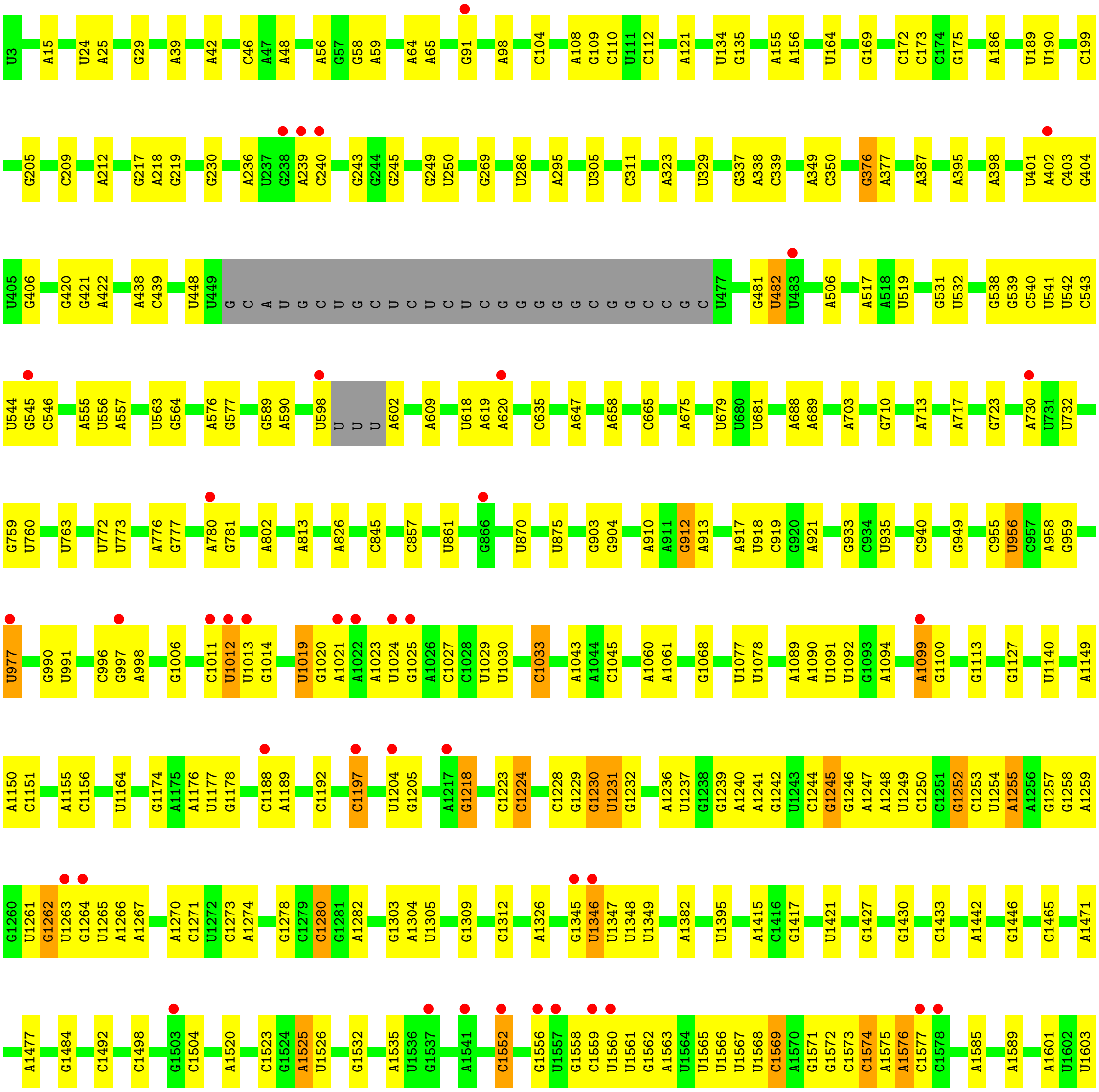
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
87	1	9	Total O 9 9	0	0
87	4	3	Total O 3 3	0	0
87	B	6	Total O 6 6	0	0
87	AS	12	Total O 12 12	0	0

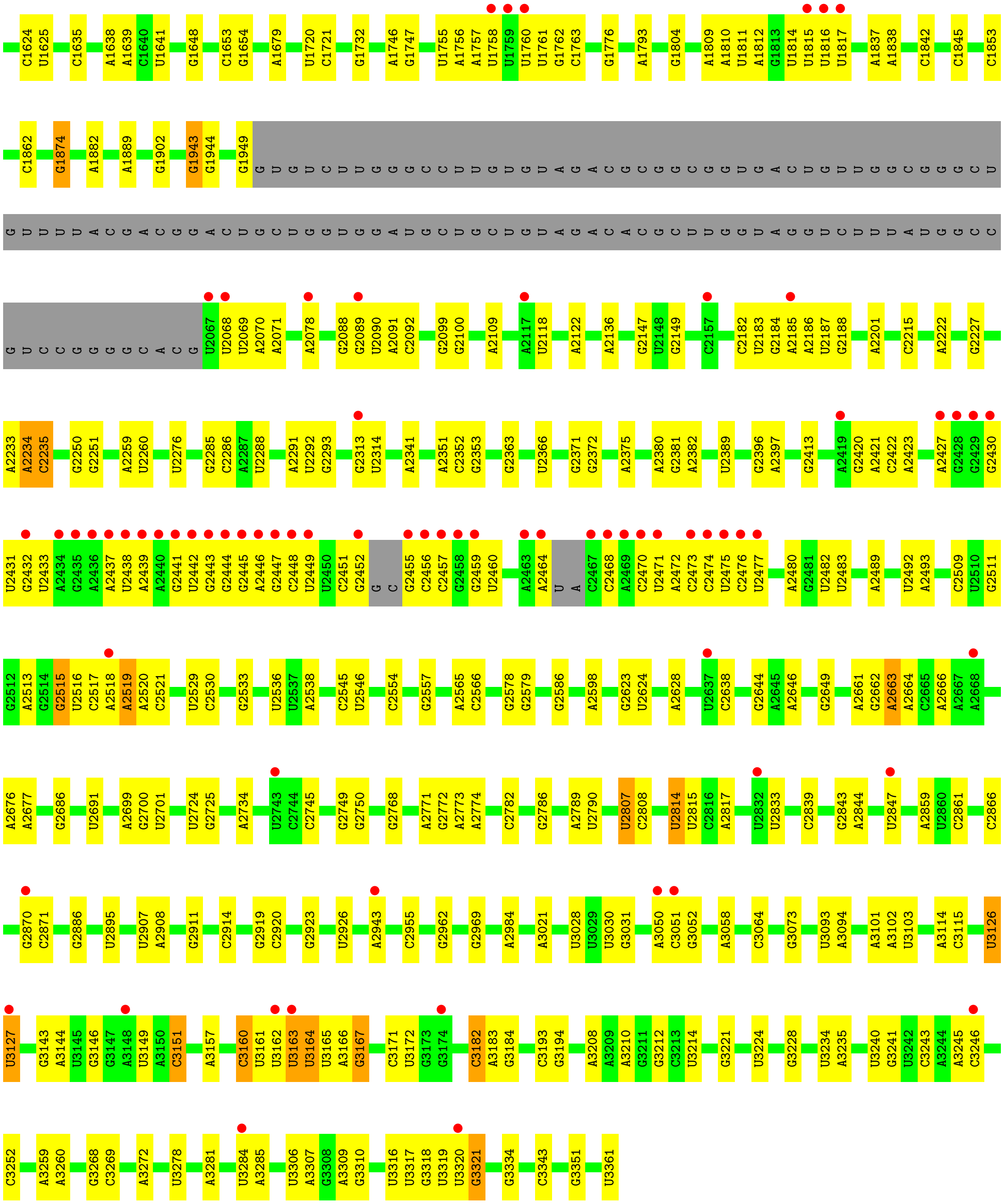
3 Residue-property plots ⓘ

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

- Molecule 1: 25S

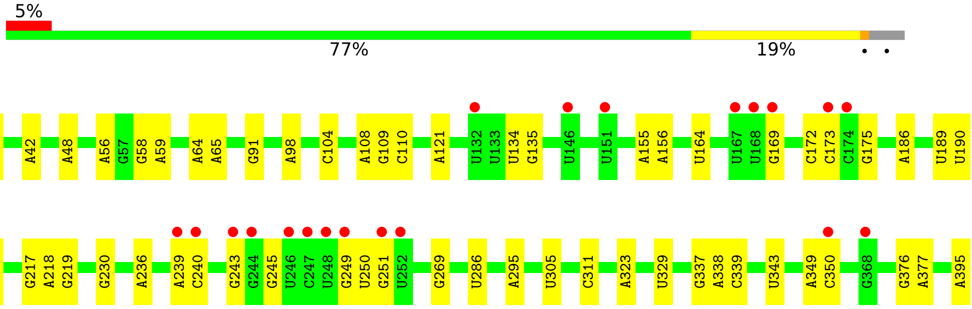
Chain 1:

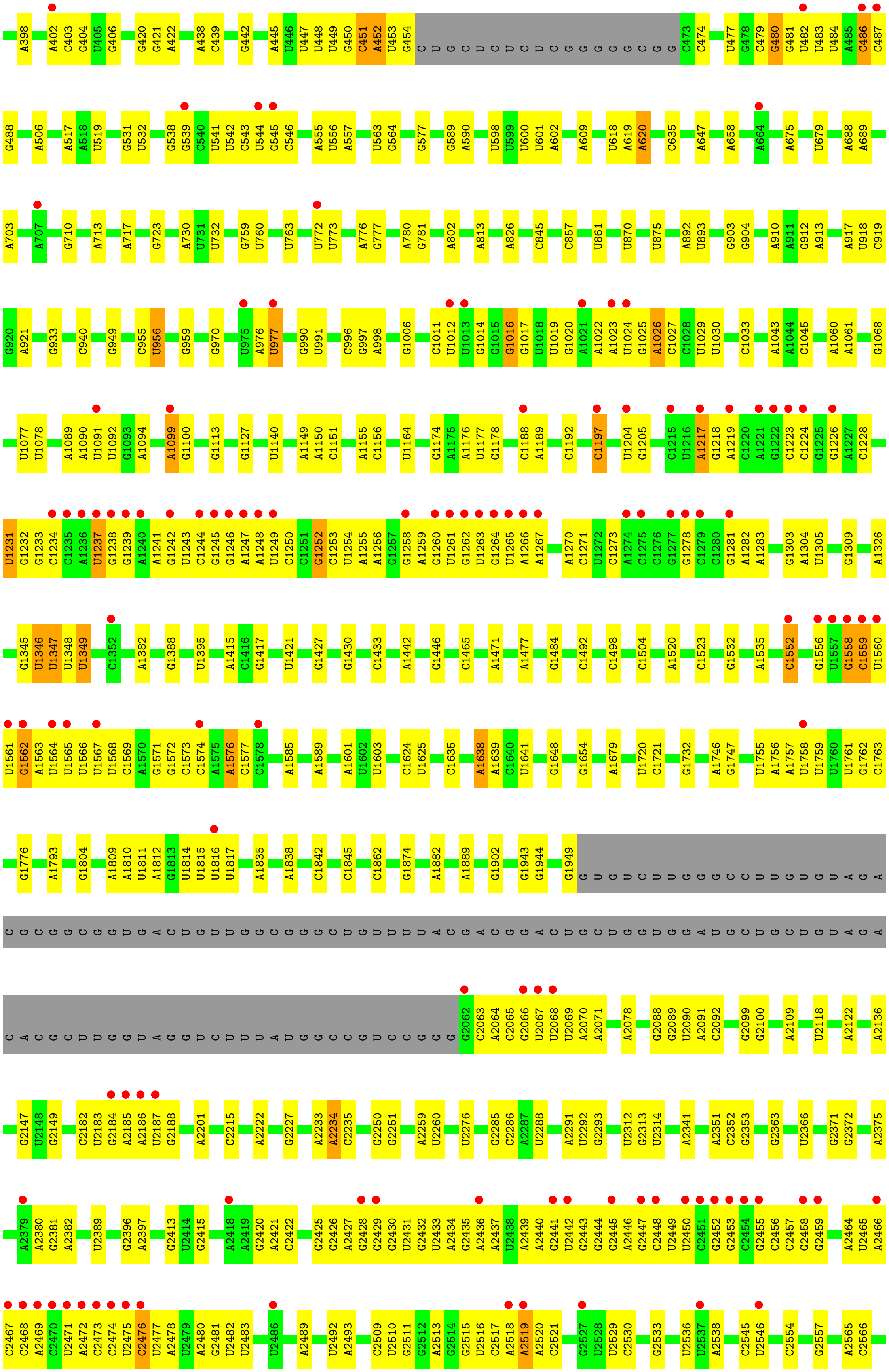


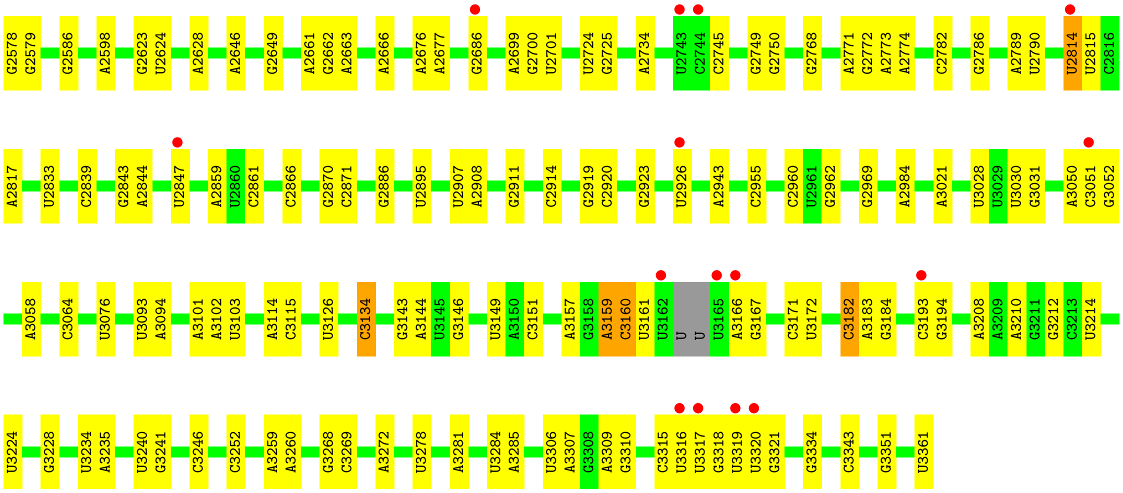


- Molecule 1: 25S

Chain AS:

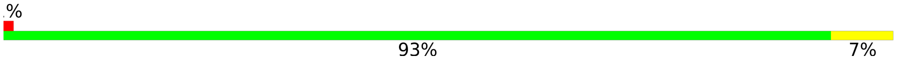


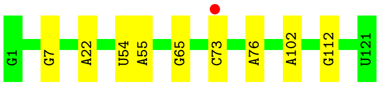

A398 A402 C403 G404 U405 G406 G420 G421 A422 A438 C439 G442 A445 U446 U447 U448 U449 G450 C451 A452 U453 G454 C U G C U C U C U C G G G G G C G G C473 C474 U477 G478 C479 G480 G481 U482 U483 U484 A485 C486 C487
G488 A506 A517 A518 U519 G531 U532 G538 G539 C540 U541 U542 C543 U544 G545 C546 A555 U556 A557 U563 G564 G577 G589 A590 U598 U599 U600 U601 A602 A609 U618 A619 A620 C635 A647 A658 A664 A675 U679 A688 A689
A703 A707 G710 A713 A717 G723 A730 U731 U732 G759 U760 U763 U772 U773 A776 G777 A780 G781 A802 A813 A826 C845 C857 U861 U870 U875 A892 U893 G903 G904 A910 A911 G912 A913 A917 U918 C919
G920 A921 G933 C940 G949 C955 U956 G959 G970 U975 A976 U977 G990 U991 C996 G997 A998 G1006 C1011 U1012 U1013 G1014 G1015 G1016 G1017 U1018 U1019 G1020 A1021 A1022 A1023 U1024 G1025 A1026 C1027 C1028 U1029 U1030 C1033 A1043 A1044 C1045 A1060 A1061 G1068
U1077 U1078 A1089 A1090 U1091 U1092 G1093 A1094 A1099 G1100 G1113 G1127 U1140 A1149 A1150 C1151 A1155 C1156 U1164 G1174 A1175 A1176 U1177 G1178 C1188 A1189 C1192 C1197 U1204 G1205 C1215 U1216 A1217 G1218 A1219 C1220 A1221 G1222 C1223 C1224 G1225 G1226 A1227 C1228
U1231 G1232 G1233 C1234 C1235 A1236 U1237 G1238 G1239 A1240 A1241 G1242 U1243 C1244 G1245 G1246 A1247 A1248 U1249 C1250 C1251 G1252 C1253 U1254 A1255 A1256 G1257 G1258 A1259 G1260 U1261 G1262 U1263 G1264 U1265 A1266 A1267 A1270 C1271 U1272 C1273 A1274 C1275 C1276 G1277 G1278 C1279 C1280 G1281 A1282 A1283 G1303 A1304 U1305 G1309 A1326
G1345 U1346 U1347 U1348 U1349 C1352 A1382 G1388 U1395 A1415 C1416 G1417 U1421 G1427 G1430 C1433 A1442 G1446 C1465 A1471 A1477 G1484 C1492 C1498 C1504 A1520 C1523 G1532 A1535 C1552 G1556 U1557 G1558 C1559 U1560
U1561 G1562 A1563 U1564 U1565 U1566 U1567 U1568 C1569 A1570 G1571 G1572 C1573 C1574 A1575 A1576 C1577 C1578 A1585 A1589 A1601 U1602 U1603 C1624 U1625 C1635 A1638 A1639 C1640 U1641 G1648 G1654 A1679 U1720 C1721 G1732 A1746 G1747 U1755 A1756 A1757 U1758 U1759 U1760 U1761 G1762 C1763
G1776 A1793 G1804 A1809 A1810 U1811 A1812 G1813 U1814 U1815 U1816 U1817 A1835 A1838 C1842 C1845 C1862 G1874 A1882 A1889 G1902 G1943 G1944 G1949 G U G U C U U G G G C C U U G U G U A G A
C G C G G C G G U G A C U G U U G G C G G G C U G U U U U A C G A C G G A C U G C U G G U G G A U G C U G C U G U A G A
C A C G C U U G G U A G G U C U U U A U G G C C G U C C G G G G2062 C2063 A2064 C2065 G2066 U2067 U2068 U2069 A2070 A2071 A2078 G2088 G2089 U2090 A2091 C2092 G2099 G2100 A2109 U2118 A2122 A2136
G2147 U2148 G2149 C2182 U2183 G2184 A2185 A2186 U2187 G2188 A2201 C2215 A2222 G2227 A2233 A2234 C2235 G2250 G2251 A2259 U2260 U2276 G2285 C2286 A2287 U2288 A2291 U2292 G2293 U2312 G2313 U2314 A2341 A2351 C2352 G2353 G2363 U2366 G2371 G2372 A2375
A2379 A2380 G2381 A2382 U2389 G2396 A2397 G2413 U2414 G2415 A2418 A2419 G2420 A2421 C2422 G2425 G2426 A2427 G2428 G2429 G2430 U2431 G2432 U2433 A2434 C2435 A2436 A2437 U2438 A2439 A2440 G2441 U2442 G2443 G2444 C2445 A2446 G2447 C2448 U2449 U2450 C2451 G2452 G2453 C2454 G2455 C2456 C2457 G2458 G2459 A2464 U2465 A2466
C2467 C2468 A2469 C2470 U2471 A2472 C2473 C2474 U2475 C2476 U2477 A2478 U2479 A2480 G2481 U2482 U2483 U2486 A2489 U2492 A2493 C2509 U2510 G2511 G2512 A2513 G2514 G2515 U2516 C2517 A2518 A2519 A2520 C2521 G2527 U2528 U2529 C2530 G2533 U2536 U2537 A2538 C2545 U2546 C2554 G2557 A2565 C2566



- Molecule 2: 5S

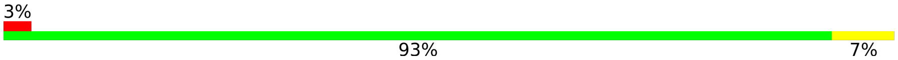
Chain 3:

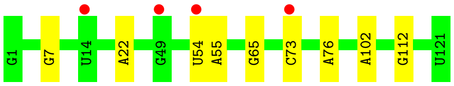




- Molecule 2: 5S

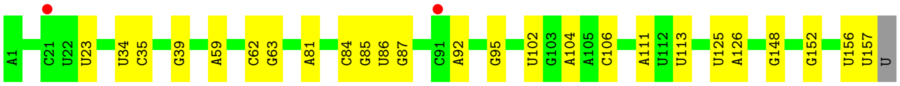
Chain AT:





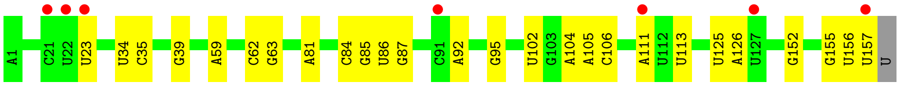
- Molecule 3: 5.8S

Chain 4:



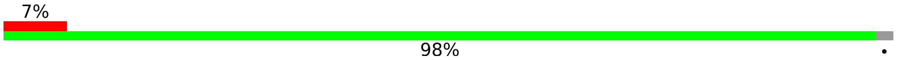
- Molecule 3: 5.8S

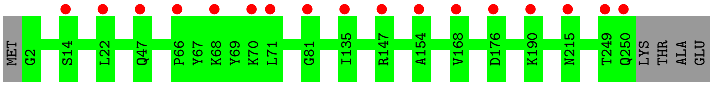
Chain AU:



- Molecule 4: 60S ribosomal protein L2-B

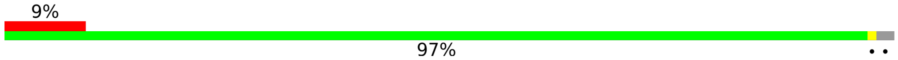
Chain j:

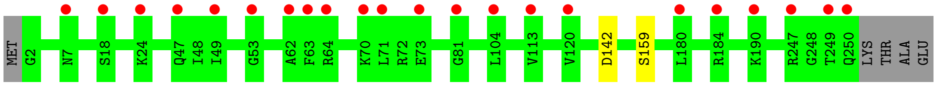




- Molecule 4: 60S ribosomal protein L2-B

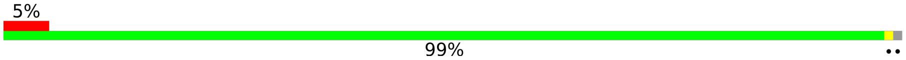
Chain AW:

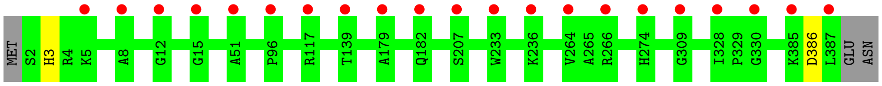




- Molecule 5: 60S ribosomal protein L3

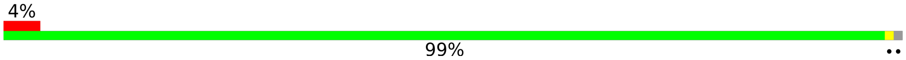
Chain k:

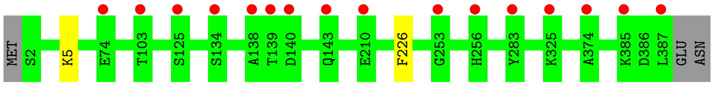




- Molecule 5: 60S ribosomal protein L3

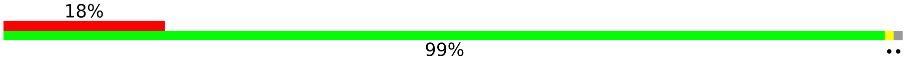
Chain AX:

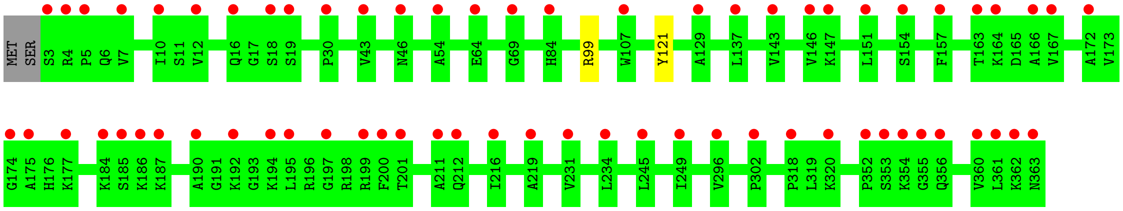




- Molecule 6: 60S ribosomal protein L4-B

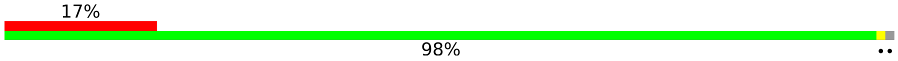
Chain l:

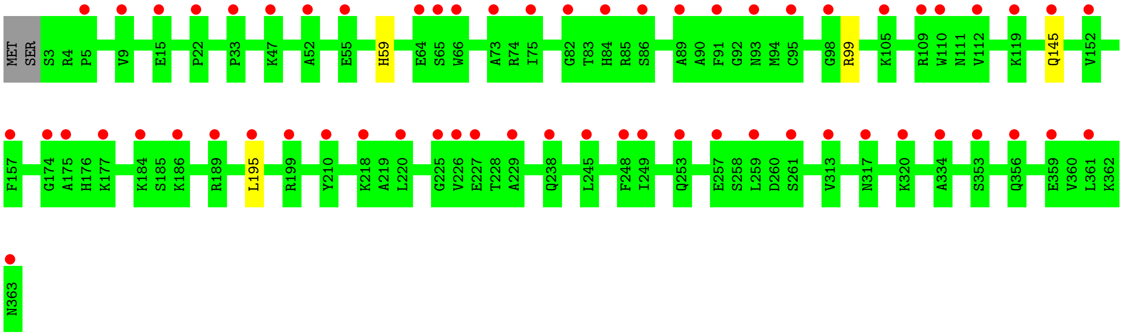




- Molecule 6: 60S ribosomal protein L4-B

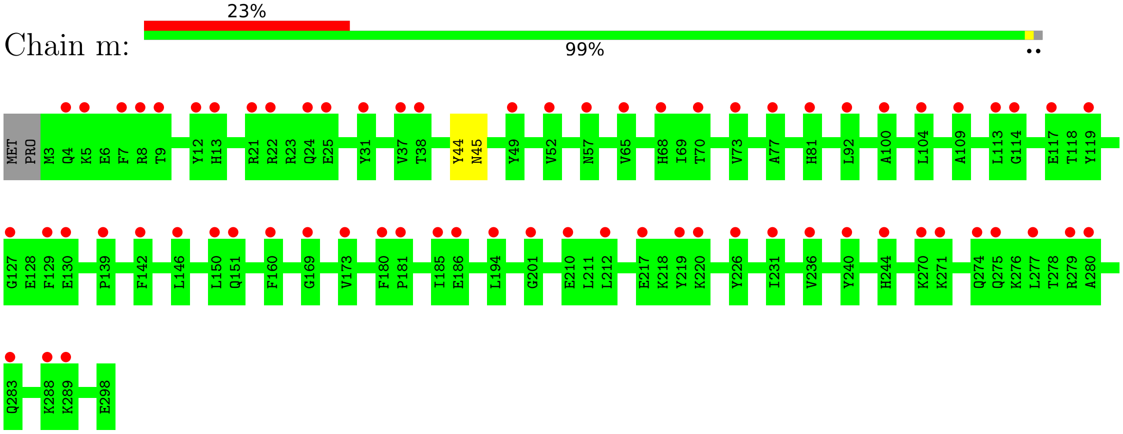
Chain AY:





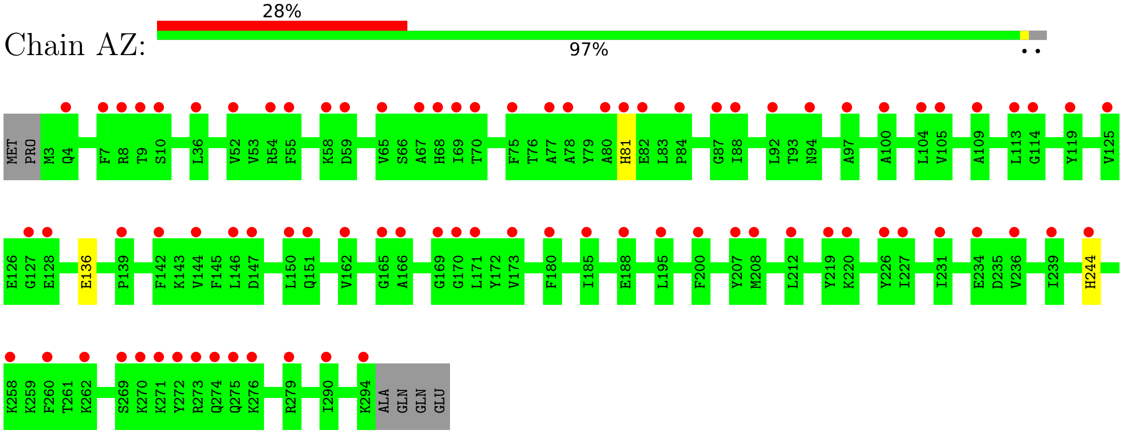
- Molecule 7: Uncharacterized protein CaJ7.0206

Chain m:



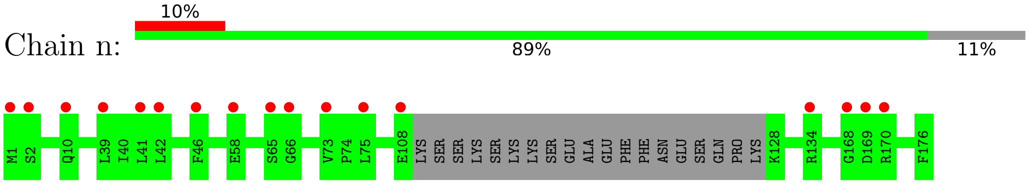
- Molecule 7: Uncharacterized protein CaJ7.0206

Chain AZ:



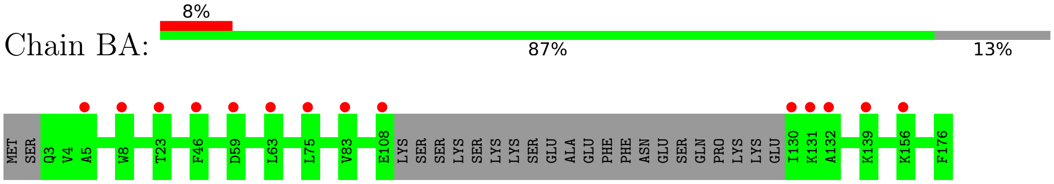
- Molecule 8: 60S ribosomal protein L6

Chain n:



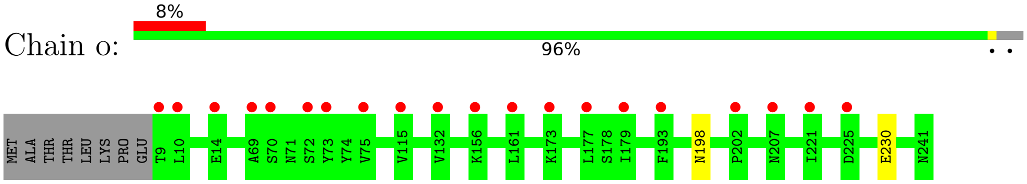
- Molecule 8: 60S ribosomal protein L6

Chain BA:



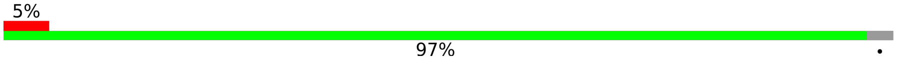
- Molecule 9: 60S ribosomal protein L7-A

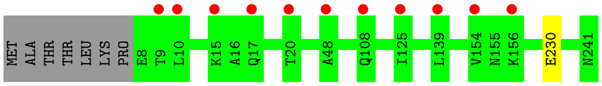
Chain o:



- Molecule 9: 60S ribosomal protein L7-A

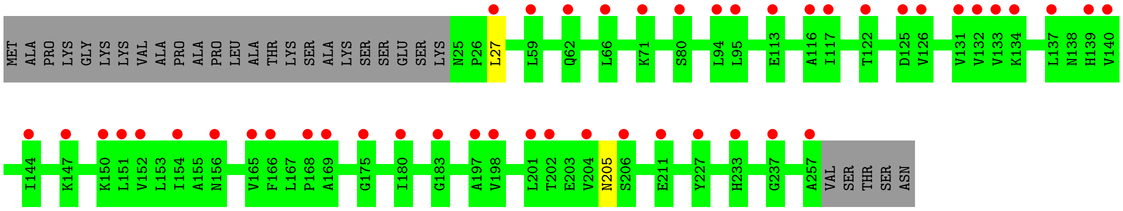
Chain BB:





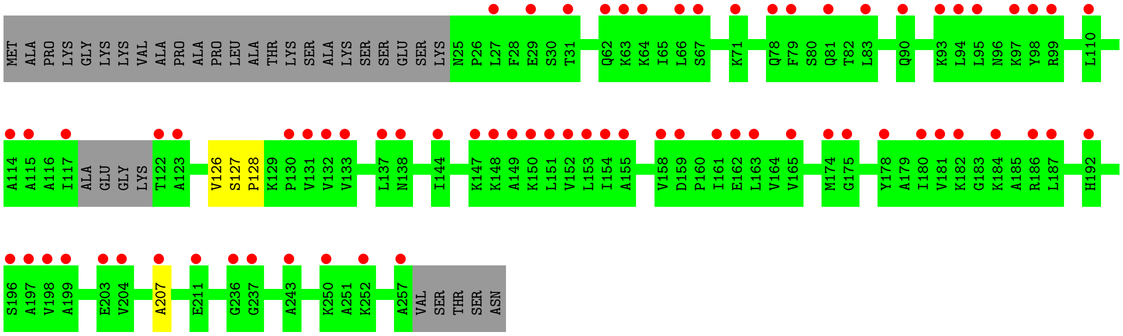
- Molecule 10: 60S ribosomal protein L8

Chain p:



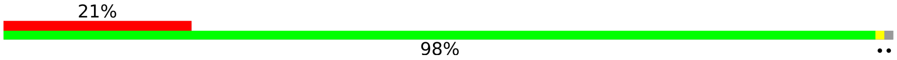
- Molecule 10: 60S ribosomal protein L8

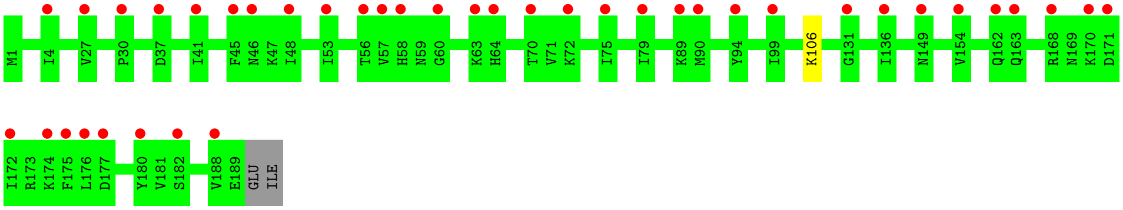
Chain BC:



- Molecule 11: 60S ribosomal protein L9-B

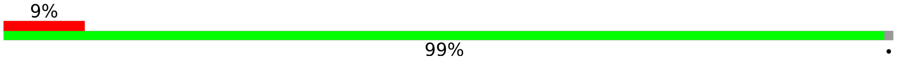
Chain q:

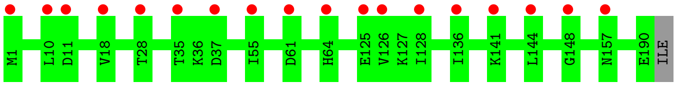




- Molecule 11: 60S ribosomal protein L9-B

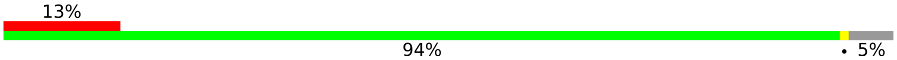
Chain BD:

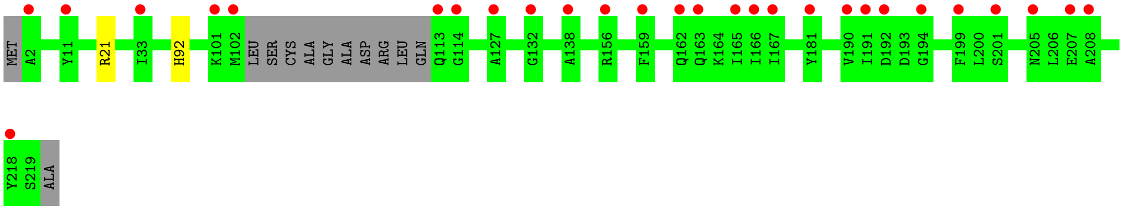




- Molecule 12: 60S ribosomal protein L10

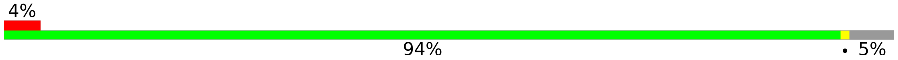
Chain r:

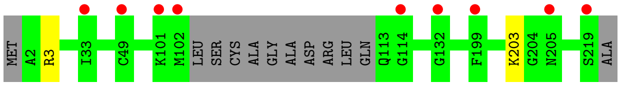




- Molecule 12: 60S ribosomal protein L10

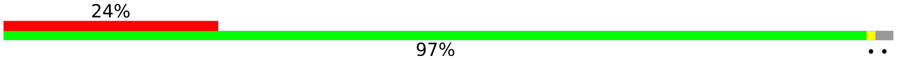
Chain BE:

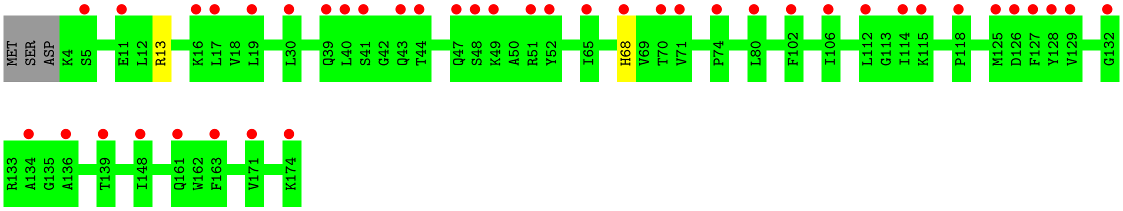




- Molecule 13: 60S ribosomal protein L11-B

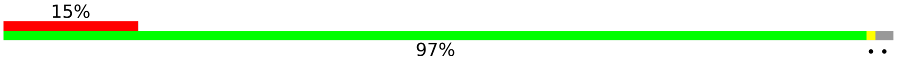
Chain s:

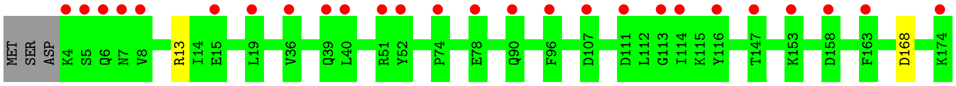




- Molecule 13: 60S ribosomal protein L11-B

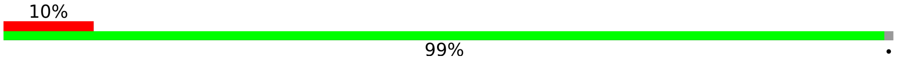
Chain BF:

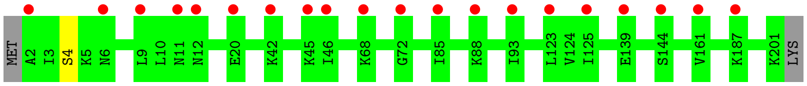




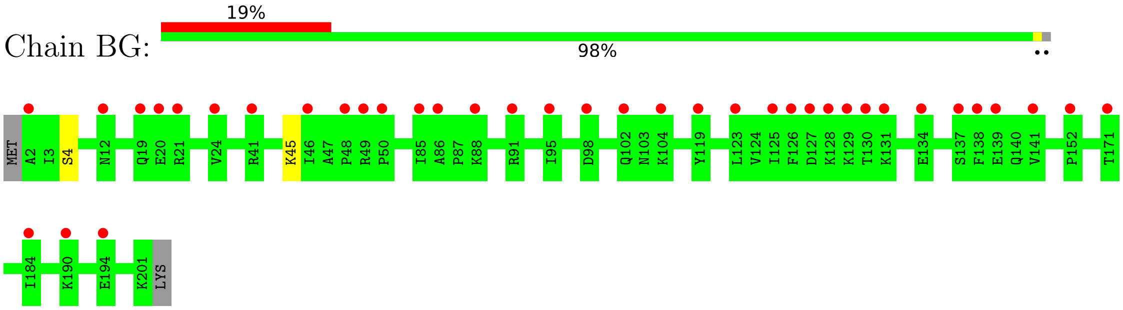
- Molecule 14: 60S ribosomal protein L13

Chain t:

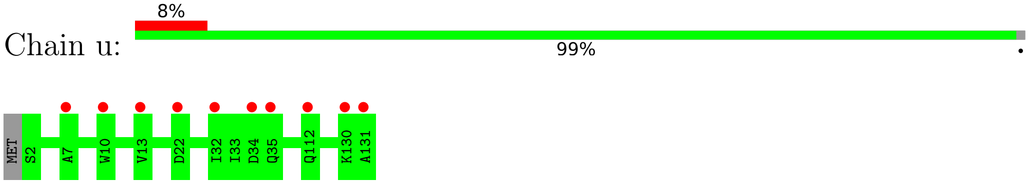




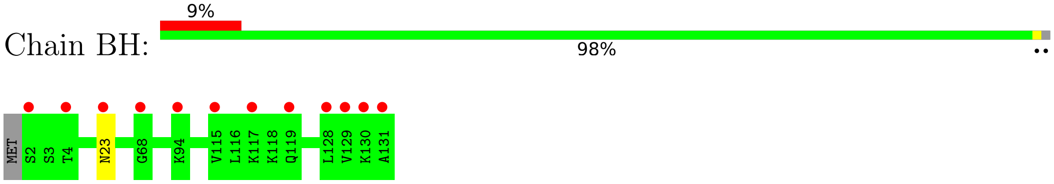
- Molecule 14: 60S ribosomal protein L13



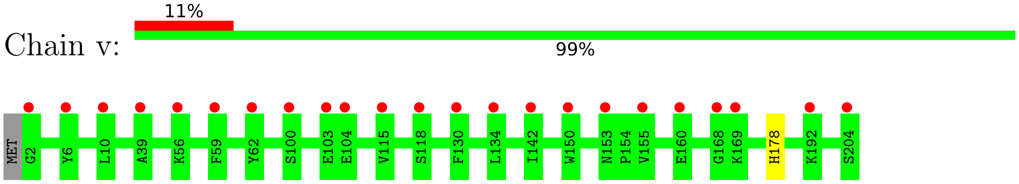
• Molecule 15: 60S ribosomal protein L14-B



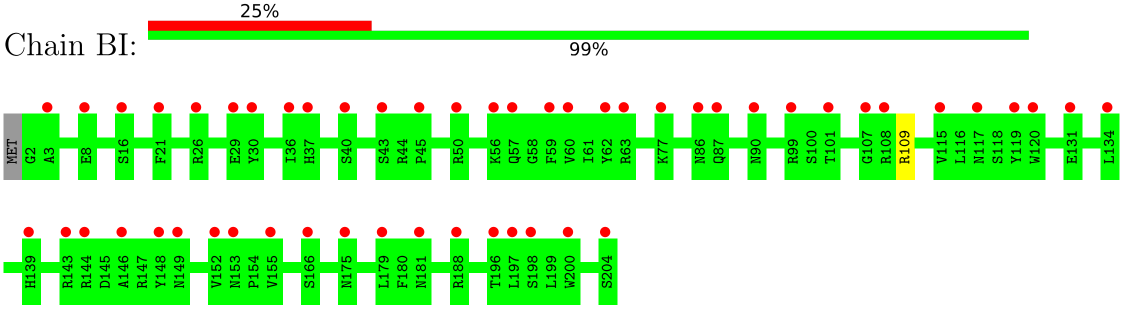
• Molecule 15: 60S ribosomal protein L14-B



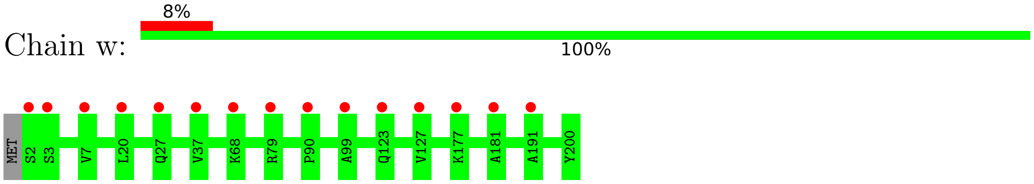
• Molecule 16: 60S ribosomal protein L15-A



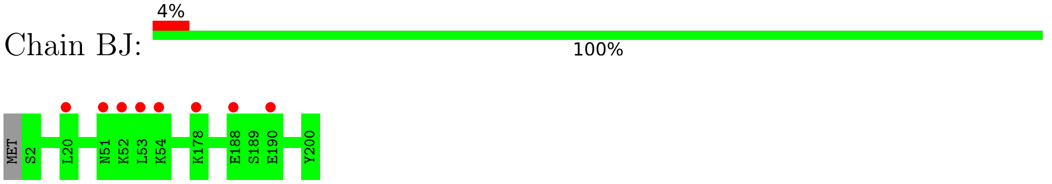
• Molecule 16: 60S ribosomal protein L15-A



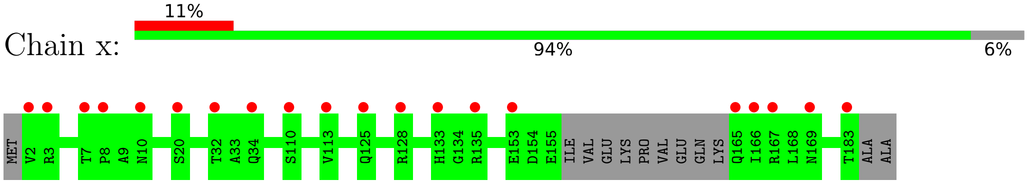
• Molecule 17: Ribosomal protein L13



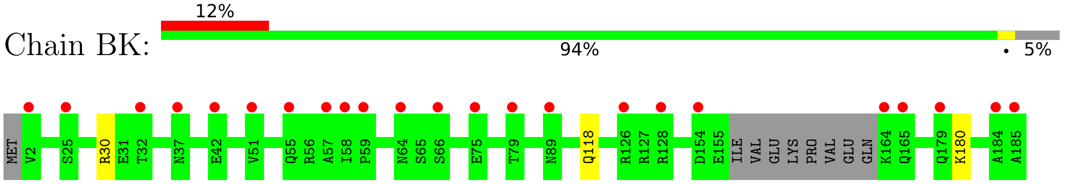
- Molecule 17: Ribosomal protein L13



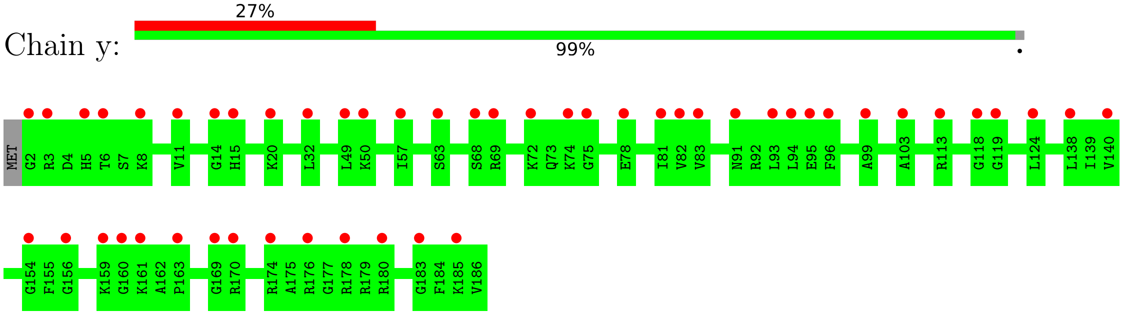
- Molecule 18: Ribosomal protein L22



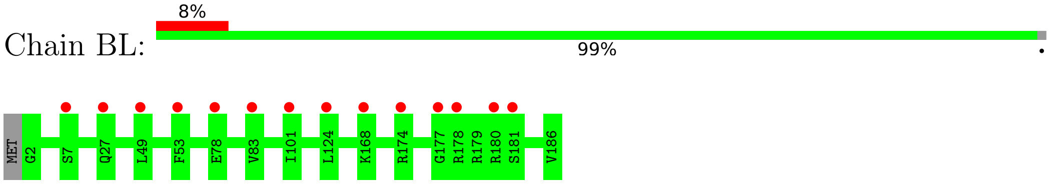
- Molecule 18: Ribosomal protein L22



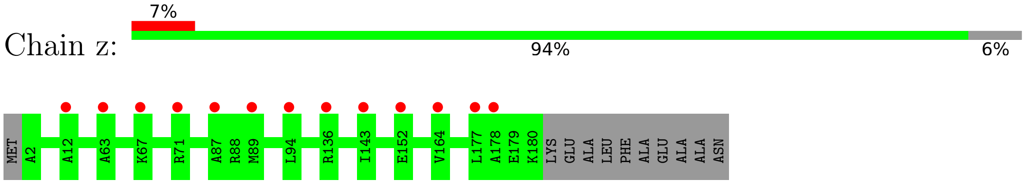
- Molecule 19: 60S ribosomal protein L18-A



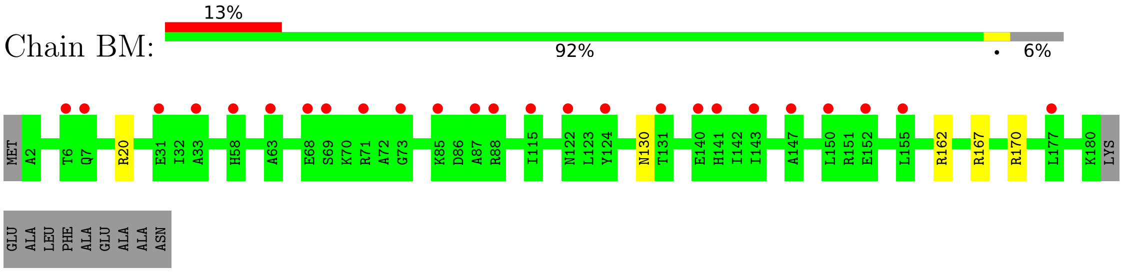
- Molecule 19: 60S ribosomal protein L18-A



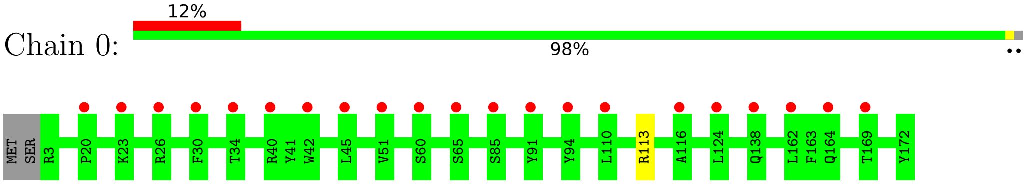
- Molecule 20: 60S ribosomal protein L19-A



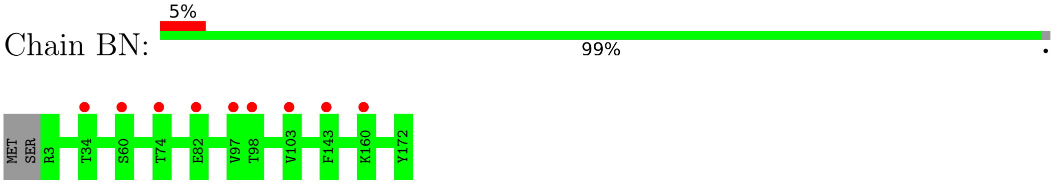
- Molecule 20: 60S ribosomal protein L19-A



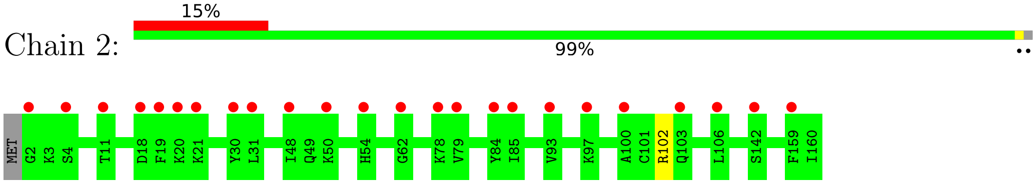
- Molecule 21: 60S ribosomal protein L20



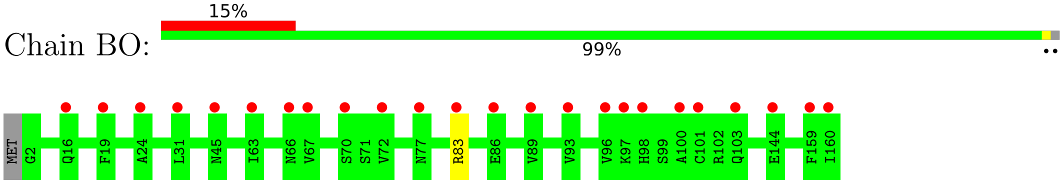
- Molecule 21: 60S ribosomal protein L20



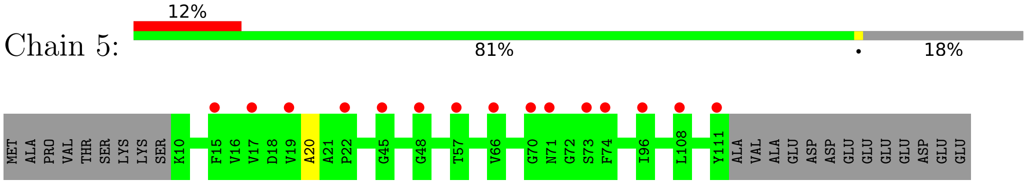
- Molecule 22: 60S ribosomal protein L21-A



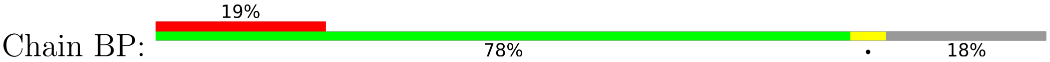
- Molecule 22: 60S ribosomal protein L21-A

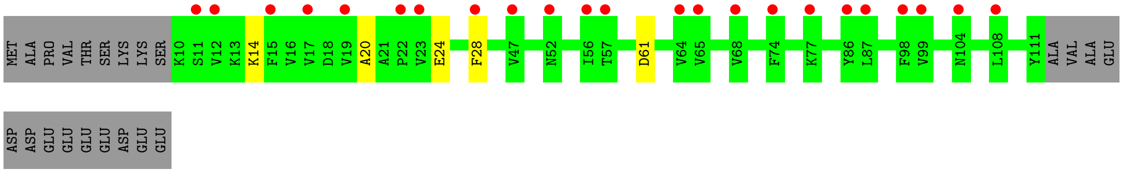


- Molecule 23: 60S ribosomal protein L22-B



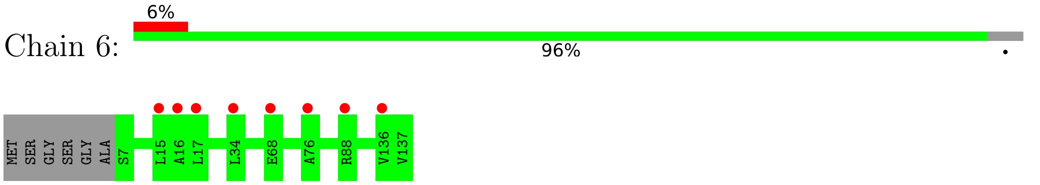
- Molecule 23: 60S ribosomal protein L22-B





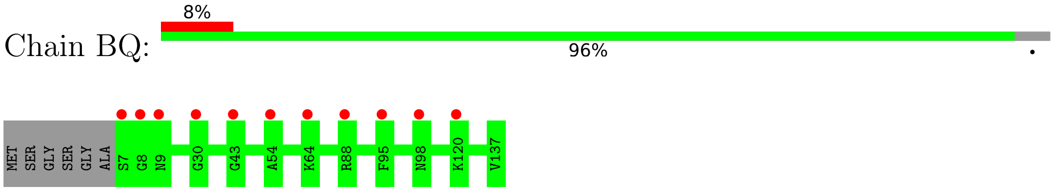
- Molecule 24: 60S ribosomal protein L23-A

Chain 6:



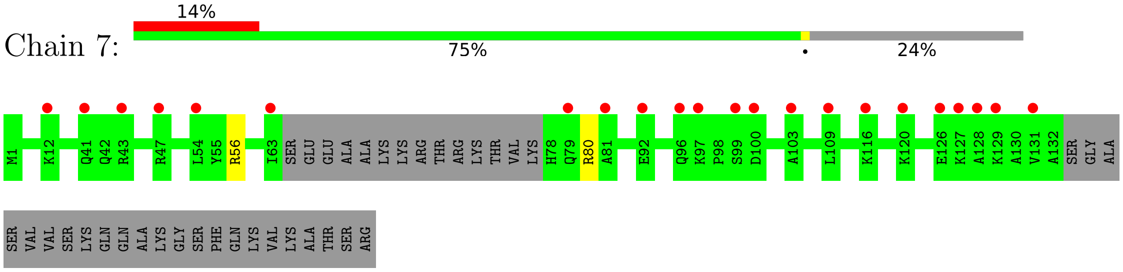
- Molecule 24: 60S ribosomal protein L23-A

Chain BQ:



- Molecule 25: 60S ribosomal protein L24-A

Chain 7:



- Molecule 25: 60S ribosomal protein L24-A

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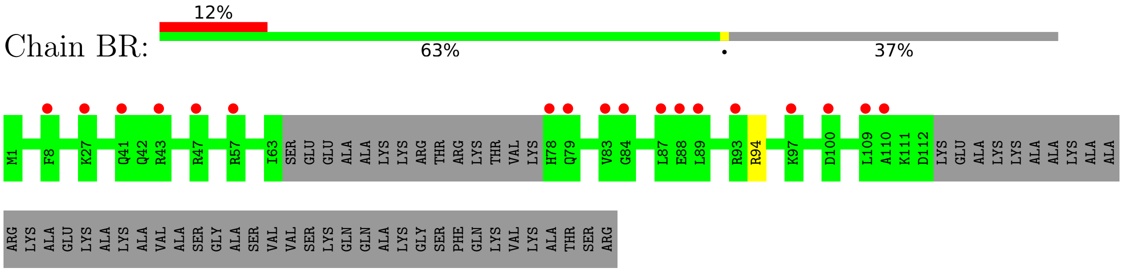
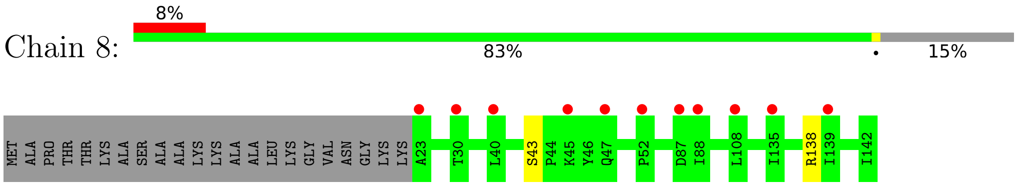


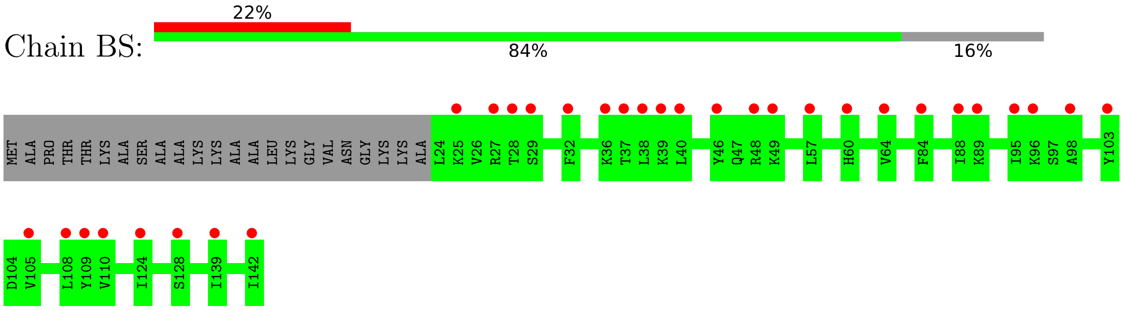
- Molecule 26: 60S ribosomal protein L25

Chain 8:



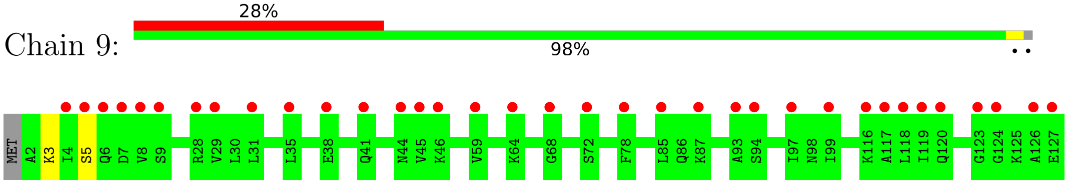
- Molecule 26: 60S ribosomal protein L25

Chain BS:



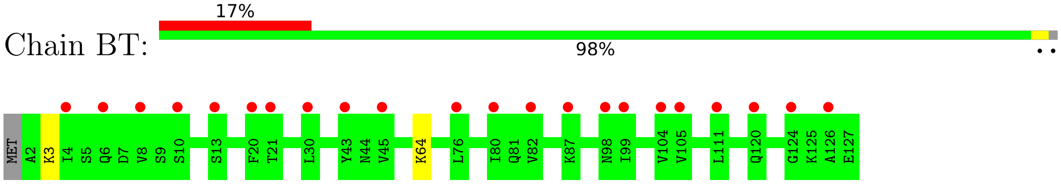
• Molecule 27: Ribosomal protein L24

Chain 9:



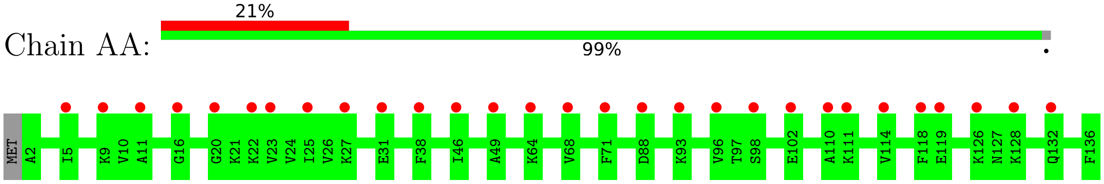
• Molecule 27: Ribosomal protein L24

Chain BT:



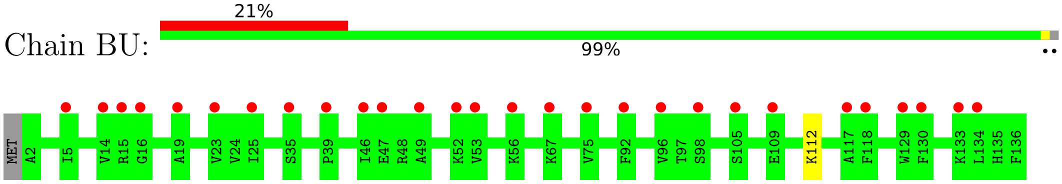
• Molecule 28: 60S ribosomal protein L27

Chain AA:



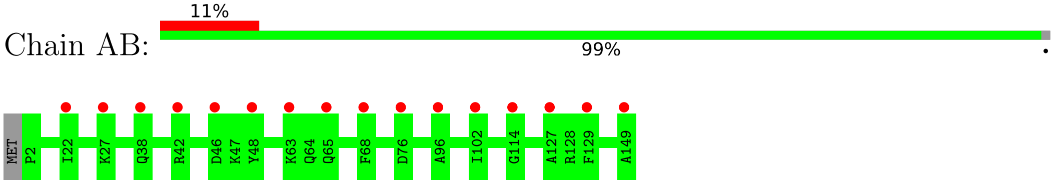
• Molecule 28: 60S ribosomal protein L27

Chain BU:



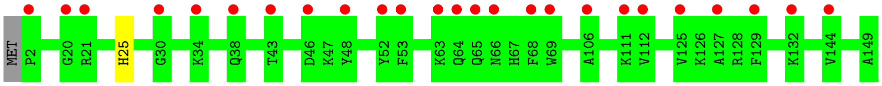
• Molecule 29: 60S ribosomal protein L28

Chain AB:



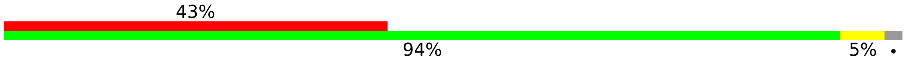
• Molecule 29: 60S ribosomal protein L28

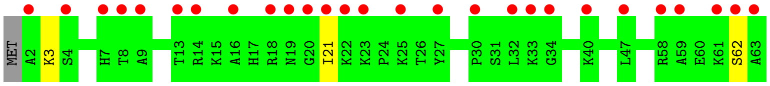
Chain BV:



• Molecule 30: 60S ribosomal protein L29

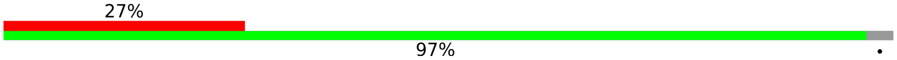
Chain AC:

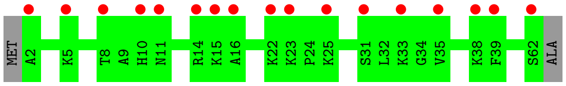




• Molecule 30: 60S ribosomal protein L29

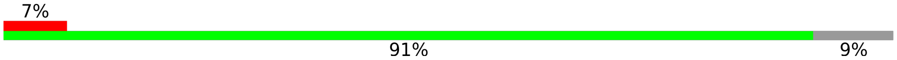
Chain BW:

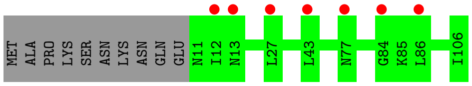




• Molecule 31: 60S ribosomal protein L30

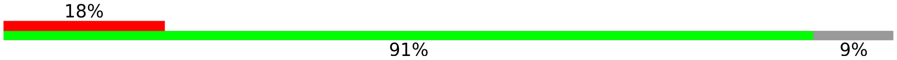
Chain AD:

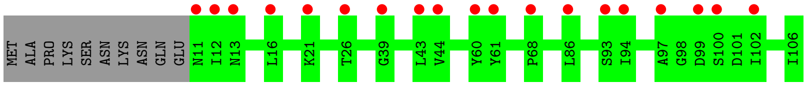




• Molecule 31: 60S ribosomal protein L30

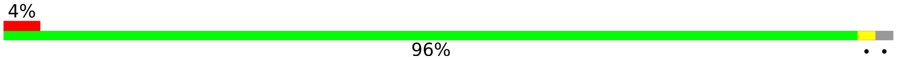
Chain BX:

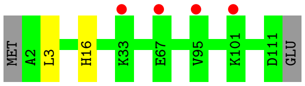




• Molecule 32: 60S ribosomal protein L31-B

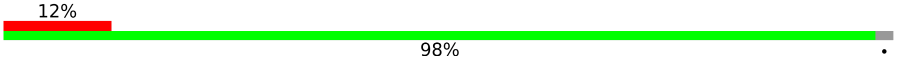
Chain AE:

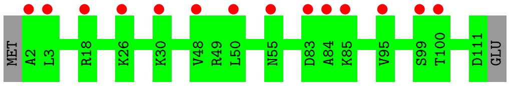




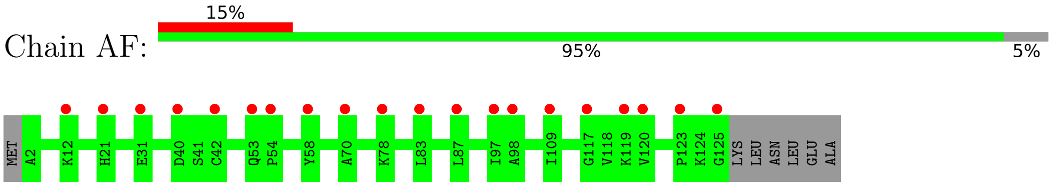
• Molecule 32: 60S ribosomal protein L31-B

Chain BY:

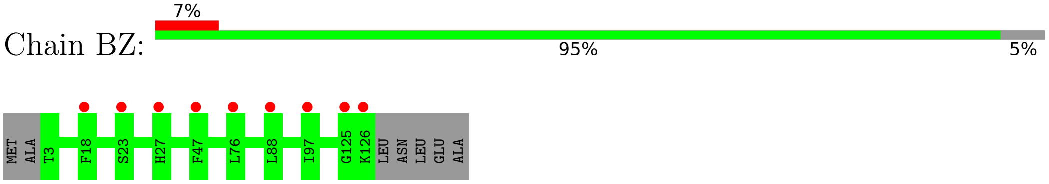




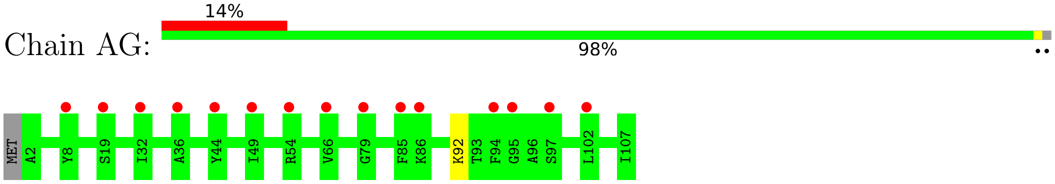
• Molecule 33: 60S ribosomal protein L32



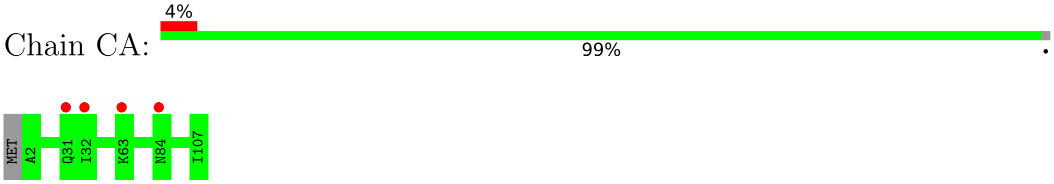
- Molecule 33: 60S ribosomal protein L32



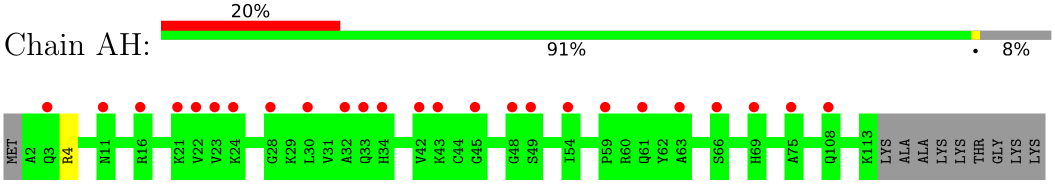
- Molecule 34: 60S ribosomal protein L33-A



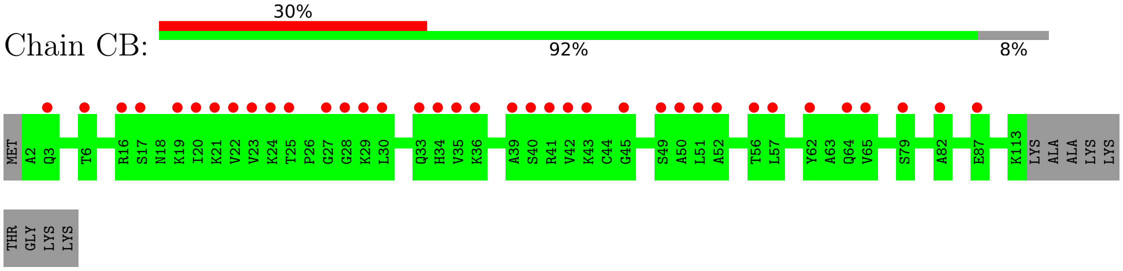
- Molecule 34: 60S ribosomal protein L33-A



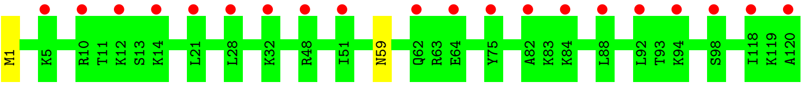
- Molecule 35: 60S ribosomal protein L34-B



- Molecule 35: 60S ribosomal protein L34-B

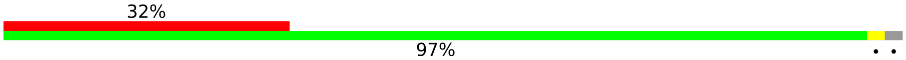


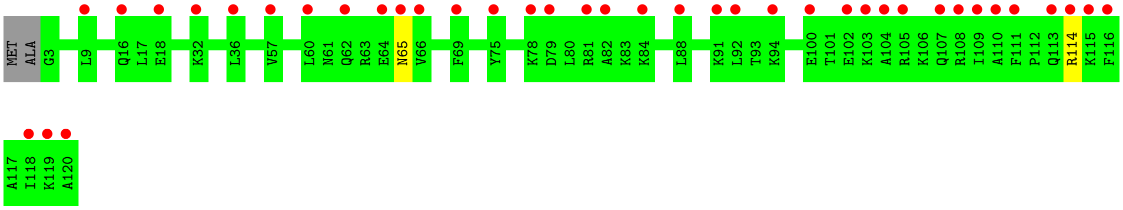
- Molecule 36: Ribosomal protein L29



- Molecule 36: Ribosomal protein L29

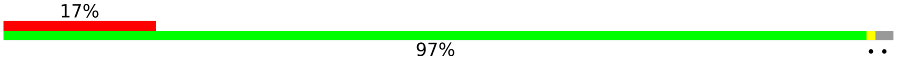
Chain CC:

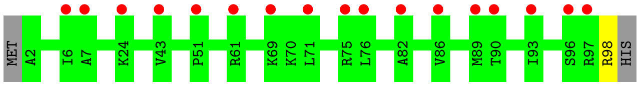




- Molecule 37: 60S ribosomal protein L36

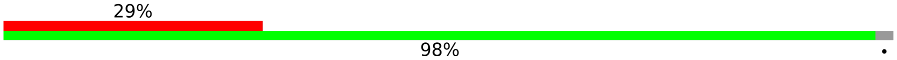
Chain AJ:

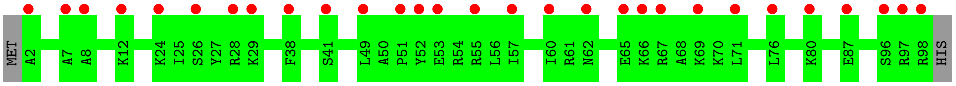




- Molecule 37: 60S ribosomal protein L36

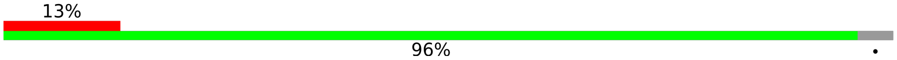
Chain CD:

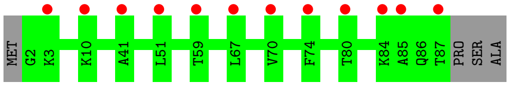




- Molecule 38: 60S ribosomal protein L37-B

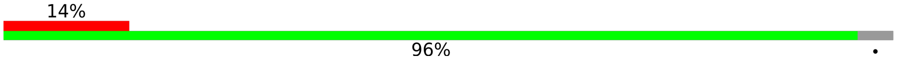
Chain AK:

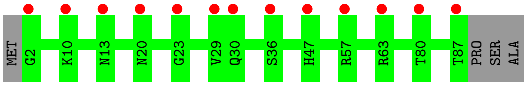




- Molecule 38: 60S ribosomal protein L37-B

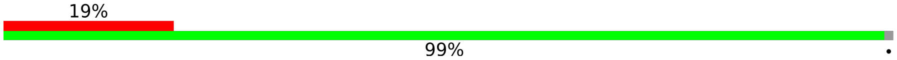
Chain CE:

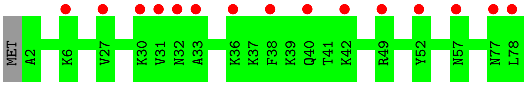




- Molecule 39: 60S ribosomal protein L38

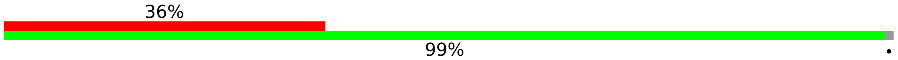
Chain AL:

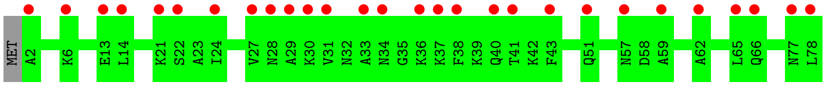




- Molecule 39: 60S ribosomal protein L38

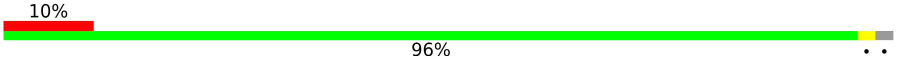
Chain CF:

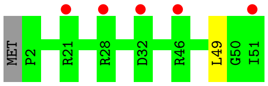




- Molecule 40: 60S ribosomal protein L39

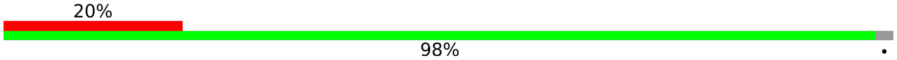
Chain AM:

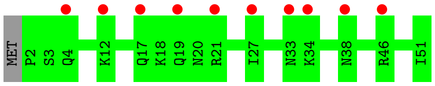




- Molecule 40: 60S ribosomal protein L39

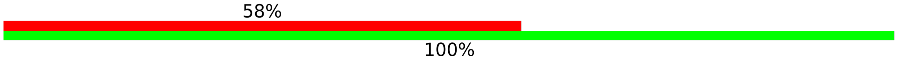
Chain CG:

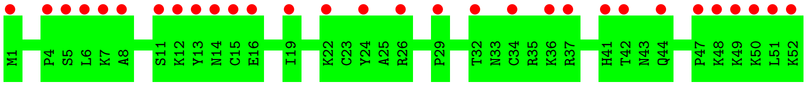




- Molecule 41: 60S ribosomal protein L40-B

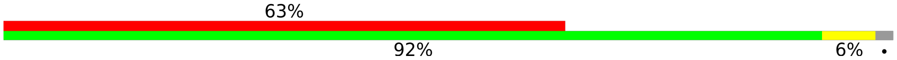
Chain AN:

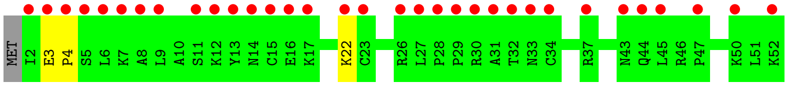




- Molecule 41: 60S ribosomal protein L40-B

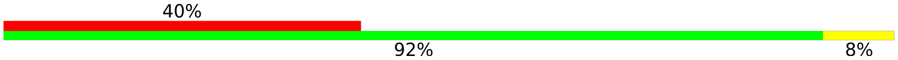
Chain CH:

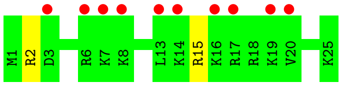




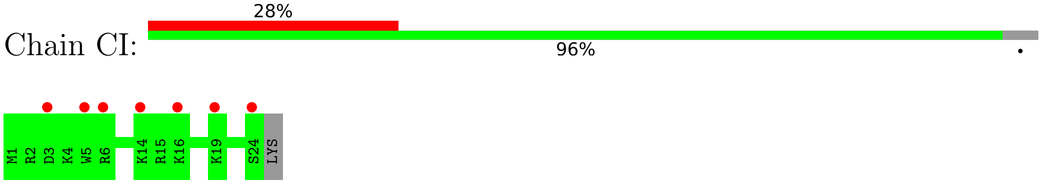
- Molecule 42: 60S ribosomal protein L41

Chain AO:

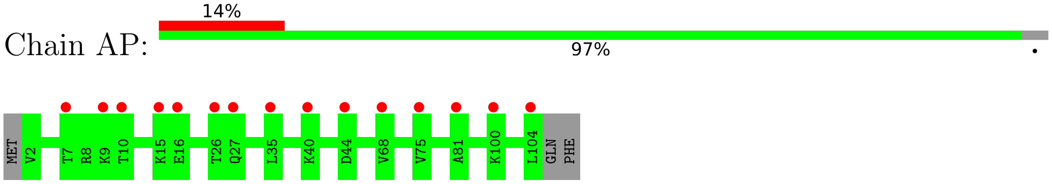




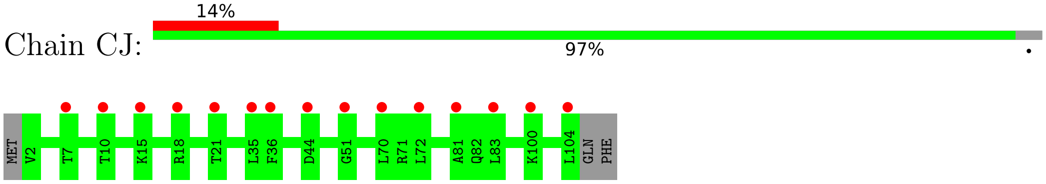
- Molecule 42: 60S ribosomal protein L41



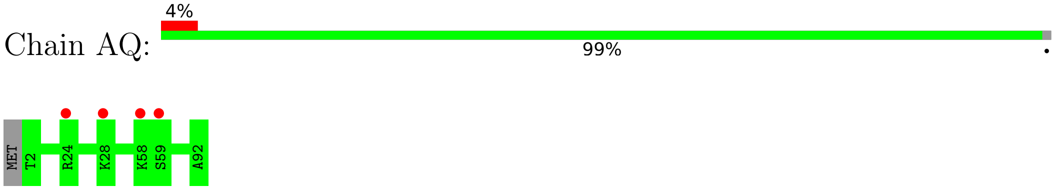
- Molecule 43: 60S ribosomal protein L42-B



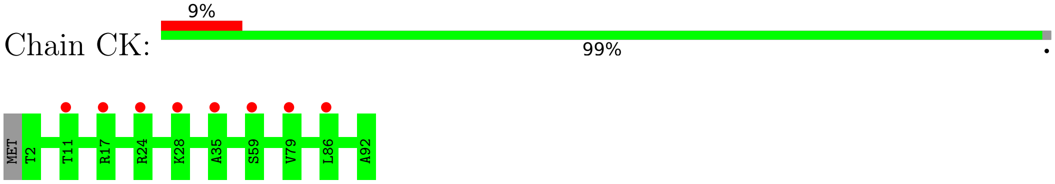
- Molecule 43: 60S ribosomal protein L42-B



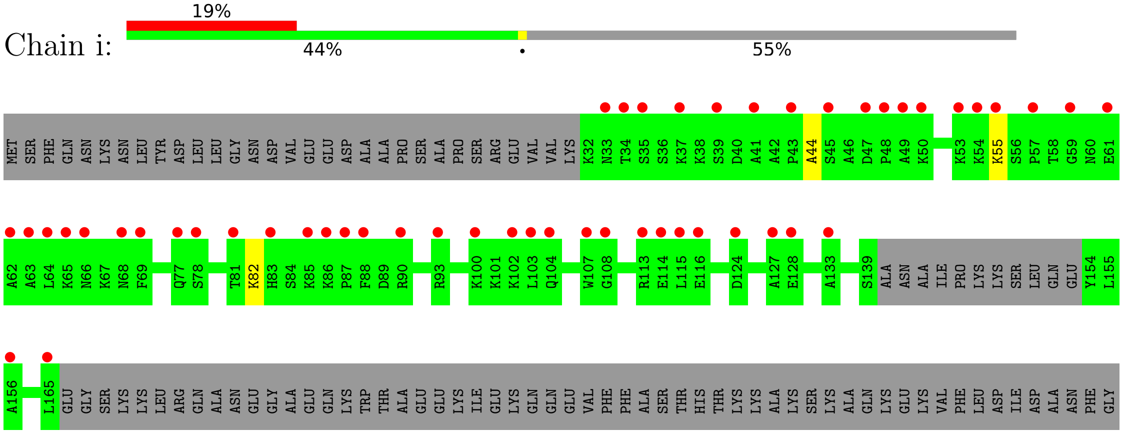
- Molecule 44: 60S ribosomal protein L43-A

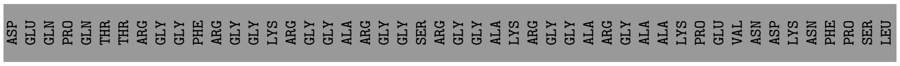


- Molecule 44: 60S ribosomal protein L43-A

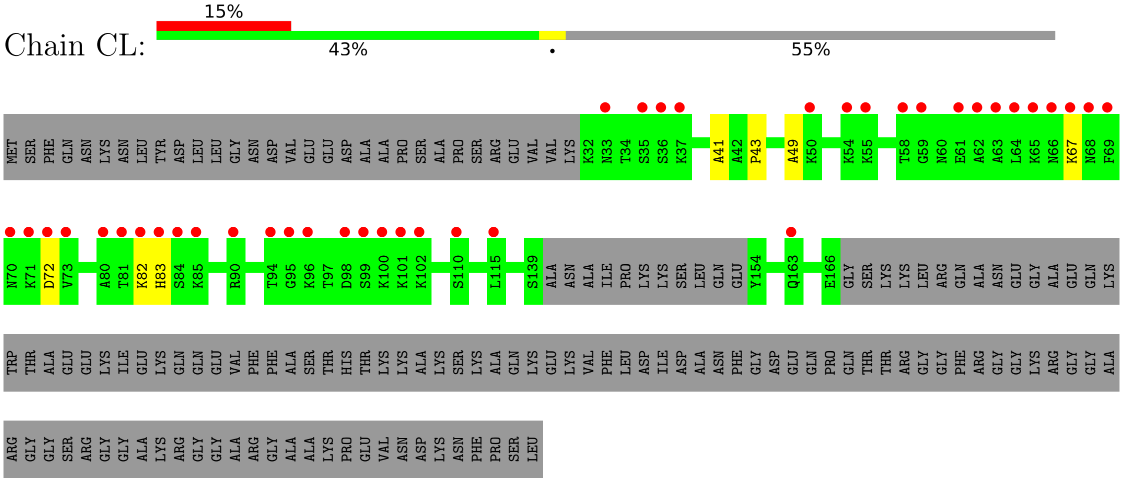


- Molecule 45: 60S ribosomal protein CAALFM_C304810CA

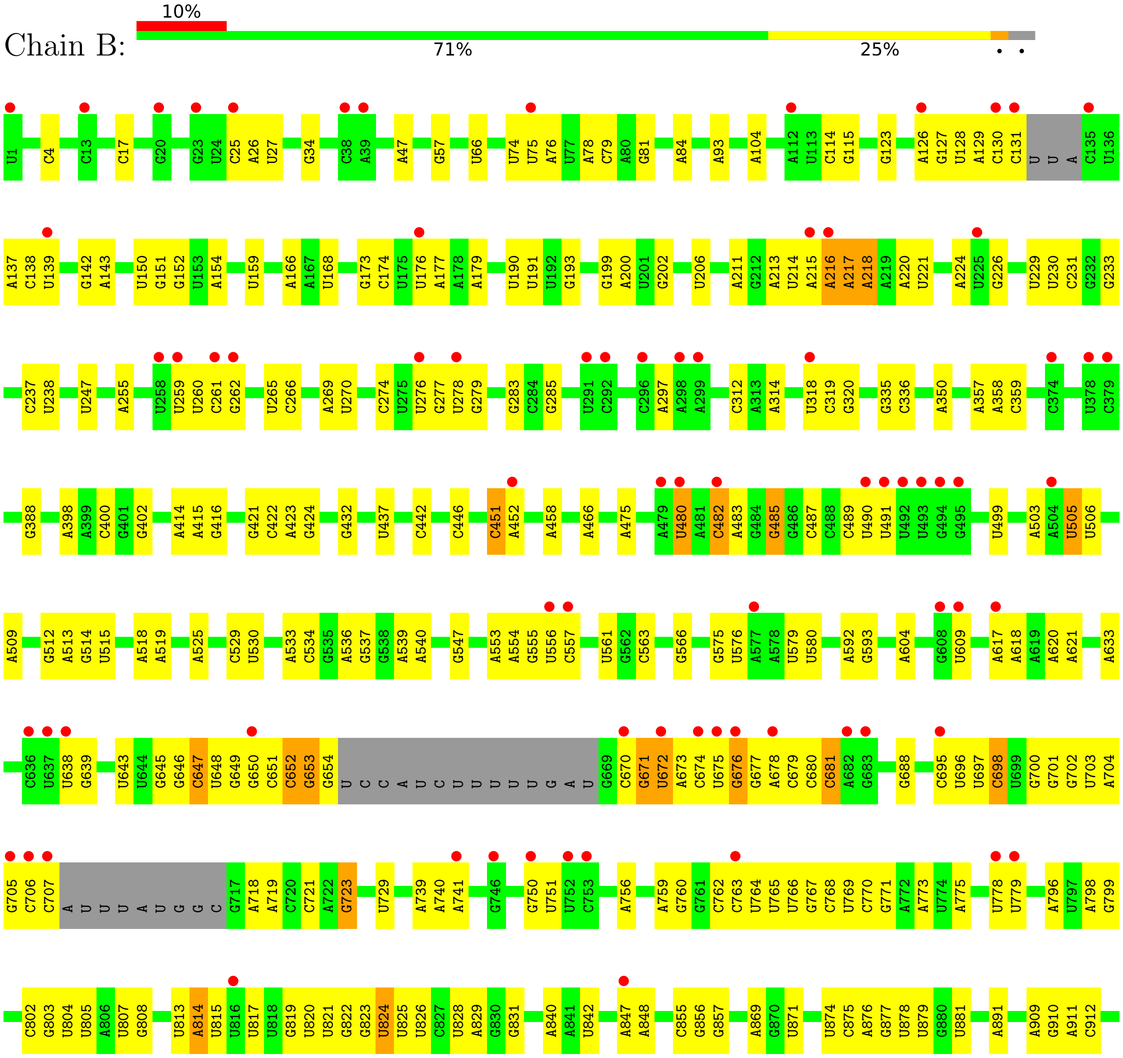


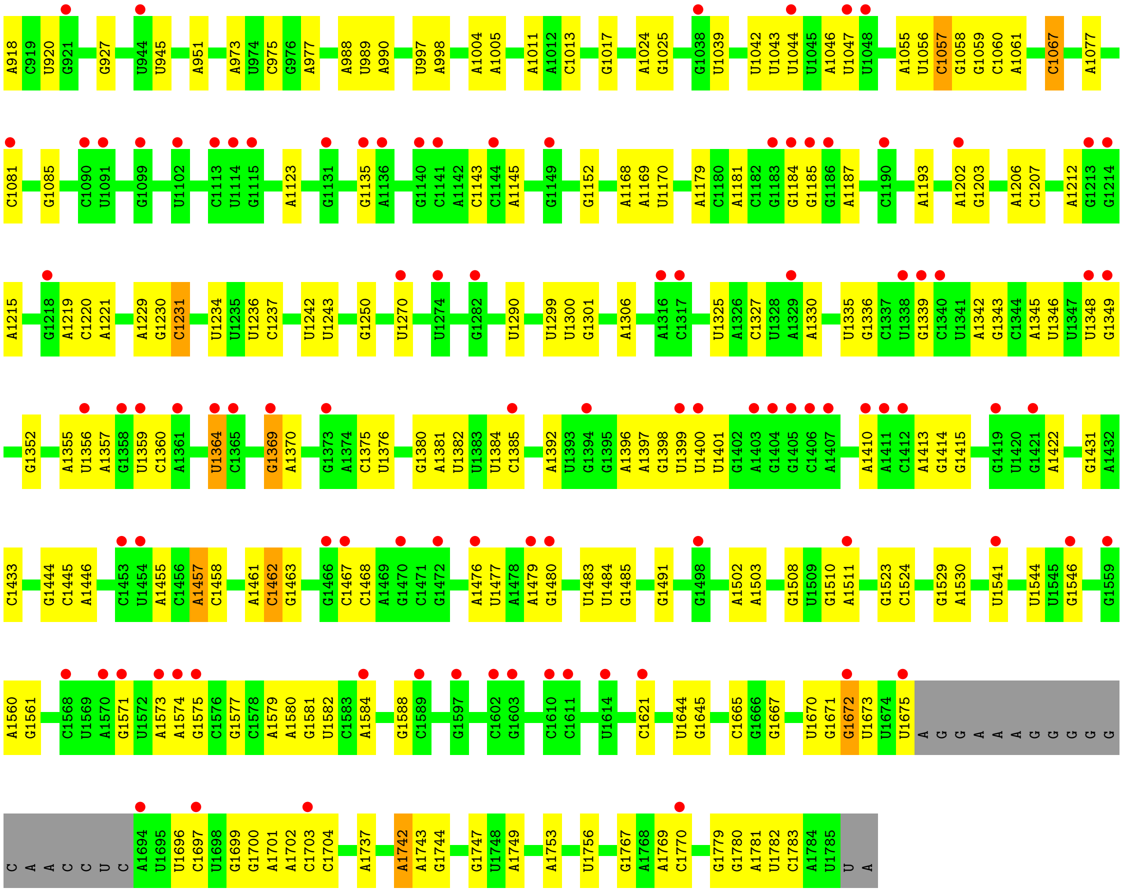


- Molecule 45: 60S ribosomal protein CAALFM_C304810CA

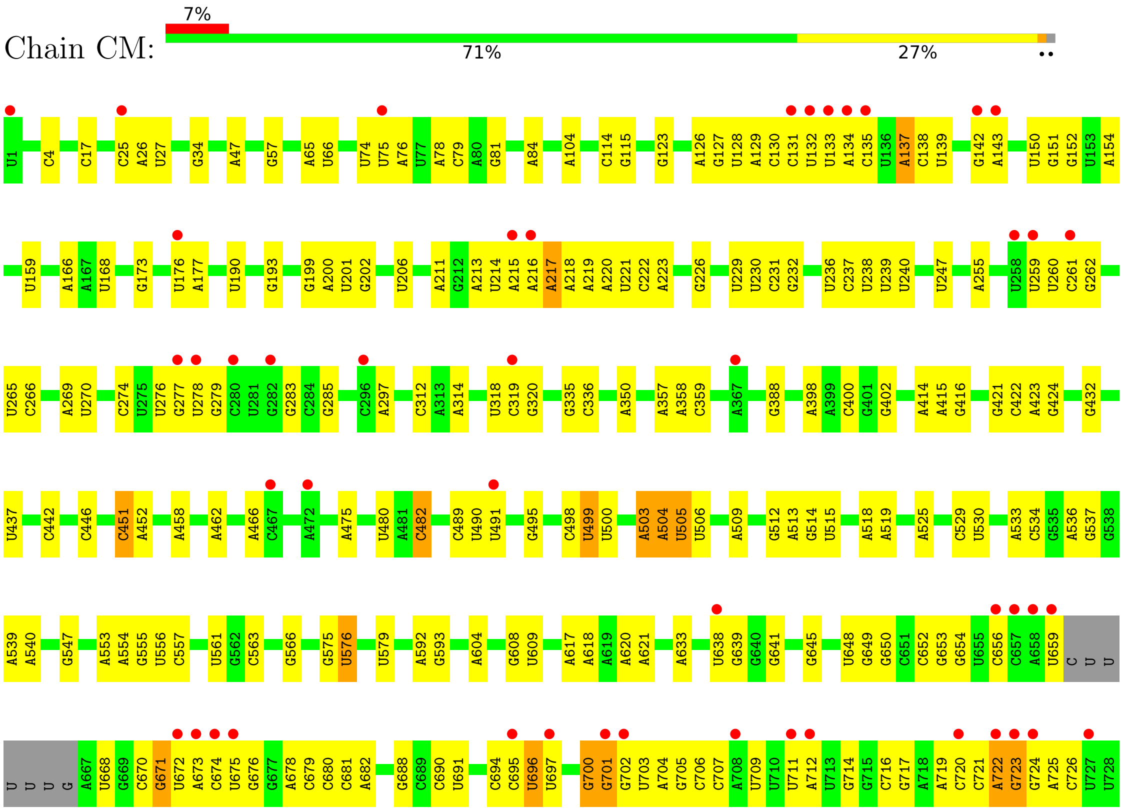


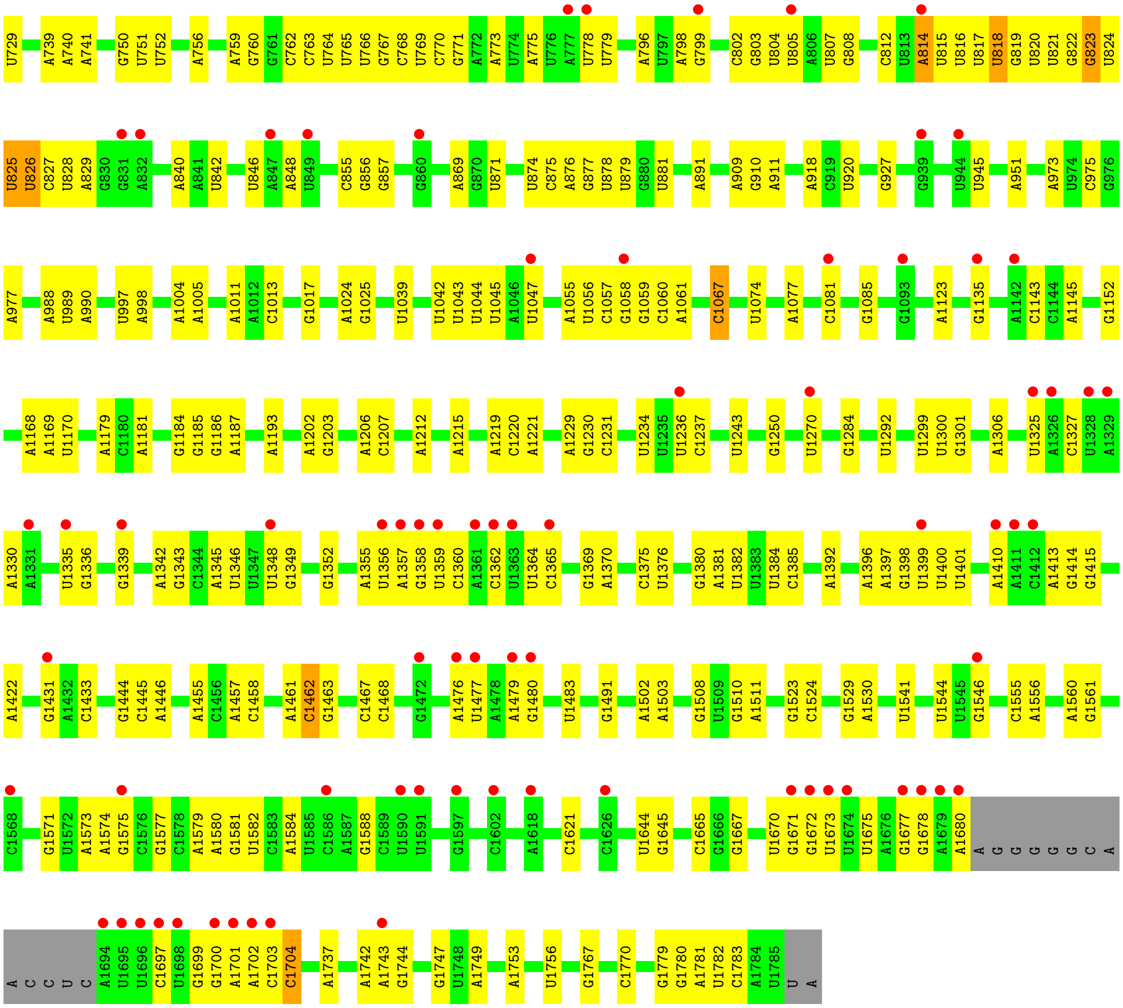
- Molecule 46: 18S





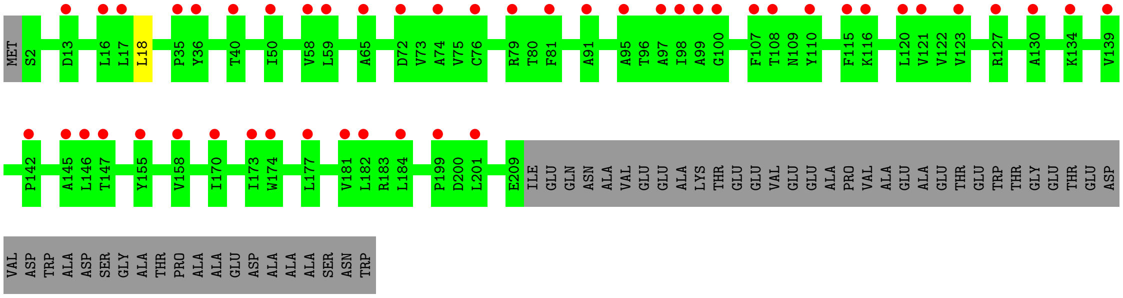
- Molecule 46: 18S





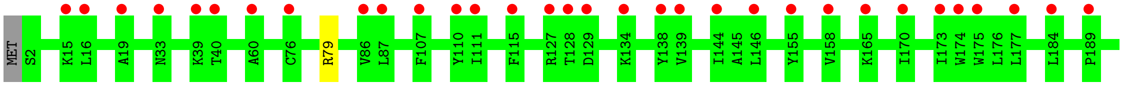
- Molecule 47: 40S ribosomal protein S0

Chain C:

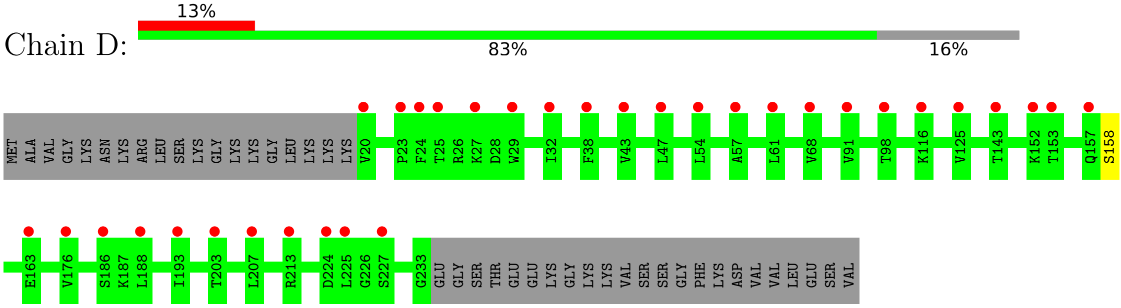


- Molecule 47: 40S ribosomal protein S0

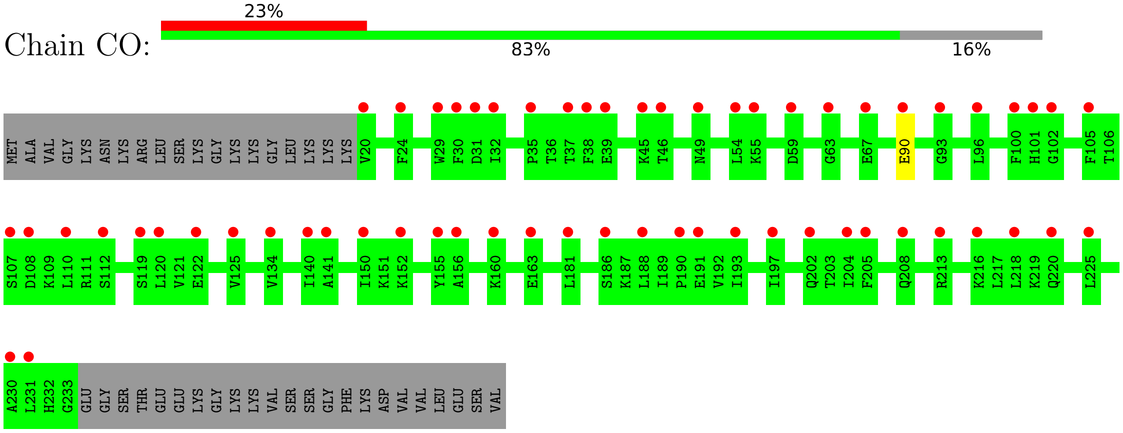
Chain CN:



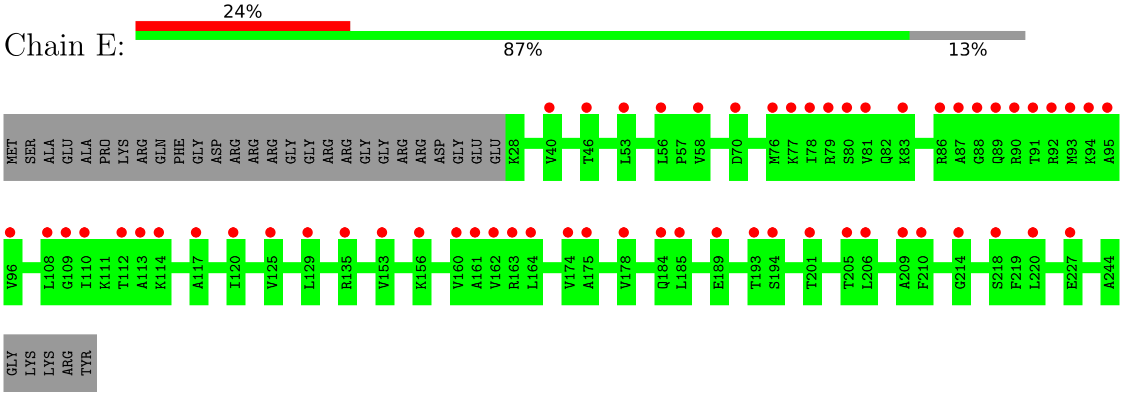
- Molecule 48: 40S ribosomal protein S1



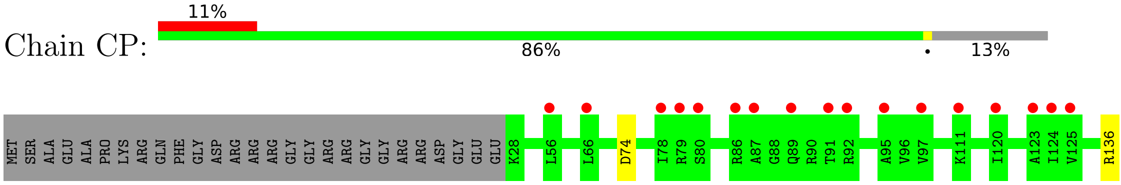
- Molecule 48: 40S ribosomal protein S1

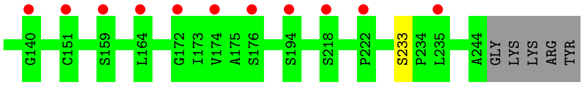


- Molecule 49: Ribosomal protein S5



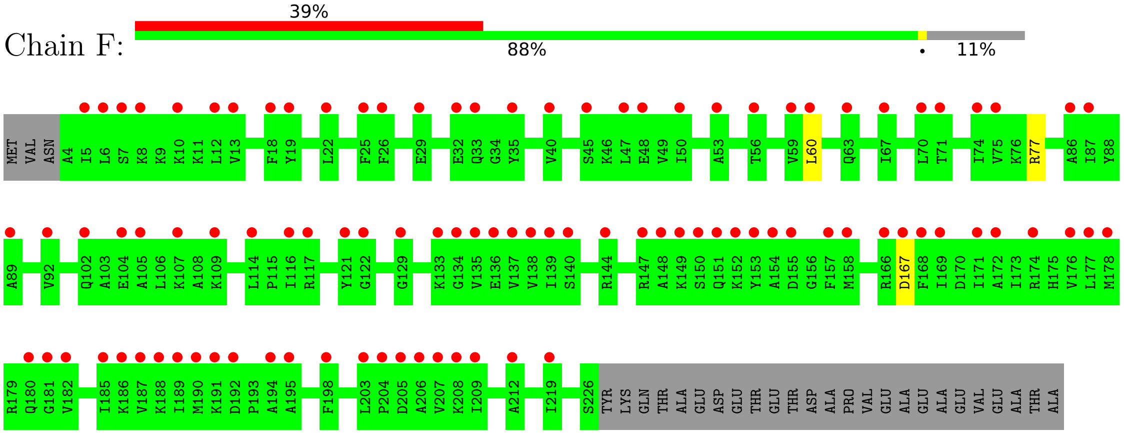
- Molecule 49: Ribosomal protein S5





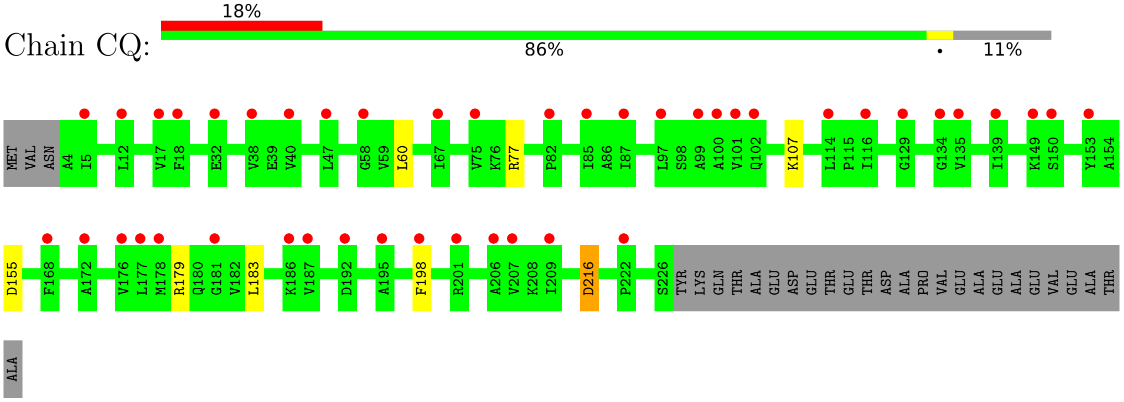
- Molecule 50: Ribosomal protein S3

Chain F:



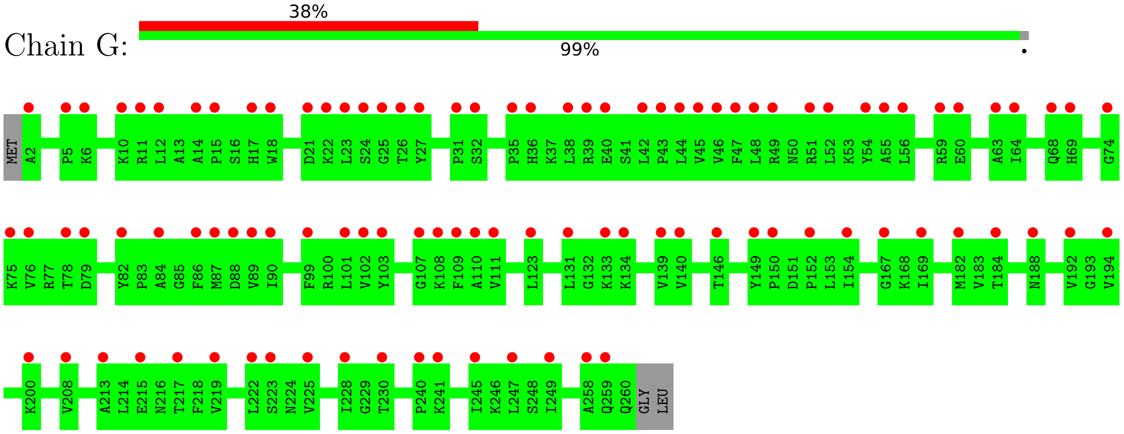
- Molecule 50: Ribosomal protein S3

Chain CQ:



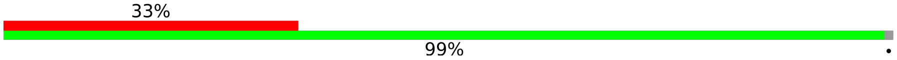
- Molecule 51: 40S ribosomal protein S4

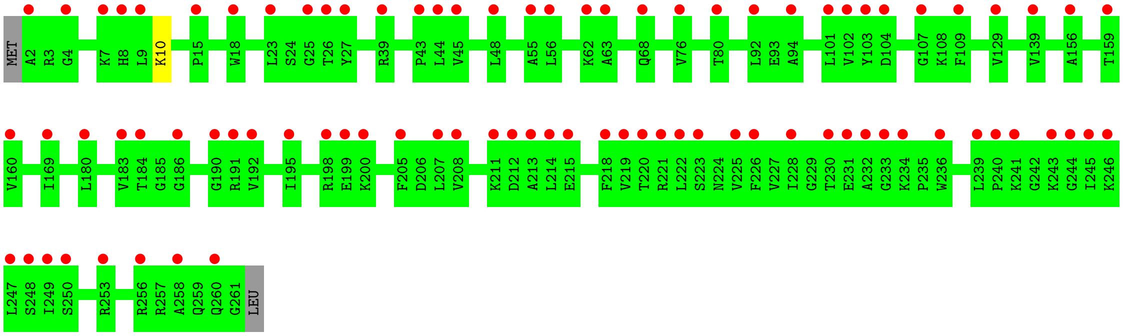
Chain G:



- Molecule 51: 40S ribosomal protein S4

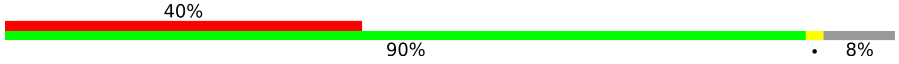
Chain CR:

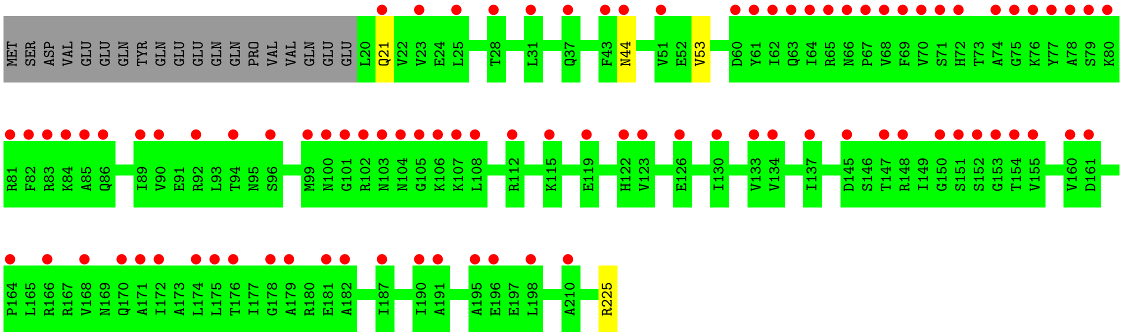




- Molecule 52: Ribosomal protein S7

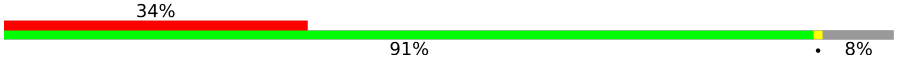
Chain H:

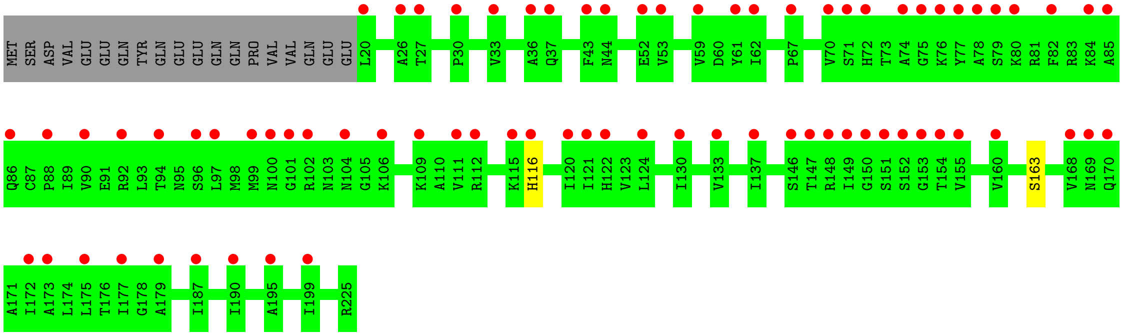




- Molecule 52: Ribosomal protein S7

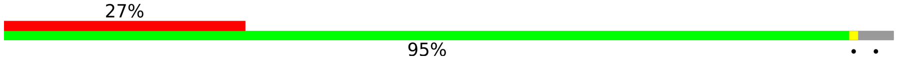
Chain CS:

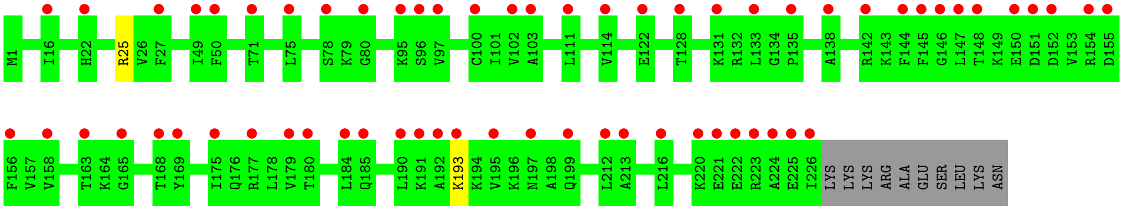




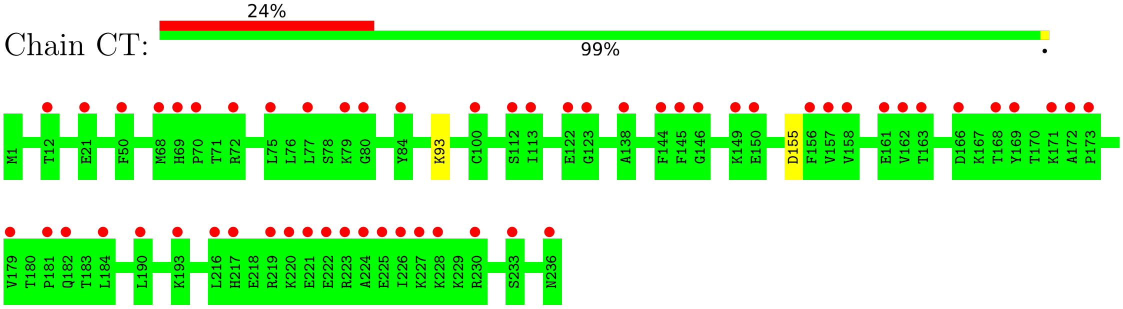
- Molecule 53: 40S ribosomal protein S6

Chain I:

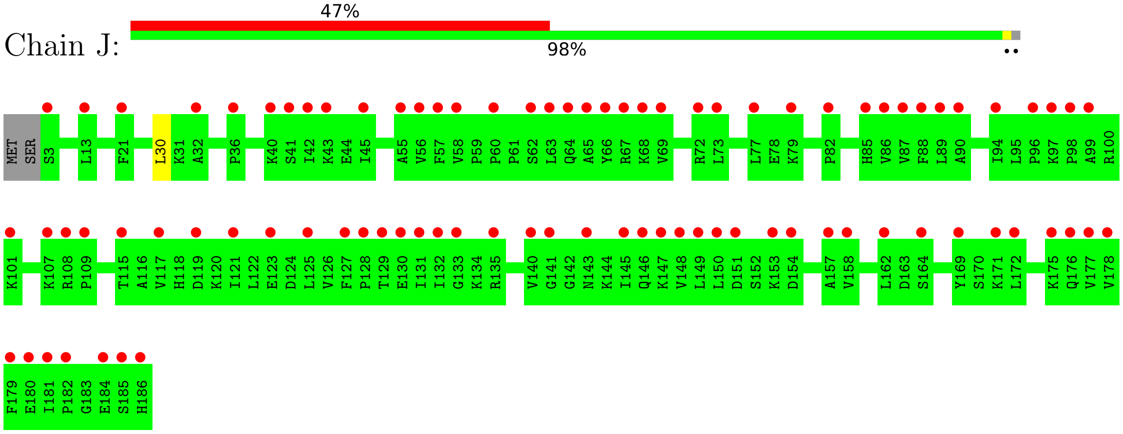




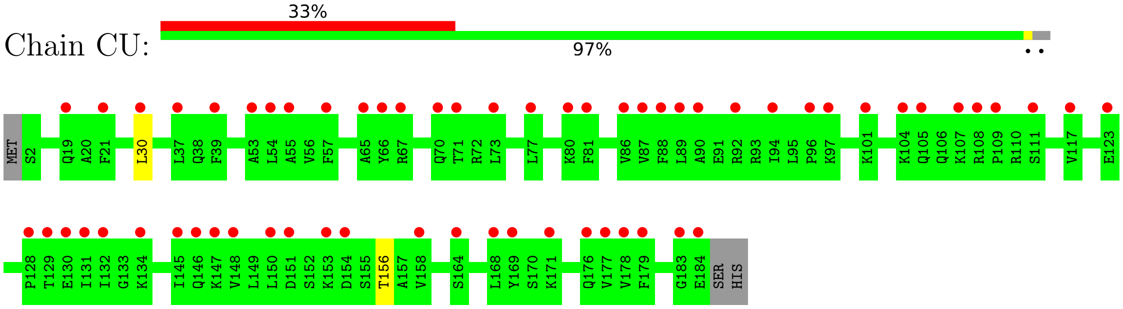
- Molecule 53: 40S ribosomal protein S6



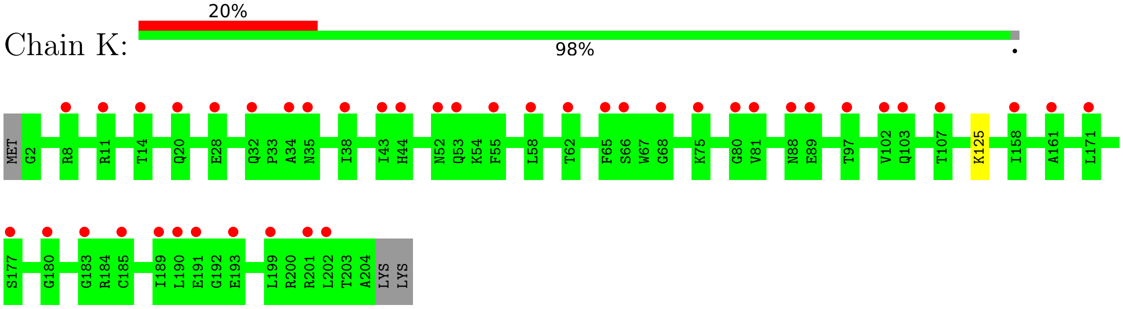
- Molecule 54: 40S ribosomal protein S7



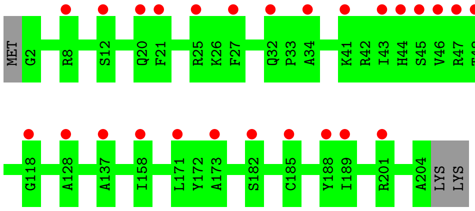
- Molecule 54: 40S ribosomal protein S7



- Molecule 55: 40S ribosomal protein S8

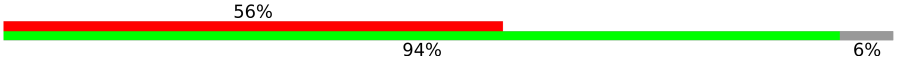


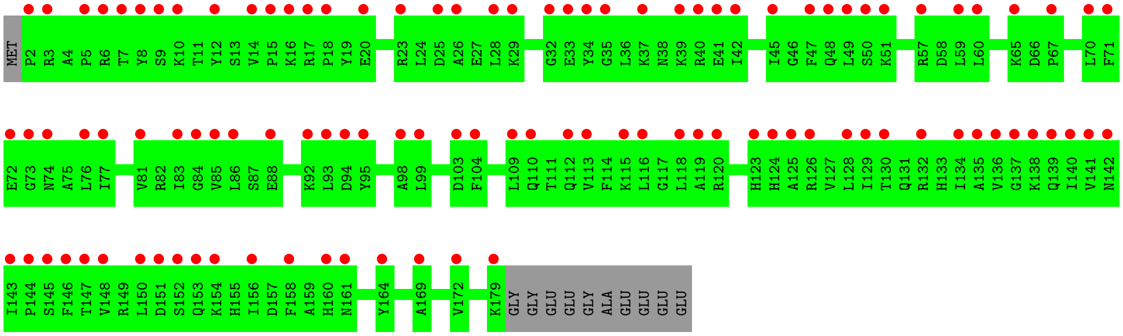
- Molecule 55: 40S ribosomal protein S8



- Molecule 56: Ribosomal protein S4

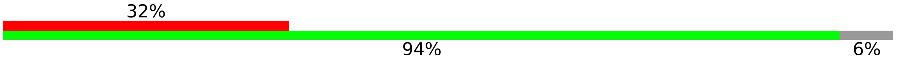
Chain L:

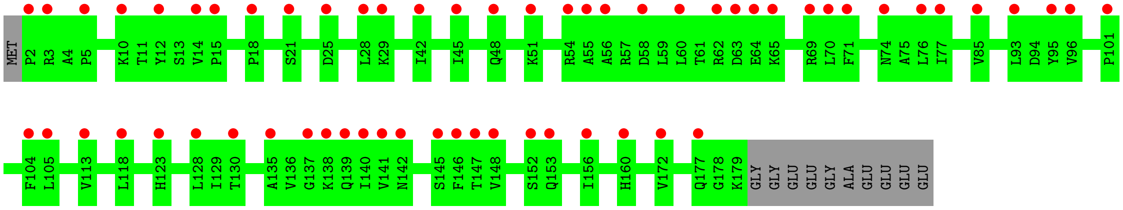




- Molecule 56: Ribosomal protein S4

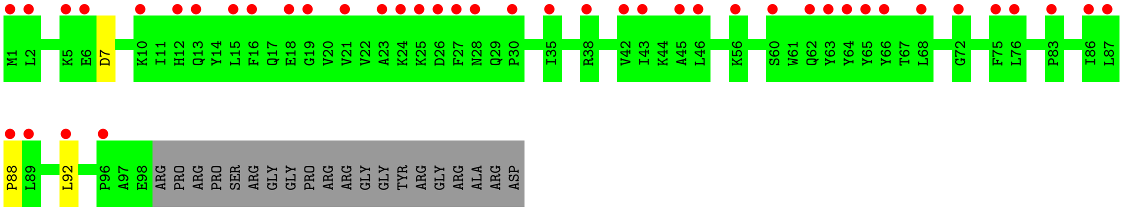
Chain CW:





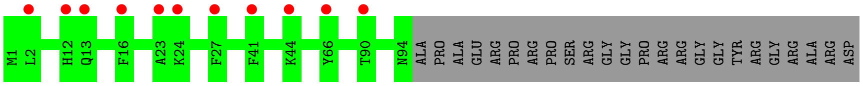
- Molecule 57: 40S ribosomal protein S10-A

Chain M:



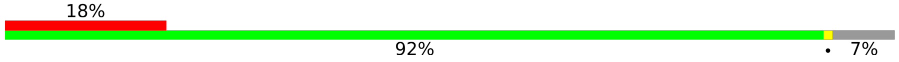
- Molecule 57: 40S ribosomal protein S10-A

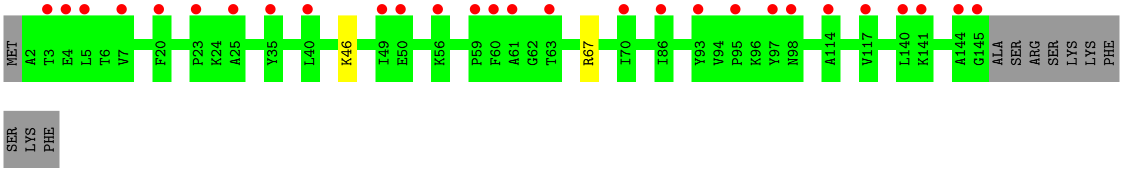
Chain CX:



- Molecule 58: 40S ribosomal protein S11A

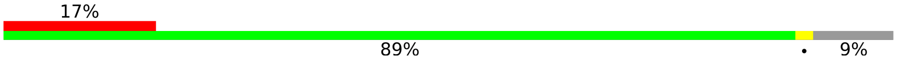
Chain N:

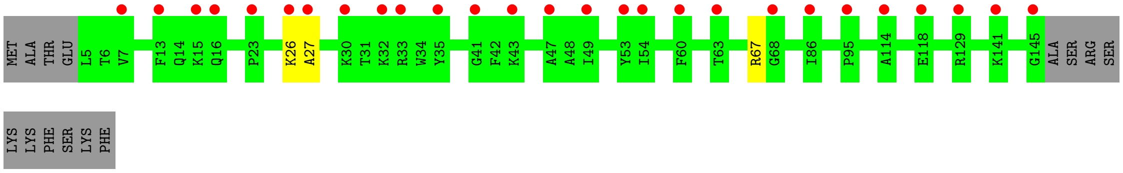




- Molecule 58: 40S ribosomal protein S11A

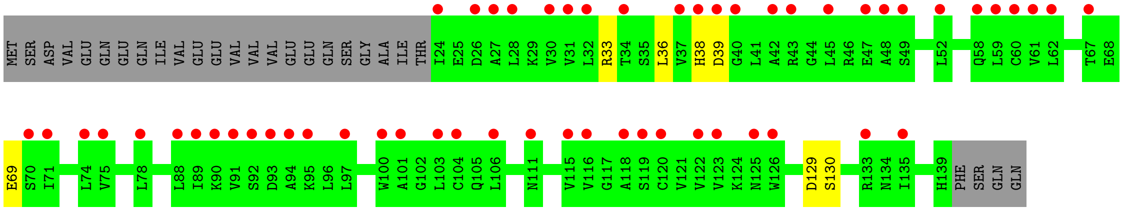
Chain CY:





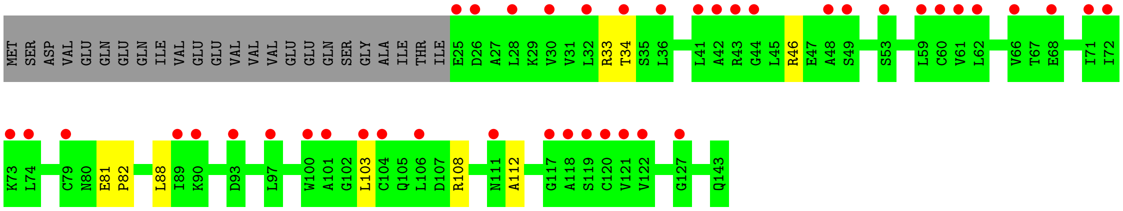
- Molecule 59: 40S ribosomal protein S12

Chain O:



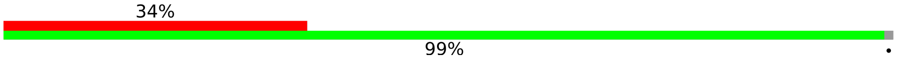
- Molecule 59: 40S ribosomal protein S12

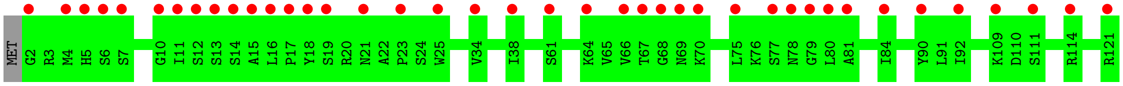
Chain CZ:

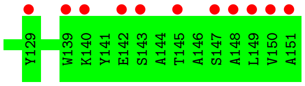


- Molecule 60: 40S ribosomal protein S13

Chain P:

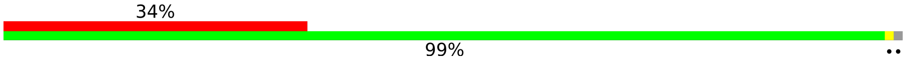


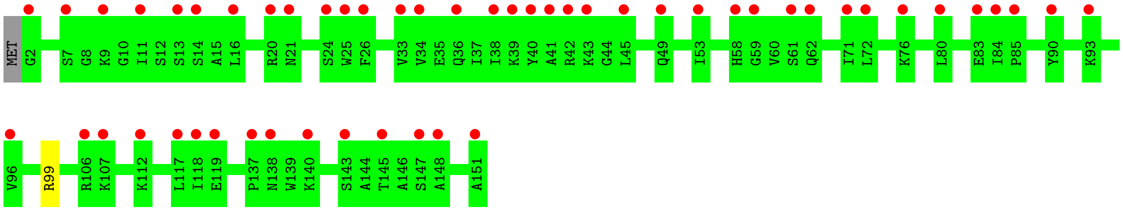




- Molecule 60: 40S ribosomal protein S13

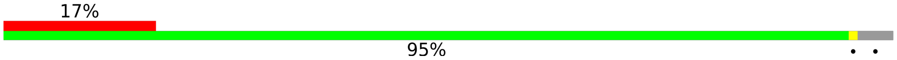
Chain DA:

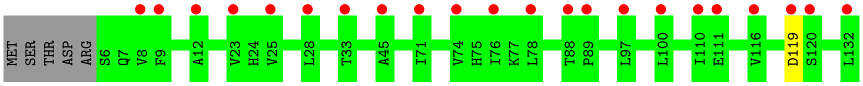




- Molecule 61: 40S ribosomal protein S14-A

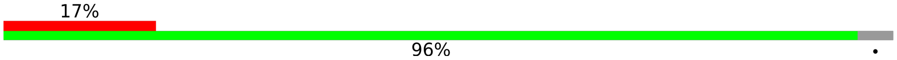
Chain Q:

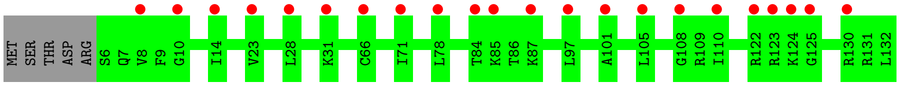




- Molecule 61: 40S ribosomal protein S14-A

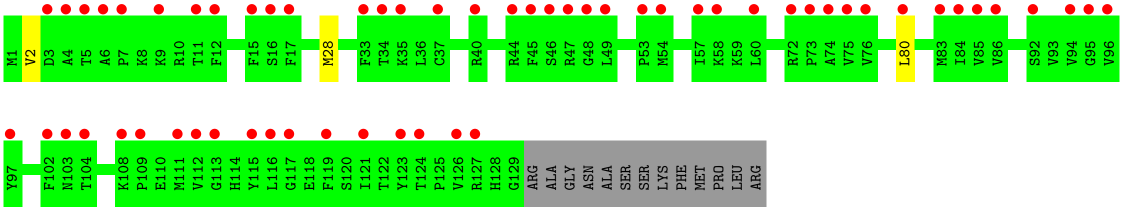
Chain DB:





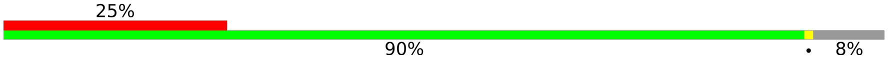
- Molecule 62: 40S ribosomal protein S15

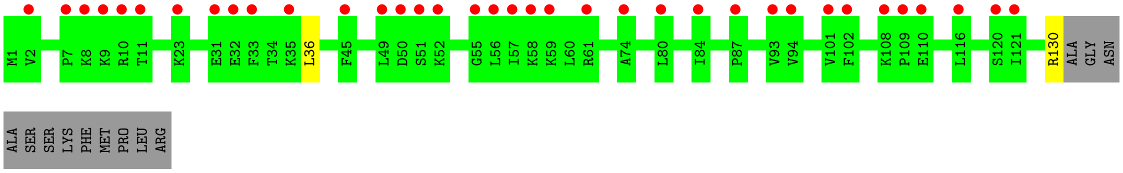
Chain R:



- Molecule 62: 40S ribosomal protein S15

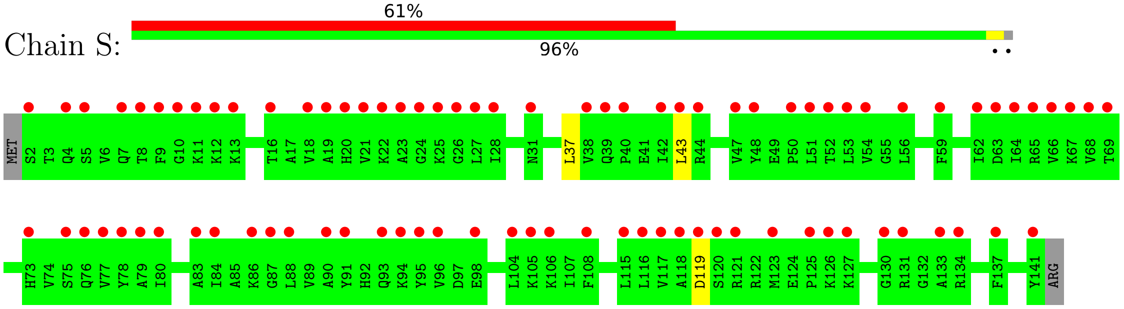
Chain DC:





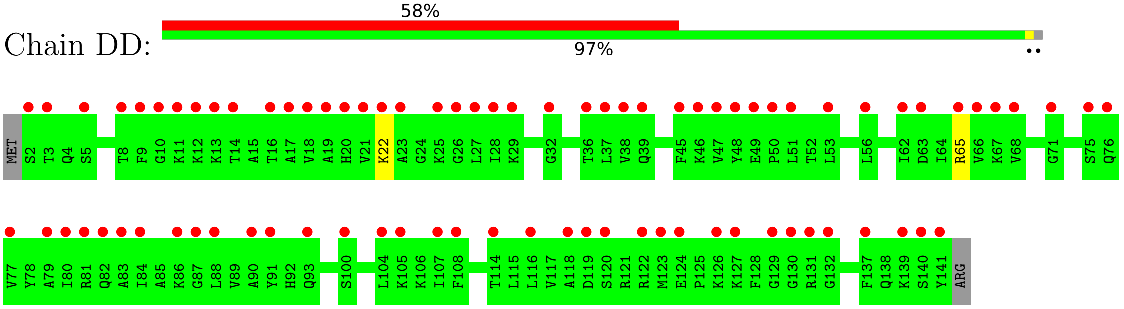
- Molecule 63: 40S ribosomal protein S16

Chain S:



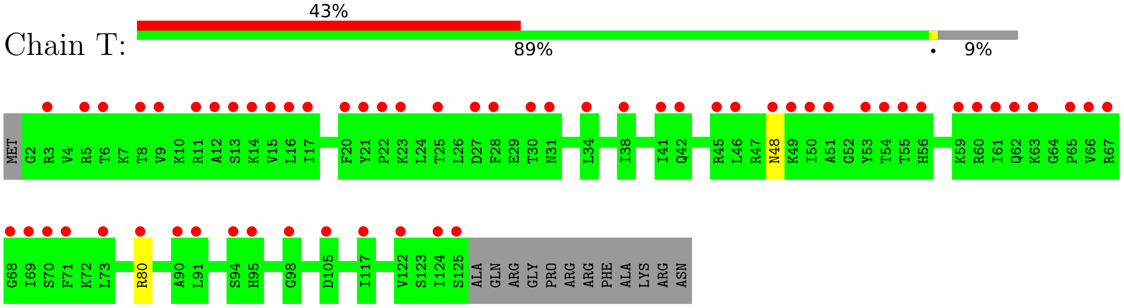
- Molecule 63: 40S ribosomal protein S16

Chain DD:



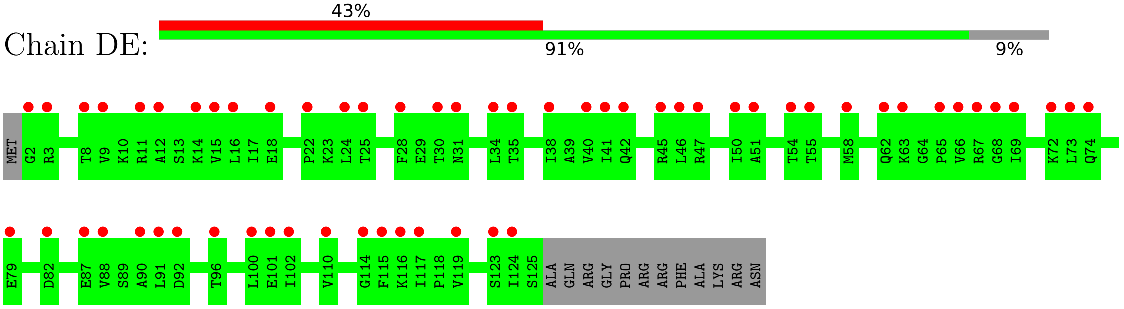
- Molecule 64: 40S ribosomal protein S17-B

Chain T:



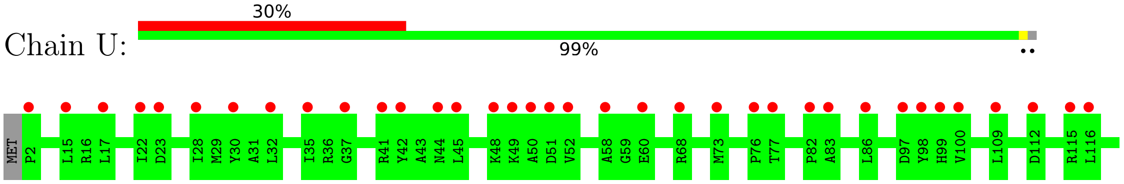
- Molecule 64: 40S ribosomal protein S17-B

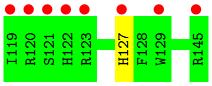
Chain DE:



- Molecule 65: 40S ribosomal protein S18-B

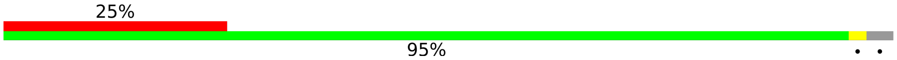
Chain U:

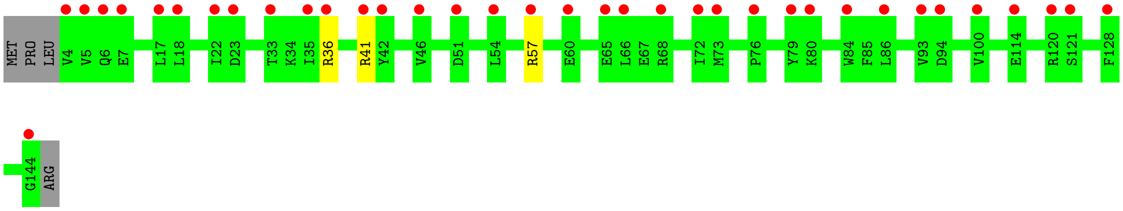




- Molecule 65: 40S ribosomal protein S18-B

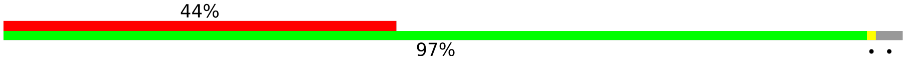
Chain DF:

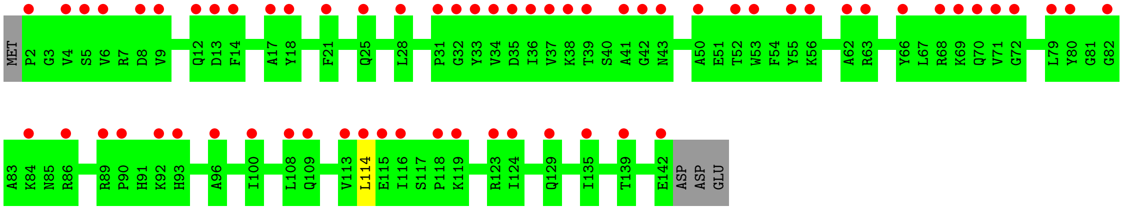




- Molecule 66: 40S ribosomal protein S19-A

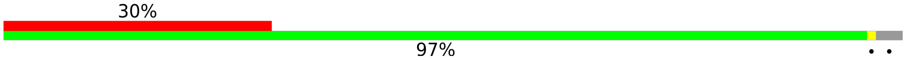
Chain V:

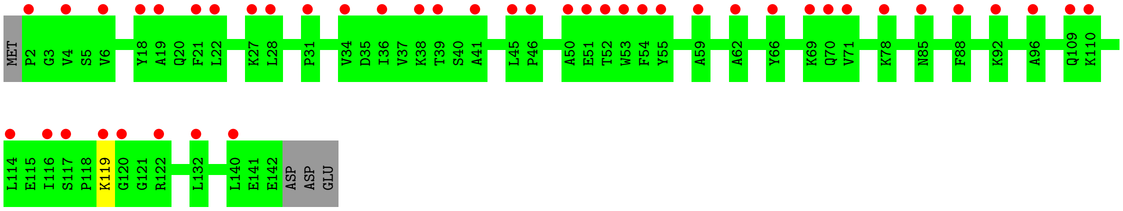




- Molecule 66: 40S ribosomal protein S19-A

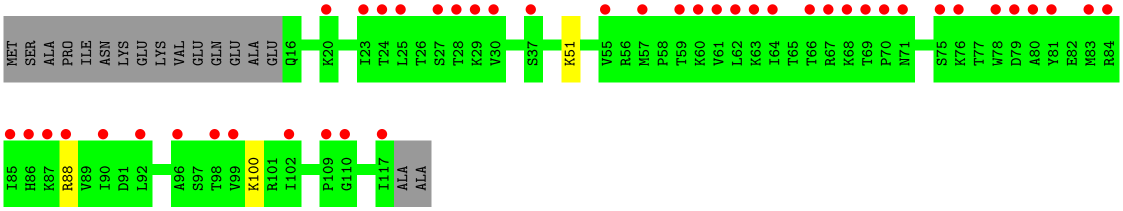
Chain DG:





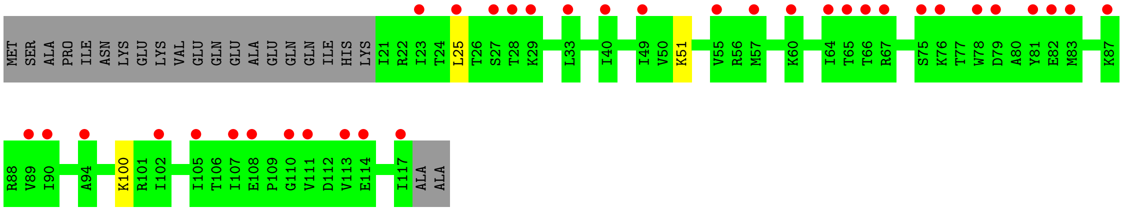
- Molecule 67: Ribosomal protein S10

Chain W:



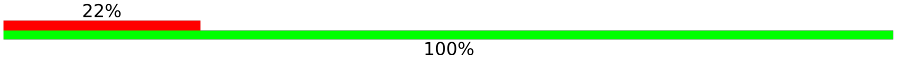
- Molecule 67: Ribosomal protein S10

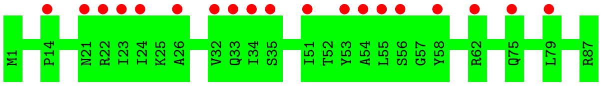
Chain DH:



- Molecule 68: 40S ribosomal protein S21

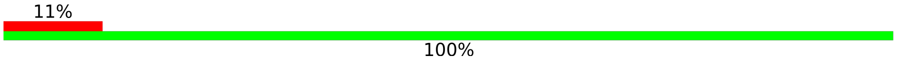
Chain X:

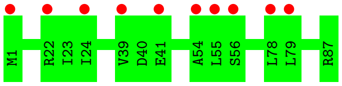




- Molecule 68: 40S ribosomal protein S21

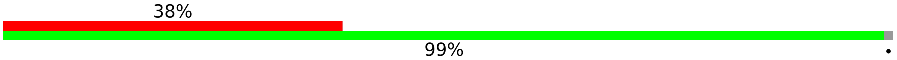
Chain DI:

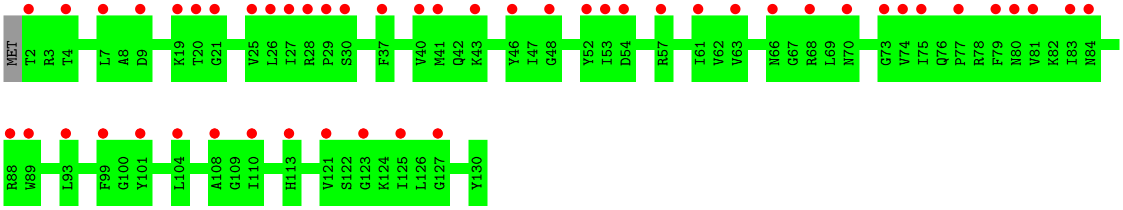




- Molecule 69: 40S ribosomal protein S22-A

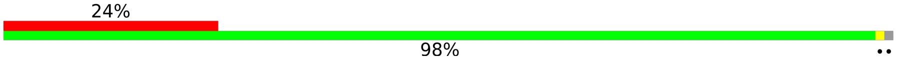
Chain Y:

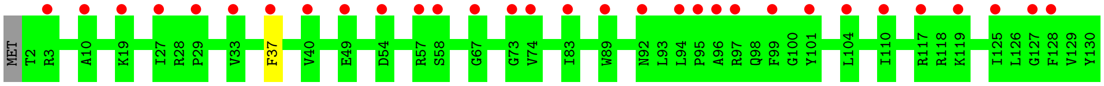




- Molecule 69: 40S ribosomal protein S22-A

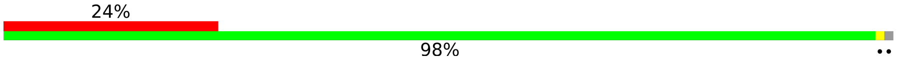
Chain DJ:

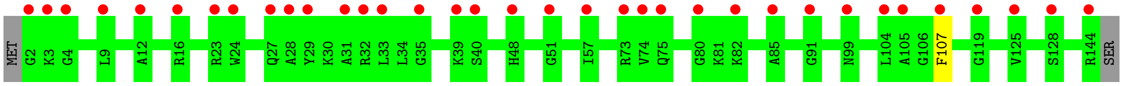




- Molecule 70: Ribosomal protein S23 (S12)

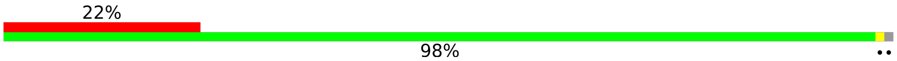
Chain Z:

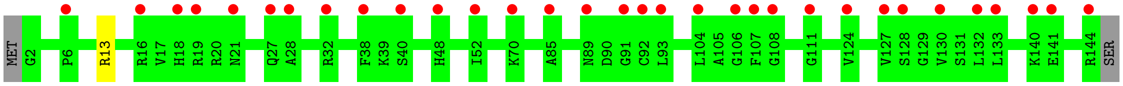




- Molecule 70: Ribosomal protein S23 (S12)

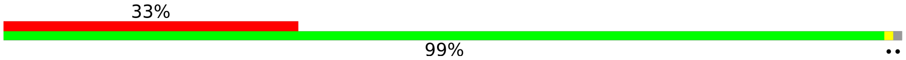
Chain DK:

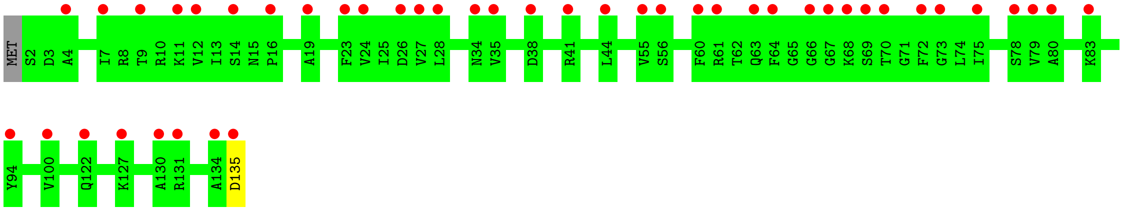




- Molecule 71: 40S ribosomal protein S24

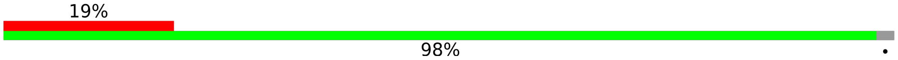
Chain a:

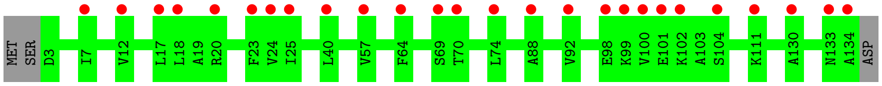




- Molecule 71: 40S ribosomal protein S24

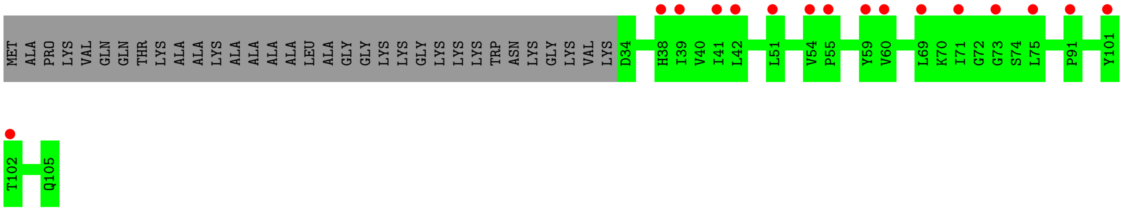
Chain DL:





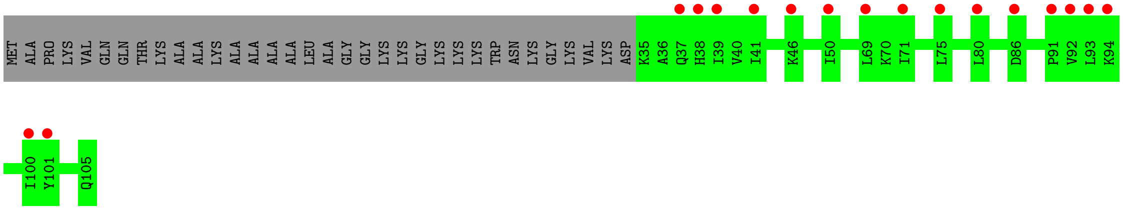
- Molecule 72: 40S ribosomal protein S25

Chain b:



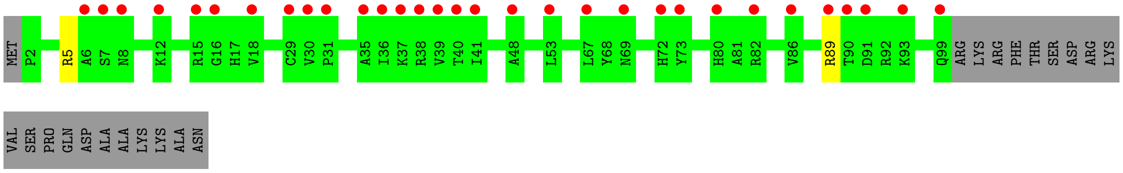
- Molecule 72: 40S ribosomal protein S25

Chain DM:



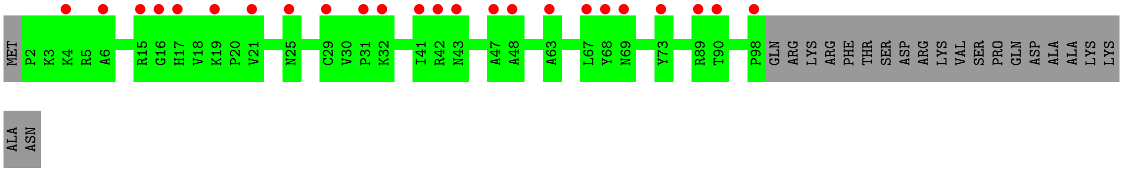
- Molecule 73: 40S ribosomal protein S26

Chain c:



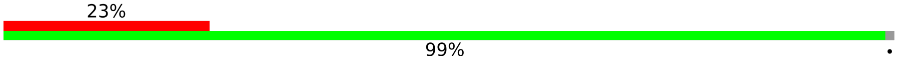
- Molecule 73: 40S ribosomal protein S26

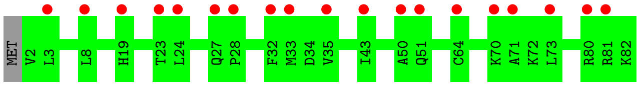
Chain DN:



- Molecule 74: 40S ribosomal protein S27

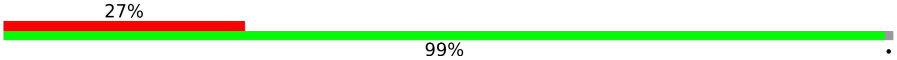
Chain d:

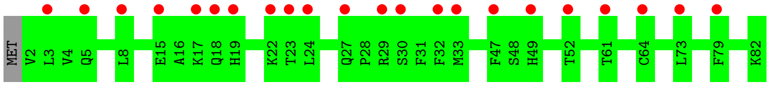




- Molecule 74: 40S ribosomal protein S27

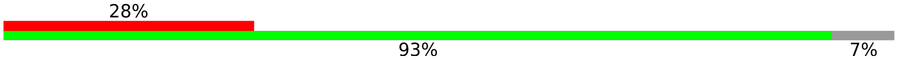
Chain DO:

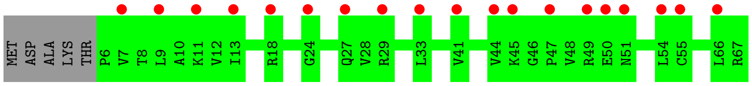




- Molecule 75: 40S ribosomal protein S28-B

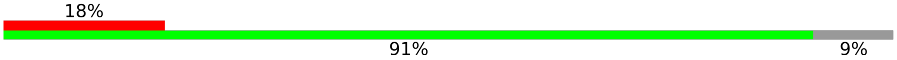
Chain e:

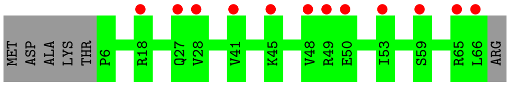




- Molecule 75: 40S ribosomal protein S28-B

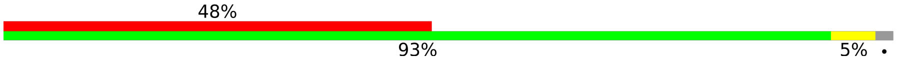
Chain DP:

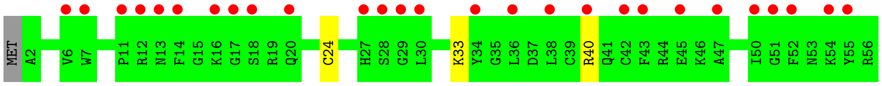




- Molecule 76: 40S ribosomal protein S29A

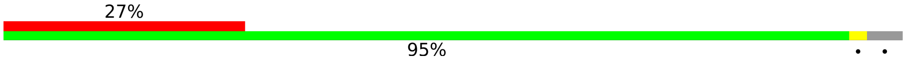
Chain f:

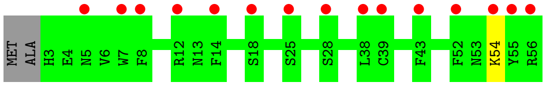




- Molecule 76: 40S ribosomal protein S29A

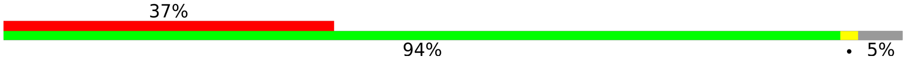
Chain DQ:

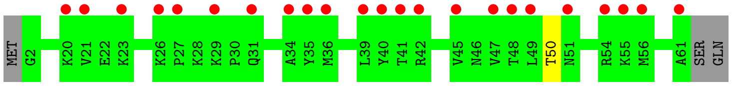




- Molecule 77: 40S ribosomal protein S30

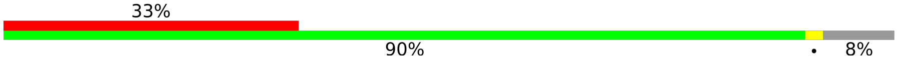
Chain g:

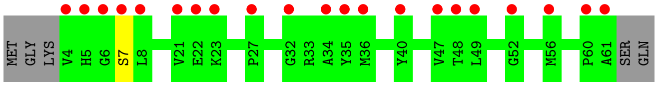




- Molecule 77: 40S ribosomal protein S30

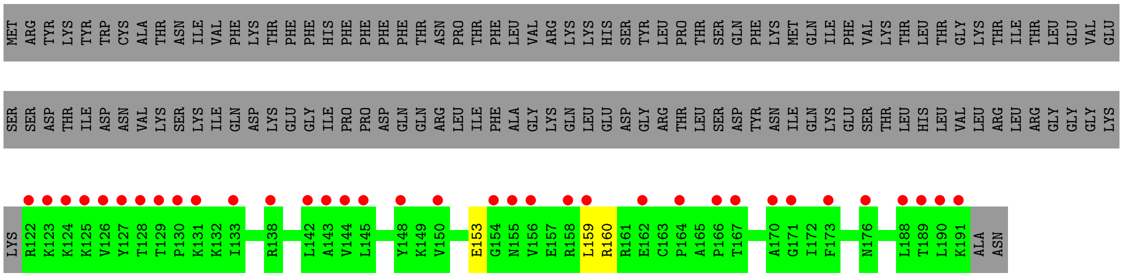
Chain DR:





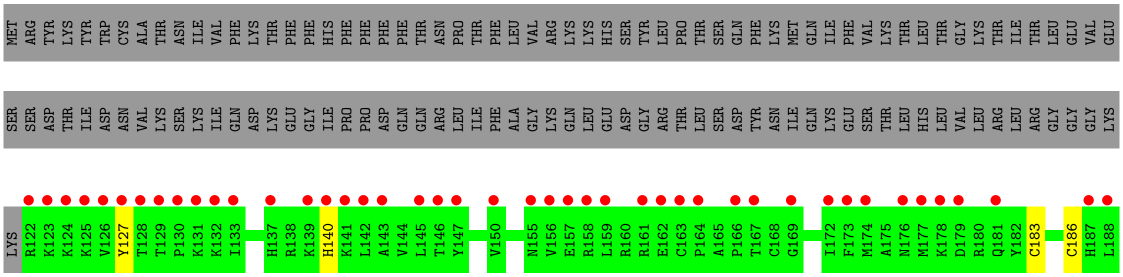
- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

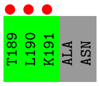
Chain h:



- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

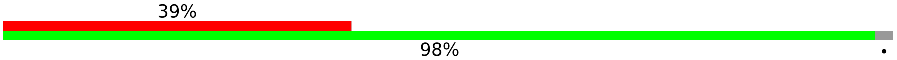
Chain DS:

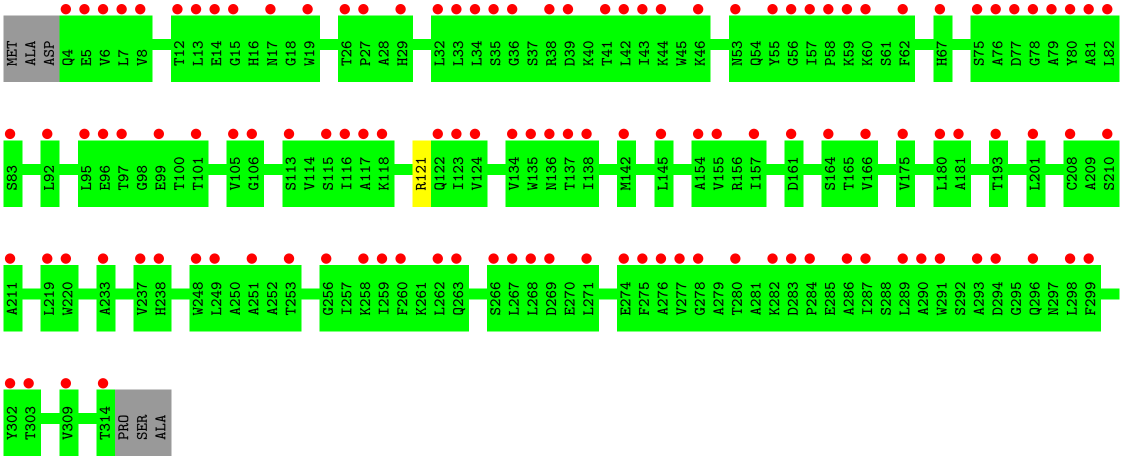




- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

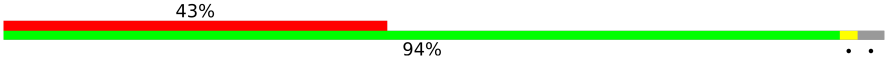
Chain AR:

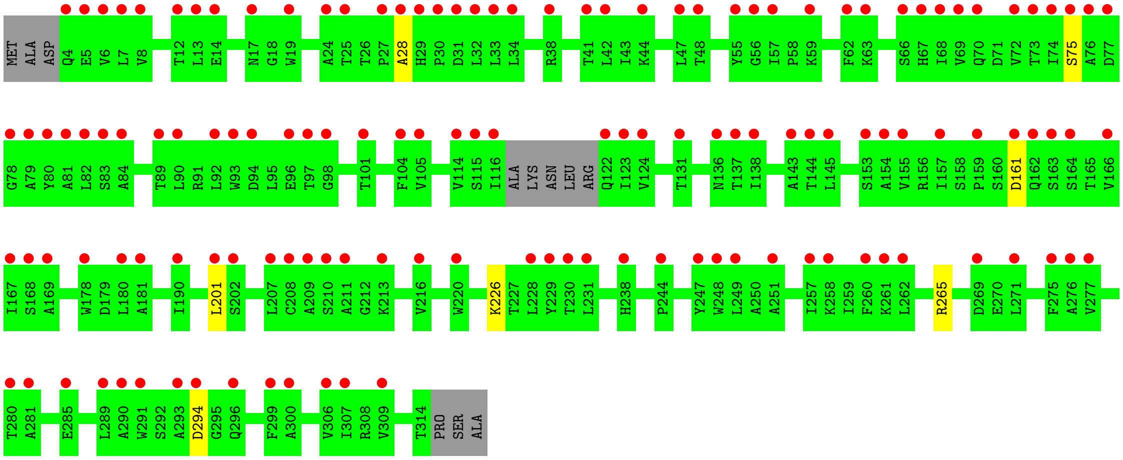




- Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

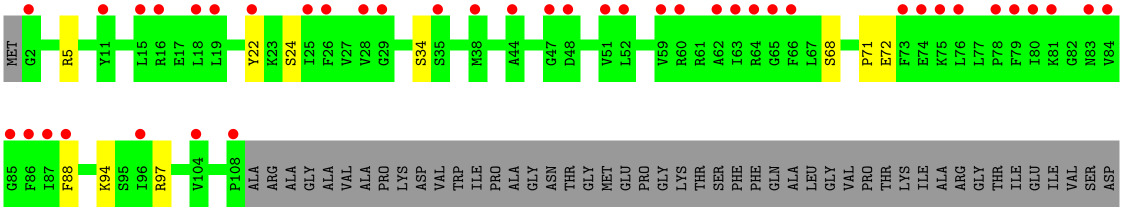
Chain DT:

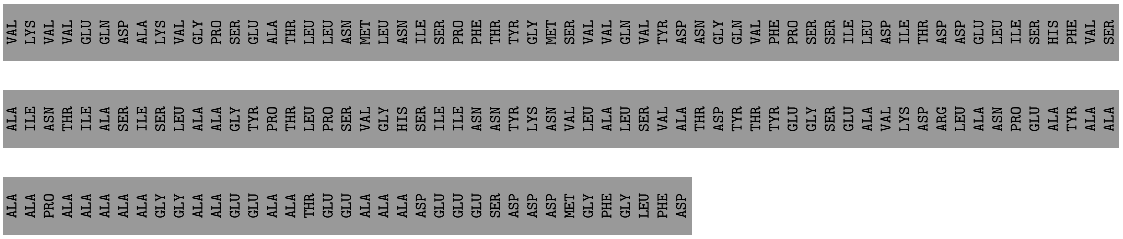




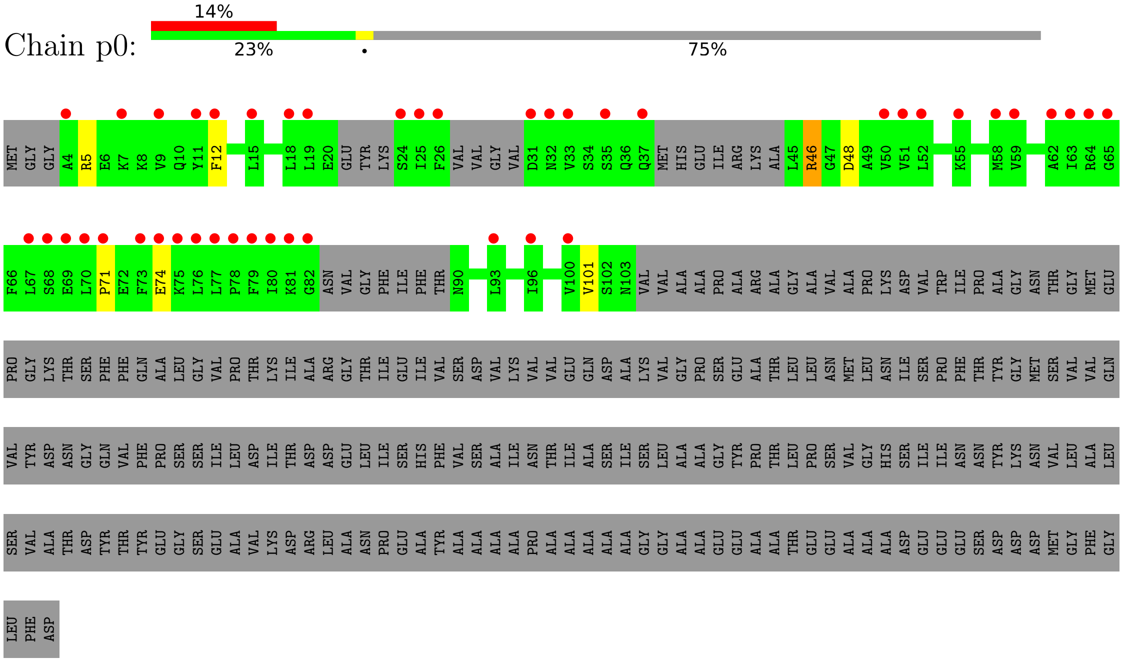
- Molecule 80: 60S acidic ribosomal protein P0

Chain P0:

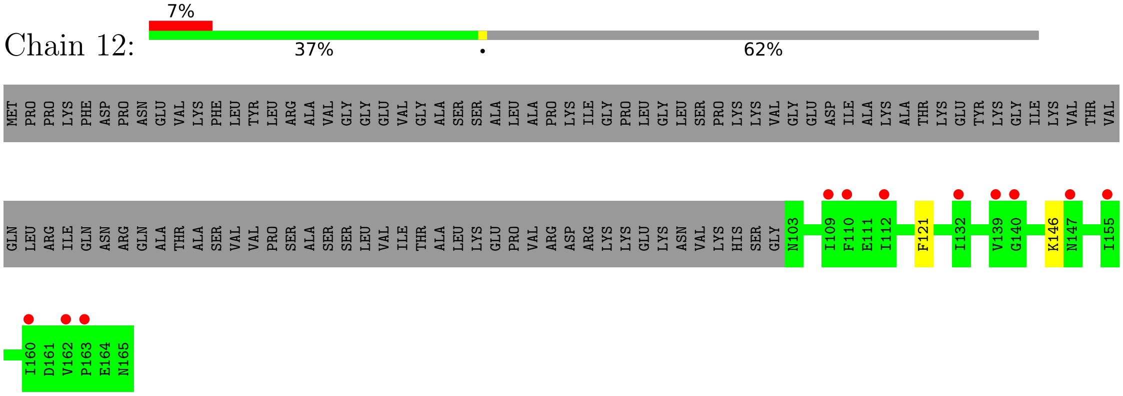




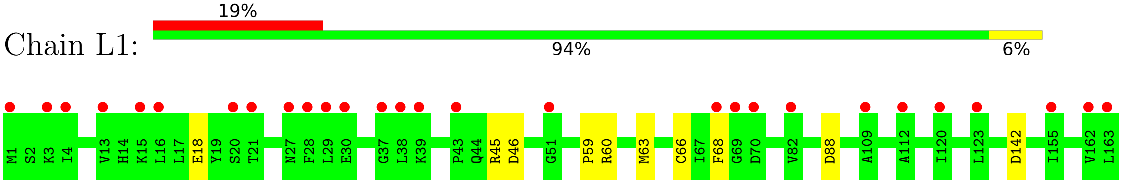
- Molecule 80: 60S acidic ribosomal protein P0

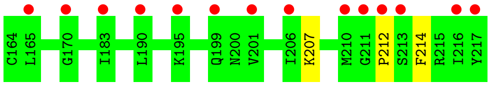


- Molecule 81: 60S ribosomal protein L12-A



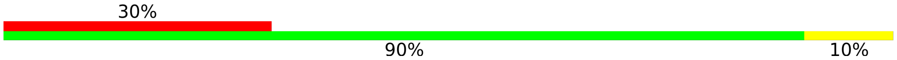
- Molecule 82: Ribosomal protein

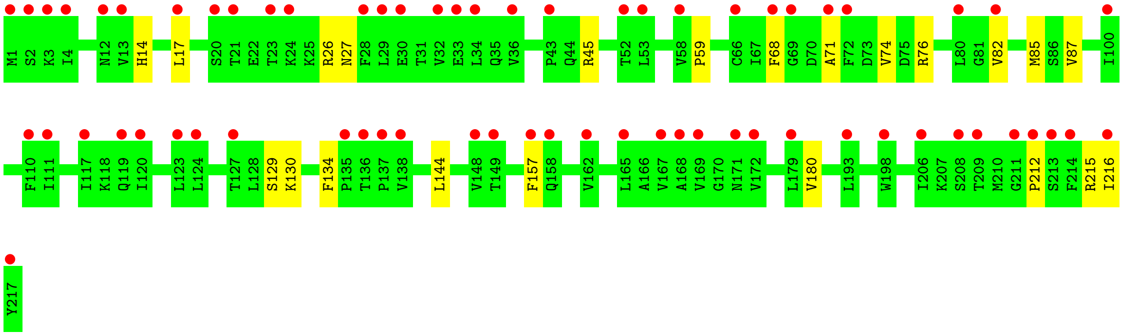




- Molecule 82: Ribosomal protein

Chain l1:





4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	298.81Å 292.84Å 450.18Å 90.00° 100.11° 90.00°	Depositor
Resolution (Å)	163.72 – 3.05 163.72 – 3.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (163.72-3.05) 89.6 (163.72-3.05)	Depositor EDS
R_{merge}	0.84	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.19rc4_4035: ???)	Depositor
R, R_{free}	0.283 , 0.307 0.283 , 0.307	Depositor DCC
R_{free} test set	2000 reflections (0.14%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	408804	wwPDB-VP
Average B, all atoms (Å^2)	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.31% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 3K5, ZN, HYG, MG

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	1	0.30	0/76756	0.90	107/119655 (0.1%)
1	AS	0.29	0/77209	0.89	86/120366 (0.1%)
2	3	0.25	0/2884	0.78	0/4492
2	AT	0.25	0/2884	0.78	0/4492
3	4	0.25	0/3724	0.80	1/5798 (0.0%)
3	AU	0.24	0/3724	0.81	2/5798 (0.0%)
4	AW	0.27	0/1922	0.56	0/2581
4	j	0.27	0/1922	0.59	0/2581
5	AX	0.27	0/3145	0.57	0/4231
5	k	0.27	0/3145	0.57	0/4231
6	AY	0.26	0/2799	0.53	0/3777
6	l	0.28	0/2799	0.55	0/3777
7	AZ	0.26	0/2447	0.51	0/3294
7	m	0.27	0/2479	0.53	0/3337
8	BA	0.27	0/1231	0.55	0/1662
8	n	0.28	0/1263	0.54	0/1703
9	BB	0.27	0/1918	0.50	0/2575
9	o	0.28	0/1909	0.52	0/2563
10	BC	0.30	0/1807	0.50	0/2434
10	p	0.28	0/1835	0.50	0/2472
11	BD	0.26	0/1537	0.54	0/2067
11	q	0.28	0/1528	0.58	0/2055
12	BE	0.27	0/1724	0.57	0/2314
12	r	0.29	0/1724	0.57	0/2314
13	BF	0.26	0/1390	0.58	0/1861
13	s	0.27	0/1390	0.57	0/1861
14	BG	0.27	0/1637	0.55	0/2195
14	t	0.27	0/1637	0.56	0/2195
15	BH	0.26	0/1044	0.54	0/1407
15	u	0.27	0/1044	0.56	0/1407
16	BI	0.26	0/1753	0.60	0/2347
16	v	0.27	0/1753	0.60	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	BJ	0.28	0/1620	0.53	0/2167
17	w	0.27	0/1620	0.52	0/2167
18	BK	0.26	0/1429	0.57	0/1920
18	x	0.26	0/1410	0.57	0/1895
19	BL	0.27	0/1482	0.57	0/1985
19	y	0.27	0/1482	0.58	0/1985
20	BM	0.26	0/1475	0.59	0/1961
20	z	0.27	0/1475	0.60	0/1961
21	0	0.26	0/1457	0.57	0/1962
21	BN	0.27	0/1457	0.54	0/1962
22	2	0.28	0/1285	0.54	0/1723
22	BO	0.26	0/1285	0.54	0/1723
23	5	0.32	0/841	0.49	0/1133
23	BP	0.28	0/841	0.51	0/1133
24	6	0.27	0/993	0.57	0/1339
24	BQ	0.27	0/993	0.57	0/1339
25	7	0.27	0/958	0.53	0/1267
25	BR	0.26	0/814	0.55	0/1079
26	8	0.26	0/981	0.53	0/1326
26	BS	0.24	0/976	0.51	0/1319
27	9	0.25	0/999	0.52	0/1334
27	BT	0.25	0/999	0.53	0/1334
28	AA	0.27	0/1112	0.49	0/1488
28	BU	0.26	0/1112	0.49	0/1488
29	AB	0.26	0/1199	0.53	0/1607
29	BV	0.27	0/1199	0.54	0/1607
30	AC	0.26	0/503	0.58	0/668
30	BW	0.24	0/498	0.52	0/661
31	AD	0.27	0/738	0.48	0/994
31	BX	0.27	0/738	0.49	0/994
32	AE	0.25	0/907	0.56	1/1219 (0.1%)
32	BY	0.25	0/907	0.56	0/1219
33	AF	0.27	0/1021	0.54	0/1368
33	BZ	0.26	0/1025	0.55	0/1372
34	AG	0.27	0/866	0.54	0/1165
34	CA	0.29	0/866	0.53	0/1165
35	AH	0.26	0/896	0.58	0/1195
35	CB	0.26	0/896	0.58	0/1195
36	AI	0.26	0/1003	0.56	0/1336
36	CC	0.25	0/990	0.55	0/1319
37	AJ	0.35	0/763	0.60	0/1012
37	CD	0.26	0/763	0.56	0/1012
38	AK	0.27	0/690	0.61	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	CE	0.28	0/690	0.61	0/916
39	AL	0.26	0/623	0.50	0/831
39	CF	0.28	0/623	0.56	0/831
40	AM	0.26	0/447	0.58	0/594
40	CG	0.27	0/447	0.62	0/594
41	AN	0.31	0/425	0.61	0/563
41	CH	0.32	0/417	0.62	0/553
42	AO	0.31	0/237	0.72	0/304
42	CI	0.27	0/228	0.69	0/293
43	AP	0.27	0/840	0.55	0/1110
43	CJ	0.28	0/840	0.54	0/1110
44	AQ	0.28	0/705	0.60	0/940
44	CK	0.26	0/705	0.59	0/940
45	CL	0.36	0/942	0.64	0/1258
45	i	0.35	0/933	0.68	0/1246
46	B	0.31	0/41511	0.95	83/64681 (0.1%)
46	CM	0.31	0/42081	0.94	72/65573 (0.1%)
47	C	0.25	0/1666	0.49	0/2273
47	CN	0.26	0/1666	0.51	0/2273
48	CO	0.26	0/1750	0.58	0/2354
48	D	0.25	0/1750	0.53	0/2354
49	CP	0.27	0/1657	0.53	0/2248
49	E	0.25	0/1657	0.50	0/2248
50	CQ	0.28	0/1731	0.65	3/2324 (0.1%)
50	F	0.27	0/1731	0.60	1/2324 (0.0%)
51	CR	0.26	0/2096	0.55	0/2822
51	G	0.26	0/2092	0.55	0/2817
52	CS	0.27	0/1631	0.54	0/2199
52	H	0.31	0/1631	0.58	0/2199
53	CT	0.27	0/1929	0.57	0/2571
53	I	0.26	0/1845	0.55	0/2464
54	CU	0.32	0/1499	0.57	0/2016
54	J	0.26	0/1510	0.55	0/2031
55	CV	0.27	0/1606	0.61	0/2150
55	K	0.28	0/1606	0.59	0/2150
56	CW	0.26	0/1478	0.56	0/1978
56	L	0.26	0/1478	0.56	0/1978
57	CX	0.29	0/809	0.58	0/1092
57	M	0.28	0/836	0.62	0/1130
58	CY	0.28	0/1154	0.57	0/1553
58	N	0.27	0/1175	0.57	0/1582
59	CZ	0.31	0/921	0.84	1/1240 (0.1%)
59	O	0.36	0/892	0.81	0/1203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	DA	0.25	0/1210	0.53	0/1631
60	P	0.25	0/1210	0.50	0/1631
61	DB	0.27	0/953	0.62	0/1279
61	Q	0.32	0/953	0.62	0/1279
62	DC	0.29	0/1049	0.60	0/1409
62	R	0.31	0/1038	0.62	1/1395 (0.1%)
63	DD	0.25	0/1109	0.54	0/1486
63	S	0.33	0/1109	0.68	2/1486 (0.1%)
64	DE	0.27	0/1009	0.62	0/1354
64	T	0.27	0/1009	0.63	0/1354
65	DF	0.28	0/1178	0.59	0/1579
65	U	0.27	0/1205	0.57	0/1615
66	DG	0.26	0/1120	0.55	0/1508
66	V	0.27	0/1120	0.59	1/1508 (0.1%)
67	DH	0.27	0/772	0.59	1/1045 (0.1%)
67	W	0.26	0/818	0.55	0/1106
68	DI	0.30	0/683	0.59	0/918
68	X	0.26	0/683	0.57	0/918
69	DJ	0.27	0/1049	0.56	0/1412
69	Y	0.25	0/1049	0.54	0/1412
70	DK	0.27	0/1128	0.59	0/1505
70	Z	0.26	0/1128	0.61	0/1505
71	DL	0.27	0/1086	0.58	0/1447
71	a	0.26	0/1100	0.56	0/1466
72	DM	0.26	0/577	0.56	0/778
72	b	0.25	0/585	0.52	0/789
73	DN	0.25	0/782	0.60	0/1048
73	c	0.27	0/791	0.60	0/1060
74	DO	0.28	0/624	0.56	0/843
74	d	0.25	0/624	0.53	0/843
75	DP	0.27	0/478	0.69	0/640
75	e	0.27	0/489	0.67	0/654
76	DQ	0.30	0/461	0.58	0/613
76	f	0.28	0/466	0.58	0/620
77	DR	0.34	0/469	0.77	0/626
77	g	0.30	0/482	0.66	1/642 (0.2%)
78	DS	0.39	0/585	0.84	0/778
78	h	0.34	0/585	0.69	0/778
79	AR	0.25	0/2451	0.54	0/3337
79	DT	0.27	0/2409	0.60	1/3280 (0.0%)
80	P0	0.26	0/857	0.57	0/1148
80	p0	0.37	0/638	0.72	0/845
81	12	0.26	0/486	0.51	0/653

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
82	L1	0.30	0/1737	0.54	0/2335
82	l1	0.33	0/1737	0.59	1/2335 (0.0%)
All	All	0.29	0/437098	0.79	365/641006 (0.1%)

There are no bond length outliers.

The worst 5 of 365 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	B	653	G	O5'-P-OP2	-22.09	84.20	110.70
46	B	1742	A	O4'-C1'-N9	13.61	119.08	108.20
1	AS	1576	A	O4'-C1'-N9	12.61	118.28	108.20
1	1	1576	A	O4'-C1'-N9	12.17	117.94	108.20
46	B	653	G	O5'-P-OP1	11.61	124.63	110.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
4	AW	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
4	j	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
5	AX	384/389 (99%)	372 (97%)	12 (3%)	0	100	100
5	k	384/389 (99%)	372 (97%)	12 (3%)	0	100	100
6	AY	359/363 (99%)	349 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	l	359/363 (99%)	348 (97%)	11 (3%)	0	100	100
7	AZ	290/298 (97%)	278 (96%)	12 (4%)	0	100	100
7	m	294/298 (99%)	281 (96%)	12 (4%)	1 (0%)	37	64
8	BA	149/176 (85%)	147 (99%)	2 (1%)	0	100	100
8	n	153/176 (87%)	150 (98%)	3 (2%)	0	100	100
9	BB	232/241 (96%)	226 (97%)	5 (2%)	1 (0%)	30	58
9	o	231/241 (96%)	223 (96%)	7 (3%)	1 (0%)	30	58
10	BC	225/262 (86%)	210 (93%)	11 (5%)	4 (2%)	7	25
10	p	231/262 (88%)	223 (96%)	7 (3%)	1 (0%)	30	58
11	BD	188/191 (98%)	184 (98%)	4 (2%)	0	100	100
11	q	187/191 (98%)	182 (97%)	5 (3%)	0	100	100
12	BE	204/220 (93%)	199 (98%)	5 (2%)	0	100	100
12	r	204/220 (93%)	201 (98%)	3 (2%)	0	100	100
13	BF	169/174 (97%)	163 (96%)	6 (4%)	0	100	100
13	s	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
14	BG	198/202 (98%)	193 (98%)	5 (2%)	0	100	100
14	t	198/202 (98%)	196 (99%)	2 (1%)	0	100	100
15	BH	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
15	u	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
16	BI	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
16	v	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	BJ	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
17	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	BK	172/185 (93%)	167 (97%)	5 (3%)	0	100	100
18	x	169/185 (91%)	166 (98%)	3 (2%)	0	100	100
19	BL	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
19	y	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
20	BM	177/190 (93%)	173 (98%)	4 (2%)	0	100	100
20	z	177/190 (93%)	174 (98%)	3 (2%)	0	100	100
21	0	168/172 (98%)	166 (99%)	2 (1%)	0	100	100
21	BN	168/172 (98%)	166 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	2	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
22	BO	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
23	5	100/124 (81%)	89 (89%)	10 (10%)	1 (1%)	13	38
23	BP	100/124 (81%)	87 (87%)	11 (11%)	2 (2%)	6	22
24	6	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
24	BQ	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
25	7	114/155 (74%)	103 (90%)	11 (10%)	0	100	100
25	BR	94/155 (61%)	90 (96%)	4 (4%)	0	100	100
26	8	118/142 (83%)	116 (98%)	2 (2%)	0	100	100
26	BS	117/142 (82%)	115 (98%)	2 (2%)	0	100	100
27	9	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
27	BT	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
28	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
28	BU	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
29	BV	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
30	AC	60/63 (95%)	57 (95%)	1 (2%)	2 (3%)	3	14
30	BW	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
31	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
31	BX	94/106 (89%)	92 (98%)	2 (2%)	0	100	100
32	AE	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
32	BY	108/112 (96%)	103 (95%)	5 (5%)	0	100	100
33	AF	122/131 (93%)	122 (100%)	0	0	100	100
33	BZ	122/131 (93%)	122 (100%)	0	0	100	100
34	AG	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
34	CA	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
35	AH	110/122 (90%)	108 (98%)	2 (2%)	0	100	100
35	CB	110/122 (90%)	107 (97%)	3 (3%)	0	100	100
36	AI	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
36	CC	116/120 (97%)	114 (98%)	2 (2%)	0	100	100
37	AJ	95/99 (96%)	93 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	CD	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
38	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
38	CE	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
39	AL	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
39	CF	75/78 (96%)	68 (91%)	7 (9%)	0	100	100
40	AM	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5	21
40	CG	48/51 (94%)	48 (100%)	0	0	100	100
41	AN	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
41	CH	49/52 (94%)	46 (94%)	1 (2%)	2 (4%)	2	11
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	CI	22/25 (88%)	22 (100%)	0	0	100	100
43	AP	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
43	CJ	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
44	CK	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	CL	117/267 (44%)	91 (78%)	22 (19%)	4 (3%)	3	13
45	i	116/267 (43%)	91 (78%)	23 (20%)	2 (2%)	7	26
47	C	206/261 (79%)	201 (98%)	5 (2%)	0	100	100
47	CN	206/261 (79%)	198 (96%)	8 (4%)	0	100	100
48	CO	212/256 (83%)	204 (96%)	8 (4%)	0	100	100
48	D	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
49	CP	215/249 (86%)	209 (97%)	6 (3%)	0	100	100
49	E	215/249 (86%)	210 (98%)	5 (2%)	0	100	100
50	CQ	221/251 (88%)	211 (96%)	10 (4%)	0	100	100
50	F	221/251 (88%)	213 (96%)	8 (4%)	0	100	100
51	CR	258/262 (98%)	254 (98%)	4 (2%)	0	100	100
51	G	257/262 (98%)	253 (98%)	4 (2%)	0	100	100
52	CS	204/225 (91%)	196 (96%)	8 (4%)	0	100	100
52	H	204/225 (91%)	185 (91%)	17 (8%)	2 (1%)	13	38
53	CT	234/236 (99%)	231 (99%)	3 (1%)	0	100	100
53	I	224/236 (95%)	221 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	CU	181/186 (97%)	171 (94%)	9 (5%)	1 (1%)	22	49
54	J	182/186 (98%)	172 (94%)	10 (6%)	0	100	100
55	CV	201/206 (98%)	199 (99%)	2 (1%)	0	100	100
55	K	201/206 (98%)	200 (100%)	1 (0%)	0	100	100
56	CW	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
56	L	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
57	CX	92/118 (78%)	86 (94%)	6 (6%)	0	100	100
57	M	96/118 (81%)	81 (84%)	13 (14%)	2 (2%)	5	21
58	CY	139/155 (90%)	133 (96%)	4 (3%)	2 (1%)	9	30
58	N	142/155 (92%)	137 (96%)	5 (4%)	0	100	100
59	CZ	117/143 (82%)	90 (77%)	22 (19%)	5 (4%)	2	10
59	O	114/143 (80%)	89 (78%)	23 (20%)	2 (2%)	7	25
60	DA	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
60	P	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
61	DB	125/132 (95%)	120 (96%)	5 (4%)	0	100	100
61	Q	125/132 (95%)	119 (95%)	5 (4%)	1 (1%)	16	43
62	DC	128/142 (90%)	111 (87%)	17 (13%)	0	100	100
62	R	127/142 (89%)	115 (91%)	11 (9%)	1 (1%)	16	43
63	DD	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
63	S	138/142 (97%)	132 (96%)	6 (4%)	0	100	100
64	DE	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
64	T	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
65	DF	139/145 (96%)	133 (96%)	5 (4%)	1 (1%)	19	46
65	U	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
66	DG	139/145 (96%)	133 (96%)	5 (4%)	1 (1%)	19	46
66	V	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
67	DH	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
67	W	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
68	DI	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	X	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
69	DJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	DK	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
70	Z	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
71	DL	130/135 (96%)	130 (100%)	0	0	100	100
71	a	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
72	DM	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
72	b	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
73	DN	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
73	c	96/119 (81%)	93 (97%)	3 (3%)	0	100	100
74	DO	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
74	d	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
75	DP	59/67 (88%)	53 (90%)	6 (10%)	0	100	100
75	e	60/67 (90%)	57 (95%)	3 (5%)	0	100	100
76	DQ	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
76	f	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
77	DR	56/63 (89%)	52 (93%)	3 (5%)	1 (2%)	7	25
77	g	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
78	DS	68/193 (35%)	57 (84%)	10 (15%)	1 (2%)	8	29
78	h	68/193 (35%)	55 (81%)	13 (19%)	0	100	100
79	AR	309/317 (98%)	292 (94%)	17 (6%)	0	100	100
79	DT	302/317 (95%)	281 (93%)	19 (6%)	2 (1%)	19	46
80	P0	105/312 (34%)	81 (77%)	21 (20%)	3 (3%)	3	16
80	p0	69/312 (22%)	46 (67%)	20 (29%)	3 (4%)	2	10
81	12	61/165 (37%)	36 (59%)	25 (41%)	0	100	100
82	L1	215/217 (99%)	166 (77%)	46 (21%)	3 (1%)	9	30
82	l1	215/217 (99%)	131 (61%)	72 (34%)	12 (6%)	1	7
All	All	22749/25499 (89%)	21733 (96%)	951 (4%)	65 (0%)	37	64

5 of 65 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	AC	21	ILE
40	AM	49	LEU

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Mol	Chain	Res	Type
45	i	55	LYS
59	O	130	SER
41	CH	3	GLU

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	
4	AW	190/194 (98%)	188 (99%)	2 (1%)	70	83
4	j	190/194 (98%)	190 (100%)	0	100	100
5	AX	325/328 (99%)	323 (99%)	2 (1%)	84	90
5	k	325/328 (99%)	323 (99%)	2 (1%)	84	90
6	AY	290/292 (99%)	286 (99%)	4 (1%)	62	79
6	l	290/292 (99%)	288 (99%)	2 (1%)	81	89
7	AZ	247/252 (98%)	244 (99%)	3 (1%)	67	82
7	m	250/252 (99%)	249 (100%)	1 (0%)	89	93
8	BA	132/154 (86%)	132 (100%)	0	100	100
8	n	136/154 (88%)	136 (100%)	0	100	100
9	BB	198/204 (97%)	198 (100%)	0	100	100
9	o	197/204 (97%)	196 (100%)	1 (0%)	86	91
10	BC	191/216 (88%)	191 (100%)	0	100	100
10	p	193/216 (89%)	192 (100%)	1 (0%)	86	91
11	BD	169/170 (99%)	169 (100%)	0	100	100
11	q	168/170 (99%)	167 (99%)	1 (1%)	84	90
12	BE	178/186 (96%)	176 (99%)	2 (1%)	70	83
12	r	178/186 (96%)	176 (99%)	2 (1%)	70	83
13	BF	146/149 (98%)	144 (99%)	2 (1%)	62	79
13	s	146/149 (98%)	144 (99%)	2 (1%)	62	79
14	BG	166/168 (99%)	164 (99%)	2 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	t	166/168 (99%)	165 (99%)	1 (1%)	84	90
15	BH	108/109 (99%)	107 (99%)	1 (1%)	75	86
15	u	108/109 (99%)	108 (100%)	0	100	100
16	BI	177/178 (99%)	176 (99%)	1 (1%)	84	90
16	v	177/178 (99%)	176 (99%)	1 (1%)	84	90
17	BJ	166/167 (99%)	166 (100%)	0	100	100
17	w	166/167 (99%)	166 (100%)	0	100	100
18	BK	145/154 (94%)	142 (98%)	3 (2%)	48	69
18	x	144/154 (94%)	144 (100%)	0	100	100
19	BL	153/154 (99%)	153 (100%)	0	100	100
19	y	153/154 (99%)	153 (100%)	0	100	100
20	BM	146/153 (95%)	141 (97%)	5 (3%)	32	59
20	z	146/153 (95%)	146 (100%)	0	100	100
21	0	155/157 (99%)	154 (99%)	1 (1%)	84	90
21	BN	155/157 (99%)	155 (100%)	0	100	100
22	2	133/134 (99%)	132 (99%)	1 (1%)	79	88
22	BO	133/134 (99%)	132 (99%)	1 (1%)	79	88
23	5	93/112 (83%)	93 (100%)	0	100	100
23	BP	93/112 (83%)	90 (97%)	3 (3%)	34	60
24	6	101/104 (97%)	101 (100%)	0	100	100
24	BQ	101/104 (97%)	101 (100%)	0	100	100
25	7	97/127 (76%)	95 (98%)	2 (2%)	48	69
25	BR	86/127 (68%)	85 (99%)	1 (1%)	67	82
26	8	107/121 (88%)	105 (98%)	2 (2%)	52	72
26	BS	107/121 (88%)	107 (100%)	0	100	100
27	9	111/112 (99%)	109 (98%)	2 (2%)	54	74
27	BT	111/112 (99%)	109 (98%)	2 (2%)	54	74
28	AA	117/118 (99%)	117 (100%)	0	100	100
28	BU	117/118 (99%)	116 (99%)	1 (1%)	75	86
29	AB	120/121 (99%)	120 (100%)	0	100	100
29	BV	120/121 (99%)	119 (99%)	1 (1%)	79	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	AC	48/49 (98%)	47 (98%)	1 (2%)	48	69
30	BW	48/49 (98%)	48 (100%)	0	100	100
31	AD	81/90 (90%)	81 (100%)	0	100	100
31	BX	81/90 (90%)	81 (100%)	0	100	100
32	AE	98/100 (98%)	97 (99%)	1 (1%)	73	85
32	BY	98/100 (98%)	98 (100%)	0	100	100
33	AF	109/115 (95%)	109 (100%)	0	100	100
33	BZ	110/115 (96%)	110 (100%)	0	100	100
34	AG	91/92 (99%)	90 (99%)	1 (1%)	70	83
34	CA	91/92 (99%)	91 (100%)	0	100	100
35	AH	95/102 (93%)	94 (99%)	1 (1%)	70	83
35	CB	95/102 (93%)	95 (100%)	0	100	100
36	AI	106/106 (100%)	104 (98%)	2 (2%)	52	72
36	CC	105/106 (99%)	103 (98%)	2 (2%)	52	72
37	AJ	77/79 (98%)	76 (99%)	1 (1%)	65	80
37	CD	77/79 (98%)	77 (100%)	0	100	100
38	AK	70/73 (96%)	70 (100%)	0	100	100
38	CE	70/73 (96%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	68 (100%)	0	100	100
39	CF	68/69 (99%)	68 (100%)	0	100	100
40	AM	46/47 (98%)	46 (100%)	0	100	100
40	CG	46/47 (98%)	46 (100%)	0	100	100
41	AN	47/47 (100%)	47 (100%)	0	100	100
41	CH	46/47 (98%)	45 (98%)	1 (2%)	47	68
42	AO	24/24 (100%)	22 (92%)	2 (8%)	9	29
42	CI	23/24 (96%)	23 (100%)	0	100	100
43	AP	88/91 (97%)	88 (100%)	0	100	100
43	CJ	88/91 (97%)	88 (100%)	0	100	100
44	AQ	72/73 (99%)	72 (100%)	0	100	100
44	CK	72/73 (99%)	72 (100%)	0	100	100
45	CL	100/212 (47%)	97 (97%)	3 (3%)	36	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	i	99/212 (47%)	98 (99%)	1 (1%)	73	85
47	C	176/215 (82%)	175 (99%)	1 (1%)	84	90
47	CN	176/215 (82%)	174 (99%)	2 (1%)	70	83
48	CO	194/229 (85%)	193 (100%)	1 (0%)	86	91
48	D	194/229 (85%)	193 (100%)	1 (0%)	86	91
49	CP	175/198 (88%)	172 (98%)	3 (2%)	56	75
49	E	175/198 (88%)	175 (100%)	0	100	100
50	CQ	174/196 (89%)	168 (97%)	6 (3%)	32	59
50	F	174/196 (89%)	172 (99%)	2 (1%)	70	83
51	CR	218/220 (99%)	217 (100%)	1 (0%)	86	91
51	G	218/220 (99%)	218 (100%)	0	100	100
52	CS	178/197 (90%)	176 (99%)	2 (1%)	70	83
52	H	178/197 (90%)	176 (99%)	2 (1%)	70	83
53	CT	204/204 (100%)	202 (99%)	2 (1%)	73	85
53	I	195/204 (96%)	193 (99%)	2 (1%)	73	85
54	CU	164/167 (98%)	163 (99%)	1 (1%)	84	90
54	J	165/167 (99%)	164 (99%)	1 (1%)	84	90
55	CV	157/160 (98%)	157 (100%)	0	100	100
55	K	157/160 (98%)	156 (99%)	1 (1%)	84	90
56	CW	153/160 (96%)	153 (100%)	0	100	100
56	L	153/160 (96%)	153 (100%)	0	100	100
57	CX	88/104 (85%)	88 (100%)	0	100	100
57	M	90/104 (86%)	89 (99%)	1 (1%)	70	83
58	CY	122/134 (91%)	121 (99%)	1 (1%)	79	88
58	N	124/134 (92%)	122 (98%)	2 (2%)	58	76
59	CZ	101/123 (82%)	98 (97%)	3 (3%)	36	61
59	O	98/123 (80%)	93 (95%)	5 (5%)	20	46
60	DA	129/130 (99%)	128 (99%)	1 (1%)	79	88
60	P	129/130 (99%)	129 (100%)	0	100	100
61	DB	97/102 (95%)	97 (100%)	0	100	100
61	Q	97/102 (95%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	DC	112/121 (93%)	110 (98%)	2 (2%)	54	74
62	R	111/121 (92%)	110 (99%)	1 (1%)	75	86
63	DD	114/116 (98%)	112 (98%)	2 (2%)	54	74
63	S	114/116 (98%)	113 (99%)	1 (1%)	75	86
64	DE	112/122 (92%)	112 (100%)	0	100	100
64	T	112/122 (92%)	110 (98%)	2 (2%)	54	74
65	DF	125/129 (97%)	123 (98%)	2 (2%)	58	76
65	U	128/129 (99%)	127 (99%)	1 (1%)	79	88
66	DG	113/117 (97%)	113 (100%)	0	100	100
66	V	113/117 (97%)	113 (100%)	0	100	100
67	DH	87/105 (83%)	85 (98%)	2 (2%)	45	67
67	W	92/105 (88%)	89 (97%)	3 (3%)	33	59
68	DI	71/71 (100%)	71 (100%)	0	100	100
68	X	71/71 (100%)	71 (100%)	0	100	100
69	DJ	112/113 (99%)	111 (99%)	1 (1%)	75	86
69	Y	112/113 (99%)	112 (100%)	0	100	100
70	DK	116/118 (98%)	115 (99%)	1 (1%)	75	86
70	Z	116/118 (98%)	115 (99%)	1 (1%)	75	86
71	DL	109/112 (97%)	109 (100%)	0	100	100
71	a	111/112 (99%)	110 (99%)	1 (1%)	75	86
72	DM	63/85 (74%)	63 (100%)	0	100	100
72	b	64/85 (75%)	64 (100%)	0	100	100
73	DN	83/102 (81%)	83 (100%)	0	100	100
73	c	84/102 (82%)	82 (98%)	2 (2%)	44	67
74	DO	72/73 (99%)	72 (100%)	0	100	100
74	d	72/73 (99%)	72 (100%)	0	100	100
75	DP	53/58 (91%)	53 (100%)	0	100	100
75	e	54/58 (93%)	54 (100%)	0	100	100
76	DQ	47/48 (98%)	46 (98%)	1 (2%)	48	69
76	f	47/48 (98%)	44 (94%)	3 (6%)	14	38
77	DR	50/54 (93%)	50 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	g	51/54 (94%)	51 (100%)	0	100	100
78	DS	62/175 (35%)	59 (95%)	3 (5%)	21	48
78	h	62/175 (35%)	59 (95%)	3 (5%)	21	48
79	AR	259/263 (98%)	258 (100%)	1 (0%)	89	93
79	DT	255/263 (97%)	251 (98%)	4 (2%)	58	76
80	P0	92/247 (37%)	85 (92%)	7 (8%)	11	32
80	p0	71/247 (29%)	66 (93%)	5 (7%)	12	35
81	12	53/137 (39%)	51 (96%)	2 (4%)	28	55
82	L1	196/196 (100%)	186 (95%)	10 (5%)	20	46
82	l1	196/196 (100%)	187 (95%)	9 (5%)	23	49
All	All	19544/21471 (91%)	19359 (99%)	185 (1%)	75	86

5 of 185 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	CP	136	ARG
70	DK	13	ARG
50	CQ	155	ASP
59	CZ	33	ARG
79	DT	265	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
9	BB	17	GLN
63	DD	138	GLN
12	BE	95	HIS
82	l1	12	ASN
48	CO	232	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3203/3359 (95%)	594 (18%)	44 (1%)
1	AS	3223/3359 (95%)	625 (19%)	52 (1%)
2	3	120/121 (99%)	9 (7%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	AT	120/121 (99%)	9 (7%)	0
3	4	156/158 (98%)	23 (14%)	3 (1%)
3	AU	156/158 (98%)	23 (14%)	3 (1%)
46	B	1736/1787 (97%)	433 (24%)	42 (2%)
46	CM	1762/1787 (98%)	454 (25%)	55 (3%)
All	All	10476/10850 (96%)	2170 (20%)	199 (1%)

5 of 2170 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	15	A
1	1	24	U
1	1	25	A
1	1	29	G
1	1	39	A

5 of 199 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AS	2183	U
3	AU	156	U
1	AS	2447	G
1	AS	2789	A
46	CM	176	U

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1231 ligands modelled in this entry, 1227 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	$\#\|Z\| > 2$
86	HYG	B	1953	83	35,39,39	0.40	0	43,60,60	1.09	4 (9%)
86	HYG	CM	1902	83	35,39,39	0.47	0	43,60,60	1.22	5 (11%)
84	3K5	AS	3401	-	62,63,63	0.24	0	82,95,95	0.99	4 (4%)
84	3K5	1	3402	-	62,63,63	0.30	0	82,95,95	0.90	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
86	HYG	B	1953	83	-	5/12/87/87	0/4/4/4
86	HYG	CM	1902	83	-	6/12/87/87	0/4/4/4
84	3K5	AS	3401	-	-	3/29/121/121	0/7/7/7
84	3K5	1	3402	-	-	6/29/121/121	0/7/7/7

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
84	AS	3401	3K5	O14-C34-C33	4.71	118.45	107.70
84	AS	3401	3K5	C34-O14-C38	3.80	123.60	117.72
86	CM	1902	HYG	C16-C17-C12	-3.68	104.56	113.50
86	B	1953	HYG	C16-C17-C12	-3.36	105.34	113.50
86	B	1953	HYG	O22-C17-C16	3.23	119.08	111.22

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

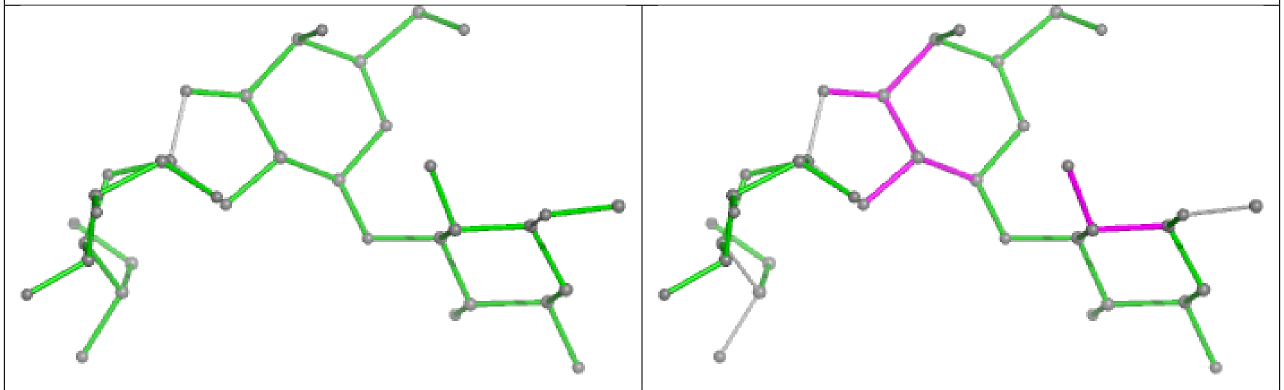
Mol	Chain	Res	Type	Atoms
84	1	3402	3K5	O15-C38-O14-C34
84	AS	3401	3K5	O15-C38-O14-C34
86	B	1953	HYG	N36-C33-C34-O35
86	CM	1902	HYG	O28-C27-C33-C34
86	CM	1902	HYG	N36-C33-C34-O35

There are no ring outliers.

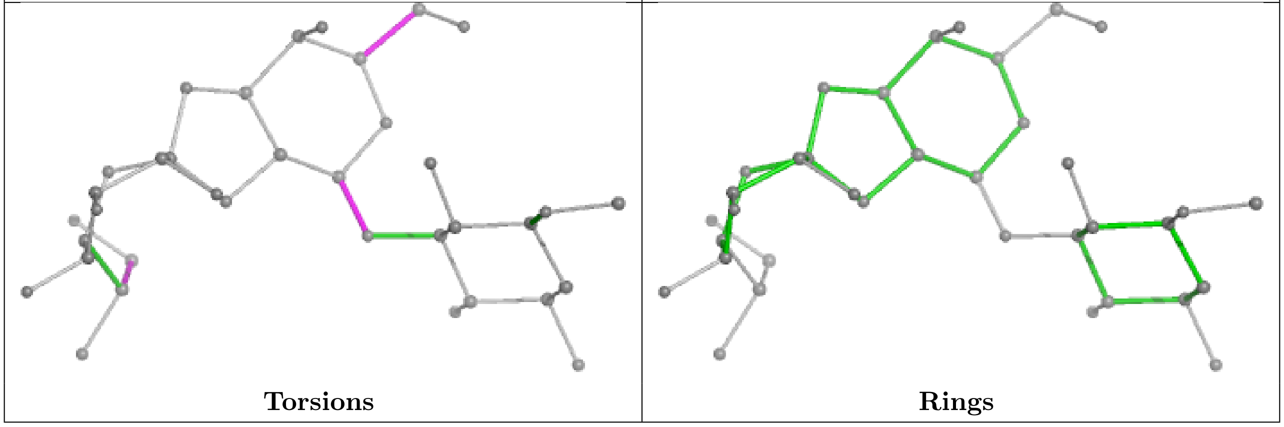
No monomer is involved in short contacts.

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

Ligand HYG B 1953

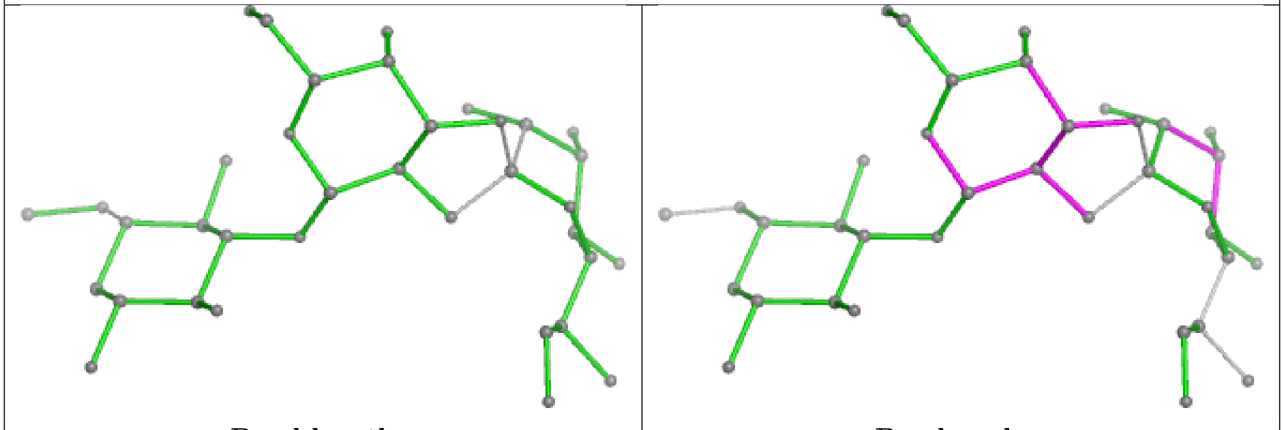


Bond lengths **Bond angles**

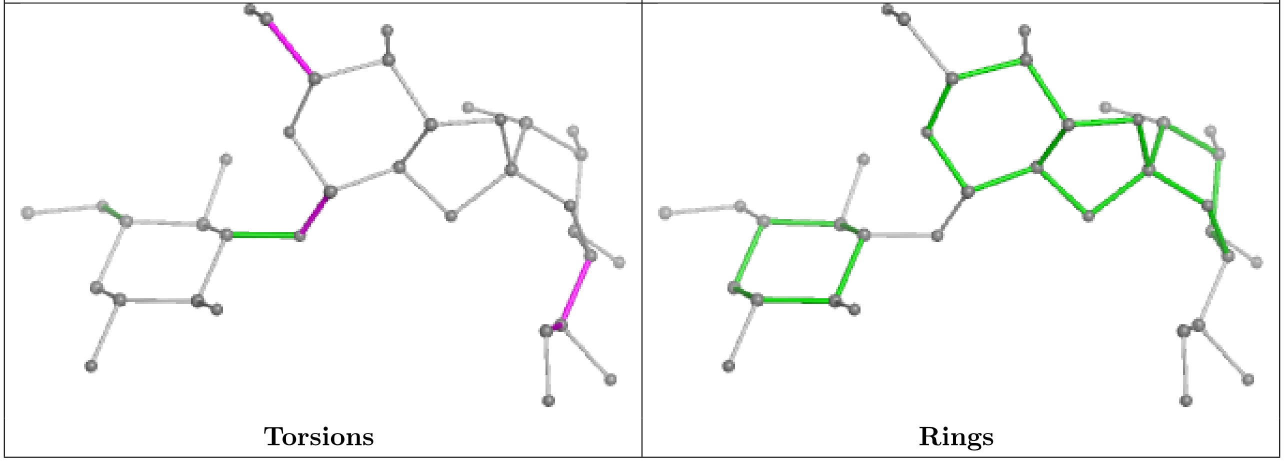


Torsions **Rings**

Ligand HYG CM 1902

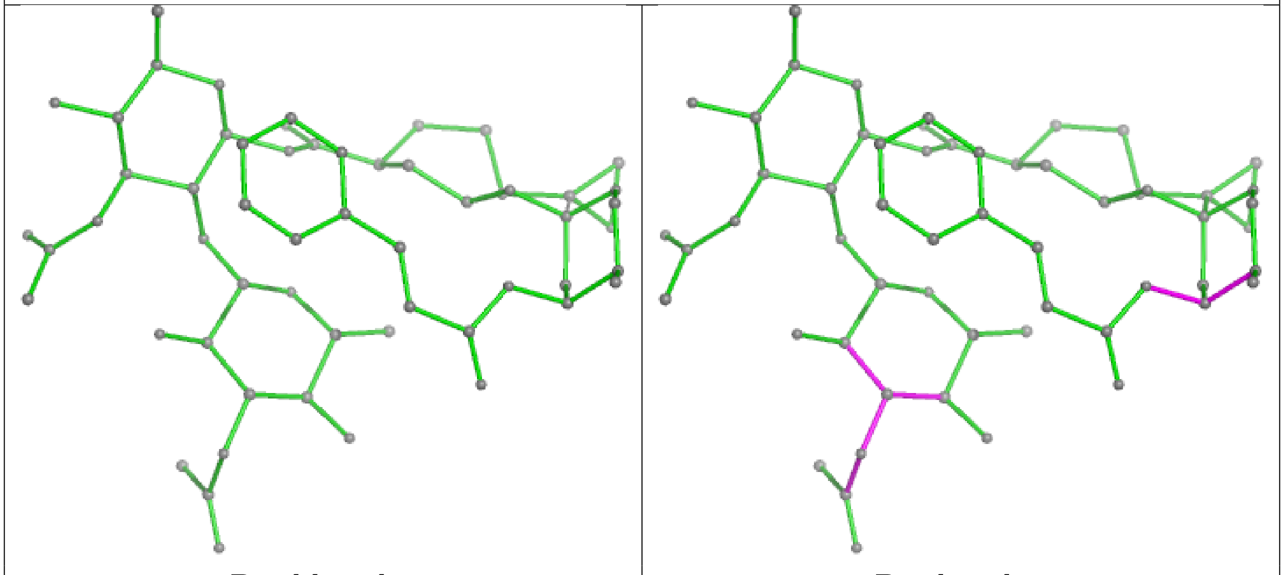


Bond lengths **Bond angles**

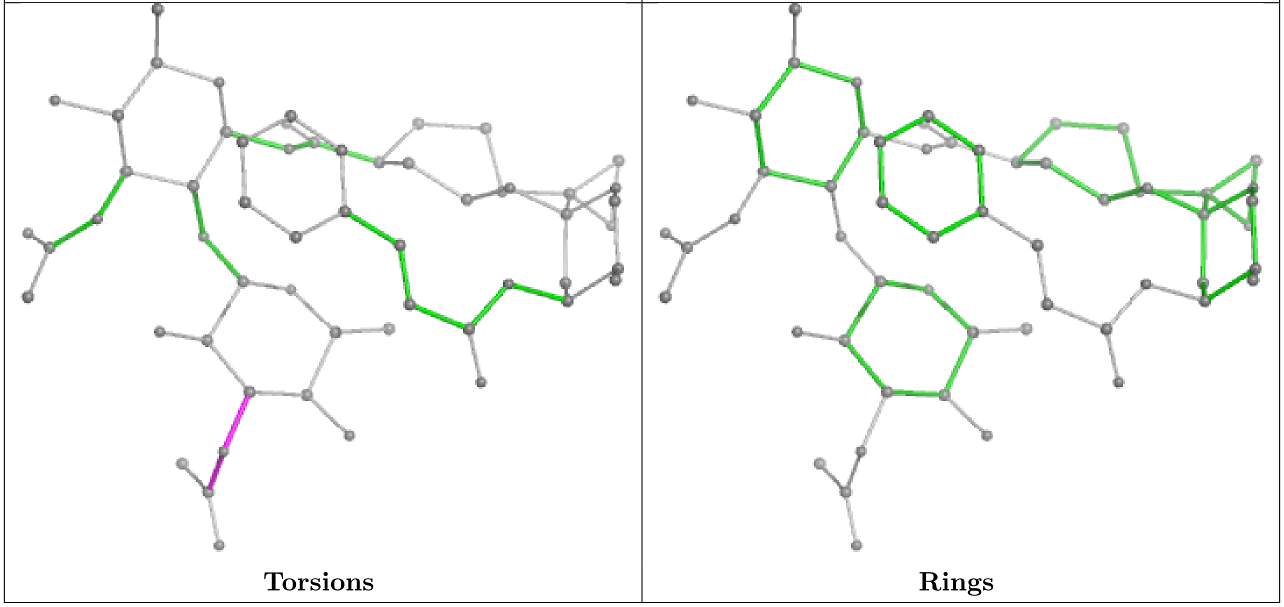


Torsions **Rings**

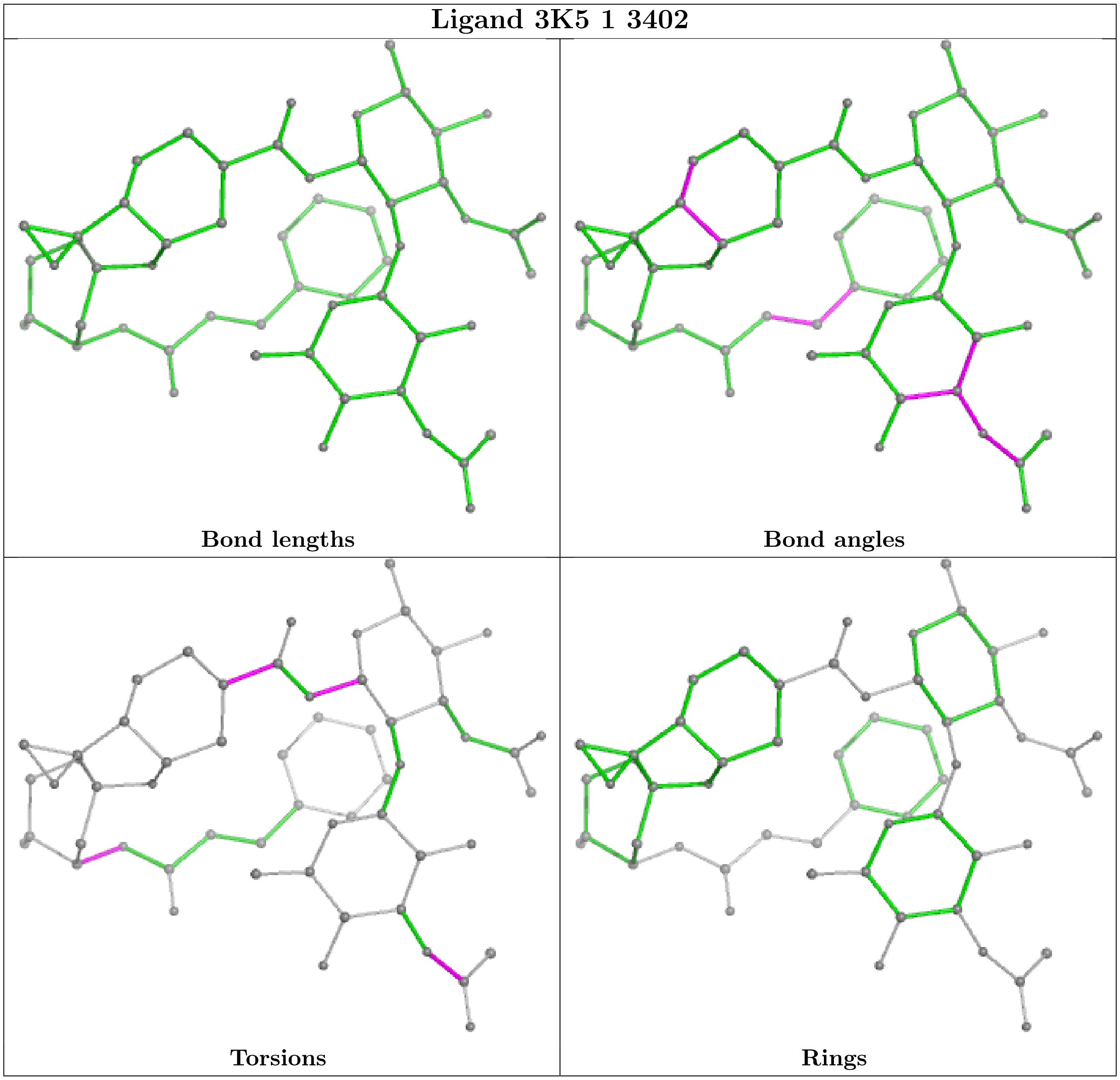
Ligand 3K5 AS 3401



Bond lengths **Bond angles**



Torsions **Rings**



Ligand 3K5 1 3402

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1	3208/3359 (95%)	0.47	112 (3%)	47	28	32, 64, 173, 334	0
1	AS	3227/3359 (96%)	0.47	153 (4%)	37	21	34, 69, 204, 323	0
2	3	121/121 (100%)	0.46	1 (0%)	82	66	50, 78, 100, 136	0
2	AT	121/121 (100%)	0.35	4 (3%)	49	30	39, 70, 93, 145	0
3	4	157/158 (99%)	0.27	2 (1%)	74	56	46, 67, 117, 169	0
3	AU	157/158 (99%)	0.63	7 (4%)	39	22	55, 89, 136, 219	0
4	AW	249/254 (98%)	0.90	22 (8%)	17	9	37, 72, 95, 108	0
4	j	249/254 (98%)	0.85	17 (6%)	25	14	28, 52, 74, 143	0
5	AX	386/389 (99%)	0.57	16 (4%)	42	24	34, 56, 85, 150	0
5	k	386/389 (99%)	0.70	21 (5%)	32	19	29, 58, 78, 116	0
6	AY	361/363 (99%)	1.24	61 (16%)	5	3	44, 73, 101, 132	0
6	l	361/363 (99%)	1.16	66 (18%)	4	2	35, 70, 105, 135	0
7	AZ	292/298 (97%)	1.62	83 (28%)	1	1	44, 93, 124, 140	0
7	m	296/298 (99%)	1.42	68 (22%)	2	1	50, 87, 119, 141	0
8	BA	153/176 (86%)	0.93	14 (9%)	16	9	48, 68, 103, 132	0
8	n	157/176 (89%)	0.99	17 (10%)	12	7	53, 75, 101, 138	0
9	BB	234/241 (97%)	0.62	11 (4%)	37	21	35, 55, 113, 167	0
9	o	233/241 (96%)	1.01	20 (8%)	18	10	38, 63, 123, 164	0
10	BC	229/262 (87%)	1.65	72 (31%)	1	1	76, 117, 159, 188	0
10	p	233/262 (88%)	1.21	46 (19%)	3	2	51, 76, 125, 148	0
11	BD	190/191 (99%)	1.12	18 (9%)	15	8	48, 74, 106, 155	0
11	q	189/191 (98%)	1.35	40 (21%)	3	2	52, 77, 97, 127	0
12	BE	208/220 (94%)	0.63	9 (4%)	40	23	33, 51, 99, 134	0
12	r	208/220 (94%)	0.99	28 (13%)	8	4	40, 65, 101, 119	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	BF	171/174 (98%)	1.17	26 (15%) 6 3	53, 81, 114, 127	0
13	s	171/174 (98%)	1.53	42 (24%) 2 1	58, 92, 116, 131	0
14	BG	200/202 (99%)	1.30	38 (19%) 4 2	48, 92, 133, 154	0
14	t	200/202 (99%)	0.92	20 (10%) 14 8	43, 75, 110, 143	0
15	BH	130/131 (99%)	0.80	12 (9%) 16 9	43, 65, 96, 128	0
15	u	130/131 (99%)	0.94	10 (7%) 21 11	52, 70, 89, 103	0
16	BI	203/204 (99%)	1.63	52 (25%) 2 1	54, 84, 106, 118	0
16	v	203/204 (99%)	1.17	23 (11%) 11 7	36, 57, 71, 85	0
17	BJ	199/200 (99%)	0.53	8 (4%) 43 25	34, 51, 86, 120	0
17	w	199/200 (99%)	0.83	15 (7%) 22 12	33, 55, 82, 103	0
18	BK	176/185 (95%)	1.11	23 (13%) 8 5	44, 63, 91, 123	0
18	x	173/185 (93%)	0.99	20 (11%) 11 6	33, 59, 92, 120	0
19	BL	185/186 (99%)	0.92	14 (7%) 21 11	45, 69, 85, 104	0
19	y	185/186 (99%)	1.49	50 (27%) 2 1	41, 66, 85, 100	0
20	BM	179/190 (94%)	1.07	25 (13%) 7 4	48, 77, 137, 169	0
20	z	179/190 (94%)	0.97	13 (7%) 22 12	45, 68, 126, 145	0
21	0	170/172 (98%)	1.03	21 (12%) 9 5	46, 64, 87, 137	0
21	BN	170/172 (98%)	0.69	9 (5%) 33 19	39, 58, 77, 105	0
22	2	159/160 (99%)	1.15	24 (15%) 6 3	44, 63, 111, 147	0
22	BO	159/160 (99%)	1.08	24 (15%) 6 3	37, 60, 113, 147	0
23	5	102/124 (82%)	1.17	15 (14%) 7 3	73, 109, 140, 160	0
23	BP	102/124 (82%)	1.37	23 (22%) 3 1	89, 125, 151, 162	0
24	6	131/137 (95%)	0.78	8 (6%) 28 16	37, 55, 76, 86	0
24	BQ	131/137 (95%)	0.83	11 (8%) 18 10	32, 53, 77, 116	0
25	7	118/155 (76%)	1.09	22 (18%) 4 2	38, 76, 126, 143	0
25	BR	98/155 (63%)	1.17	18 (18%) 4 2	39, 70, 128, 138	0
26	8	120/142 (84%)	0.99	11 (9%) 16 9	53, 71, 91, 98	0
26	BS	119/142 (83%)	1.45	31 (26%) 2 1	62, 93, 113, 128	0
27	9	126/127 (99%)	1.58	35 (27%) 2 1	55, 80, 98, 113	0
27	BT	126/127 (99%)	1.24	22 (17%) 5 2	59, 91, 123, 140	0
28	AA	135/136 (99%)	1.36	29 (21%) 3 1	56, 84, 111, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
28	BU	135/136 (99%)	1.45	28 (20%) 3 2	78, 113, 137, 159	0
29	AB	148/149 (99%)	1.16	16 (10%) 12 7	34, 63, 95, 123	0
29	BV	148/149 (99%)	1.27	25 (16%) 5 3	44, 73, 96, 118	0
30	AC	62/63 (98%)	1.83	27 (43%) 1 0	39, 77, 122, 143	0
30	BW	61/63 (96%)	1.57	17 (27%) 2 1	38, 76, 112, 135	0
31	AD	96/106 (90%)	0.83	7 (7%) 22 12	53, 73, 95, 108	0
31	BX	96/106 (90%)	1.30	19 (19%) 3 2	78, 103, 128, 152	0
32	AE	110/112 (98%)	0.76	4 (3%) 46 28	46, 64, 109, 134	0
32	BY	110/112 (98%)	1.04	14 (12%) 9 5	42, 72, 120, 146	0
33	AF	124/131 (94%)	1.19	20 (16%) 5 3	33, 65, 83, 94	0
33	BZ	124/131 (94%)	0.90	9 (7%) 22 12	37, 63, 87, 107	0
34	AG	106/107 (99%)	1.15	15 (14%) 7 4	45, 61, 78, 99	0
34	CA	106/107 (99%)	0.63	4 (3%) 44 26	36, 51, 73, 91	0
35	AH	112/122 (91%)	1.42	25 (22%) 3 1	46, 70, 113, 139	0
35	CB	112/122 (91%)	1.63	37 (33%) 1 0	50, 95, 128, 158	0
36	AI	120/120 (100%)	1.28	20 (16%) 5 3	60, 83, 106, 128	0
36	CC	118/120 (98%)	1.65	39 (33%) 1 0	74, 100, 125, 135	0
37	AJ	97/99 (97%)	1.18	17 (17%) 5 2	50, 70, 102, 166	0
37	CD	97/99 (97%)	1.57	29 (29%) 1 1	77, 98, 125, 155	0
38	AK	86/90 (95%)	0.93	12 (13%) 7 4	28, 54, 95, 109	0
38	CE	86/90 (95%)	1.22	13 (15%) 6 3	48, 71, 100, 135	0
39	AL	77/78 (98%)	1.37	15 (19%) 4 2	72, 94, 125, 153	0
39	CF	77/78 (98%)	1.73	28 (36%) 1 0	83, 115, 157, 165	0
40	AM	50/51 (98%)	1.15	5 (10%) 14 8	42, 61, 84, 95	0
40	CG	50/51 (98%)	1.60	10 (20%) 3 2	55, 76, 97, 105	0
41	AN	52/52 (100%)	2.36	30 (57%) 0 0	65, 96, 120, 128	0
41	CH	51/52 (98%)	2.59	33 (64%) 0 0	60, 95, 115, 127	0
42	AO	25/25 (100%)	1.89	10 (40%) 1 0	55, 66, 82, 88	0
42	CI	24/25 (96%)	1.58	7 (29%) 1 1	43, 58, 68, 74	0
43	AP	103/106 (97%)	0.98	15 (14%) 7 4	36, 62, 100, 118	0
43	CJ	103/106 (97%)	1.12	15 (14%) 7 4	44, 72, 107, 121	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
44	AQ	91/92 (98%)	0.87	4 (4%) 39 23	39, 57, 97, 108	0
44	CK	91/92 (98%)	0.96	8 (8%) 17 9	48, 72, 104, 123	0
45	CL	121/267 (45%)	1.65	40 (33%) 1 0	59, 88, 120, 144	0
45	i	120/267 (44%)	2.03	51 (42%) 1 0	59, 103, 135, 152	0
46	B	1741/1787 (97%)	0.97	174 (9%) 14 8	48, 89, 173, 457	0
46	CM	1765/1787 (98%)	0.82	121 (6%) 24 13	41, 79, 180, 457	0
47	C	208/261 (79%)	1.43	48 (23%) 2 1	80, 109, 137, 148	0
47	CN	208/261 (79%)	1.34	32 (15%) 6 3	53, 97, 127, 165	0
48	CO	214/256 (83%)	1.62	60 (28%) 2 1	65, 113, 138, 164	0
48	D	214/256 (83%)	1.20	33 (15%) 6 3	58, 92, 111, 131	0
49	CP	217/249 (87%)	1.04	28 (12%) 9 5	42, 73, 102, 120	0
49	E	217/249 (87%)	1.62	59 (27%) 2 1	69, 97, 121, 146	0
50	CQ	223/251 (88%)	1.30	44 (19%) 3 2	49, 76, 133, 174	0
50	F	223/251 (88%)	1.94	99 (44%) 1 0	70, 107, 152, 178	0
51	CR	260/262 (99%)	1.74	86 (33%) 1 0	58, 88, 110, 151	0
51	G	259/262 (98%)	1.87	100 (38%) 1 0	63, 96, 116, 156	0
52	CS	206/225 (91%)	1.89	76 (36%) 1 0	65, 99, 137, 191	0
52	H	206/225 (91%)	2.04	91 (44%) 1 0	67, 103, 143, 168	0
53	CT	236/236 (100%)	1.44	56 (23%) 2 1	54, 94, 139, 159	0
53	I	226/236 (95%)	1.40	63 (27%) 2 1	59, 96, 142, 175	0
54	CU	183/186 (98%)	1.66	61 (33%) 1 0	67, 124, 165, 174	0
54	J	184/186 (98%)	2.14	87 (47%) 0 0	76, 126, 156, 173	0
55	CV	203/206 (98%)	1.43	47 (23%) 2 1	38, 70, 120, 148	0
55	K	203/206 (98%)	1.29	42 (20%) 3 2	43, 79, 123, 140	0
56	CW	178/189 (94%)	1.85	60 (33%) 1 0	59, 93, 121, 136	0
56	L	178/189 (94%)	2.33	106 (59%) 0 0	74, 108, 129, 143	0
57	CX	94/118 (79%)	1.16	11 (11%) 10 6	62, 85, 123, 142	0
57	M	98/118 (83%)	1.96	43 (43%) 1 0	84, 117, 142, 158	0
58	CY	141/155 (90%)	1.36	27 (19%) 4 2	39, 67, 95, 149	0
58	N	144/155 (92%)	1.35	28 (19%) 4 2	48, 77, 113, 139	0
59	CZ	119/143 (83%)	1.72	42 (35%) 1 0	124, 157, 177, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
59	O	116/143 (81%)	2.02	56 (48%)	0	0	136, 175, 196, 203	0
60	DA	150/151 (99%)	1.70	52 (34%)	1	0	54, 89, 117, 134	0
60	P	150/151 (99%)	1.70	51 (34%)	1	0	46, 88, 116, 122	0
61	DB	127/132 (96%)	1.30	22 (17%)	5	2	57, 97, 123, 132	0
61	Q	127/132 (96%)	1.14	22 (17%)	5	2	44, 79, 96, 107	0
62	DC	130/142 (91%)	1.57	36 (27%)	2	1	50, 89, 130, 144	0
62	R	129/142 (90%)	1.99	59 (45%)	1	0	63, 100, 137, 151	0
63	DD	140/142 (98%)	2.37	82 (58%)	0	0	58, 98, 130, 143	0
63	S	140/142 (98%)	2.60	86 (61%)	0	0	67, 112, 148, 152	0
64	DE	124/137 (90%)	2.10	59 (47%)	0	0	67, 108, 158, 166	0
64	T	124/137 (90%)	2.34	59 (47%)	0	0	80, 121, 166, 176	0
65	DF	141/145 (97%)	1.53	36 (25%)	2	1	54, 92, 124, 156	0
65	U	144/145 (99%)	1.71	44 (30%)	1	1	62, 90, 114, 157	0
66	DG	141/145 (97%)	1.73	44 (31%)	1	1	60, 90, 119, 148	0
66	V	141/145 (97%)	2.11	64 (45%)	1	0	79, 107, 140, 162	0
67	DH	97/119 (81%)	1.82	35 (36%)	1	0	49, 94, 122, 150	0
67	W	102/119 (85%)	2.04	44 (43%)	1	0	71, 121, 149, 158	0
68	DI	87/87 (100%)	1.07	10 (11%)	11	6	61, 83, 114, 149	0
68	X	87/87 (100%)	1.33	19 (21%)	3	1	76, 102, 126, 133	0
69	DJ	129/130 (99%)	1.45	31 (24%)	2	1	50, 69, 87, 96	0
69	Y	129/130 (99%)	1.93	50 (38%)	1	0	59, 84, 105, 113	0
70	DK	143/145 (98%)	1.34	32 (22%)	3	1	43, 64, 88, 116	0
70	Z	143/145 (98%)	1.48	35 (24%)	2	1	56, 78, 97, 115	0
71	DL	132/135 (97%)	1.39	26 (19%)	3	2	71, 110, 133, 174	0
71	a	134/135 (99%)	1.73	44 (32%)	1	1	68, 112, 130, 144	0
72	DM	71/105 (67%)	1.39	17 (23%)	2	1	89, 120, 143, 148	0
72	b	72/105 (68%)	1.50	16 (22%)	3	1	85, 111, 134, 154	0
73	DN	97/119 (81%)	1.54	24 (24%)	2	1	52, 75, 129, 137	0
73	c	98/119 (82%)	1.64	31 (31%)	1	1	53, 83, 123, 135	0
74	DO	81/82 (98%)	1.66	22 (27%)	2	1	73, 99, 160, 173	0
74	d	81/82 (98%)	1.58	19 (23%)	2	1	73, 99, 156, 170	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
75	DP	61/67 (91%)	1.26	12 (19%)	3	2	78, 101, 129, 148	0
75	e	62/67 (92%)	1.70	19 (30%)	1	1	91, 111, 131, 138	0
76	DQ	54/56 (96%)	1.51	15 (27%)	2	1	51, 65, 93, 103	0
76	f	55/56 (98%)	2.03	27 (49%)	0	0	75, 92, 118, 141	0
77	DR	58/63 (92%)	1.79	21 (36%)	1	0	63, 101, 161, 173	0
77	g	60/63 (95%)	1.90	23 (38%)	1	0	75, 105, 154, 169	0
78	DS	70/193 (36%)	2.81	47 (67%)	0	0	95, 163, 181, 196	0
78	h	70/193 (36%)	2.28	35 (50%)	0	0	113, 160, 185, 191	0
79	AR	311/317 (98%)	1.92	124 (39%)	1	0	114, 155, 178, 192	0
79	DT	306/317 (96%)	2.01	135 (44%)	1	0	100, 145, 174, 196	0
80	P0	107/312 (34%)	1.79	42 (39%)	1	0	104, 127, 144, 157	0
80	p0	79/312 (25%)	2.57	44 (55%)	0	0	119, 138, 155, 161	0
81	12	63/165 (38%)	1.17	11 (17%)	5	2	98, 132, 151, 157	0
82	L1	217/217 (100%)	1.19	42 (19%)	4	2	91, 127, 164, 224	0
82	l1	217/217 (100%)	1.62	65 (29%)	1	1	109, 137, 164, 197	0
All	All	33588/36349 (92%)	1.14	5883 (17%)	5	2	28, 80, 154, 457	0

The worst 5 of 5883 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	G	110	ALA	9.8
67	W	81	TYR	9.8
50	F	206	ALA	9.6
78	DS	127	TYR	9.4
1	AS	1263	U	9.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3715	1/1	0.10	0.43	76,76,76,76	0
83	MG	1	3921	1/1	0.12	0.22	67,67,67,67	0
83	MG	B	1928	1/1	0.16	0.35	108,108,108,108	0
83	MG	J	201	1/1	0.27	0.17	129,129,129,129	0
83	MG	1	3841	1/1	0.31	0.21	73,73,73,73	0
83	MG	B	1851	1/1	0.39	0.24	53,53,53,53	0
83	MG	CM	1819	1/1	0.43	0.28	74,74,74,74	0
83	MG	8	201	1/1	0.47	0.29	62,62,62,62	0
83	MG	8	202	1/1	0.49	0.66	79,79,79,79	0
83	MG	1	3651	1/1	0.53	0.42	77,77,77,77	0
83	MG	9	202	1/1	0.53	0.30	81,81,81,81	0
85	ZN	d	101	1/1	0.53	0.19	285,285,285,285	0
83	MG	1	3868	1/1	0.54	0.22	54,54,54,54	0
83	MG	1	3803	1/1	0.55	0.30	92,92,92,92	0
83	MG	AS	3676	1/1	0.55	0.18	72,72,72,72	0
83	MG	Y	201	1/1	0.59	0.15	58,58,58,58	0
83	MG	B	1898	1/1	0.59	0.33	60,60,60,60	0
83	MG	1	3669	1/1	0.59	0.37	76,76,76,76	0
83	MG	u	202	1/1	0.59	0.14	51,51,51,51	0
83	MG	1	3527	1/1	0.60	0.37	72,72,72,72	0
83	MG	AS	3601	1/1	0.61	0.17	124,124,124,124	0
83	MG	CM	1876	1/1	0.61	0.22	51,51,51,51	0
83	MG	1	3930	1/1	0.61	0.26	81,81,81,81	0
83	MG	1	3470	1/1	0.62	0.30	53,53,53,53	0
83	MG	4	207	1/1	0.63	0.32	64,64,64,64	0
83	MG	1	3722	1/1	0.63	0.23	61,61,61,61	0
83	MG	DB	203	1/1	0.63	0.16	52,52,52,52	0
83	MG	1	3699	1/1	0.63	0.23	54,54,54,54	0
83	MG	1	3630	1/1	0.64	0.41	59,59,59,59	0
83	MG	1	3867	1/1	0.64	0.22	51,51,51,51	0
83	MG	1	3688	1/1	0.64	0.43	82,82,82,82	0
83	MG	a	201	1/1	0.64	0.14	76,76,76,76	0
83	MG	B	1924	1/1	0.64	0.32	69,69,69,69	0
83	MG	1	3716	1/1	0.65	0.14	77,77,77,77	0
83	MG	G	302	1/1	0.65	0.37	63,63,63,63	0
83	MG	1	3476	1/1	0.65	0.18	58,58,58,58	0
83	MG	1	3796	1/1	0.65	0.17	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	4	203	1/1	0.65	0.19	57,57,57,57	0
83	MG	f	102	1/1	0.65	0.16	81,81,81,81	0
83	MG	B	1941	1/1	0.66	0.15	58,58,58,58	0
83	MG	DG	201	1/1	0.66	0.32	52,52,52,52	0
83	MG	B	1875	1/1	0.66	0.33	75,75,75,75	0
83	MG	AG	201	1/1	0.67	0.29	86,86,86,86	0
83	MG	AJ	101	1/1	0.67	0.27	82,82,82,82	0
83	MG	1	3432	1/1	0.67	0.17	48,48,48,48	0
83	MG	1	3914	1/1	0.67	0.18	57,57,57,57	0
83	MG	B	1922	1/1	0.68	0.21	66,66,66,66	0
83	MG	AS	3631	1/1	0.68	0.17	66,66,66,66	0
83	MG	s	201	1/1	0.68	0.22	62,62,62,62	0
83	MG	1	3713	1/1	0.68	0.14	51,51,51,51	0
83	MG	1	3655	1/1	0.69	0.22	54,54,54,54	0
83	MG	k	404	1/1	0.69	0.19	79,79,79,79	0
83	MG	1	3797	1/1	0.69	0.21	77,77,77,77	0
83	MG	AS	3519	1/1	0.69	0.26	42,42,42,42	0
83	MG	9	201	1/1	0.70	0.83	70,70,70,70	0
83	MG	CM	1880	1/1	0.70	0.19	66,66,66,66	0
83	MG	1	3543	1/1	0.70	0.27	62,62,62,62	0
83	MG	1	3890	1/1	0.70	0.22	46,46,46,46	0
83	MG	CM	1864	1/1	0.70	0.19	73,73,73,73	0
83	MG	CL	301	1/1	0.71	0.18	40,40,40,40	0
83	MG	r	302	1/1	0.71	0.20	50,50,50,50	0
83	MG	CM	1859	1/1	0.71	0.20	60,60,60,60	0
83	MG	B	1896	1/1	0.71	0.10	61,61,61,61	0
83	MG	B	1829	1/1	0.71	0.16	64,64,64,64	0
83	MG	I	301	1/1	0.71	0.28	99,99,99,99	0
83	MG	AS	3627	1/1	0.71	0.18	57,57,57,57	0
83	MG	1	3483	1/1	0.71	0.14	38,38,38,38	0
83	MG	B	1856	1/1	0.71	0.16	47,47,47,47	0
83	MG	1	3842	1/1	0.72	0.12	63,63,63,63	0
83	MG	B	1862	1/1	0.72	0.19	68,68,68,68	0
83	MG	1	3856	1/1	0.72	0.16	66,66,66,66	0
83	MG	1	3681	1/1	0.72	0.23	52,52,52,52	0
83	MG	1	3931	1/1	0.72	0.17	61,61,61,61	0
83	MG	AS	3673	1/1	0.72	0.15	45,45,45,45	0
83	MG	1	3837	1/1	0.72	0.13	34,34,34,34	0
83	MG	1	3776	1/1	0.72	0.42	57,57,57,57	0
83	MG	AS	3597	1/1	0.73	0.11	28,28,28,28	0
83	MG	o	303	1/1	0.73	0.20	57,57,57,57	0
83	MG	CM	1882	1/1	0.73	0.24	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	BF	201	1/1	0.74	0.14	44,44,44,44	0
83	MG	1	3783	1/1	0.74	0.20	48,48,48,48	0
83	MG	AS	3493	1/1	0.74	0.23	51,51,51,51	0
83	MG	CM	1836	1/1	0.74	0.16	48,48,48,48	0
83	MG	B	1939	1/1	0.74	0.16	78,78,78,78	0
83	MG	1	3564	1/1	0.74	0.17	57,57,57,57	0
83	MG	1	3597	1/1	0.74	0.36	60,60,60,60	0
83	MG	AS	3615	1/1	0.74	0.18	50,50,50,50	0
83	MG	1	3909	1/1	0.74	0.20	79,79,79,79	0
83	MG	B	1810	1/1	0.74	0.27	45,45,45,45	0
83	MG	1	3913	1/1	0.74	0.21	55,55,55,55	0
83	MG	1	3598	1/1	0.74	0.24	56,56,56,56	0
83	MG	1	3587	1/1	0.75	0.16	58,58,58,58	0
83	MG	1	3468	1/1	0.75	0.22	38,38,38,38	0
83	MG	AS	3585	1/1	0.75	0.22	44,44,44,44	0
83	MG	CM	1822	1/1	0.75	0.20	44,44,44,44	0
83	MG	1	3876	1/1	0.75	0.14	42,42,42,42	0
83	MG	B	1890	1/1	0.75	0.17	53,53,53,53	0
83	MG	1	3438	1/1	0.75	0.20	31,31,31,31	0
83	MG	AS	3622	1/1	0.75	0.11	47,47,47,47	0
83	MG	1	3674	1/1	0.75	0.22	83,83,83,83	0
83	MG	B	1899	1/1	0.75	0.20	73,73,73,73	0
83	MG	AS	3637	1/1	0.75	0.27	97,97,97,97	0
83	MG	1	3517	1/1	0.75	0.17	58,58,58,58	0
83	MG	j	302	1/1	0.75	0.14	53,53,53,53	0
83	MG	1	3873	1/1	0.76	0.11	40,40,40,40	0
83	MG	1	3694	1/1	0.76	0.15	39,39,39,39	0
83	MG	1	3854	1/1	0.76	0.30	61,61,61,61	0
83	MG	1	3781	1/1	0.76	0.13	82,82,82,82	0
83	MG	B	1866	1/1	0.76	0.22	78,78,78,78	0
83	MG	B	1926	1/1	0.76	0.21	41,41,41,41	0
83	MG	1	3545	1/1	0.76	0.26	51,51,51,51	0
83	MG	1	3746	1/1	0.76	0.14	66,66,66,66	0
83	MG	CM	1816	1/1	0.77	0.22	27,27,27,27	0
83	MG	1	3631	1/1	0.77	0.27	64,64,64,64	0
83	MG	1	3923	1/1	0.77	0.25	64,64,64,64	0
83	MG	1	3902	1/1	0.77	0.27	51,51,51,51	0
83	MG	CM	1853	1/1	0.77	0.28	72,72,72,72	0
83	MG	V	201	1/1	0.77	0.29	48,48,48,48	0
83	MG	1	3553	1/1	0.77	0.26	54,54,54,54	0
83	MG	3	202	1/1	0.77	0.11	59,59,59,59	0
83	MG	B	1877	1/1	0.77	0.24	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AS	3414	1/1	0.77	0.30	47,47,47,47	0
83	MG	1	3584	1/1	0.77	0.15	41,41,41,41	0
83	MG	1	3838	1/1	0.77	0.16	61,61,61,61	0
83	MG	B	1943	1/1	0.77	0.08	68,68,68,68	0
83	MG	BZ	202	1/1	0.78	0.14	66,66,66,66	0
83	MG	0	204	1/1	0.78	0.18	45,45,45,45	0
83	MG	1	3861	1/1	0.78	0.13	56,56,56,56	0
83	MG	1	3726	1/1	0.78	0.21	43,43,43,43	0
83	MG	AS	3621	1/1	0.78	0.16	53,53,53,53	0
83	MG	1	3727	1/1	0.78	0.11	38,38,38,38	0
83	MG	1	3652	1/1	0.78	0.19	43,43,43,43	0
83	MG	1	3848	1/1	0.78	0.21	78,78,78,78	0
83	MG	1	3607	1/1	0.78	0.14	51,51,51,51	0
83	MG	AS	3652	1/1	0.78	0.12	51,51,51,51	0
83	MG	AS	3666	1/1	0.78	0.13	53,53,53,53	0
83	MG	1	3893	1/1	0.78	0.19	52,52,52,52	0
83	MG	B	1944	1/1	0.78	0.13	76,76,76,76	0
83	MG	1	3552	1/1	0.78	0.19	50,50,50,50	0
83	MG	BN	201	1/1	0.78	0.12	59,59,59,59	0
83	MG	1	3754	1/1	0.79	0.24	61,61,61,61	0
83	MG	CL	302	1/1	0.79	0.40	59,59,59,59	0
83	MG	CM	1808	1/1	0.79	0.22	58,58,58,58	0
83	MG	1	3700	1/1	0.79	0.25	47,47,47,47	0
83	MG	AS	3629	1/1	0.79	0.16	38,38,38,38	0
83	MG	1	3830	1/1	0.79	0.26	43,43,43,43	0
83	MG	AH	202	1/1	0.79	0.16	55,55,55,55	0
83	MG	AS	3641	1/1	0.79	0.31	48,48,48,48	0
83	MG	1	3832	1/1	0.79	0.20	56,56,56,56	0
83	MG	CM	1860	1/1	0.79	0.21	41,41,41,41	0
83	MG	AS	3562	1/1	0.79	0.14	50,50,50,50	0
83	MG	1	3594	1/1	0.79	0.29	72,72,72,72	0
83	MG	0	201	1/1	0.79	0.24	70,70,70,70	0
83	MG	AT	207	1/1	0.79	0.22	68,68,68,68	0
83	MG	DA	201	1/1	0.79	0.28	57,57,57,57	0
83	MG	1	3524	1/1	0.79	0.27	44,44,44,44	0
83	MG	1	3648	1/1	0.79	0.14	44,44,44,44	0
83	MG	1	3871	1/1	0.79	0.20	67,67,67,67	0
83	MG	1	3729	1/1	0.80	0.41	50,50,50,50	0
83	MG	AT	202	1/1	0.80	0.27	55,55,55,55	0
83	MG	1	3800	1/1	0.80	0.21	62,62,62,62	0
83	MG	1	3732	1/1	0.80	0.13	26,26,26,26	0
83	MG	B	1806	1/1	0.80	0.15	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3554	1/1	0.80	0.12	40,40,40,40	0
83	MG	AS	3573	1/1	0.80	0.15	30,30,30,30	0
83	MG	AS	3581	1/1	0.80	0.12	46,46,46,46	0
83	MG	CM	1806	1/1	0.80	0.11	28,28,28,28	0
83	MG	B	1927	1/1	0.80	0.15	57,57,57,57	0
83	MG	B	1817	1/1	0.80	0.26	45,45,45,45	0
83	MG	CM	1818	1/1	0.80	0.20	38,38,38,38	0
83	MG	B	1934	1/1	0.80	0.16	102,102,102,102	0
83	MG	CM	1821	1/1	0.80	0.17	35,35,35,35	0
83	MG	AS	3602	1/1	0.80	0.15	59,59,59,59	0
83	MG	B	1938	1/1	0.80	0.28	70,70,70,70	0
83	MG	1	3747	1/1	0.80	0.09	45,45,45,45	0
83	MG	B	1850	1/1	0.80	0.12	24,24,24,24	0
83	MG	1	3591	1/1	0.80	0.17	58,58,58,58	0
83	MG	1	3625	1/1	0.80	0.41	95,95,95,95	0
83	MG	1	3502	1/1	0.80	0.15	41,41,41,41	0
83	MG	6	203	1/1	0.80	0.17	42,42,42,42	0
83	MG	1	3466	1/1	0.80	0.22	43,43,43,43	0
83	MG	CM	1898	1/1	0.80	0.13	44,44,44,44	0
83	MG	3	214	1/1	0.80	0.15	82,82,82,82	0
83	MG	AS	3662	1/1	0.80	0.09	57,57,57,57	0
83	MG	1	3671	1/1	0.80	0.22	52,52,52,52	0
83	MG	1	3895	1/1	0.80	0.14	44,44,44,44	0
83	MG	AS	3624	1/1	0.81	0.13	41,41,41,41	0
83	MG	1	3595	1/1	0.81	0.15	42,42,42,42	0
83	MG	3	210	1/1	0.81	0.21	59,59,59,59	0
83	MG	1	3672	1/1	0.81	0.12	57,57,57,57	0
83	MG	1	3547	1/1	0.81	0.13	42,42,42,42	0
83	MG	CM	1820	1/1	0.81	0.21	27,27,27,27	0
83	MG	1	3911	1/1	0.81	0.16	63,63,63,63	0
83	MG	AS	3646	1/1	0.81	0.13	35,35,35,35	0
83	MG	1	3677	1/1	0.81	0.22	55,55,55,55	0
83	MG	AE	202	1/1	0.81	0.09	63,63,63,63	0
83	MG	AS	3580	1/1	0.81	0.13	42,42,42,42	0
83	MG	1	3442	1/1	0.81	0.34	52,52,52,52	0
83	MG	1	3489	1/1	0.81	0.14	49,49,49,49	0
83	MG	CM	1874	1/1	0.81	0.16	66,66,66,66	0
83	MG	1	3692	1/1	0.81	0.14	176,176,176,176	0
83	MG	1	3928	1/1	0.81	0.21	59,59,59,59	0
83	MG	1	3495	1/1	0.81	0.23	68,68,68,68	0
83	MG	B	1902	1/1	0.81	0.34	60,60,60,60	0
83	MG	CO	301	1/1	0.81	0.26	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AS	3618	1/1	0.81	0.20	45,45,45,45	0
83	MG	B	1916	1/1	0.81	0.19	69,69,69,69	0
83	MG	1	3555	1/1	0.81	0.10	46,46,46,46	0
83	MG	CL	303	1/1	0.81	0.21	41,41,41,41	0
83	MG	1	3794	1/1	0.82	0.26	68,68,68,68	0
83	MG	1	3686	1/1	0.82	0.19	60,60,60,60	0
83	MG	B	1893	1/1	0.82	0.34	43,43,43,43	0
83	MG	5	201	1/1	0.82	0.13	64,64,64,64	0
83	MG	CM	1811	1/1	0.82	0.25	59,59,59,59	0
83	MG	1	3753	1/1	0.82	0.30	55,55,55,55	0
83	MG	B	1827	1/1	0.82	0.14	37,37,37,37	0
83	MG	1	3798	1/1	0.82	0.14	41,41,41,41	0
83	MG	B	1911	1/1	0.82	0.26	60,60,60,60	0
83	MG	B	1912	1/1	0.82	0.14	81,81,81,81	0
83	MG	B	1846	1/1	0.82	0.11	57,57,57,57	0
83	MG	B	1918	1/1	0.82	0.16	59,59,59,59	0
83	MG	CM	1837	1/1	0.82	0.20	39,39,39,39	0
83	MG	AS	3427	1/1	0.82	0.12	43,43,43,43	0
83	MG	AS	3490	1/1	0.82	0.15	35,35,35,35	0
83	MG	AS	3661	1/1	0.82	0.23	64,64,64,64	0
83	MG	AS	3491	1/1	0.82	0.22	64,64,64,64	0
83	MG	1	3563	1/1	0.82	0.22	50,50,50,50	0
83	MG	1	3675	1/1	0.82	0.22	52,52,52,52	0
83	MG	1	3891	1/1	0.82	0.21	65,65,65,65	0
83	MG	B	1859	1/1	0.82	0.17	34,34,34,34	0
83	MG	AT	206	1/1	0.82	0.16	61,61,61,61	0
83	MG	1	3645	1/1	0.82	0.27	47,47,47,47	0
83	MG	B	1865	1/1	0.82	0.15	25,25,25,25	0
83	MG	1	3518	1/1	0.82	0.27	57,57,57,57	0
83	MG	1	3862	1/1	0.82	0.16	80,80,80,80	0
83	MG	B	1940	1/1	0.82	0.16	76,76,76,76	0
83	MG	AS	3632	1/1	0.83	0.17	38,38,38,38	0
83	MG	AS	3516	1/1	0.83	0.26	40,40,40,40	0
83	MG	1	3537	1/1	0.83	0.20	51,51,51,51	0
83	MG	AS	3539	1/1	0.83	0.20	59,59,59,59	0
83	MG	B	1942	1/1	0.83	0.17	67,67,67,67	0
83	MG	B	1907	1/1	0.83	0.10	44,44,44,44	0
83	MG	3	206	1/1	0.83	0.12	47,47,47,47	0
83	MG	1	3683	1/1	0.83	0.14	104,104,104,104	0
83	MG	AH	203	1/1	0.83	0.14	29,29,29,29	0
83	MG	CM	1848	1/1	0.83	0.30	52,52,52,52	0
83	MG	AS	3675	1/1	0.83	0.12	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	CM	1858	1/1	0.83	0.15	42,42,42,42	0
83	MG	1	3858	1/1	0.83	0.17	48,48,48,48	0
83	MG	AS	3600	1/1	0.83	0.16	46,46,46,46	0
83	MG	AT	204	1/1	0.83	0.22	64,64,64,64	0
83	MG	1	3877	1/1	0.83	0.12	52,52,52,52	0
83	MG	1	3419	1/1	0.83	0.17	47,47,47,47	0
83	MG	1	3618	1/1	0.83	0.15	34,34,34,34	0
83	MG	B	1886	1/1	0.83	0.16	95,95,95,95	0
83	MG	1	3866	1/1	0.83	0.09	62,62,62,62	0
83	MG	1	3668	1/1	0.83	0.14	32,32,32,32	0
83	MG	AS	3474	1/1	0.83	0.24	41,41,41,41	0
83	MG	B	1844	1/1	0.83	0.16	55,55,55,55	0
83	MG	1	3583	1/1	0.83	0.22	52,52,52,52	0
83	MG	AB	202	1/1	0.83	0.25	76,76,76,76	0
83	MG	Z	202	1/1	0.84	0.16	58,58,58,58	0
83	MG	1	3839	1/1	0.84	0.10	55,55,55,55	0
83	MG	1	3526	1/1	0.84	0.16	48,48,48,48	0
83	MG	1	3639	1/1	0.84	0.20	54,54,54,54	0
83	MG	B	1864	1/1	0.84	0.19	42,42,42,42	0
83	MG	1	3766	1/1	0.84	0.15	44,44,44,44	0
83	MG	1	3926	1/1	0.84	0.26	53,53,53,53	0
83	MG	1	3849	1/1	0.84	0.27	47,47,47,47	0
83	MG	B	1802	1/1	0.84	0.26	45,45,45,45	0
83	MG	AS	3638	1/1	0.84	0.21	59,59,59,59	0
83	MG	B	1935	1/1	0.84	0.20	56,56,56,56	0
83	MG	CM	1835	1/1	0.84	0.24	54,54,54,54	0
83	MG	AS	3518	1/1	0.84	0.20	43,43,43,43	0
83	MG	1	3464	1/1	0.84	0.28	48,48,48,48	0
83	MG	AS	3538	1/1	0.84	0.11	32,32,32,32	0
83	MG	0	202	1/1	0.84	0.11	39,39,39,39	0
83	MG	AS	3540	1/1	0.84	0.20	37,37,37,37	0
83	MG	AS	3560	1/1	0.84	0.10	52,52,52,52	0
83	MG	1	3827	1/1	0.84	0.18	50,50,50,50	0
83	MG	1	3714	1/1	0.84	0.21	43,43,43,43	0
83	MG	AS	3677	1/1	0.84	0.18	45,45,45,45	0
83	MG	1	3455	1/1	0.84	0.30	32,32,32,32	0
83	MG	CM	1877	1/1	0.84	0.14	47,47,47,47	0
83	MG	B	1836	1/1	0.84	0.21	51,51,51,51	0
83	MG	1	3836	1/1	0.84	0.18	31,31,31,31	0
83	MG	1	3908	1/1	0.84	0.10	23,23,23,23	0
83	MG	CM	1899	1/1	0.84	0.18	31,31,31,31	0
83	MG	AW	304	1/1	0.84	0.28	84,84,84,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
83	MG	B	1909	1/1	0.84	0.16	35,35,35,35	0
83	MG	B	1910	1/1	0.84	0.12	54,54,54,54	0
83	MG	1	3525	1/1	0.84	0.19	44,44,44,44	0
83	MG	1	3720	1/1	0.84	0.19	23,23,23,23	0
83	MG	AS	3482	1/1	0.85	0.14	67,67,67,67	0
83	MG	1	3444	1/1	0.85	0.28	45,45,45,45	0
83	MG	1	3724	1/1	0.85	0.19	49,49,49,49	0
83	MG	w	302	1/1	0.85	0.36	52,52,52,52	0
83	MG	1	3929	1/1	0.85	0.11	77,77,77,77	0
83	MG	1	3568	1/1	0.85	0.23	44,44,44,44	0
83	MG	AS	3642	1/1	0.85	0.19	46,46,46,46	0
83	MG	B	1897	1/1	0.85	0.12	42,42,42,42	0
83	MG	1	3569	1/1	0.85	0.26	38,38,38,38	0
83	MG	B	1833	1/1	0.85	0.28	32,32,32,32	0
83	MG	1	3491	1/1	0.85	0.17	32,32,32,32	0
83	MG	1	3559	1/1	0.85	0.18	46,46,46,46	0
83	MG	CM	1850	1/1	0.85	0.15	58,58,58,58	0
83	MG	B	1949	1/1	0.85	0.18	47,47,47,47	0
83	MG	1	3740	1/1	0.85	0.19	53,53,53,53	0
83	MG	1	3701	1/1	0.85	0.20	59,59,59,59	0
83	MG	1	3603	1/1	0.85	0.14	50,50,50,50	0
83	MG	4	206	1/1	0.85	0.16	24,24,24,24	0
83	MG	CM	1872	1/1	0.85	0.21	45,45,45,45	0
83	MG	1	3585	1/1	0.85	0.21	44,44,44,44	0
83	MG	1	3530	1/1	0.85	0.20	52,52,52,52	0
83	MG	B	1919	1/1	0.85	0.28	50,50,50,50	0
83	MG	k	401	1/1	0.85	0.12	58,58,58,58	0
83	MG	BB	301	1/1	0.85	0.12	28,28,28,28	0
83	MG	1	3622	1/1	0.85	0.25	42,42,42,42	0
83	MG	AS	3616	1/1	0.85	0.16	45,45,45,45	0
83	MG	1	3719	1/1	0.85	0.08	27,27,27,27	0
83	MG	AS	3450	1/1	0.85	0.21	38,38,38,38	0
83	MG	AS	3467	1/1	0.85	0.14	57,57,57,57	0
83	MG	AS	3473	1/1	0.85	0.12	16,16,16,16	0
83	MG	1	3657	1/1	0.85	0.17	22,22,22,22	0
86	HYG	B	1953	36/36	0.85	0.16	49,77,94,99	0
83	MG	1	3924	1/1	0.86	0.15	69,69,69,69	0
83	MG	1	3428	1/1	0.86	0.33	47,47,47,47	0
83	MG	1	3457	1/1	0.86	0.10	20,20,20,20	0
83	MG	1	3617	1/1	0.86	0.10	37,37,37,37	0
83	MG	AS	3630	1/1	0.86	0.07	50,50,50,50	0
83	MG	1	3575	1/1	0.86	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3593	1/1	0.86	0.17	35,35,35,35	0
83	MG	1	3682	1/1	0.86	0.21	85,85,85,85	0
83	MG	1	3579	1/1	0.86	0.11	36,36,36,36	0
83	MG	AS	3512	1/1	0.86	0.17	20,20,20,20	0
83	MG	CM	1827	1/1	0.86	0.22	34,34,34,34	0
83	MG	1	3721	1/1	0.86	0.18	43,43,43,43	0
83	MG	AS	3644	1/1	0.86	0.19	59,59,59,59	0
83	MG	1	3892	1/1	0.86	0.10	53,53,53,53	0
83	MG	CM	1845	1/1	0.86	0.13	29,29,29,29	0
83	MG	B	1882	1/1	0.86	0.21	49,49,49,49	0
83	MG	AS	3653	1/1	0.86	0.16	68,68,68,68	0
83	MG	1	3661	1/1	0.86	0.10	33,33,33,33	0
83	MG	1	3843	1/1	0.86	0.30	62,62,62,62	0
83	MG	1	3896	1/1	0.86	0.17	43,43,43,43	0
83	MG	AS	3544	1/1	0.86	0.13	28,28,28,28	0
83	MG	4	209	1/1	0.86	0.08	54,54,54,54	0
83	MG	B	1946	1/1	0.86	0.23	32,32,32,32	0
83	MG	1	3793	1/1	0.86	0.12	18,18,18,18	0
83	MG	1	3723	1/1	0.86	0.08	16,16,16,16	0
83	MG	AT	203	1/1	0.86	0.21	57,57,57,57	0
83	MG	B	1807	1/1	0.86	0.21	40,40,40,40	0
83	MG	1	3663	1/1	0.86	0.17	54,54,54,54	0
83	MG	1	3664	1/1	0.86	0.22	32,32,32,32	0
83	MG	1	3580	1/1	0.86	0.21	61,61,61,61	0
83	MG	1	3799	1/1	0.86	0.10	33,33,33,33	0
83	MG	1	3920	1/1	0.86	0.21	49,49,49,49	0
83	MG	1	3515	1/1	0.86	0.20	21,21,21,21	0
83	MG	AS	3412	1/1	0.86	0.16	23,23,23,23	0
83	MG	w	303	1/1	0.86	0.15	56,56,56,56	0
85	ZN	CB	201	1/1	0.86	0.15	202,202,202,202	0
83	MG	1	3529	1/1	0.86	0.10	38,38,38,38	0
83	MG	1	3872	1/1	0.87	0.14	48,48,48,48	0
83	MG	1	3807	1/1	0.87	0.11	54,54,54,54	0
83	MG	AS	3599	1/1	0.87	0.31	50,50,50,50	0
83	MG	BJ	303	1/1	0.87	0.12	30,30,30,30	0
83	MG	1	3875	1/1	0.87	0.13	42,42,42,42	0
83	MG	1	3844	1/1	0.87	0.16	48,48,48,48	0
83	MG	1	3812	1/1	0.87	0.23	46,46,46,46	0
83	MG	AS	3605	1/1	0.87	0.24	38,38,38,38	0
83	MG	1	3879	1/1	0.87	0.13	39,39,39,39	0
83	MG	B	1835	1/1	0.87	0.20	21,21,21,21	0
83	MG	AS	3413	1/1	0.87	0.19	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3884	1/1	0.87	0.14	65,65,65,65	0
83	MG	AS	3426	1/1	0.87	0.19	30,30,30,30	0
83	MG	1	3815	1/1	0.87	0.17	30,30,30,30	0
83	MG	AS	3428	1/1	0.87	0.25	37,37,37,37	0
83	MG	AS	3628	1/1	0.87	0.16	33,33,33,33	0
83	MG	AS	3449	1/1	0.87	0.16	40,40,40,40	0
83	MG	B	1845	1/1	0.87	0.20	35,35,35,35	0
83	MG	CM	1823	1/1	0.87	0.17	34,34,34,34	0
83	MG	AS	3455	1/1	0.87	0.10	29,29,29,29	0
83	MG	1	3853	1/1	0.87	0.14	33,33,33,33	0
83	MG	0	205	1/1	0.87	0.39	55,55,55,55	0
83	MG	1	3653	1/1	0.87	0.07	39,39,39,39	0
83	MG	3	203	1/1	0.87	0.16	31,31,31,31	0
83	MG	1	3855	1/1	0.87	0.12	43,43,43,43	0
83	MG	AS	3643	1/1	0.87	0.16	39,39,39,39	0
83	MG	3	209	1/1	0.87	0.20	48,48,48,48	0
83	MG	1	3434	1/1	0.87	0.23	41,41,41,41	0
83	MG	AS	3648	1/1	0.87	0.17	32,32,32,32	0
83	MG	AS	3649	1/1	0.87	0.14	48,48,48,48	0
83	MG	AS	3504	1/1	0.87	0.26	50,50,50,50	0
83	MG	3	212	1/1	0.87	0.16	59,59,59,59	0
83	MG	1	3562	1/1	0.87	0.16	48,48,48,48	0
83	MG	AE	201	1/1	0.87	0.12	62,62,62,62	0
83	MG	1	3498	1/1	0.87	0.22	39,39,39,39	0
83	MG	AS	3667	1/1	0.87	0.12	92,92,92,92	0
83	MG	B	1879	1/1	0.87	0.22	46,46,46,46	0
83	MG	CM	1883	1/1	0.87	0.13	45,45,45,45	0
83	MG	CM	1884	1/1	0.87	0.21	54,54,54,54	0
83	MG	CM	1891	1/1	0.87	0.22	26,26,26,26	0
83	MG	1	3906	1/1	0.87	0.15	27,27,27,27	0
83	MG	1	3548	1/1	0.87	0.17	43,43,43,43	0
83	MG	B	1887	1/1	0.87	0.23	47,47,47,47	0
83	MG	AS	3678	1/1	0.87	0.12	42,42,42,42	0
83	MG	1	3413	1/1	0.87	0.23	31,31,31,31	0
83	MG	1	3503	1/1	0.87	0.09	32,32,32,32	0
83	MG	DG	202	1/1	0.87	0.12	63,63,63,63	0
83	MG	B	1952	1/1	0.87	0.23	48,48,48,48	0
83	MG	1	3540	1/1	0.87	0.24	42,42,42,42	0
85	ZN	DQ	102	1/1	0.87	0.28	118,118,118,118	0
83	MG	1	3494	1/1	0.87	0.19	13,13,13,13	0
83	MG	B	1892	1/1	0.88	0.15	40,40,40,40	0
83	MG	B	1815	1/1	0.88	0.26	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	B	1947	1/1	0.88	0.18	63,63,63,63	0
83	MG	1	3889	1/1	0.88	0.13	69,69,69,69	0
83	MG	1	3679	1/1	0.88	0.15	27,27,27,27	0
83	MG	1	3647	1/1	0.88	0.14	45,45,45,45	0
83	MG	B	1830	1/1	0.88	0.22	46,46,46,46	0
83	MG	AS	3547	1/1	0.88	0.12	35,35,35,35	0
83	MG	1	3835	1/1	0.88	0.09	25,25,25,25	0
83	MG	AS	3657	1/1	0.88	0.18	17,17,17,17	0
83	MG	Q	201	1/1	0.88	0.21	49,49,49,49	0
83	MG	B	1905	1/1	0.88	0.14	38,38,38,38	0
83	MG	1	3401	1/1	0.88	0.31	30,30,30,30	0
83	MG	B	1908	1/1	0.88	0.21	46,46,46,46	0
83	MG	1	3500	1/1	0.88	0.18	37,37,37,37	0
83	MG	AS	3596	1/1	0.88	0.08	37,37,37,37	0
83	MG	B	1843	1/1	0.88	0.21	21,21,21,21	0
83	MG	1	3411	1/1	0.88	0.17	10,10,10,10	0
83	MG	1	3423	1/1	0.88	0.19	42,42,42,42	0
83	MG	1	3905	1/1	0.88	0.12	27,27,27,27	0
83	MG	1	3725	1/1	0.88	0.19	40,40,40,40	0
83	MG	1	3773	1/1	0.88	0.14	32,32,32,32	0
83	MG	1	3691	1/1	0.88	0.21	22,22,22,22	0
83	MG	AS	3441	1/1	0.88	0.22	29,29,29,29	0
83	MG	1	3778	1/1	0.88	0.21	57,57,57,57	0
83	MG	1	3845	1/1	0.88	0.16	37,37,37,37	0
83	MG	BE	302	1/1	0.88	0.12	48,48,48,48	0
83	MG	1	3654	1/1	0.88	0.16	70,70,70,70	0
83	MG	1	3918	1/1	0.88	0.13	43,43,43,43	0
83	MG	AS	3626	1/1	0.88	0.20	40,40,40,40	0
83	MG	1	3817	1/1	0.88	0.12	32,32,32,32	0
83	MG	DB	201	1/1	0.88	0.14	38,38,38,38	0
83	MG	1	3824	1/1	0.88	0.12	47,47,47,47	0
83	MG	AM	101	1/1	0.88	0.17	54,54,54,54	0
83	MG	1	3881	1/1	0.88	0.20	25,25,25,25	0
83	MG	B	1805	1/1	0.88	0.20	57,57,57,57	0
83	MG	1	3718	1/1	0.88	0.13	35,35,35,35	0
83	MG	1	3885	1/1	0.88	0.10	53,53,53,53	0
83	MG	1	3887	1/1	0.88	0.08	58,58,58,58	0
83	MG	B	1825	1/1	0.89	0.16	32,32,32,32	0
83	MG	1	3599	1/1	0.89	0.17	36,36,36,36	0
83	MG	AS	3481	1/1	0.89	0.14	25,25,25,25	0
83	MG	B	1891	1/1	0.89	0.12	41,41,41,41	0
83	MG	1	3804	1/1	0.89	0.13	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
83	MG	1	3558	1/1	0.89	0.14	47,47,47,47	0
83	MG	1	3775	1/1	0.89	0.15	32,32,32,32	0
83	MG	1	3662	1/1	0.89	0.16	42,42,42,42	0
83	MG	1	3407	1/1	0.89	0.31	23,23,23,23	0
83	MG	AS	3515	1/1	0.89	0.14	31,31,31,31	0
83	MG	1	3818	1/1	0.89	0.12	38,38,38,38	0
83	MG	B	1900	1/1	0.89	0.27	50,50,50,50	0
83	MG	CM	1825	1/1	0.89	0.26	31,31,31,31	0
83	MG	1	3611	1/1	0.89	0.28	24,24,24,24	0
83	MG	CM	1833	1/1	0.89	0.26	42,42,42,42	0
83	MG	AS	3537	1/1	0.89	0.21	41,41,41,41	0
83	MG	1	3735	1/1	0.89	0.25	33,33,33,33	0
83	MG	k	403	1/1	0.89	0.14	57,57,57,57	0
83	MG	CM	1839	1/1	0.89	0.19	36,36,36,36	0
83	MG	1	3829	1/1	0.89	0.12	25,25,25,25	0
83	MG	1	3433	1/1	0.89	0.32	45,45,45,45	0
83	MG	B	1855	1/1	0.89	0.19	79,79,79,79	0
83	MG	Y	202	1/1	0.89	0.19	71,71,71,71	0
83	MG	1	3643	1/1	0.89	0.13	27,27,27,27	0
83	MG	AS	3568	1/1	0.89	0.18	39,39,39,39	0
83	MG	1	3860	1/1	0.89	0.12	46,46,46,46	0
83	MG	AS	3671	1/1	0.89	0.13	32,32,32,32	0
83	MG	CM	1865	1/1	0.89	0.18	45,45,45,45	0
83	MG	CM	1866	1/1	0.89	0.10	25,25,25,25	0
83	MG	CM	1868	1/1	0.89	0.20	64,64,64,64	0
83	MG	1	3833	1/1	0.89	0.21	41,41,41,41	0
83	MG	AR	401	1/1	0.89	0.18	48,48,48,48	0
83	MG	1	3539	1/1	0.89	0.10	24,24,24,24	0
83	MG	1	3894	1/1	0.89	0.17	57,57,57,57	0
83	MG	1	3706	1/1	0.89	0.12	36,36,36,36	0
83	MG	AS	3417	1/1	0.89	0.21	23,23,23,23	0
83	MG	B	1868	1/1	0.89	0.09	59,59,59,59	0
83	MG	B	1869	1/1	0.89	0.18	41,41,41,41	0
83	MG	1	3684	1/1	0.89	0.28	54,54,54,54	0
83	MG	AS	3603	1/1	0.89	0.17	38,38,38,38	0
83	MG	AT	209	1/1	0.89	0.16	52,52,52,52	0
83	MG	B	1814	1/1	0.89	0.14	53,53,53,53	0
83	MG	AS	3606	1/1	0.89	0.07	32,32,32,32	0
83	MG	AS	3442	1/1	0.89	0.23	45,45,45,45	0
83	MG	B	1933	1/1	0.89	0.12	57,57,57,57	0
83	MG	BH	201	1/1	0.89	0.10	43,43,43,43	0
83	MG	1	3763	1/1	0.89	0.17	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3765	1/1	0.89	0.14	38,38,38,38	0
83	MG	B	1824	1/1	0.89	0.21	26,26,26,26	0
83	MG	CK	102	1/1	0.89	0.15	32,32,32,32	0
83	MG	AS	3468	1/1	0.89	0.12	37,37,37,37	0
83	MG	k	402	1/1	0.90	0.13	54,54,54,54	0
83	MG	1	3614	1/1	0.90	0.20	86,86,86,86	0
83	MG	1	3774	1/1	0.90	0.11	29,29,29,29	0
83	MG	B	1823	1/1	0.90	0.16	31,31,31,31	0
83	MG	1	3523	1/1	0.90	0.23	42,42,42,42	0
83	MG	CJ	202	1/1	0.90	0.09	21,21,21,21	0
83	MG	r	301	1/1	0.90	0.20	34,34,34,34	0
83	MG	AS	3404	1/1	0.90	0.28	19,19,19,19	0
83	MG	AS	3405	1/1	0.90	0.25	16,16,16,16	0
83	MG	B	1903	1/1	0.90	0.18	87,87,87,87	0
83	MG	1	3680	1/1	0.90	0.08	30,30,30,30	0
83	MG	B	1828	1/1	0.90	0.18	39,39,39,39	0
83	MG	1	3507	1/1	0.90	0.18	9,9,9,9	0
83	MG	AS	3419	1/1	0.90	0.13	27,27,27,27	0
83	MG	AS	3420	1/1	0.90	0.12	15,15,15,15	0
83	MG	1	3619	1/1	0.90	0.14	33,33,33,33	0
83	MG	v	303	1/1	0.90	0.11	72,72,72,72	0
83	MG	1	3731	1/1	0.90	0.11	37,37,37,37	0
83	MG	1	3790	1/1	0.90	0.11	49,49,49,49	0
83	MG	B	1839	1/1	0.90	0.34	48,48,48,48	0
83	MG	CM	1824	1/1	0.90	0.09	28,28,28,28	0
83	MG	AS	3447	1/1	0.90	0.38	48,48,48,48	0
83	MG	1	3514	1/1	0.90	0.18	30,30,30,30	0
83	MG	1	3925	1/1	0.90	0.11	37,37,37,37	0
83	MG	1	3734	1/1	0.90	0.16	14,14,14,14	0
83	MG	1	3600	1/1	0.90	0.14	35,35,35,35	0
83	MG	2	203	1/1	0.90	0.09	37,37,37,37	0
83	MG	1	3736	1/1	0.90	0.17	39,39,39,39	0
83	MG	1	3484	1/1	0.90	0.14	34,34,34,34	0
83	MG	B	1931	1/1	0.90	0.18	47,47,47,47	0
83	MG	1	3717	1/1	0.90	0.19	42,42,42,42	0
83	MG	1	3497	1/1	0.90	0.18	11,11,11,11	0
83	MG	1	3673	1/1	0.90	0.16	47,47,47,47	0
83	MG	3	204	1/1	0.90	0.19	32,32,32,32	0
83	MG	AS	3496	1/1	0.90	0.22	40,40,40,40	0
83	MG	AS	3500	1/1	0.90	0.13	32,32,32,32	0
83	MG	1	3637	1/1	0.90	0.10	49,49,49,49	0
83	MG	AS	3507	1/1	0.90	0.16	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3755	1/1	0.90	0.15	34,34,34,34	0
83	MG	CM	1870	1/1	0.90	0.15	30,30,30,30	0
83	MG	AS	3658	1/1	0.90	0.10	28,28,28,28	0
83	MG	1	3810	1/1	0.90	0.13	20,20,20,20	0
83	MG	3	211	1/1	0.90	0.17	34,34,34,34	0
83	MG	B	1870	1/1	0.90	0.10	42,42,42,42	0
83	MG	AG	202	1/1	0.90	0.14	52,52,52,52	0
83	MG	AS	3536	1/1	0.90	0.12	35,35,35,35	0
83	MG	1	3759	1/1	0.90	0.10	49,49,49,49	0
83	MG	1	3762	1/1	0.90	0.14	31,31,31,31	0
83	MG	CM	1885	1/1	0.90	0.11	26,26,26,26	0
83	MG	CM	1890	1/1	0.90	0.11	24,24,24,24	0
83	MG	1	3693	1/1	0.90	0.11	37,37,37,37	0
83	MG	CM	1897	1/1	0.90	0.21	41,41,41,41	0
83	MG	1	3904	1/1	0.90	0.16	32,32,32,32	0
83	MG	1	3429	1/1	0.90	0.24	24,24,24,24	0
83	MG	1	3697	1/1	0.90	0.10	50,50,50,50	0
83	MG	CP	301	1/1	0.90	0.24	32,32,32,32	0
83	MG	AS	3550	1/1	0.90	0.20	19,19,19,19	0
83	MG	AS	3552	1/1	0.90	0.17	27,27,27,27	0
83	MG	4	212	1/1	0.90	0.10	60,60,60,60	0
83	MG	K	301	1/1	0.90	0.06	27,27,27,27	0
83	MG	AS	3565	1/1	0.90	0.23	31,31,31,31	0
84	3K5	1	3402	57/57	0.90	0.18	26,53,74,90	0
84	3K5	AS	3401	57/57	0.90	0.17	41,66,88,90	0
83	MG	AS	3567	1/1	0.90	0.12	45,45,45,45	0
85	ZN	h	201	1/1	0.90	0.10	209,209,209,209	0
83	MG	1	3907	1/1	0.90	0.19	74,74,74,74	0
83	MG	BE	301	1/1	0.90	0.17	33,33,33,33	0
83	MG	1	3771	1/1	0.90	0.14	38,38,38,38	0
86	HYG	CM	1902	36/36	0.90	0.13	34,53,79,89	0
83	MG	CM	1805	1/1	0.91	0.13	18,18,18,18	0
83	MG	1	3586	1/1	0.91	0.13	47,47,47,47	0
83	MG	CM	1807	1/1	0.91	0.22	37,37,37,37	0
83	MG	1	3880	1/1	0.91	0.26	58,58,58,58	0
83	MG	1	3698	1/1	0.91	0.22	58,58,58,58	0
83	MG	B	1951	1/1	0.91	0.12	29,29,29,29	0
83	MG	1	3780	1/1	0.91	0.19	32,32,32,32	0
83	MG	G	301	1/1	0.91	0.14	72,72,72,72	0
83	MG	AS	3497	1/1	0.91	0.13	26,26,26,26	0
83	MG	1	3851	1/1	0.91	0.07	19,19,19,19	0
83	MG	AS	3502	1/1	0.91	0.18	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AD	201	1/1	0.91	0.17	59,59,59,59	0
83	MG	B	1842	1/1	0.91	0.17	25,25,25,25	0
83	MG	j	303	1/1	0.91	0.10	19,19,19,19	0
83	MG	AS	3514	1/1	0.91	0.18	22,22,22,22	0
83	MG	1	3490	1/1	0.91	0.16	44,44,44,44	0
83	MG	R	201	1/1	0.91	0.13	83,83,83,83	0
83	MG	B	1904	1/1	0.91	0.08	36,36,36,36	0
83	MG	1	3820	1/1	0.91	0.07	29,29,29,29	0
83	MG	AS	3523	1/1	0.91	0.19	29,29,29,29	0
83	MG	AS	3534	1/1	0.91	0.17	38,38,38,38	0
83	MG	1	3567	1/1	0.91	0.08	20,20,20,20	0
83	MG	CM	1849	1/1	0.91	0.15	50,50,50,50	0
83	MG	Z	201	1/1	0.91	0.33	54,54,54,54	0
83	MG	CM	1851	1/1	0.91	0.14	28,28,28,28	0
83	MG	B	1847	1/1	0.91	0.14	35,35,35,35	0
83	MG	1	3510	1/1	0.91	0.12	23,23,23,23	0
83	MG	1	3792	1/1	0.91	0.16	32,32,32,32	0
83	MG	1	3705	1/1	0.91	0.12	34,34,34,34	0
83	MG	1	3430	1/1	0.91	0.11	50,50,50,50	0
83	MG	B	1858	1/1	0.91	0.15	66,66,66,66	0
83	MG	AS	3408	1/1	0.91	0.09	28,28,28,28	0
83	MG	AS	3672	1/1	0.91	0.09	29,29,29,29	0
83	MG	1	3760	1/1	0.91	0.11	55,55,55,55	0
83	MG	B	1860	1/1	0.91	0.10	78,78,78,78	0
83	MG	B	1803	1/1	0.91	0.16	28,28,28,28	0
83	MG	1	3658	1/1	0.91	0.11	39,39,39,39	0
83	MG	1	3901	1/1	0.91	0.10	29,29,29,29	0
83	MG	AT	201	1/1	0.91	0.13	21,21,21,21	0
83	MG	1	3690	1/1	0.91	0.08	25,25,25,25	0
83	MG	AS	3421	1/1	0.91	0.35	19,19,19,19	0
83	MG	1	3621	1/1	0.91	0.12	54,54,54,54	0
83	MG	AS	3584	1/1	0.91	0.19	37,37,37,37	0
83	MG	CM	1888	1/1	0.91	0.09	47,47,47,47	0
83	MG	B	1930	1/1	0.91	0.15	60,60,60,60	0
83	MG	AT	208	1/1	0.91	0.13	27,27,27,27	0
83	MG	AS	3588	1/1	0.91	0.10	21,21,21,21	0
83	MG	AS	3593	1/1	0.91	0.09	16,16,16,16	0
83	MG	1	3446	1/1	0.91	0.11	71,71,71,71	0
83	MG	BB	302	1/1	0.91	0.14	53,53,53,53	0
83	MG	1	3608	1/1	0.91	0.38	67,67,67,67	0
83	MG	0	203	1/1	0.91	0.13	75,75,75,75	0
83	MG	B	1818	1/1	0.91	0.10	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	B	1821	1/1	0.91	0.21	31,31,31,31	0
83	MG	BJ	302	1/1	0.91	0.17	58,58,58,58	0
83	MG	1	3628	1/1	0.91	0.27	48,48,48,48	0
83	MG	B	1884	1/1	0.91	0.09	97,97,97,97	0
83	MG	BZ	201	1/1	0.91	0.18	41,41,41,41	0
85	ZN	AH	201	1/1	0.91	0.11	138,138,138,138	0
85	ZN	AP	201	1/1	0.91	0.09	181,181,181,181	0
83	MG	AS	3604	1/1	0.91	0.26	46,46,46,46	0
83	MG	AS	3465	1/1	0.91	0.15	19,19,19,19	0
83	MG	1	3695	1/1	0.91	0.22	32,32,32,32	0
83	MG	3	213	1/1	0.91	0.15	49,49,49,49	0
83	MG	1	3809	1/1	0.91	0.07	57,57,57,57	0
83	MG	1	3739	1/1	0.91	0.19	28,28,28,28	0
83	MG	1	3531	1/1	0.92	0.17	39,39,39,39	0
83	MG	AS	3591	1/1	0.92	0.17	52,52,52,52	0
83	MG	B	1923	1/1	0.92	0.17	57,57,57,57	0
83	MG	1	3758	1/1	0.92	0.15	33,33,33,33	0
83	MG	1	3813	1/1	0.92	0.12	27,27,27,27	0
83	MG	1	3535	1/1	0.92	0.14	34,34,34,34	0
83	MG	1	3431	1/1	0.92	0.18	20,20,20,20	0
83	MG	1	3644	1/1	0.92	0.08	20,20,20,20	0
83	MG	CM	1801	1/1	0.92	0.24	41,41,41,41	0
83	MG	1	3513	1/1	0.92	0.18	23,23,23,23	0
83	MG	AS	3459	1/1	0.92	0.14	50,50,50,50	0
83	MG	AS	3460	1/1	0.92	0.16	51,51,51,51	0
83	MG	AS	3462	1/1	0.92	0.25	31,31,31,31	0
83	MG	1	3443	1/1	0.92	0.19	44,44,44,44	0
83	MG	CM	1813	1/1	0.92	0.25	35,35,35,35	0
83	MG	1	3825	1/1	0.92	0.11	39,39,39,39	0
83	MG	1	3542	1/1	0.92	0.17	28,28,28,28	0
83	MG	AS	3469	1/1	0.92	0.27	25,25,25,25	0
83	MG	AS	3472	1/1	0.92	0.26	36,36,36,36	0
83	MG	AC	101	1/1	0.92	0.12	41,41,41,41	0
83	MG	AS	3623	1/1	0.92	0.23	32,32,32,32	0
83	MG	1	3649	1/1	0.92	0.19	38,38,38,38	0
83	MG	AS	3476	1/1	0.92	0.24	34,34,34,34	0
83	MG	1	3493	1/1	0.92	0.20	30,30,30,30	0
83	MG	1	3883	1/1	0.92	0.09	28,28,28,28	0
83	MG	CM	1828	1/1	0.92	0.25	22,22,22,22	0
83	MG	CM	1832	1/1	0.92	0.20	14,14,14,14	0
83	MG	AS	3487	1/1	0.92	0.16	20,20,20,20	0
83	MG	1	3576	1/1	0.92	0.16	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3687	1/1	0.92	0.13	39,39,39,39	0
83	MG	1	3577	1/1	0.92	0.14	12,12,12,12	0
83	MG	AS	3634	1/1	0.92	0.09	52,52,52,52	0
83	MG	CM	1841	1/1	0.92	0.33	45,45,45,45	0
83	MG	CM	1843	1/1	0.92	0.10	26,26,26,26	0
83	MG	1	3427	1/1	0.92	0.24	16,16,16,16	0
83	MG	1	3469	1/1	0.92	0.17	28,28,28,28	0
83	MG	AS	3640	1/1	0.92	0.16	46,46,46,46	0
83	MG	1	3415	1/1	0.92	0.24	23,23,23,23	0
83	MG	B	1950	1/1	0.92	0.09	40,40,40,40	0
83	MG	AP	203	1/1	0.92	0.14	73,73,73,73	0
83	MG	CM	1855	1/1	0.92	0.17	29,29,29,29	0
83	MG	CM	1857	1/1	0.92	0.12	48,48,48,48	0
83	MG	4	205	1/1	0.92	0.08	33,33,33,33	0
83	MG	1	3551	1/1	0.92	0.10	36,36,36,36	0
83	MG	1	3840	1/1	0.92	0.06	14,14,14,14	0
83	MG	1	3787	1/1	0.92	0.23	23,23,23,23	0
83	MG	1	3788	1/1	0.92	0.18	23,23,23,23	0
83	MG	1	3789	1/1	0.92	0.16	21,21,21,21	0
83	MG	AS	3655	1/1	0.92	0.20	55,55,55,55	0
83	MG	1	3900	1/1	0.92	0.16	29,29,29,29	0
83	MG	CM	1871	1/1	0.92	0.17	22,22,22,22	0
83	MG	1	3730	1/1	0.92	0.25	55,55,55,55	0
83	MG	AS	3524	1/1	0.92	0.22	27,27,27,27	0
83	MG	AS	3525	1/1	0.92	0.24	32,32,32,32	0
83	MG	AS	3665	1/1	0.92	0.14	51,51,51,51	0
83	MG	AS	3528	1/1	0.92	0.14	41,41,41,41	0
83	MG	1	3620	1/1	0.92	0.14	21,21,21,21	0
83	MG	AS	3535	1/1	0.92	0.19	27,27,27,27	0
83	MG	1	3846	1/1	0.92	0.09	44,44,44,44	0
83	MG	1	3473	1/1	0.92	0.19	13,13,13,13	0
83	MG	o	301	1/1	0.92	0.07	21,21,21,21	0
83	MG	1	3451	1/1	0.92	0.11	26,26,26,26	0
83	MG	1	3623	1/1	0.92	0.10	40,40,40,40	0
83	MG	1	3624	1/1	0.92	0.20	24,24,24,24	0
83	MG	1	3425	1/1	0.92	0.12	36,36,36,36	0
83	MG	1	3426	1/1	0.92	0.14	24,24,24,24	0
83	MG	1	3702	1/1	0.92	0.15	33,33,33,33	0
83	MG	AS	3556	1/1	0.92	0.18	37,37,37,37	0
83	MG	1	3463	1/1	0.92	0.16	18,18,18,18	0
83	MG	1	3751	1/1	0.92	0.18	43,43,43,43	0
83	MG	x	201	1/1	0.92	0.18	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
83	MG	AS	3566	1/1	0.92	0.14	26,26,26,26	0
83	MG	AW	302	1/1	0.92	0.09	29,29,29,29	0
83	MG	x	202	1/1	0.92	0.06	20,20,20,20	0
83	MG	B	1913	1/1	0.92	0.11	49,49,49,49	0
83	MG	B	1914	1/1	0.92	0.07	47,47,47,47	0
83	MG	AS	3574	1/1	0.92	0.07	17,17,17,17	0
83	MG	AS	3575	1/1	0.92	0.10	33,33,33,33	0
83	MG	1	3508	1/1	0.92	0.17	33,33,33,33	0
83	MG	1	3710	1/1	0.92	0.10	38,38,38,38	0
83	MG	BJ	301	1/1	0.92	0.16	22,22,22,22	0
83	MG	AS	3425	1/1	0.92	0.19	17,17,17,17	0
83	MG	1	3922	1/1	0.92	0.25	42,42,42,42	0
83	MG	1	3626	1/1	0.93	0.16	46,46,46,46	0
83	MG	1	3601	1/1	0.93	0.11	61,61,61,61	0
83	MG	1	3424	1/1	0.93	0.19	14,14,14,14	0
83	MG	CM	1804	1/1	0.93	0.22	25,25,25,25	0
83	MG	AS	3612	1/1	0.93	0.11	25,25,25,25	0
83	MG	2	202	1/1	0.93	0.10	34,34,34,34	0
83	MG	AS	3495	1/1	0.93	0.24	33,33,33,33	0
83	MG	B	1901	1/1	0.93	0.13	43,43,43,43	0
83	MG	CM	1810	1/1	0.93	0.13	46,46,46,46	0
83	MG	3	208	1/1	0.93	0.09	47,47,47,47	0
83	MG	1	3462	1/1	0.93	0.15	19,19,19,19	0
83	MG	CM	1814	1/1	0.93	0.12	19,19,19,19	0
83	MG	CM	1815	1/1	0.93	0.15	28,28,28,28	0
83	MG	1	3741	1/1	0.93	0.23	18,18,18,18	0
83	MG	AS	3503	1/1	0.93	0.15	21,21,21,21	0
83	MG	1	3857	1/1	0.93	0.10	40,40,40,40	0
83	MG	AS	3505	1/1	0.93	0.07	12,12,12,12	0
83	MG	Y	203	1/1	0.93	0.25	41,41,41,41	0
83	MG	1	3784	1/1	0.93	0.16	30,30,30,30	0
83	MG	1	3859	1/1	0.93	0.13	77,77,77,77	0
83	MG	1	3633	1/1	0.93	0.12	40,40,40,40	0
83	MG	1	3496	1/1	0.93	0.11	31,31,31,31	0
83	MG	1	3565	1/1	0.93	0.17	44,44,44,44	0
83	MG	AS	3635	1/1	0.93	0.22	44,44,44,44	0
83	MG	1	3863	1/1	0.93	0.13	29,29,29,29	0
83	MG	AS	3520	1/1	0.93	0.15	20,20,20,20	0
83	MG	AS	3522	1/1	0.93	0.11	30,30,30,30	0
83	MG	B	1848	1/1	0.93	0.15	30,30,30,30	0
83	MG	1	3831	1/1	0.93	0.18	80,80,80,80	0
83	MG	CM	1838	1/1	0.93	0.14	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
83	MG	1	3485	1/1	0.93	0.12	37,37,37,37	0
83	MG	1	3615	1/1	0.93	0.17	51,51,51,51	0
83	MG	AS	3529	1/1	0.93	0.10	55,55,55,55	0
83	MG	AS	3533	1/1	0.93	0.19	40,40,40,40	0
83	MG	1	3910	1/1	0.93	0.09	64,64,64,64	0
83	MG	1	3590	1/1	0.93	0.12	17,17,17,17	0
83	MG	1	3646	1/1	0.93	0.21	48,48,48,48	0
83	MG	AS	3654	1/1	0.93	0.06	17,17,17,17	0
83	MG	1	3487	1/1	0.93	0.07	11,11,11,11	0
83	MG	1	3915	1/1	0.93	0.07	17,17,17,17	0
83	MG	B	1863	1/1	0.93	0.20	58,58,58,58	0
83	MG	AS	3659	1/1	0.93	0.09	18,18,18,18	0
83	MG	AS	3660	1/1	0.93	0.09	27,27,27,27	0
83	MG	1	3403	1/1	0.93	0.22	25,25,25,25	0
83	MG	CM	1861	1/1	0.93	0.09	24,24,24,24	0
83	MG	CM	1862	1/1	0.93	0.13	29,29,29,29	0
83	MG	1	3919	1/1	0.93	0.35	51,51,51,51	0
83	MG	AS	3546	1/1	0.93	0.15	15,15,15,15	0
83	MG	1	3471	1/1	0.93	0.14	21,21,21,21	0
83	MG	AS	3549	1/1	0.93	0.34	33,33,33,33	0
83	MG	CM	1869	1/1	0.93	0.13	17,17,17,17	0
83	MG	AS	3434	1/1	0.93	0.18	18,18,18,18	0
83	MG	AS	3435	1/1	0.93	0.24	30,30,30,30	0
83	MG	1	3538	1/1	0.93	0.16	48,48,48,48	0
83	MG	AS	3674	1/1	0.93	0.20	44,44,44,44	0
83	MG	1	3454	1/1	0.93	0.06	9,9,9,9	0
83	MG	AS	3444	1/1	0.93	0.15	15,15,15,15	0
83	MG	CM	1878	1/1	0.93	0.18	33,33,33,33	0
83	MG	1	3704	1/1	0.93	0.13	30,30,30,30	0
83	MG	CM	1881	1/1	0.93	0.08	11,11,11,11	0
83	MG	B	1937	1/1	0.93	0.18	47,47,47,47	0
83	MG	B	1874	1/1	0.93	0.17	37,37,37,37	0
83	MG	B	1808	1/1	0.93	0.14	29,29,29,29	0
83	MG	AS	3457	1/1	0.93	0.10	23,23,23,23	0
83	MG	u	201	1/1	0.93	0.11	28,28,28,28	0
83	MG	1	3769	1/1	0.93	0.12	21,21,21,21	0
83	MG	AS	3577	1/1	0.93	0.24	30,30,30,30	0
83	MG	CM	1895	1/1	0.93	0.20	21,21,21,21	0
83	MG	AS	3578	1/1	0.93	0.20	27,27,27,27	0
83	MG	AS	3579	1/1	0.93	0.19	38,38,38,38	0
83	MG	AU	202	1/1	0.93	0.20	31,31,31,31	0
83	MG	CM	1901	1/1	0.93	0.09	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3882	1/1	0.93	0.16	39,39,39,39	0
83	MG	1	3770	1/1	0.93	0.12	46,46,46,46	0
83	MG	1	3578	1/1	0.93	0.21	27,27,27,27	0
83	MG	B	1820	1/1	0.93	0.12	22,22,22,22	0
83	MG	B	1888	1/1	0.93	0.22	52,52,52,52	0
83	MG	AS	3589	1/1	0.93	0.17	21,21,21,21	0
83	MG	AS	3590	1/1	0.93	0.17	33,33,33,33	0
83	MG	AS	3470	1/1	0.93	0.19	31,31,31,31	0
83	MG	1	3505	1/1	0.93	0.06	22,22,22,22	0
83	MG	AS	3594	1/1	0.93	0.10	34,34,34,34	0
83	MG	1	3847	1/1	0.93	0.07	36,36,36,36	0
83	MG	1	3733	1/1	0.93	0.22	11,11,11,11	0
83	MG	1	3439	1/1	0.93	0.18	20,20,20,20	0
83	MG	AS	3480	1/1	0.93	0.11	29,29,29,29	0
85	ZN	CJ	201	1/1	0.93	0.11	211,211,211,211	0
83	MG	D	301	1/1	0.93	0.16	38,38,38,38	0
83	MG	B	1826	1/1	0.93	0.14	43,43,43,43	0
83	MG	AS	3486	1/1	0.93	0.12	28,28,28,28	0
83	MG	AS	3415	1/1	0.94	0.23	22,22,22,22	0
83	MG	1	3602	1/1	0.94	0.07	28,28,28,28	0
83	MG	AS	3636	1/1	0.94	0.11	42,42,42,42	0
83	MG	AS	3532	1/1	0.94	0.27	23,23,23,23	0
83	MG	1	3886	1/1	0.94	0.09	27,27,27,27	0
83	MG	AS	3639	1/1	0.94	0.12	37,37,37,37	0
83	MG	1	3467	1/1	0.94	0.20	37,37,37,37	0
83	MG	3	205	1/1	0.94	0.16	27,27,27,27	0
83	MG	1	3604	1/1	0.94	0.15	25,25,25,25	0
83	MG	1	3660	1/1	0.94	0.08	25,25,25,25	0
83	MG	CM	1826	1/1	0.94	0.10	34,34,34,34	0
83	MG	1	3606	1/1	0.94	0.13	58,58,58,58	0
83	MG	1	3801	1/1	0.94	0.09	29,29,29,29	0
83	MG	AS	3647	1/1	0.94	0.16	45,45,45,45	0
83	MG	B	1852	1/1	0.94	0.11	26,26,26,26	0
83	MG	AS	3542	1/1	0.94	0.17	37,37,37,37	0
83	MG	AS	3651	1/1	0.94	0.07	17,17,17,17	0
83	MG	B	1853	1/1	0.94	0.20	27,27,27,27	0
83	MG	AS	3437	1/1	0.94	0.16	33,33,33,33	0
83	MG	1	3761	1/1	0.94	0.09	18,18,18,18	0
83	MG	1	3519	1/1	0.94	0.15	41,41,41,41	0
83	MG	1	3520	1/1	0.94	0.17	25,25,25,25	0
83	MG	B	1929	1/1	0.94	0.11	37,37,37,37	0
83	MG	CM	1847	1/1	0.94	0.16	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
83	MG	AS	3554	1/1	0.94	0.16	18,18,18,18	0
83	MG	1	3634	1/1	0.94	0.11	43,43,43,43	0
83	MG	1	3665	1/1	0.94	0.06	24,24,24,24	0
83	MG	B	1861	1/1	0.94	0.10	45,45,45,45	0
83	MG	4	204	1/1	0.94	0.15	25,25,25,25	0
83	MG	1	3609	1/1	0.94	0.06	20,20,20,20	0
83	MG	1	3610	1/1	0.94	0.20	47,47,47,47	0
83	MG	AS	3669	1/1	0.94	0.21	56,56,56,56	0
83	MG	1	3903	1/1	0.94	0.13	56,56,56,56	0
83	MG	AS	3569	1/1	0.94	0.16	33,33,33,33	0
83	MG	AS	3571	1/1	0.94	0.17	14,14,14,14	0
83	MG	1	3814	1/1	0.94	0.07	33,33,33,33	0
83	MG	B	1867	1/1	0.94	0.09	49,49,49,49	0
83	MG	4	210	1/1	0.94	0.07	34,34,34,34	0
83	MG	1	3670	1/1	0.94	0.09	47,47,47,47	0
83	MG	j	301	1/1	0.94	0.07	15,15,15,15	0
83	MG	B	1873	1/1	0.94	0.16	48,48,48,48	0
83	MG	B	1945	1/1	0.94	0.21	56,56,56,56	0
83	MG	1	3816	1/1	0.94	0.17	28,28,28,28	0
83	MG	1	3459	1/1	0.94	0.10	20,20,20,20	0
83	MG	CM	1873	1/1	0.94	0.21	40,40,40,40	0
83	MG	1	3574	1/1	0.94	0.12	22,22,22,22	0
83	MG	CM	1875	1/1	0.94	0.08	18,18,18,18	0
83	MG	B	1878	1/1	0.94	0.17	14,14,14,14	0
83	MG	1	3592	1/1	0.94	0.22	43,43,43,43	0
83	MG	1	3821	1/1	0.94	0.22	43,43,43,43	0
83	MG	AU	201	1/1	0.94	0.09	40,40,40,40	0
83	MG	B	1883	1/1	0.94	0.17	23,23,23,23	0
83	MG	1	3864	1/1	0.94	0.14	41,41,41,41	0
83	MG	B	1813	1/1	0.94	0.13	19,19,19,19	0
83	MG	1	3460	1/1	0.94	0.17	15,15,15,15	0
83	MG	o	302	1/1	0.94	0.12	16,16,16,16	0
83	MG	CM	1886	1/1	0.94	0.23	40,40,40,40	0
83	MG	1	3777	1/1	0.94	0.19	21,21,21,21	0
83	MG	1	3703	1/1	0.94	0.23	48,48,48,48	0
83	MG	1	3916	1/1	0.94	0.09	45,45,45,45	0
83	MG	AS	3501	1/1	0.94	0.12	40,40,40,40	0
83	MG	1	3779	1/1	0.94	0.22	33,33,33,33	0
83	MG	1	3441	1/1	0.94	0.21	29,29,29,29	0
83	MG	1	3445	1/1	0.94	0.17	25,25,25,25	0
83	MG	1	3678	1/1	0.94	0.15	19,19,19,19	0
83	MG	CM	1903	1/1	0.94	0.09	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AS	3610	1/1	0.94	0.07	35,35,35,35	0
83	MG	1	3709	1/1	0.94	0.16	25,25,25,25	0
83	MG	AS	3614	1/1	0.94	0.09	16,16,16,16	0
83	MG	AS	3508	1/1	0.94	0.06	46,46,46,46	0
83	MG	DB	202	1/1	0.94	0.15	57,57,57,57	0
83	MG	AS	3511	1/1	0.94	0.27	50,50,50,50	0
83	MG	1	3453	1/1	0.94	0.13	33,33,33,33	0
83	MG	1	3878	1/1	0.94	0.15	34,34,34,34	0
83	MG	DQ	101	1/1	0.94	0.10	42,42,42,42	0
83	MG	1	3744	1/1	0.94	0.18	23,23,23,23	0
83	MG	CM	1802	1/1	0.94	0.26	15,15,15,15	0
83	MG	y	201	1/1	0.94	0.09	12,12,12,12	0
83	MG	AS	3403	1/1	0.94	0.19	5,5,5,5	0
83	MG	1	3560	1/1	0.94	0.14	24,24,24,24	0
83	MG	B	1834	1/1	0.94	0.11	29,29,29,29	0
83	MG	1	3458	1/1	0.94	0.21	8,8,8,8	0
83	MG	1	3749	1/1	0.94	0.15	20,20,20,20	0
83	MG	1	3546	1/1	0.94	0.12	36,36,36,36	0
83	MG	1	3482	1/1	0.94	0.24	23,23,23,23	0
83	MG	AS	3526	1/1	0.94	0.08	27,27,27,27	0
83	MG	1	3782	1/1	0.95	0.12	28,28,28,28	0
83	MG	1	3549	1/1	0.95	0.18	32,32,32,32	0
83	MG	B	1857	1/1	0.95	0.16	37,37,37,37	0
83	MG	1	3737	1/1	0.95	0.16	15,15,15,15	0
83	MG	1	3738	1/1	0.95	0.11	21,21,21,21	0
83	MG	AS	3541	1/1	0.95	0.09	49,49,49,49	0
83	MG	1	3504	1/1	0.95	0.10	21,21,21,21	0
83	MG	1	3888	1/1	0.95	0.17	28,28,28,28	0
83	MG	AS	3545	1/1	0.95	0.22	15,15,15,15	0
83	MG	1	3452	1/1	0.95	0.16	19,19,19,19	0
83	MG	CM	1830	1/1	0.95	0.18	25,25,25,25	0
83	MG	1	3506	1/1	0.95	0.07	26,26,26,26	0
83	MG	AS	3650	1/1	0.95	0.08	7,7,7,7	0
83	MG	1	3743	1/1	0.95	0.11	25,25,25,25	0
83	MG	4	201	1/1	0.95	0.25	41,41,41,41	0
83	MG	1	3642	1/1	0.95	0.19	16,16,16,16	0
83	MG	AS	3553	1/1	0.95	0.11	46,46,46,46	0
83	MG	1	3406	1/1	0.95	0.24	26,26,26,26	0
83	MG	AS	3461	1/1	0.95	0.17	23,23,23,23	0
83	MG	1	3795	1/1	0.95	0.15	37,37,37,37	0
83	MG	CM	1844	1/1	0.95	0.13	26,26,26,26	0
83	MG	AS	3464	1/1	0.95	0.18	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3412	1/1	0.95	0.25	19,19,19,19	0
83	MG	B	1801	1/1	0.95	0.07	69,69,69,69	0
83	MG	B	1872	1/1	0.95	0.13	40,40,40,40	0
83	MG	1	3748	1/1	0.95	0.15	28,28,28,28	0
83	MG	1	3897	1/1	0.95	0.19	52,52,52,52	0
83	MG	CM	1852	1/1	0.95	0.07	24,24,24,24	0
83	MG	AS	3471	1/1	0.95	0.24	51,51,51,51	0
83	MG	1	3898	1/1	0.95	0.07	16,16,16,16	0
83	MG	4	211	1/1	0.95	0.08	11,11,11,11	0
83	MG	1	3557	1/1	0.95	0.15	34,34,34,34	0
83	MG	1	3711	1/1	0.95	0.06	22,22,22,22	0
83	MG	AS	3479	1/1	0.95	0.13	30,30,30,30	0
83	MG	1	3850	1/1	0.95	0.07	22,22,22,22	0
83	MG	B	1811	1/1	0.95	0.17	27,27,27,27	0
83	MG	CM	1863	1/1	0.95	0.12	44,44,44,44	0
83	MG	1	3712	1/1	0.95	0.11	41,41,41,41	0
83	MG	B	1885	1/1	0.95	0.08	45,45,45,45	0
83	MG	1	3612	1/1	0.95	0.10	27,27,27,27	0
83	MG	AS	3587	1/1	0.95	0.10	14,14,14,14	0
83	MG	1	3405	1/1	0.95	0.23	21,21,21,21	0
83	MG	1	3532	1/1	0.95	0.15	15,15,15,15	0
83	MG	1	3616	1/1	0.95	0.18	22,22,22,22	0
83	MG	AS	3494	1/1	0.95	0.16	31,31,31,31	0
83	MG	1	3808	1/1	0.95	0.12	28,28,28,28	0
83	MG	1	3650	1/1	0.95	0.11	34,34,34,34	0
83	MG	1	3512	1/1	0.95	0.17	49,49,49,49	0
83	MG	1	3561	1/1	0.95	0.07	26,26,26,26	0
83	MG	AW	301	1/1	0.95	0.11	30,30,30,30	0
83	MG	1	3456	1/1	0.95	0.07	6,6,6,6	0
83	MG	AW	303	1/1	0.95	0.08	34,34,34,34	0
83	MG	1	3414	1/1	0.95	0.21	20,20,20,20	0
83	MG	1	3410	1/1	0.95	0.19	7,7,7,7	0
83	MG	1	3768	1/1	0.95	0.08	27,27,27,27	0
83	MG	1	3917	1/1	0.95	0.08	79,79,79,79	0
83	MG	1	3516	1/1	0.95	0.16	30,30,30,30	0
83	MG	1	3416	1/1	0.95	0.16	25,25,25,25	0
83	MG	CM	1887	1/1	0.95	0.19	16,16,16,16	0
83	MG	1	3819	1/1	0.95	0.19	13,13,13,13	0
83	MG	AS	3607	1/1	0.95	0.13	37,37,37,37	0
83	MG	AS	3609	1/1	0.95	0.06	8,8,8,8	0
83	MG	1	3869	1/1	0.95	0.07	37,37,37,37	0
83	MG	AS	3611	1/1	0.95	0.12	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
83	MG	AS	3513	1/1	0.95	0.14	28,28,28,28	0
83	MG	1	3870	1/1	0.95	0.14	43,43,43,43	0
83	MG	AS	3406	1/1	0.95	0.23	17,17,17,17	0
83	MG	1	3659	1/1	0.95	0.11	24,24,24,24	0
83	MG	1	3436	1/1	0.95	0.16	23,23,23,23	0
83	MG	1	3823	1/1	0.95	0.11	34,34,34,34	0
83	MG	1	3448	1/1	0.95	0.16	14,14,14,14	0
83	MG	1	3571	1/1	0.95	0.14	15,15,15,15	0
83	MG	2	201	1/1	0.95	0.17	75,75,75,75	0
83	MG	1	3450	1/1	0.95	0.17	32,32,32,32	0
83	MG	1	3696	1/1	0.95	0.11	19,19,19,19	0
83	MG	1	3418	1/1	0.95	0.15	33,33,33,33	0
83	MG	AS	3527	1/1	0.95	0.09	35,35,35,35	0
83	MG	1	3486	1/1	0.95	0.17	18,18,18,18	0
83	MG	CM	1809	1/1	0.95	0.13	67,67,67,67	0
83	MG	B	1921	1/1	0.95	0.08	24,24,24,24	0
83	MG	AS	3530	1/1	0.95	0.17	34,34,34,34	0
83	MG	CM	1812	1/1	0.95	0.14	41,41,41,41	0
83	MG	AS	3633	1/1	0.95	0.05	43,43,43,43	0
83	MG	1	3666	1/1	0.95	0.09	27,27,27,27	0
83	MG	1	3667	1/1	0.95	0.05	16,16,16,16	0
83	MG	AS	3430	1/1	0.95	0.29	31,31,31,31	0
83	MG	CM	1817	1/1	0.95	0.11	19,19,19,19	0
83	MG	AS	3432	1/1	0.95	0.14	12,12,12,12	0
83	MG	AS	3509	1/1	0.96	0.10	29,29,29,29	0
83	MG	AS	3613	1/1	0.96	0.10	28,28,28,28	0
83	MG	AS	3510	1/1	0.96	0.15	28,28,28,28	0
83	MG	1	3786	1/1	0.96	0.08	24,24,24,24	0
83	MG	AS	3409	1/1	0.96	0.12	9,9,9,9	0
83	MG	AS	3617	1/1	0.96	0.07	25,25,25,25	0
83	MG	AS	3410	1/1	0.96	0.19	26,26,26,26	0
83	MG	1	3828	1/1	0.96	0.08	36,36,36,36	0
83	MG	1	3581	1/1	0.96	0.09	24,24,24,24	0
83	MG	1	3750	1/1	0.96	0.16	39,39,39,39	0
83	MG	1	3632	1/1	0.96	0.12	20,20,20,20	0
83	MG	AS	3625	1/1	0.96	0.18	42,42,42,42	0
83	MG	AF	201	1/1	0.96	0.12	23,23,23,23	0
83	MG	AS	3418	1/1	0.96	0.25	19,19,19,19	0
83	MG	1	3752	1/1	0.96	0.12	39,39,39,39	0
83	MG	B	1917	1/1	0.96	0.11	24,24,24,24	0
83	MG	1	3791	1/1	0.96	0.13	46,46,46,46	0
83	MG	AS	3424	1/1	0.96	0.19	15,15,15,15	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	1	3834	1/1	0.96	0.19	21,21,21,21	0
83	MG	1	3521	1/1	0.96	0.14	26,26,26,26	0
83	MG	1	3541	1/1	0.96	0.08	34,34,34,34	0
83	MG	1	3522	1/1	0.96	0.07	24,24,24,24	0
83	MG	CM	1829	1/1	0.96	0.13	25,25,25,25	0
83	MG	AS	3429	1/1	0.96	0.16	17,17,17,17	0
83	MG	AS	3531	1/1	0.96	0.12	45,45,45,45	0
83	MG	1	3756	1/1	0.96	0.14	31,31,31,31	0
83	MG	CM	1834	1/1	0.96	0.22	28,28,28,28	0
83	MG	AS	3431	1/1	0.96	0.19	8,8,8,8	0
83	MG	1	3638	1/1	0.96	0.15	9,9,9,9	0
83	MG	1	3422	1/1	0.96	0.22	14,14,14,14	0
83	MG	1	3544	1/1	0.96	0.28	19,19,19,19	0
83	MG	AS	3436	1/1	0.96	0.16	10,10,10,10	0
83	MG	B	1804	1/1	0.96	0.15	14,14,14,14	0
83	MG	CM	1842	1/1	0.96	0.09	45,45,45,45	0
83	MG	AS	3439	1/1	0.96	0.13	32,32,32,32	0
83	MG	AS	3440	1/1	0.96	0.17	17,17,17,17	0
83	MG	1	3589	1/1	0.96	0.13	16,16,16,16	0
83	MG	CM	1846	1/1	0.96	0.08	18,18,18,18	0
83	MG	1	3613	1/1	0.96	0.18	24,24,24,24	0
83	MG	1	3404	1/1	0.96	0.14	30,30,30,30	0
83	MG	AS	3446	1/1	0.96	0.21	22,22,22,22	0
83	MG	1	3447	1/1	0.96	0.12	10,10,10,10	0
83	MG	B	1809	1/1	0.96	0.07	79,79,79,79	0
83	MG	AS	3548	1/1	0.96	0.13	26,26,26,26	0
83	MG	B	1936	1/1	0.96	0.09	25,25,25,25	0
83	MG	CM	1854	1/1	0.96	0.20	27,27,27,27	0
83	MG	1	3927	1/1	0.96	0.07	22,22,22,22	0
83	MG	B	1871	1/1	0.96	0.12	63,63,63,63	0
83	MG	1	3511	1/1	0.96	0.19	14,14,14,14	0
83	MG	v	302	1/1	0.96	0.07	19,19,19,19	0
83	MG	AS	3555	1/1	0.96	0.15	11,11,11,11	0
83	MG	1	3805	1/1	0.96	0.07	27,27,27,27	0
83	MG	AS	3663	1/1	0.96	0.19	42,42,42,42	0
83	MG	AS	3558	1/1	0.96	0.05	25,25,25,25	0
83	MG	w	301	1/1	0.96	0.09	22,22,22,22	0
83	MG	AS	3561	1/1	0.96	0.19	18,18,18,18	0
83	MG	AS	3463	1/1	0.96	0.18	34,34,34,34	0
83	MG	AS	3563	1/1	0.96	0.14	17,17,17,17	0
83	MG	B	1876	1/1	0.96	0.12	54,54,54,54	0
83	MG	1	3461	1/1	0.96	0.14	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AS	3466	1/1	0.96	0.14	25,25,25,25	0
83	MG	1	3474	1/1	0.96	0.26	21,21,21,21	0
83	MG	B	1819	1/1	0.96	0.20	16,16,16,16	0
83	MG	B	1881	1/1	0.96	0.12	51,51,51,51	0
83	MG	B	1948	1/1	0.96	0.18	22,22,22,22	0
83	MG	1	3437	1/1	0.96	0.19	19,19,19,19	0
83	MG	1	3596	1/1	0.96	0.11	36,36,36,36	0
83	MG	AS	3576	1/1	0.96	0.15	24,24,24,24	0
83	MG	B	1822	1/1	0.96	0.18	22,22,22,22	0
83	MG	AT	205	1/1	0.96	0.16	22,22,22,22	0
83	MG	x	203	1/1	0.96	0.15	24,24,24,24	0
83	MG	AS	3475	1/1	0.96	0.09	22,22,22,22	0
83	MG	1	3573	1/1	0.96	0.11	23,23,23,23	0
83	MG	AS	3478	1/1	0.96	0.11	16,16,16,16	0
83	MG	AS	3583	1/1	0.96	0.24	30,30,30,30	0
83	MG	1	3501	1/1	0.96	0.16	12,12,12,12	0
83	MG	1	3488	1/1	0.96	0.25	9,9,9,9	0
83	MG	AS	3586	1/1	0.96	0.17	15,15,15,15	0
83	MG	3	207	1/1	0.96	0.11	51,51,51,51	0
83	MG	CM	1893	1/1	0.96	0.10	17,17,17,17	0
83	MG	1	3477	1/1	0.96	0.10	14,14,14,14	0
83	MG	CM	1896	1/1	0.96	0.06	4,4,4,4	0
83	MG	1	3656	1/1	0.96	0.12	28,28,28,28	0
83	MG	L	201	1/1	0.96	0.19	41,41,41,41	0
83	MG	AS	3488	1/1	0.96	0.28	15,15,15,15	0
83	MG	AS	3592	1/1	0.96	0.12	20,20,20,20	0
83	MG	AS	3489	1/1	0.96	0.08	29,29,29,29	0
83	MG	1	3742	1/1	0.96	0.12	32,32,32,32	0
83	MG	AS	3595	1/1	0.96	0.18	31,31,31,31	0
83	MG	B	1894	1/1	0.96	0.12	27,27,27,27	0
83	MG	B	1895	1/1	0.96	0.10	37,37,37,37	0
83	MG	BK	201	1/1	0.96	0.16	11,11,11,11	0
83	MG	AS	3598	1/1	0.96	0.04	24,24,24,24	0
83	MG	B	1832	1/1	0.96	0.17	19,19,19,19	0
83	MG	1	3899	1/1	0.96	0.17	31,31,31,31	0
83	MG	CA	201	1/1	0.96	0.10	33,33,33,33	0
83	MG	1	3478	1/1	0.96	0.12	20,20,20,20	0
83	MG	1	3556	1/1	0.96	0.06	35,35,35,35	0
83	MG	1	3745	1/1	0.96	0.15	30,30,30,30	0
83	MG	B	1837	1/1	0.96	0.13	26,26,26,26	0
83	MG	B	1838	1/1	0.96	0.14	20,20,20,20	0
83	MG	1	3479	1/1	0.96	0.16	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
83	MG	1	3481	1/1	0.96	0.11	12,12,12,12	0
83	MG	CM	1803	1/1	0.96	0.14	13,13,13,13	0
83	MG	1	3689	1/1	0.96	0.07	33,33,33,33	0
83	MG	1	3785	1/1	0.96	0.14	20,20,20,20	0
83	MG	AB	201	1/1	0.96	0.07	9,9,9,9	0
83	MG	AS	3448	1/1	0.97	0.11	33,33,33,33	0
83	MG	B	1889	1/1	0.97	0.16	37,37,37,37	0
83	MG	AS	3572	1/1	0.97	0.14	16,16,16,16	0
83	MG	B	1816	1/1	0.97	0.22	17,17,17,17	0
83	MG	AS	3451	1/1	0.97	0.15	26,26,26,26	0
83	MG	BQ	201	1/1	0.97	0.13	14,14,14,14	0
83	MG	AS	3454	1/1	0.97	0.09	20,20,20,20	0
83	MG	1	3912	1/1	0.97	0.06	26,26,26,26	0
83	MG	1	3480	1/1	0.97	0.16	16,16,16,16	0
83	MG	AS	3402	1/1	0.97	0.06	46,46,46,46	0
83	MG	B	1932	1/1	0.97	0.08	18,18,18,18	0
83	MG	1	3627	1/1	0.97	0.14	11,11,11,11	0
83	MG	1	3533	1/1	0.97	0.15	25,25,25,25	0
83	MG	AS	3582	1/1	0.97	0.15	16,16,16,16	0
83	MG	1	3629	1/1	0.97	0.09	25,25,25,25	0
83	MG	AS	3521	1/1	0.97	0.23	28,28,28,28	0
83	MG	1	3435	1/1	0.97	0.09	0,0,0,0	0
83	MG	v	301	1/1	0.97	0.07	21,21,21,21	0
83	MG	1	3757	1/1	0.97	0.23	19,19,19,19	0
83	MG	AS	3411	1/1	0.97	0.22	13,13,13,13	0
83	MG	1	3536	1/1	0.97	0.16	15,15,15,15	0
83	MG	1	3707	1/1	0.97	0.04	3,3,3,3	0
83	MG	1	3822	1/1	0.97	0.06	23,23,23,23	0
83	MG	1	3492	1/1	0.97	0.10	31,31,31,31	0
83	MG	1	3417	1/1	0.97	0.09	13,13,13,13	0
83	MG	CM	1879	1/1	0.97	0.12	26,26,26,26	0
83	MG	1	3802	1/1	0.97	0.13	19,19,19,19	0
83	MG	B	1831	1/1	0.97	0.15	23,23,23,23	0
83	MG	B	1906	1/1	0.97	0.11	12,12,12,12	0
83	MG	AK	102	1/1	0.97	0.06	12,12,12,12	0
83	MG	AS	3477	1/1	0.97	0.13	14,14,14,14	0
83	MG	AS	3422	1/1	0.97	0.07	20,20,20,20	0
83	MG	AS	3423	1/1	0.97	0.14	25,25,25,25	0
83	MG	4	208	1/1	0.97	0.11	8,8,8,8	0
83	MG	1	3874	1/1	0.97	0.11	45,45,45,45	0
83	MG	1	3826	1/1	0.97	0.06	36,36,36,36	0
83	MG	AS	3484	1/1	0.97	0.04	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
83	MG	AS	3485	1/1	0.97	0.16	15,15,15,15	0
83	MG	AS	3543	1/1	0.97	0.09	23,23,23,23	0
83	MG	1	3421	1/1	0.97	0.22	3,3,3,3	0
83	MG	1	3728	1/1	0.97	0.18	18,18,18,18	0
83	MG	1	3852	1/1	0.97	0.14	24,24,24,24	0
83	MG	1	3764	1/1	0.97	0.15	18,18,18,18	0
83	MG	CM	1900	1/1	0.97	0.13	35,35,35,35	0
83	MG	B	1915	1/1	0.97	0.10	31,31,31,31	0
83	MG	1	3806	1/1	0.97	0.07	32,32,32,32	0
83	MG	AS	3492	1/1	0.97	0.10	16,16,16,16	0
83	MG	AS	3551	1/1	0.97	0.12	23,23,23,23	0
83	MG	CQ	301	1/1	0.97	0.06	3,3,3,3	0
83	MG	I	302	1/1	0.97	0.06	31,31,31,31	0
83	MG	1	3409	1/1	0.97	0.04	12,12,12,12	0
83	MG	1	3570	1/1	0.97	0.17	28,28,28,28	0
83	MG	AS	3619	1/1	0.97	0.10	20,20,20,20	0
83	MG	AS	3620	1/1	0.97	0.16	26,26,26,26	0
83	MG	1	3509	1/1	0.97	0.18	20,20,20,20	0
83	MG	CM	1840	1/1	0.97	0.20	24,24,24,24	0
83	MG	B	1920	1/1	0.97	0.07	68,68,68,68	0
83	MG	AS	3499	1/1	0.97	0.07	6,6,6,6	0
83	MG	6	201	1/1	0.97	0.13	23,23,23,23	0
83	MG	6	202	1/1	0.97	0.14	27,27,27,27	0
85	ZN	AQ	101	1/1	0.97	0.06	65,65,65,65	0
83	MG	B	1812	1/1	0.97	0.11	17,17,17,17	0
83	MG	AS	3443	1/1	0.97	0.19	11,11,11,11	0
83	MG	AS	3564	1/1	0.97	0.05	12,12,12,12	0
85	ZN	CH	101	1/1	0.97	0.11	75,75,75,75	0
83	MG	1	3640	1/1	0.97	0.21	27,27,27,27	0
83	MG	1	3641	1/1	0.97	0.16	7,7,7,7	0
85	ZN	DS	201	1/1	0.97	0.07	134,134,134,134	0
83	MG	AS	3506	1/1	0.97	0.11	18,18,18,18	0
83	MG	1	3685	1/1	0.97	0.17	33,33,33,33	0
83	MG	1	3550	1/1	0.98	0.12	9,9,9,9	0
83	MG	CM	1831	1/1	0.98	0.08	44,44,44,44	0
83	MG	AS	3445	1/1	0.98	0.05	22,22,22,22	0
83	MG	1	3499	1/1	0.98	0.18	13,13,13,13	0
83	MG	1	3528	1/1	0.98	0.10	32,32,32,32	0
83	MG	B	1854	1/1	0.98	0.06	58,58,58,58	0
83	MG	1	3534	1/1	0.98	0.05	15,15,15,15	0
83	MG	BV	201	1/1	0.98	0.21	25,25,25,25	0
83	MG	AS	3664	1/1	0.98	0.10	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
83	MG	1	3865	1/1	0.98	0.03	25,25,25,25	0
83	MG	AS	3483	1/1	0.98	0.11	13,13,13,13	0
83	MG	AS	3517	1/1	0.98	0.09	22,22,22,22	0
83	MG	CM	1889	1/1	0.98	0.13	33,33,33,33	0
83	MG	AS	3668	1/1	0.98	0.06	63,63,63,63	0
83	MG	4	202	1/1	0.98	0.18	10,10,10,10	0
83	MG	AS	3670	1/1	0.98	0.08	11,11,11,11	0
83	MG	CM	1894	1/1	0.98	0.25	16,16,16,16	0
83	MG	AS	3452	1/1	0.98	0.14	19,19,19,19	0
83	MG	AS	3453	1/1	0.98	0.14	14,14,14,14	0
83	MG	1	3420	1/1	0.98	0.13	17,17,17,17	0
83	MG	B	1880	1/1	0.98	0.12	20,20,20,20	0
83	MG	AS	3557	1/1	0.98	0.09	20,20,20,20	0
83	MG	B	1925	1/1	0.98	0.06	28,28,28,28	0
83	MG	AS	3559	1/1	0.98	0.09	8,8,8,8	0
83	MG	AS	3458	1/1	0.98	0.15	1,1,1,1	0
83	MG	AS	3679	1/1	0.98	0.06	28,28,28,28	0
83	MG	1	3635	1/1	0.98	0.07	37,37,37,37	0
83	MG	1	3636	1/1	0.98	0.05	22,22,22,22	0
83	MG	CM	1856	1/1	0.98	0.12	24,24,24,24	0
83	MG	B	1840	1/1	0.98	0.15	38,38,38,38	0
83	MG	B	1841	1/1	0.98	0.19	36,36,36,36	0
83	MG	1	3605	1/1	0.98	0.05	22,22,22,22	0
83	MG	AS	3407	1/1	0.98	0.05	0,0,0,0	0
83	MG	AS	3433	1/1	0.98	0.23	17,17,17,17	0
83	MG	AS	3498	1/1	0.98	0.10	26,26,26,26	0
83	MG	1	3465	1/1	0.98	0.10	10,10,10,10	0
83	MG	AS	3645	1/1	0.98	0.10	26,26,26,26	0
83	MG	AS	3570	1/1	0.98	0.14	16,16,16,16	0
85	ZN	AK	101	1/1	0.98	0.08	55,55,55,55	0
85	ZN	AN	101	1/1	0.98	0.06	73,73,73,73	0
83	MG	AS	3608	1/1	0.98	0.04	21,21,21,21	0
83	MG	CM	1867	1/1	0.98	0.10	34,34,34,34	0
83	MG	1	3767	1/1	0.98	0.04	26,26,26,26	0
85	ZN	f	101	1/1	0.98	0.07	71,71,71,71	0
83	MG	1	3811	1/1	0.98	0.06	6,6,6,6	0
83	MG	1	3588	1/1	0.98	0.10	26,26,26,26	0
83	MG	AS	3438	1/1	0.98	0.20	17,17,17,17	0
83	MG	1	3676	1/1	0.98	0.09	41,41,41,41	0
85	ZN	DN	201	1/1	0.98	0.03	59,59,59,59	0
83	MG	1	3449	1/1	0.98	0.15	11,11,11,11	0
83	MG	B	1849	1/1	0.98	0.13	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
83	MG	1	3572	1/1	0.98	0.10	11,11,11,11	0
83	MG	AS	3416	1/1	0.98	0.05	47,47,47,47	0
83	MG	1	3475	1/1	0.99	0.17	3,3,3,3	0
85	ZN	c	201	1/1	0.99	0.03	51,51,51,51	0
83	MG	AS	3656	1/1	0.99	0.04	45,45,45,45	0
83	MG	AS	3456	1/1	0.99	0.16	7,7,7,7	0
83	MG	1	3772	1/1	0.99	0.12	18,18,18,18	0
83	MG	1	3472	1/1	0.99	0.10	10,10,10,10	0
85	ZN	CE	101	1/1	0.99	0.04	66,66,66,66	0
83	MG	1	3440	1/1	0.99	0.18	2,2,2,2	0
83	MG	1	3566	1/1	0.99	0.10	3,3,3,3	0
85	ZN	CK	101	1/1	0.99	0.03	84,84,84,84	0
83	MG	1	3582	1/1	0.99	0.20	31,31,31,31	0
83	MG	1	3408	1/1	0.99	0.03	47,47,47,47	0
83	MG	CM	1892	1/1	0.99	0.14	9,9,9,9	0
83	MG	3	201	1/1	0.99	0.12	0,0,0,0	0
83	MG	AP	202	1/1	0.99	0.03	12,12,12,12	0
83	MG	1	3708	1/1	1.00	0.08	11,11,11,11	0

6.5 Other polymers ⓘ

There are no such residues in this entry.