



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 06:50 PM UTC

PDB ID : 8OJ3 / pdb_00008oj3
Title : Crystal structure of the Candida albicans 80S ribosome in complex with geneticin G418 (rotated state)
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on : 2023-03-23
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

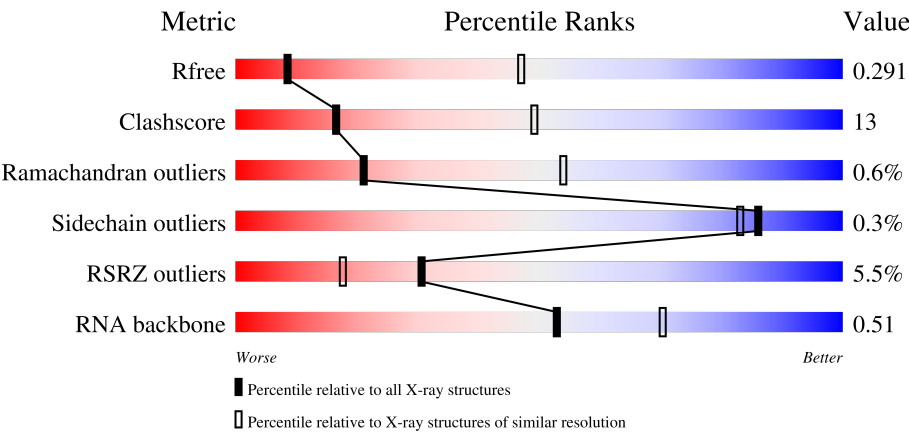
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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

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

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Mol	Chain	Length	Quality of chain
3	4	158	
3	AU	158	
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	r	219	
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	
16	v	204	
17	BJ	200	
17	w	200	
18	BK	185	
18	x	185	
19	BL	186	
19	y	186	
20	BM	190	
20	z	190	
21	0	172	
21	BN	172	
22	2	160	
22	BO	160	
23	5	124	
23	BP	124	
24	6	137	
24	BQ	137	
25	7	155	
25	BR	155	
26	8	142	
26	BS	142	
27	9	127	
27	BT	127	
28	AA	136	

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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	
41	CH	52	
42	AO	25	
42	CI	25	
43	AP	106	
43	CJ	106	
44	AQ	92	
44	CK	92	
45	CL	267	
45	i	267	
46	B	1787	
46	CM	1787	
47	C	261	
47	CN	261	
48	CO	256	
48	D	256	
49	CP	249	
49	E	249	
50	CQ	251	
50	F	251	
51	CR	262	
51	G	262	
52	CS	225	
52	H	225	
53	CT	236	

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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	
79	AR	317	
79	DT	317	
80	BE	220	
81	P0	312	
82	12	165	

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
84	MG	1	3508	-	-	-	X
84	MG	1	3731	-	-	-	X
84	MG	1	3870	-	-	-	X
84	MG	AS	3535	-	-	-	X
84	MG	AS	3641	-	-	-	X
84	MG	AS	3654	-	-	-	X
84	MG	CL	301	-	-	-	X

2 Entry composition

There are 86 unique types of molecules in this entry. The entry contains 400037 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 ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3218	Total	C	N	O	P	0	0	0
			68791	30731	12364	22478	3218			
1	AS	3101	Total	C	N	O	P	0	0	0
			66291	29614	11913	21663	3101			

- Molecule 2 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 3 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	156	Total	C	N	O	P	0	0	0
			3313	1482	581	1094	156			
3	AU	158	Total	C	N	O	P	0	0	0
			3353	1500	585	1110	158			

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

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

- 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	0	0	0
			3077	1950	582	538	7			
5	AX	386	Total	C	N	O	S	0	0	0
			3077	1950	582	538	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	l	359	Total	C	N	O	S	0	0	0
			2734	1720	524	487	3			
6	AY	359	Total	C	N	O	S	0	0	0
			2734	1720	524	487	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	294	Total	C	N	O	S	0	0	0
			2409	1534	419	455	1			
7	AZ	292	Total	C	N	O	S	0	0	0
			2394	1526	416	450	2			

- 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	0	0	0
			1242	796	226	219	1			
8	BA	153	Total	C	N	O		0	0	0
			1210	777	221	212				

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	o	229	Total	C	N	O	S	0	0	0
			1843	1182	338	322	1			
9	BB	226	Total	C	N	O	S	0	0	0
			1816	1165	333	317	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	236	Total	C	N	O	S	0	0	0
			1825	1168	324	330	3			

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	r	207	Total	C	N	O	S	0	0	0
			1681	1064	321	290	6			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	u	128	Total	C	N	O	S	0	0	0
			1015	651	190	173	1			
15	BH	130	Total	C	N	O	S	0	0	0
			1029	660	193	175	1			

- 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	0	0	0
			1713	1075	356	280	2			
16	BI	203	Total	C	N	O	S	0	0	0
			1713	1075	356	280	2			

- Molecule 17 is a protein called Ribosomal protein L13.

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

- Molecule 18 is a protein called Ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	x	169	Total	C	N	O	0	0	0
			1352	835	273	244			
18	BK	174	Total	C	N	O	0	0	0
			1396	862	282	252			

- 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	0	0	0
			1458	916	297	245			
19	BL	185	Total	C	N	O	0	0	0
			1458	916	297	245			

- 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	0	0	0
			1457	901	310	243	3			
20	BM	179	Total	C	N	O	S	0	0	0
			1457	901	310	243	3			

- 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	0	0	0
			1423	921	258	241	3			

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

- 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	0	0	0
			1262	798	241	221	2			
22	BO	159	Total	C	N	O	S	0	0	0
			1262	798	241	221	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	5	100	Total	C	N	O	S	0	0	0
			803	518	135	150				
23	BP	99	Total	C	N	O	S	0	0	0
			794	512	133	149				

- 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	0	0	0
			977	615	183	171	8			
24	BQ	131	Total	C	N	O	S	0	0	0
			977	615	183	171	8			

- 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	0	0	0
			945	591	192	161	1			
25	BR	109	Total	C	N	O	S	0	0	0
			877	549	178	149	1			

- 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	0	0	0
			965	616	173	175	1			
26	BS	119	Total	C	N	O	S	0	0	0
			960	613	172	174	1			

- Molecule 27 is a protein called Ribosomal protein L24.

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

- 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	0	0	0
			1087	705	197	183	2			
28	BU	135	Total	C	N	O	S	0	0	0
			1087	705	197	183	2			

- 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	0	0	0
			1170	741	231	197	1			
29	BV	148	Total	C	N	O	S	0	0	0
			1170	741	231	197	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	AC	58	Total	C	N	O	0	0	0
			464	290	100	74			
30	BW	60	Total	C	N	O	0	0	0
			482	301	103	78			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	AD	98	Total	C	N	O	S	0	0	0
			747	479	124	142	2			
31	BX	94	Total	C	N	O	S	0	0	0
			715	460	119	134	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AE	108	Total	C	N	O	S	0	0	0
			881	556	166	157	2			
32	BY	108	Total	C	N	O	S	0	0	0
			881	556	166	157	2			

- 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	0	0	0
			1000	638	194	167	1			
33	BZ	122	Total	C	N	O	S	0	0	0
			991	633	192	165	1			

- 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	0	0	0
			847	543	161	142	1			
34	CA	106	Total	C	N	O	S	0	0	0
			847	543	161	142	1			

- 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	0	0	0
			887	547	182	154	4			
35	CB	110	Total	C	N	O	S	0	0	0
			869	536	179	150	4			

- Molecule 36 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
36	AI	115	Total	C	N	O	0	0	0
			963	611	190	162			
36	CC	117	Total	C	N	O	0	0	0
			974	618	192	164			

- 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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	CD	95	Total	C	N	O	S	0	0	0
			736	459	148	128	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	50	Total	C	N	O	S	0	0	0
			402	249	83	65	5			
41	CH	50	Total	C	N	O	S	0	0	0
			403	249	84	65	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			
42	CI	24	Total	C	N	O	S	0	0	0
			227	138	61	27	1			

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	i	106	Total	C	N	O	0	0	0
			805	483	147	175			
45	CL	120	Total	C	N	O	0	0	0
			919	554	165	200			

- Molecule 46 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B	1708	Total	C	N	O	P	0	0	0
			36410	16276	6460	11966	1708			
46	CM	1728	Total	C	N	O	P	0	0	0
			36839	16468	6538	12105	1728			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	D	214	Total	C	N	O	S	0	0	0
			1724	1094	313	313	4			
48	CO	213	Total	C	N	O	S	0	0	0
			1717	1089	312	312	4			

- Molecule 49 is a protein called Ribosomal protein S5.

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

- Molecule 50 is a protein called Ribosomal protein S3.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	G	258	Total	C	N	O	S	0	0	0
			2042	1299	383	355	5			
51	CR	260	Total	C	N	O	S	0	0	0
			2055	1306	386	358	5			

- Molecule 52 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	H	206	Total	C	N	O	S	0	0	0
			1614	1008	301	301	4			
52	CS	205	Total	C	N	O	S	0	0	0
			1606	1002	300	300	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	I	223	Total	C	N	O	S	0	0	0
			1798	1119	348	325	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	182	Total	C	N	O	S	0	0	0
			1466	939	264	263				
54	CU	179	Total	C	N	O	S	0	0	0
			1449	929	261	259				

- 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			
58	CY	141	Total	C	N	O	S	0	0	0
			1129	722	212	192	3			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
60	P	148	Total	C	N	O	S	0	0	0
			1175	749	217	208	1			
60	DA	150	Total	C	N	O	S	0	0	0
			1187	757	219	210	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
61	Q	127	Total	C	N	O	S	0	0	0
			942	579	186	174	3			
61	DB	122	Total	C	N	O	S	0	0	0
			905	555	180	167	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
62	R	131	Total	C	N	O	S	0	0	0
			1034	658	190	179	7			
62	DC	130	Total	C	N	O	S	0	0	0
			1029	655	189	178	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
63	S	139	Total	C	N	O	S	0	0	0
			1085	697	197	190	1			
63	DD	139	Total	C	N	O	S	0	0	0
			1085	697	197	190	1			

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

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

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

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

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

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

- Molecule 67 is a protein called Ribosomal protein S10.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	e	60	Total	C	N	O	S	0	0	0
			468	287	93	86	2			
75	DP	61	Total	C	N	O	S	0	0	0
			476	293	94	87	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	g	60	Total	C	N	O	S	0	0	0
			474	297	96	79	2			
77	DR	59	Total	C	N	O	S	0	0	0
			470	295	95	78	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	h	70	Total	C	N	O	S	0	0	0
			574	362	113	93	6			
78	DS	68	Total	C	N	O	S	0	0	0
			555	350	108	91	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	AR	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			
79	DT	307	Total	C	N	O	S	0	0	0
			2362	1498	403	456	5			

- Molecule 80 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
80	BE	205	Total	C	N	O	S	0	0	0
			1662	1052	318	285	7			

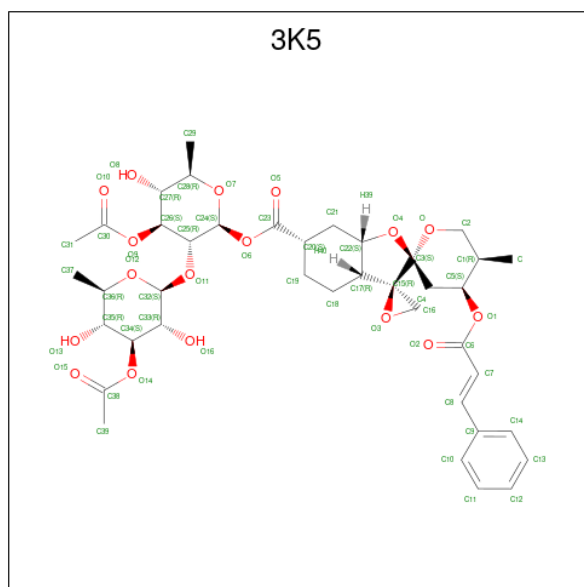
- Molecule 81 is a protein called 60S acidic ribosomal protein P0.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
81	P0	107	Total	C	N	O	S	0	0	0
			845	542	150	150	3			

- Molecule 82 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	12	63	Total	C	N	O	S	0	0	0
			480	297	85	96	2			

- Molecule 83 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 (CCD ID: 3K5) (formula: C₄₀H₅₂O₁₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
83	1	1	Total	C	O	0	0
			57	40	17		
83	AS	1	Total	C	O	0	0
			57	40	17		

- Molecule 84 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	1	469	Total Mg 469 469	0	0
84	3	7	Total Mg 7 7	0	0
84	4	1	Total Mg 1 1	0	0
84	j	1	Total Mg 1 1	0	0
84	k	3	Total Mg 3 3	0	0
84	m	1	Total Mg 1 1	0	0
84	o	4	Total Mg 4 4	0	0
84	r	1	Total Mg 1 1	0	0
84	u	1	Total Mg 1 1	0	0
84	v	2	Total Mg 2 2	0	0
84	w	1	Total Mg 1 1	0	0
84	x	1	Total Mg 1 1	0	0
84	y	3	Total Mg 3 3	0	0
84	0	4	Total Mg 4 4	0	0
84	2	1	Total Mg 1 1	0	0
84	6	1	Total Mg 1 1	0	0
84	AB	2	Total Mg 2 2	0	0
84	AC	1	Total Mg 1 1	0	0
84	AD	1	Total Mg 1 1	0	0
84	AJ	1	Total Mg 1 1	0	0
84	AP	2	Total Mg 2 2	0	0
84	B	99	Total Mg 99 99	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	C	1	Total 1	Mg 1	0	0
84	D	1	Total 1	Mg 1	0	0
84	E	1	Total 1	Mg 1	0	0
84	F	1	Total 1	Mg 1	0	0
84	G	1	Total 1	Mg 1	0	0
84	K	1	Total 1	Mg 1	0	0
84	L	1	Total 1	Mg 1	0	0
84	Q	2	Total 2	Mg 2	0	0
84	R	4	Total 4	Mg 4	0	0
84	T	1	Total 1	Mg 1	0	0
84	Y	2	Total 2	Mg 2	0	0
84	a	1	Total 1	Mg 1	0	0
84	AS	389	Total 389	Mg 389	0	0
84	AT	5	Total 5	Mg 5	0	0
84	AU	5	Total 5	Mg 5	0	0
84	AW	1	Total 1	Mg 1	0	0
84	AX	3	Total 3	Mg 3	0	0
84	AY	2	Total 2	Mg 2	0	0
84	AZ	1	Total 1	Mg 1	0	0
84	BB	2	Total 2	Mg 2	0	0
84	BC	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	BE	1	Total 1	Mg 1	0	0
84	BI	1	Total 1	Mg 1	0	0
84	BK	1	Total 1	Mg 1	0	0
84	BL	2	Total 2	Mg 2	0	0
84	BO	1	Total 1	Mg 1	0	0
84	BQ	1	Total 1	Mg 1	0	0
84	BZ	1	Total 1	Mg 1	0	0
84	CA	1	Total 1	Mg 1	0	0
84	CB	1	Total 1	Mg 1	0	0
84	CG	1	Total 1	Mg 1	0	0
84	CL	2	Total 2	Mg 2	0	0
84	CM	78	Total 78	Mg 78	0	0
84	CW	1	Total 1	Mg 1	0	0
84	DA	1	Total 1	Mg 1	0	0
84	DG	1	Total 1	Mg 1	0	0
84	DH	1	Total 1	Mg 1	0	0
84	DK	2	Total 2	Mg 2	0	0
84	P0	1	Total 1	Mg 1	0	0

- Molecule 85 is ZINC ION (CCD ID: ZN) (formula: Zn).

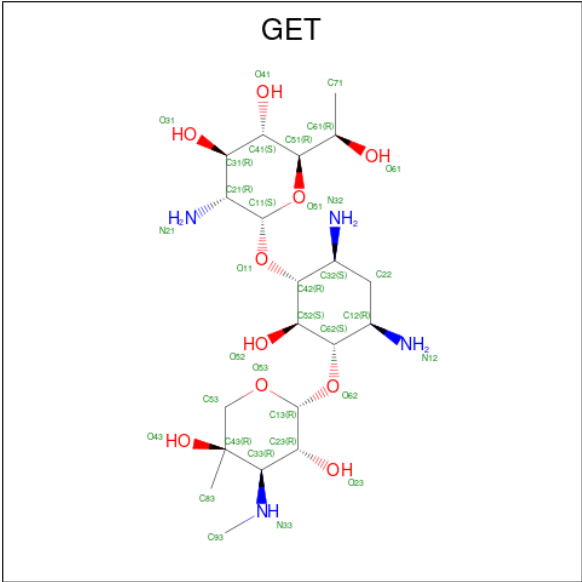
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AH	1	Total 1	Zn 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	AK	1	Total	Zn	0	0
			1	1		
85	AN	1	Total	Zn	0	0
			1	1		
85	AP	1	Total	Zn	0	0
			1	1		
85	AQ	1	Total	Zn	0	0
			1	1		
85	c	1	Total	Zn	0	0
			1	1		
85	d	1	Total	Zn	0	0
			1	1		
85	f	1	Total	Zn	0	0
			1	1		
85	h	1	Total	Zn	0	0
			1	1		
85	CB	1	Total	Zn	0	0
			1	1		
85	CE	1	Total	Zn	0	0
			1	1		
85	CH	1	Total	Zn	0	0
			1	1		
85	CJ	1	Total	Zn	0	0
			1	1		
85	CK	1	Total	Zn	0	0
			1	1		
85	DN	1	Total	Zn	0	0
			1	1		
85	DQ	1	Total	Zn	0	0
			1	1		
85	DS	1	Total	Zn	0	0
			1	1		

- Molecule 86 is GENETICIN (CCD ID: GET) (formula: $C_{20}H_{40}N_4O_{10}$) (labeled as "Ligand of Interest" by depositor).

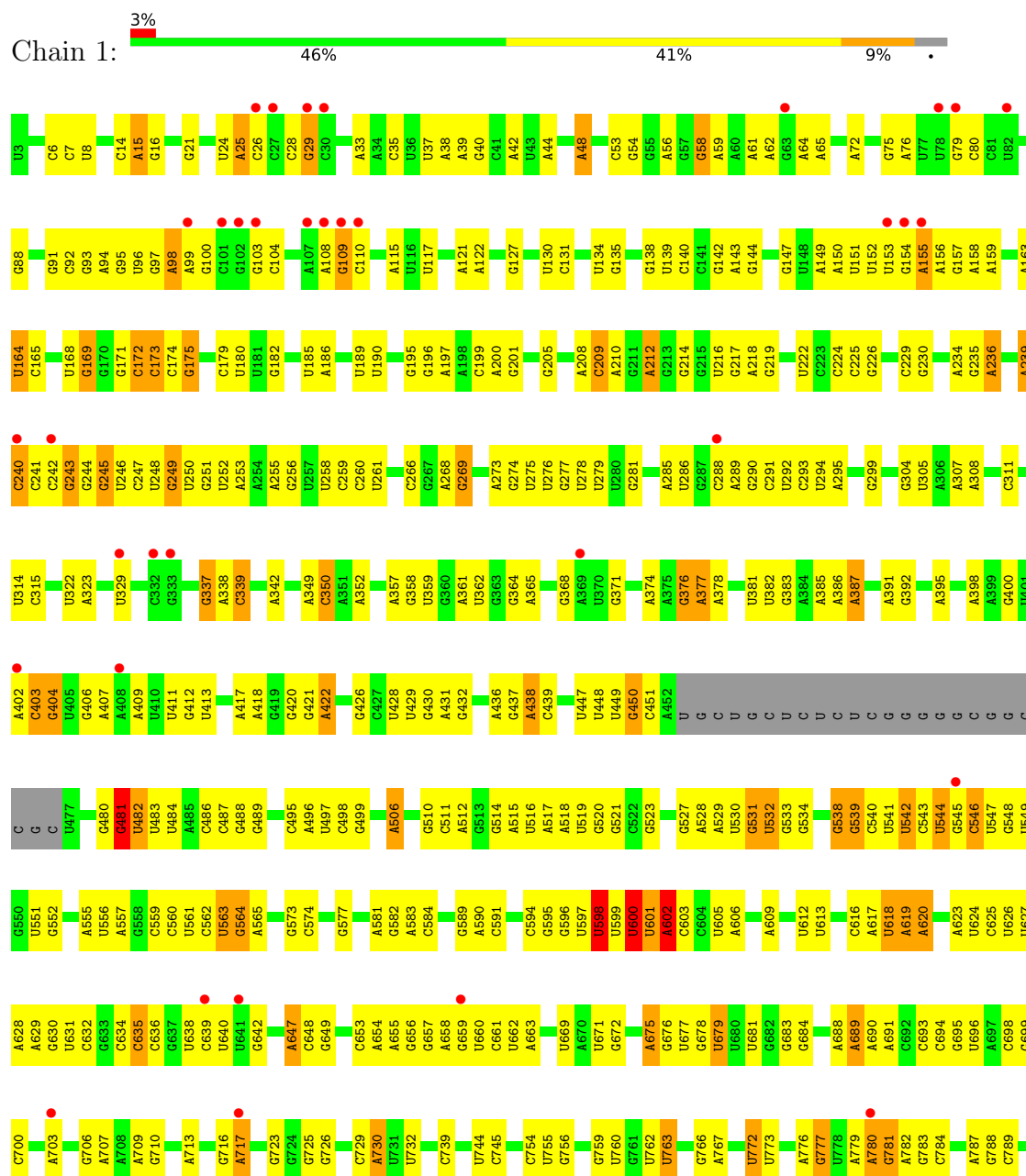


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
86	B	1	Total	C	N	O	0	0
			34	20	4	10		
86	CM	1	Total	C	N	O	0	0
			34	20	4	10		

3 Residue-property plots [i](#)

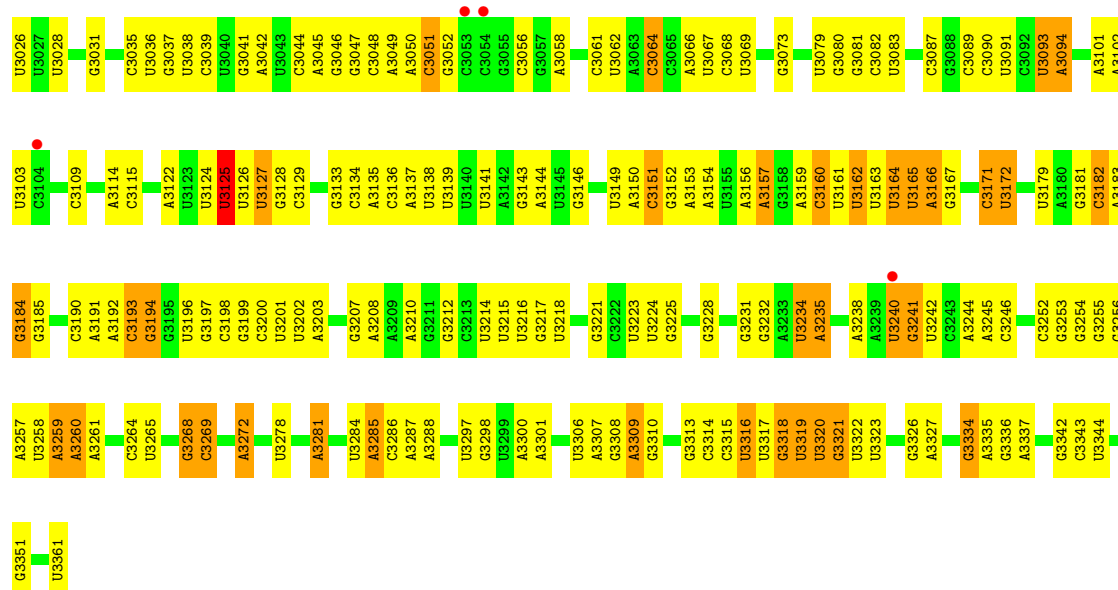
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 ribosomal RNA

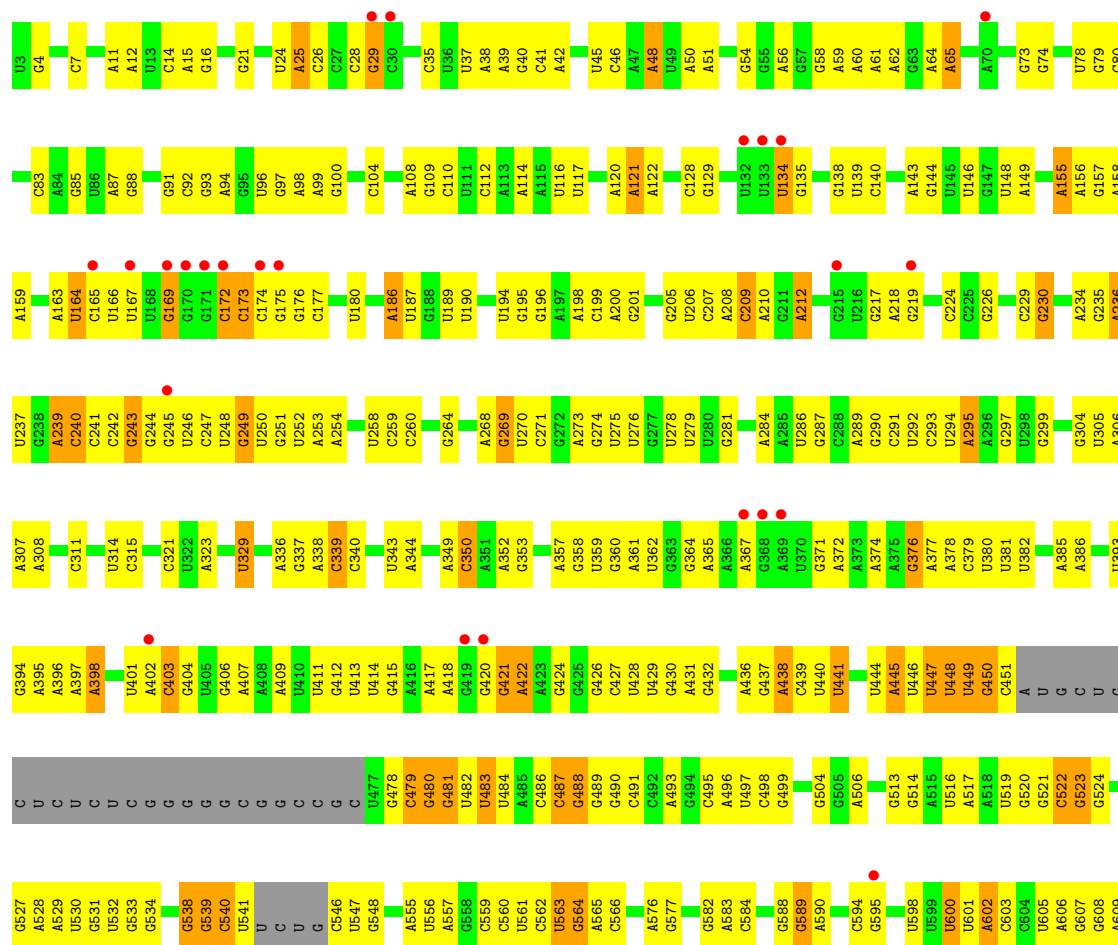


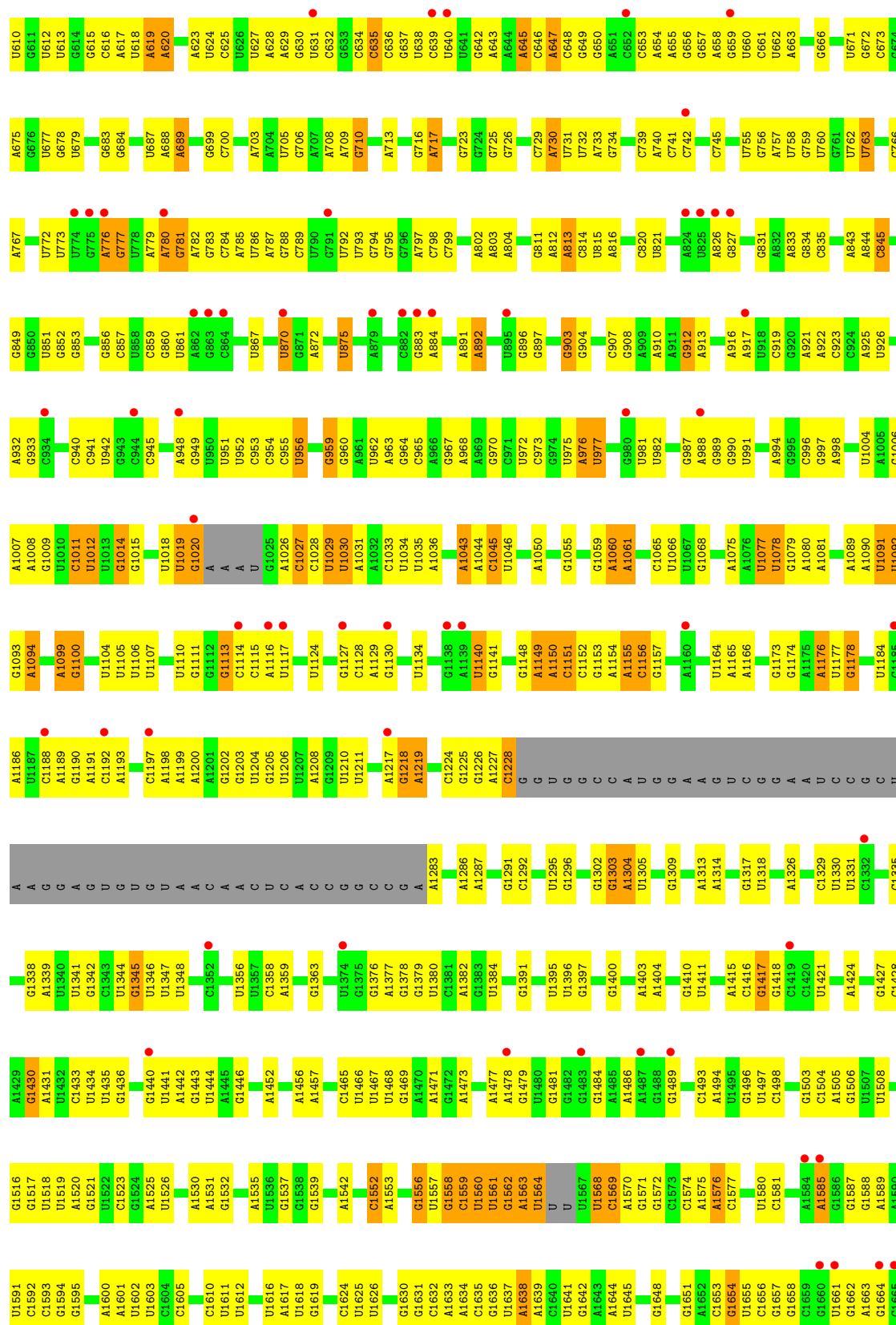
G1808	A1809	A1810	U1811	A1812	G1813	U1814	U1815	U1816	G1817	A1825	G1826	A1831	A1832	A1833	A1835	U1836	A1837	U1838	A1838	G1841	G1842	C1845	U1851	C1852	C1853	G1857	U1858	U1859	A1860	A1861	C1862	A1863	A1864	U1865	C1866	U1867	G1874	U1791	G1792	A1793	A1794	A1795	C1796	C1799	A1800	C1801	A1802	G1803	G1804	A1805	C1900	G1901				
U1568	C1569	A1570	G1571	C1572	G1573	A1574	C1575	A1576	C1577	G1578	C1579	A1580	C1581	A1584	A1585	G1586	G1587	C1588	A1589	G1590	C1591	A1592	C1593	G1594	G1595	A1596	U1597	C1598	A1599	G1600	U1601	C1602	U1603	U1611	U1612	A1617	G1618	G1619	U1620	A1621	C1624	U1625	G1626	A1627	A1628	C1629	G1630	G1714	G1715	A1633	A1634	C1635	U1636	U1637	A1638	
A1639	C1640	U1641	G1642	A1643	G1644	U1645	G1648	G1651	A1652	C1653	G1654	U1655	C1656	G1657	G1658	U1661	G1662	A1663	G1664	A1672	G1673	G1674	A1675	G1676	U1677	G1678	A1679	U1680	C1681	U1682	U1683	U1684	U1685	U1690	A1695	G1696	C1697	C1705	C1706	U1713	G1714	G1715	U1718	A1719	U1720	A1806	C1907									
A1725	G1732	U1738	C1741	U1742	G1743	A1745	A1746	G1747	A1748	G1754	U1755	A1756	A1757	U1758	U1759	U1760	U1761	G1762	C1763	G1767	U1768	G1774	G1775	G1776	U1779	U1780	G1781	G1782	A1783	G1786	U1787	C1788	U1789	U1790	U1791	A1792	A1793	A1794	A1795	A1796	C1799	A1800	C1801	A1802	G1803	G1804	A1805	C1900	G1901							
G1397	G1400	A1403	A1404	G1405	C1406	A1415	C1416	G1417	G1418	U1421	A1424	G1427	C1428	G1430	C1433	U1434	U1435	G1436	G1437	G1440	U1441	A1442	G1443	U1444	G1445	G1446	A1456	A1457	G1460	A1461	G1462	C1465	U1466	U1467	U1468	G1469	A1470	A1471	G1472	A1473	G1476	A1477	A1478	U1479	U1480	G1481										
U1301	G1302	G1303	A1304	U1305	C1308	G1309	C1312	A1313	A1314	A1322	C1323	U1324	A1325	A1326	U1327	U1330	U1331	C1332	G1338	A1339	U1344	G1345	U1346	U1347	U1348	A1350	U1351	C1352	U1357	C1358	A1359	G1363	U1364	A1365	G1376	U1377	G1378	G1379	A1382	G1383	A1386	A1389	A1390	G1391	U1395	U1396										
U1230	U1231	G1232	G1233	C1234	C1235	A1236	U1237	G1238	C1239	A1240	A1241	G1242	U1243	C1244	G1245	G1246	A1247	A1248	U1249	C1250	C1251	G1252	C1253	U1254	A1255	A1256	G1257	G1258	A1259	U1262	U1263	G1264	U1265	A1266	A1267	C1268	A1269	A1270	C1271	U1272	G1273	U1274	C1275	C1276	G1277	G1278	C1279	C1280	A1286	A1287	G1291	C1292	C1293	C1294	A1297	A1298
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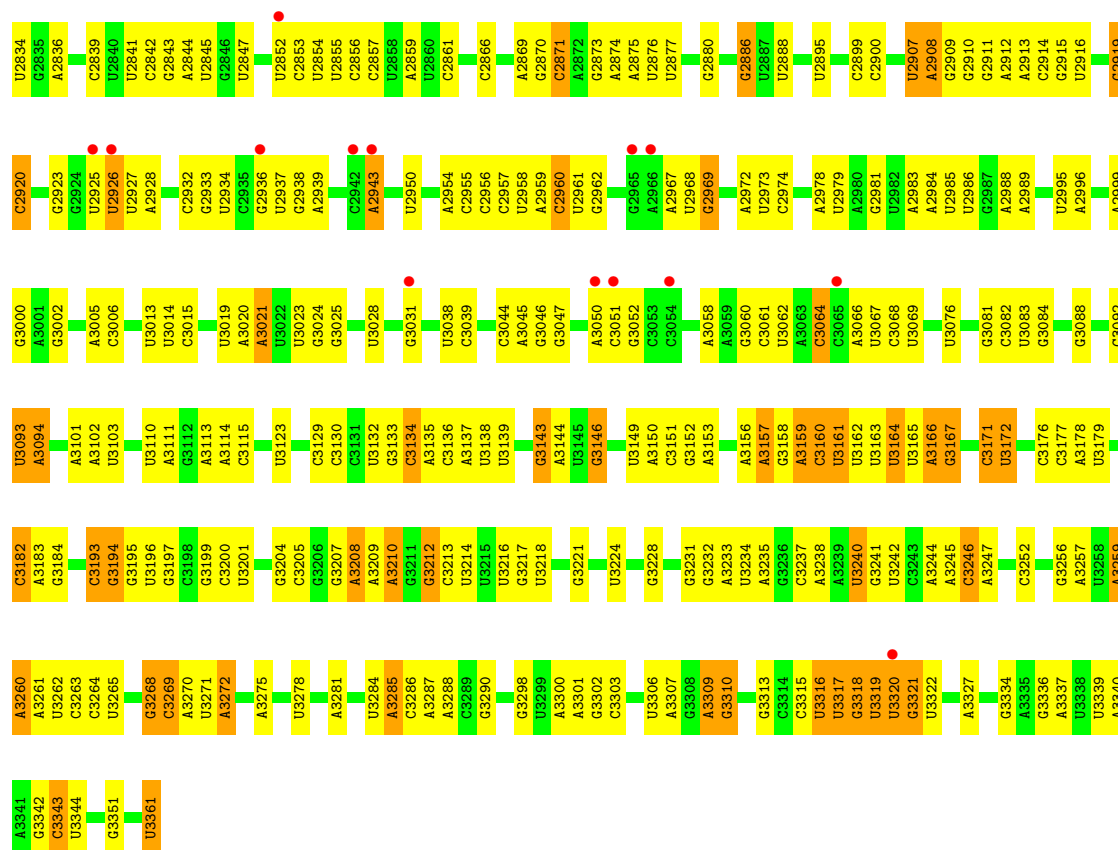


• Molecule 1: 25S ribosomal RNA

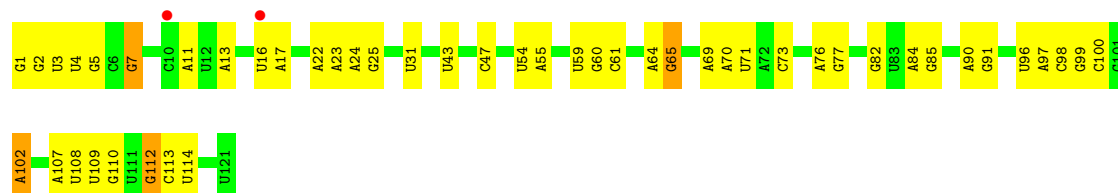




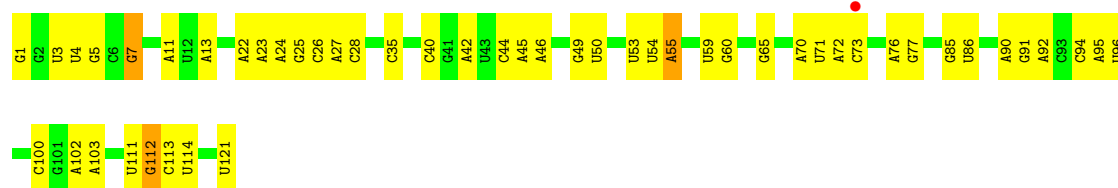




• Molecule 2: 5S ribosomal RNA

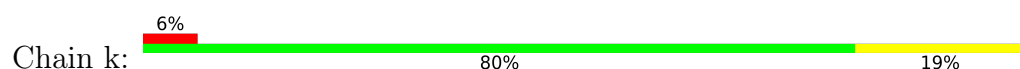


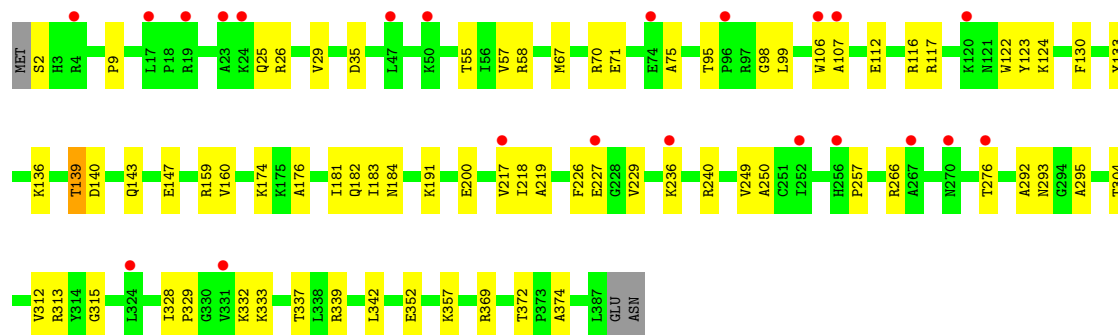
• Molecule 2: 5S ribosomal RNA



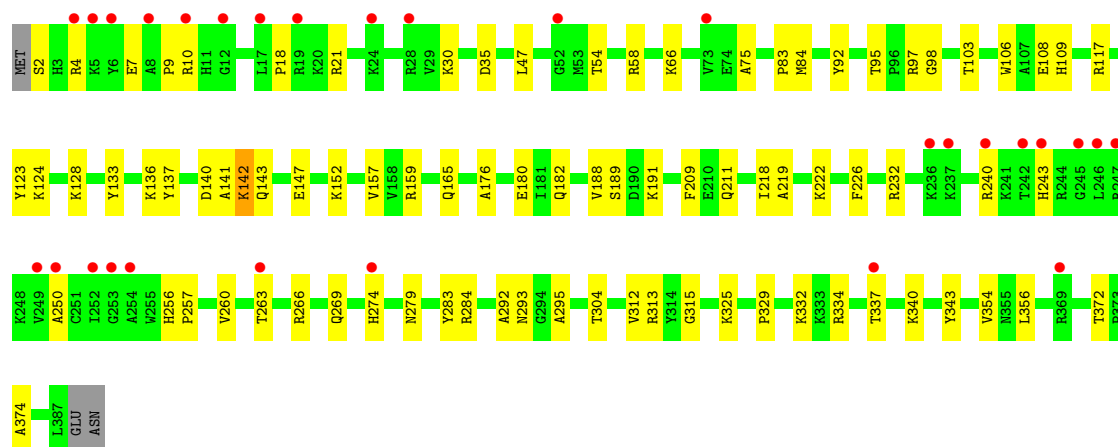
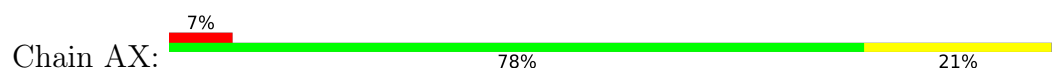
• Molecule 3: 5.8S ribosomal RNA



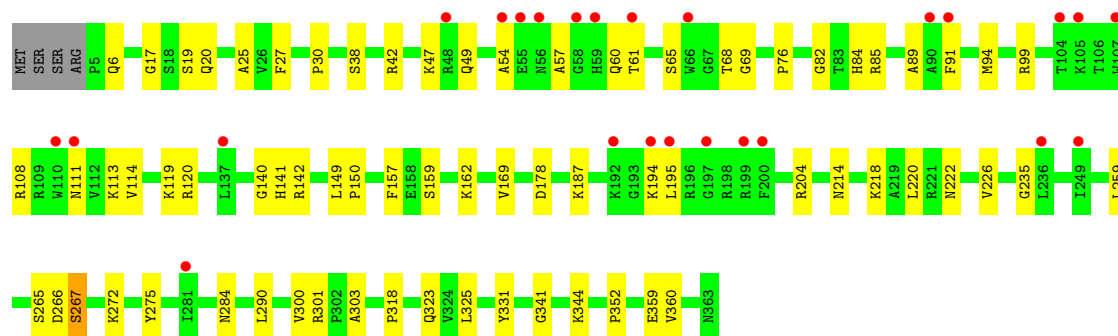
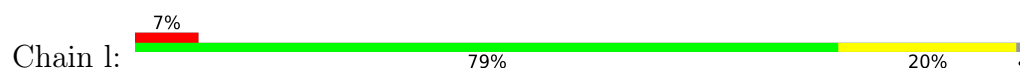




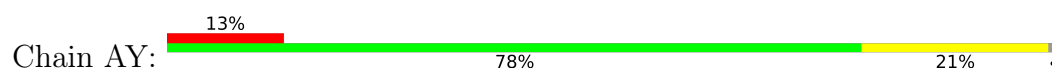
• Molecule 5: 60S ribosomal protein L3

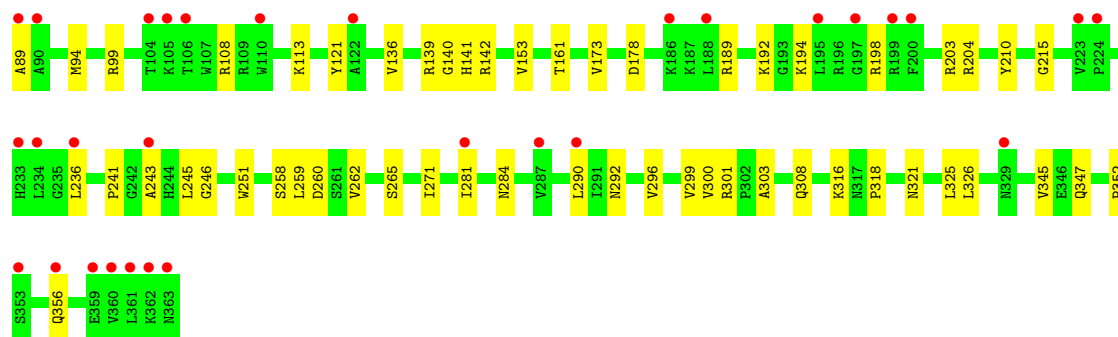


• Molecule 6: 60S ribosomal protein L4-B

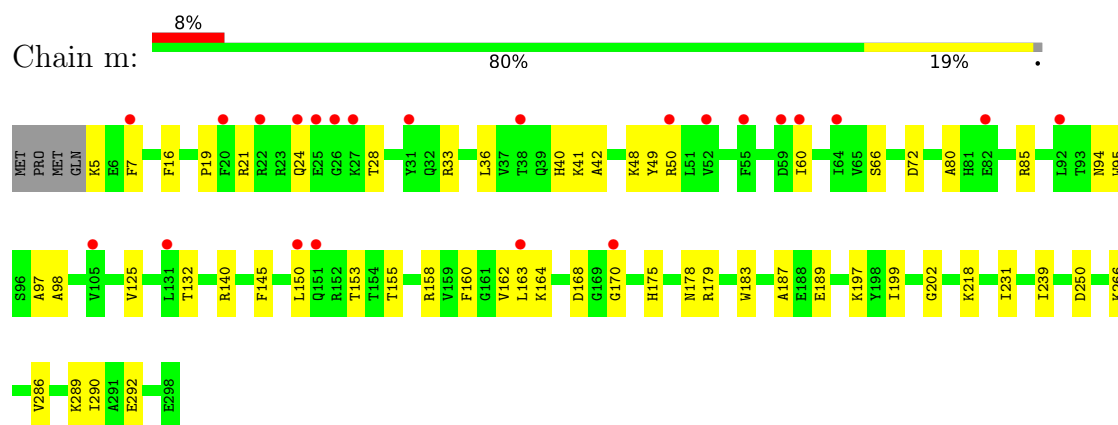


• Molecule 6: 60S ribosomal protein L4-B

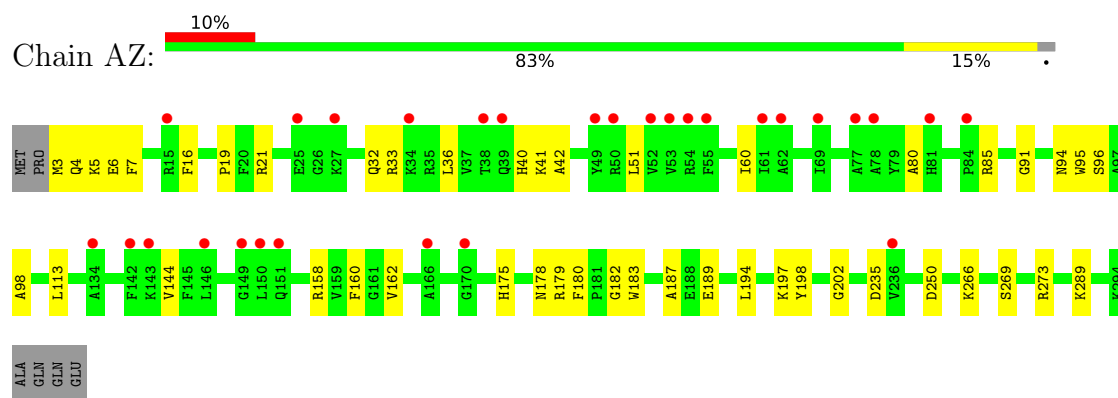




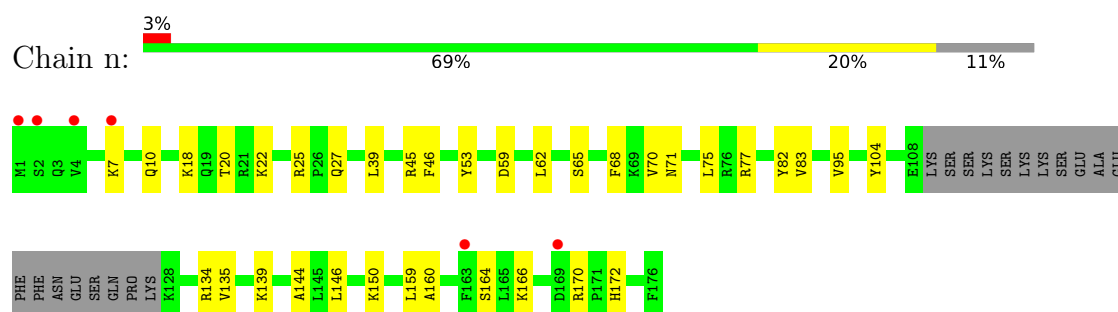
• Molecule 7: Uncharacterized protein CaJ7.0206



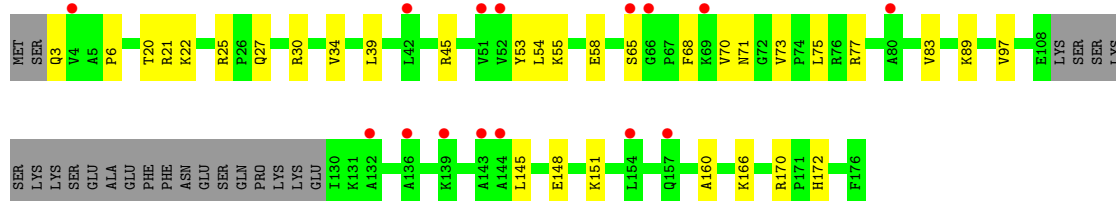
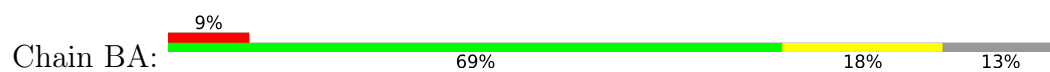
• Molecule 7: Uncharacterized protein CaJ7.0206



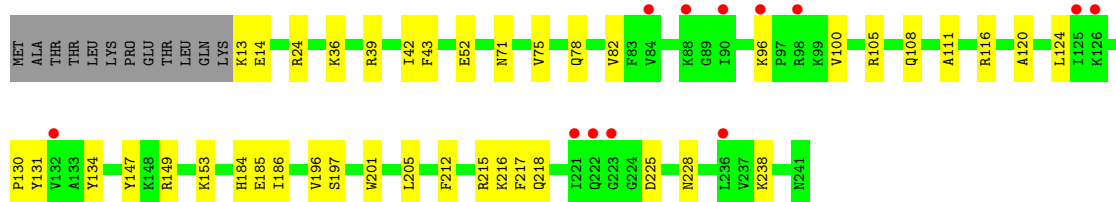
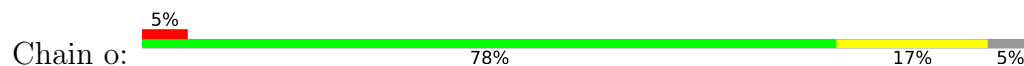
• Molecule 8: 60S ribosomal protein L6



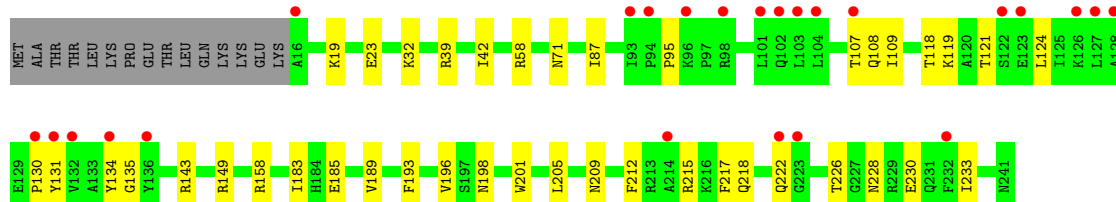
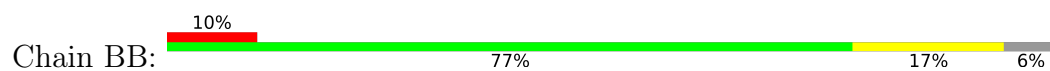
• Molecule 8: 60S ribosomal protein L6



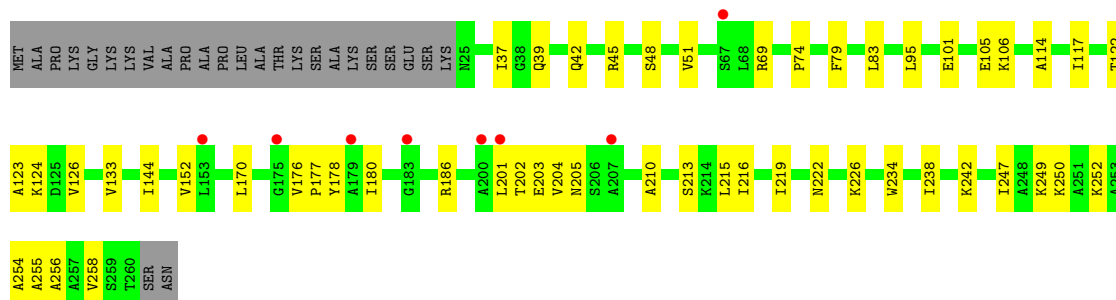
• Molecule 9: 60S ribosomal protein L7-A



• Molecule 9: 60S ribosomal protein L7-A

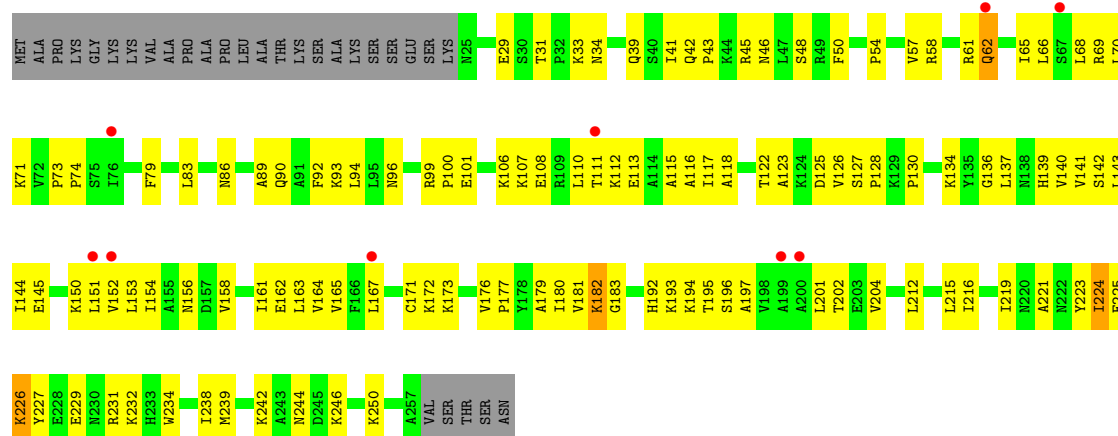


• Molecule 10: 60S ribosomal protein L8

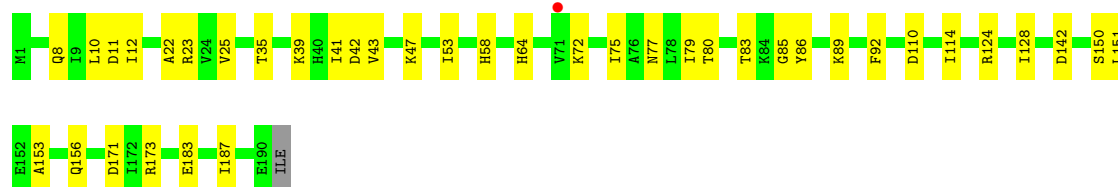
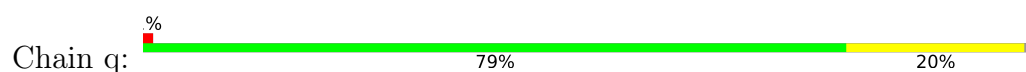


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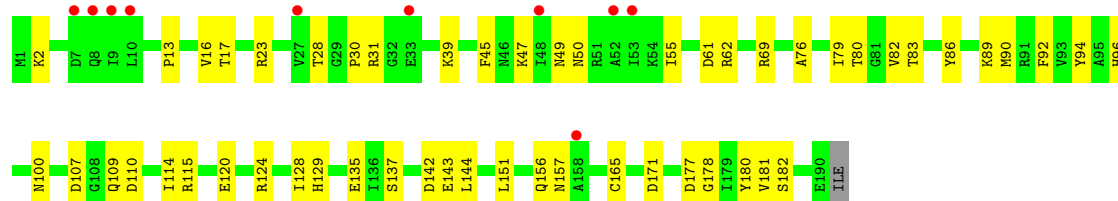
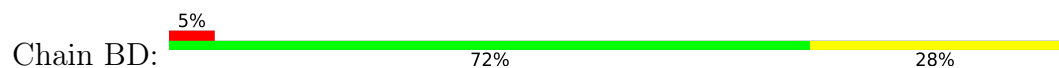




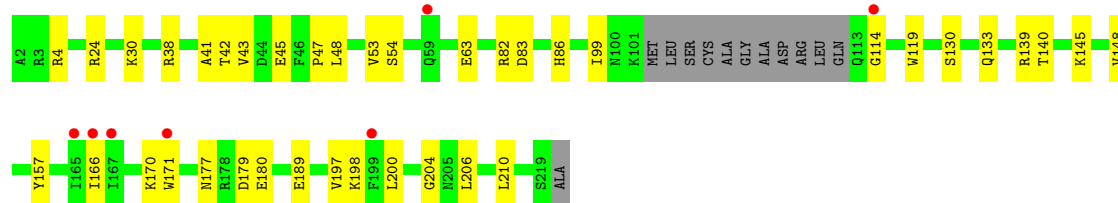
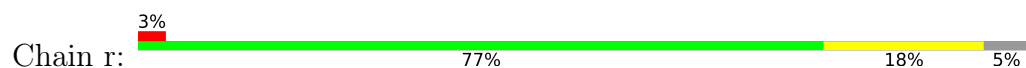
• Molecule 11: 60S ribosomal protein L9-B



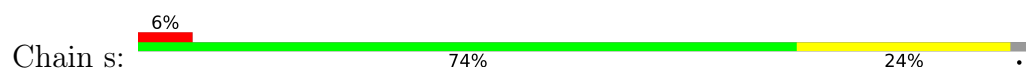
• Molecule 11: 60S ribosomal protein L9-B

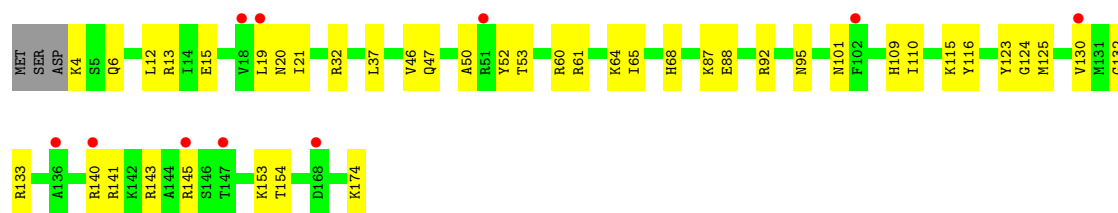


• Molecule 12: 60S ribosomal protein L10

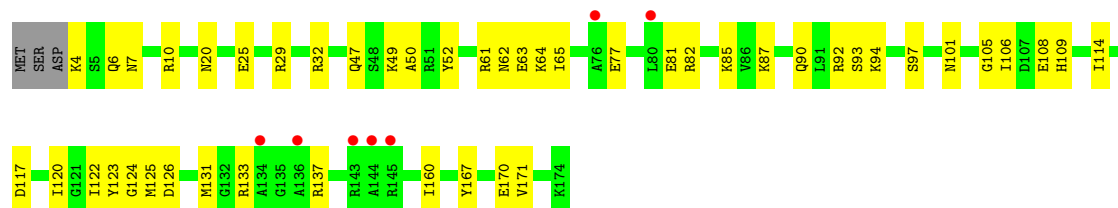
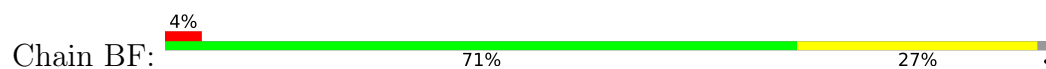


• Molecule 13: 60S ribosomal protein L11-B

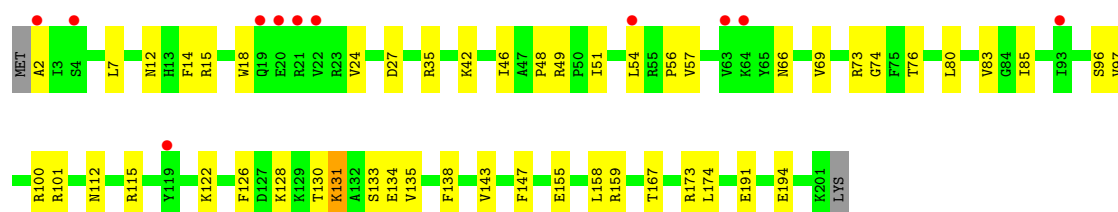
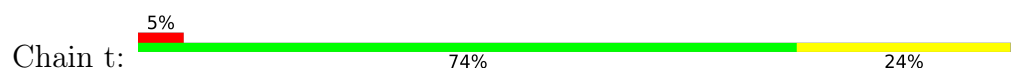




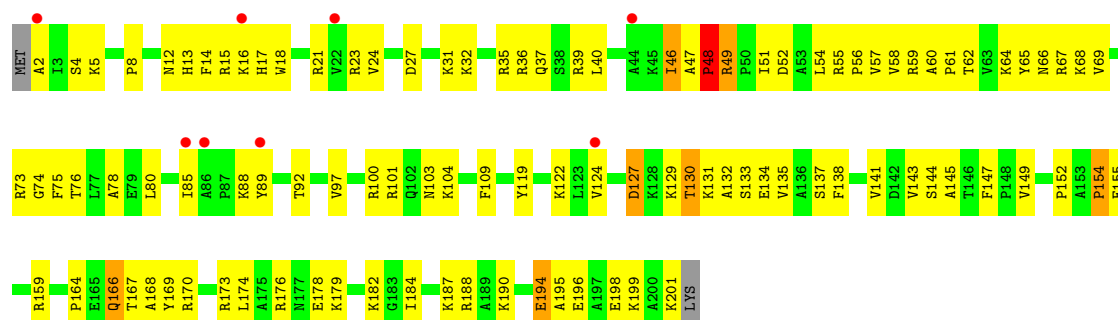
• Molecule 13: 60S ribosomal protein L11-B



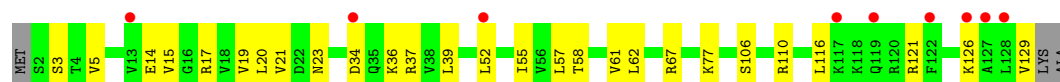
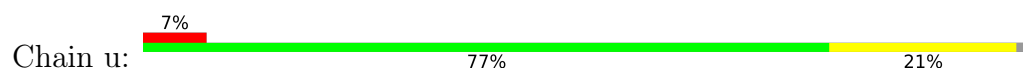
• Molecule 14: 60S ribosomal protein L13



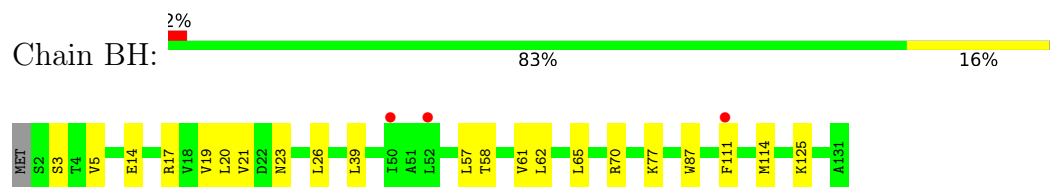
• Molecule 14: 60S ribosomal protein L13



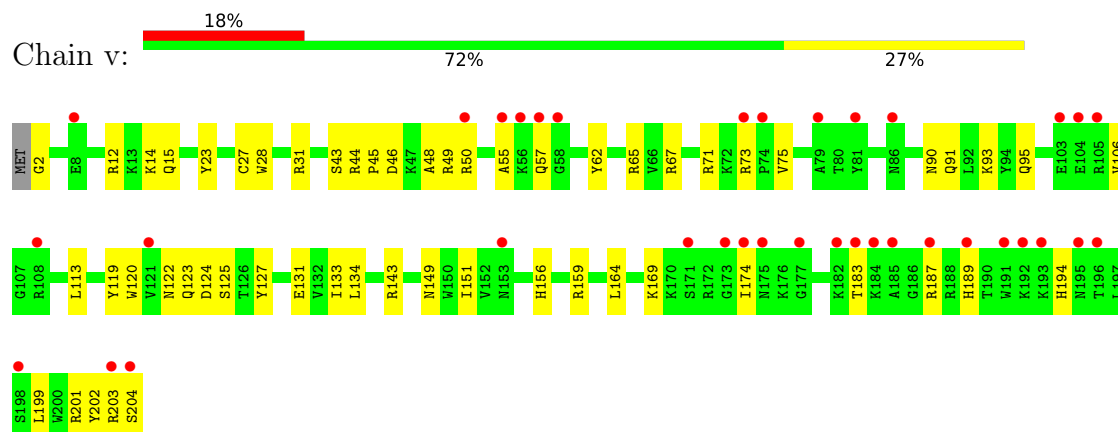
• Molecule 15: 60S ribosomal protein L14-B



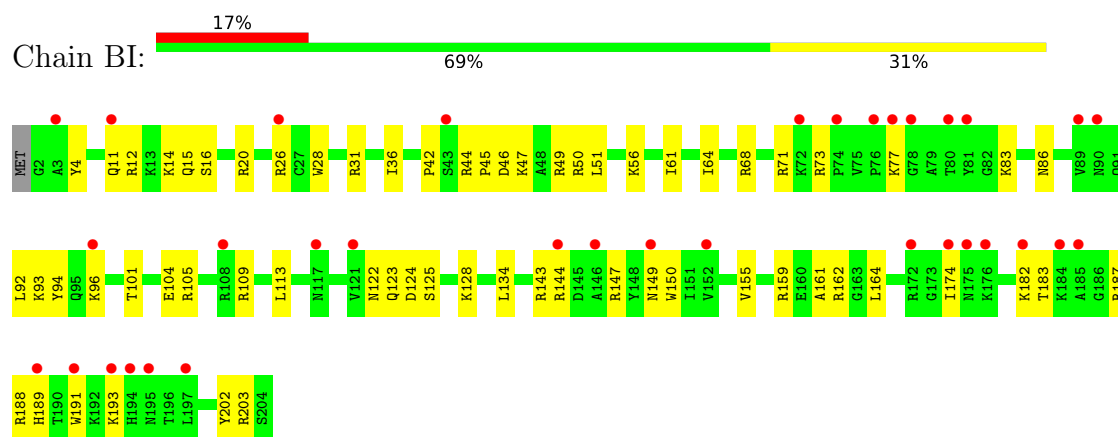
- Molecule 15: 60S ribosomal protein L14-B



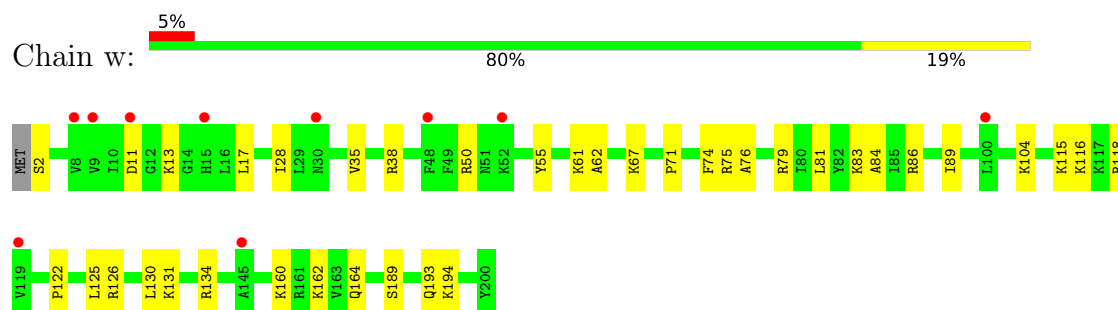
- Molecule 16: 60S ribosomal protein L15-A



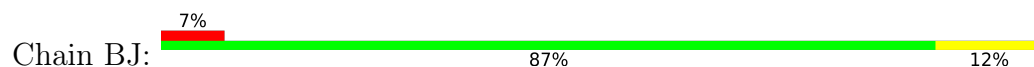
- Molecule 16: 60S ribosomal protein L15-A

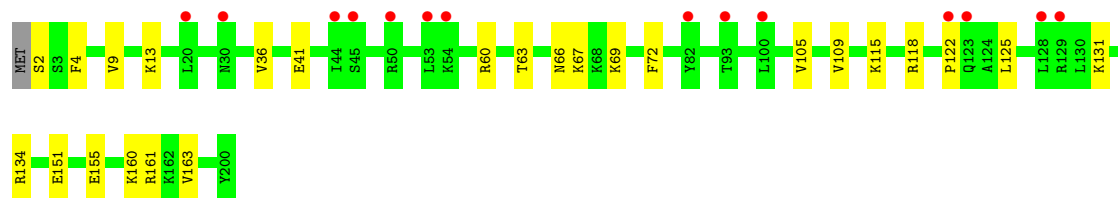


- Molecule 17: Ribosomal protein L13

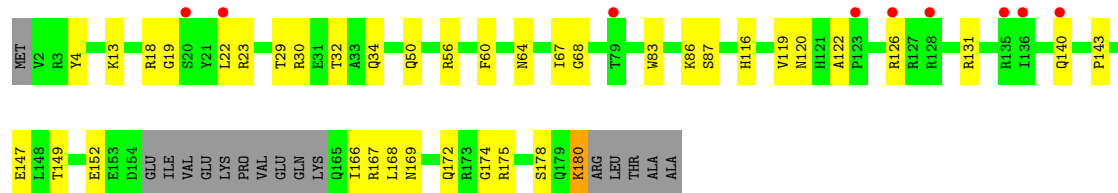


- Molecule 17: Ribosomal protein L13

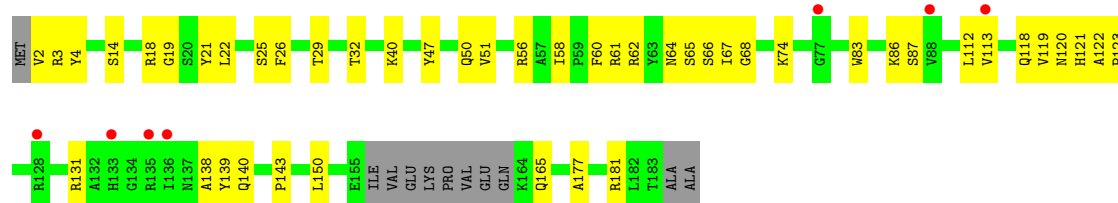




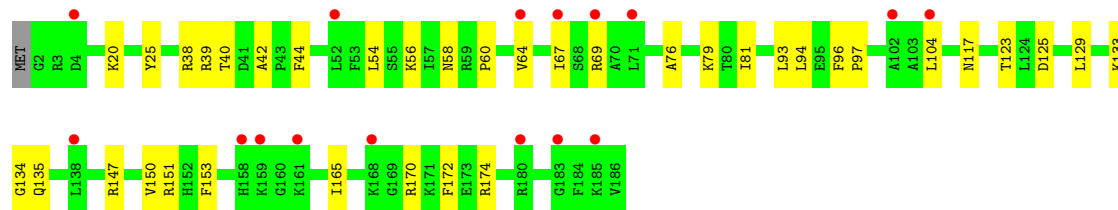
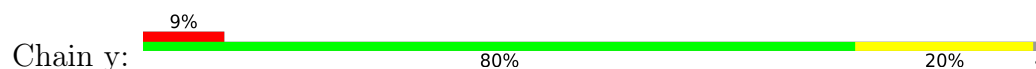
• Molecule 18: Ribosomal protein L22



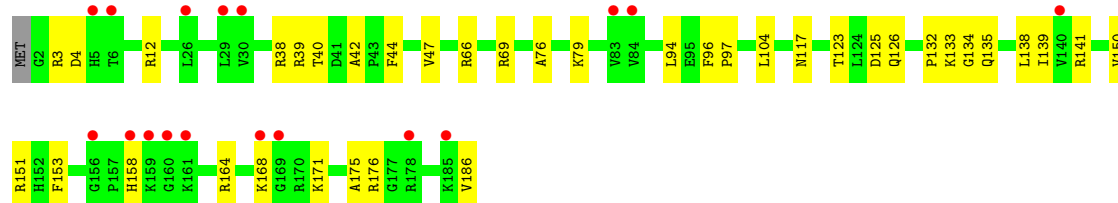
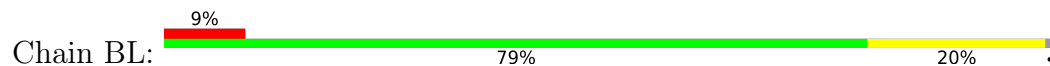
• Molecule 18: Ribosomal protein L22



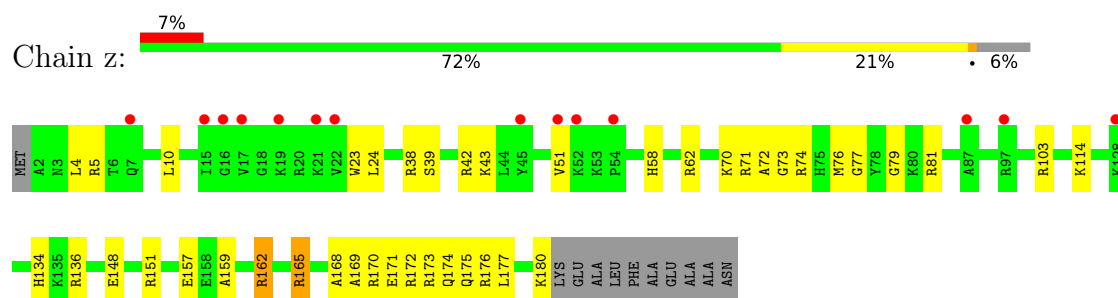
• Molecule 19: 60S ribosomal protein L18-A



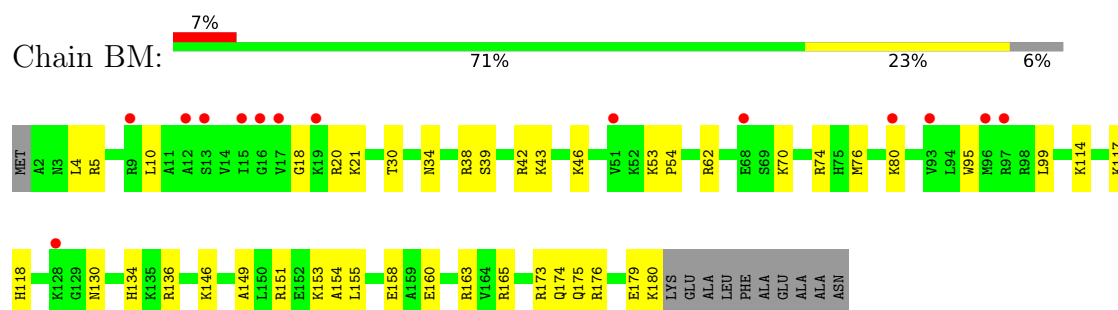
• Molecule 19: 60S ribosomal protein L18-A



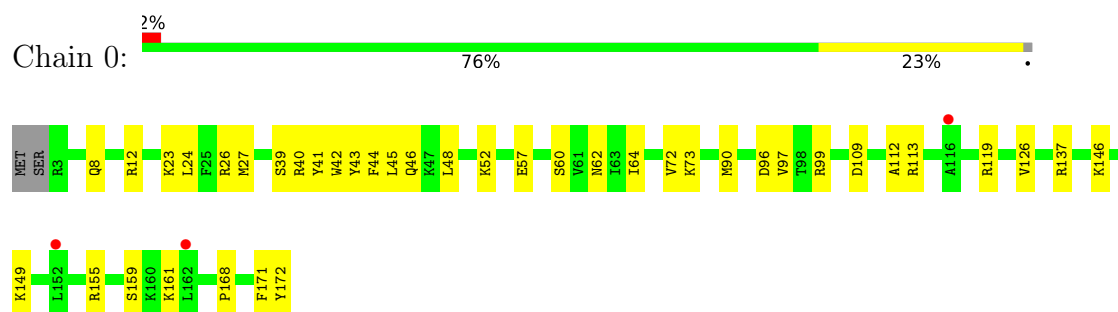
- Molecule 20: 60S ribosomal protein L19-A



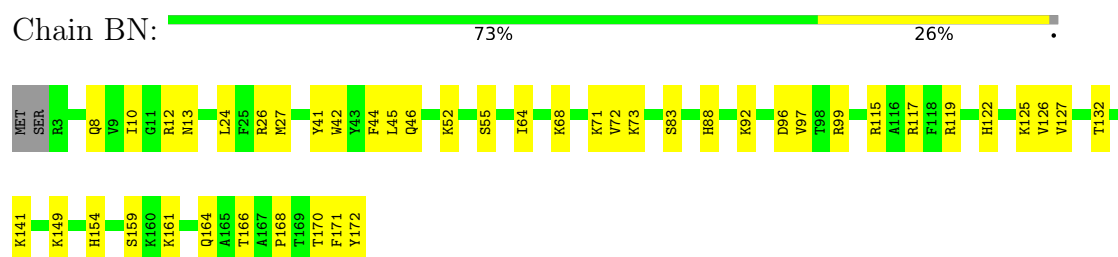
- Molecule 20: 60S ribosomal protein L19-A



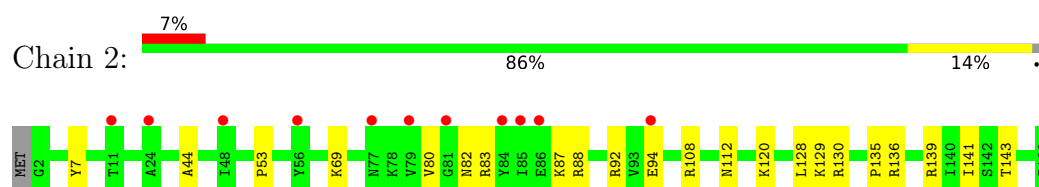
- Molecule 21: 60S ribosomal protein L20



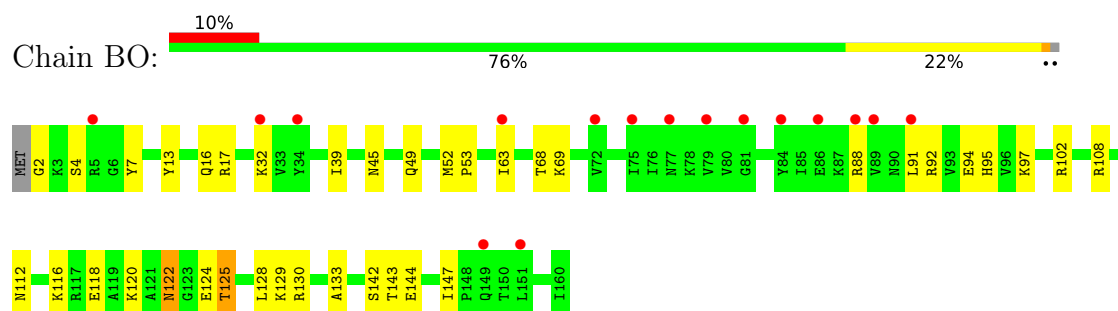
- Molecule 21: 60S ribosomal protein L20



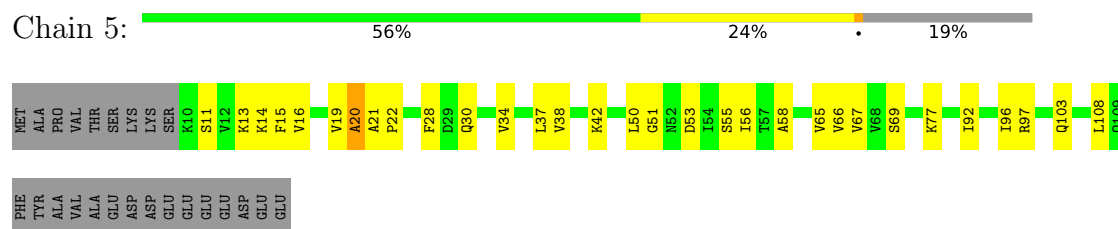
- Molecule 22: 60S ribosomal protein L21-A



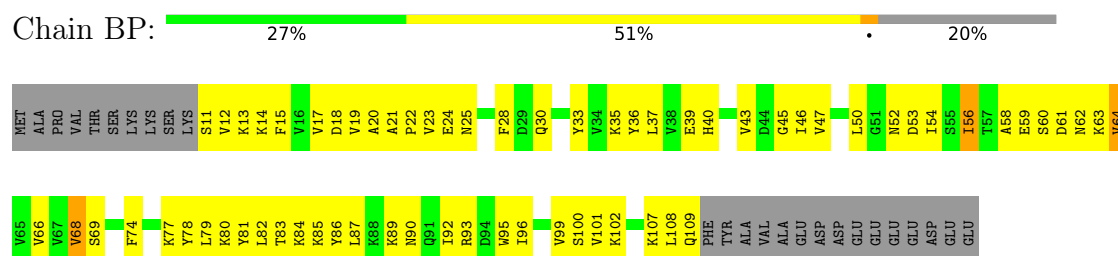
- Molecule 22: 60S ribosomal protein L21-A



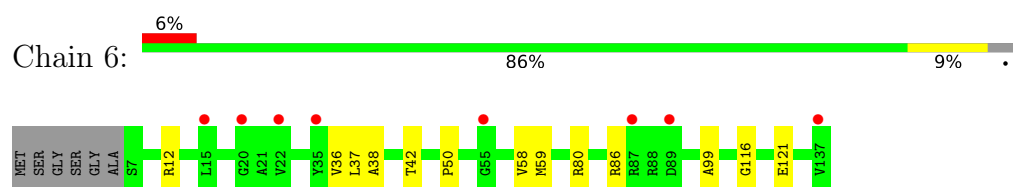
- Molecule 23: 60S ribosomal protein L22-B



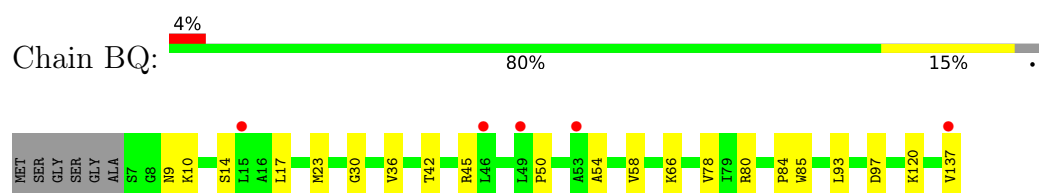
- Molecule 23: 60S ribosomal protein L22-B



- Molecule 24: 60S ribosomal protein L23-A



- Molecule 24: 60S ribosomal protein L23-A

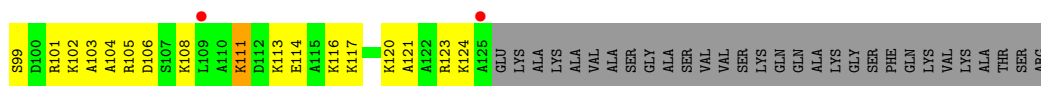


- Molecule 25: 60S ribosomal protein L24-A





Chain BR: 3% 43% 26% 30%



Chain 8:



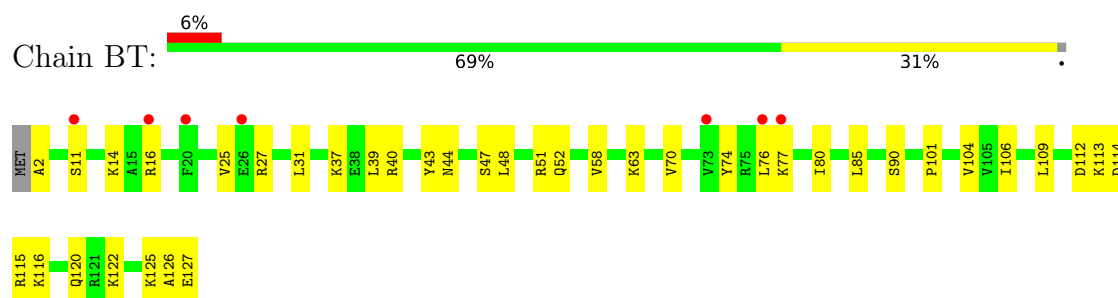
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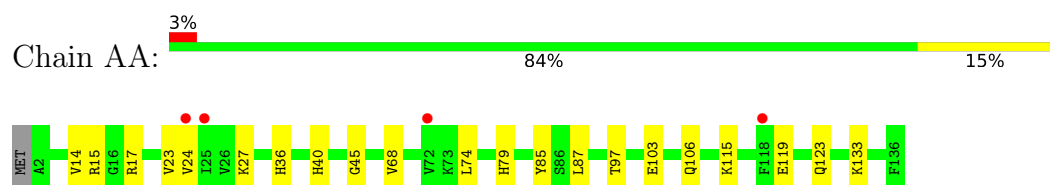
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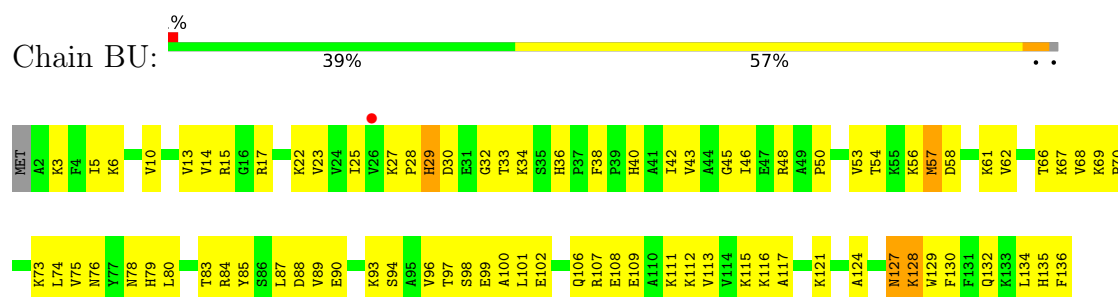
- Molecule 27: Ribosomal protein L24



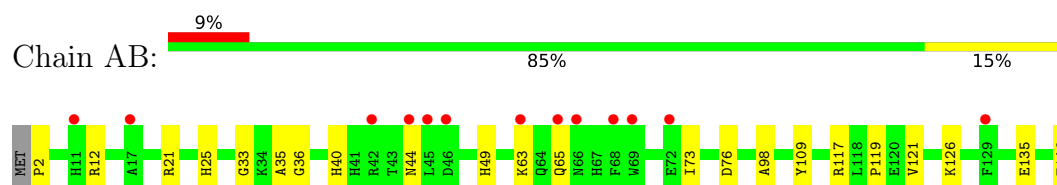
- Molecule 28: 60S ribosomal protein L27



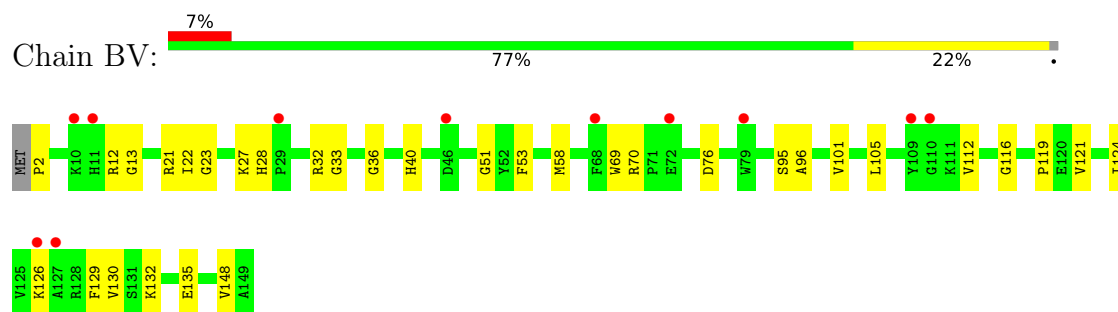
- Molecule 28: 60S ribosomal protein L27



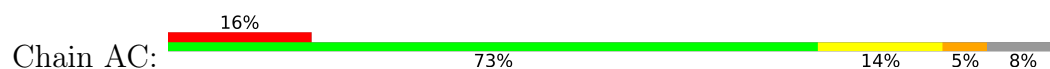
- Molecule 29: 60S ribosomal protein L28

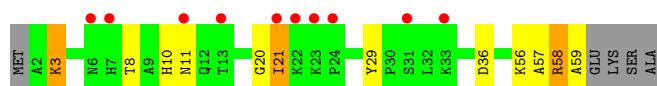


- Molecule 29: 60S ribosomal protein L28

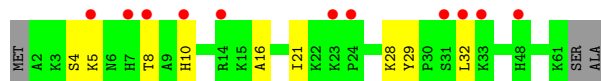
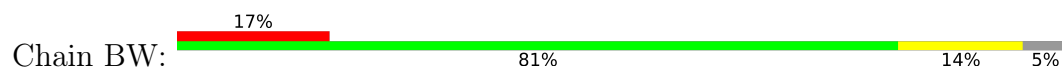


- Molecule 30: 60S ribosomal protein L29

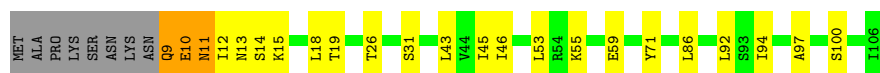




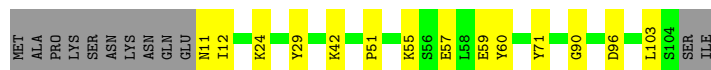
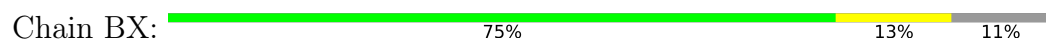
- Molecule 30: 60S ribosomal protein L29



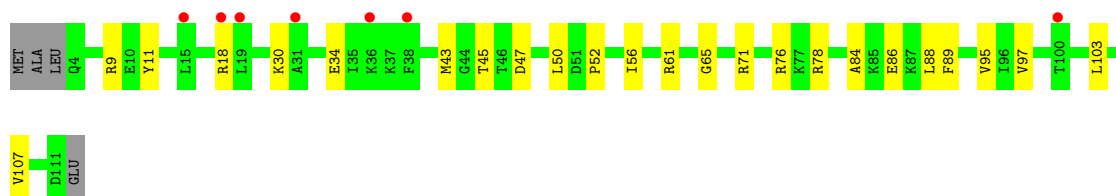
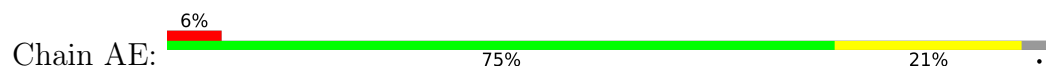
- Molecule 31: 60S ribosomal protein L30



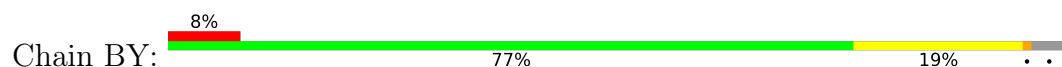
- Molecule 31: 60S ribosomal protein L30



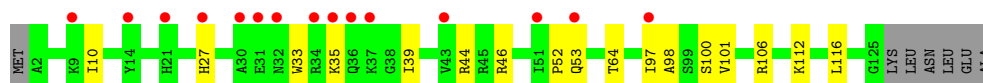
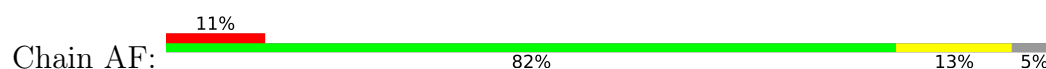
- Molecule 32: 60S ribosomal protein L31-B



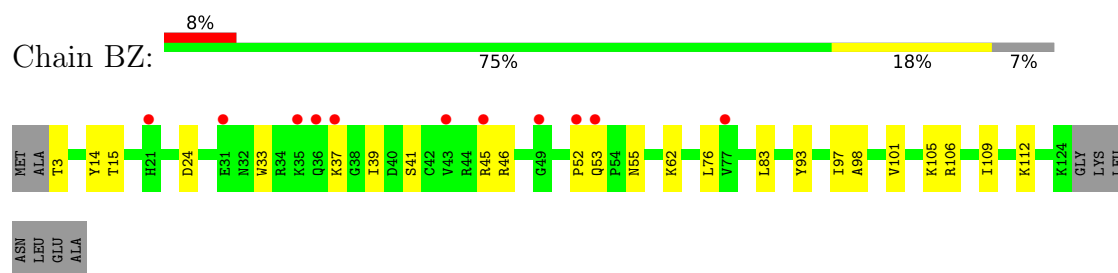
- Molecule 32: 60S ribosomal protein L31-B



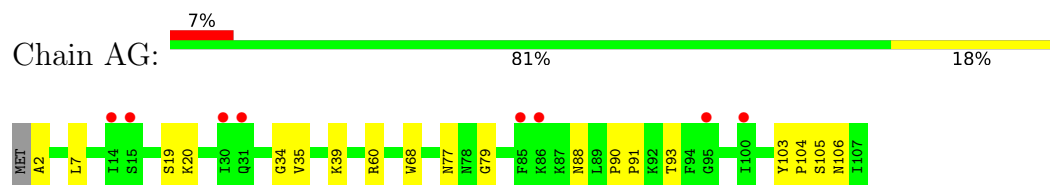
- Molecule 33: 60S ribosomal protein L32



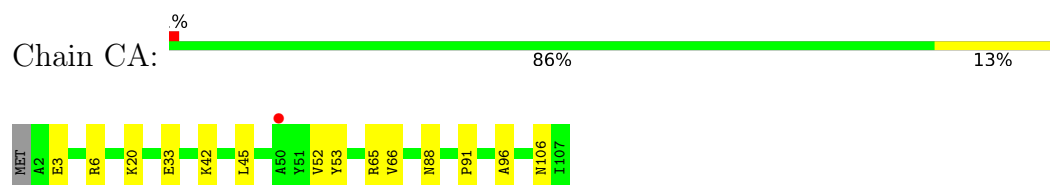
- Molecule 33: 60S ribosomal protein L32



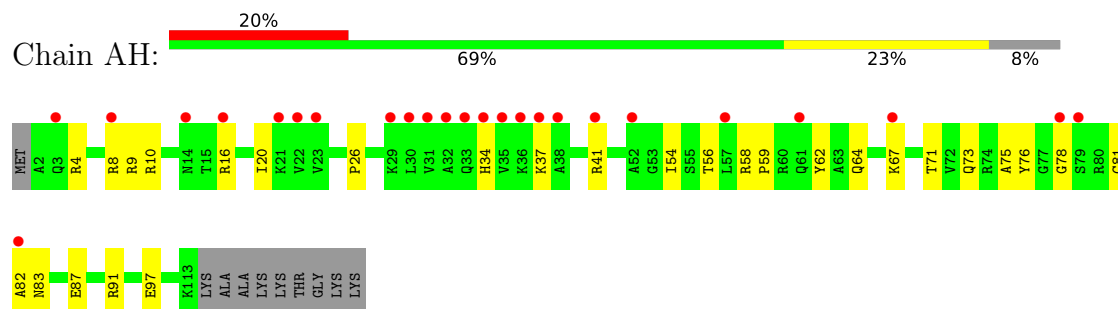
- Molecule 34: 60S ribosomal protein L33-A



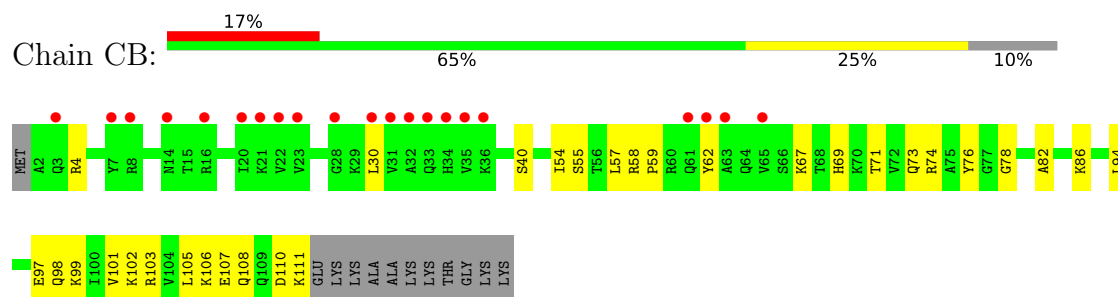
- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-B

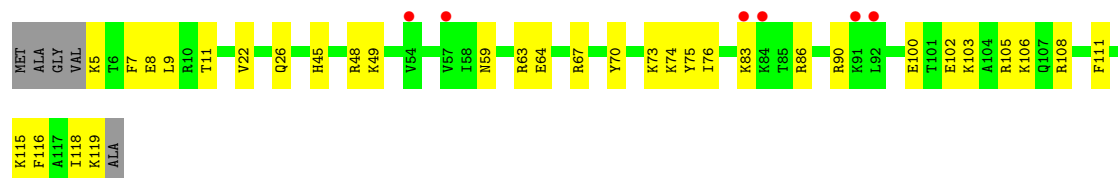


- Molecule 35: 60S ribosomal protein L34-B

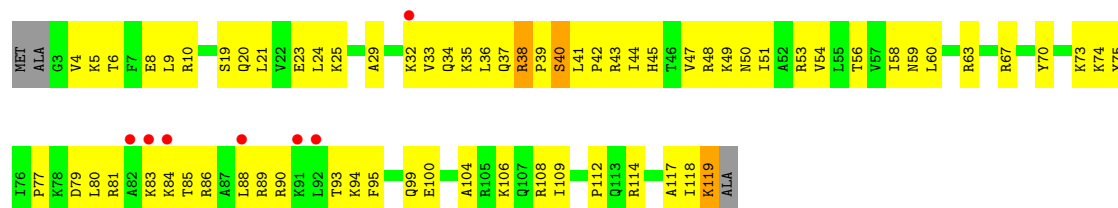
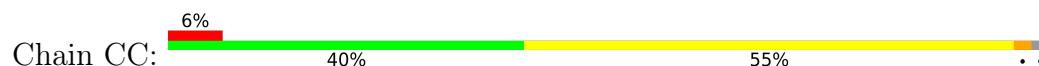


- Molecule 36: Ribosomal protein L29

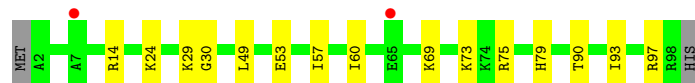
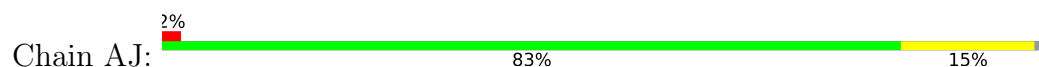




• Molecule 36: Ribosomal protein L29



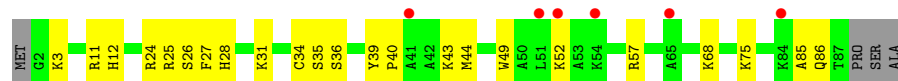
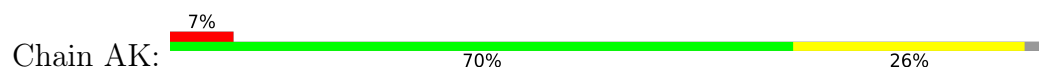
• Molecule 37: 60S ribosomal protein L36



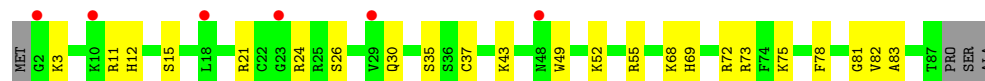
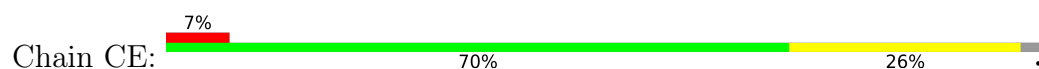
• Molecule 37: 60S ribosomal protein L36



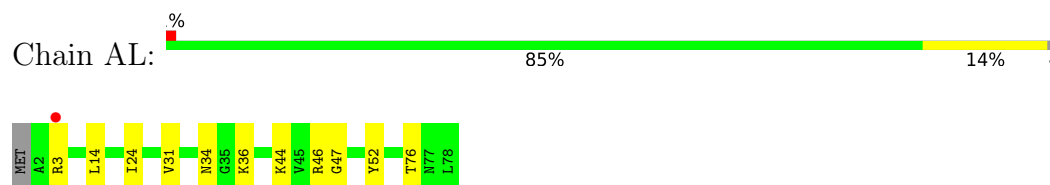
• Molecule 38: 60S ribosomal protein L37-B



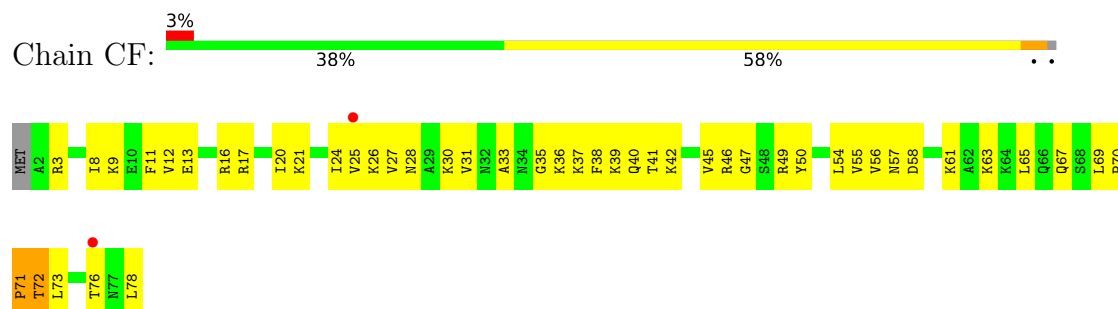
• Molecule 38: 60S ribosomal protein L37-B



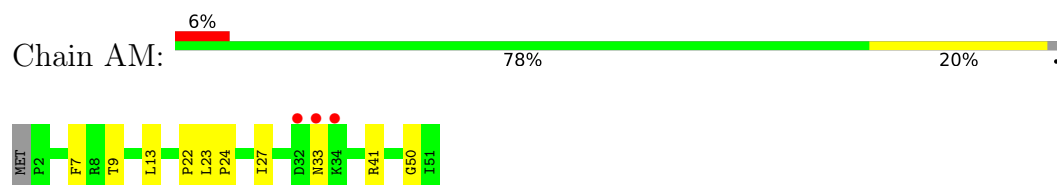
- Molecule 39: 60S ribosomal protein L38



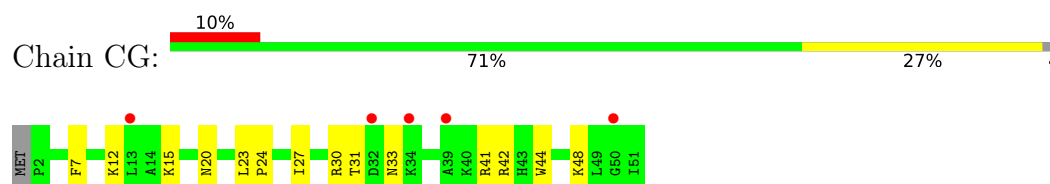
- Molecule 39: 60S ribosomal protein L38



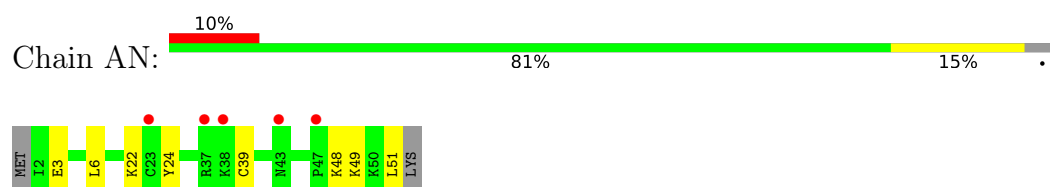
- Molecule 40: 60S ribosomal protein L39



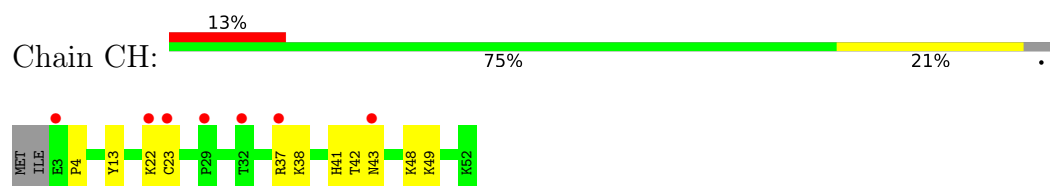
- Molecule 40: 60S ribosomal protein L39



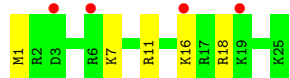
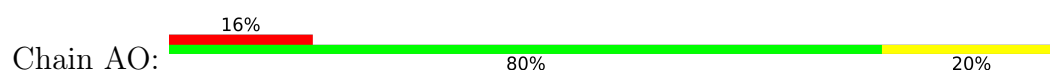
- Molecule 41: 60S ribosomal protein L40-B



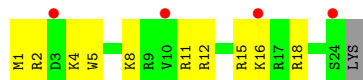
- Molecule 41: 60S ribosomal protein L40-B



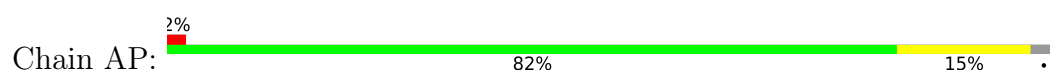
- Molecule 42: 60S ribosomal protein L41



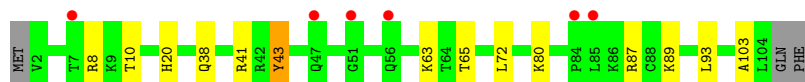
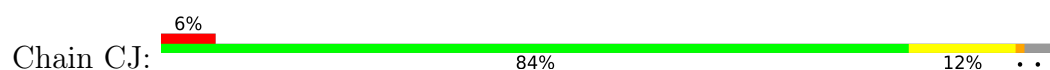
- Molecule 42: 60S ribosomal protein L41



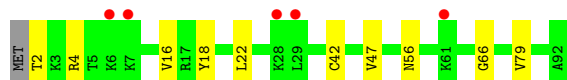
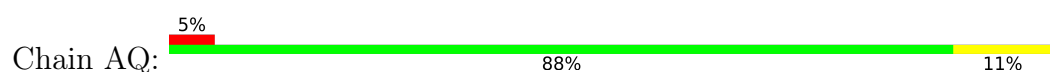
- Molecule 43: 60S ribosomal protein L42-B



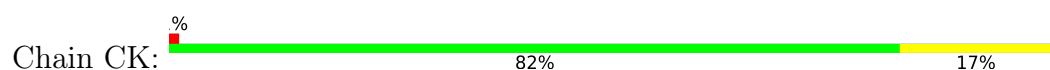
- Molecule 43: 60S ribosomal protein L42-B



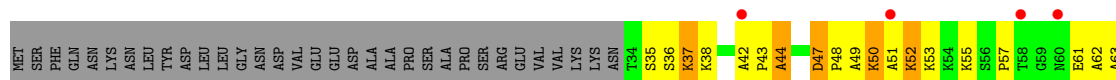
- Molecule 44: 60S ribosomal protein L43-A



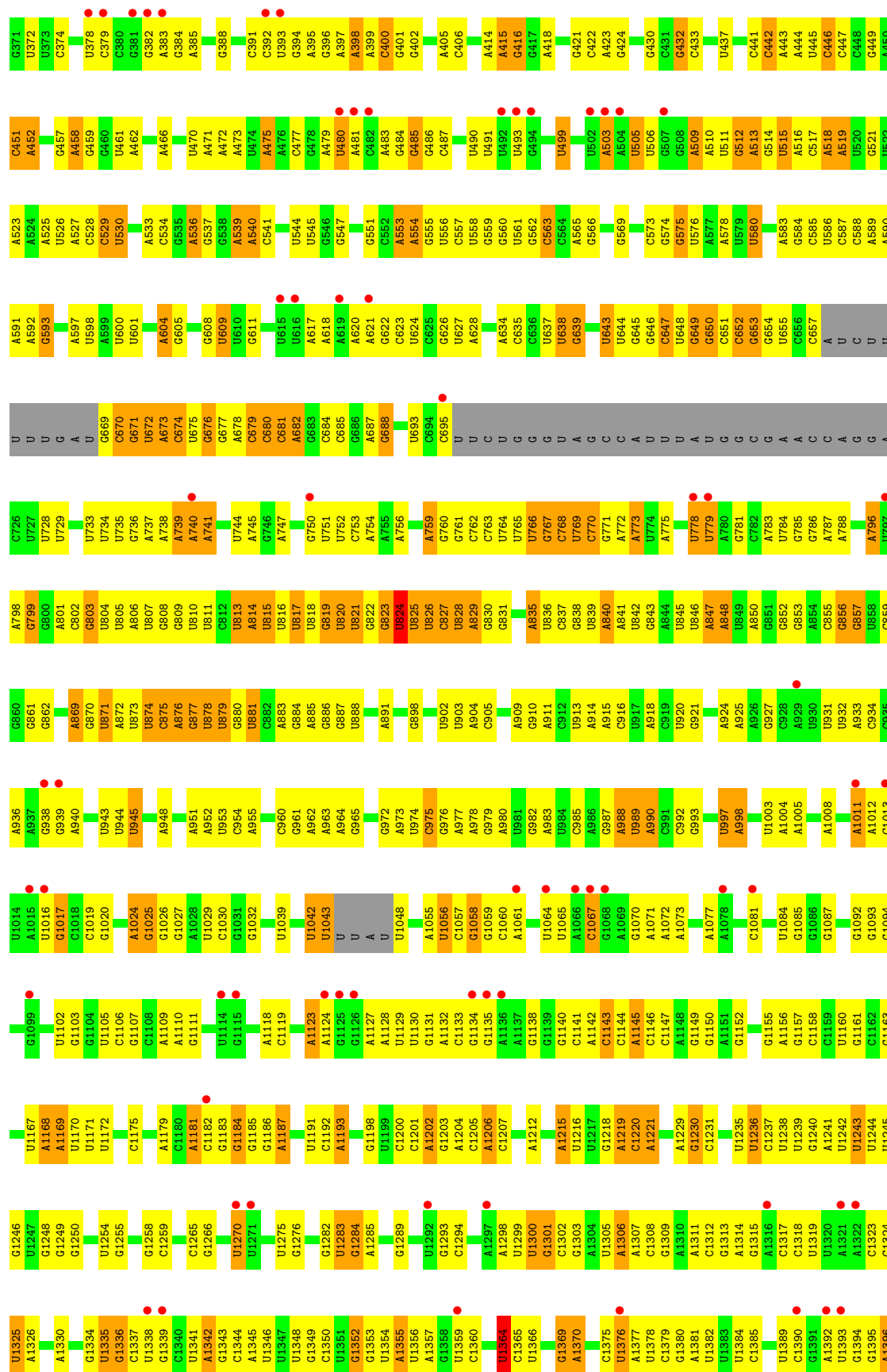
- Molecule 44: 60S ribosomal protein L43-A

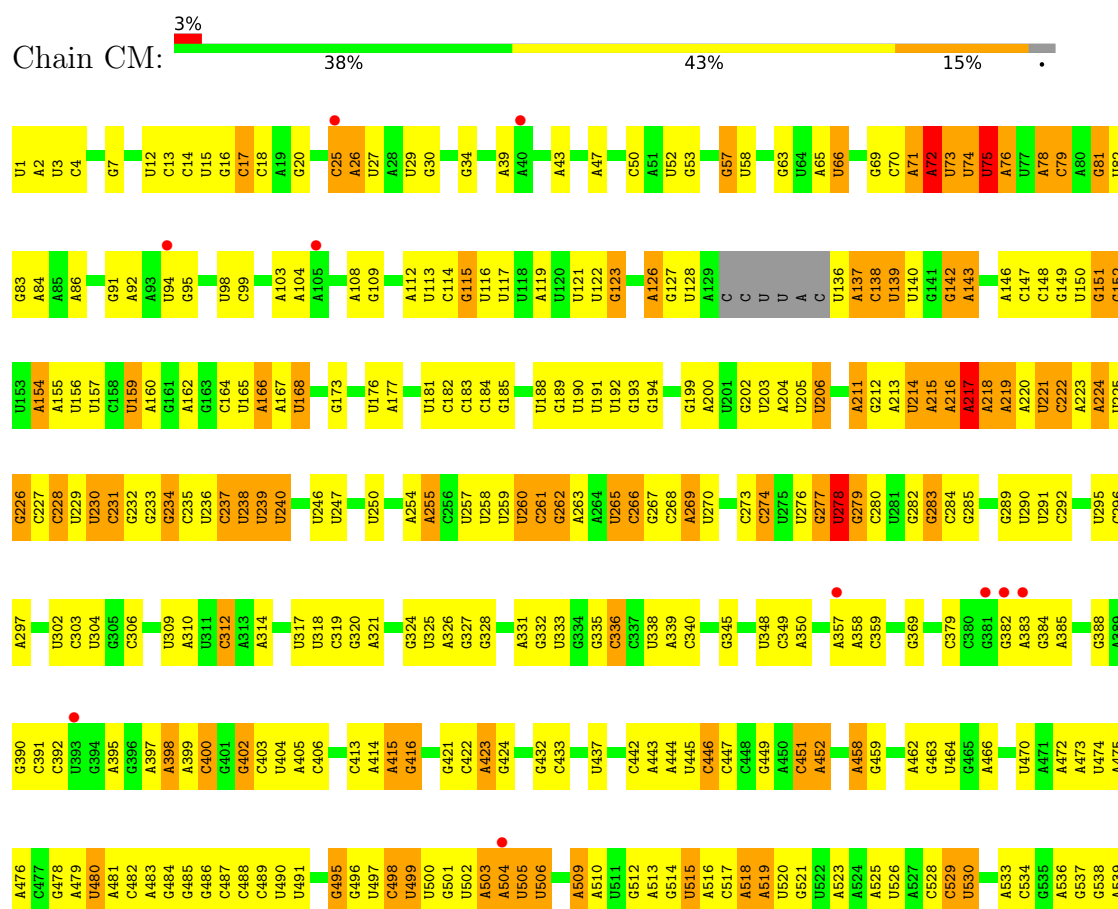
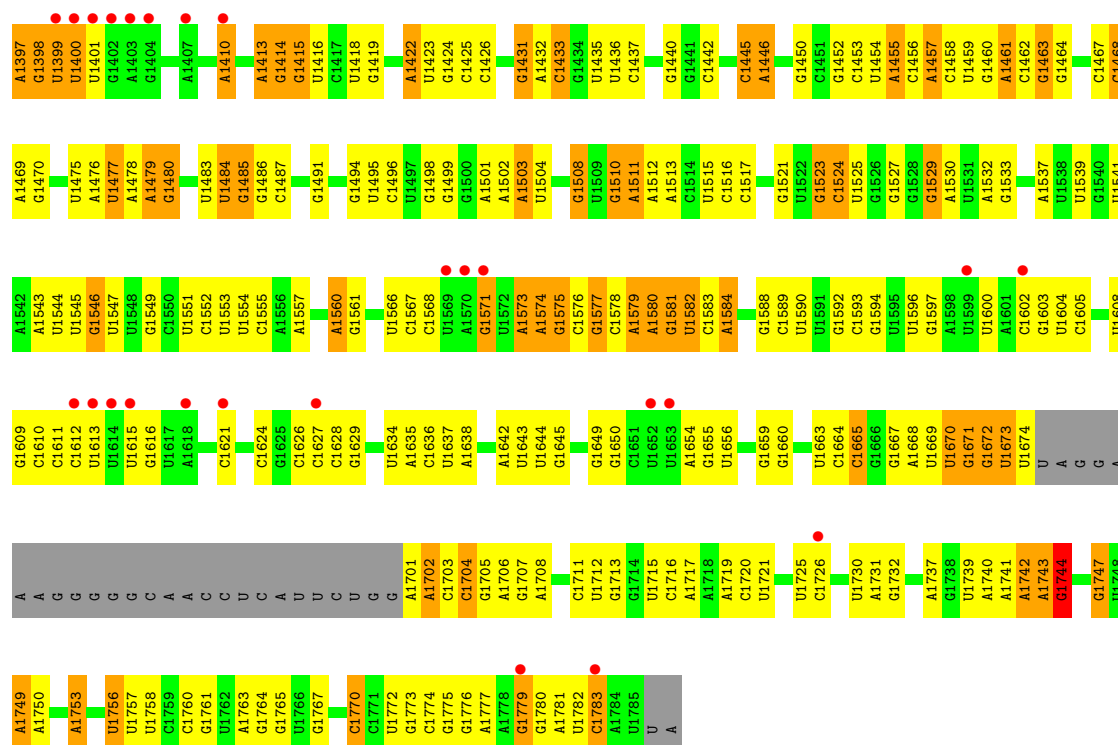


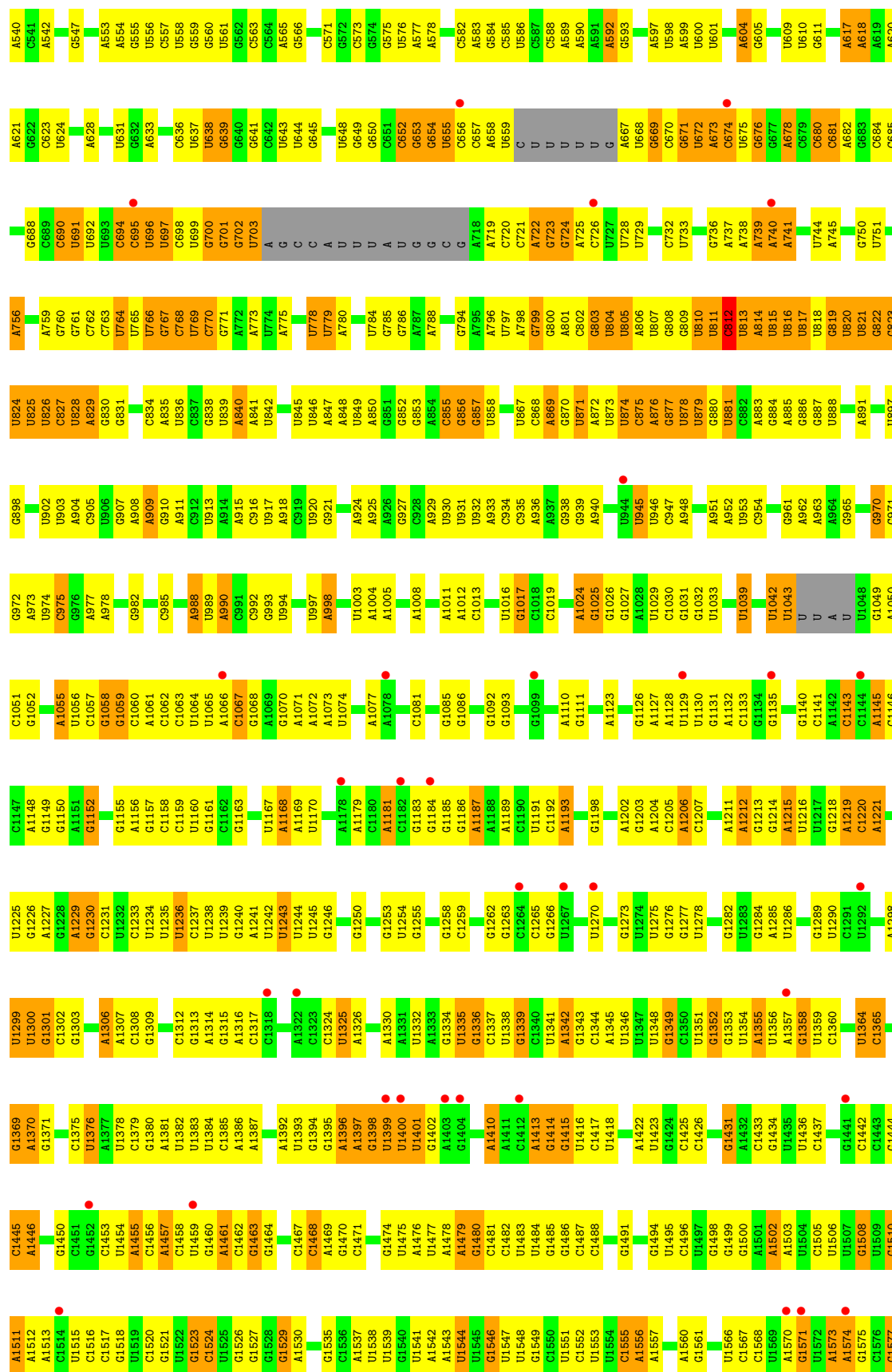
- Molecule 45: 60S ribosomal protein CAALFM_C304810CA

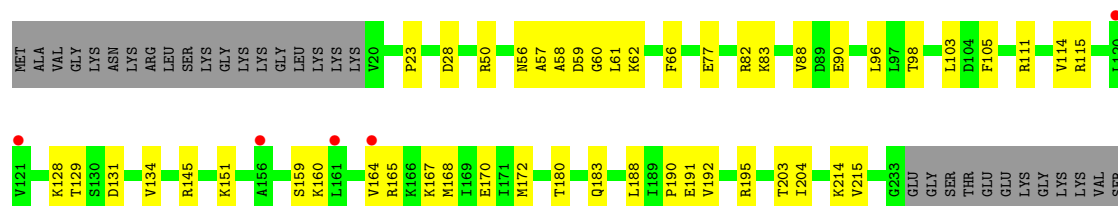


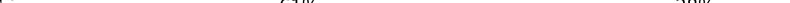


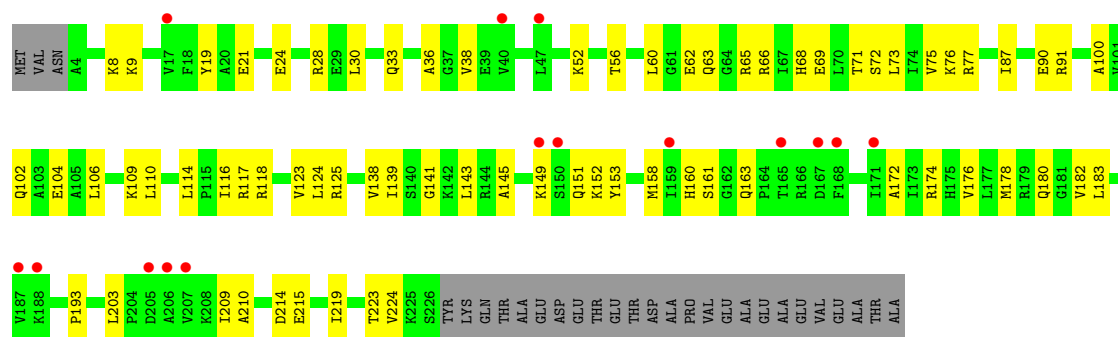




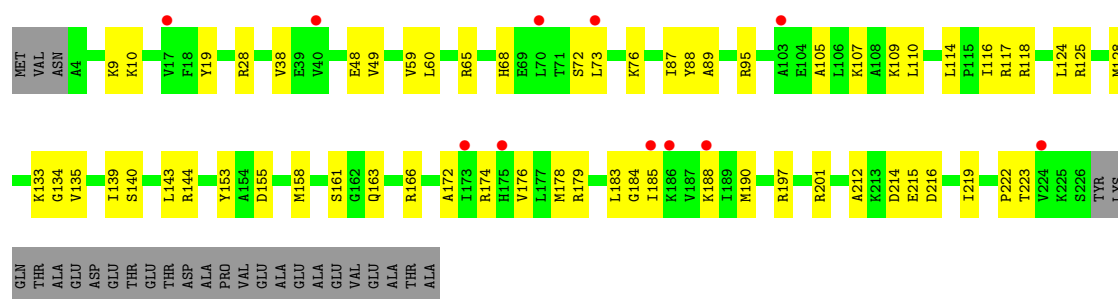




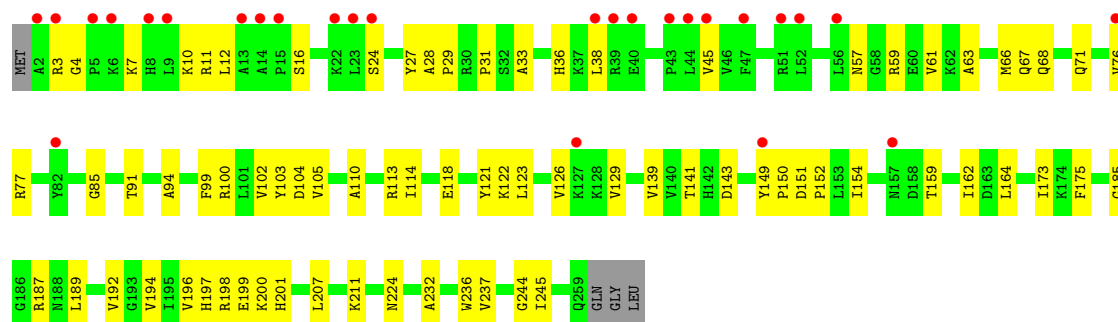
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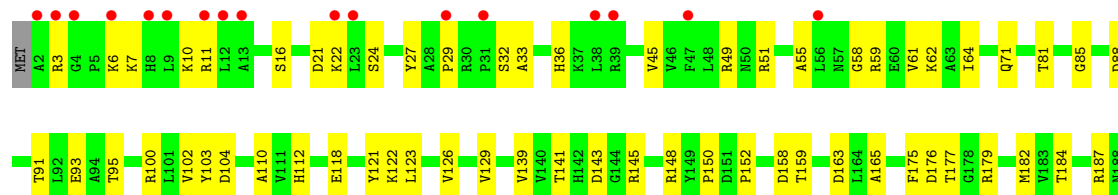
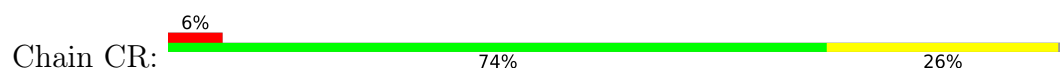
• Molecule 50: Ribosomal protein S3



• Molecule 51: 40S ribosomal protein S4

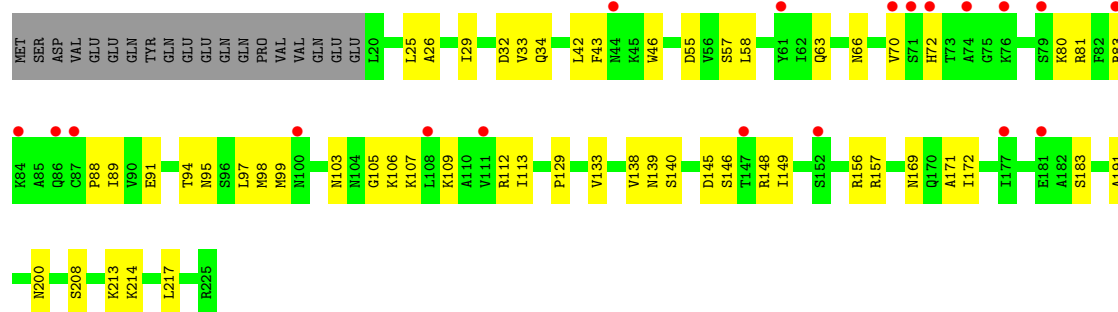


• Molecule 51: 40S ribosomal protein S4

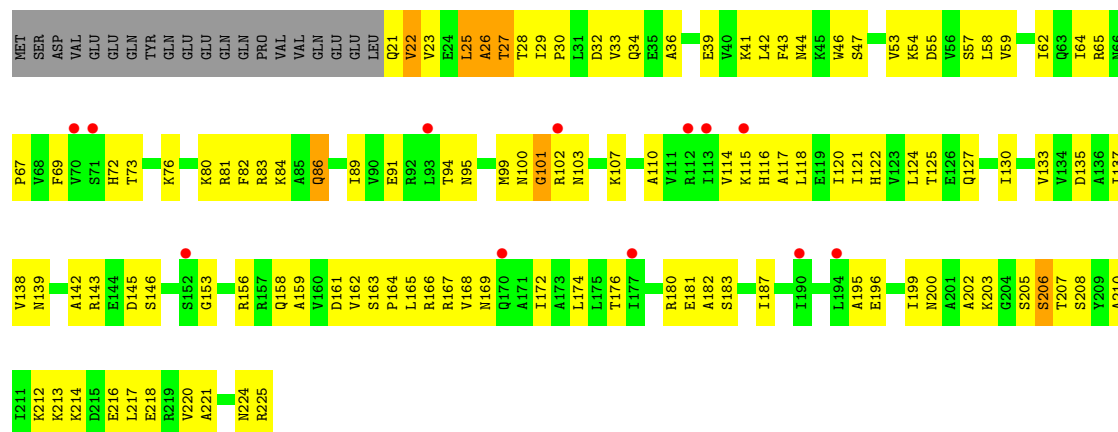




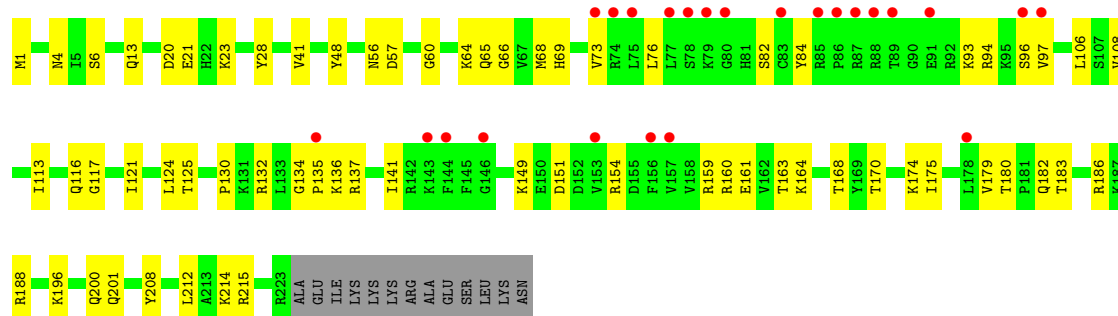
• Molecule 52: Ribosomal protein S7



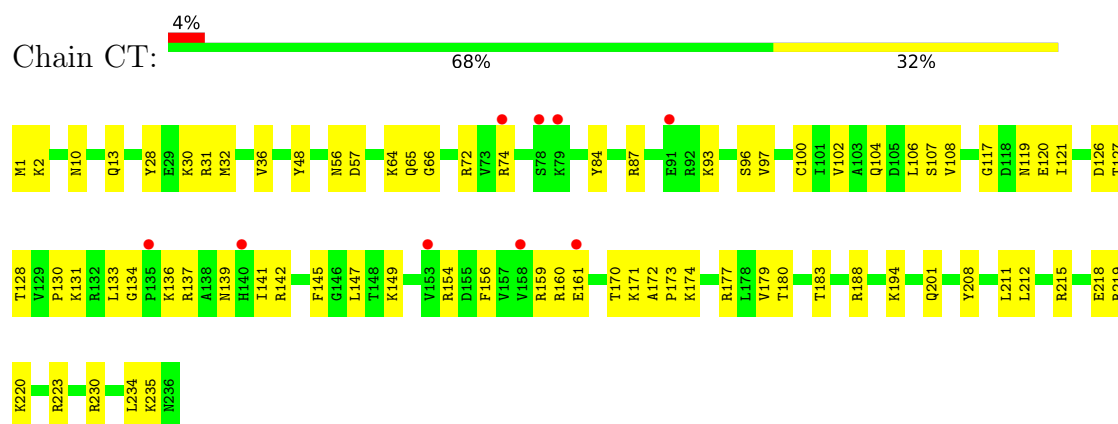
• Molecule 52: Ribosomal protein S7



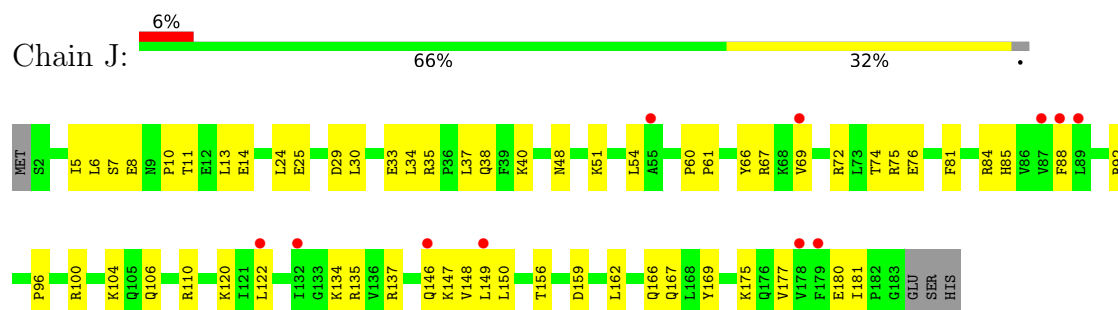
• Molecule 53: 40S ribosomal protein S6



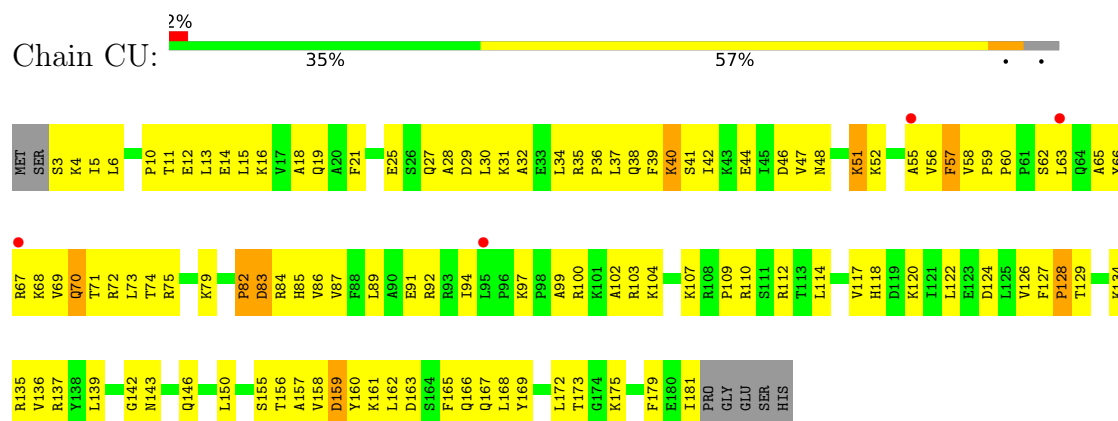
• Molecule 53: 40S ribosomal protein S6



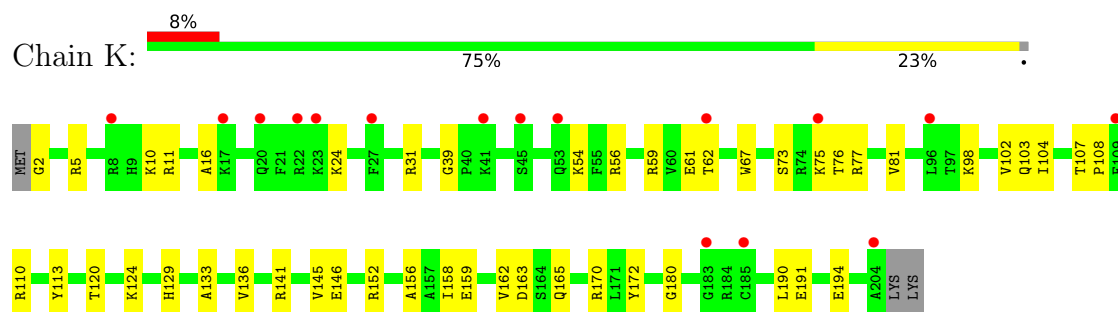
- Molecule 54: 40S ribosomal protein S7



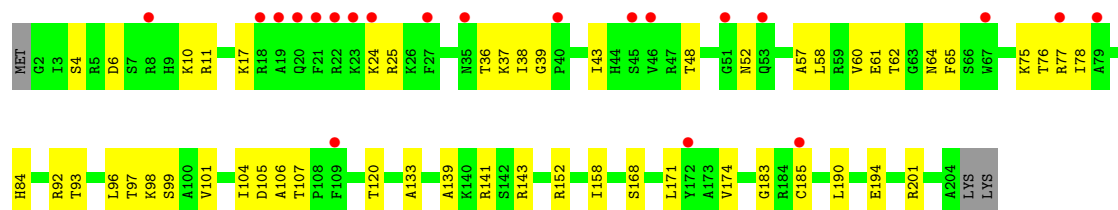
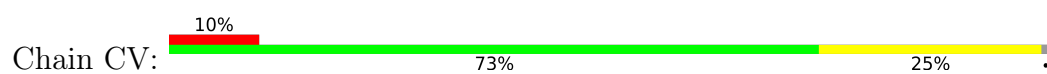
- Molecule 54: 40S ribosomal protein S7



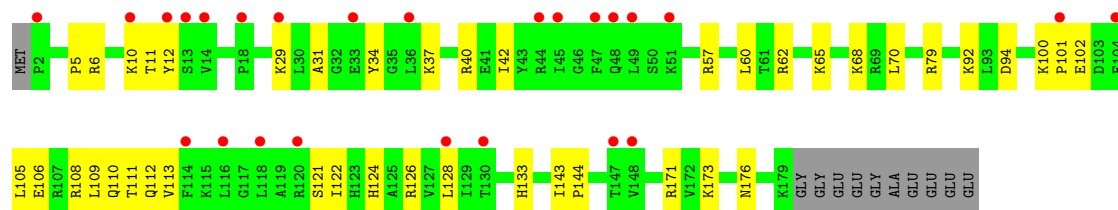
- Molecule 55: 40S ribosomal protein S8



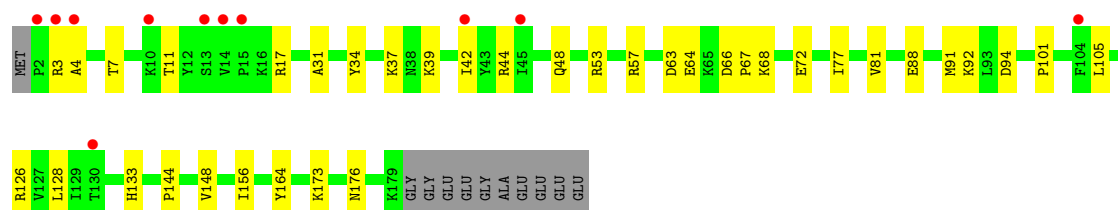
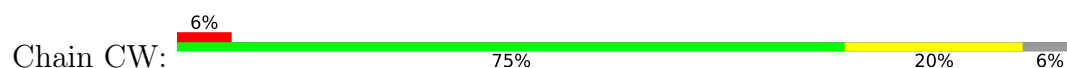
- Molecule 55: 40S ribosomal protein S8



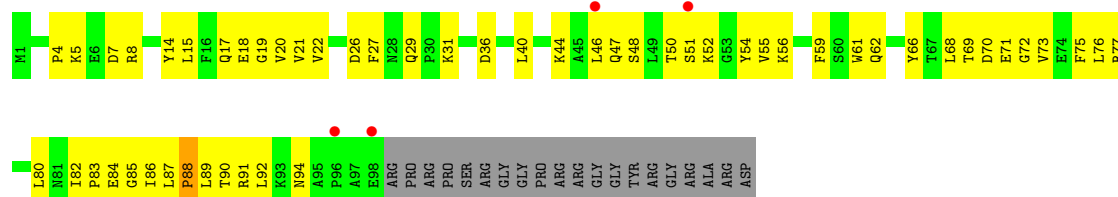
• Molecule 56: Ribosomal protein S4



• Molecule 56: Ribosomal protein S4

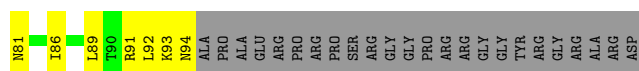


• Molecule 57: 40S ribosomal protein S10-A

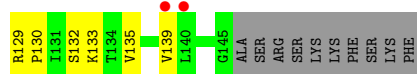


• Molecule 57: 40S ribosomal protein S10-A

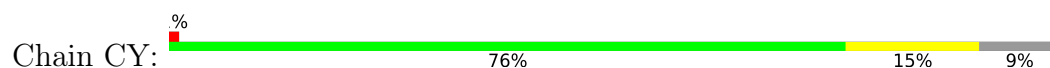




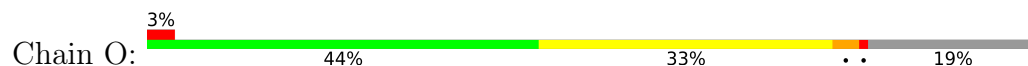
- Molecule 58: 40S ribosomal protein S11A



- Molecule 58: 40S ribosomal protein S11A



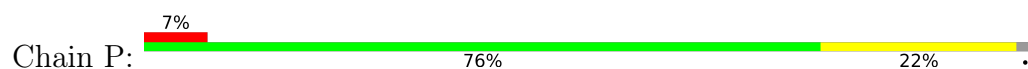
- Molecule 59: 40S ribosomal protein S12

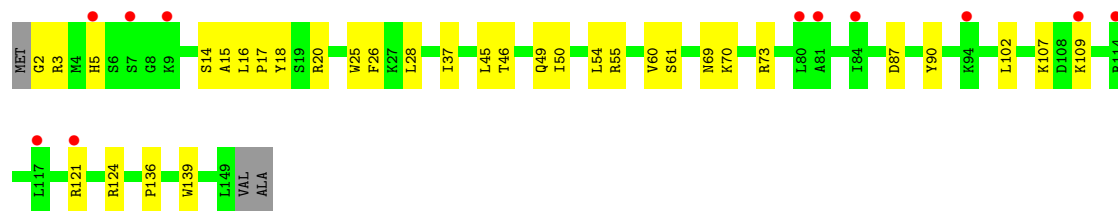


- Molecule 59: 40S ribosomal protein S12

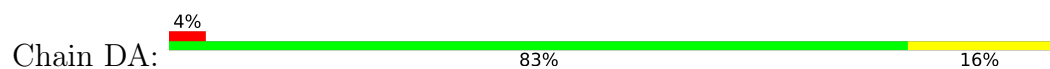


- Molecule 60: 40S ribosomal protein S13

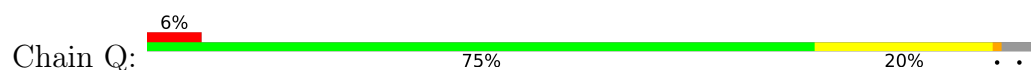




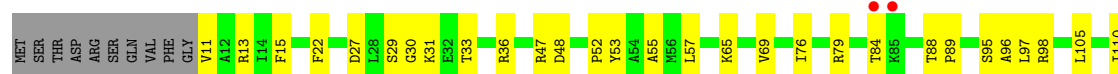
- Molecule 60: 40S ribosomal protein S13



- Molecule 61: 40S ribosomal protein S14-A



- Molecule 61: 40S ribosomal protein S14-A

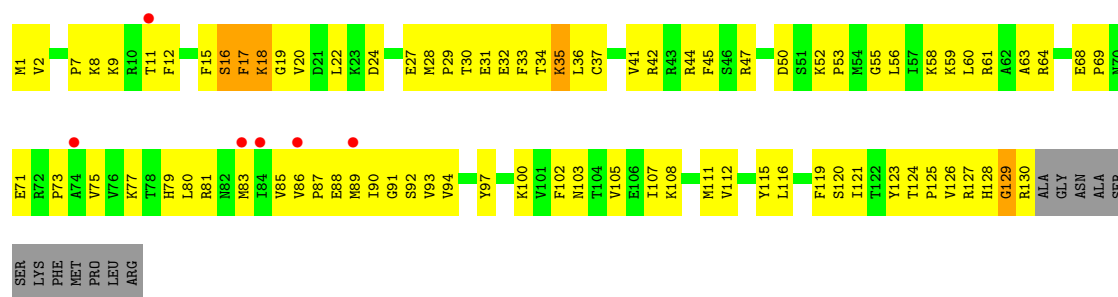


- Molecule 62: 40S ribosomal protein S15

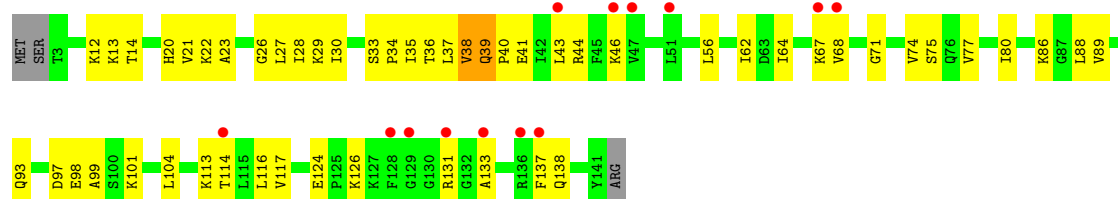


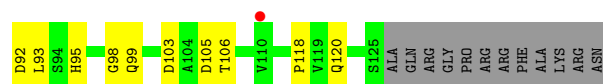
- Molecule 62: 40S ribosomal protein S15



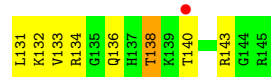
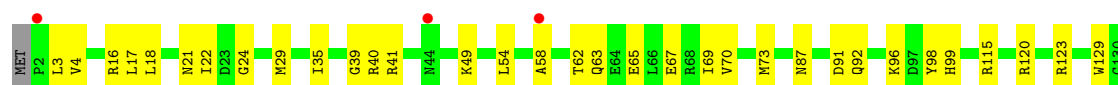


• Molecule 63: 40S ribosomal protein S16

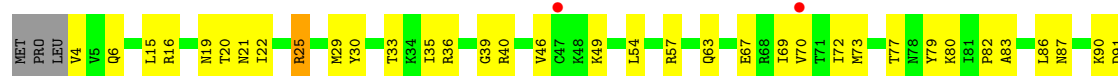




- Molecule 65: 40S ribosomal protein S18-B



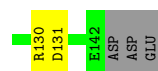
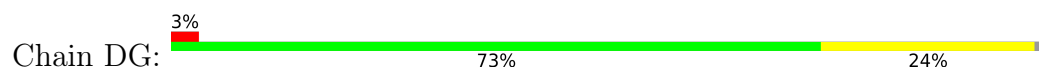
- Molecule 65: 40S ribosomal protein S18-B



- Molecule 66: 40S ribosomal protein S19-A

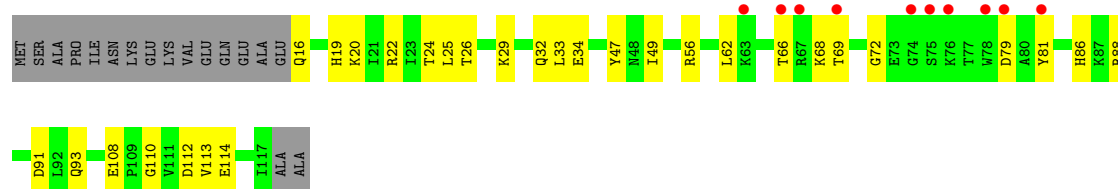


- Molecule 66: 40S ribosomal protein S19-A



- Molecule 67: Ribosomal protein S10

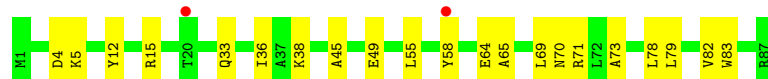
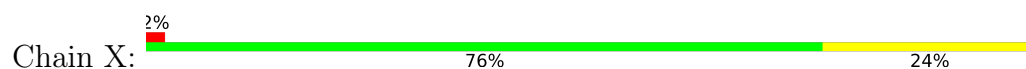




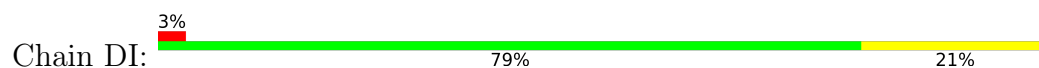
• Molecule 67: Ribosomal protein S10



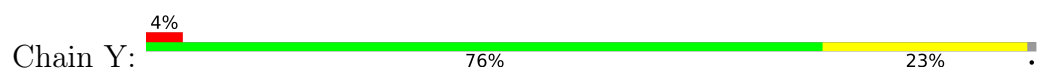
• Molecule 68: 40S ribosomal protein S21



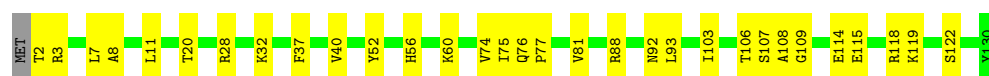
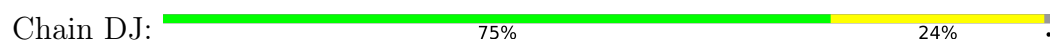
• Molecule 68: 40S ribosomal protein S21



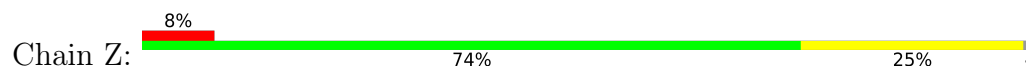
• Molecule 69: 40S ribosomal protein S22-A

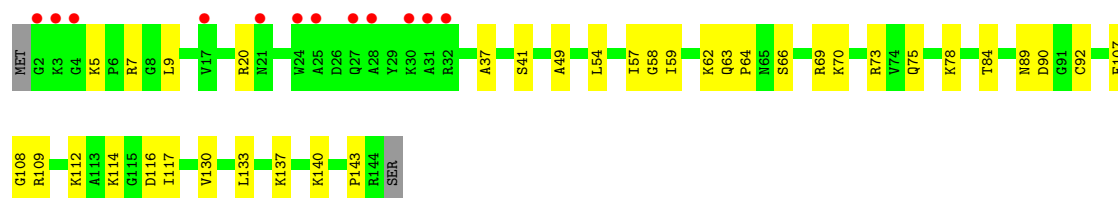


• Molecule 69: 40S ribosomal protein S22-A

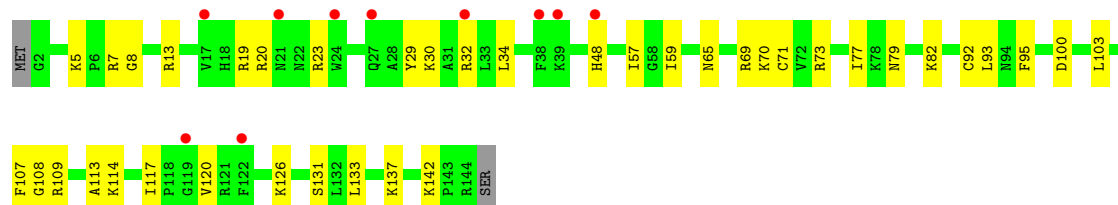
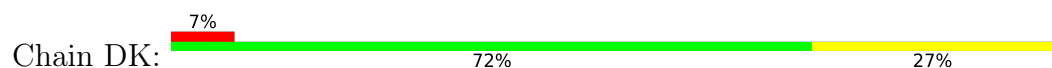


• Molecule 70: Ribosomal protein S23 (S12)

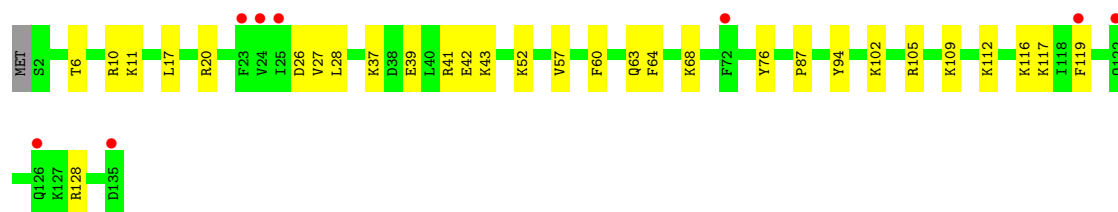
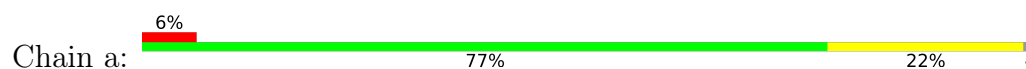




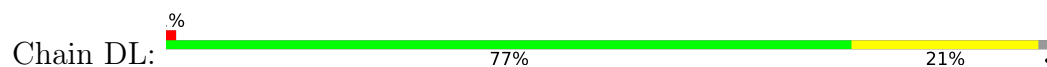
• Molecule 70: Ribosomal protein S23 (S12)



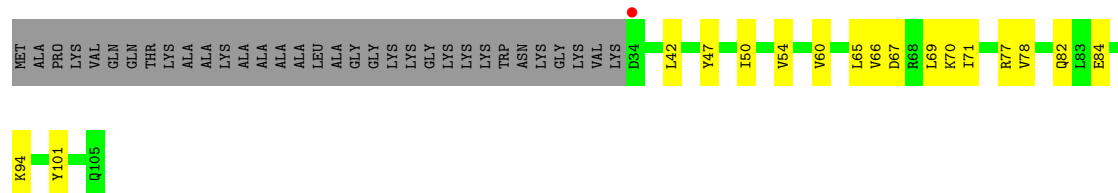
• Molecule 71: 40S ribosomal protein S24



• Molecule 71: 40S ribosomal protein S24

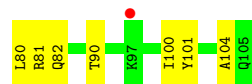
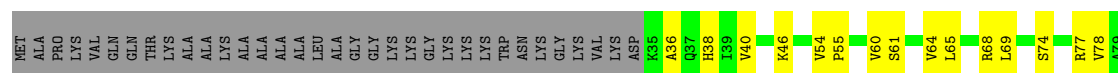


• Molecule 72: 40S ribosomal protein S25



• Molecule 72: 40S ribosomal protein S25

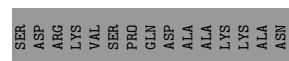




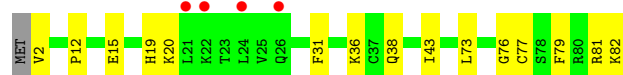
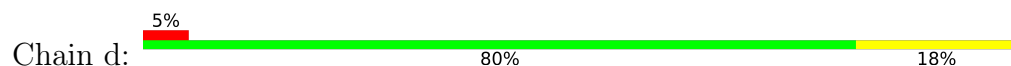
- Molecule 73: 40S ribosomal protein S26



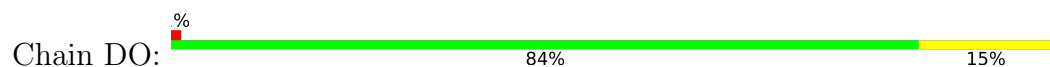
- Molecule 73: 40S ribosomal protein S26



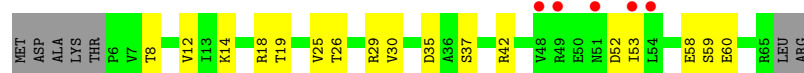
- Molecule 74: 40S ribosomal protein S27



- Molecule 74: 40S ribosomal protein S27

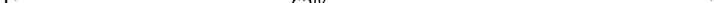


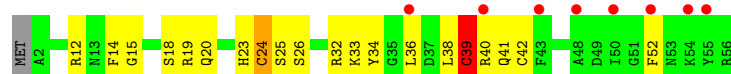
- Molecule 75: 40S ribosomal protein S28-B

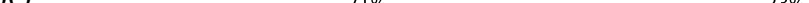


- Molecule 75: 40S ribosomal protein S28-B

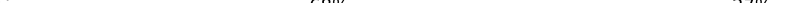


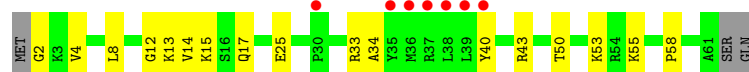
- Chain f: 

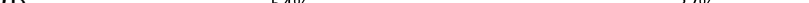


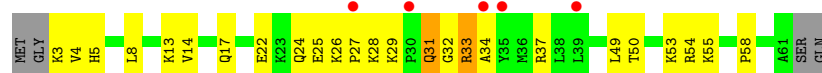
- Chain DQ: 

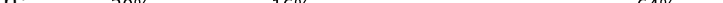


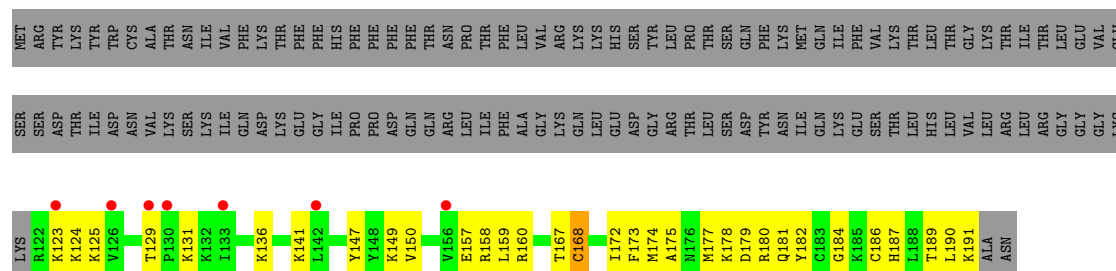
- Chain g: 



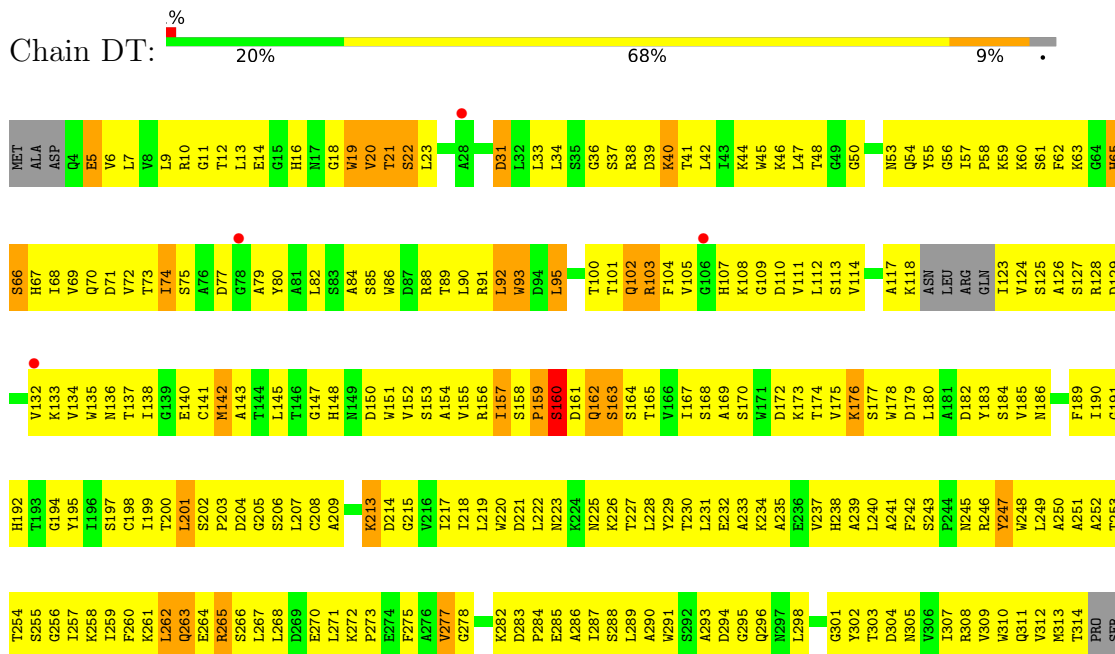
- Chain DR: 



- Chain h: 

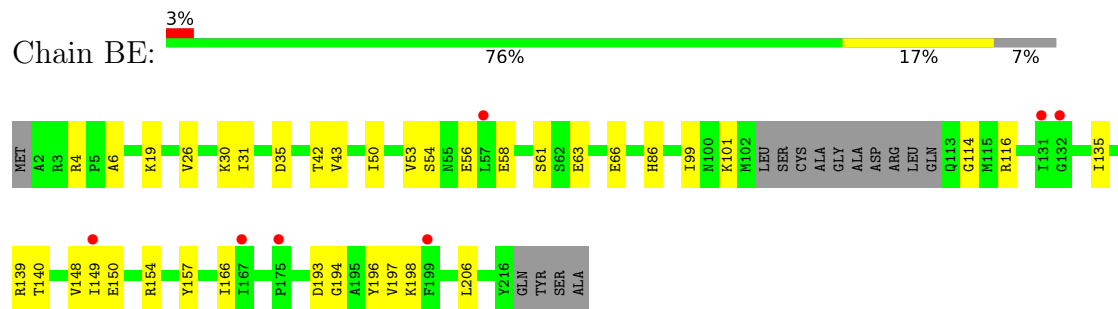


- 
- WORLD WIDE
PDB
PROTEIN DATA BANK

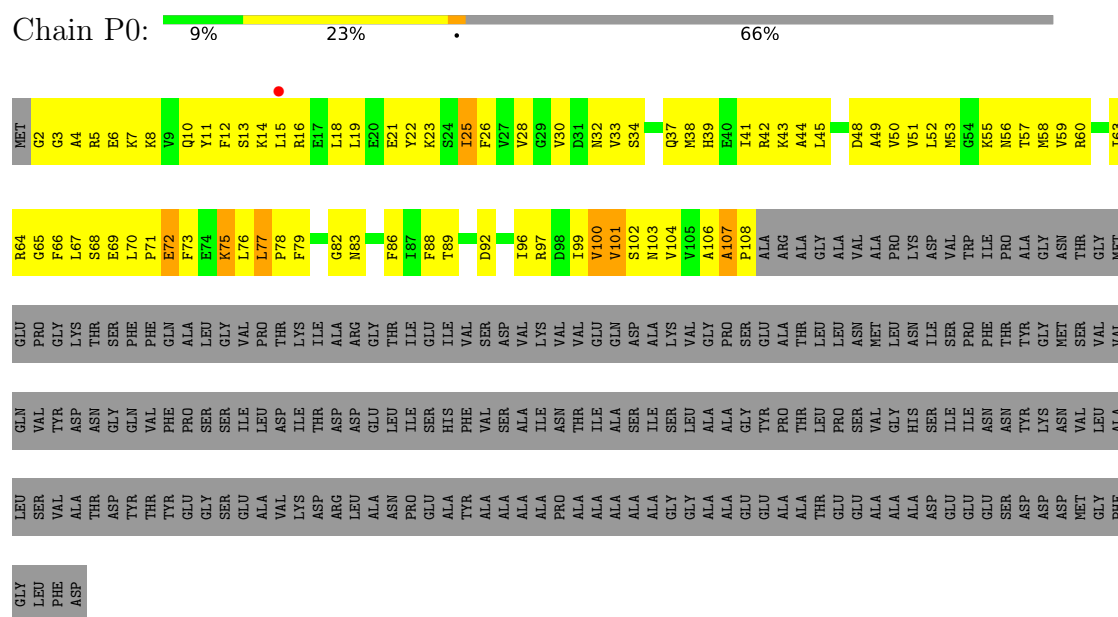


ALA

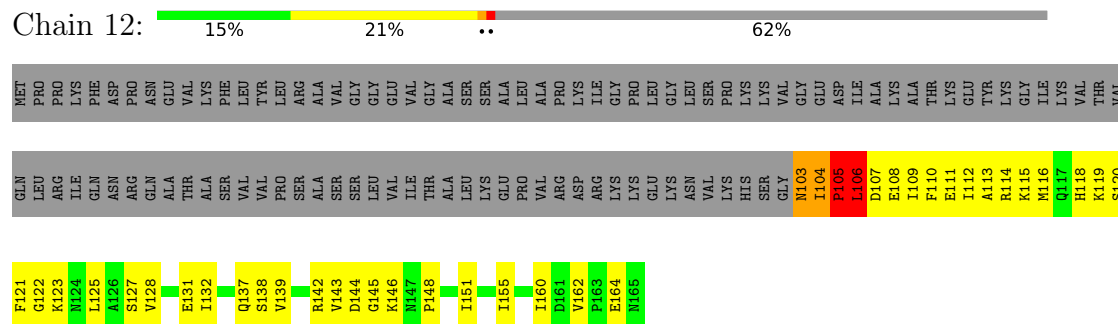
- Molecule 80: 60S ribosomal protein L10



- Molecule 81: 60S acidic ribosomal protein P0



- Molecule 82: 60S ribosomal protein L12-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	300.29Å 294.06Å 442.55Å 90.00° 99.77° 90.00°	Depositor
Resolution (Å)	266.82 – 3.50 266.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	97.9 (266.82-3.50) 86.6 (266.82-3.50)	Depositor EDS
R_{merge}	0.52	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.69 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.249 , 0.293 0.249 , 0.291	Depositor DCC
R_{free} test set	2000 reflections (0.16%)	wwPDB-VP
Wilson B-factor (Å ²)	67.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 91.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	400037	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GET, ZN, 3K5, 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	0.20	0/76993	0.48	17/120031 (0.0%)
1	AS	0.20	0/74190	0.48	11/115649 (0.0%)
2	3	0.16	0/2884	0.36	0/4492
2	AT	0.18	0/2884	0.37	0/4492
3	4	0.16	0/3702	0.41	0/5764
3	AU	0.21	0/3746	0.49	4/5832 (0.1%)
4	AW	0.16	0/1922	0.44	0/2581
4	j	0.17	0/1922	0.46	0/2581
5	AX	0.21	0/3145	0.52	2/4231 (0.0%)
5	k	0.20	0/3145	0.51	0/4231
6	AY	0.16	0/2782	0.47	0/3754
6	l	0.18	0/2782	0.51	0/3754
7	AZ	0.17	0/2447	0.45	0/3294
7	m	0.17	0/2462	0.48	0/3315
8	BA	0.17	0/1231	0.50	0/1662
8	n	0.18	0/1263	0.50	0/1703
9	BB	0.16	0/1849	0.48	0/2485
9	o	0.19	0/1876	0.49	0/2519
10	BC	0.48	0/1835	1.00	1/2472 (0.0%)
10	p	0.25	0/1855	0.62	3/2500 (0.1%)
11	BD	0.18	0/1537	0.46	0/2067
11	q	0.19	0/1537	0.49	0/2067
12	r	0.19	0/1716	0.47	0/2304
13	BF	0.18	0/1390	0.50	0/1861
13	s	0.18	0/1390	0.51	0/1861
14	BG	0.47	0/1637	0.99	6/2195 (0.3%)
14	t	0.24	0/1637	0.63	3/2195 (0.1%)
15	BH	0.18	0/1044	0.47	0/1407
15	u	0.22	0/1030	0.49	0/1389
16	BI	0.17	0/1753	0.46	0/2347
16	v	0.17	0/1753	0.47	0/2347
17	BJ	0.20	0/1620	0.46	0/2167

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	w	0.20	0/1620	0.51	0/2167
18	BK	0.16	0/1419	0.45	0/1906
18	x	0.23	0/1375	0.56	0/1848
19	BL	0.16	0/1482	0.46	0/1985
19	y	0.24	1/1482 (0.1%)	0.46	0/1985
20	BM	0.25	0/1475	0.63	0/1961
20	z	0.30	0/1475	0.66	2/1961 (0.1%)
21	0	0.18	0/1457	0.47	0/1962
21	BN	0.17	0/1457	0.42	0/1962
22	2	0.16	0/1285	0.45	0/1723
22	BO	0.33	0/1285	0.72	2/1723 (0.1%)
23	5	0.24	0/816	0.62	0/1099
23	BP	0.48	0/807	1.10	1/1088 (0.1%)
24	6	0.17	0/993	0.48	0/1339
24	BQ	0.18	0/993	0.48	0/1339
25	7	0.29	0/958	0.53	0/1267
25	BR	0.26	0/889	0.57	1/1175 (0.1%)
26	8	0.19	0/981	0.49	0/1326
26	BS	0.55	0/976	1.02	4/1319 (0.3%)
27	9	0.26	0/999	0.57	0/1334
27	BT	0.17	0/999	0.47	0/1334
28	AA	0.15	0/1112	0.41	0/1488
28	BU	0.52	1/1112 (0.1%)	1.05	5/1488 (0.3%)
29	AB	0.15	0/1199	0.46	0/1607
29	BV	0.17	0/1199	0.46	0/1607
30	AC	0.21	0/474	0.71	0/630
30	BW	0.21	0/492	0.50	0/653
31	AD	0.23	0/756	0.46	0/1018
31	BX	0.15	0/724	0.45	0/975
32	AE	0.17	0/894	0.47	0/1201
32	BY	0.15	0/894	0.48	0/1201
33	AF	0.16	0/1021	0.48	0/1368
33	BZ	0.17	0/1012	0.51	0/1356
34	AG	0.17	0/866	0.47	0/1165
34	CA	0.20	0/866	0.43	0/1165
35	AH	0.17	0/896	0.47	0/1195
35	CB	0.23	0/878	0.58	0/1172
36	AI	0.16	0/974	0.47	0/1297
36	CC	0.50	0/985	0.97	1/1312 (0.1%)
37	AJ	0.15	0/763	0.43	0/1012
37	CD	0.49	0/741	1.08	1/984 (0.1%)
38	AK	0.18	0/690	0.52	0/916
38	CE	0.18	0/690	0.50	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
39	AL	0.13	0/623	0.46	0/831
39	CF	0.50	0/623	0.99	0/831
40	AM	0.17	0/447	0.46	0/594
40	CG	0.18	0/447	0.51	0/594
41	AN	0.14	0/408	0.42	0/542
41	CH	0.25	0/409	0.50	0/542
42	AO	0.20	0/237	0.48	0/304
42	CI	0.22	0/228	0.44	0/293
43	AP	0.18	0/840	0.49	0/1110
43	CJ	0.17	0/840	0.53	1/1110 (0.1%)
44	AQ	0.18	0/705	0.48	0/940
44	CK	0.16	0/705	0.45	0/940
45	CL	0.48	0/929	1.13	5/1240 (0.4%)
45	i	0.53	0/816	1.24	6/1091 (0.5%)
46	B	0.20	0/40724	0.50	8/63452 (0.0%)
46	CM	0.22	0/41205	0.52	14/64202 (0.0%)
47	C	0.16	0/1666	0.44	0/2273
47	CN	0.16	0/1666	0.46	0/2273
48	CO	0.63	0/1743	1.17	4/2344 (0.2%)
48	D	0.18	0/1750	0.51	0/2354
49	CP	0.15	0/1657	0.44	0/2248
49	E	0.15	0/1657	0.43	0/2248
50	CQ	0.19	0/1731	0.58	0/2324
50	F	0.20	0/1731	0.58	0/2324
51	CR	0.18	0/2096	0.45	0/2822
51	G	0.37	1/2083 (0.0%)	0.46	0/2805
52	CS	0.61	0/1623	1.16	8/2188 (0.4%)
52	H	0.16	0/1631	0.45	0/2199
53	CT	0.19	0/1929	0.61	0/2571
53	I	0.15	0/1823	0.44	0/2434
54	CU	0.51	0/1472	1.13	4/1979 (0.2%)
54	J	0.17	0/1490	0.46	0/2004
55	CV	0.18	0/1606	0.47	0/2150
55	K	0.15	0/1606	0.44	0/2150
56	CW	0.15	0/1478	0.43	0/1978
56	L	0.15	0/1478	0.45	0/1978
57	CX	0.20	0/809	0.62	0/1092
57	M	0.22	0/836	0.76	1/1130 (0.1%)
58	CY	0.20	0/1154	0.51	2/1553 (0.1%)
58	N	0.16	0/1175	0.46	0/1582
59	CZ	0.54	0/921	1.22	3/1240 (0.2%)
59	O	0.31	0/892	0.86	1/1203 (0.1%)
60	DA	0.15	0/1210	0.43	0/1631

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	P	0.16	0/1198	0.45	0/1614
61	DB	0.17	0/915	0.49	0/1228
61	Q	0.19	0/953	0.52	0/1279
62	DC	0.49	0/1049	1.12	2/1409 (0.1%)
62	R	0.25	0/1054	0.69	2/1416 (0.1%)
63	DD	0.17	0/1103	0.50	0/1478
63	S	0.23	0/1103	0.51	0/1478
64	DE	0.20	0/1009	0.62	0/1354
64	T	0.17	0/1009	0.50	0/1354
65	DF	0.21	0/1178	0.53	0/1579
65	U	0.19	0/1205	0.54	0/1615
66	DG	0.18	0/1120	0.52	0/1508
66	V	0.18	0/1120	0.57	0/1508
67	DH	0.17	0/772	0.52	0/1045
67	W	0.18	0/818	0.51	0/1106
68	DI	0.19	0/683	0.53	0/918
68	X	0.17	0/683	0.47	0/918
69	DJ	0.17	0/1049	0.44	0/1412
69	Y	0.16	0/1049	0.41	0/1412
70	DK	0.18	0/1128	0.54	0/1505
70	Z	0.18	0/1128	0.57	0/1505
71	DL	0.15	0/1086	0.44	0/1447
71	a	0.14	0/1100	0.43	0/1466
72	DM	0.34	0/577	0.56	0/778
72	b	0.17	0/585	0.45	0/789
73	DN	0.15	0/791	0.51	0/1060
73	c	0.17	0/782	0.49	0/1048
74	DO	0.19	0/624	0.56	0/843
74	d	0.16	0/624	0.46	0/843
75	DP	0.21	0/478	0.65	0/640
75	e	0.18	0/470	0.53	0/629
76	DQ	0.23	0/461	0.57	0/613
76	f	0.35	0/466	0.85	2/620 (0.3%)
77	DR	0.37	0/478	0.77	0/637
77	g	0.19	0/482	0.54	0/642
78	DS	0.53	0/564	1.40	4/749 (0.5%)
78	h	0.22	0/585	0.73	0/778
79	AR	0.16	0/2451	0.46	0/3337
79	DT	0.62	1/2414 (0.0%)	1.26	16/3286 (0.5%)
80	BE	0.18	0/1696	0.47	0/2276
81	P0	0.36	0/857	0.75	0/1148
82	12	0.40	0/486	0.76	2/653 (0.3%)
All	All	0.23	4/427902 (0.0%)	0.54	149/627694 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	G	149	TYR	C-O	-14.47	1.17	1.23
19	y	60	PRO	CA-C	-6.84	1.48	1.51
28	BU	29	HIS	C-N	-5.87	1.26	1.33
79	DT	201	LEU	C-N	5.18	1.41	1.33

The worst 5 of 149 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	AU	102	U	P-O3'-C3'	-9.29	106.26	120.20
1	AS	524	G	P-O3'-C3'	-8.88	106.89	120.20
46	CM	72	A	P-O3'-C3'	-8.84	106.94	120.20
79	DT	40	LYS	CD-CE-NZ	8.66	139.60	111.90
1	AS	523	G	P-O3'-C3'	-8.63	107.25	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	68791	0	34571	1315	0
1	AS	66291	0	33318	1281	0
2	3	2579	0	1303	42	0
2	AT	2579	0	1304	40	0
3	4	3313	0	1674	67	0
3	AU	3353	0	1694	88	0
4	AW	1888	0	1962	54	0
4	j	1888	0	1962	48	0
5	AX	3077	0	3166	70	0
5	k	3077	0	3166	55	0
6	AY	2734	0	2862	63	0
6	l	2734	0	2862	64	0
7	AZ	2394	0	2361	40	0
7	m	2409	0	2372	45	0
8	BA	1210	0	1285	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	n	1242	0	1321	32	0
9	BB	1816	0	1900	32	0
9	o	1843	0	1932	30	0
10	BC	1805	0	1925	108	0
10	p	1825	0	1946	30	0
11	BD	1519	0	1588	39	0
11	q	1519	0	1588	27	0
12	r	1681	0	1722	30	0
13	BF	1371	0	1410	39	0
13	s	1371	0	1410	33	0
14	BG	1610	0	1686	108	0
14	t	1610	0	1686	41	0
15	BH	1029	0	1116	22	0
15	u	1015	0	1098	28	0
16	BI	1713	0	1764	61	0
16	v	1713	0	1764	51	0
17	BJ	1590	0	1705	21	0
17	w	1590	0	1705	32	0
18	BK	1396	0	1421	40	0
18	x	1352	0	1371	32	0
19	BL	1458	0	1556	39	0
19	y	1458	0	1556	28	0
20	BM	1457	0	1564	43	0
20	z	1457	0	1564	38	0
21	0	1423	0	1480	40	0
21	BN	1423	0	1480	33	0
22	2	1262	0	1314	18	0
22	BO	1262	0	1314	34	0
23	5	803	0	825	22	0
23	BP	794	0	812	73	0
24	6	977	0	1025	9	0
24	BQ	977	0	1026	13	0
25	7	945	0	1010	45	0
25	BR	877	0	939	43	0
26	8	965	0	1019	17	0
26	BS	960	0	1014	63	0
27	9	989	0	1064	31	0
27	BT	989	0	1064	37	0
28	AA	1087	0	1154	16	0
28	BU	1087	0	1154	83	0
29	AB	1170	0	1203	20	0
29	BV	1170	0	1203	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	AC	464	0	491	14	0
30	BW	482	0	510	7	0
31	AD	747	0	789	20	0
31	BX	715	0	759	12	0
32	AE	881	0	925	16	0
32	BY	881	0	925	15	0
33	AF	1000	0	1069	12	0
33	BZ	991	0	1061	21	0
34	AG	847	0	893	18	0
34	CA	847	0	893	15	0
35	AH	887	0	947	28	0
35	CB	869	0	928	32	0
36	AI	963	0	1059	34	0
36	CC	974	0	1071	71	0
37	AJ	758	0	838	11	0
37	CD	736	0	812	42	0
38	AK	677	0	697	20	0
38	CE	677	0	697	26	0
39	AL	617	0	675	7	0
39	CF	617	0	675	45	0
40	AM	438	0	475	9	0
40	CG	438	0	475	13	0
41	AN	402	0	435	7	0
41	CH	403	0	437	9	0
42	AO	236	0	285	6	0
42	CI	227	0	272	8	0
43	AP	828	0	894	17	0
43	CJ	828	0	893	12	0
44	AQ	698	0	734	12	0
44	CK	698	0	734	15	0
45	CL	919	0	899	66	0
45	i	805	0	782	78	0
46	B	36410	0	18322	910	0
46	CM	36839	0	18535	963	0
47	C	1627	0	1644	48	0
47	CN	1627	0	1644	41	0
48	CO	1717	0	1796	180	0
48	D	1724	0	1805	35	0
49	CP	1629	0	1728	31	0
49	E	1629	0	1728	36	0
50	CQ	1707	0	1807	64	0
50	F	1707	0	1807	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	CR	2055	0	2137	55	0
51	G	2042	0	2126	60	0
52	CS	1606	0	1677	111	0
52	H	1614	0	1688	43	0
53	CT	1904	0	1994	80	0
53	I	1798	0	1874	56	0
54	CU	1449	0	1546	144	0
54	J	1466	0	1561	47	0
55	CV	1579	0	1602	43	0
55	K	1579	0	1602	42	0
56	CW	1453	0	1532	34	0
56	L	1453	0	1532	37	0
57	CX	791	0	805	45	0
57	M	817	0	828	50	0
58	CY	1129	0	1183	20	0
58	N	1150	0	1201	26	0
59	CZ	913	0	934	103	0
59	O	885	0	915	50	0
60	DA	1187	0	1249	18	0
60	P	1175	0	1235	31	0
61	DB	905	0	947	38	0
61	Q	942	0	981	21	0
62	DC	1029	0	1078	98	0
62	R	1034	0	1083	51	0
63	DD	1085	0	1150	38	0
63	S	1085	0	1150	54	0
64	DE	997	0	1053	45	0
64	T	997	0	1053	36	0
65	DF	1161	0	1205	46	0
65	U	1187	0	1237	35	0
66	DG	1100	0	1114	34	0
66	V	1100	0	1114	33	0
67	DH	763	0	824	22	0
67	W	808	0	871	27	0
68	DI	676	0	677	18	0
68	X	676	0	677	19	0
69	DJ	1032	0	1066	33	0
69	Y	1032	0	1066	25	0
70	DK	1110	0	1182	34	0
70	Z	1110	0	1182	31	0
71	DL	1072	0	1123	26	0
71	a	1086	0	1132	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
72	DM	570	0	609	19	0
72	b	578	0	613	14	0
73	DN	779	0	833	25	0
73	c	770	0	824	17	0
74	DO	614	0	630	9	0
74	d	614	0	627	10	0
75	DP	476	0	510	26	0
75	e	468	0	499	12	0
76	DQ	449	0	426	14	0
76	f	454	0	430	18	0
77	DR	470	0	512	26	0
77	g	474	0	515	16	0
78	DS	555	0	585	61	0
78	h	574	0	606	30	0
79	AR	2398	0	2374	75	0
79	DT	2362	0	2335	332	0
80	BE	1662	0	1709	28	0
81	P0	845	0	884	94	0
82	12	480	0	477	54	0
83	1	57	0	52	6	0
83	AS	57	0	52	7	0
84	0	4	0	0	0	0
84	1	469	0	0	0	0
84	2	1	0	0	0	0
84	3	7	0	0	0	0
84	4	1	0	0	0	0
84	6	1	0	0	0	0
84	AB	2	0	0	0	0
84	AC	1	0	0	0	0
84	AD	1	0	0	0	0
84	AJ	1	0	0	0	0
84	AP	2	0	0	0	0
84	AS	389	0	0	0	0
84	AT	5	0	0	0	0
84	AU	5	0	0	0	0
84	AW	1	0	0	0	0
84	AX	3	0	0	0	0
84	AY	2	0	0	0	0
84	AZ	1	0	0	0	0
84	B	99	0	0	0	0
84	BB	2	0	0	0	0
84	BC	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
84	BE	1	0	0	0	0
84	BI	1	0	0	0	0
84	BK	1	0	0	0	0
84	BL	2	0	0	0	0
84	BO	1	0	0	0	0
84	BQ	1	0	0	0	0
84	BZ	1	0	0	0	0
84	C	1	0	0	0	0
84	CA	1	0	0	0	0
84	CB	1	0	0	0	0
84	CG	1	0	0	0	0
84	CL	2	0	0	0	0
84	CM	78	0	0	0	0
84	CW	1	0	0	0	0
84	D	1	0	0	0	0
84	DA	1	0	0	0	0
84	DG	1	0	0	0	0
84	DH	1	0	0	0	0
84	DK	2	0	0	0	0
84	E	1	0	0	0	0
84	F	1	0	0	0	0
84	G	1	0	0	0	0
84	K	1	0	0	0	0
84	L	1	0	0	0	0
84	P0	1	0	0	1	0
84	Q	2	0	0	0	0
84	R	4	0	0	0	0
84	T	1	0	0	0	0
84	Y	2	0	0	0	0
84	a	1	0	0	0	0
84	j	1	0	0	0	0
84	k	3	0	0	0	0
84	m	1	0	0	0	0
84	o	4	0	0	0	0
84	r	1	0	0	0	0
84	u	1	0	0	0	0
84	v	2	0	0	0	0
84	w	1	0	0	0	0
84	x	1	0	0	0	0
84	y	3	0	0	0	0
85	AH	1	0	0	0	0
85	AK	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
85	AN	1	0	0	0	0
85	AP	1	0	0	0	0
85	AQ	1	0	0	0	0
85	CB	1	0	0	0	0
85	CE	1	0	0	0	0
85	CH	1	0	0	0	0
85	CJ	1	0	0	0	0
85	CK	1	0	0	0	0
85	DN	1	0	0	0	0
85	DQ	1	0	0	0	0
85	DS	1	0	0	0	0
85	c	1	0	0	0	0
85	d	1	0	0	0	0
85	f	1	0	0	0	0
85	h	1	0	0	0	0
86	B	34	0	40	6	0
86	CM	34	0	40	5	0
All	All	400037	0	297473	8914	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 8914 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:DS:162:GLU:HA	78:DS:173:PHE:HA	1.29	1.14
79:DT:226:LYS:HD2	79:DT:227:THR:H	1.14	1.11
20:BM:176:ARG:HH12	20:BM:180:LYS:HB2	1.17	1.03
79:DT:126:ALA:HB2	79:DT:155:VAL:HG13	1.40	1.03
10:BC:62:GLN:HG3	16:BI:28:TRP:CH2	1.95	1.02

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AW	247/254 (97%)	240 (97%)	7 (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%)	374 (97%)	9 (2%)	1 (0%)	36	67
6	AY	357/363 (98%)	349 (98%)	8 (2%)	0	100	100
6	l	357/363 (98%)	346 (97%)	10 (3%)	1 (0%)	36	67
7	AZ	290/298 (97%)	280 (97%)	10 (3%)	0	100	100
7	m	292/298 (98%)	281 (96%)	11 (4%)	0	100	100
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	224/241 (93%)	218 (97%)	5 (2%)	1 (0%)	30	62
9	o	227/241 (94%)	220 (97%)	7 (3%)	0	100	100
10	BC	231/262 (88%)	210 (91%)	16 (7%)	5 (2%)	5	30
10	p	234/262 (89%)	225 (96%)	8 (3%)	1 (0%)	30	62
11	BD	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
11	q	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
12	r	203/219 (93%)	201 (99%)	2 (1%)	0	100	100
13	BF	169/174 (97%)	162 (96%)	7 (4%)	0	100	100
13	s	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
14	BG	198/202 (98%)	179 (90%)	12 (6%)	7 (4%)	3	23
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	126/131 (96%)	123 (98%)	3 (2%)	0	100	100
16	BI	201/204 (98%)	198 (98%)	3 (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	170/185 (92%)	166 (98%)	4 (2%)	0	100	100
18	x	165/185 (89%)	160 (97%)	5 (3%)	0	100	100
19	BL	183/186 (98%)	179 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	y	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
20	BM	177/190 (93%)	174 (98%)	3 (2%)	0	100	100
20	z	177/190 (93%)	172 (97%)	5 (3%)	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
22	2	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
22	BO	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
23	5	98/124 (79%)	90 (92%)	6 (6%)	2 (2%)	6	32
23	BP	97/124 (78%)	75 (77%)	16 (16%)	6 (6%)	1	12
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%)	89 (78%)	25 (22%)	0	100	100
25	BR	105/155 (68%)	90 (86%)	14 (13%)	1 (1%)	12	44
26	8	118/142 (83%)	117 (99%)	1 (1%)	0	100	100
26	BS	117/142 (82%)	111 (95%)	5 (4%)	1 (1%)	14	47
27	9	124/127 (98%)	120 (97%)	4 (3%)	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%)	116 (87%)	15 (11%)	2 (2%)	8	37
29	AB	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
29	BV	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
30	AC	56/63 (89%)	52 (93%)	1 (2%)	3 (5%)	1	14
30	BW	58/63 (92%)	57 (98%)	1 (2%)	0	100	100
31	AD	96/106 (91%)	92 (96%)	4 (4%)	0	100	100
31	BX	92/106 (87%)	90 (98%)	2 (2%)	0	100	100
32	AE	106/112 (95%)	104 (98%)	2 (2%)	0	100	100
32	BY	106/112 (95%)	103 (97%)	2 (2%)	1 (1%)	14	47
33	AF	122/131 (93%)	121 (99%)	1 (1%)	0	100	100
33	BZ	120/131 (92%)	120 (100%)	0	0	100	100
34	AG	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
34	CA	104/107 (97%)	101 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	AH	110/122 (90%)	108 (98%)	2 (2%)	0	100	100
35	CB	108/122 (88%)	105 (97%)	3 (3%)	0	100	100
36	AI	113/120 (94%)	112 (99%)	1 (1%)	0	100	100
36	CC	115/120 (96%)	111 (96%)	3 (3%)	1 (1%)	14	47
37	AJ	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
37	CD	93/99 (94%)	85 (91%)	8 (9%)	0	100	100
38	AK	84/90 (93%)	80 (95%)	4 (5%)	0	100	100
38	CE	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
39	AL	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
39	CF	75/78 (96%)	65 (87%)	7 (9%)	3 (4%)	2	19
40	AM	48/51 (94%)	48 (100%)	0	0	100	100
40	CG	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
41	AN	48/52 (92%)	48 (100%)	0	0	100	100
41	CH	48/52 (92%)	46 (96%)	1 (2%)	1 (2%)	5	31
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%)	99 (98%)	2 (2%)	0	100	100
43	CJ	101/106 (95%)	99 (98%)	2 (2%)	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	116/267 (43%)	72 (62%)	34 (29%)	10 (9%)	0	7
45	i	104/267 (39%)	51 (49%)	35 (34%)	18 (17%)	0	2
47	C	206/261 (79%)	200 (97%)	6 (3%)	0	100	100
47	CN	206/261 (79%)	199 (97%)	7 (3%)	0	100	100
48	CO	211/256 (82%)	191 (90%)	14 (7%)	6 (3%)	4	26
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%)	208 (97%)	7 (3%)	0	100	100
50	CQ	221/251 (88%)	211 (96%)	10 (4%)	0	100	100
50	F	221/251 (88%)	214 (97%)	7 (3%)	0	100	100
51	CR	258/262 (98%)	255 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	G	256/262 (98%)	252 (98%)	4 (2%)	0	100	100
52	CS	203/225 (90%)	180 (89%)	20 (10%)	3 (2%)	8	37
52	H	204/225 (91%)	193 (95%)	11 (5%)	0	100	100
53	CT	234/236 (99%)	228 (97%)	6 (3%)	0	100	100
53	I	221/236 (94%)	217 (98%)	4 (2%)	0	100	100
54	CU	177/186 (95%)	150 (85%)	21 (12%)	6 (3%)	3	23
54	J	180/186 (97%)	171 (95%)	9 (5%)	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%)	174 (99%)	2 (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%)	82 (85%)	12 (12%)	2 (2%)	5	31
58	CY	139/155 (90%)	133 (96%)	6 (4%)	0	100	100
58	N	142/155 (92%)	136 (96%)	6 (4%)	0	100	100
59	CZ	117/143 (82%)	75 (64%)	36 (31%)	6 (5%)	1	15
59	O	114/143 (80%)	88 (77%)	24 (21%)	2 (2%)	6	34
60	DA	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
60	P	146/151 (97%)	144 (99%)	2 (1%)	0	100	100
61	DB	120/132 (91%)	114 (95%)	6 (5%)	0	100	100
61	Q	125/132 (95%)	121 (97%)	3 (2%)	1 (1%)	16	49
62	DC	128/142 (90%)	97 (76%)	27 (21%)	4 (3%)	3	25
62	R	129/142 (91%)	110 (85%)	17 (13%)	2 (2%)	7	36
63	DD	137/142 (96%)	133 (97%)	4 (3%)	0	100	100
63	S	137/142 (96%)	130 (95%)	7 (5%)	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%)	6 (4%)	0	100	100
65	U	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
66	DG	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
66	V	139/145 (96%)	136 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	124 (98%)	3 (2%)	0	100	100
69	Y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	DK	141/145 (97%)	138 (98%)	3 (2%)	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%)	129 (98%)	3 (2%)	0	100	100
72	DM	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
72	b	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
73	DN	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
73	c	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
74	DO	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
74	d	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
75	DP	59/67 (88%)	54 (92%)	5 (8%)	0	100	100
75	e	58/67 (87%)	55 (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	57/63 (90%)	50 (88%)	6 (10%)	1 (2%)	6	34
77	g	58/63 (92%)	53 (91%)	5 (9%)	0	100	100
78	DS	64/193 (33%)	31 (48%)	23 (36%)	10 (16%)	0	2
78	h	68/193 (35%)	56 (82%)	11 (16%)	1 (2%)	8	37
79	AR	309/317 (98%)	291 (94%)	17 (6%)	1 (0%)	36	67
79	DT	303/317 (96%)	221 (73%)	65 (22%)	17 (6%)	1	13
80	BE	201/220 (91%)	197 (98%)	4 (2%)	0	100	100
81	P0	105/312 (34%)	69 (66%)	27 (26%)	9 (9%)	0	7
82	12	61/165 (37%)	36 (59%)	22 (36%)	3 (5%)	1	16
All	All	22176/24752 (90%)	21009 (95%)	1028 (5%)	139 (1%)	21	54

5 of 139 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	l	267	SER
10	p	205	ASN
45	i	36	SER
45	i	37	LYS
45	i	44	ALA

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%)	190 (100%)	0	100	100
4	j	190/194 (98%)	190 (100%)	0	100	100
5	AX	325/328 (99%)	325 (100%)	0	100	100
5	k	325/328 (99%)	325 (100%)	0	100	100
6	AY	288/292 (99%)	288 (100%)	0	100	100
6	l	288/292 (99%)	288 (100%)	0	100	100
7	AZ	247/252 (98%)	247 (100%)	0	100	100
7	m	248/252 (98%)	248 (100%)	0	100	100
8	BA	132/154 (86%)	132 (100%)	0	100	100
8	n	136/154 (88%)	136 (100%)	0	100	100
9	BB	190/204 (93%)	190 (100%)	0	100	100
9	o	193/204 (95%)	193 (100%)	0	100	100
10	BC	193/216 (89%)	191 (99%)	2 (1%)	68	75
10	p	196/216 (91%)	196 (100%)	0	100	100
11	BD	169/170 (99%)	169 (100%)	0	100	100
11	q	169/170 (99%)	169 (100%)	0	100	100
12	r	177/185 (96%)	177 (100%)	0	100	100
13	BF	146/149 (98%)	146 (100%)	0	100	100
13	s	146/149 (98%)	146 (100%)	0	100	100
14	BG	166/168 (99%)	164 (99%)	2 (1%)	63	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	t	166/168 (99%)	166 (100%)	0	100	100
15	BH	108/109 (99%)	108 (100%)	0	100	100
15	u	107/109 (98%)	107 (100%)	0	100	100
16	BI	177/178 (99%)	177 (100%)	0	100	100
16	v	177/178 (99%)	177 (100%)	0	100	100
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%)	145 (100%)	0	100	100
18	x	140/154 (91%)	139 (99%)	1 (1%)	76	78
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%)	144 (99%)	2 (1%)	59	71
20	z	146/153 (95%)	144 (99%)	2 (1%)	59	71
21	0	155/157 (99%)	155 (100%)	0	100	100
21	BN	155/157 (99%)	154 (99%)	1 (1%)	78	79
22	2	133/134 (99%)	133 (100%)	0	100	100
22	BO	133/134 (99%)	133 (100%)	0	100	100
23	5	91/112 (81%)	89 (98%)	2 (2%)	45	65
23	BP	90/112 (80%)	90 (100%)	0	100	100
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%)	94 (97%)	3 (3%)	35	59
25	BR	91/127 (72%)	91 (100%)	0	100	100
26	8	107/121 (88%)	107 (100%)	0	100	100
26	BS	107/121 (88%)	107 (100%)	0	100	100
27	9	111/112 (99%)	111 (100%)	0	100	100
27	BT	111/112 (99%)	111 (100%)	0	100	100
28	AA	117/118 (99%)	117 (100%)	0	100	100
28	BU	117/118 (99%)	117 (100%)	0	100	100
29	AB	120/121 (99%)	120 (100%)	0	100	100
29	BV	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	AC	45/49 (92%)	45 (100%)	0	100	100
30	BW	47/49 (96%)	47 (100%)	0	100	100
31	AD	83/90 (92%)	80 (96%)	3 (4%)	31	57
31	BX	79/90 (88%)	79 (100%)	0	100	100
32	AE	97/100 (97%)	97 (100%)	0	100	100
32	BY	97/100 (97%)	97 (100%)	0	100	100
33	AF	109/115 (95%)	109 (100%)	0	100	100
33	BZ	109/115 (95%)	109 (100%)	0	100	100
34	AG	91/92 (99%)	91 (100%)	0	100	100
34	CA	91/92 (99%)	91 (100%)	0	100	100
35	AH	95/102 (93%)	95 (100%)	0	100	100
35	CB	93/102 (91%)	93 (100%)	0	100	100
36	AI	104/106 (98%)	104 (100%)	0	100	100
36	CC	105/106 (99%)	103 (98%)	2 (2%)	50	68
37	AJ	77/79 (98%)	77 (100%)	0	100	100
37	CD	75/79 (95%)	74 (99%)	1 (1%)	61	72
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	45/47 (96%)	45 (100%)	0	100	100
41	CH	45/47 (96%)	45 (100%)	0	100	100
42	AO	24/24 (100%)	24 (100%)	0	100	100
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	99/212 (47%)	97 (98%)	2 (2%)	48	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	i	86/212 (41%)	83 (96%)	3 (4%)	32	57
47	C	176/215 (82%)	176 (100%)	0	100	100
47	CN	176/215 (82%)	176 (100%)	0	100	100
48	CO	193/229 (84%)	192 (100%)	1 (0%)	81	80
48	D	194/229 (85%)	194 (100%)	0	100	100
49	CP	175/198 (88%)	175 (100%)	0	100	100
49	E	175/198 (88%)	175 (100%)	0	100	100
50	CQ	174/196 (89%)	174 (100%)	0	100	100
50	F	174/196 (89%)	174 (100%)	0	100	100
51	CR	218/220 (99%)	218 (100%)	0	100	100
51	G	217/220 (99%)	217 (100%)	0	100	100
52	CS	177/197 (90%)	172 (97%)	5 (3%)	38	61
52	H	178/197 (90%)	178 (100%)	0	100	100
53	CT	204/204 (100%)	204 (100%)	0	100	100
53	I	193/204 (95%)	193 (100%)	0	100	100
54	CU	161/167 (96%)	161 (100%)	0	100	100
54	J	163/167 (98%)	163 (100%)	0	100	100
55	CV	157/160 (98%)	157 (100%)	0	100	100
55	K	157/160 (98%)	157 (100%)	0	100	100
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%)	65	74
58	CY	122/134 (91%)	121 (99%)	1 (1%)	73	77
58	N	124/134 (92%)	124 (100%)	0	100	100
59	CZ	101/123 (82%)	101 (100%)	0	100	100
59	O	98/123 (80%)	94 (96%)	4 (4%)	27	53
60	DA	129/130 (99%)	129 (100%)	0	100	100
60	P	128/130 (98%)	128 (100%)	0	100	100
61	DB	93/102 (91%)	93 (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%)	112 (100%)	0	100	100
62	R	112/121 (93%)	112 (100%)	0	100	100
63	DD	113/116 (97%)	113 (100%)	0	100	100
63	S	113/116 (97%)	111 (98%)	2 (2%)	51	69
64	DE	112/122 (92%)	112 (100%)	0	100	100
64	T	112/122 (92%)	112 (100%)	0	100	100
65	DF	125/129 (97%)	123 (98%)	2 (2%)	55	70
65	U	128/129 (99%)	127 (99%)	1 (1%)	73	77
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%)	87 (100%)	0	100	100
67	W	92/105 (88%)	92 (100%)	0	100	100
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%)	112 (100%)	0	100	100
69	Y	112/113 (99%)	112 (100%)	0	100	100
70	DK	116/118 (98%)	116 (100%)	0	100	100
70	Z	116/118 (98%)	116 (100%)	0	100	100
71	DL	109/112 (97%)	109 (100%)	0	100	100
71	a	111/112 (99%)	111 (100%)	0	100	100
72	DM	63/85 (74%)	63 (100%)	0	100	100
72	b	64/85 (75%)	64 (100%)	0	100	100
73	DN	84/102 (82%)	84 (100%)	0	100	100
73	c	83/102 (81%)	83 (100%)	0	100	100
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	52/58 (90%)	52 (100%)	0	100	100
76	DQ	47/48 (98%)	46 (98%)	1 (2%)	47	66
76	f	47/48 (98%)	43 (92%)	4 (8%)	10	34
77	DR	51/54 (94%)	49 (96%)	2 (4%)	28	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	g	51/54 (94%)	51 (100%)	0	100	100
78	DS	60/175 (34%)	59 (98%)	1 (2%)	53	70
78	h	62/175 (35%)	61 (98%)	1 (2%)	55	70
79	AR	259/263 (98%)	259 (100%)	0	100	100
79	DT	255/263 (97%)	248 (97%)	7 (3%)	39	62
80	BE	175/186 (94%)	175 (100%)	0	100	100
81	P0	92/247 (37%)	92 (100%)	0	100	100
82	12	53/137 (39%)	50 (94%)	3 (6%)	18	45
All	All	19011/20831 (91%)	18949 (100%)	62 (0%)	86	83

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	BC	224	ILE
79	DT	66	SER
36	CC	40	SER
79	DT	65	HIS
82	12	103	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 202 such sidechains are listed below:

Mol	Chain	Res	Type
10	BC	244	ASN
28	BU	122	HIS
81	P0	10	GLN
13	BF	47	GLN
20	BM	130	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3215/3359 (95%)	607 (18%)	45 (1%)
1	AS	3093/3359 (92%)	528 (17%)	39 (1%)
2	3	120/121 (99%)	9 (7%)	0
2	AT	120/121 (99%)	9 (7%)	0
3	4	155/158 (98%)	22 (14%)	2 (1%)
3	AU	157/158 (99%)	23 (14%)	3 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	B	1702/1787 (95%)	405 (23%)	45 (2%)
46	CM	1722/1787 (96%)	430 (24%)	48 (2%)
All	All	10284/10850 (94%)	2033 (19%)	182 (1%)

5 of 2033 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 182 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AS	2515	G
46	CM	259	U
1	AS	2789	A
1	AS	3317	U
46	CM	518	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1152 ligands modelled in this entry, 1148 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
83	3K5	AS	3401	-	63,63,63	0.35	0	84,95,95	0.91	3 (3%)
86	GET	B	1851	-	35,36,36	0.44	0	43,55,55	0.63	1 (2%)
83	3K5	1	3401	-	63,63,63	0.26	0	84,95,95	0.46	1 (1%)
86	GET	CM	1822	-	35,36,36	0.44	0	43,55,55	0.66	1 (2%)

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
83	3K5	AS	3401	-	-	4/29/121/121	0/7/7/7
86	GET	B	1851	-	-	5/13/74/74	0/3/3/3
83	3K5	1	3401	-	-	4/29/121/121	0/7/7/7
86	GET	CM	1822	-	-	2/13/74/74	0/3/3/3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	AS	3401	3K5	C34-O14-C38	4.25	124.32	117.72
83	AS	3401	3K5	O14-C34-C35	3.90	116.71	107.76
86	CM	1822	GET	O11-C11-C21	3.44	113.70	108.08
83	AS	3401	3K5	O14-C34-C33	3.37	115.51	107.76
86	B	1851	GET	O11-C11-C21	2.81	112.67	108.08

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

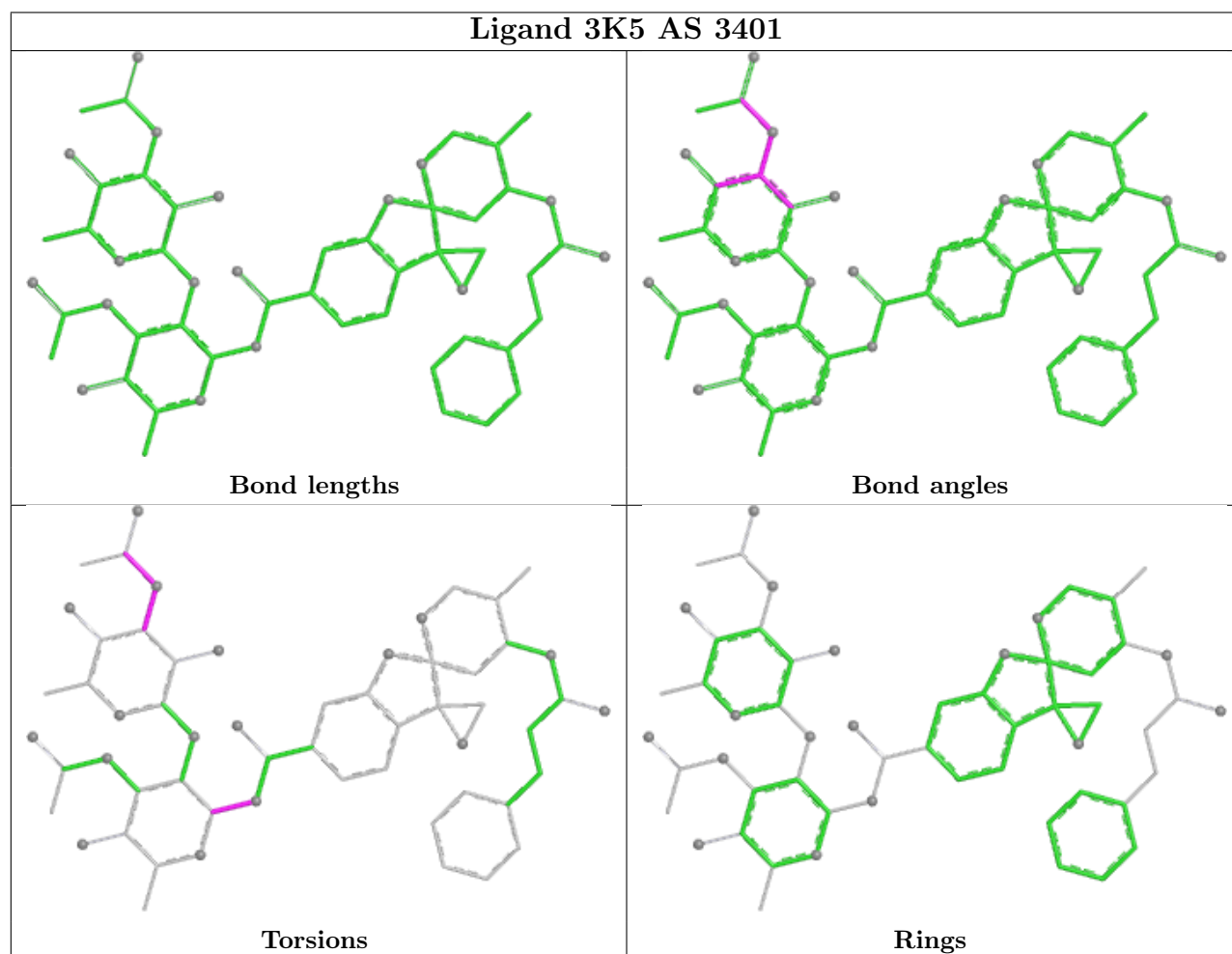
Mol	Chain	Res	Type	Atoms
86	B	1851	GET	O51-C51-C61-O61
86	B	1851	GET	C23-C33-N33-C93
83	1	3401	3K5	C39-C38-O14-C34
83	1	3401	3K5	C31-C30-O9-C26
83	1	3401	3K5	O15-C38-O14-C34

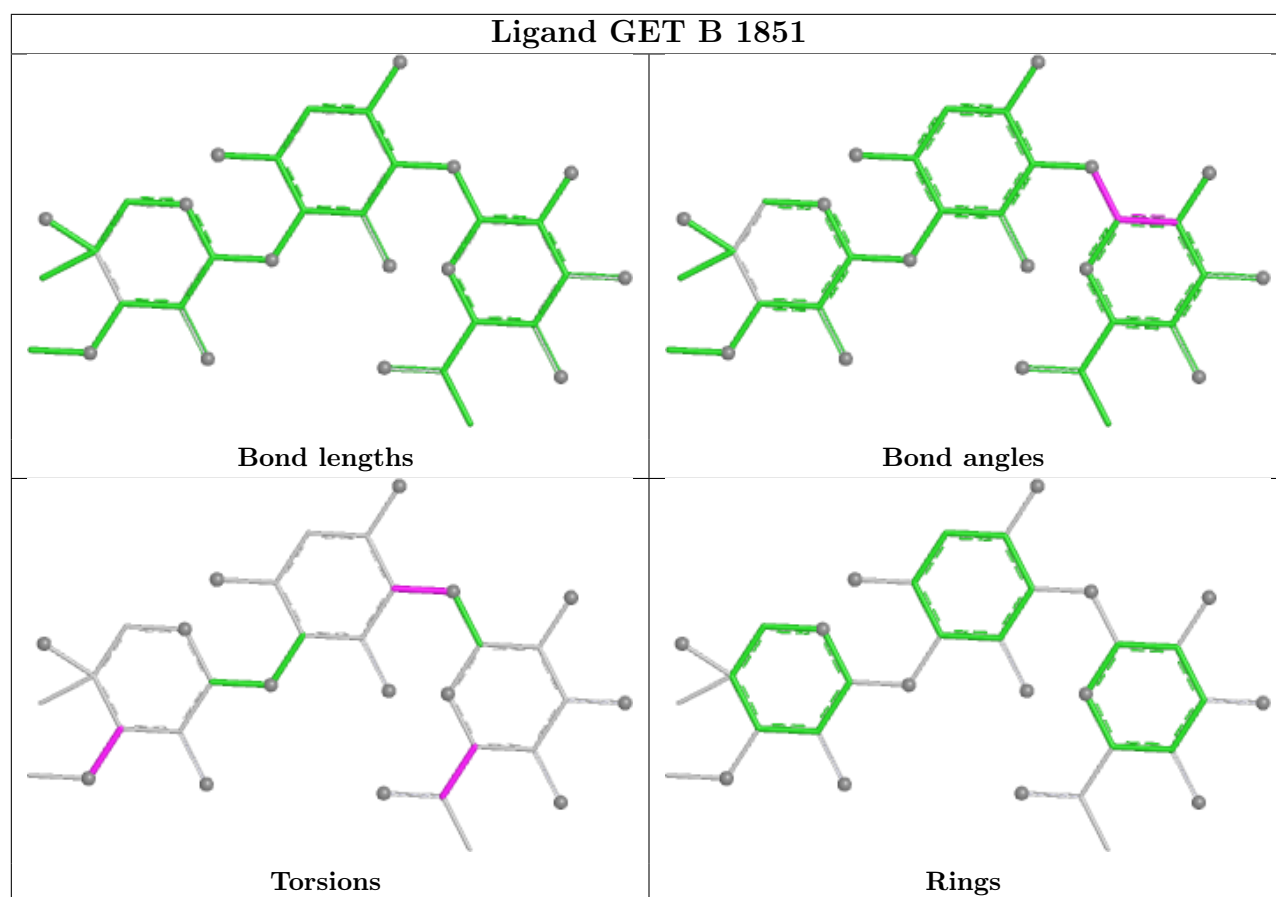
There are no ring outliers.

4 monomers are involved in 24 short contacts:

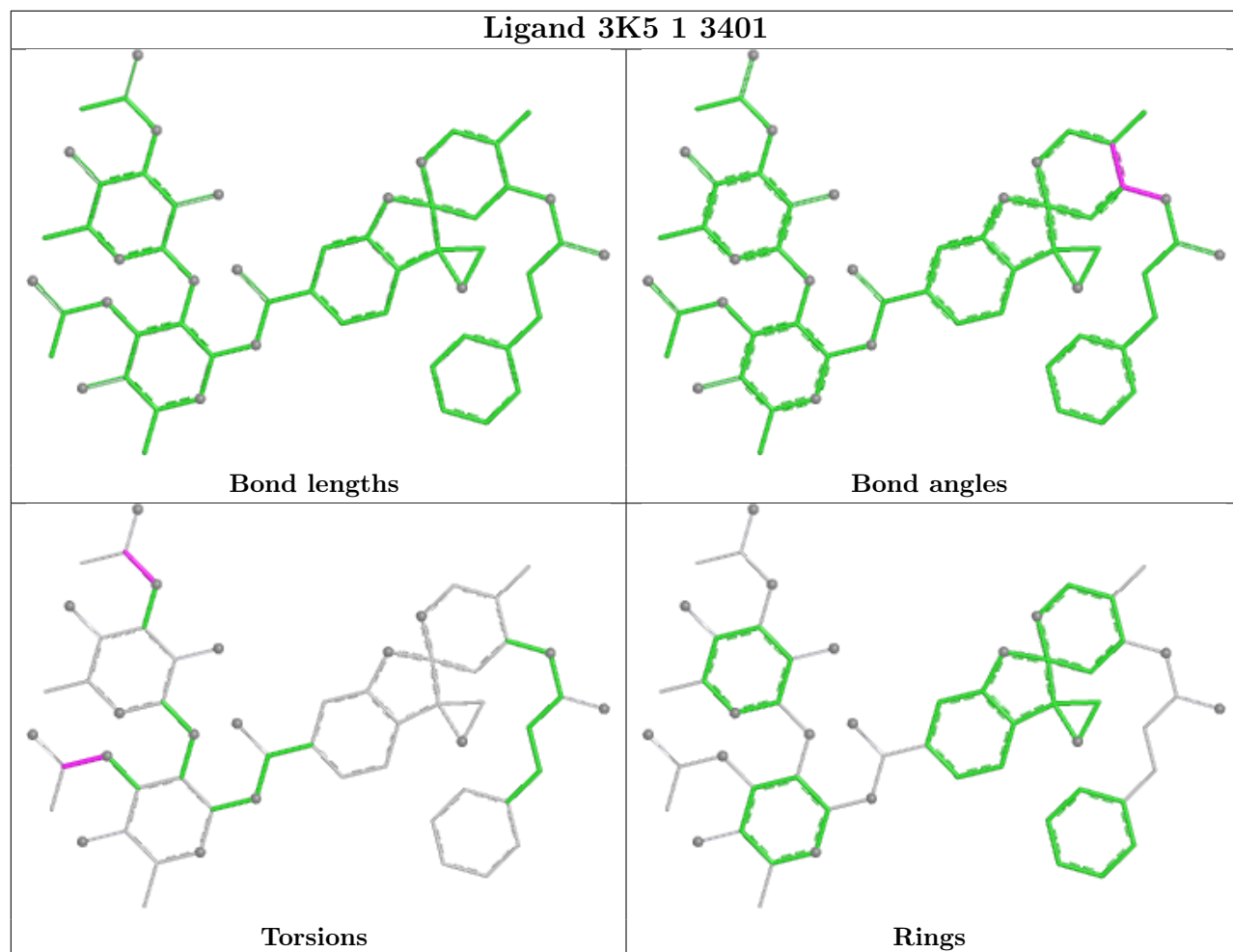
Mol	Chain	Res	Type	Clashes	Symm-Clashes
83	AS	3401	3K5	7	0
86	B	1851	GET	6	0
83	1	3401	3K5	6	0
86	CM	1822	GET	5	0

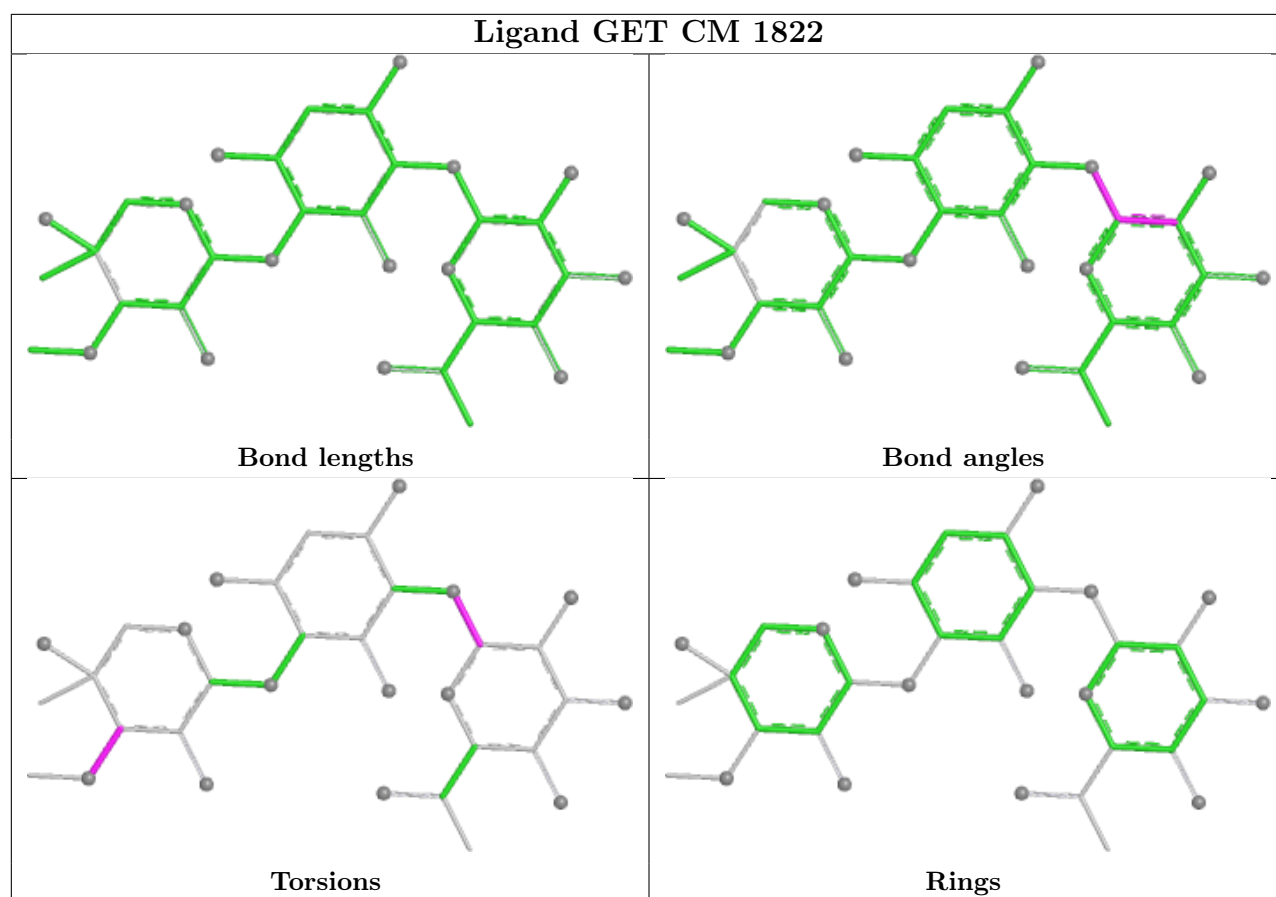
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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





Ligand 3K5 1 3401





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	1	3218/3359 (95%)	0.17	104 (3%)	50	29	67, 107, 226, 432	0
1	AS	3101/3359 (92%)	0.29	142 (4%)	37	20	74, 119, 222, 327	0
2	3	121/121 (100%)	-0.11	2 (1%)	69	43	81, 112, 128, 178	0
2	AT	121/121 (100%)	0.03	1 (0%)	82	60	86, 122, 141, 189	0
3	4	156/158 (98%)	0.08	4 (2%)	57	33	88, 119, 158, 213	0
3	AU	158/158 (100%)	0.26	7 (4%)	39	21	103, 142, 189, 269	0
4	AW	249/254 (98%)	0.51	24 (9%)	13	9	88, 128, 152, 164	0
4	j	249/254 (98%)	0.50	16 (6%)	25	15	67, 103, 134, 178	0
5	AX	386/389 (99%)	0.43	29 (7%)	20	13	61, 100, 137, 204	0
5	k	386/389 (99%)	0.42	22 (5%)	29	17	59, 100, 127, 167	0
6	AY	359/363 (98%)	0.70	47 (13%)	7	6	76, 125, 157, 177	0
6	l	359/363 (98%)	0.58	25 (6%)	22	14	58, 111, 144, 177	0
7	AZ	292/298 (97%)	0.70	29 (9%)	13	8	88, 141, 175, 185	0
7	m	294/298 (98%)	0.28	23 (7%)	19	12	88, 123, 160, 181	0
8	BA	153/176 (86%)	0.64	15 (9%)	13	9	92, 129, 157, 192	0
8	n	157/176 (89%)	0.32	6 (3%)	44	24	93, 124, 156, 186	0
9	BB	226/241 (93%)	0.54	24 (10%)	11	8	75, 107, 144, 180	0
9	o	229/241 (95%)	0.26	12 (5%)	33	19	70, 97, 140, 210	0
10	BC	233/262 (88%)	0.30	9 (3%)	43	23	132, 169, 208, 223	0
10	p	236/262 (90%)	0.21	8 (3%)	48	27	101, 134, 180, 207	0
11	BD	190/191 (99%)	0.23	10 (5%)	32	18	97, 127, 155, 192	0
11	q	190/191 (99%)	0.17	1 (0%)	87	68	84, 115, 139, 174	0
12	r	207/219 (94%)	0.23	7 (3%)	48	27	57, 93, 137, 168	0
13	BF	171/174 (98%)	0.24	7 (4%)	41	22	91, 132, 162, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	s	171/174 (98%)	0.33	10 (5%) 29 17	82, 126, 154, 168	0
14	BG	200/202 (99%)	0.30	8 (4%) 42 23	88, 140, 182, 202	0
14	t	200/202 (99%)	0.20	11 (5%) 30 18	68, 122, 169, 194	0
15	BH	130/131 (99%)	0.23	3 (2%) 61 37	90, 123, 153, 167	0
15	u	128/131 (97%)	0.23	9 (7%) 22 14	87, 112, 136, 151	0
16	BI	203/204 (99%)	1.21	34 (16%) 4 4	93, 134, 156, 171	0
16	v	203/204 (99%)	1.03	36 (17%) 4 4	74, 104, 123, 140	0
17	BJ	199/200 (99%)	0.43	14 (7%) 22 14	74, 100, 145, 164	0
17	w	199/200 (99%)	0.44	10 (5%) 34 19	69, 96, 136, 157	0
18	BK	174/185 (94%)	0.50	7 (4%) 42 23	82, 114, 142, 165	0
18	x	169/185 (91%)	0.57	9 (5%) 32 18	75, 105, 153, 171	0
19	BL	185/186 (99%)	0.73	17 (9%) 14 9	91, 120, 141, 159	0
19	y	185/186 (99%)	0.55	16 (8%) 16 11	75, 106, 131, 150	0
20	BM	179/190 (94%)	0.47	14 (7%) 19 12	103, 134, 198, 217	0
20	z	179/190 (94%)	0.61	14 (7%) 19 12	91, 120, 185, 204	0
21	0	170/172 (98%)	0.16	3 (1%) 67 42	75, 96, 124, 174	0
21	BN	170/172 (98%)	0.21	0 100 100	81, 110, 135, 159	0
22	2	159/160 (99%)	0.41	11 (6%) 23 14	74, 97, 165, 186	0
22	BO	159/160 (99%)	0.74	16 (10%) 12 8	80, 109, 165, 203	0
23	5	100/124 (80%)	0.02	0 100 100	122, 159, 188, 195	0
23	BP	99/124 (79%)	-0.23	0 100 100	137, 175, 196, 243	0
24	6	131/137 (95%)	0.57	8 (6%) 27 16	69, 92, 121, 137	0
24	BQ	131/137 (95%)	0.45	5 (3%) 44 24	58, 94, 121, 142	0
25	7	118/155 (76%)	0.03	0 100 100	80, 126, 175, 186	0
25	BR	109/155 (70%)	0.20	5 (4%) 37 20	84, 117, 150, 174	0
26	8	120/142 (84%)	0.48	13 (10%) 11 8	93, 123, 143, 156	0
26	BS	119/142 (83%)	0.38	6 (5%) 34 19	118, 146, 163, 176	0
27	9	126/127 (99%)	0.32	2 (1%) 70 45	92, 126, 155, 164	0
27	BT	126/127 (99%)	0.45	7 (5%) 30 17	110, 143, 174, 191	0
28	AA	135/136 (99%)	0.25	4 (2%) 52 30	112, 141, 166, 198	0
28	BU	135/136 (99%)	0.03	1 (0%) 84 63	138, 171, 197, 224	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
29	AB	148/149 (99%)	0.66	13 (8%)	15 10	70, 101, 132, 161	0
29	BV	148/149 (99%)	0.67	11 (7%)	20 13	77, 124, 153, 170	0
30	AC	58/63 (92%)	0.69	10 (17%)	4 4	69, 114, 142, 164	0
30	BW	60/63 (95%)	0.96	11 (18%)	3 4	87, 130, 167, 194	0
31	AD	98/106 (92%)	0.16	0	100 100	99, 130, 149, 153	0
31	BX	94/106 (88%)	-0.01	0	100 100	129, 160, 181, 199	0
32	AE	108/112 (96%)	0.33	7 (6%)	25 15	86, 115, 163, 184	0
32	BY	108/112 (96%)	0.52	9 (8%)	17 11	87, 120, 164, 203	0
33	AF	124/131 (94%)	0.84	15 (12%)	8 6	64, 105, 131, 151	0
33	BZ	122/131 (93%)	0.85	11 (9%)	15 10	88, 112, 140, 154	0
34	AG	106/107 (99%)	0.51	8 (7%)	20 13	76, 102, 120, 142	0
34	CA	106/107 (99%)	0.29	1 (0%)	81 58	85, 106, 127, 144	0
35	AH	112/122 (91%)	1.08	25 (22%)	2 2	87, 121, 168, 190	0
35	CB	110/122 (90%)	1.10	21 (19%)	3 3	112, 146, 194, 201	0
36	AI	115/120 (95%)	0.33	6 (5%)	33 19	105, 131, 157, 175	0
36	CC	117/120 (97%)	0.45	7 (5%)	27 16	127, 155, 175, 210	0
37	AJ	97/99 (97%)	0.10	2 (2%)	63 38	103, 119, 155, 199	0
37	CD	95/99 (95%)	0.20	2 (2%)	63 38	115, 148, 174, 197	0
38	AK	86/90 (95%)	0.62	6 (6%)	22 14	81, 102, 141, 152	0
38	CE	86/90 (95%)	0.60	6 (6%)	22 14	88, 120, 160, 169	0
39	AL	77/78 (98%)	0.38	1 (1%)	75 50	113, 152, 178, 207	0
39	CF	77/78 (98%)	0.04	2 (2%)	57 33	140, 167, 202, 208	0
40	AM	50/51 (98%)	0.68	3 (6%)	27 16	84, 111, 135, 143	0
40	CG	50/51 (98%)	0.72	5 (10%)	12 8	95, 125, 143, 147	0
41	AN	50/52 (96%)	0.85	5 (10%)	12 8	113, 149, 165, 169	0
41	CH	50/52 (96%)	0.95	7 (14%)	6 5	121, 154, 169, 181	0
42	AO	25/25 (100%)	1.15	4 (16%)	5 4	99, 107, 123, 130	0
42	CI	24/25 (96%)	1.18	4 (16%)	4 4	93, 112, 125, 132	0
43	AP	103/106 (97%)	0.22	2 (1%)	66 41	73, 100, 143, 158	0
43	CJ	103/106 (97%)	0.42	6 (5%)	29 17	91, 124, 160, 171	0
44	AQ	91/92 (98%)	0.44	5 (5%)	30 18	79, 111, 140, 165	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	CK	91/92 (98%)	0.04	1 (1%) 78 54	106, 130, 160, 174	0
45	CL	120/267 (44%)	0.17	6 (5%) 34 19	100, 143, 178, 186	0
45	i	106/267 (39%)	0.50	7 (6%) 24 15	108, 150, 178, 201	0
46	B	1708/1787 (95%)	0.33	100 (5%) 28 16	83, 128, 212, 439	0
46	CM	1728/1787 (96%)	0.16	55 (3%) 50 29	86, 131, 222, 410	0
47	C	208/261 (79%)	0.33	10 (4%) 35 19	127, 161, 191, 201	0
47	CN	208/261 (79%)	0.25	9 (4%) 40 21	101, 152, 181, 215	0
48	CO	213/256 (83%)	-0.08	5 (2%) 61 37	124, 173, 195, 212	0
48	D	214/256 (83%)	0.15	5 (2%) 61 37	110, 144, 167, 178	0
49	CP	217/249 (87%)	0.24	10 (4%) 37 20	83, 124, 152, 171	0
49	E	217/249 (87%)	0.38	18 (8%) 17 11	106, 137, 164, 187	0
50	CQ	223/251 (88%)	0.23	11 (4%) 35 19	99, 130, 186, 216	0
50	F	223/251 (88%)	0.48	15 (6%) 24 15	103, 143, 197, 215	0
51	CR	260/262 (99%)	0.20	17 (6%) 25 15	103, 130, 156, 184	0
51	G	258/262 (98%)	0.78	27 (10%) 11 8	110, 145, 166, 192	0
52	CS	205/225 (91%)	0.21	12 (5%) 28 16	124, 155, 189, 241	0
52	H	206/225 (91%)	0.54	19 (9%) 14 9	107, 146, 181, 213	0
53	CT	236/236 (100%)	0.32	9 (3%) 44 24	94, 143, 182, 203	0
53	I	223/236 (94%)	0.47	24 (10%) 11 8	97, 143, 178, 222	0
54	CU	179/186 (96%)	-0.02	4 (2%) 62 37	123, 179, 214, 226	0
54	J	182/186 (97%)	0.40	11 (6%) 27 16	118, 180, 204, 219	0
55	CV	203/206 (98%)	0.57	21 (10%) 12 8	82, 121, 170, 195	0
55	K	203/206 (98%)	0.34	16 (7%) 18 12	89, 129, 173, 189	0
56	CW	178/189 (94%)	0.34	11 (6%) 26 16	101, 137, 167, 188	0
56	L	178/189 (94%)	0.78	25 (14%) 6 5	118, 151, 173, 185	0
57	CX	94/118 (79%)	-0.04	0 100 100	104, 147, 177, 208	0
57	M	98/118 (83%)	0.35	4 (4%) 41 22	108, 154, 188, 204	0
58	CY	141/155 (90%)	0.16	1 (0%) 84 63	83, 118, 151, 197	0
58	N	144/155 (92%)	0.50	12 (8%) 17 11	102, 129, 165, 189	0
59	CZ	119/143 (83%)	0.03	1 (0%) 82 60	178, 214, 225, 231	0
59	O	116/143 (81%)	0.21	5 (4%) 40 21	193, 225, 239, 248	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
60	DA	150/151 (99%)	0.29	6 (4%)	42	23	103, 146, 173, 183	0
60	P	148/151 (98%)	0.56	11 (7%)	20	13	101, 140, 167, 179	0
61	DB	122/132 (92%)	0.09	3 (2%)	58	35	98, 153, 179, 189	0
61	Q	127/132 (96%)	0.38	8 (6%)	26	15	97, 129, 152, 162	0
62	DC	130/142 (91%)	0.51	6 (4%)	37	20	115, 155, 184, 195	0
62	R	131/142 (92%)	0.41	8 (6%)	27	16	94, 138, 178, 202	0
63	DD	139/142 (97%)	0.69	16 (11%)	9	6	108, 152, 179, 189	0
63	S	139/142 (97%)	0.59	13 (9%)	14	9	110, 149, 184, 201	0
64	DE	124/137 (90%)	0.43	6 (4%)	35	19	104, 163, 207, 216	0
64	T	124/137 (90%)	0.44	7 (5%)	30	17	128, 167, 217, 226	0
65	DF	141/145 (97%)	0.31	2 (1%)	73	48	115, 153, 182, 210	0
65	U	144/145 (99%)	0.28	4 (2%)	55	32	96, 126, 165, 179	0
66	DG	141/145 (97%)	0.30	4 (2%)	55	32	117, 150, 175, 193	0
66	V	141/145 (97%)	0.31	3 (2%)	63	38	110, 137, 176, 196	0
67	DH	97/119 (81%)	0.58	9 (9%)	14	9	97, 147, 182, 194	0
67	W	102/119 (85%)	0.65	10 (9%)	13	9	96, 164, 192, 198	0
68	DI	87/87 (100%)	0.15	3 (3%)	48	27	106, 144, 173, 193	0
68	X	87/87 (100%)	0.14	2 (2%)	61	37	111, 147, 172, 181	0
69	DJ	129/130 (99%)	0.28	0	100	100	104, 127, 144, 151	0
69	Y	129/130 (99%)	0.58	5 (3%)	43	23	112, 133, 148, 154	0
70	DK	143/145 (98%)	0.52	10 (6%)	22	14	79, 104, 131, 156	0
70	Z	143/145 (98%)	0.58	12 (8%)	17	11	85, 110, 132, 158	0
71	DL	132/135 (97%)	0.02	2 (1%)	72	47	114, 150, 176, 204	0
71	a	134/135 (99%)	0.25	8 (5%)	27	16	115, 152, 175, 189	0
72	DM	71/105 (67%)	0.04	1 (1%)	73	48	149, 175, 195, 201	0
72	b	72/105 (68%)	-0.06	1 (1%)	73	48	120, 150, 179, 193	0
73	DN	98/119 (82%)	0.31	6 (6%)	27	16	109, 136, 188, 195	0
73	c	97/119 (81%)	0.49	9 (9%)	14	9	100, 133, 168, 197	0
74	DO	81/82 (98%)	0.02	1 (1%)	76	52	125, 163, 219, 233	0
74	d	81/82 (98%)	0.35	4 (4%)	35	19	120, 154, 198, 218	0
75	DP	61/67 (91%)	-0.12	1 (1%)	70	45	133, 162, 183, 192	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	e	60/67 (89%)	0.32	5 (8%) 17 11	125, 156, 185, 191	0
76	DQ	54/56 (96%)	0.50	3 (5%) 30 17	95, 116, 149, 169	0
76	f	55/56 (98%)	0.89	8 (14%) 6 5	98, 118, 141, 175	0
77	DR	59/63 (93%)	0.48	5 (8%) 16 11	98, 140, 207, 220	0
77	g	60/63 (95%)	0.64	7 (11%) 9 6	117, 147, 202, 222	0
78	DS	68/193 (35%)	0.20	4 (5%) 28 16	154, 226, 246, 252	0
78	h	70/193 (36%)	0.47	7 (10%) 12 8	163, 211, 237, 252	0
79	AR	311/317 (98%)	0.27	8 (2%) 57 33	162, 200, 225, 242	0
79	DT	307/317 (96%)	-0.01	4 (1%) 75 50	162, 200, 221, 236	0
80	BE	205/220 (93%)	0.19	7 (3%) 48 27	64, 97, 143, 172	0
81	P0	107/312 (34%)	-0.05	1 (0%) 81 58	155, 176, 191, 202	0
82	12	63/165 (38%)	-0.10	0 100 100	159, 180, 196, 207	0
All	All	32813/35602 (92%)	0.34	1793 (5%) 30 18	57, 128, 201, 439	0

The worst 5 of 1793 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	G	39	ARG	9.7
53	I	79	LYS	9.0
53	CT	79	LYS	8.9
6	l	55	GLU	8.6
35	CB	33	GLN	8.5

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides 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
84	MG	AS	3650	1/1	0.08	0.09	115,115,115,115	0
84	MG	BL	202	1/1	0.09	0.24	107,107,107,107	0
84	MG	1	3751	1/1	0.10	0.26	111,111,111,111	0
84	MG	B	1886	1/1	0.27	0.13	66,66,66,66	0
84	MG	AS	3517	1/1	0.28	0.25	106,106,106,106	0
84	MG	AS	3536	1/1	0.28	0.34	110,110,110,110	0
84	MG	BC	301	1/1	0.29	0.32	125,125,125,125	0
84	MG	AS	3715	1/1	0.32	0.31	158,158,158,158	0
84	MG	AS	3713	1/1	0.33	0.25	95,95,95,95	0
84	MG	1	3570	1/1	0.34	0.22	112,112,112,112	0
84	MG	AS	3576	1/1	0.35	0.20	97,97,97,97	0
84	MG	AS	3641	1/1	0.36	1.19	81,81,81,81	0
84	MG	1	3778	1/1	0.36	0.24	80,80,80,80	0
84	MG	AS	3756	1/1	0.37	0.20	69,69,69,69	0
84	MG	1	3726	1/1	0.39	0.13	96,96,96,96	0
84	MG	AS	3649	1/1	0.39	0.17	101,101,101,101	0
84	MG	1	3837	1/1	0.39	0.24	82,82,82,82	0
84	MG	1	3595	1/1	0.39	0.30	89,89,89,89	0
84	MG	AS	3692	1/1	0.41	0.18	86,86,86,86	0
84	MG	CM	1830	1/1	0.41	0.24	96,96,96,96	0
84	MG	1	3761	1/1	0.42	0.31	106,106,106,106	0
84	MG	AS	3765	1/1	0.43	0.22	96,96,96,96	0
84	MG	1	3800	1/1	0.43	0.11	70,70,70,70	0
84	MG	AS	3489	1/1	0.44	0.34	57,57,57,57	0
84	MG	1	3481	1/1	0.44	0.39	113,113,113,113	0
84	MG	1	3770	1/1	0.44	0.22	85,85,85,85	0
84	MG	AS	3585	1/1	0.45	0.27	78,78,78,78	0
84	MG	AS	3716	1/1	0.47	0.19	86,86,86,86	0
84	MG	AS	3560	1/1	0.47	0.32	96,96,96,96	0
84	MG	DK	201	1/1	0.47	0.16	91,91,91,91	0
84	MG	AS	3703	1/1	0.48	0.15	77,77,77,77	0
84	MG	o	304	1/1	0.48	0.17	75,75,75,75	0
84	MG	1	3870	1/1	0.49	0.43	87,87,87,87	0
84	MG	1	3741	1/1	0.49	0.25	98,98,98,98	0
84	MG	1	3747	1/1	0.49	0.28	82,82,82,82	0
84	MG	AS	3651	1/1	0.49	0.17	122,122,122,122	0
84	MG	AS	3678	1/1	0.49	0.17	108,108,108,108	0
84	MG	AS	3735	1/1	0.49	0.24	89,89,89,89	0
84	MG	AS	3673	1/1	0.50	0.14	79,79,79,79	0
84	MG	AS	3752	1/1	0.50	0.21	115,115,115,115	0
84	MG	1	3756	1/1	0.51	0.15	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	B	1803	1/1	0.51	0.26	113,113,113,113	0
84	MG	AY	402	1/1	0.52	0.19	120,120,120,120	0
84	MG	AS	3614	1/1	0.52	0.12	74,74,74,74	0
84	MG	AS	3569	1/1	0.52	0.27	89,89,89,89	0
84	MG	1	3567	1/1	0.52	0.25	87,87,87,87	0
84	MG	CM	1878	1/1	0.52	0.11	58,58,58,58	0
84	MG	AS	3481	1/1	0.52	0.29	76,76,76,76	0
84	MG	1	3711	1/1	0.53	0.17	64,64,64,64	0
84	MG	1	3505	1/1	0.53	0.16	77,77,77,77	0
84	MG	AS	3710	1/1	0.53	0.20	69,69,69,69	0
84	MG	1	3408	1/1	0.53	0.17	71,71,71,71	0
84	MG	1	3441	1/1	0.54	0.32	71,71,71,71	0
84	MG	1	3605	1/1	0.54	0.17	60,60,60,60	0
84	MG	1	3799	1/1	0.54	0.10	78,78,78,78	0
84	MG	1	3576	1/1	0.54	0.16	58,58,58,58	0
84	MG	AS	3518	1/1	0.55	0.23	88,88,88,88	0
84	MG	AS	3529	1/1	0.55	0.12	88,88,88,88	0
84	MG	1	3423	1/1	0.55	0.22	103,103,103,103	0
84	MG	1	3675	1/1	0.56	0.26	77,77,77,77	0
84	MG	AS	3588	1/1	0.56	0.28	72,72,72,72	0
84	MG	1	3476	1/1	0.56	0.25	80,80,80,80	0
84	MG	AS	3789	1/1	0.56	0.14	94,94,94,94	0
84	MG	AS	3580	1/1	0.56	0.13	80,80,80,80	0
84	MG	B	1850	1/1	0.57	0.26	198,198,198,198	0
84	MG	1	3508	1/1	0.57	0.60	123,123,123,123	0
84	MG	CL	301	1/1	0.57	0.49	85,85,85,85	0
84	MG	1	3662	1/1	0.57	0.12	88,88,88,88	0
84	MG	AS	3729	1/1	0.57	0.12	71,71,71,71	0
84	MG	B	1834	1/1	0.57	0.23	63,63,63,63	0
84	MG	1	3754	1/1	0.58	0.16	108,108,108,108	0
84	MG	C	301	1/1	0.58	0.10	89,89,89,89	0
84	MG	1	3824	1/1	0.58	0.20	80,80,80,80	0
84	MG	AS	3755	1/1	0.58	0.15	64,64,64,64	0
84	MG	1	3415	1/1	0.58	0.15	69,69,69,69	0
84	MG	AS	3601	1/1	0.58	0.23	78,78,78,78	0
84	MG	1	3492	1/1	0.58	0.32	72,72,72,72	0
84	MG	1	3723	1/1	0.59	0.28	72,72,72,72	0
84	MG	1	3742	1/1	0.59	0.15	69,69,69,69	0
84	MG	1	3678	1/1	0.59	0.21	75,75,75,75	0
84	MG	1	3730	1/1	0.59	0.32	70,70,70,70	0
84	MG	1	3776	1/1	0.59	0.27	66,66,66,66	0
84	MG	B	1859	1/1	0.59	0.23	85,85,85,85	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3490	1/1	0.60	0.24	47,47,47,47	0
84	MG	1	3744	1/1	0.60	0.16	84,84,84,84	0
84	MG	B	1821	1/1	0.60	0.24	80,80,80,80	0
84	MG	1	3722	1/1	0.60	0.12	82,82,82,82	0
84	MG	1	3785	1/1	0.61	0.21	35,35,35,35	0
84	MG	1	3731	1/1	0.61	0.45	82,82,82,82	0
84	MG	1	3470	1/1	0.61	0.25	77,77,77,77	0
84	MG	AS	3618	1/1	0.61	0.17	73,73,73,73	0
84	MG	1	3593	1/1	0.61	0.23	83,83,83,83	0
84	MG	AS	3539	1/1	0.61	0.23	95,95,95,95	0
84	MG	AS	3584	1/1	0.62	0.19	99,99,99,99	0
84	MG	1	3405	1/1	0.62	0.22	85,85,85,85	0
84	MG	1	3665	1/1	0.62	0.20	70,70,70,70	0
84	MG	1	3698	1/1	0.62	0.20	79,79,79,79	0
84	MG	1	3825	1/1	0.62	0.18	104,104,104,104	0
84	MG	1	3794	1/1	0.62	0.13	71,71,71,71	0
84	MG	AS	3717	1/1	0.62	0.30	79,79,79,79	0
84	MG	AS	3674	1/1	0.63	0.10	94,94,94,94	0
84	MG	AS	3568	1/1	0.63	0.20	81,81,81,81	0
84	MG	AS	3790	1/1	0.63	0.24	98,98,98,98	0
84	MG	1	3787	1/1	0.63	0.11	76,76,76,76	0
84	MG	1	3821	1/1	0.63	0.17	64,64,64,64	0
84	MG	AS	3739	1/1	0.63	0.34	93,93,93,93	0
84	MG	CG	101	1/1	0.63	0.14	101,101,101,101	0
84	MG	AS	3751	1/1	0.63	0.13	81,81,81,81	0
84	MG	3	206	1/1	0.63	0.20	83,83,83,83	0
84	MG	AS	3663	1/1	0.63	0.17	103,103,103,103	0
84	MG	AS	3525	1/1	0.63	0.16	46,46,46,46	0
84	MG	AS	3759	1/1	0.64	0.29	81,81,81,81	0
84	MG	AS	3662	1/1	0.64	0.17	78,78,78,78	0
84	MG	1	3823	1/1	0.64	0.14	99,99,99,99	0
84	MG	1	3451	1/1	0.64	0.13	50,50,50,50	0
84	MG	AS	3512	1/1	0.64	0.27	78,78,78,78	0
84	MG	1	3543	1/1	0.64	0.21	58,58,58,58	0
84	MG	1	3599	1/1	0.64	0.13	72,72,72,72	0
84	MG	AS	3744	1/1	0.64	0.29	71,71,71,71	0
84	MG	1	3547	1/1	0.64	0.19	72,72,72,72	0
84	MG	AS	3709	1/1	0.64	0.06	90,90,90,90	0
84	MG	1	3681	1/1	0.64	0.15	63,63,63,63	0
84	MG	1	3689	1/1	0.64	0.22	78,78,78,78	0
84	MG	1	3733	1/1	0.65	0.38	83,83,83,83	0
84	MG	AS	3433	1/1	0.65	0.23	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3740	1/1	0.65	0.22	79,79,79,79	0
84	MG	CM	1826	1/1	0.65	0.15	69,69,69,69	0
84	MG	AS	3705	1/1	0.65	0.23	78,78,78,78	0
84	MG	CM	1850	1/1	0.65	0.15	63,63,63,63	0
84	MG	1	3697	1/1	0.65	0.16	74,74,74,74	0
84	MG	1	3691	1/1	0.65	0.10	73,73,73,73	0
84	MG	AS	3783	1/1	0.66	0.20	84,84,84,84	0
84	MG	1	3585	1/1	0.66	0.18	98,98,98,98	0
84	MG	1	3546	1/1	0.66	0.14	82,82,82,82	0
84	MG	1	3841	1/1	0.66	0.15	71,71,71,71	0
84	MG	AS	3511	1/1	0.66	0.20	75,75,75,75	0
84	MG	1	3417	1/1	0.66	0.24	82,82,82,82	0
84	MG	1	3788	1/1	0.66	0.23	78,78,78,78	0
84	MG	1	3565	1/1	0.66	0.11	49,49,49,49	0
84	MG	CM	1816	1/1	0.66	0.24	67,67,67,67	0
84	MG	B	1900	1/1	0.66	0.18	101,101,101,101	0
84	MG	AS	3714	1/1	0.66	0.20	54,54,54,54	0
84	MG	B	1802	1/1	0.66	0.25	67,67,67,67	0
84	MG	AS	3764	1/1	0.66	0.12	86,86,86,86	0
84	MG	DG	201	1/1	0.66	0.16	121,121,121,121	0
84	MG	AS	3532	1/1	0.66	0.31	65,65,65,65	0
84	MG	AS	3542	1/1	0.67	0.28	61,61,61,61	0
84	MG	AX	401	1/1	0.67	0.08	76,76,76,76	0
84	MG	1	3768	1/1	0.67	0.10	62,62,62,62	0
84	MG	CM	1846	1/1	0.67	0.23	69,69,69,69	0
84	MG	CM	1847	1/1	0.67	0.17	85,85,85,85	0
84	MG	1	3535	1/1	0.67	0.27	86,86,86,86	0
84	MG	CM	1871	1/1	0.67	0.20	76,76,76,76	0
84	MG	AS	3720	1/1	0.67	0.19	60,60,60,60	0
84	MG	AS	3721	1/1	0.67	0.11	83,83,83,83	0
84	MG	AS	3633	1/1	0.67	0.27	43,43,43,43	0
84	MG	B	1885	1/1	0.68	0.15	100,100,100,100	0
84	MG	1	3732	1/1	0.68	0.28	65,65,65,65	0
84	MG	B	1820	1/1	0.68	0.11	66,66,66,66	0
84	MG	1	3847	1/1	0.68	0.13	68,68,68,68	0
84	MG	AS	3472	1/1	0.69	0.25	64,64,64,64	0
84	MG	AS	3554	1/1	0.69	0.20	85,85,85,85	0
84	MG	1	3506	1/1	0.69	0.13	49,49,49,49	0
84	MG	AS	3426	1/1	0.69	0.20	56,56,56,56	0
84	MG	1	3571	1/1	0.69	0.07	94,94,94,94	0
84	MG	AS	3725	1/1	0.69	0.06	89,89,89,89	0
84	MG	1	3763	1/1	0.70	0.11	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3807	1/1	0.70	0.28	65,65,65,65	0
84	MG	1	3845	1/1	0.70	0.25	60,60,60,60	0
84	MG	1	3817	1/1	0.70	0.23	101,101,101,101	0
84	MG	CM	1805	1/1	0.70	0.33	63,63,63,63	0
84	MG	1	3856	1/1	0.70	0.24	91,91,91,91	0
84	MG	1	3609	1/1	0.70	0.13	82,82,82,82	0
84	MG	AS	3570	1/1	0.70	0.18	87,87,87,87	0
84	MG	1	3624	1/1	0.70	0.09	63,63,63,63	0
84	MG	1	3606	1/1	0.70	0.32	67,67,67,67	0
84	MG	AS	3667	1/1	0.70	0.07	70,70,70,70	0
84	MG	1	3717	1/1	0.70	0.25	54,54,54,54	0
84	MG	Y	202	1/1	0.70	0.17	108,108,108,108	0
84	MG	1	3830	1/1	0.70	0.14	49,49,49,49	0
84	MG	AS	3428	1/1	0.70	0.18	71,71,71,71	0
84	MG	AX	402	1/1	0.71	0.12	81,81,81,81	0
84	MG	AS	3737	1/1	0.71	0.33	107,107,107,107	0
84	MG	B	1835	1/1	0.71	0.13	67,67,67,67	0
84	MG	AS	3741	1/1	0.71	0.16	85,85,85,85	0
84	MG	1	3548	1/1	0.71	0.24	48,48,48,48	0
84	MG	AS	3749	1/1	0.71	0.24	73,73,73,73	0
84	MG	1	3591	1/1	0.71	0.10	45,45,45,45	0
84	MG	B	1860	1/1	0.71	0.20	73,73,73,73	0
84	MG	1	3482	1/1	0.71	0.12	99,99,99,99	0
84	MG	1	3745	1/1	0.71	0.24	80,80,80,80	0
84	MG	1	3572	1/1	0.71	0.29	45,45,45,45	0
84	MG	1	3748	1/1	0.71	0.23	86,86,86,86	0
84	MG	1	3661	1/1	0.71	0.15	102,102,102,102	0
84	MG	1	3412	1/1	0.71	0.15	66,66,66,66	0
84	MG	B	1831	1/1	0.71	0.18	79,79,79,79	0
84	MG	1	3850	1/1	0.71	0.07	57,57,57,57	0
84	MG	AS	3443	1/1	0.71	0.25	62,62,62,62	0
84	MG	AS	3460	1/1	0.72	0.15	48,48,48,48	0
84	MG	B	1868	1/1	0.72	0.15	64,64,64,64	0
84	MG	1	3461	1/1	0.72	0.26	59,59,59,59	0
84	MG	1	3692	1/1	0.72	0.20	56,56,56,56	0
84	MG	B	1897	1/1	0.72	0.20	94,94,94,94	0
84	MG	1	3418	1/1	0.72	0.10	64,64,64,64	0
84	MG	CM	1823	1/1	0.72	0.28	44,44,44,44	0
84	MG	1	3516	1/1	0.72	0.09	86,86,86,86	0
84	MG	E	301	1/1	0.72	0.11	54,54,54,54	0
84	MG	CM	1843	1/1	0.72	0.16	80,80,80,80	0
84	MG	1	3528	1/1	0.72	0.16	94,94,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3806	1/1	0.72	0.18	44,44,44,44	0
84	MG	1	3587	1/1	0.72	0.16	96,96,96,96	0
84	MG	AS	3592	1/1	0.72	0.21	66,66,66,66	0
84	MG	AD	201	1/1	0.72	0.26	58,58,58,58	0
84	MG	1	3813	1/1	0.72	0.08	69,69,69,69	0
84	MG	AS	3615	1/1	0.72	0.12	102,102,102,102	0
84	MG	AS	3654	1/1	0.73	0.41	87,87,87,87	0
84	MG	AS	3575	1/1	0.73	0.14	38,38,38,38	0
84	MG	AS	3435	1/1	0.73	0.22	72,72,72,72	0
84	MG	1	3534	1/1	0.73	0.28	54,54,54,54	0
84	MG	B	1806	1/1	0.73	0.23	99,99,99,99	0
84	MG	1	3530	1/1	0.73	0.10	61,61,61,61	0
84	MG	1	3709	1/1	0.73	0.10	53,53,53,53	0
84	MG	AS	3484	1/1	0.73	0.16	64,64,64,64	0
84	MG	AS	3745	1/1	0.73	0.13	104,104,104,104	0
84	MG	AS	3697	1/1	0.73	0.19	65,65,65,65	0
84	MG	a	201	1/1	0.73	0.13	78,78,78,78	0
84	MG	AS	3552	1/1	0.73	0.20	77,77,77,77	0
84	MG	1	3625	1/1	0.73	0.32	86,86,86,86	0
84	MG	1	3538	1/1	0.73	0.17	59,59,59,59	0
84	MG	AS	3625	1/1	0.73	0.09	66,66,66,66	0
84	MG	AS	3567	1/1	0.73	0.14	82,82,82,82	0
84	MG	AS	3515	1/1	0.73	0.24	66,66,66,66	0
84	MG	AS	3516	1/1	0.73	0.12	90,90,90,90	0
84	MG	1	3693	1/1	0.73	0.16	53,53,53,53	0
84	MG	AS	3572	1/1	0.73	0.22	94,94,94,94	0
84	MG	AS	3612	1/1	0.74	0.21	77,77,77,77	0
84	MG	AS	3563	1/1	0.74	0.18	75,75,75,75	0
84	MG	1	3545	1/1	0.74	0.12	50,50,50,50	0
84	MG	1	3641	1/1	0.74	0.14	71,71,71,71	0
84	MG	1	3654	1/1	0.74	0.23	102,102,102,102	0
84	MG	1	3411	1/1	0.74	0.15	90,90,90,90	0
84	MG	AS	3757	1/1	0.74	0.23	65,65,65,65	0
84	MG	B	1892	1/1	0.74	0.23	81,81,81,81	0
84	MG	CM	1877	1/1	0.74	0.12	97,97,97,97	0
84	MG	AS	3642	1/1	0.74	0.09	62,62,62,62	0
84	MG	1	3832	1/1	0.74	0.22	62,62,62,62	0
84	MG	AS	3686	1/1	0.74	0.17	75,75,75,75	0
84	MG	AS	3718	1/1	0.75	0.11	60,60,60,60	0
84	MG	AS	3527	1/1	0.75	0.15	77,77,77,77	0
84	MG	1	3672	1/1	0.75	0.23	68,68,68,68	0
84	MG	AS	3656	1/1	0.75	0.16	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	B	1804	1/1	0.75	0.15	77,77,77,77	0
84	MG	1	3704	1/1	0.75	0.17	60,60,60,60	0
84	MG	1	3752	1/1	0.75	0.20	77,77,77,77	0
84	MG	B	1895	1/1	0.75	0.15	78,78,78,78	0
84	MG	AS	3545	1/1	0.75	0.23	84,84,84,84	0
84	MG	AS	3611	1/1	0.75	0.23	56,56,56,56	0
84	MG	1	3804	1/1	0.75	0.18	85,85,85,85	0
84	MG	1	3828	1/1	0.75	0.27	81,81,81,81	0
84	MG	AS	3509	1/1	0.75	0.12	62,62,62,62	0
84	MG	1	3504	1/1	0.75	0.18	65,65,65,65	0
84	MG	1	3647	1/1	0.75	0.21	49,49,49,49	0
84	MG	AS	3630	1/1	0.75	0.16	74,74,74,74	0
84	MG	B	1845	1/1	0.75	0.13	89,89,89,89	0
84	MG	y	201	1/1	0.75	0.11	63,63,63,63	0
84	MG	B	1857	1/1	0.75	0.21	50,50,50,50	0
84	MG	AS	3645	1/1	0.75	0.23	72,72,72,72	0
84	MG	1	3495	1/1	0.75	0.20	91,91,91,91	0
84	MG	1	3685	1/1	0.75	0.09	96,96,96,96	0
84	MG	1	3414	1/1	0.76	0.29	72,72,72,72	0
84	MG	1	3489	1/1	0.76	0.35	67,67,67,67	0
84	MG	AZ	301	1/1	0.76	0.16	82,82,82,82	0
84	MG	AS	3620	1/1	0.76	0.13	62,62,62,62	0
84	MG	AS	3622	1/1	0.76	0.15	74,74,74,74	0
84	MG	BZ	201	1/1	0.76	0.10	70,70,70,70	0
84	MG	1	3782	1/1	0.76	0.11	76,76,76,76	0
84	MG	1	3558	1/1	0.76	0.13	69,69,69,69	0
84	MG	0	201	1/1	0.76	0.13	87,87,87,87	0
84	MG	B	1844	1/1	0.76	0.12	45,45,45,45	0
84	MG	1	3758	1/1	0.76	0.17	67,67,67,67	0
84	MG	1	3683	1/1	0.76	0.19	74,74,74,74	0
84	MG	1	3559	1/1	0.76	0.09	23,23,23,23	0
84	MG	CM	1841	1/1	0.76	0.09	42,42,42,42	0
84	MG	1	3749	1/1	0.76	0.16	77,77,77,77	0
84	MG	CM	1844	1/1	0.76	0.20	78,78,78,78	0
84	MG	CM	1845	1/1	0.76	0.12	57,57,57,57	0
84	MG	AS	3596	1/1	0.76	0.11	70,70,70,70	0
84	MG	AS	3412	1/1	0.76	0.25	84,84,84,84	0
84	MG	AS	3602	1/1	0.76	0.17	76,76,76,76	0
84	MG	CM	1857	1/1	0.76	0.10	83,83,83,83	0
84	MG	CM	1869	1/1	0.76	0.25	64,64,64,64	0
84	MG	1	3674	1/1	0.76	0.17	67,67,67,67	0
84	MG	B	1809	1/1	0.76	0.19	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	AS	3665	1/1	0.76	0.12	75,75,75,75	0
84	MG	AS	3724	1/1	0.76	0.12	87,87,87,87	0
84	MG	B	1872	1/1	0.76	0.20	95,95,95,95	0
84	MG	1	3614	1/1	0.77	0.13	83,83,83,83	0
84	MG	AS	3631	1/1	0.77	0.22	53,53,53,53	0
84	MG	B	1855	1/1	0.77	0.14	67,67,67,67	0
84	MG	AS	3634	1/1	0.77	0.17	58,58,58,58	0
84	MG	AS	3635	1/1	0.77	0.23	76,76,76,76	0
84	MG	AY	401	1/1	0.77	0.20	82,82,82,82	0
84	MG	AS	3638	1/1	0.77	0.16	76,76,76,76	0
84	MG	B	1856	1/1	0.77	0.15	148,148,148,148	0
84	MG	1	3568	1/1	0.77	0.26	67,67,67,67	0
84	MG	1	3579	1/1	0.77	0.23	93,93,93,93	0
84	MG	1	3630	1/1	0.77	0.10	39,39,39,39	0
84	MG	B	1812	1/1	0.77	0.19	52,52,52,52	0
84	MG	1	3789	1/1	0.77	0.09	67,67,67,67	0
84	MG	AS	3530	1/1	0.77	0.26	68,68,68,68	0
84	MG	AS	3437	1/1	0.77	0.17	68,68,68,68	0
84	MG	AS	3535	1/1	0.77	0.40	111,111,111,111	0
84	MG	1	3700	1/1	0.77	0.22	77,77,77,77	0
84	MG	AS	3446	1/1	0.77	0.12	55,55,55,55	0
84	MG	CM	1838	1/1	0.77	0.19	101,101,101,101	0
84	MG	1	3765	1/1	0.77	0.25	98,98,98,98	0
84	MG	1	3703	1/1	0.77	0.17	59,59,59,59	0
84	MG	1	3670	1/1	0.77	0.20	77,77,77,77	0
84	MG	B	1841	1/1	0.77	0.34	73,73,73,73	0
84	MG	AS	3681	1/1	0.77	0.23	82,82,82,82	0
84	MG	AS	3682	1/1	0.77	0.24	67,67,67,67	0
84	MG	AS	3485	1/1	0.77	0.14	91,91,91,91	0
84	MG	B	1899	1/1	0.77	0.11	83,83,83,83	0
84	MG	AS	3695	1/1	0.77	0.14	67,67,67,67	0
84	MG	AS	3758	1/1	0.77	0.23	77,77,77,77	0
84	MG	1	3582	1/1	0.77	0.16	49,49,49,49	0
84	MG	1	3536	1/1	0.77	0.26	73,73,73,73	0
84	MG	AS	3704	1/1	0.77	0.11	75,75,75,75	0
84	MG	AS	3776	1/1	0.77	0.17	88,88,88,88	0
84	MG	1	3803	1/1	0.78	0.09	63,63,63,63	0
84	MG	AS	3556	1/1	0.78	0.09	76,76,76,76	0
84	MG	1	3827	1/1	0.78	0.22	50,50,50,50	0
84	MG	1	3687	1/1	0.78	0.12	83,83,83,83	0
84	MG	1	3583	1/1	0.78	0.10	81,81,81,81	0
84	MG	1	3610	1/1	0.78	0.14	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3809	1/1	0.78	0.11	179,179,179,179	0
84	MG	CM	1831	1/1	0.78	0.25	58,58,58,58	0
84	MG	AS	3670	1/1	0.78	0.14	98,98,98,98	0
84	MG	AS	3528	1/1	0.78	0.20	83,83,83,83	0
84	MG	1	3553	1/1	0.78	0.08	66,66,66,66	0
84	MG	1	3791	1/1	0.78	0.09	51,51,51,51	0
84	MG	1	3820	1/1	0.78	0.34	88,88,88,88	0
84	MG	AS	3534	1/1	0.78	0.15	113,113,113,113	0
84	MG	1	3578	1/1	0.78	0.30	72,72,72,72	0
84	MG	1	3779	1/1	0.78	0.11	60,60,60,60	0
84	MG	B	1814	1/1	0.78	0.26	40,40,40,40	0
84	MG	AS	3406	1/1	0.78	0.12	122,122,122,122	0
84	MG	B	1818	1/1	0.78	0.20	57,57,57,57	0
84	MG	BB	302	1/1	0.78	0.19	83,83,83,83	0
84	MG	AS	3547	1/1	0.78	0.13	98,98,98,98	0
84	MG	AS	3748	1/1	0.78	0.15	67,67,67,67	0
84	MG	1	3694	1/1	0.78	0.13	84,84,84,84	0
85	ZN	d	101	1/1	0.78	0.09	314,314,314,314	0
84	MG	B	1861	1/1	0.79	0.21	52,52,52,52	0
84	MG	AS	3696	1/1	0.79	0.27	78,78,78,78	0
84	MG	B	1807	1/1	0.79	0.26	48,48,48,48	0
84	MG	1	3468	1/1	0.79	0.13	40,40,40,40	0
84	MG	AT	203	1/1	0.79	0.18	70,70,70,70	0
84	MG	AS	3623	1/1	0.79	0.12	70,70,70,70	0
84	MG	B	1884	1/1	0.79	0.18	58,58,58,58	0
84	MG	AS	3707	1/1	0.79	0.17	42,42,42,42	0
84	MG	1	3573	1/1	0.79	0.14	76,76,76,76	0
84	MG	1	3575	1/1	0.79	0.11	59,59,59,59	0
84	MG	1	3496	1/1	0.79	0.29	69,69,69,69	0
84	MG	AS	3504	1/1	0.79	0.10	74,74,74,74	0
84	MG	AS	3505	1/1	0.79	0.12	90,90,90,90	0
84	MG	1	3533	1/1	0.79	0.25	37,37,37,37	0
84	MG	1	3771	1/1	0.79	0.17	64,64,64,64	0
84	MG	B	1828	1/1	0.79	0.18	70,70,70,70	0
84	MG	1	3431	1/1	0.79	0.23	41,41,41,41	0
84	MG	B	1832	1/1	0.79	0.12	92,92,92,92	0
84	MG	1	3485	1/1	0.79	0.09	69,69,69,69	0
84	MG	1	3427	1/1	0.79	0.20	64,64,64,64	0
84	MG	AS	3519	1/1	0.79	0.16	110,110,110,110	0
84	MG	AS	3655	1/1	0.79	0.21	99,99,99,99	0
84	MG	o	301	1/1	0.79	0.30	67,67,67,67	0
84	MG	AS	3658	1/1	0.79	0.21	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3478	1/1	0.79	0.18	53,53,53,53	0
84	MG	1	3514	1/1	0.79	0.22	87,87,87,87	0
84	MG	1	3637	1/1	0.79	0.21	65,65,65,65	0
84	MG	1	3639	1/1	0.79	0.11	61,61,61,61	0
84	MG	1	3480	1/1	0.79	0.10	57,57,57,57	0
84	MG	AS	3606	1/1	0.79	0.20	83,83,83,83	0
84	MG	CM	1856	1/1	0.79	0.21	88,88,88,88	0
84	MG	1	3592	1/1	0.79	0.17	73,73,73,73	0
84	MG	CM	1868	1/1	0.79	0.25	74,74,74,74	0
84	MG	1	3519	1/1	0.79	0.26	80,80,80,80	0
84	MG	AS	3613	1/1	0.79	0.23	71,71,71,71	0
84	MG	AS	3439	1/1	0.79	0.27	67,67,67,67	0
84	MG	AS	3683	1/1	0.79	0.19	61,61,61,61	0
84	MG	AS	3684	1/1	0.79	0.19	63,63,63,63	0
84	MG	1	3795	1/1	0.79	0.09	68,68,68,68	0
84	MG	AS	3616	1/1	0.79	0.21	61,61,61,61	0
84	MG	v	302	1/1	0.80	0.14	77,77,77,77	0
84	MG	1	3769	1/1	0.80	0.12	51,51,51,51	0
84	MG	AS	3422	1/1	0.80	0.45	36,36,36,36	0
84	MG	B	1846	1/1	0.80	0.18	64,64,64,64	0
84	MG	1	3580	1/1	0.80	0.27	60,60,60,60	0
84	MG	AB	201	1/1	0.80	0.10	55,55,55,55	0
84	MG	AS	3786	1/1	0.80	0.09	70,70,70,70	0
84	MG	1	3562	1/1	0.80	0.07	66,66,66,66	0
84	MG	1	3598	1/1	0.80	0.25	78,78,78,78	0
84	MG	1	3802	1/1	0.80	0.13	54,54,54,54	0
84	MG	AS	3699	1/1	0.80	0.24	79,79,79,79	0
84	MG	AS	3700	1/1	0.80	0.17	95,95,95,95	0
84	MG	1	3669	1/1	0.80	0.19	83,83,83,83	0
84	MG	1	3497	1/1	0.80	0.33	78,78,78,78	0
84	MG	B	1862	1/1	0.80	0.21	76,76,76,76	0
84	MG	BB	301	1/1	0.80	0.22	60,60,60,60	0
84	MG	AS	3555	1/1	0.80	0.10	80,80,80,80	0
84	MG	AS	3708	1/1	0.80	0.10	71,71,71,71	0
84	MG	1	3603	1/1	0.80	0.24	54,54,54,54	0
84	MG	1	3783	1/1	0.80	0.09	66,66,66,66	0
84	MG	CB	202	1/1	0.80	0.12	65,65,65,65	0
84	MG	AS	3712	1/1	0.80	0.11	94,94,94,94	0
84	MG	1	3515	1/1	0.80	0.17	70,70,70,70	0
84	MG	AS	3564	1/1	0.80	0.11	60,60,60,60	0
84	MG	1	3849	1/1	0.80	0.09	70,70,70,70	0
84	MG	1	3810	1/1	0.80	0.17	144,144,144,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3853	1/1	0.80	0.09	106,106,106,106	0
84	MG	B	1893	1/1	0.80	0.18	87,87,87,87	0
84	MG	AS	3646	1/1	0.80	0.23	74,74,74,74	0
84	MG	AS	3571	1/1	0.80	0.15	84,84,84,84	0
84	MG	1	3762	1/1	0.80	0.19	82,82,82,82	0
84	MG	B	1896	1/1	0.80	0.10	78,78,78,78	0
84	MG	B	1826	1/1	0.80	0.11	76,76,76,76	0
84	MG	AS	3731	1/1	0.80	0.22	77,77,77,77	0
84	MG	1	3499	1/1	0.80	0.36	50,50,50,50	0
84	MG	AS	3583	1/1	0.80	0.34	60,60,60,60	0
84	MG	1	3466	1/1	0.80	0.12	79,79,79,79	0
84	MG	AS	3659	1/1	0.80	0.15	63,63,63,63	0
84	MG	1	3790	1/1	0.80	0.18	56,56,56,56	0
84	MG	AS	3586	1/1	0.80	0.24	61,61,61,61	0
84	MG	o	303	1/1	0.80	0.28	56,56,56,56	0
84	MG	AS	3666	1/1	0.80	0.12	74,74,74,74	0
84	MG	R	201	1/1	0.80	0.28	61,61,61,61	0
84	MG	Y	201	1/1	0.80	0.22	85,85,85,85	0
84	MG	1	3527	1/1	0.80	0.14	75,75,75,75	0
84	MG	v	301	1/1	0.80	0.15	56,56,56,56	0
84	MG	AS	3603	1/1	0.80	0.23	38,38,38,38	0
84	MG	AS	3610	1/1	0.81	0.14	83,83,83,83	0
84	MG	1	3457	1/1	0.81	0.24	43,43,43,43	0
84	MG	AS	3770	1/1	0.81	0.08	61,61,61,61	0
84	MG	AS	3691	1/1	0.81	0.09	59,59,59,59	0
84	MG	1	3638	1/1	0.81	0.15	89,89,89,89	0
84	MG	AS	3408	1/1	0.81	0.10	87,87,87,87	0
84	MG	AS	3788	1/1	0.81	0.11	63,63,63,63	0
84	MG	1	3402	1/1	0.81	0.29	69,69,69,69	0
84	MG	AS	3420	1/1	0.81	0.15	50,50,50,50	0
84	MG	AT	201	1/1	0.81	0.12	59,59,59,59	0
84	MG	B	1858	1/1	0.81	0.12	48,48,48,48	0
84	MG	1	3542	1/1	0.81	0.26	55,55,55,55	0
84	MG	1	3646	1/1	0.81	0.17	86,86,86,86	0
84	MG	AS	3621	1/1	0.81	0.07	61,61,61,61	0
84	MG	B	1810	1/1	0.81	0.22	78,78,78,78	0
84	MG	1	3684	1/1	0.81	0.11	86,86,86,86	0
84	MG	B	1867	1/1	0.81	0.18	62,62,62,62	0
84	MG	1	3863	1/1	0.81	0.20	83,83,83,83	0
84	MG	AS	3440	1/1	0.81	0.22	42,42,42,42	0
84	MG	BL	201	1/1	0.81	0.15	66,66,66,66	0
84	MG	1	3463	1/1	0.81	0.26	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	B	1878	1/1	0.81	0.19	102,102,102,102	0
84	MG	1	3650	1/1	0.81	0.23	59,59,59,59	0
84	MG	j	301	1/1	0.81	0.14	65,65,65,65	0
84	MG	AS	3475	1/1	0.81	0.10	62,62,62,62	0
84	MG	AS	3478	1/1	0.81	0.09	74,74,74,74	0
84	MG	1	3651	1/1	0.81	0.25	55,55,55,55	0
84	MG	1	3560	1/1	0.81	0.09	66,66,66,66	0
84	MG	B	1829	1/1	0.81	0.15	56,56,56,56	0
84	MG	1	3544	1/1	0.81	0.10	58,58,58,58	0
84	MG	AS	3491	1/1	0.81	0.07	39,39,39,39	0
84	MG	CM	1832	1/1	0.81	0.19	99,99,99,99	0
84	MG	AS	3498	1/1	0.81	0.21	48,48,48,48	0
84	MG	AS	3500	1/1	0.81	0.20	80,80,80,80	0
84	MG	AS	3503	1/1	0.81	0.15	83,83,83,83	0
84	MG	AS	3579	1/1	0.81	0.18	45,45,45,45	0
84	MG	1	3793	1/1	0.81	0.08	46,46,46,46	0
84	MG	AS	3740	1/1	0.81	0.10	40,40,40,40	0
84	MG	1	3444	1/1	0.81	0.22	50,50,50,50	0
84	MG	1	3737	1/1	0.81	0.15	57,57,57,57	0
84	MG	B	1839	1/1	0.81	0.08	69,69,69,69	0
84	MG	1	3618	1/1	0.81	0.19	63,63,63,63	0
84	MG	1	3426	1/1	0.81	0.27	51,51,51,51	0
84	MG	G	301	1/1	0.81	0.10	68,68,68,68	0
84	MG	AC	101	1/1	0.81	0.07	59,59,59,59	0
84	MG	R	204	1/1	0.81	0.23	55,55,55,55	0
84	MG	1	3597	1/1	0.81	0.21	97,97,97,97	1
84	MG	CM	1879	1/1	0.81	0.15	61,61,61,61	0
84	MG	DA	201	1/1	0.81	0.17	86,86,86,86	0
84	MG	1	3493	1/1	0.81	0.23	65,65,65,65	0
84	MG	AS	3526	1/1	0.81	0.17	80,80,80,80	0
84	MG	AS	3609	1/1	0.81	0.19	98,98,98,98	0
84	MG	AS	3719	1/1	0.82	0.17	95,95,95,95	0
84	MG	AS	3688	1/1	0.82	0.06	120,120,120,120	0
84	MG	1	3555	1/1	0.82	0.25	70,70,70,70	0
84	MG	AS	3780	1/1	0.82	0.07	35,35,35,35	0
84	MG	1	3846	1/1	0.82	0.16	99,99,99,99	0
84	MG	AS	3784	1/1	0.82	0.07	57,57,57,57	0
84	MG	AS	3451	1/1	0.82	0.23	72,72,72,72	0
84	MG	CM	1836	1/1	0.82	0.14	57,57,57,57	0
84	MG	AS	3787	1/1	0.82	0.16	96,96,96,96	0
84	MG	1	3406	1/1	0.82	0.17	46,46,46,46	0
84	MG	1	3563	1/1	0.82	0.23	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3735	1/1	0.82	0.10	87,87,87,87	0
84	MG	1	3640	1/1	0.82	0.16	48,48,48,48	0
84	MG	1	3725	1/1	0.82	0.16	90,90,90,90	0
84	MG	AS	3587	1/1	0.82	0.17	83,83,83,83	0
84	MG	AS	3524	1/1	0.82	0.11	83,83,83,83	0
84	MG	1	3859	1/1	0.82	0.24	59,59,59,59	0
84	MG	1	3767	1/1	0.82	0.07	58,58,58,58	0
84	MG	CM	1861	1/1	0.82	0.09	92,92,92,92	0
84	MG	AS	3599	1/1	0.82	0.11	50,50,50,50	0
84	MG	1	3869	1/1	0.82	0.12	95,95,95,95	0
84	MG	AS	3711	1/1	0.82	0.20	78,78,78,78	0
84	MG	AS	3431	1/1	0.82	0.14	60,60,60,60	0
84	MG	1	3796	1/1	0.82	0.10	105,105,105,105	0
84	MG	1	3835	1/1	0.82	0.13	65,65,65,65	0
84	MG	1	3425	1/1	0.82	0.29	36,36,36,36	0
84	MG	1	3642	1/1	0.82	0.09	51,51,51,51	0
84	MG	1	3842	1/1	0.82	0.13	88,88,88,88	0
84	MG	AS	3573	1/1	0.82	0.17	68,68,68,68	0
84	MG	AS	3597	1/1	0.83	0.15	70,70,70,70	0
84	MG	1	3644	1/1	0.83	0.12	62,62,62,62	0
84	MG	R	202	1/1	0.83	0.16	61,61,61,61	0
84	MG	1	3707	1/1	0.83	0.17	44,44,44,44	0
84	MG	AS	3562	1/1	0.83	0.24	61,61,61,61	0
84	MG	1	3680	1/1	0.83	0.20	70,70,70,70	0
84	MG	AS	3607	1/1	0.83	0.23	56,56,56,56	0
84	MG	CM	1821	1/1	0.83	0.30	77,77,77,77	0
84	MG	AS	3453	1/1	0.83	0.08	54,54,54,54	0
84	MG	CM	1825	1/1	0.83	0.21	51,51,51,51	0
84	MG	1	3581	1/1	0.83	0.16	70,70,70,70	0
84	MG	o	302	1/1	0.83	0.14	46,46,46,46	0
84	MG	AS	3403	1/1	0.83	0.07	84,84,84,84	0
84	MG	1	3714	1/1	0.83	0.13	77,77,77,77	0
84	MG	CM	1834	1/1	0.83	0.22	130,130,130,130	0
84	MG	B	1811	1/1	0.83	0.16	54,54,54,54	0
84	MG	AS	3410	1/1	0.83	0.37	50,50,50,50	0
84	MG	1	3458	1/1	0.83	0.21	65,65,65,65	0
84	MG	1	3805	1/1	0.83	0.10	84,84,84,84	0
84	MG	1	3753	1/1	0.83	0.42	79,79,79,79	0
84	MG	AS	3423	1/1	0.83	0.21	61,61,61,61	0
84	MG	1	3552	1/1	0.83	0.14	64,64,64,64	0
84	MG	AS	3677	1/1	0.83	0.21	49,49,49,49	0
84	MG	AS	3581	1/1	0.83	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3584	1/1	0.83	0.17	81,81,81,81	0
84	MG	AS	3627	1/1	0.83	0.29	72,72,72,72	0
84	MG	B	1823	1/1	0.83	0.20	60,60,60,60	0
84	MG	AS	3726	1/1	0.83	0.13	80,80,80,80	0
84	MG	1	3860	1/1	0.83	0.12	54,54,54,54	0
84	MG	AS	3685	1/1	0.83	0.23	67,67,67,67	0
84	MG	CM	1876	1/1	0.83	0.05	76,76,76,76	0
84	MG	1	3449	1/1	0.83	0.34	54,54,54,54	0
84	MG	AS	3551	1/1	0.83	0.10	74,74,74,74	0
84	MG	AS	3738	1/1	0.83	0.23	43,43,43,43	0
84	MG	1	3865	1/1	0.83	0.15	60,60,60,60	0
84	MG	AS	3553	1/1	0.83	0.11	96,96,96,96	0
84	MG	1	3586	1/1	0.83	0.26	71,71,71,71	0
84	MG	AS	3743	1/1	0.83	0.21	73,73,73,73	0
84	MG	AS	3742	1/1	0.84	0.22	93,93,93,93	0
84	MG	1	3750	1/1	0.84	0.09	91,91,91,91	0
84	MG	1	3858	1/1	0.84	0.08	81,81,81,81	0
84	MG	AS	3507	1/1	0.84	0.12	80,80,80,80	0
84	MG	AS	3508	1/1	0.84	0.15	71,71,71,71	0
84	MG	1	3797	1/1	0.84	0.13	48,48,48,48	0
84	MG	AS	3648	1/1	0.84	0.16	55,55,55,55	0
84	MG	AS	3441	1/1	0.84	0.18	39,39,39,39	0
84	MG	1	3628	1/1	0.84	0.12	99,99,99,99	0
84	MG	B	1888	1/1	0.84	0.10	59,59,59,59	0
84	MG	AS	3653	1/1	0.84	0.15	54,54,54,54	0
84	MG	1	3839	1/1	0.84	0.32	80,80,80,80	0
84	MG	1	3517	1/1	0.84	0.10	50,50,50,50	0
84	MG	AS	3458	1/1	0.84	0.11	83,83,83,83	0
84	MG	1	3673	1/1	0.84	0.29	68,68,68,68	0
84	MG	AS	3767	1/1	0.84	0.17	54,54,54,54	0
84	MG	AS	3520	1/1	0.84	0.15	66,66,66,66	0
84	MG	AS	3523	1/1	0.84	0.13	103,103,103,103	0
84	MG	1	3636	1/1	0.84	0.19	43,43,43,43	0
84	MG	AS	3474	1/1	0.84	0.10	72,72,72,72	0
84	MG	AS	3413	1/1	0.84	0.36	71,71,71,71	0
84	MG	AS	3785	1/1	0.84	0.14	59,59,59,59	0
84	MG	3	201	1/1	0.84	0.22	63,63,63,63	0
84	MG	AS	3668	1/1	0.84	0.17	68,68,68,68	0
84	MG	1	3659	1/1	0.84	0.11	69,69,69,69	0
84	MG	1	3454	1/1	0.84	0.25	59,59,59,59	0
84	MG	k	401	1/1	0.84	0.09	71,71,71,71	0
84	MG	CM	1862	1/1	0.84	0.07	66,66,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	AS	3577	1/1	0.84	0.11	63,63,63,63	0
84	MG	1	3434	1/1	0.84	0.45	47,47,47,47	0
84	MG	AS	3680	1/1	0.84	0.06	108,108,108,108	0
84	MG	CM	1875	1/1	0.84	0.07	57,57,57,57	0
84	MG	AS	3429	1/1	0.84	0.22	83,83,83,83	0
84	MG	AS	3497	1/1	0.84	0.14	51,51,51,51	0
84	MG	AS	3628	1/1	0.84	0.17	67,67,67,67	0
84	MG	1	3511	1/1	0.84	0.26	38,38,38,38	0
84	MG	B	1838	1/1	0.84	0.18	38,38,38,38	0
84	MG	1	3648	1/1	0.84	0.09	63,63,63,63	0
84	MG	AS	3543	1/1	0.84	0.12	66,66,66,66	0
84	MG	AS	3544	1/1	0.84	0.25	52,52,52,52	0
85	ZN	CB	201	1/1	0.84	0.06	296,296,296,296	0
84	MG	AS	3411	1/1	0.85	0.18	69,69,69,69	0
84	MG	1	3617	1/1	0.85	0.20	33,33,33,33	0
84	MG	AS	3538	1/1	0.85	0.14	98,98,98,98	0
84	MG	CA	201	1/1	0.85	0.11	58,58,58,58	0
84	MG	1	3677	1/1	0.85	0.12	68,68,68,68	0
84	MG	AS	3496	1/1	0.85	0.20	52,52,52,52	0
84	MG	B	1880	1/1	0.85	0.11	88,88,88,88	0
84	MG	AS	3591	1/1	0.85	0.26	68,68,68,68	0
84	MG	AS	3746	1/1	0.85	0.23	79,79,79,79	0
84	MG	AS	3643	1/1	0.85	0.10	47,47,47,47	0
84	MG	1	3743	1/1	0.85	0.09	81,81,81,81	0
84	MG	AS	3698	1/1	0.85	0.13	51,51,51,51	0
84	MG	1	3814	1/1	0.85	0.25	56,56,56,56	0
84	MG	1	3764	1/1	0.85	0.30	74,74,74,74	0
84	MG	1	3818	1/1	0.85	0.30	70,70,70,70	0
84	MG	1	3494	1/1	0.85	0.18	48,48,48,48	0
84	MG	1	3623	1/1	0.85	0.13	66,66,66,66	0
84	MG	AB	202	1/1	0.85	0.11	70,70,70,70	0
84	MG	1	3602	1/1	0.85	0.09	57,57,57,57	0
84	MG	1	3699	1/1	0.85	0.13	44,44,44,44	0
84	MG	1	3500	1/1	0.85	0.44	58,58,58,58	0
84	MG	1	3702	1/1	0.85	0.11	76,76,76,76	0
84	MG	1	3864	1/1	0.85	0.06	46,46,46,46	0
84	MG	AS	3660	1/1	0.85	0.11	95,95,95,95	0
84	MG	1	3550	1/1	0.85	0.32	56,56,56,56	0
84	MG	B	1854	1/1	0.85	0.17	64,64,64,64	0
84	MG	1	3867	1/1	0.85	0.10	48,48,48,48	0
84	MG	1	3594	1/1	0.85	0.07	76,76,76,76	0
84	MG	AS	3454	1/1	0.85	0.13	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3734	1/1	0.85	0.09	73,73,73,73	0
84	MG	1	3834	1/1	0.85	0.14	90,90,90,90	0
84	MG	1	3529	1/1	0.85	0.27	57,57,57,57	0
84	MG	AS	3722	1/1	0.85	0.07	90,90,90,90	0
84	MG	CM	1873	1/1	0.85	0.15	81,81,81,81	0
84	MG	CM	1874	1/1	0.85	0.10	68,68,68,68	0
84	MG	1	3755	1/1	0.85	0.10	55,55,55,55	0
84	MG	AT	204	1/1	0.85	0.23	54,54,54,54	0
84	MG	AS	3676	1/1	0.85	0.11	61,61,61,61	0
84	MG	B	1815	1/1	0.85	0.08	64,64,64,64	0
84	MG	AS	3477	1/1	0.85	0.09	50,50,50,50	0
84	MG	CW	201	1/1	0.85	0.16	81,81,81,81	0
84	MG	AS	3626	1/1	0.85	0.23	52,52,52,52	0
84	MG	AS	3734	1/1	0.85	0.15	80,80,80,80	0
84	MG	1	3523	1/1	0.85	0.14	84,84,84,84	0
85	ZN	AH	201	1/1	0.85	0.08	232,232,232,232	0
84	MG	k	402	1/1	0.85	0.27	98,98,98,98	0
84	MG	1	3532	1/1	0.85	0.17	44,44,44,44	0
84	MG	B	1891	1/1	0.86	0.14	86,86,86,86	0
84	MG	1	3819	1/1	0.86	0.17	84,84,84,84	0
84	MG	1	3474	1/1	0.86	0.10	58,58,58,58	0
84	MG	CM	1829	1/1	0.86	0.10	52,52,52,52	0
84	MG	AS	3469	1/1	0.86	0.12	42,42,42,42	0
84	MG	1	3403	1/1	0.86	0.27	56,56,56,56	0
84	MG	1	3604	1/1	0.86	0.08	49,49,49,49	0
84	MG	AS	3558	1/1	0.86	0.11	58,58,58,58	0
84	MG	AS	3421	1/1	0.86	0.25	54,54,54,54	0
84	MG	AS	3521	1/1	0.86	0.18	54,54,54,54	0
84	MG	CM	1840	1/1	0.86	0.11	60,60,60,60	0
84	MG	AP	203	1/1	0.86	0.16	86,86,86,86	0
84	MG	B	1898	1/1	0.86	0.10	67,67,67,67	0
84	MG	AS	3608	1/1	0.86	0.24	46,46,46,46	0
84	MG	1	3455	1/1	0.86	0.20	45,45,45,45	0
84	MG	AS	3693	1/1	0.86	0.17	63,63,63,63	0
84	MG	AT	202	1/1	0.86	0.06	64,64,64,64	0
84	MG	1	3537	1/1	0.86	0.16	27,27,27,27	0
84	MG	1	3607	1/1	0.86	0.20	72,72,72,72	0
84	MG	AS	3486	1/1	0.86	0.21	46,46,46,46	0
84	MG	1	3705	1/1	0.86	0.14	68,68,68,68	0
84	MG	AX	403	1/1	0.86	0.27	45,45,45,45	0
84	MG	1	3479	1/1	0.86	0.32	49,49,49,49	0
84	MG	AS	3657	1/1	0.86	0.14	78,78,78,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3541	1/1	0.86	0.13	26,26,26,26	0
84	MG	AS	3436	1/1	0.86	0.21	65,65,65,65	0
84	MG	1	3746	1/1	0.86	0.05	71,71,71,71	0
84	MG	1	3759	1/1	0.86	0.13	74,74,74,74	0
84	MG	BK	201	1/1	0.86	0.11	73,73,73,73	0
84	MG	B	1843	1/1	0.86	0.14	75,75,75,75	0
84	MG	B	1882	1/1	0.86	0.20	76,76,76,76	0
84	MG	1	3815	1/1	0.86	0.17	44,44,44,44	0
84	MG	AS	3754	1/1	0.86	0.10	106,106,106,106	0
84	MG	x	201	1/1	0.86	0.16	53,53,53,53	0
84	MG	AS	3447	1/1	0.86	0.17	55,55,55,55	0
84	MG	DH	201	1/1	0.86	0.07	53,53,53,53	0
84	MG	1	3760	1/1	0.86	0.13	83,83,83,83	0
84	MG	AS	3671	1/1	0.86	0.10	48,48,48,48	0
84	MG	1	3420	1/1	0.86	0.15	21,21,21,21	0
84	MG	AS	3550	1/1	0.86	0.20	71,71,71,71	0
84	MG	B	1879	1/1	0.87	0.15	58,58,58,58	0
84	MG	CM	1807	1/1	0.87	0.12	72,72,72,72	0
84	MG	1	3855	1/1	0.87	0.09	43,43,43,43	0
84	MG	AS	3459	1/1	0.87	0.11	66,66,66,66	0
84	MG	1	3833	1/1	0.87	0.13	47,47,47,47	0
84	MG	AS	3462	1/1	0.87	0.14	60,60,60,60	0
84	MG	AS	3466	1/1	0.87	0.07	44,44,44,44	0
84	MG	B	1840	1/1	0.87	0.23	47,47,47,47	0
84	MG	1	3667	1/1	0.87	0.15	37,37,37,37	0
84	MG	AS	3768	1/1	0.87	0.10	62,62,62,62	0
84	MG	1	3715	1/1	0.87	0.16	47,47,47,47	0
84	MG	1	3649	1/1	0.87	0.07	85,85,85,85	0
84	MG	AS	3417	1/1	0.87	0.21	47,47,47,47	0
84	MG	u	201	1/1	0.87	0.13	83,83,83,83	0
84	MG	1	3862	1/1	0.87	0.23	77,77,77,77	0
84	MG	1	3838	1/1	0.87	0.10	53,53,53,53	0
84	MG	CM	1842	1/1	0.87	0.16	67,67,67,67	0
84	MG	1	3792	1/1	0.87	0.11	150,150,150,150	0
84	MG	B	1819	1/1	0.87	0.12	50,50,50,50	0
84	MG	1	3539	1/1	0.87	0.15	53,53,53,53	0
84	MG	1	3780	1/1	0.87	0.07	103,103,103,103	0
84	MG	1	3868	1/1	0.87	0.34	70,70,70,70	0
84	MG	AS	3540	1/1	0.87	0.17	108,108,108,108	0
84	MG	1	3686	1/1	0.87	0.09	103,103,103,103	0
84	MG	AS	3434	1/1	0.87	0.29	64,64,64,64	0
84	MG	B	1827	1/1	0.87	0.17	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	AS	3636	1/1	0.87	0.13	60,60,60,60	0
84	MG	AS	3637	1/1	0.87	0.10	46,46,46,46	0
84	MG	1	3671	1/1	0.87	0.12	75,75,75,75	0
84	MG	AS	3640	1/1	0.87	0.12	76,76,76,76	0
84	MG	1	3738	1/1	0.87	0.20	67,67,67,67	0
84	MG	Q	202	1/1	0.87	0.17	57,57,57,57	0
84	MG	B	1863	1/1	0.87	0.17	53,53,53,53	0
84	MG	3	202	1/1	0.87	0.11	45,45,45,45	0
84	MG	AS	3600	1/1	0.87	0.09	76,76,76,76	0
84	MG	AS	3647	1/1	0.87	0.28	54,54,54,54	0
84	MG	1	3440	1/1	0.87	0.13	67,67,67,67	0
84	MG	B	1870	1/1	0.87	0.12	63,63,63,63	0
84	MG	BO	201	1/1	0.87	0.10	91,91,91,91	0
84	MG	1	3439	1/1	0.87	0.20	43,43,43,43	0
84	MG	1	3816	1/1	0.87	0.25	59,59,59,59	0
84	MG	AS	3652	1/1	0.87	0.21	105,105,105,105	0
84	MG	AS	3753	1/1	0.87	0.28	74,74,74,74	0
84	MG	AS	3402	1/1	0.87	0.14	75,75,75,75	0
84	MG	CM	1802	1/1	0.87	0.22	53,53,53,53	0
84	MG	CM	1824	1/1	0.88	0.19	62,62,62,62	0
84	MG	AS	3679	1/1	0.88	0.15	61,61,61,61	0
84	MG	1	3472	1/1	0.88	0.11	60,60,60,60	0
84	MG	K	301	1/1	0.88	0.06	63,63,63,63	0
84	MG	1	3695	1/1	0.88	0.10	44,44,44,44	0
84	MG	1	3801	1/1	0.88	0.16	55,55,55,55	0
84	MG	1	3668	1/1	0.88	0.06	23,23,23,23	0
84	MG	1	3682	1/1	0.88	0.19	44,44,44,44	0
84	MG	AS	3488	1/1	0.88	0.25	32,32,32,32	0
84	MG	1	3509	1/1	0.88	0.07	11,11,11,11	0
84	MG	AS	3690	1/1	0.88	0.07	46,46,46,46	0
84	MG	1	3518	1/1	0.88	0.20	69,69,69,69	0
84	MG	B	1883	1/1	0.88	0.08	47,47,47,47	0
84	MG	1	3829	1/1	0.88	0.11	42,42,42,42	0
84	MG	1	3459	1/1	0.88	0.21	43,43,43,43	0
84	MG	AU	205	1/1	0.88	0.10	54,54,54,54	0
84	MG	AS	3574	1/1	0.88	0.09	87,87,87,87	0
84	MG	1	3727	1/1	0.88	0.30	61,61,61,61	0
84	MG	AS	3502	1/1	0.88	0.15	74,74,74,74	0
84	MG	CM	1853	1/1	0.88	0.13	80,80,80,80	0
84	MG	1	3728	1/1	0.88	0.13	59,59,59,59	0
84	MG	1	3521	1/1	0.88	0.20	57,57,57,57	0
84	MG	AS	3701	1/1	0.88	0.20	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3498	1/1	0.88	0.11	58,58,58,58	0
84	MG	CM	1867	1/1	0.88	0.17	60,60,60,60	0
84	MG	AS	3506	1/1	0.88	0.11	74,74,74,74	0
84	MG	AS	3624	1/1	0.88	0.10	85,85,85,85	0
84	MG	CM	1870	1/1	0.88	0.17	94,94,94,94	0
84	MG	1	3836	1/1	0.88	0.23	77,77,77,77	0
84	MG	B	1822	1/1	0.88	0.16	105,105,105,105	0
84	MG	6	201	1/1	0.88	0.17	53,53,53,53	0
84	MG	AS	3419	1/1	0.88	0.18	82,82,82,82	0
84	MG	AS	3629	1/1	0.88	0.27	43,43,43,43	0
84	MG	AS	3548	1/1	0.88	0.11	91,91,91,91	0
84	MG	1	3588	1/1	0.88	0.12	71,71,71,71	0
84	MG	AS	3514	1/1	0.88	0.22	53,53,53,53	0
84	MG	AS	3760	1/1	0.88	0.14	67,67,67,67	0
84	MG	CM	1801	1/1	0.88	0.23	41,41,41,41	0
84	MG	AS	3763	1/1	0.88	0.19	65,65,65,65	0
84	MG	1	3526	1/1	0.88	0.09	103,103,103,103	0
84	MG	1	3569	1/1	0.88	0.14	54,54,54,54	0
84	MG	1	3432	1/1	0.88	0.19	78,78,78,78	0
84	MG	1	3775	1/1	0.88	0.08	55,55,55,55	0
84	MG	1	3712	1/1	0.88	0.12	50,50,50,50	0
85	ZN	DS	201	1/1	0.88	0.06	353,353,353,353	0
84	MG	B	1889	1/1	0.89	0.11	44,44,44,44	0
84	MG	1	3848	1/1	0.89	0.08	69,69,69,69	0
84	MG	CM	1809	1/1	0.89	0.19	60,60,60,60	0
84	MG	CM	1810	1/1	0.89	0.27	52,52,52,52	0
84	MG	CM	1815	1/1	0.89	0.18	43,43,43,43	0
84	MG	1	3701	1/1	0.89	0.06	87,87,87,87	0
84	MG	m	301	1/1	0.89	0.13	61,61,61,61	0
84	MG	B	1847	1/1	0.89	0.13	60,60,60,60	0
84	MG	1	3658	1/1	0.89	0.12	62,62,62,62	0
84	MG	AS	3432	1/1	0.89	0.20	92,92,92,92	0
84	MG	B	1852	1/1	0.89	0.15	57,57,57,57	0
84	MG	AS	3766	1/1	0.89	0.17	63,63,63,63	0
83	3K5	1	3401	57/57	0.89	0.19	72,107,146,164	0
84	MG	1	3520	1/1	0.89	0.15	95,95,95,95	0
84	MG	1	3447	1/1	0.89	0.07	81,81,81,81	0
84	MG	AS	3775	1/1	0.89	0.07	43,43,43,43	0
84	MG	1	3484	1/1	0.89	0.08	27,27,27,27	0
84	MG	AS	3778	1/1	0.89	0.13	60,60,60,60	0
84	MG	D	301	1/1	0.89	0.12	24,24,24,24	0
84	MG	1	3524	1/1	0.89	0.15	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3601	1/1	0.89	0.19	57,57,57,57	0
84	MG	1	3619	1/1	0.89	0.06	5,5,5,5	0
84	MG	AS	3565	1/1	0.89	0.20	68,68,68,68	0
84	MG	AS	3444	1/1	0.89	0.16	52,52,52,52	0
84	MG	Q	201	1/1	0.89	0.20	110,110,110,110	0
84	MG	1	3643	1/1	0.89	0.23	51,51,51,51	0
84	MG	CM	1848	1/1	0.89	0.11	104,104,104,104	0
84	MG	CM	1849	1/1	0.89	0.13	67,67,67,67	0
84	MG	y	203	1/1	0.89	0.20	82,82,82,82	0
84	MG	AS	3675	1/1	0.89	0.14	60,60,60,60	0
84	MG	1	3554	1/1	0.89	0.04	65,65,65,65	0
84	MG	0	202	1/1	0.89	0.20	54,54,54,54	0
84	MG	1	3716	1/1	0.89	0.14	46,46,46,46	0
84	MG	AS	3733	1/1	0.89	0.14	102,102,102,102	0
84	MG	CM	1866	1/1	0.89	0.17	83,83,83,83	0
84	MG	B	1869	1/1	0.89	0.13	65,65,65,65	0
84	MG	1	3589	1/1	0.89	0.10	75,75,75,75	0
84	MG	B	1871	1/1	0.89	0.09	40,40,40,40	0
84	MG	1	3410	1/1	0.89	0.21	77,77,77,77	0
84	MG	1	3435	1/1	0.89	0.14	44,44,44,44	0
84	MG	AS	3407	1/1	0.89	0.09	83,83,83,83	0
84	MG	AS	3473	1/1	0.89	0.21	60,60,60,60	0
84	MG	1	3629	1/1	0.89	0.12	49,49,49,49	0
84	MG	AS	3409	1/1	0.89	0.17	86,86,86,86	0
84	MG	AJ	101	1/1	0.89	0.22	100,100,100,100	0
84	MG	1	3510	1/1	0.89	0.15	56,56,56,56	0
84	MG	1	3632	1/1	0.89	0.11	51,51,51,51	0
84	MG	AS	3747	1/1	0.89	0.16	47,47,47,47	0
84	MG	AS	3537	1/1	0.89	0.19	72,72,72,72	0
84	MG	1	3635	1/1	0.89	0.23	45,45,45,45	0
84	MG	4	201	1/1	0.89	0.07	43,43,43,43	0
84	MG	AS	3595	1/1	0.89	0.12	72,72,72,72	0
84	MG	B	1842	1/1	0.89	0.16	67,67,67,67	0
85	ZN	AP	201	1/1	0.89	0.06	294,294,294,294	0
84	MG	CL	302	1/1	0.89	0.14	88,88,88,88	0
85	ZN	h	201	1/1	0.89	0.09	285,285,285,285	0
84	MG	B	1887	1/1	0.89	0.09	81,81,81,81	0
85	ZN	CJ	201	1/1	0.89	0.06	300,300,300,300	0
84	MG	1	3798	1/1	0.89	0.05	44,44,44,44	0
84	MG	1	3462	1/1	0.90	0.15	49,49,49,49	0
84	MG	AS	3456	1/1	0.90	0.10	31,31,31,31	0
84	MG	1	3611	1/1	0.90	0.15	81,81,81,81	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3421	1/1	0.90	0.13	48,48,48,48	0
84	MG	AU	203	1/1	0.90	0.08	61,61,61,61	0
84	MG	1	3615	1/1	0.90	0.13	40,40,40,40	0
84	MG	AS	3461	1/1	0.90	0.18	74,74,74,74	0
84	MG	1	3718	1/1	0.90	0.11	42,42,42,42	0
84	MG	1	3487	1/1	0.90	0.14	43,43,43,43	0
84	MG	AS	3467	1/1	0.90	0.14	79,79,79,79	0
84	MG	B	1877	1/1	0.90	0.13	47,47,47,47	0
84	MG	AS	3590	1/1	0.90	0.06	58,58,58,58	0
84	MG	AS	3669	1/1	0.90	0.11	71,71,71,71	0
84	MG	AS	3471	1/1	0.90	0.21	41,41,41,41	0
84	MG	AS	3632	1/1	0.90	0.11	85,85,85,85	0
84	MG	1	3600	1/1	0.90	0.18	55,55,55,55	0
84	MG	B	1813	1/1	0.90	0.16	74,74,74,74	0
84	MG	1	3488	1/1	0.90	0.08	51,51,51,51	0
84	MG	1	3811	1/1	0.90	0.07	90,90,90,90	0
84	MG	AS	3557	1/1	0.90	0.08	60,60,60,60	0
84	MG	CM	1865	1/1	0.90	0.06	119,119,119,119	0
84	MG	1	3812	1/1	0.90	0.16	45,45,45,45	0
84	MG	1	3513	1/1	0.90	0.22	64,64,64,64	0
84	MG	AS	3480	1/1	0.90	0.13	77,77,77,77	0
84	MG	1	3766	1/1	0.90	0.13	47,47,47,47	0
83	3K5	AS	3401	57/57	0.90	0.15	82,121,151,184	0
84	MG	AS	3644	1/1	0.90	0.17	86,86,86,86	0
84	MG	AS	3771	1/1	0.90	0.32	69,69,69,69	0
84	MG	CM	1803	1/1	0.90	0.06	192,192,192,192	0
84	MG	1	3549	1/1	0.90	0.19	66,66,66,66	0
84	MG	1	3729	1/1	0.90	0.04	56,56,56,56	0
84	MG	CM	1808	1/1	0.90	0.06	61,61,61,61	0
84	MG	AS	3487	1/1	0.90	0.15	62,62,62,62	0
84	MG	AS	3779	1/1	0.90	0.08	66,66,66,66	0
84	MG	AS	3732	1/1	0.90	0.10	85,85,85,85	0
84	MG	AS	3782	1/1	0.90	0.17	72,72,72,72	0
84	MG	CM	1820	1/1	0.90	0.15	68,68,68,68	0
84	MG	1	3424	1/1	0.90	0.07	74,74,74,74	0
84	MG	1	3706	1/1	0.90	0.10	60,60,60,60	0
84	MG	DK	202	1/1	0.90	0.10	51,51,51,51	0
84	MG	3	207	1/1	0.90	0.12	48,48,48,48	0
84	MG	1	3453	1/1	0.90	0.25	67,67,67,67	0
84	MG	1	3471	1/1	0.90	0.09	40,40,40,40	0
84	MG	CM	1828	1/1	0.90	0.15	69,69,69,69	0
84	MG	1	3428	1/1	0.90	0.27	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3633	1/1	0.90	0.24	27,27,27,27	0
84	MG	B	1864	1/1	0.90	0.19	67,67,67,67	0
86	GET	B	1851	34/34	0.90	0.09	105,127,149,167	0
84	MG	AS	3492	1/1	0.91	0.16	97,97,97,97	0
84	MG	1	3708	1/1	0.91	0.13	103,103,103,103	0
84	MG	1	3590	1/1	0.91	0.24	57,57,57,57	0
84	MG	r	301	1/1	0.91	0.09	48,48,48,48	0
84	MG	AS	3619	1/1	0.91	0.10	60,60,60,60	0
84	MG	AS	3455	1/1	0.91	0.11	64,64,64,64	0
84	MG	1	3491	1/1	0.91	0.29	52,52,52,52	0
84	MG	AS	3578	1/1	0.91	0.12	52,52,52,52	0
84	MG	1	3561	1/1	0.91	0.11	63,63,63,63	0
84	MG	1	3772	1/1	0.91	0.09	61,61,61,61	0
84	MG	1	3450	1/1	0.91	0.20	54,54,54,54	0
84	MG	1	3502	1/1	0.91	0.20	53,53,53,53	0
84	MG	B	1875	1/1	0.91	0.05	48,48,48,48	0
84	MG	AS	3465	1/1	0.91	0.12	52,52,52,52	0
84	MG	AS	3546	1/1	0.91	0.15	38,38,38,38	0
84	MG	1	3656	1/1	0.91	0.18	52,52,52,52	0
84	MG	CM	1858	1/1	0.91	0.09	111,111,111,111	0
84	MG	AS	3510	1/1	0.91	0.13	70,70,70,70	0
84	MG	1	3620	1/1	0.91	0.10	49,49,49,49	0
84	MG	1	3448	1/1	0.91	0.15	54,54,54,54	0
84	MG	AS	3513	1/1	0.91	0.08	47,47,47,47	0
84	MG	AS	3594	1/1	0.91	0.11	104,104,104,104	0
84	MG	1	3566	1/1	0.91	0.08	32,32,32,32	0
84	MG	1	3557	1/1	0.91	0.09	70,70,70,70	0
84	MG	AS	3774	1/1	0.91	0.11	37,37,37,37	0
84	MG	1	3626	1/1	0.91	0.12	65,65,65,65	0
84	MG	1	3786	1/1	0.91	0.06	45,45,45,45	0
84	MG	B	1824	1/1	0.91	0.14	49,49,49,49	0
84	MG	AS	3727	1/1	0.91	0.06	50,50,50,50	0
84	MG	1	3851	1/1	0.91	0.21	76,76,76,76	0
84	MG	1	3666	1/1	0.91	0.09	50,50,50,50	0
84	MG	1	3627	1/1	0.91	0.34	46,46,46,46	0
84	MG	CM	1817	1/1	0.91	0.07	190,190,190,190	0
84	MG	AS	3605	1/1	0.91	0.16	91,91,91,91	0
84	MG	1	3522	1/1	0.91	0.07	38,38,38,38	0
84	MG	AS	3689	1/1	0.91	0.04	59,59,59,59	0
84	MG	B	1890	1/1	0.91	0.12	54,54,54,54	0
84	MG	AS	3442	1/1	0.91	0.21	22,22,22,22	0
84	MG	1	3452	1/1	0.91	0.15	63,63,63,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	CM	1827	1/1	0.91	0.10	35,35,35,35	0
84	MG	1	3612	1/1	0.91	0.12	74,74,74,74	0
84	MG	AS	3694	1/1	0.91	0.18	45,45,45,45	0
84	MG	B	1833	1/1	0.91	0.09	72,72,72,72	0
84	MG	B	1894	1/1	0.91	0.07	98,98,98,98	0
84	MG	AS	3450	1/1	0.91	0.16	47,47,47,47	0
84	MG	AT	205	1/1	0.91	0.16	75,75,75,75	0
84	MG	CM	1835	1/1	0.91	0.08	68,68,68,68	0
84	MG	1	3596	1/1	0.92	0.05	51,51,51,51	0
84	MG	1	3774	1/1	0.92	0.07	43,43,43,43	0
84	MG	1	3486	1/1	0.92	0.19	62,62,62,62	0
84	MG	1	3688	1/1	0.92	0.09	106,106,106,106	0
84	MG	1	3422	1/1	0.92	0.14	45,45,45,45	0
84	MG	1	3690	1/1	0.92	0.11	61,61,61,61	0
84	MG	B	1816	1/1	0.92	0.07	34,34,34,34	0
84	MG	BI	301	1/1	0.92	0.05	48,48,48,48	0
84	MG	AS	3672	1/1	0.92	0.11	63,63,63,63	0
84	MG	1	3512	1/1	0.92	0.15	53,53,53,53	0
84	MG	1	3781	1/1	0.92	0.14	54,54,54,54	0
84	MG	AS	3416	1/1	0.92	0.15	41,41,41,41	0
84	MG	1	3757	1/1	0.92	0.07	44,44,44,44	0
84	MG	1	3503	1/1	0.92	0.16	70,70,70,70	0
84	MG	y	202	1/1	0.92	0.08	54,54,54,54	0
84	MG	1	3713	1/1	0.92	0.10	62,62,62,62	0
84	MG	CM	1860	1/1	0.92	0.18	69,69,69,69	0
84	MG	1	3866	1/1	0.92	0.14	86,86,86,86	0
84	MG	AS	3772	1/1	0.92	0.06	59,59,59,59	0
84	MG	CM	1863	1/1	0.92	0.14	70,70,70,70	0
84	MG	AS	3639	1/1	0.92	0.05	60,60,60,60	0
84	MG	B	1825	1/1	0.92	0.08	68,68,68,68	0
84	MG	AS	3425	1/1	0.92	0.09	68,68,68,68	0
84	MG	AS	3777	1/1	0.92	0.15	98,98,98,98	0
84	MG	1	3443	1/1	0.92	0.20	35,35,35,35	0
84	MG	1	3433	1/1	0.92	0.17	34,34,34,34	0
84	MG	1	3655	1/1	0.92	0.07	58,58,58,58	0
84	MG	CM	1872	1/1	0.92	0.07	85,85,85,85	0
84	MG	B	1866	1/1	0.92	0.12	47,47,47,47	0
84	MG	CM	1812	1/1	0.92	0.08	152,152,152,152	0
84	MG	1	3460	1/1	0.92	0.16	45,45,45,45	0
84	MG	B	1830	1/1	0.92	0.07	79,79,79,79	0
84	MG	1	3577	1/1	0.92	0.07	48,48,48,48	0
84	MG	CM	1818	1/1	0.92	0.21	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3721	1/1	0.92	0.09	86,86,86,86	0
84	MG	1	3844	1/1	0.92	0.18	74,74,74,74	0
84	MG	1	3507	1/1	0.92	0.11	50,50,50,50	0
84	MG	B	1873	1/1	0.92	0.21	61,61,61,61	0
84	MG	1	3551	1/1	0.92	0.12	52,52,52,52	0
84	MG	1	3540	1/1	0.92	0.11	72,72,72,72	0
84	MG	1	3477	1/1	0.92	0.17	41,41,41,41	0
84	MG	P0	401	1/1	0.92	0.08	200,200,200,200	0
84	MG	AS	3617	1/1	0.92	0.17	62,62,62,62	0
84	MG	AS	3533	1/1	0.92	0.14	64,64,64,64	0
84	MG	1	3404	1/1	0.92	0.12	22,22,22,22	0
84	MG	k	403	1/1	0.92	0.08	58,58,58,58	0
84	MG	AS	3495	1/1	0.92	0.24	41,41,41,41	0
84	MG	AW	301	1/1	0.92	0.10	82,82,82,82	0
84	MG	AS	3445	1/1	0.92	0.12	75,75,75,75	0
84	MG	1	3645	1/1	0.92	0.16	68,68,68,68	0
84	MG	AS	3541	1/1	0.93	0.10	55,55,55,55	0
84	MG	1	3720	1/1	0.93	0.16	58,58,58,58	0
84	MG	AS	3482	1/1	0.93	0.08	69,69,69,69	0
84	MG	1	3556	1/1	0.93	0.17	43,43,43,43	0
84	MG	w	301	1/1	0.93	0.10	49,49,49,49	0
84	MG	AS	3750	1/1	0.93	0.20	62,62,62,62	0
84	MG	1	3430	1/1	0.93	0.12	43,43,43,43	0
84	MG	1	3416	1/1	0.93	0.15	89,89,89,89	0
84	MG	CM	1864	1/1	0.93	0.06	34,34,34,34	0
84	MG	3	205	1/1	0.93	0.18	32,32,32,32	0
84	MG	1	3724	1/1	0.93	0.07	74,74,74,74	0
84	MG	CM	1819	1/1	0.93	0.09	54,54,54,54	0
84	MG	AS	3490	1/1	0.93	0.05	62,62,62,62	0
84	MG	T	201	1/1	0.93	0.11	121,121,121,121	0
84	MG	AS	3522	1/1	0.93	0.09	82,82,82,82	0
84	MG	1	3446	1/1	0.93	0.12	77,77,77,77	0
84	MG	1	3663	1/1	0.93	0.07	69,69,69,69	0
84	MG	B	1817	1/1	0.93	0.25	56,56,56,56	0
84	MG	AS	3761	1/1	0.93	0.14	89,89,89,89	0
84	MG	1	3857	1/1	0.93	0.13	92,92,92,92	0
84	MG	1	3631	1/1	0.93	0.09	48,48,48,48	0
84	MG	AS	3559	1/1	0.93	0.19	71,71,71,71	0
84	MG	AS	3728	1/1	0.93	0.06	55,55,55,55	0
84	MG	AS	3405	1/1	0.93	0.22	57,57,57,57	0
84	MG	AS	3561	1/1	0.93	0.07	78,78,78,78	0
84	MG	AS	3769	1/1	0.93	0.07	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	AS	3501	1/1	0.93	0.07	52,52,52,52	0
84	MG	1	3436	1/1	0.93	0.14	54,54,54,54	0
84	MG	AS	3664	1/1	0.93	0.13	61,61,61,61	0
84	MG	1	3773	1/1	0.93	0.12	62,62,62,62	0
84	MG	AS	3736	1/1	0.93	0.21	47,47,47,47	0
84	MG	1	3822	1/1	0.93	0.09	51,51,51,51	0
84	MG	1	3467	1/1	0.93	0.05	36,36,36,36	0
84	MG	1	3843	1/1	0.93	0.13	71,71,71,71	0
84	MG	B	1848	1/1	0.93	0.10	46,46,46,46	0
84	MG	1	3525	1/1	0.93	0.14	75,75,75,75	0
84	MG	1	3475	1/1	0.93	0.21	16,16,16,16	0
84	MG	1	3657	1/1	0.93	0.09	69,69,69,69	0
84	MG	1	3719	1/1	0.93	0.10	74,74,74,74	0
84	MG	1	3469	1/1	0.94	0.09	31,31,31,31	0
84	MG	AS	3499	1/1	0.94	0.04	70,70,70,70	0
84	MG	1	3634	1/1	0.94	0.22	41,41,41,41	0
84	MG	1	3483	1/1	0.94	0.08	112,112,112,112	0
84	MG	AS	3457	1/1	0.94	0.16	44,44,44,44	0
84	MG	AS	3582	1/1	0.94	0.07	44,44,44,44	0
84	MG	1	3622	1/1	0.94	0.05	72,72,72,72	0
84	MG	1	3608	1/1	0.94	0.11	53,53,53,53	0
84	MG	B	1836	1/1	0.94	0.12	51,51,51,51	0
84	MG	1	3429	1/1	0.94	0.14	59,59,59,59	0
84	MG	1	3840	1/1	0.94	0.09	67,67,67,67	0
84	MG	CM	1852	1/1	0.94	0.14	37,37,37,37	0
84	MG	1	3445	1/1	0.94	0.11	32,32,32,32	0
84	MG	CM	1855	1/1	0.94	0.07	45,45,45,45	0
84	MG	AS	3589	1/1	0.94	0.19	65,65,65,65	0
84	MG	AS	3424	1/1	0.94	0.09	57,57,57,57	0
84	MG	AS	3723	1/1	0.94	0.10	60,60,60,60	0
84	MG	AS	3549	1/1	0.94	0.09	60,60,60,60	0
84	MG	1	3442	1/1	0.94	0.14	45,45,45,45	0
84	MG	1	3409	1/1	0.94	0.06	52,52,52,52	0
84	MG	AS	3773	1/1	0.94	0.12	96,96,96,96	0
84	MG	B	1874	1/1	0.94	0.12	44,44,44,44	0
84	MG	1	3613	1/1	0.94	0.14	51,51,51,51	0
84	MG	AS	3430	1/1	0.94	0.17	51,51,51,51	0
84	MG	B	1876	1/1	0.94	0.12	56,56,56,56	0
84	MG	1	3710	1/1	0.94	0.13	42,42,42,42	1
84	MG	1	3531	1/1	0.94	0.12	84,84,84,84	0
84	MG	R	203	1/1	0.94	0.14	59,59,59,59	0
84	MG	AS	3781	1/1	0.94	0.03	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3676	1/1	0.94	0.14	65,65,65,65	0
84	MG	AS	3604	1/1	0.94	0.13	62,62,62,62	0
84	MG	1	3826	1/1	0.94	0.07	38,38,38,38	0
84	MG	0	204	1/1	0.94	0.10	77,77,77,77	0
84	MG	AS	3483	1/1	0.94	0.08	103,103,103,103	0
84	MG	B	1849	1/1	0.94	0.09	91,91,91,91	0
84	MG	2	201	1/1	0.94	0.11	44,44,44,44	0
84	MG	1	3564	1/1	0.94	0.14	46,46,46,46	0
84	MG	1	3808	1/1	0.94	0.09	144,144,144,144	0
84	MG	AS	3404	1/1	0.94	0.04	41,41,41,41	0
84	MG	1	3574	1/1	0.94	0.05	41,41,41,41	0
84	MG	1	3679	1/1	0.94	0.14	56,56,56,56	0
84	MG	1	3854	1/1	0.94	0.07	81,81,81,81	0
84	MG	AS	3702	1/1	0.94	0.07	66,66,66,66	0
84	MG	AU	201	1/1	0.94	0.07	64,64,64,64	0
84	MG	1	3831	1/1	0.94	0.10	51,51,51,51	0
84	MG	AU	204	1/1	0.94	0.11	82,82,82,82	0
84	MG	CM	1833	1/1	0.94	0.10	40,40,40,40	0
84	MG	AS	3494	1/1	0.94	0.06	105,105,105,105	0
84	MG	AP	202	1/1	0.94	0.16	49,49,49,49	0
84	MG	1	3456	1/1	0.94	0.19	47,47,47,47	0
84	MG	CM	1837	1/1	0.94	0.16	62,62,62,62	0
84	MG	1	3664	1/1	0.94	0.24	40,40,40,40	0
86	GET	CM	1822	34/34	0.94	0.12	107,119,148,157	0
84	MG	B	1865	1/1	0.95	0.19	65,65,65,65	0
84	MG	CM	1814	1/1	0.95	0.08	127,127,127,127	0
84	MG	AS	3449	1/1	0.95	0.05	39,39,39,39	0
84	MG	1	3777	1/1	0.95	0.18	29,29,29,29	0
84	MG	F	301	1/1	0.95	0.13	77,77,77,77	0
84	MG	BE	301	1/1	0.95	0.10	59,59,59,59	0
84	MG	AS	3598	1/1	0.95	0.11	42,42,42,42	0
84	MG	AS	3452	1/1	0.95	0.07	24,24,24,24	0
84	MG	0	203	1/1	0.95	0.04	33,33,33,33	0
84	MG	1	3465	1/1	0.95	0.13	44,44,44,44	0
84	MG	AS	3476	1/1	0.95	0.16	49,49,49,49	0
84	MG	BQ	201	1/1	0.95	0.18	54,54,54,54	0
84	MG	L	201	1/1	0.95	0.25	55,55,55,55	0
84	MG	AS	3438	1/1	0.95	0.07	46,46,46,46	0
84	MG	AS	3479	1/1	0.95	0.17	42,42,42,42	0
84	MG	1	3438	1/1	0.95	0.14	75,75,75,75	0
84	MG	1	3616	1/1	0.95	0.09	65,65,65,65	0
84	MG	1	3501	1/1	0.95	0.14	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	B	1805	1/1	0.95	0.11	38,38,38,38	0
84	MG	AS	3566	1/1	0.95	0.05	55,55,55,55	0
84	MG	B	1837	1/1	0.95	0.08	57,57,57,57	0
84	MG	1	3861	1/1	0.95	0.08	54,54,54,54	0
84	MG	AS	3463	1/1	0.95	0.08	41,41,41,41	0
84	MG	1	3473	1/1	0.95	0.10	59,59,59,59	0
84	MG	1	3413	1/1	0.95	0.15	44,44,44,44	0
84	MG	AS	3593	1/1	0.95	0.10	68,68,68,68	0
84	MG	AS	3661	1/1	0.96	0.10	66,66,66,66	0
84	MG	B	1853	1/1	0.96	0.14	47,47,47,47	0
84	MG	AS	3414	1/1	0.96	0.13	54,54,54,54	0
84	MG	B	1808	1/1	0.96	0.03	57,57,57,57	0
84	MG	AS	3464	1/1	0.96	0.07	43,43,43,43	0
84	MG	1	3784	1/1	0.96	0.12	67,67,67,67	0
84	MG	AS	3706	1/1	0.96	0.07	51,51,51,51	0
84	MG	AS	3418	1/1	0.96	0.22	39,39,39,39	0
84	MG	AS	3687	1/1	0.96	0.07	85,85,85,85	0
84	MG	CM	1851	1/1	0.96	0.05	49,49,49,49	0
84	MG	AU	202	1/1	0.96	0.05	60,60,60,60	0
84	MG	AS	3730	1/1	0.96	0.12	46,46,46,46	0
84	MG	1	3739	1/1	0.96	0.10	98,98,98,98	0
84	MG	AS	3468	1/1	0.96	0.14	42,42,42,42	0
84	MG	B	1881	1/1	0.96	0.07	52,52,52,52	0
84	MG	AS	3470	1/1	0.96	0.08	48,48,48,48	0
84	MG	3	203	1/1	0.96	0.20	54,54,54,54	0
84	MG	CM	1804	1/1	0.96	0.05	48,48,48,48	0
84	MG	B	1801	1/1	0.96	0.26	46,46,46,46	0
84	MG	3	204	1/1	0.96	0.16	30,30,30,30	0
84	MG	1	3852	1/1	0.96	0.09	71,71,71,71	0
84	MG	1	3464	1/1	0.96	0.08	8,8,8,8	0
84	MG	1	3653	1/1	0.96	0.15	30,30,30,30	0
85	ZN	DN	201	1/1	0.96	0.05	125,125,125,125	0
84	MG	CM	1811	1/1	0.96	0.09	59,59,59,59	0
84	MG	1	3419	1/1	0.96	0.03	49,49,49,49	0
84	MG	1	3407	1/1	0.96	0.12	50,50,50,50	0
84	MG	AS	3427	1/1	0.97	0.11	39,39,39,39	0
84	MG	1	3696	1/1	0.97	0.09	39,39,39,39	0
84	MG	1	3660	1/1	0.97	0.14	35,35,35,35	0
84	MG	CM	1806	1/1	0.97	0.06	38,38,38,38	0
84	MG	CM	1859	1/1	0.97	0.15	46,46,46,46	0
85	ZN	AK	101	1/1	0.97	0.06	115,115,115,115	0
84	MG	AS	3415	1/1	0.97	0.16	81,81,81,81	0

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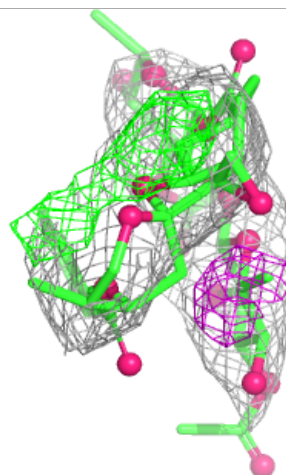
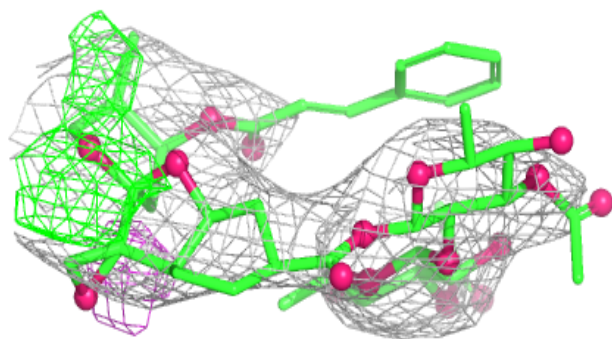
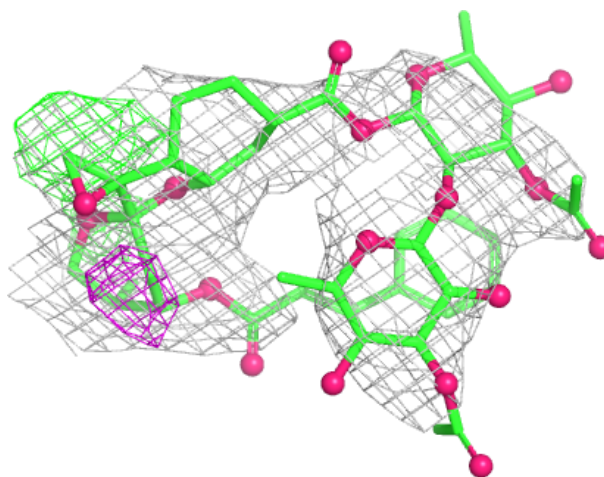
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	MG	1	3621	1/1	0.97	0.07	56,56,56,56	0
85	ZN	f	101	1/1	0.97	0.09	125,125,125,125	0
84	MG	AS	3448	1/1	0.97	0.09	73,73,73,73	0
84	MG	AS	3531	1/1	0.97	0.13	86,86,86,86	1
85	ZN	CE	101	1/1	0.97	0.05	128,128,128,128	0
84	MG	1	3652	1/1	0.97	0.09	44,44,44,44	0
84	MG	1	3437	1/1	0.97	0.08	49,49,49,49	0
85	ZN	DQ	101	1/1	0.97	0.08	121,121,121,121	0
84	MG	CM	1813	1/1	0.97	0.07	168,168,168,168	0
84	MG	CM	1839	1/1	0.97	0.05	50,50,50,50	0
84	MG	1	3736	1/1	0.97	0.09	40,40,40,40	0
84	MG	AS	3762	1/1	0.98	0.07	41,41,41,41	0
85	ZN	AN	101	1/1	0.98	0.05	110,110,110,110	0
84	MG	AS	3493	1/1	0.98	0.14	36,36,36,36	0
85	ZN	c	201	1/1	0.98	0.04	132,132,132,132	0
84	MG	CM	1854	1/1	0.98	0.15	41,41,41,41	0
85	ZN	CK	101	1/1	0.99	0.03	151,151,151,151	0
85	ZN	CH	101	1/1	0.99	0.09	117,117,117,117	0
85	ZN	AQ	101	1/1	0.99	0.08	128,128,128,128	0

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

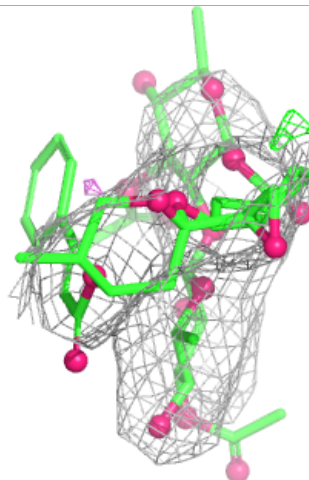
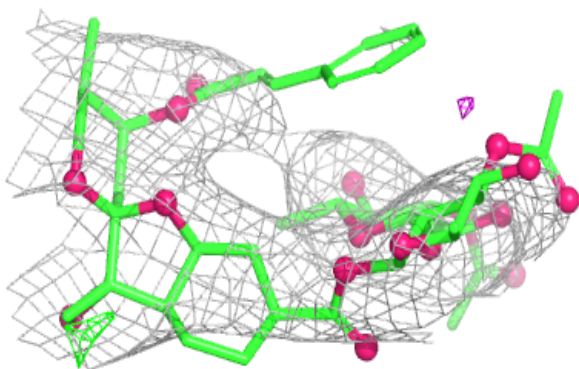
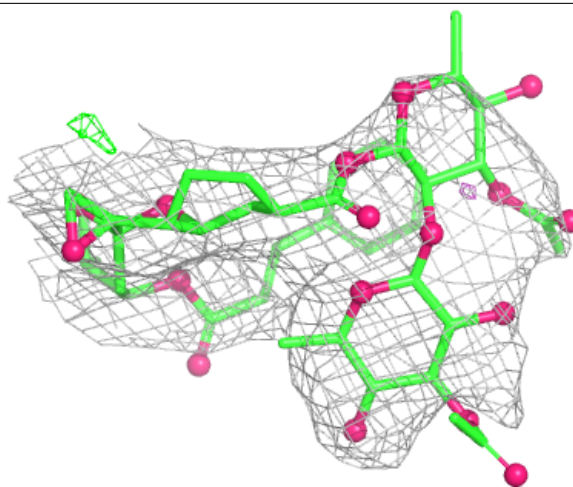
Electron density around 3K5 1 3401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



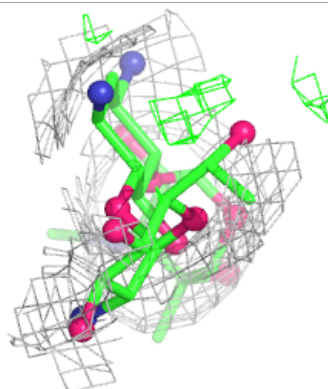
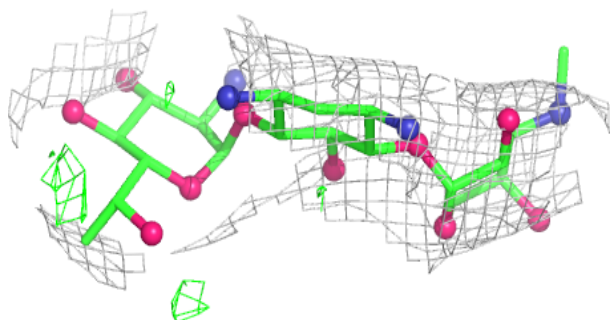
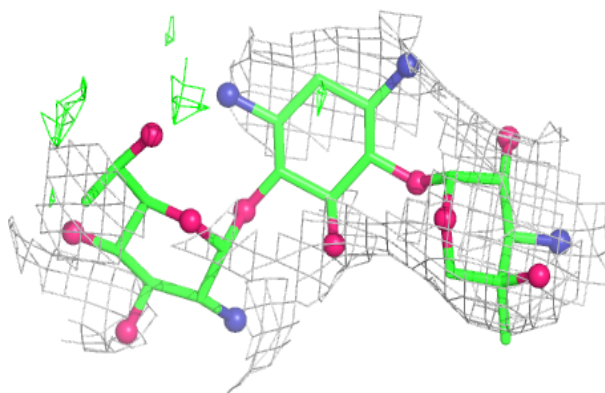
Electron density around 3K5 AS 3401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

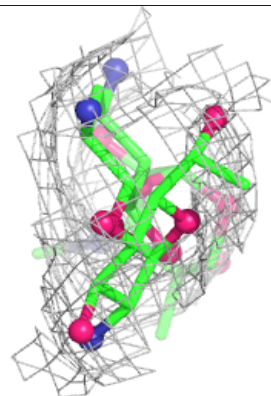
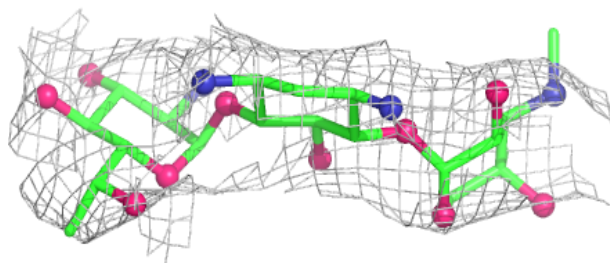
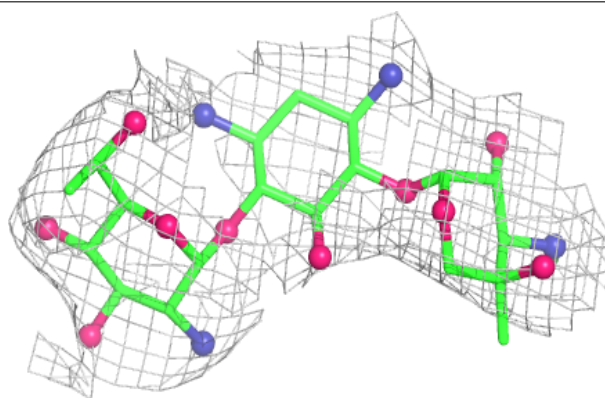


Electron density around GET B 1851:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around GET CM 1822:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.