



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 5, 2024 – 12:38 am BST

PDB ID : 8CQ7  
Title : Crystal structure of phyllanthoside bound to the *Candida albicans* 80S ribosome  
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.  
Deposited on : 2023-03-03  
Resolution : 3.20 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](mailto: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>.

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

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

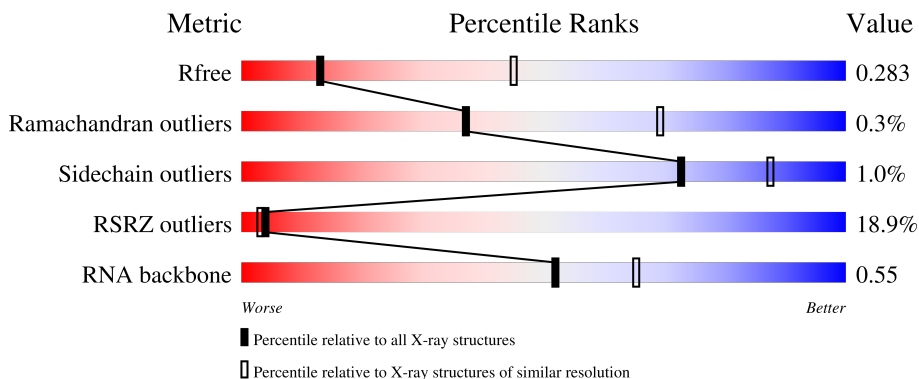
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1370 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)
RNA backbone	3690	1111 (3.50-2.90)

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  $\geq 3$ , 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	 7% 76% 18% ..
1	AS	3359	 11% 76% 18% ..
2	3	121	 % 93% 7%
2	AT	121	 5% 93% 7%
3	4	158	 2% 84% 16% .

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Mol	Chain	Length	Quality of chain
3	AU	158	9% 84% 16%
4	AW	254	20% 97%
4	j	254	9% 98%
5	AX	389	6% 99%
5	k	389	5% 99%
6	AY	363	35% 99%
6	l	363	14% 99%
7	AZ	298	37% 97%
7	m	298	26% 99%
8	BA	176	11% 87% 13%
8	n	176	13% 89% 11%
9	BB	241	10% 97%
9	o	241	5% 95%
10	BC	262	32% 87% 11%
10	p	262	18% 90% 9%
11	BD	191	20% 99%
11	q	191	6% 99%
12	BE	220	10% 94% 5%
12	r	220	14% 94% 5%
13	BF	174	22% 97%
13	s	174	20% 97%
14	BG	202	29% 98%
14	t	202	14% 99%
15	BH	131	11% 98%
15	u	131	4% 99%

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Mol	Chain	Length	Quality of chain
16	BI	204	34% 99%
16	v	204	7% 99%
17	BJ	200	12% 100%
17	w	200	4% 100%
18	BK	185	16% 94% 5%
18	x	185	10% 94% 6%
19	BL	186	19% 99% .
19	y	186	16% 99% .
20	BM	190	14% 92% 6%
20	z	190	16% 94% 6%
21	0	172	5% 98% ..
21	BN	172	6% 99% .
22	2	160	11% 99% .
22	BO	160	16% 99% ..
23	5	124	22% 82% 17%
23	BP	124	25% 77% 5% 18%
24	6	137	9% 96% .
24	BQ	137	12% 96% .
25	7	155	10% 74% 24%
25	BR	155	12% 62% 37%
26	8	142	10% 83% 15%
26	BS	142	18% 84% 16%
27	9	127	18% 98% ..
27	BT	127	28% 98% ..
28	AA	136	21% 99% .

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Mol	Chain	Length	Quality of chain
28	BU	136	42% 99%
29	AB	149	7% 99%
29	BV	149	30% 99%
30	AC	63	27% 90% 6%
30	BW	63	43% 97%
31	AD	106	5% 91% 9%
31	BX	106	15% 91% 9%
32	AE	112	7% 96%
32	BY	112	16% 96%
33	AF	131	14% 95% 5%
33	BZ	131	27% 95% 5%
34	AG	107	6% 98%
34	CA	107	7% 99%
35	AH	122	23% 90% 8%
35	CB	122	37% 92% 8%
36	AI	120	15% 99%
36	CC	120	42% 97%
37	AJ	99	3% 96%
37	CD	99	31% 98%
38	AK	90	13% 96%
38	CE	90	29% 96%
39	AL	78	22% 99%
39	CF	78	47% 99%
40	AM	51	10% 96%
40	CG	51	25% 96%

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Mol	Chain	Length	Quality of chain
41	AN	52	48% 100%
41	CH	52	77% 90% 8%
42	AO	25	20% 92% 8%
42	CI	25	12% 92%
43	AP	106	16% 97%
43	CJ	106	18% 96%
44	AQ	92	12% 99%
44	CK	92	14% 99%
45	CL	267	27% 44% 55%
45	i	267	19% 43% 55%
46	B	1787	14% 71% 26%
46	CM	1787	9% 71% 27%
47	C	261	23% 79% 20%
47	CN	261	18% 79% 20%
48	CO	256	21% 83% 16%
48	D	256	11% 83% 16%
49	CP	249	11% 86% 13%
49	E	249	27% 87% 13%
50	CQ	251	14% 87% 11%
50	F	251	28% 88% 11%
51	CR	262	24% 99%
51	G	262	34% 98%
52	CS	225	29% 90% 8%
52	H	225	22% 91% 8%
53	CT	236	26% 99%

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Mol	Chain	Length	Quality of chain
53	I	236	20% 94%
54	CU	186	27% 97%
54	J	186	37% 99%
55	CV	206	36% 99%
55	K	206	28% 98%
56	CW	189	38% 94% 6%
56	L	189	52% 94% 6%
57	CX	118	13% 80% 20%
57	M	118	30% 80% 20%
58	CY	155	13% 90% 9%
58	N	155	16% 92% 7%
59	DA	151	15% 99%
59	P	151	18% 99%
60	DB	132	20% 95%
60	Q	132	13% 94%
61	DC	142	26% 90% 8%
61	R	142	21% 88% 9%
62	DD	142	25% 98%
62	S	142	37% 96%
63	DE	137	34% 91% 9%
63	T	137	33% 88% 9%
64	DF	145	26% 95%
64	U	145	17% 98%
65	DG	145	28% 97%
65	V	145	18% 97%

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Mol	Chain	Length	Quality of chain
66	DH	119	12% 79% 18%
66	W	119	31% 83% 14%
67	DI	87	13% 99%
67	X	87	15% 100%
68	DJ	130	14% 98%
68	Y	130	25% 99%
69	DK	145	8% 97%
69	Z	145	25% 99%
70	DL	135	26% 98%
70	a	135	36% 99%
71	DM	105	21% 67% 32%
71	b	105	14% 69% 31%
72	DN	119	28% 82% 18%
72	c	119	21% 81% 18%
73	DO	82	28% 99%
73	d	82	21% 98%
74	DP	67	21% 91% 9%
74	e	67	36% 93% 7%
75	DQ	56	21% 95%
75	f	56	18% 96%
76	DR	63	30% 87% 5% 8%
76	g	63	41% 92% 5%
77	DS	193	25% 33% 64%
77	h	193	19% 34% 64%
78	AR	317	37% 97%

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Mol	Chain	Length	Quality of chain
78	DT	317	
79	CZ	143	
79	O	143	
80	P0	312	
80	p0	312	
81	12	165	
82	L1	217	
82	11	217	

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	3586	-	-	-	X
84	MG	1	3758	-	-	-	X
84	MG	AD	201	-	-	-	X
84	MG	AS	3458	-	-	-	X
84	MG	AS	3501	-	-	-	X
84	MG	AS	3503	-	-	-	X
84	MG	AS	3533	-	-	-	X
84	MG	AS	3622	-	-	-	X
84	MG	AS	3661	-	-	-	X
84	MG	AT	210	-	-	-	X
84	MG	B	1803	-	-	-	X
84	MG	CL	302	-	-	-	X
84	MG	CM	1828	-	-	-	X

## 2 Entry composition [i](#)

There are 86 unique types of molecules in this entry. The entry contains 408874 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 25S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	1	3216	Total	C	N	O	P	0	0	0
			68751	30713	12360	22462	3216			
1	AS	3222	Total	C	N	O	P	0	0	0
			68877	30769	12381	22505	3222			

- Molecule 2 is a RNA chain called 5S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	4	157	Total	C	N	O	P	0	0	0
			3333	1491	583	1102	157			
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
			Total	C	N	O	S			
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	1	0
			3084	1955	584	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	361	Total	C	N	O	S	0	0	0
			2751	1729	529	490	3			
6	AY	361	Total	C	N	O	S	0	0	0
			2751	1729	529	490	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	m	296	Total	C	N	O	S	0	0	0
			2426	1544	422	458	2			
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	231	Total	C	N	O	S	0	0	0
			1861	1193	342	325	1			
9	BB	234	Total	C	N	O	S	0	0	0
			1885	1208	345	331	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	p	238	Total	C	N	O	S	0	0	0
			1839	1175	327	334	3			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
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
			Total	C	N	O	S			
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			
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	103	Total	C	N	O	0	0	0
			831	539	138	154			
23	BP	102	Total	C	N	O	0	1	0
			837	546	138	153			

- 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	98	Total	C	N	O	S	0	0	0
			801	501	162	137	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			

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

- Molecule 27 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
30	AC	59	473	295	101	77		0	0	0
30	BW	61	488	304	104	80		0	0	0

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	AE	110	Total	C	N	O	S	0	0	0
			894	565	168	159	2			
32	BY	110	Total	C	N	O	S	0	0	0
			894	565	168	159	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	124	Total	C	N	O	S	0	0	0
			1004	641	195	167	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	112	Total	C	N	O	S	0	0	0
			887	547	182	154	4			

- Molecule 36 is a protein called Ribosomal protein L29.

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

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
37	AJ	95	Total 736	C 459	N 148	O 128	S 1	0	0	0
37	CD	97	Total 758	C 471	N 156	O 130	S 1	0	0	0

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

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

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

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

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

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

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	121	Total	C	N	O	0	0	0
			931	563	166	202			
45	CL	121	Total	C	N	O	0	0	0
			931	563	166	202			

- Molecule 46 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B	1756	Total	C	N	O	P	0	0	0
			37425	16730	6631	12308	1756			
46	CM	1765	Total	C	N	O	P	0	0	0
			37621	16818	6670	12368	1765			

- 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
			Total	C	N	O	S			
48	D	214	Total	C	N	O	S	0	0	0
			1724	1094	313	313	4			
48	CO	214	Total	C	N	O	S	0	0	0
			1724	1094	313	313	4			

- Molecule 49 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
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
			Total	C	N	O	S			
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
			Total	C	N	O	S			
51	G	259	Total	C	N	O	S	0	0	0
			2051	1304	385	357	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
			Total	C	N	O	S			
52	H	206	Total	C	N	O	S	0	0	0
			1614	1008	301	301	4			
52	CS	206	Total	C	N	O	S	0	0	0
			1614	1008	301	301	4			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	J	185	Total	C	N	O	S	0	0	0
			1491	953	269	269				
54	CU	183	Total	C	N	O	S	0	0	0
			1475	944	265	266				

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

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

- Molecule 56 is a protein called Ribosomal protein S4.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	M	94	Total	C	N	O	S	0	0	0
			785	508	131	146				
57	CX	94	Total	C	N	O	S	0	0	0
			791	515	131	144	1			

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 S13.

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

- Molecule 60 is a protein called 40S ribosomal protein S14-A.

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

- Molecule 61 is a protein called 40S ribosomal protein S15.

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

- Molecule 62 is a protein called 40S ribosomal protein S16.

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

- Molecule 63 is a protein called 40S ribosomal protein S17-B.

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

- Molecule 64 is a protein called 40S ribosomal protein S18-B.

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

- Molecule 65 is a protein called 40S ribosomal protein S19-A.

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

- Molecule 66 is a protein called Ribosomal protein S10.

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

- Molecule 67 is a protein called 40S ribosomal protein S21.

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

- Molecule 68 is a protein called 40S ribosomal protein S22-A.

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

- Molecule 69 is a protein called Ribosomal protein S23 (S12).

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

- Molecule 70 is a protein called 40S ribosomal protein S24.

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

- Molecule 71 is a protein called 40S ribosomal protein S25.

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

- Molecule 72 is a protein called 40S ribosomal protein S26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
72	c	98	Total	C	N	O	S	0	0	0
			779	482	163	128	6			
72	DN	98	Total	C	N	O	S	0	0	0
			779	482	163	128	6			

- Molecule 73 is a protein called 40S ribosomal protein S27.

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

- Molecule 74 is a protein called 40S ribosomal protein S28-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	e	62	Total	C	N	O	S	0	0	0
			487	299	98	88	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
74	DP	61	Total	C	N	O	S	0	0	0
			476	293	94	87	2			

- Molecule 75 is a protein called 40S ribosomal protein S29A.

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

- Molecule 76 is a protein called 40S ribosomal protein S30.

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

- Molecule 77 is a protein called Ubiquitin-40S ribosomal protein S31 fusion protein.

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

- Molecule 78 is a protein called Guanine nucleotide-binding protein subunit beta-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	AR	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			
78	DT	311	Total	C	N	O	S	0	0	0
			2398	1519	412	462	5			

- Molecule 79 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
79	CZ	119	Total	C	N	O	S	0	0	0
			913	566	163	179	5			
79	O	39	Total	C	N	O	S	0	0	0
			293	180	50	60	3			



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
80	P0	107	Total	C	N	O	S	0	0	0
			845	542	150	150	3			
80	p0	61	Total	C	N	O	S	0	0	0
			487	305	94	85	3			

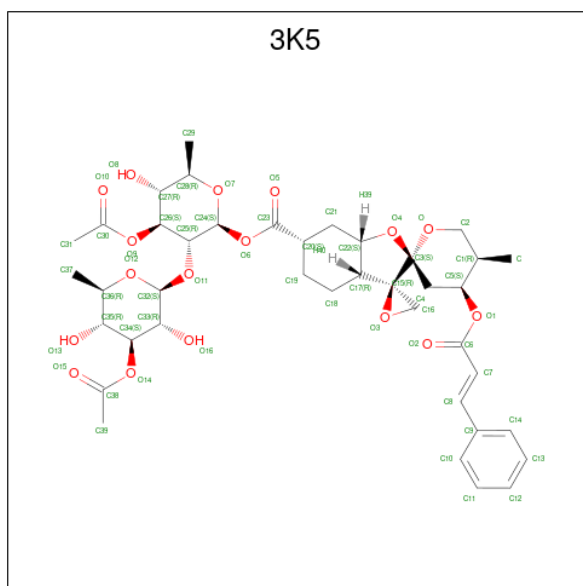
- Molecule 81 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
81	12	62	Total	C	N	O	S	0	0	0
			472	293	83	94	2			

- Molecule 82 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
82	L1	217	Total	C	N	O	S	0	0	0
			1711	1096	294	312	9			
82	11	211	Total	C	N	O	S	0	0	0
			1661	1064	287	302	8			

- 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}decahy  
 drodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose  
 (three-letter code: 3K5) (formula: C<sub>40</sub>H<sub>52</sub>O<sub>17</sub>).



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 (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	1	636	Total	Mg	0	0
			636	636		
84	3	19	Total	Mg	0	0
			19	19		
84	4	15	Total	Mg	0	0
			15	15		
84	j	3	Total	Mg	0	0
			3	3		
84	k	7	Total	Mg	0	0
			7	7		
84	o	6	Total	Mg	0	0
			6	6		
84	r	3	Total	Mg	0	0
			3	3		
84	s	1	Total	Mg	0	0
			1	1		
84	u	2	Total	Mg	0	0
			2	2		
84	v	4	Total	Mg	0	0
			4	4		
84	w	4	Total	Mg	0	0
			4	4		
84	x	3	Total	Mg	0	0
			3	3		
84	y	3	Total	Mg	0	0
			3	3		
84	z	1	Total	Mg	0	0
			1	1		
84	0	3	Total	Mg	0	0
			3	3		
84	2	2	Total	Mg	0	0
			2	2		
84	6	3	Total	Mg	0	0
			3	3		
84	8	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	9	1	Total Mg 1 1	0	0
84	AA	1	Total Mg 1 1	0	0
84	AB	2	Total Mg 2 2	0	0
84	AC	2	Total Mg 2 2	0	0
84	AD	2	Total Mg 2 2	0	0
84	AE	2	Total Mg 2 2	0	0
84	AF	2	Total Mg 2 2	0	0
84	AG	2	Total Mg 2 2	0	0
84	AH	1	Total Mg 1 1	0	0
84	AI	1	Total Mg 1 1	0	0
84	AJ	1	Total Mg 1 1	0	0
84	AM	1	Total Mg 1 1	0	0
84	AO	1	Total Mg 1 1	0	0
84	AP	2	Total Mg 2 2	0	0
84	i	1	Total Mg 1 1	0	0
84	B	197	Total Mg 197 197	0	0
84	D	2	Total Mg 2 2	0	0
84	E	1	Total Mg 1 1	0	0
84	G	1	Total Mg 1 1	0	0
84	I	1	Total Mg 1 1	0	0
84	J	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
84	K	2	Total Mg 2 2	0	0
84	Q	2	Total Mg 2 2	0	0
84	R	1	Total Mg 1 1	0	0
84	U	1	Total Mg 1 1	0	0
84	Y	3	Total Mg 3 3	0	0
84	Z	3	Total Mg 3 3	0	0
84	a	1	Total Mg 1 1	0	0
84	c	1	Total Mg 1 1	0	0
84	f	1	Total Mg 1 1	0	0
84	g	1	Total Mg 1 1	0	0
84	AR	1	Total Mg 1 1	0	0
84	AS	433	Total Mg 433 433	0	0
84	AT	14	Total Mg 14 14	0	0
84	AU	9	Total Mg 9 9	0	0
84	AW	4	Total Mg 4 4	0	0
84	AX	1	Total Mg 1 1	0	0
84	AY	1	Total Mg 1 1	0	0
84	BB	6	Total Mg 6 6	0	0
84	BE	3	Total Mg 3 3	0	0
84	BF	1	Total Mg 1 1	0	0
84	BH	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	BI	1	Total 1	Mg 1	0	0
84	BJ	4	Total 4	Mg 4	0	0
84	BK	1	Total 1	Mg 1	0	0
84	BN	3	Total 3	Mg 3	0	0
84	BO	2	Total 2	Mg 2	0	0
84	BS	2	Total 2	Mg 2	0	0
84	BV	1	Total 1	Mg 1	0	0
84	BZ	4	Total 4	Mg 4	0	0
84	CA	2	Total 2	Mg 2	0	0
84	CJ	1	Total 1	Mg 1	0	0
84	CL	4	Total 4	Mg 4	0	0
84	CM	183	Total 183	Mg 183	0	0
84	CN	1	Total 1	Mg 1	0	0
84	CO	1	Total 1	Mg 1	0	0
84	CP	1	Total 1	Mg 1	0	0
84	CQ	3	Total 3	Mg 3	0	0
84	CW	2	Total 2	Mg 2	0	0
84	CY	1	Total 1	Mg 1	0	0
84	DA	1	Total 1	Mg 1	0	0
84	DB	3	Total 3	Mg 3	0	0
84	DG	2	Total 2	Mg 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	DJ	2	Total	Mg	0	0
			2	2		

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

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

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
86	1	23	Total O 23 23	0	0
86	1	1	Total O 1 1	0	0
86	B	12	Total O 12 12	0	0
86	AS	22	Total O 22 22	0	0
86	BQ	2	Total O 2 2	0	0



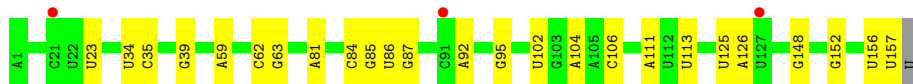
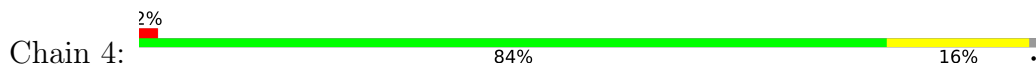




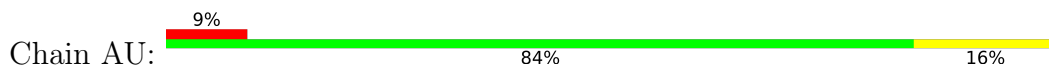




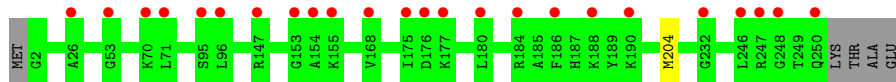
- Molecule 3: 5.8S



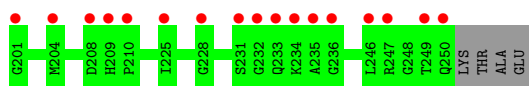
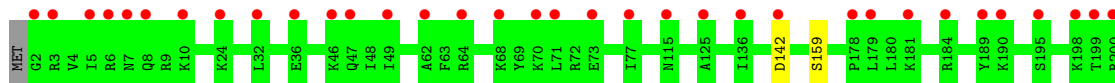
- Molecule 3: 5.8S



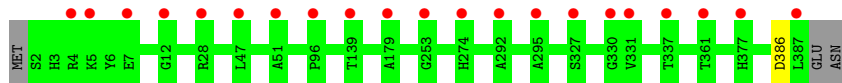
- Molecule 4: 60S ribosomal protein L2-B



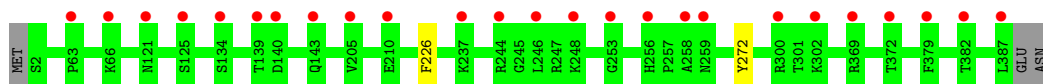
- Molecule 4: 60S ribosomal protein L2-B



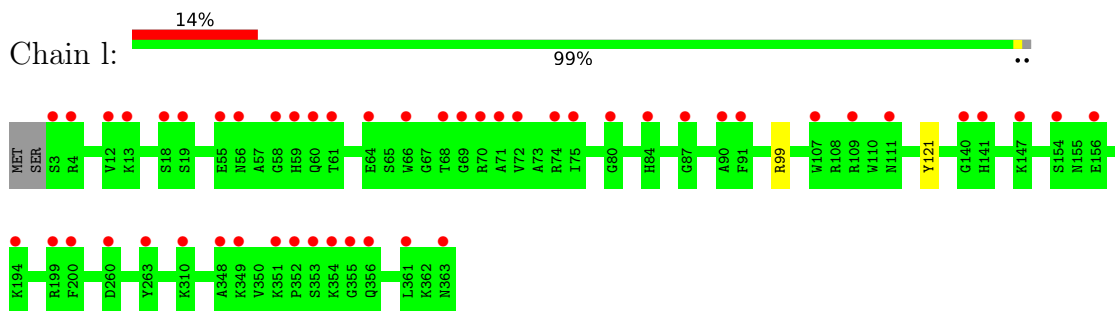
- Molecule 5: 60S ribosomal protein L3



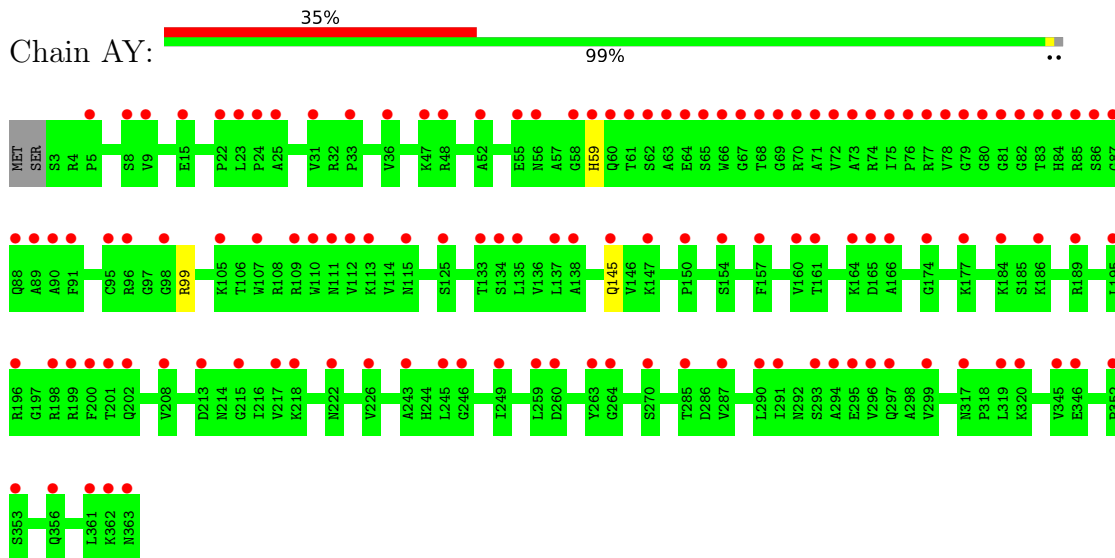
- Molecule 5: 60S ribosomal protein L3



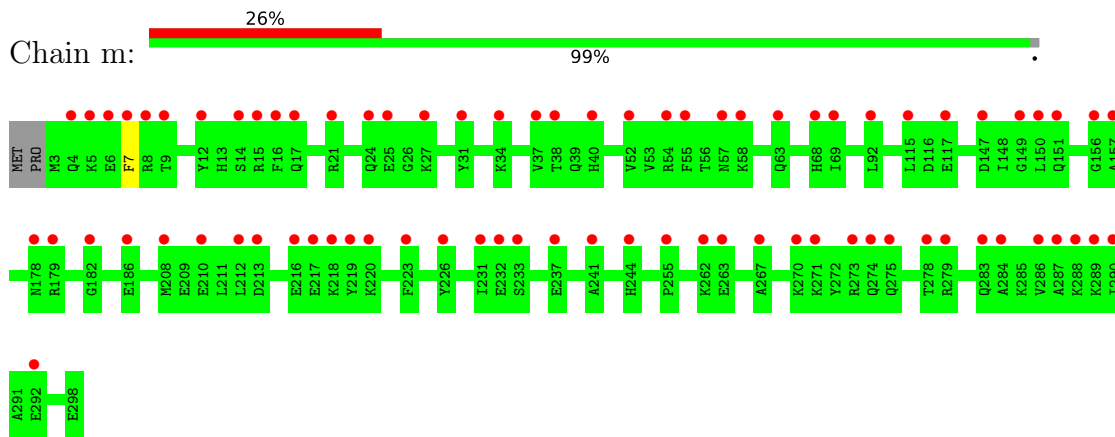
- Molecule 6: 60S ribosomal protein L4-B



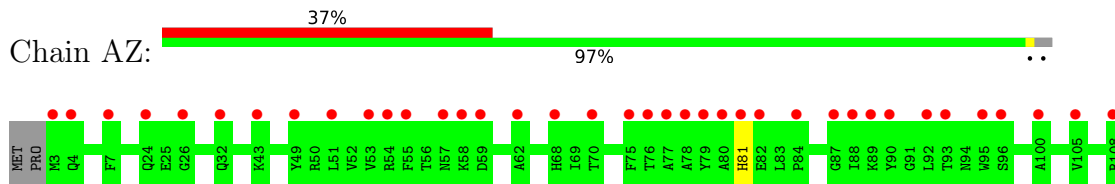
• Molecule 6: 60S ribosomal protein L4-B

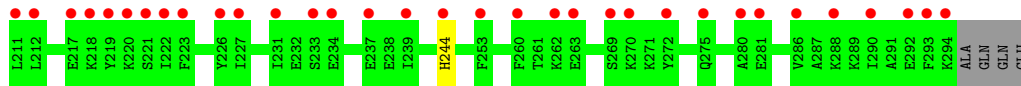
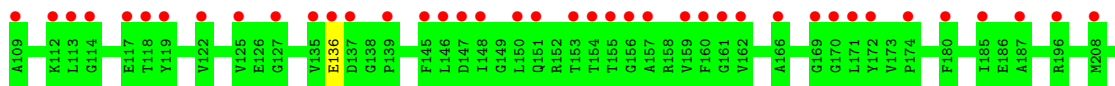


• Molecule 7: Uncharacterized protein CaJ7.0206

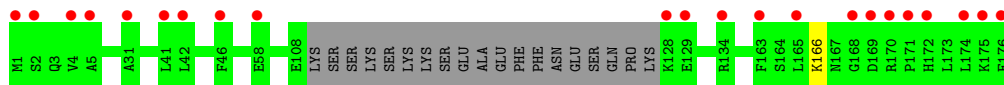
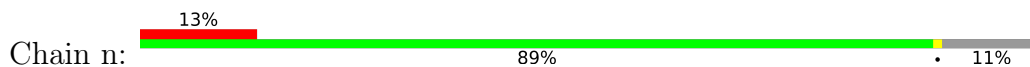


• Molecule 7: Uncharacterized protein CaJ7.0206

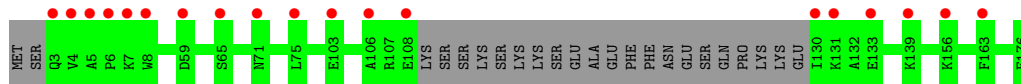
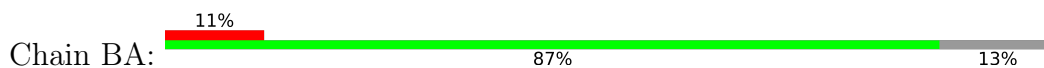




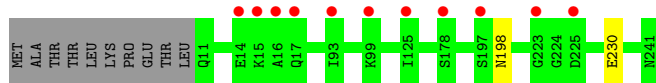
- Molecule 8: 60S ribosomal protein L6



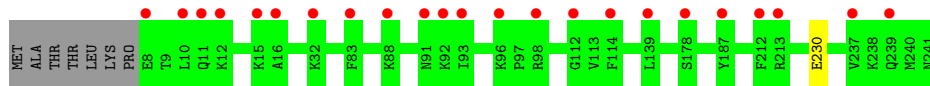
- Molecule 8: 60S ribosomal protein L6



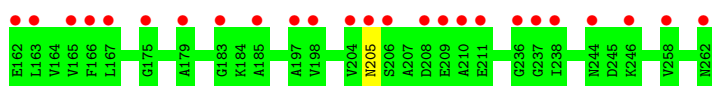
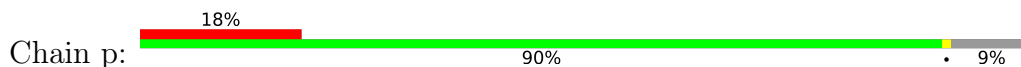
- Molecule 9: 60S ribosomal protein L7-A



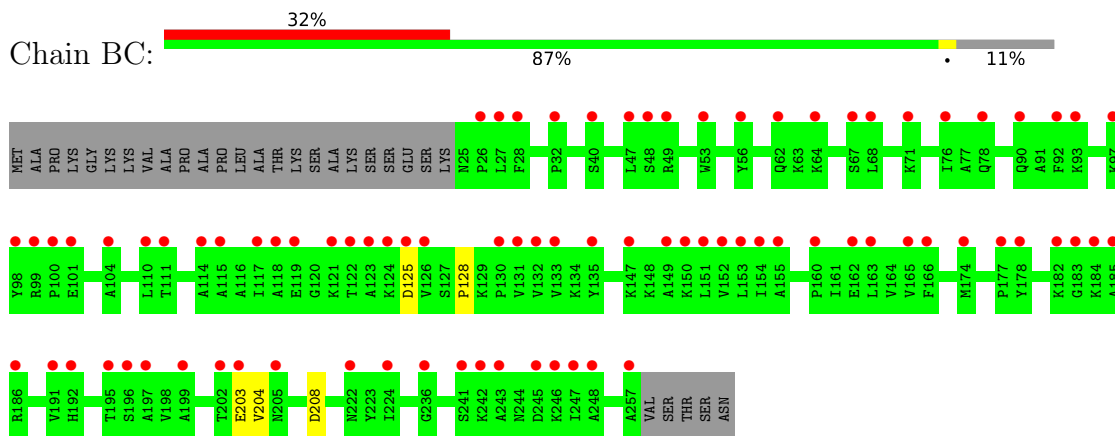
- Molecule 9: 60S ribosomal protein L7-A



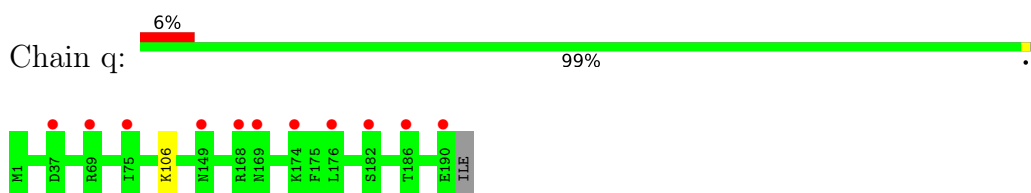
- Molecule 10: 60S ribosomal protein L8



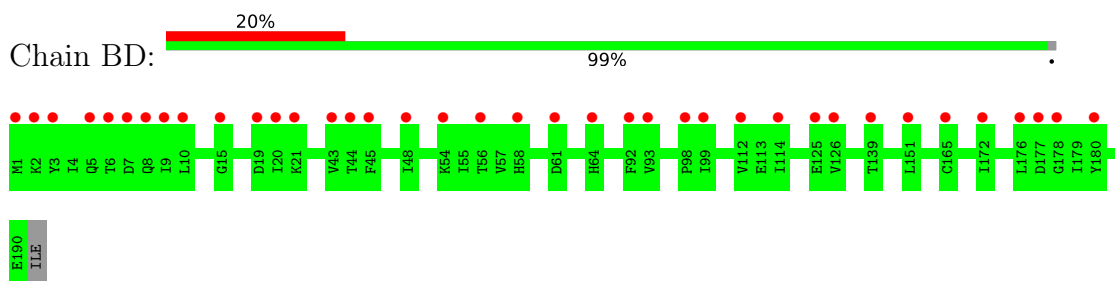
- Molecule 10: 60S ribosomal protein L8



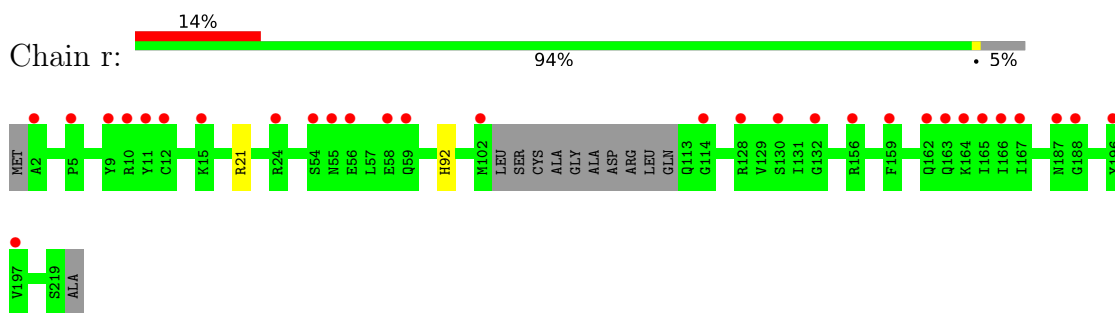
- Molecule 11: 60S ribosomal protein L9-B



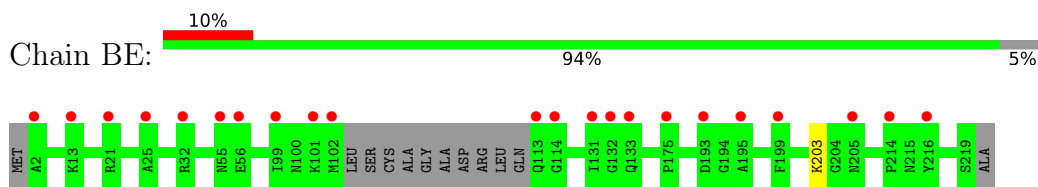
- Molecule 11: 60S ribosomal protein L9-B



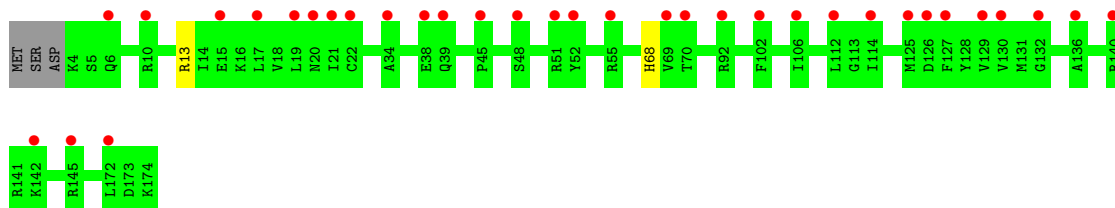
- Molecule 12: 60S ribosomal protein L10



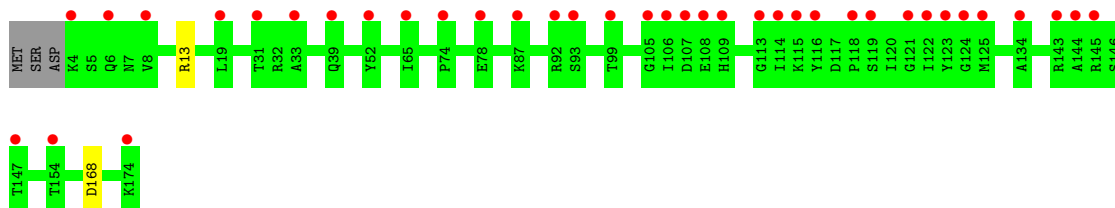
- Molecule 12: 60S ribosomal protein L10



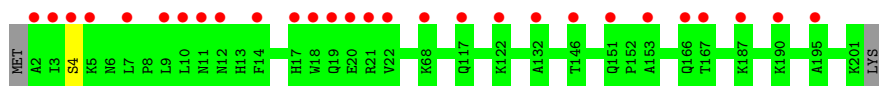
- Molecule 13: 60S ribosomal protein L11-B



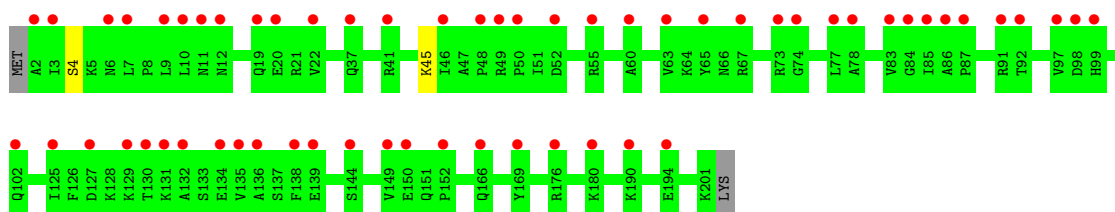
- Molecule 13: 60S ribosomal protein L11-B



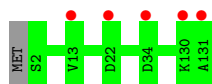
- Molecule 14: 60S ribosomal protein L13



- Molecule 14: 60S ribosomal protein L13



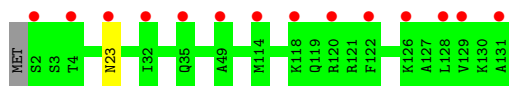
- Molecule 15: 60S ribosomal protein L14-B



- Molecule 15: 60S ribosomal protein L14-B



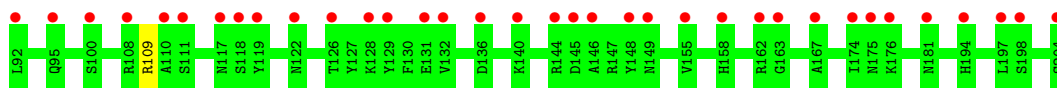
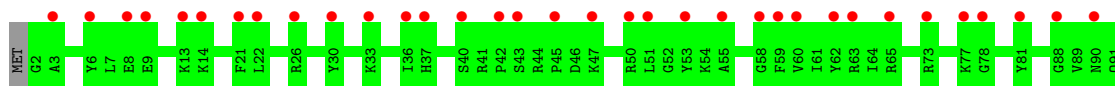




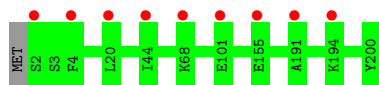
- Molecule 16: 60S ribosomal protein L15-A



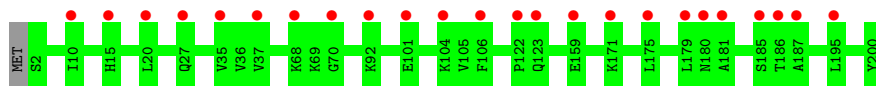
- Molecule 16: 60S ribosomal protein L15-A



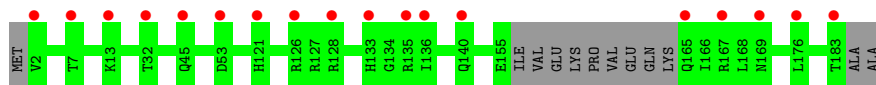
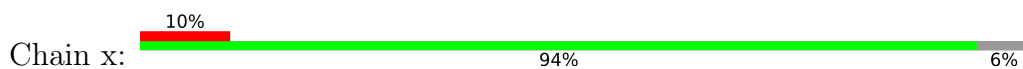
- Molecule 17: Ribosomal protein L13



- Molecule 17: Ribosomal protein L13

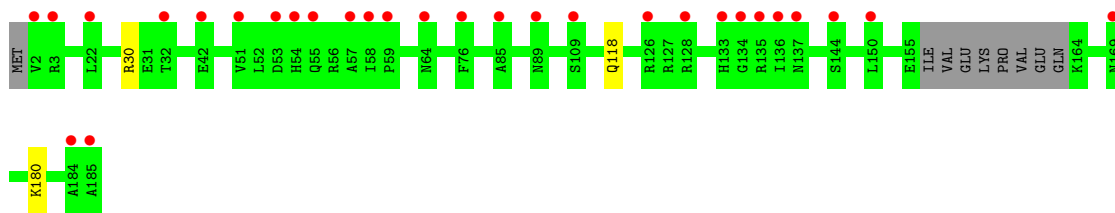


- Molecule 18: Ribosomal protein L22

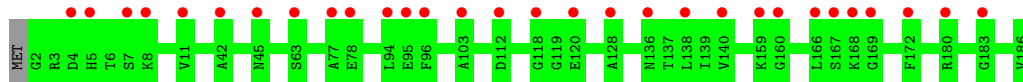


- Molecule 18: Ribosomal protein L22

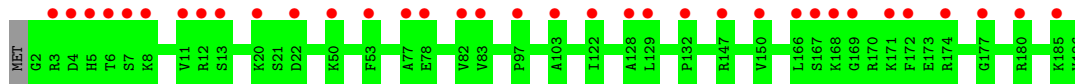




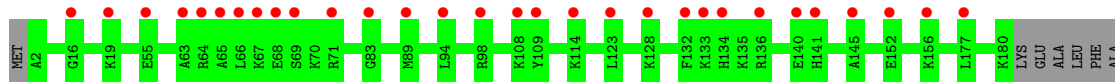
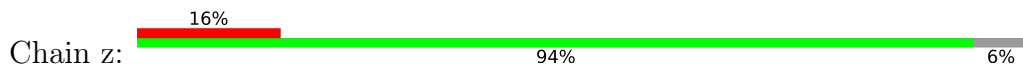
- Molecule 19: 60S ribosomal protein L18-A



- Molecule 19: 60S ribosomal protein L18-A

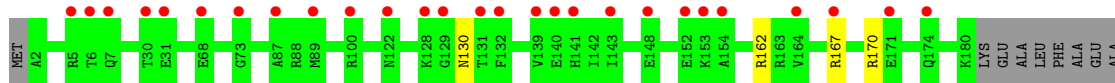


- Molecule 20: 60S ribosomal protein L19-A



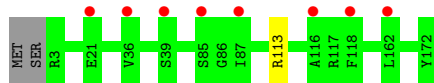
GLU  
ALA  
ALA  
ASN

- Molecule 20: 60S ribosomal protein L19-A

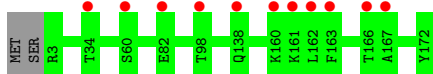


ALA  
ASN

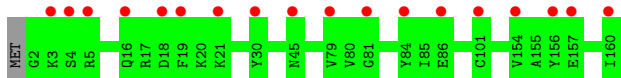
- Molecule 21: 60S ribosomal protein L20



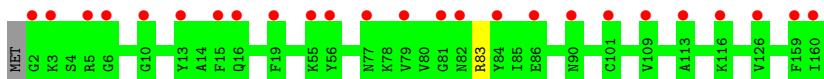
- Molecule 21: 60S ribosomal protein L20



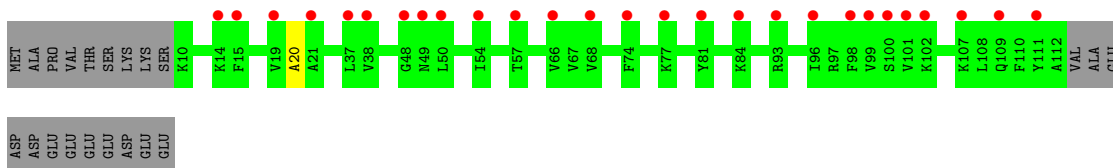
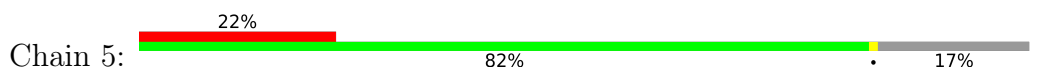
- Molecule 22: 60S ribosomal protein L21-A



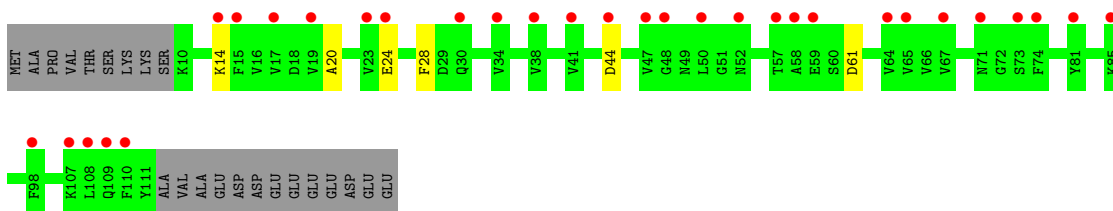
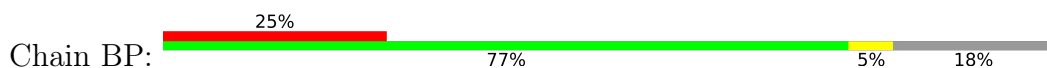
- Molecule 22: 60S ribosomal protein L21-A



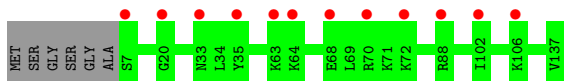
- Molecule 23: 60S ribosomal protein L22-B



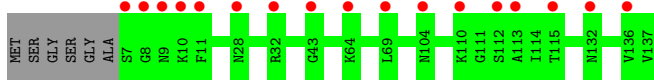
- Molecule 23: 60S ribosomal protein L22-B



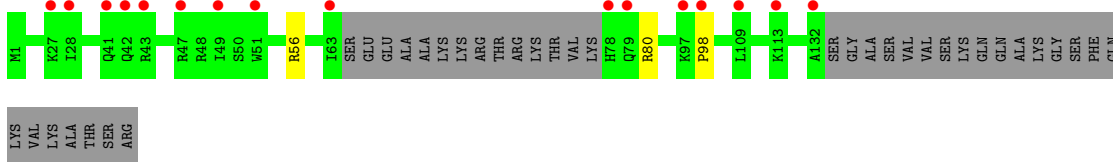
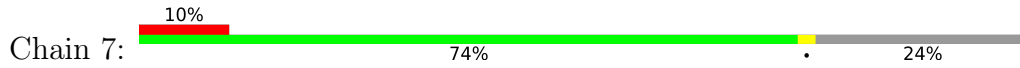
- Molecule 24: 60S ribosomal protein L23-A



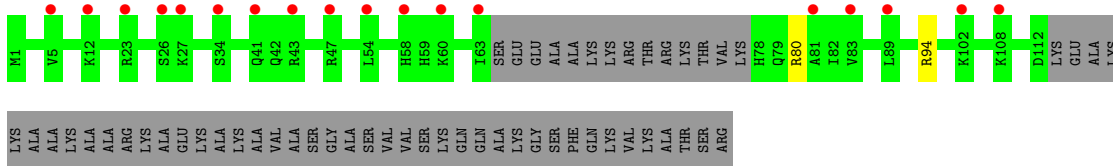
- Molecule 24: 60S ribosomal protein L23-A



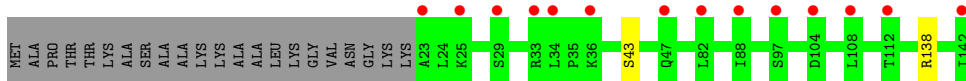
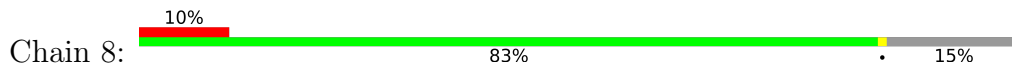
- Molecule 25: 60S ribosomal protein L24-A



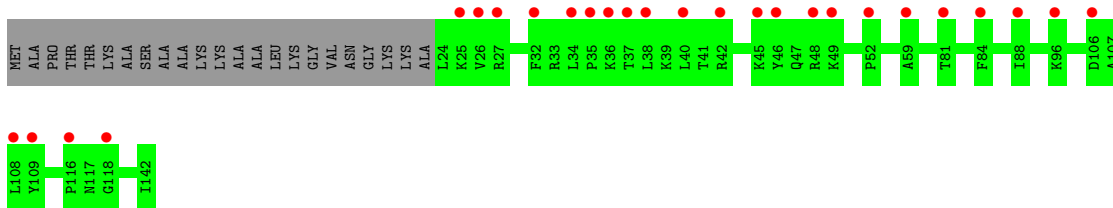
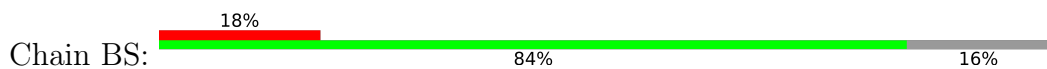
- Molecule 25: 60S ribosomal protein L24-A



- Molecule 26: 60S ribosomal protein L25

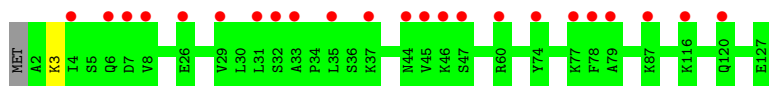


- Molecule 26: 60S ribosomal protein L25

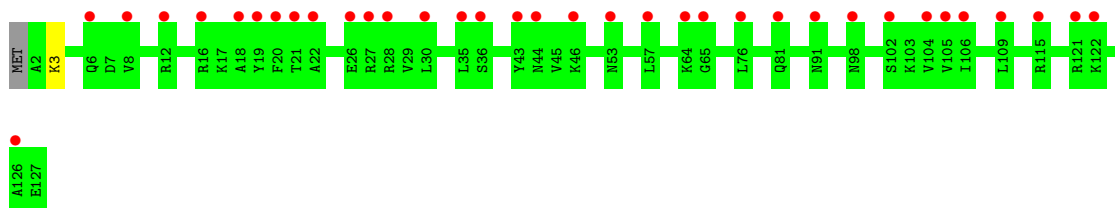


- Molecule 27: Ribosomal protein L24

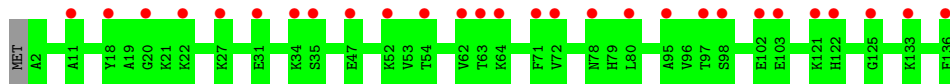




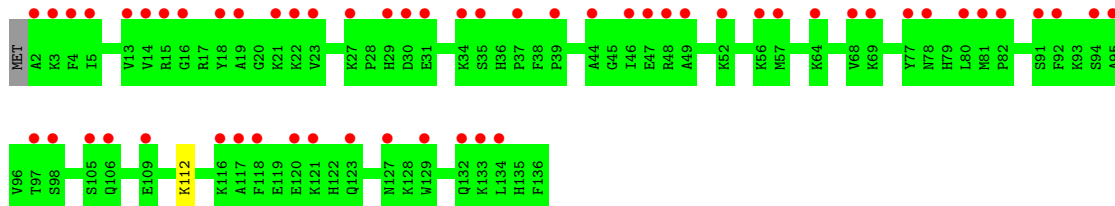
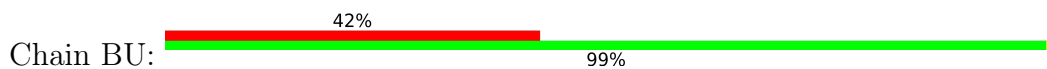
- Molecule 27: Ribosomal protein L24



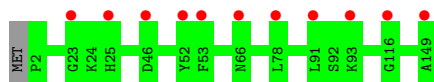
- Molecule 28: 60S ribosomal protein L27



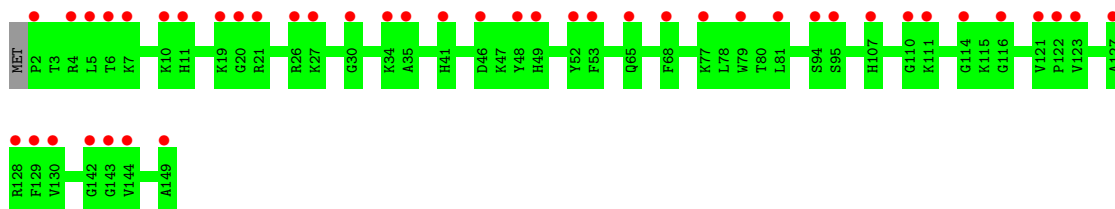
- Molecule 28: 60S ribosomal protein L27



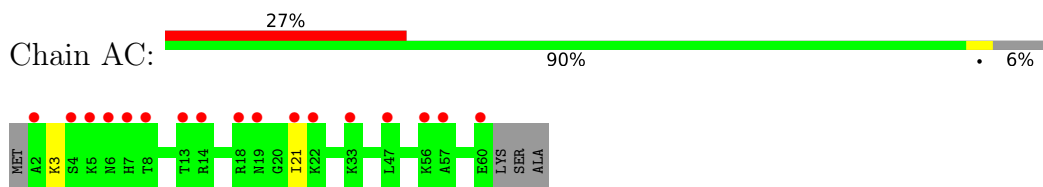
- Molecule 29: 60S ribosomal protein L28



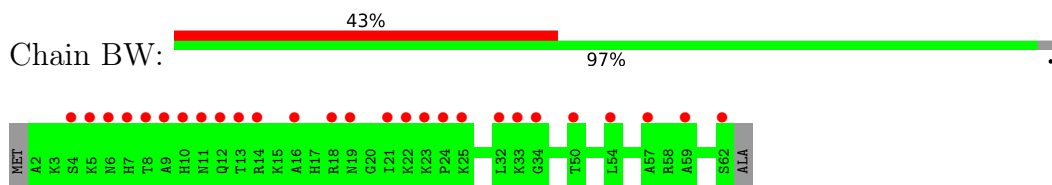
- Molecule 29: 60S ribosomal protein L28



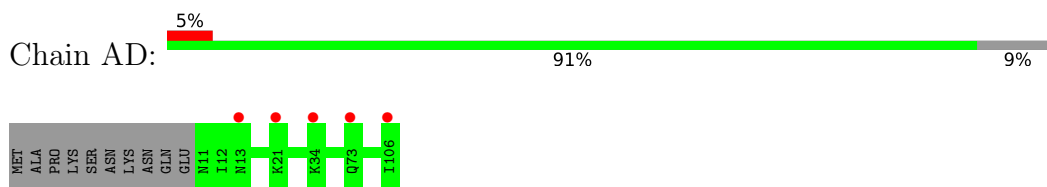
- Molecule 30: 60S ribosomal protein L29



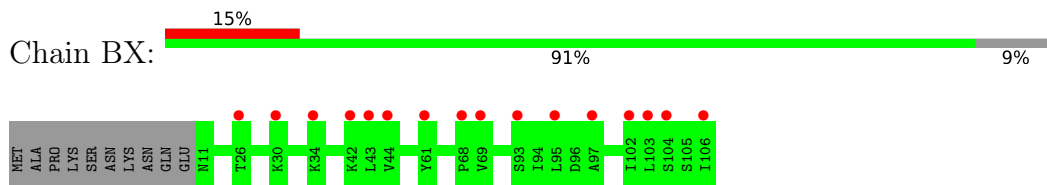
- Molecule 30: 60S ribosomal protein L29



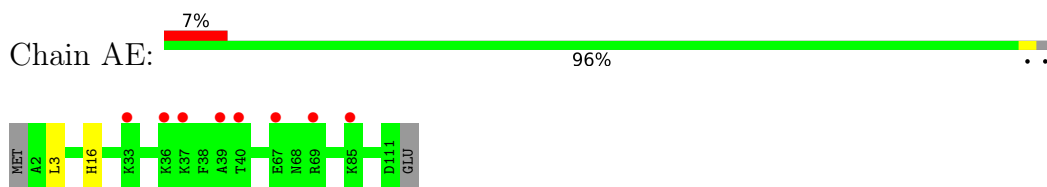
- Molecule 31: 60S ribosomal protein L30



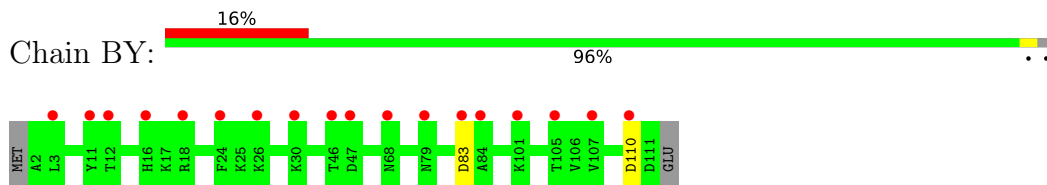
- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31-B

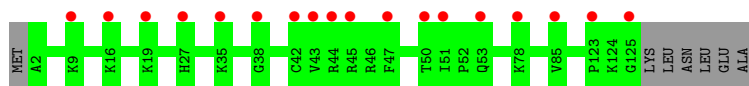


- Molecule 32: 60S ribosomal protein L31-B

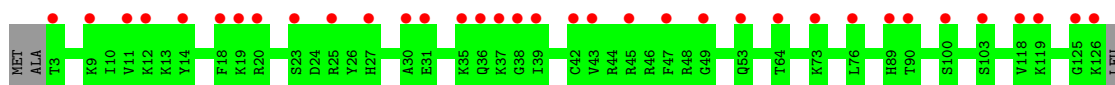


- Molecule 33: 60S ribosomal protein L32

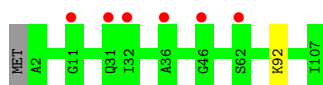




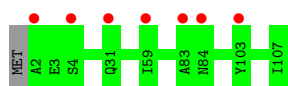
- Molecule 33: 60S ribosomal protein L32



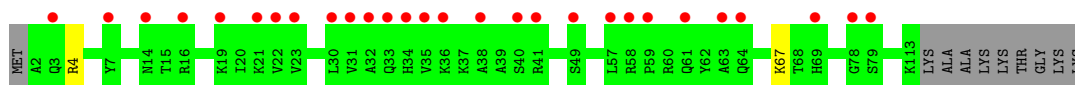
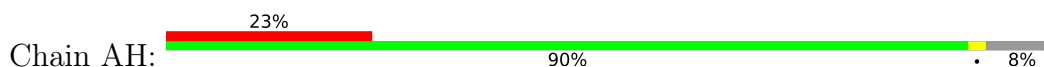
- Molecule 34: 60S ribosomal protein L33-A



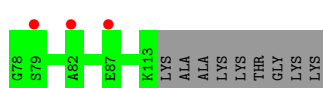
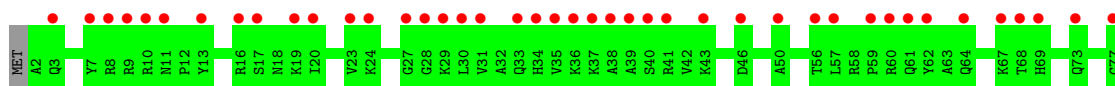
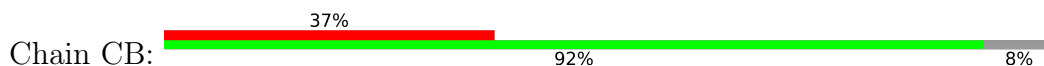
- Molecule 34: 60S ribosomal protein L33-A



- Molecule 35: 60S ribosomal protein L34-B

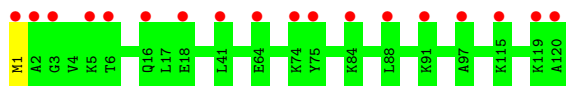


- Molecule 35: 60S ribosomal protein L34-B

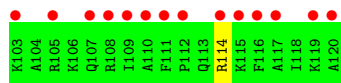
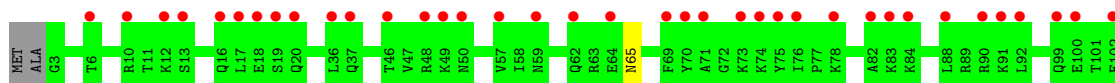
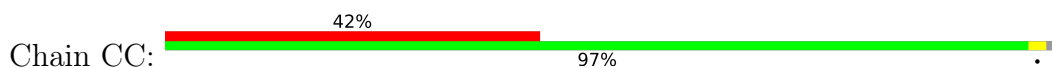


- Molecule 36: Ribosomal protein L29

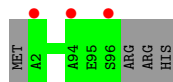




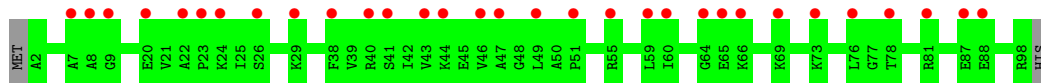
- Molecule 36: Ribosomal protein L29



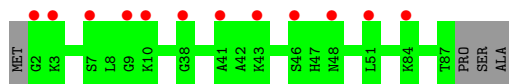
- Molecule 37: 60S ribosomal protein L36



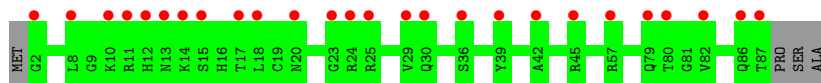
- Molecule 37: 60S ribosomal protein L36



- Molecule 38: 60S ribosomal protein L37-B



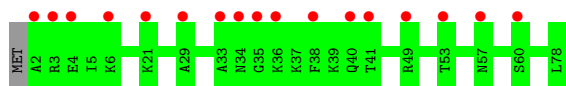
- Molecule 38: 60S ribosomal protein L37-B



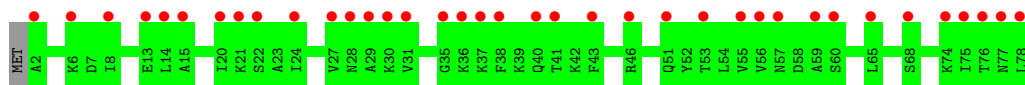
- Molecule 39: 60S ribosomal protein L38



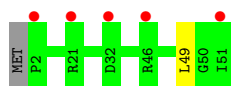




- Molecule 39: 60S ribosomal protein L38



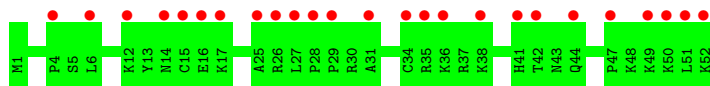
- Molecule 40: 60S ribosomal protein L39



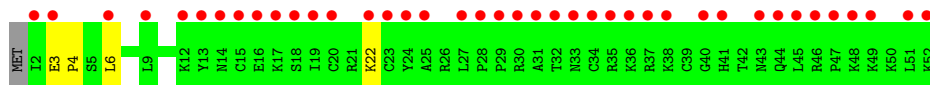
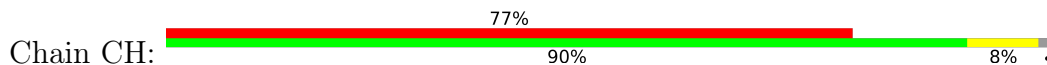
- Molecule 40: 60S ribosomal protein L39



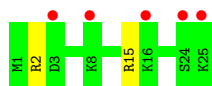
- Molecule 41: 60S ribosomal protein L40-B



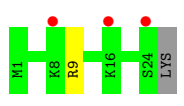
- Molecule 41: 60S ribosomal protein L40-B



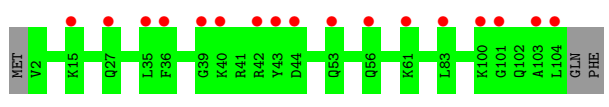
- Molecule 42: 60S ribosomal protein L41



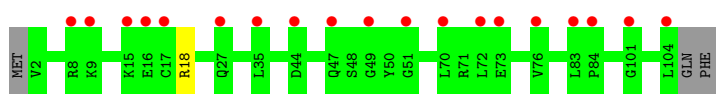
- Molecule 42: 60S ribosomal protein L41



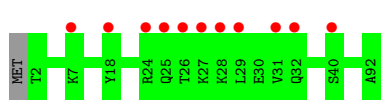
• Molecule 43: 60S ribosomal protein L42-B



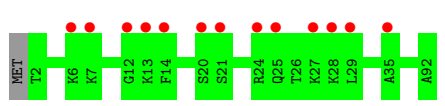
• Molecule 43: 60S ribosomal protein L42-B



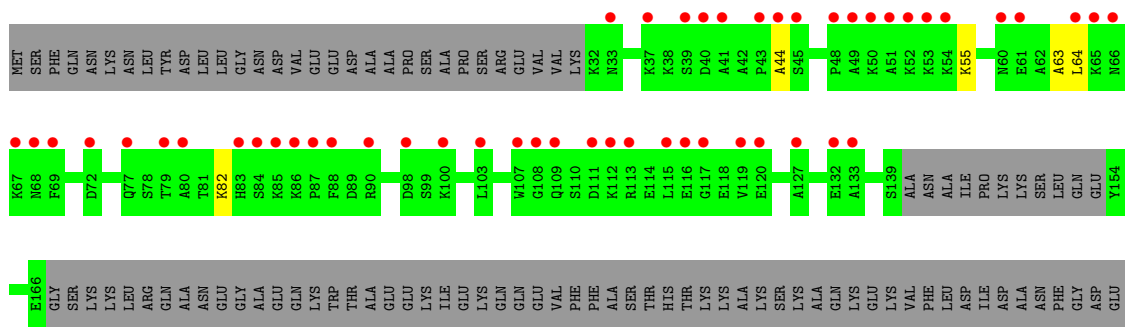
• Molecule 44: 60S ribosomal protein L43-A



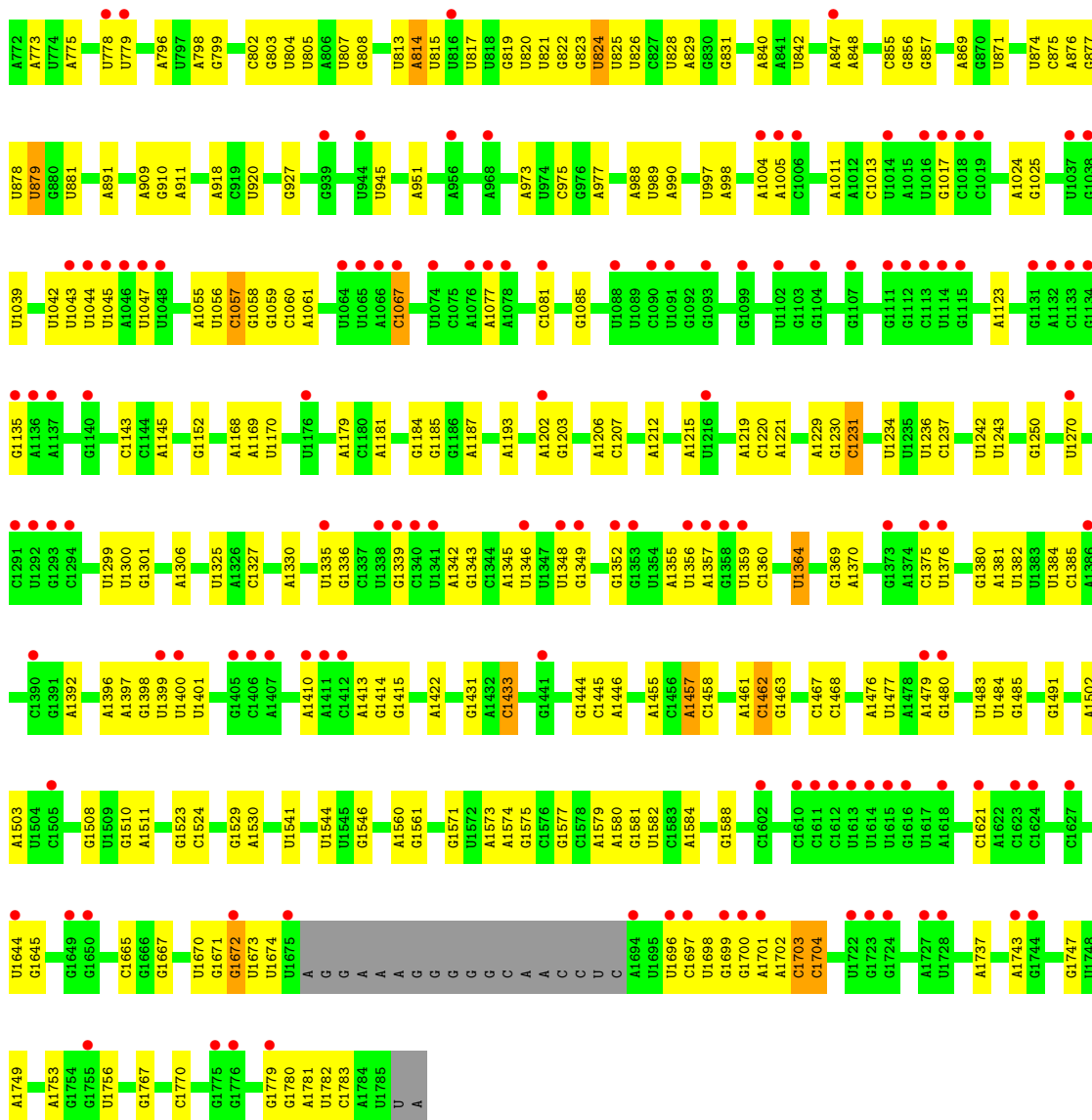
• Molecule 44: 60S ribosomal protein L43-A



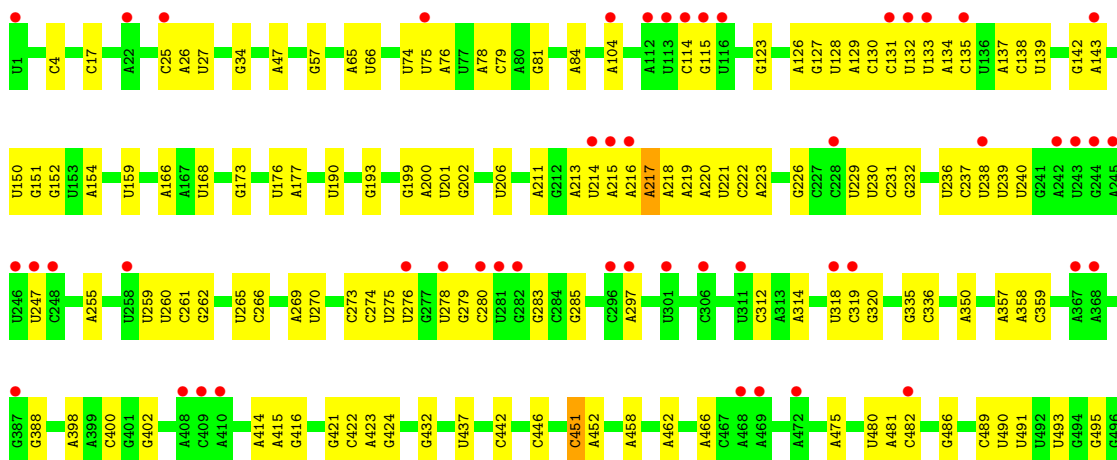
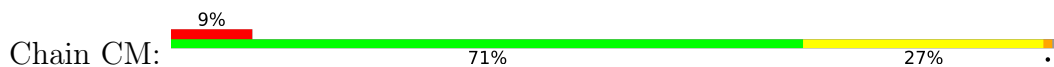
• Molecule 45: 60S ribosomal protein CAALFM\_C304810CA

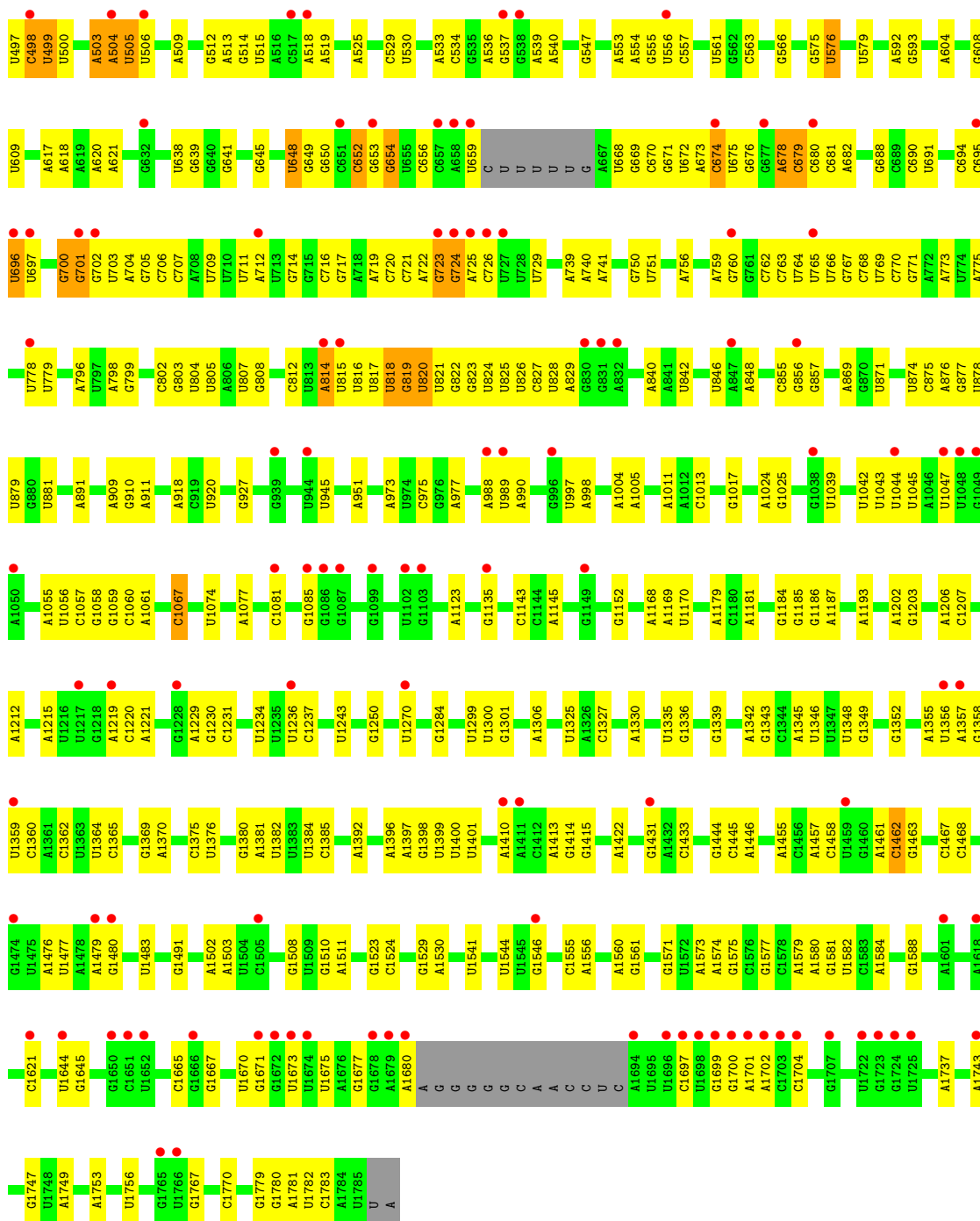




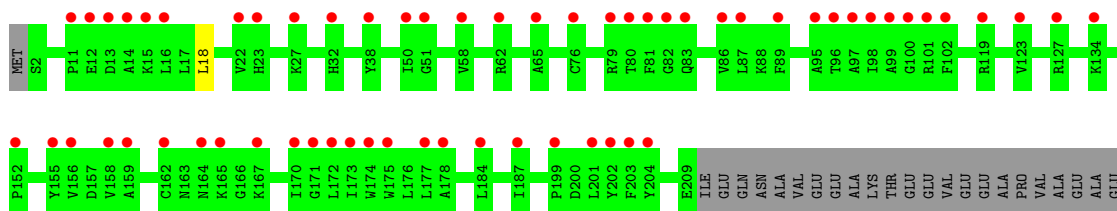
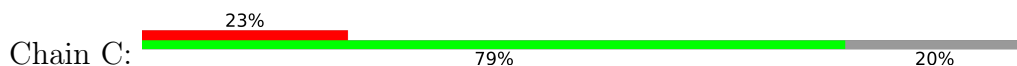


• Molecule 46: 18S





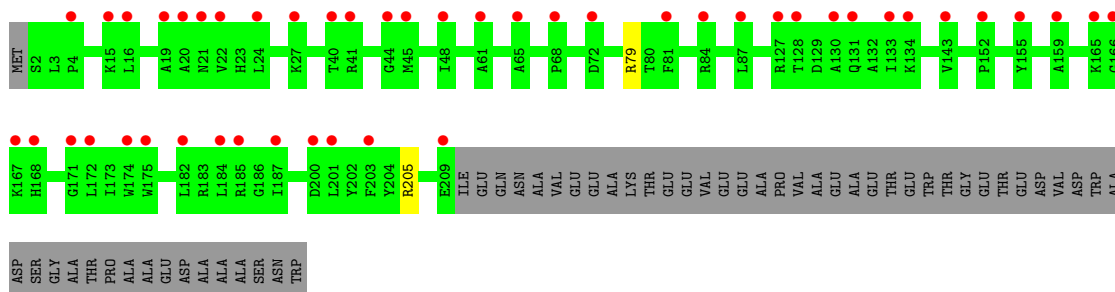
• Molecule 47: 40S ribosomal protein S0



THR  
GLU  
TRP  
TRP  
GLY  
GLU  
THR  
GLU  
VAL  
ASP  
VAL  
ASP  
TRP  
ALA  
ALA  
ASP  
SER  
GLY  
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GLU  
ASP  
ALA  
ALA  
ALA  
ASN  
TRP

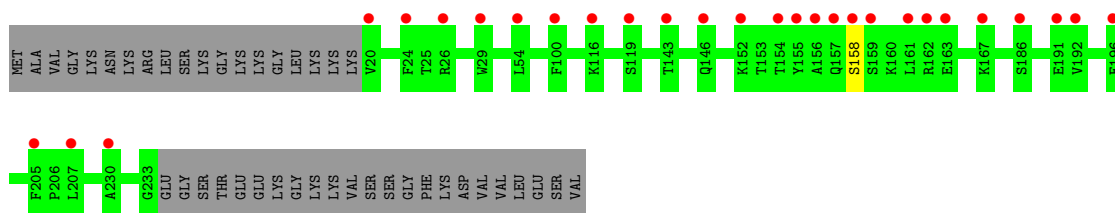
• Molecule 47: 40S ribosomal protein S0

Chain CN: 18% 79% 20%



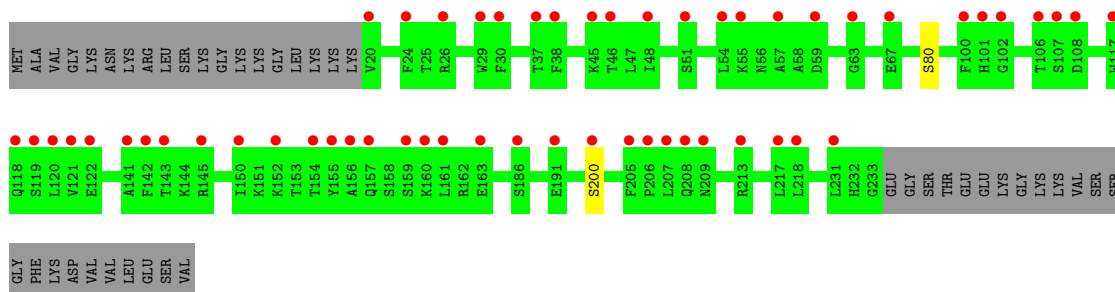
• Molecule 48: 40S ribosomal protein S1

Chain D: 11% 83% 16%



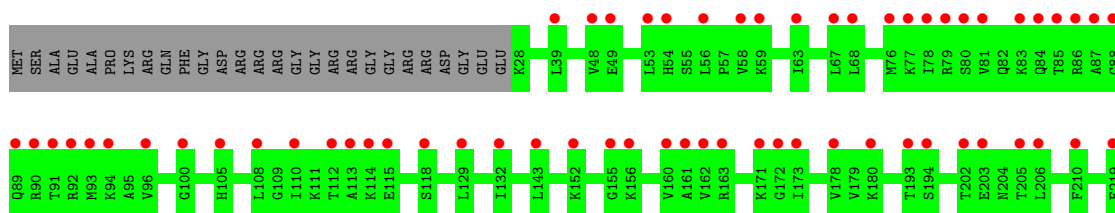
• Molecule 48: 40S ribosomal protein S1

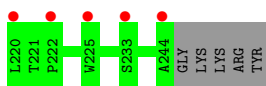
Chain CO: 21% 83% 16%



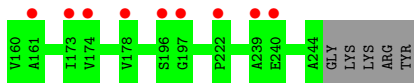
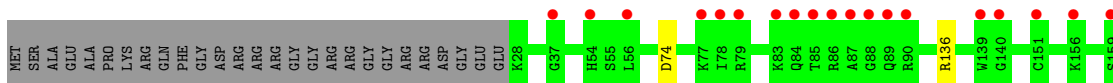
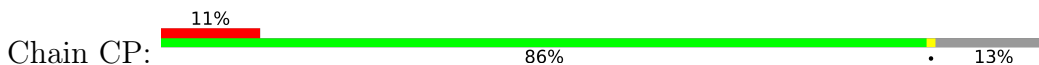
• Molecule 49: Ribosomal protein S5

Chain E: 27% 87% 13%

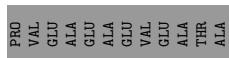
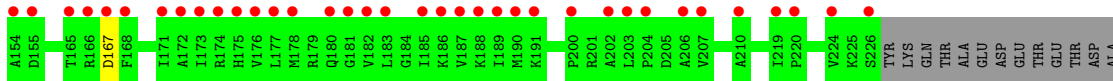
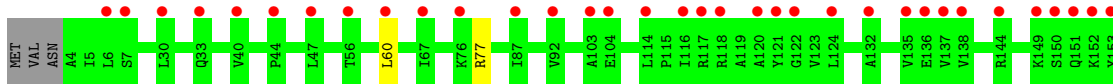
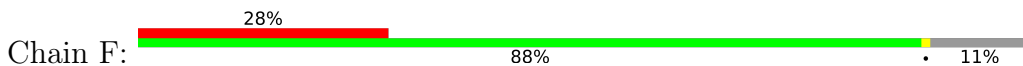




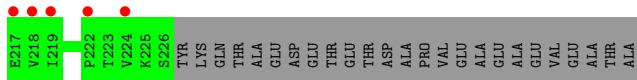
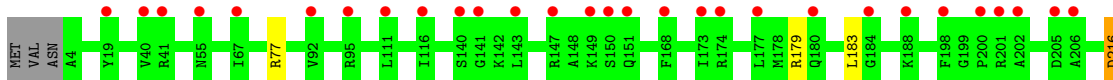
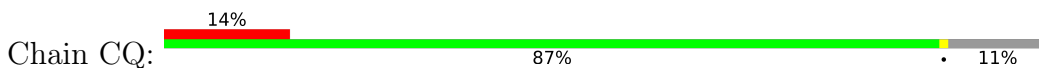
• Molecule 49: Ribosomal protein S5



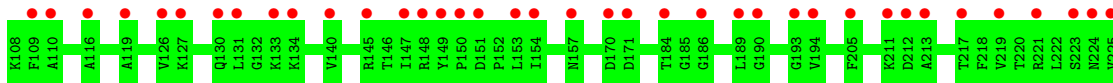
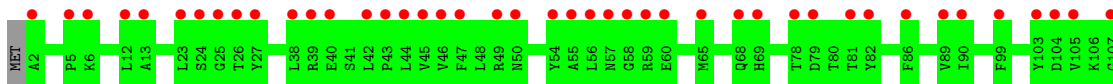
• Molecule 50: Ribosomal protein S3

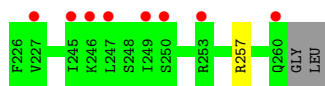


• Molecule 50: Ribosomal protein S3



• Molecule 51: 40S ribosomal protein S4

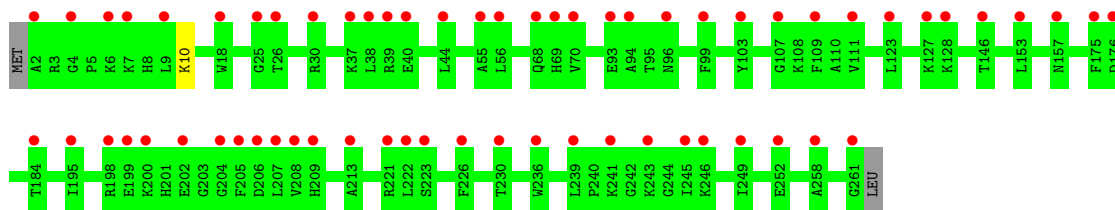




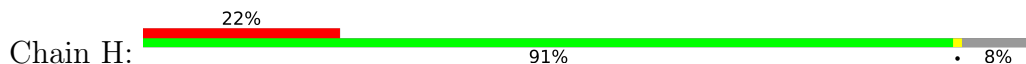
• Molecule 51: 40S ribosomal protein S4



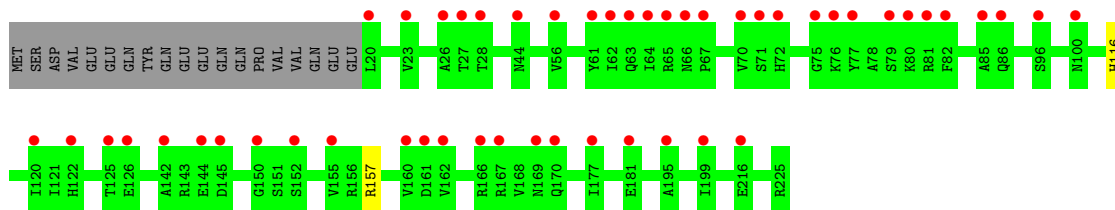
Chain CR:



• Molecule 52: Ribosomal protein S7



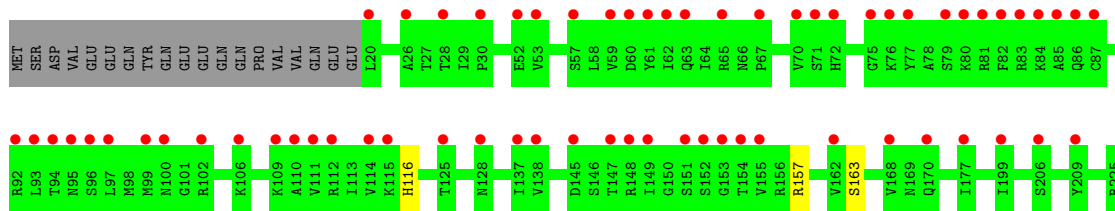
Chain H:



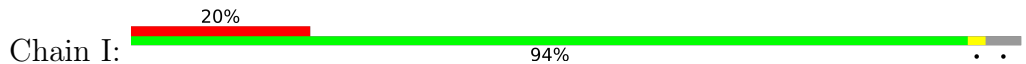
• Molecule 52: Ribosomal protein S7



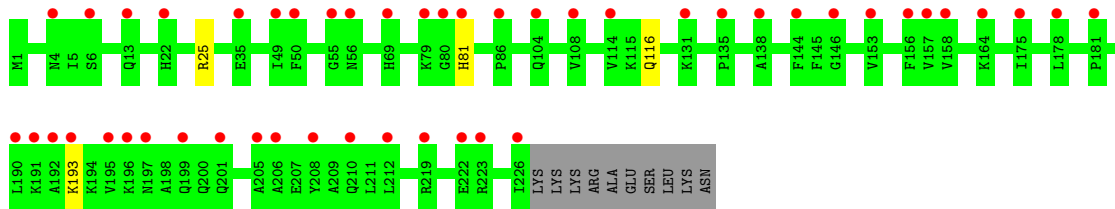
Chain CS:



• Molecule 53: 40S ribosomal protein S6



Chain I:



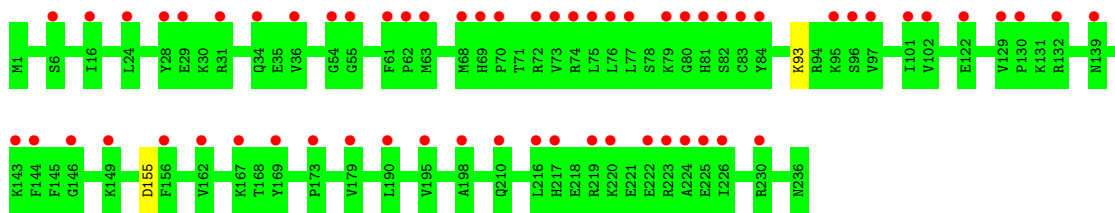
• Molecule 53: 40S ribosomal protein S6



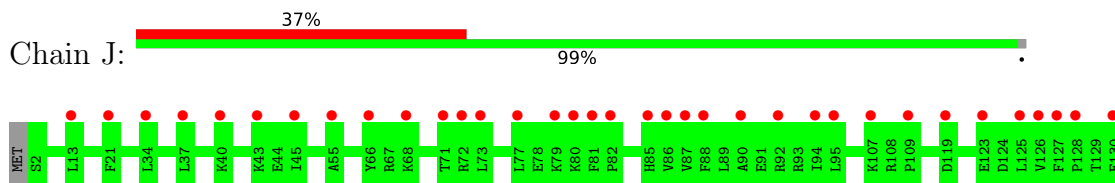
Chain CT:



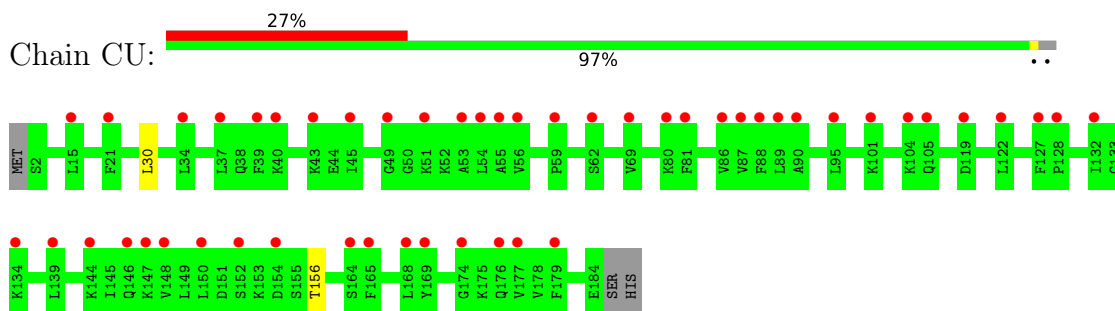




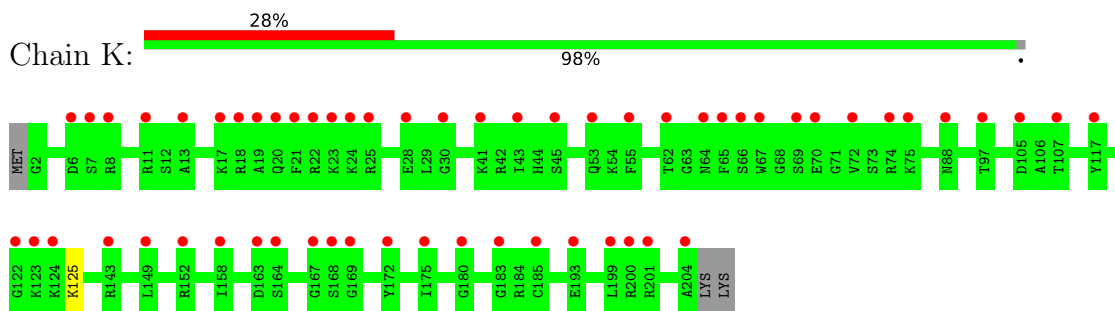
- Molecule 54: 40S ribosomal protein S7



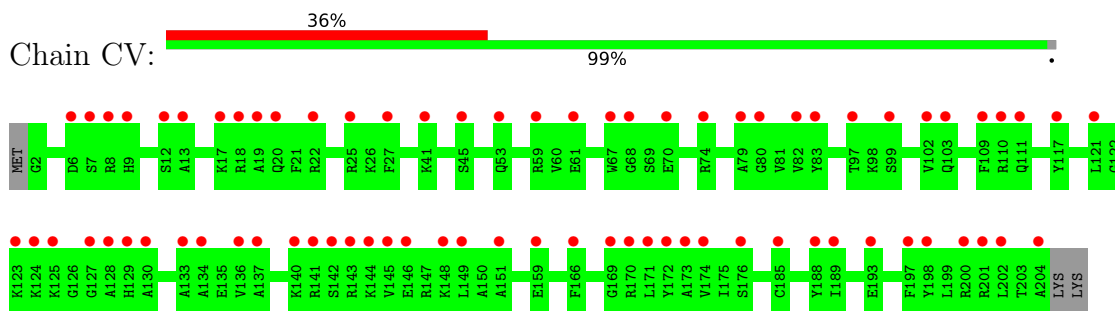
- Molecule 54: 40S ribosomal protein S7



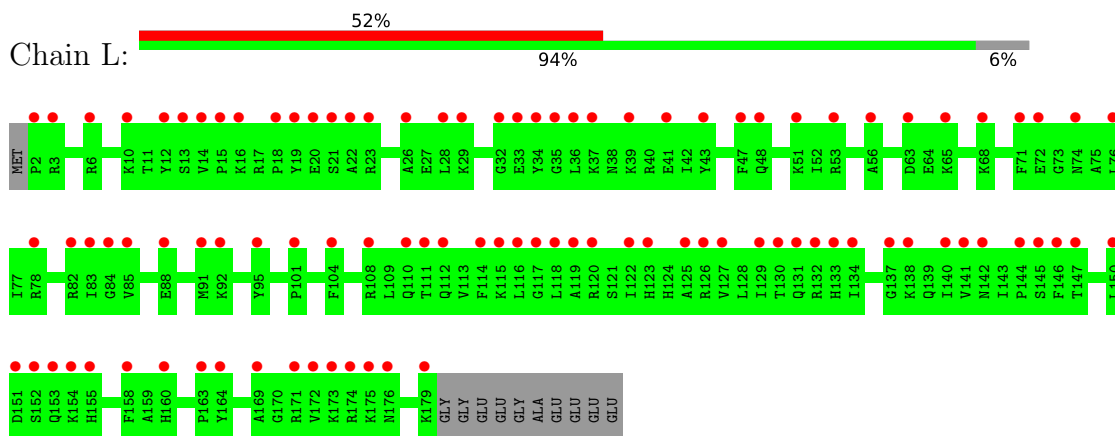
- Molecule 55: 40S ribosomal protein S8



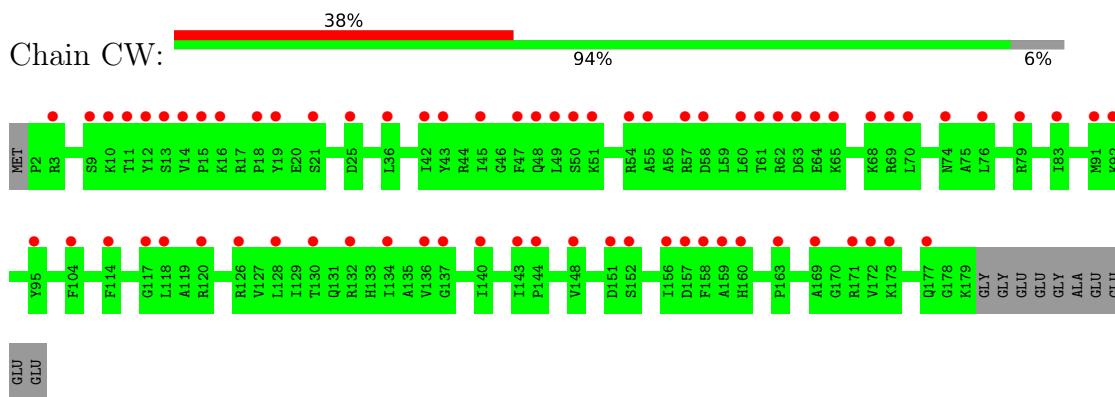
- Molecule 55: 40S ribosomal protein S8



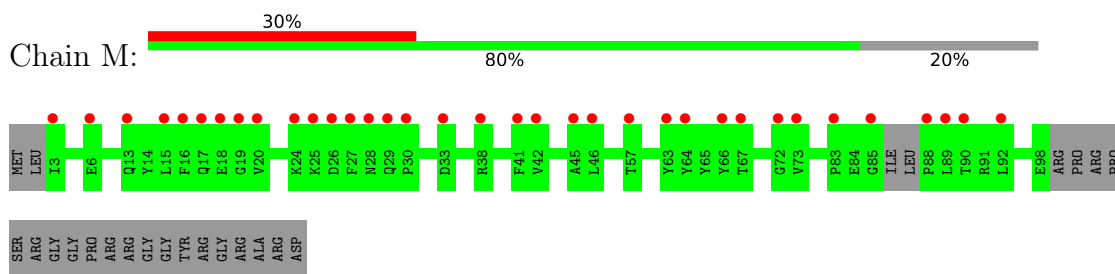
- Molecule 56: Ribosomal protein S4



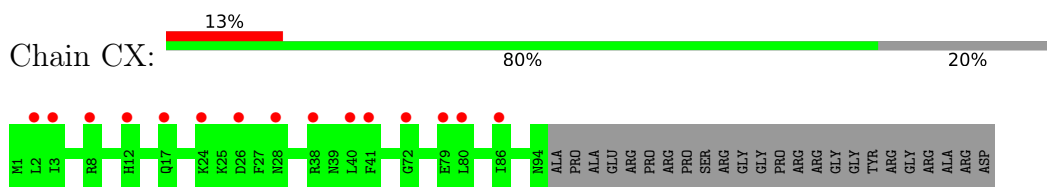
- Molecule 56: Ribosomal protein S4



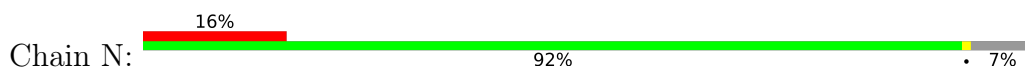
- Molecule 57: 40S ribosomal protein S10-A



- Molecule 57: 40S ribosomal protein S10-A

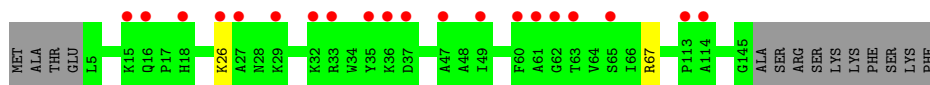


- Molecule 58: 40S ribosomal protein S11A

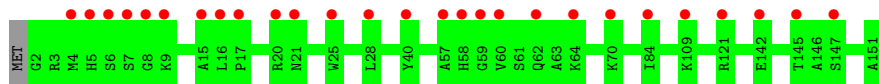




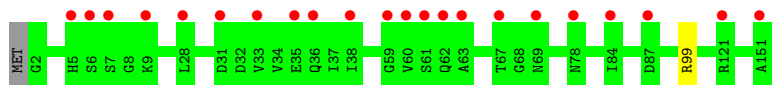
• Molecule 58: 40S ribosomal protein S11A



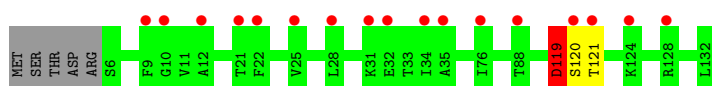
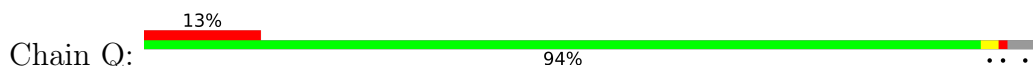
• Molecule 59: 40S ribosomal protein S13



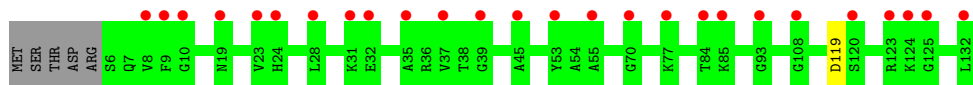
• Molecule 59: 40S ribosomal protein S13



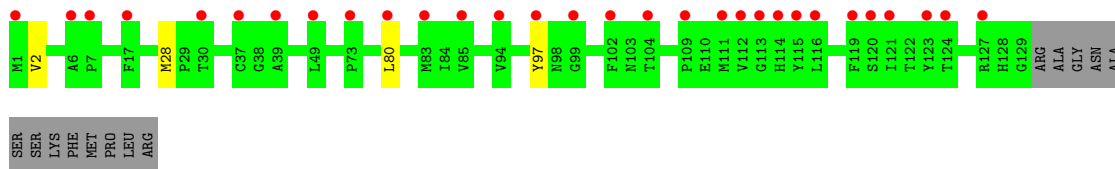
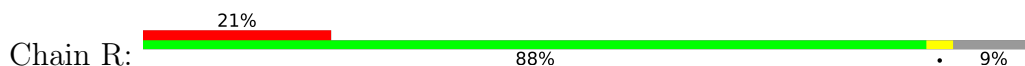
• Molecule 60: 40S ribosomal protein S14-A



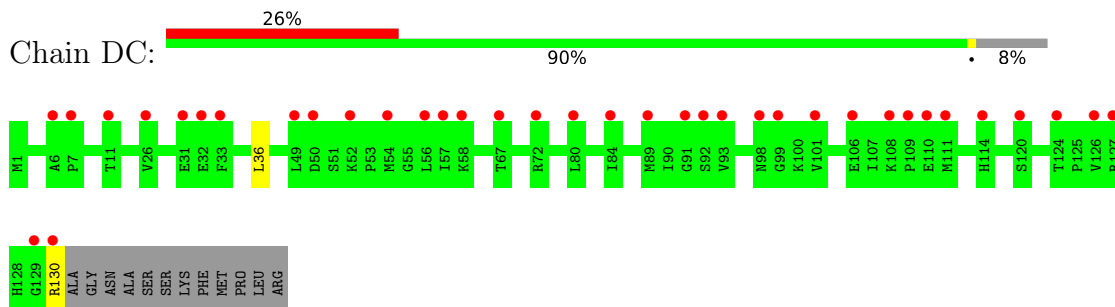
• Molecule 60: 40S ribosomal protein S14-A



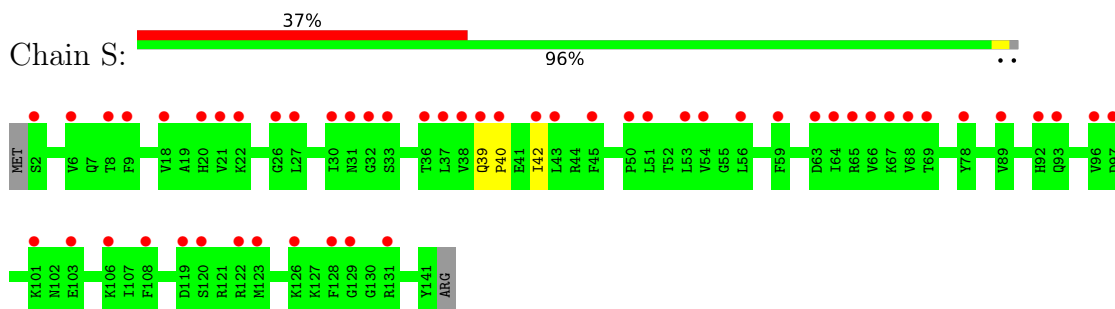
• Molecule 61: 40S ribosomal protein S15



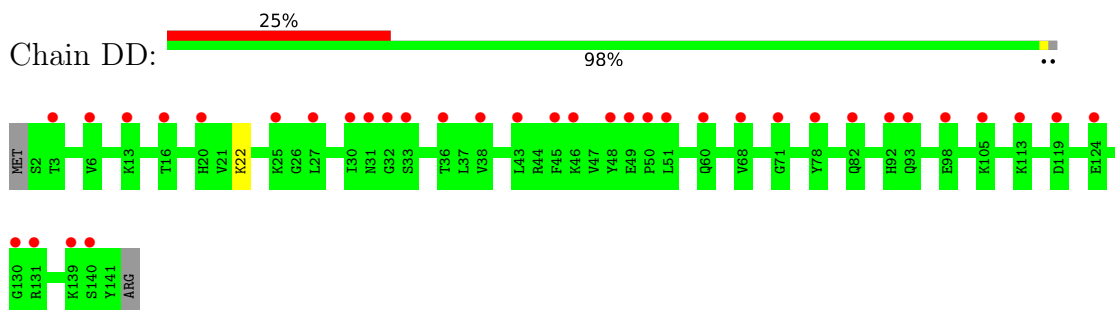
- Molecule 61: 40S ribosomal protein S15



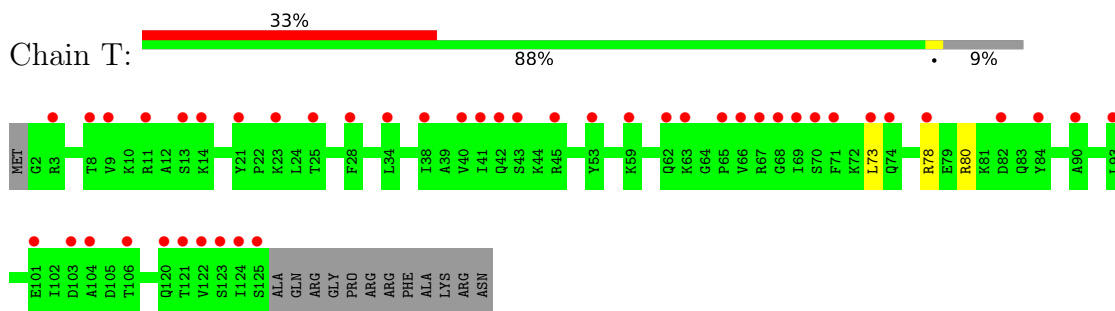
- Molecule 62: 40S ribosomal protein S16



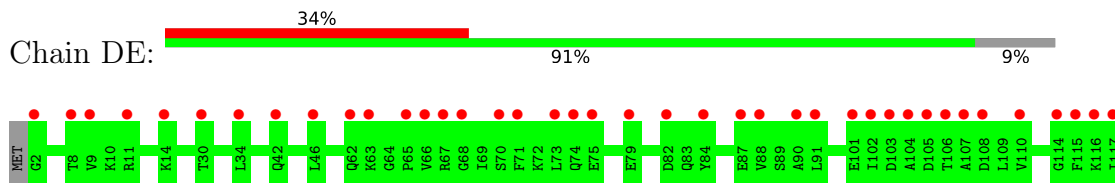
- Molecule 62: 40S ribosomal protein S16



- Molecule 63: 40S ribosomal protein S17-B

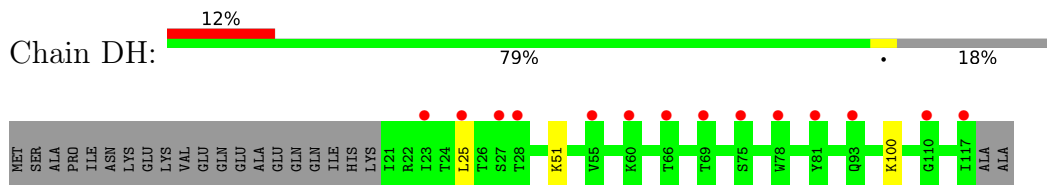


- Molecule 63: 40S ribosomal protein S17-B

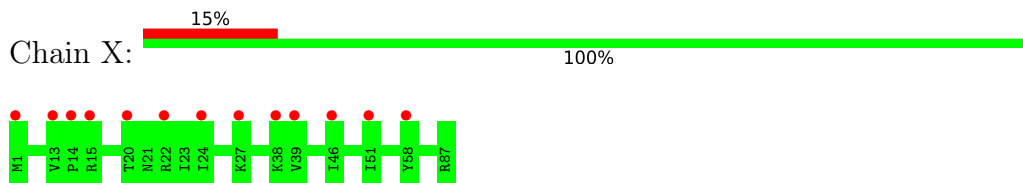




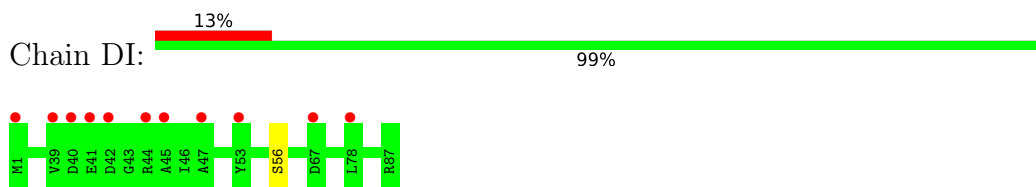
- Molecule 66: Ribosomal protein S10



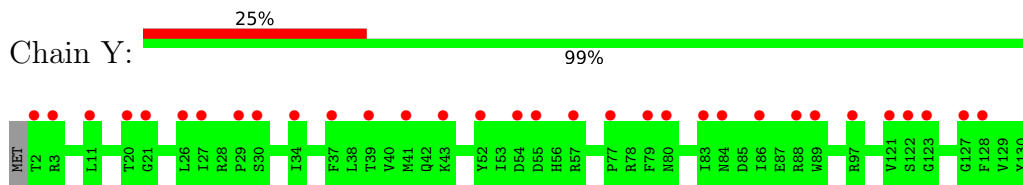
- Molecule 67: 40S ribosomal protein S21



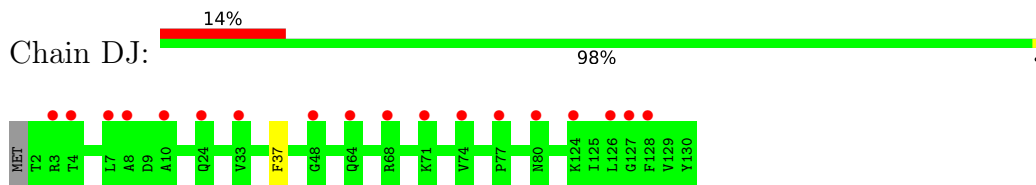
- Molecule 67: 40S ribosomal protein S21



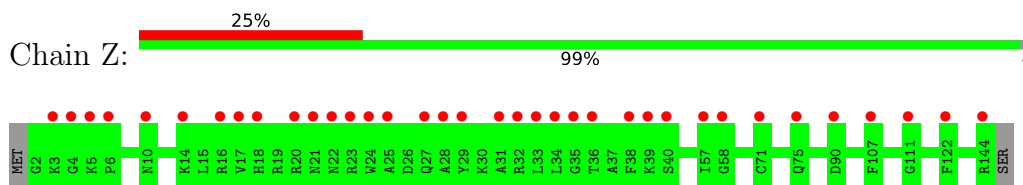
- Molecule 68: 40S ribosomal protein S22-A



- Molecule 68: 40S ribosomal protein S22-A



- Molecule 69: Ribosomal protein S23 (S12)

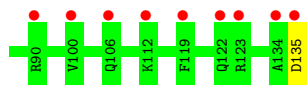
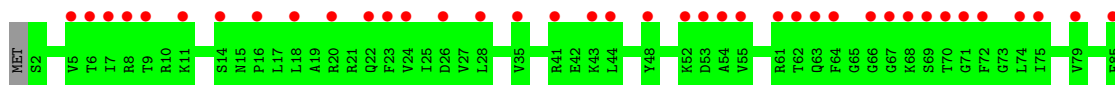


- Molecule 69: Ribosomal protein S23 (S12)

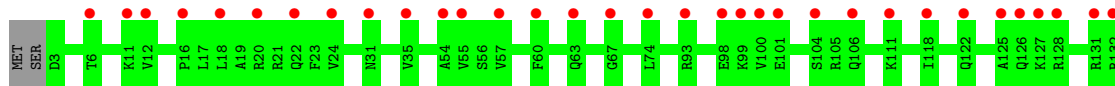




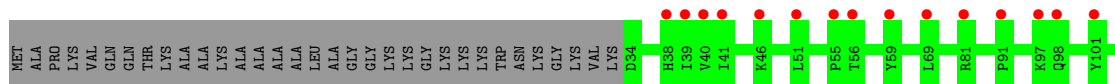
- Molecule 70: 40S ribosomal protein S24



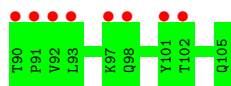
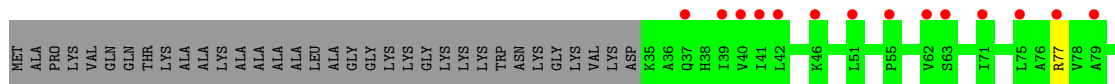
- Molecule 70: 40S ribosomal protein S24



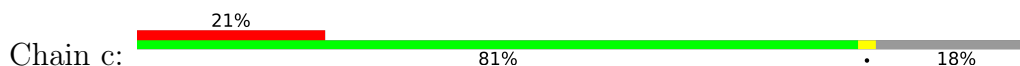
- Molecule 71: 40S ribosomal protein S25

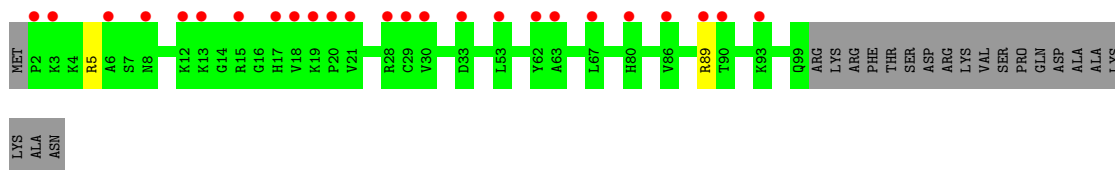


- Molecule 71: 40S ribosomal protein S25

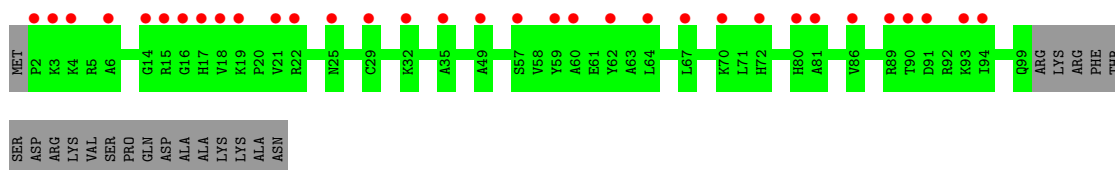
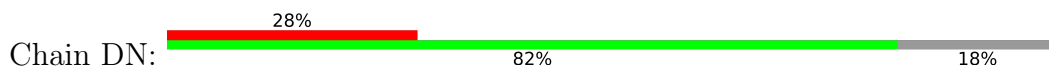


- Molecule 72: 40S ribosomal protein S26

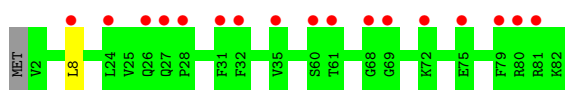




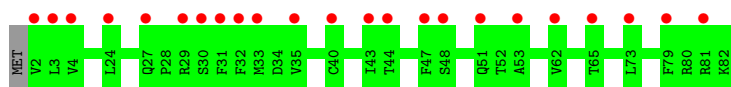
• Molecule 72: 40S ribosomal protein S26



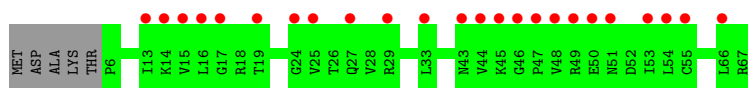
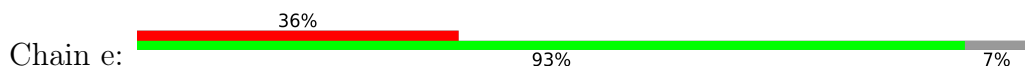
• Molecule 73: 40S ribosomal protein S27



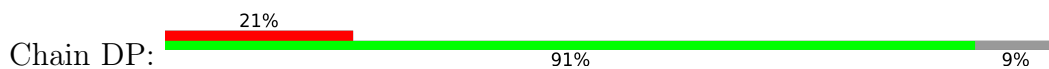
• Molecule 73: 40S ribosomal protein S27



• Molecule 74: 40S ribosomal protein S28-B



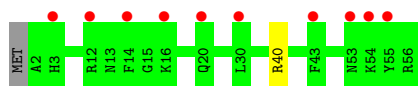
• Molecule 74: 40S ribosomal protein S28-B



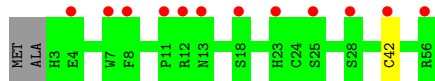
• Molecule 75: 40S ribosomal protein S29A



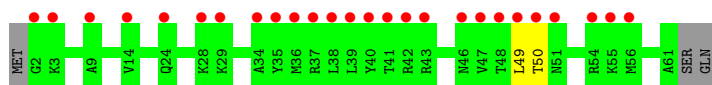
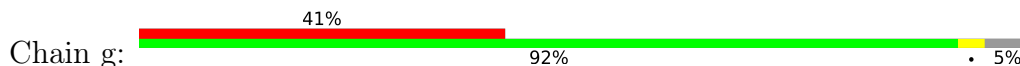




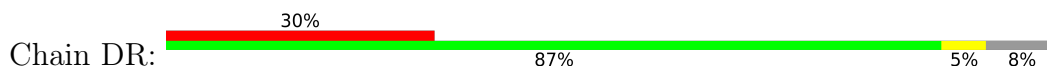
- Molecule 75: 40S ribosomal protein S29A



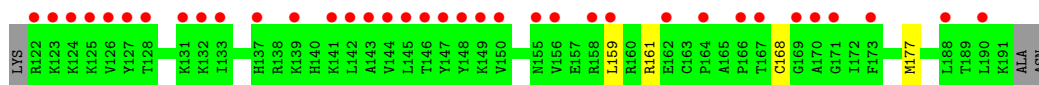
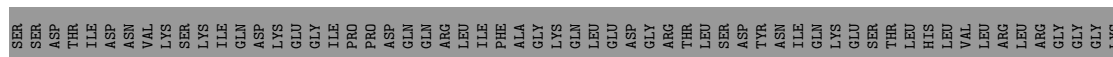
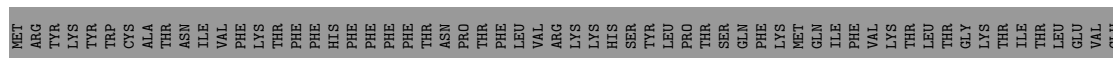
- Molecule 76: 40S ribosomal protein S30



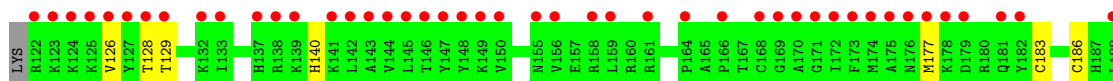
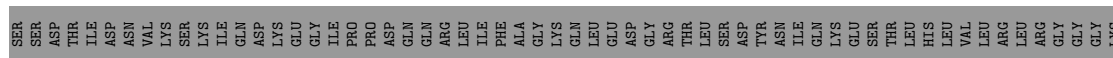
- Molecule 76: 40S ribosomal protein S30

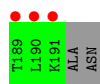


- Molecule 77: Ubiquitin-40S ribosomal protein S31 fusion protein

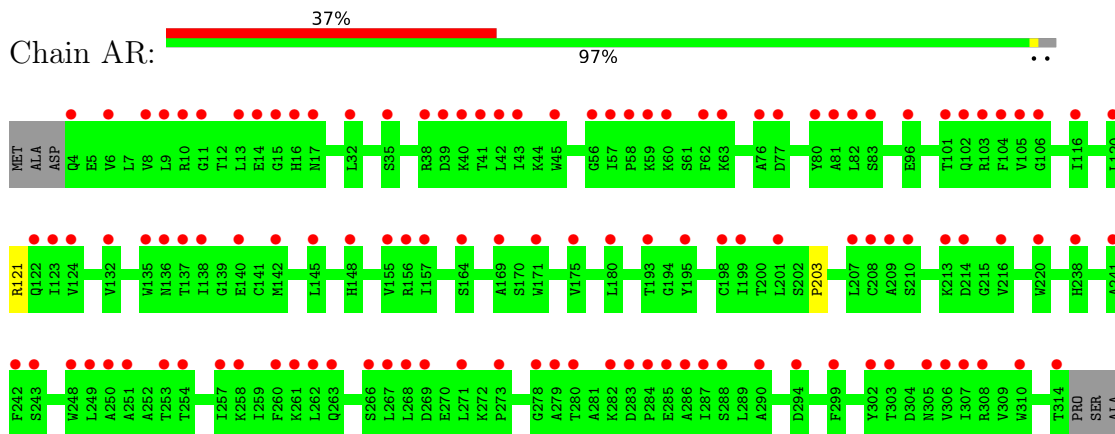


- Molecule 77: Ubiquitin-40S ribosomal protein S31 fusion protein

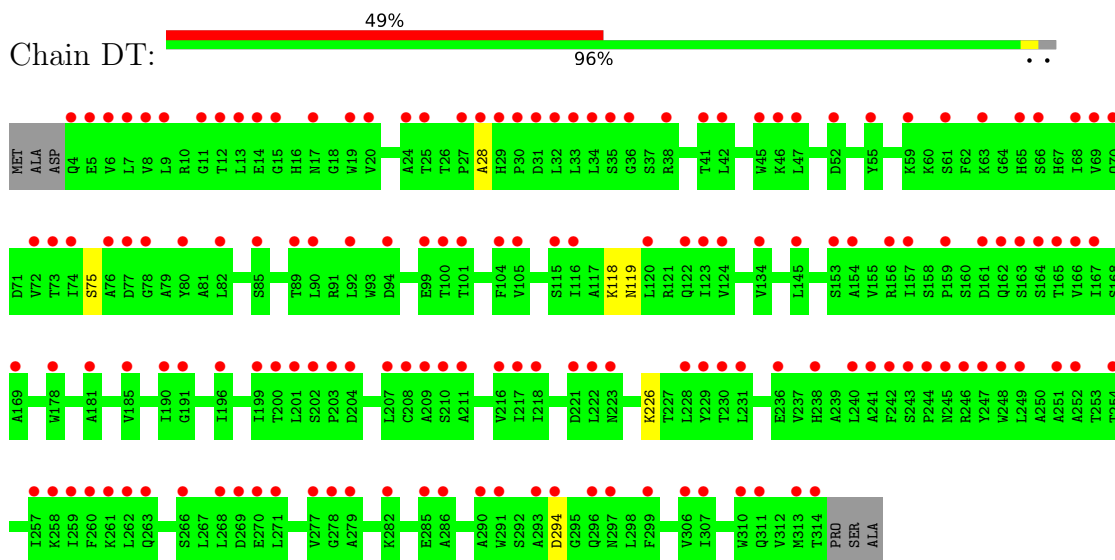




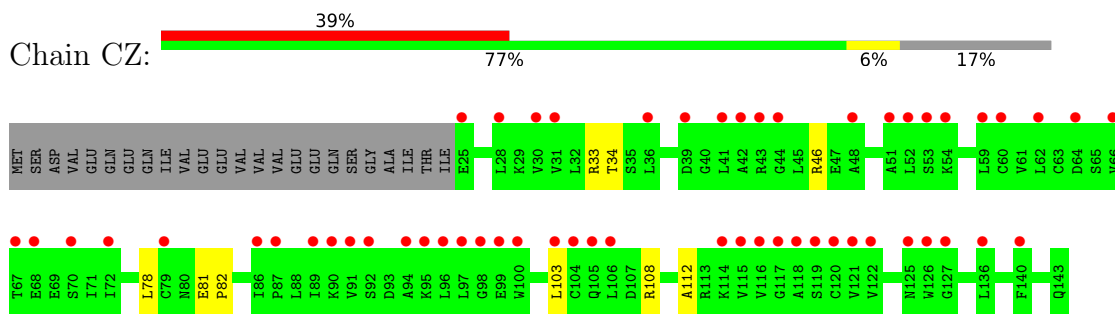
• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein



• Molecule 78: Guanine nucleotide-binding protein subunit beta-like protein

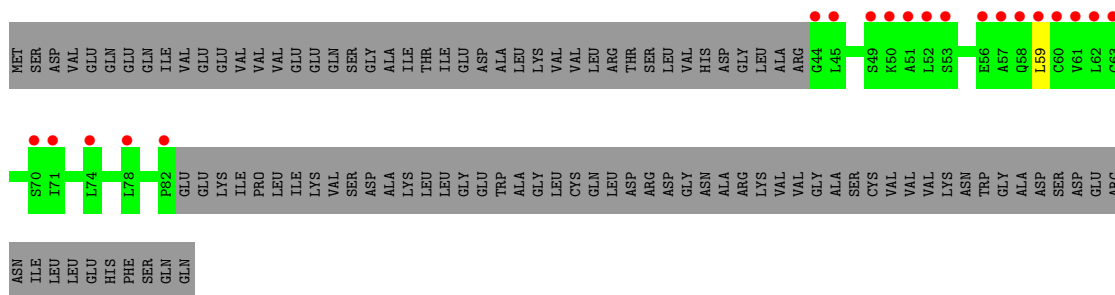


• Molecule 79: 40S ribosomal protein S12

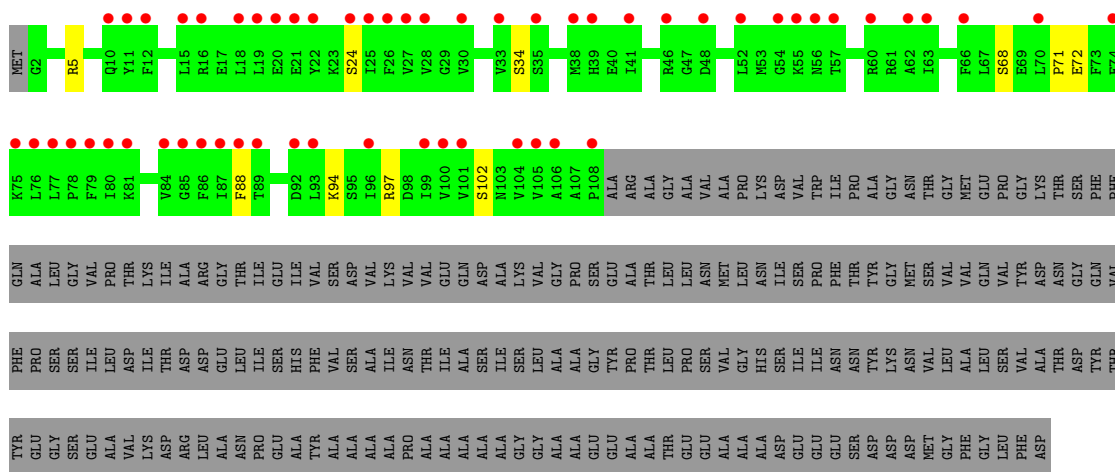


• Molecule 79: 40S ribosomal protein S12

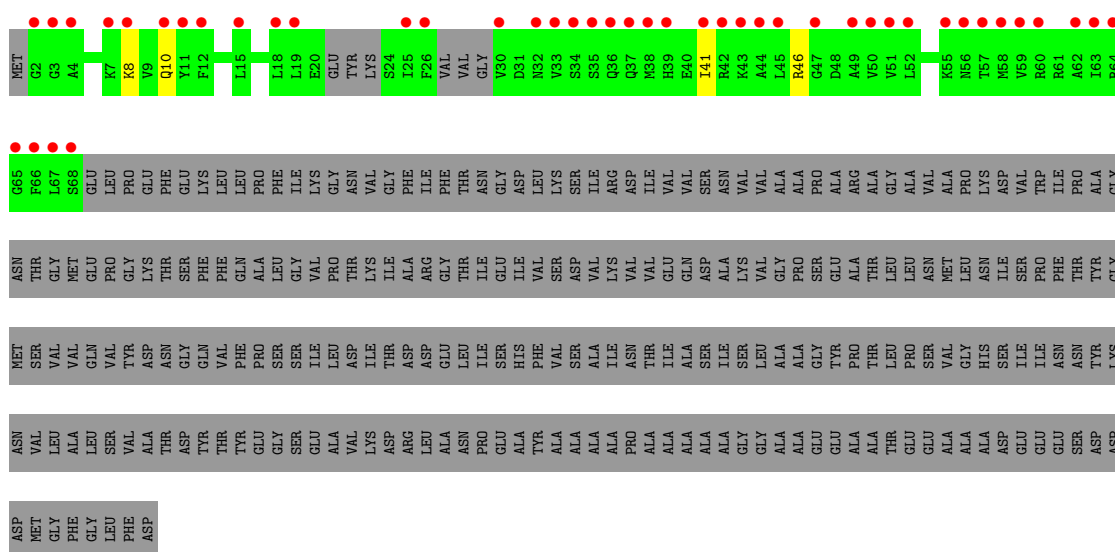




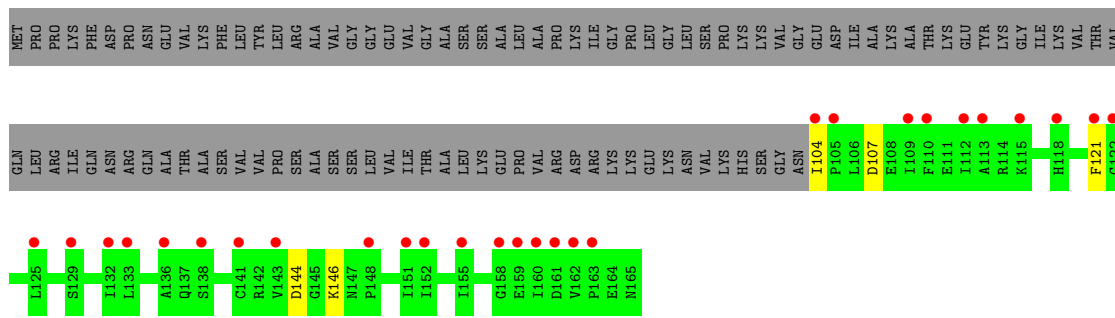
● Molecule 80: 60S acidic ribosomal protein P0



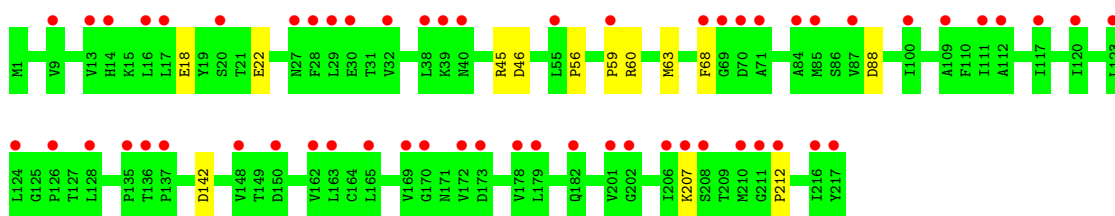
● Molecule 80: 60S acidic ribosomal protein P0



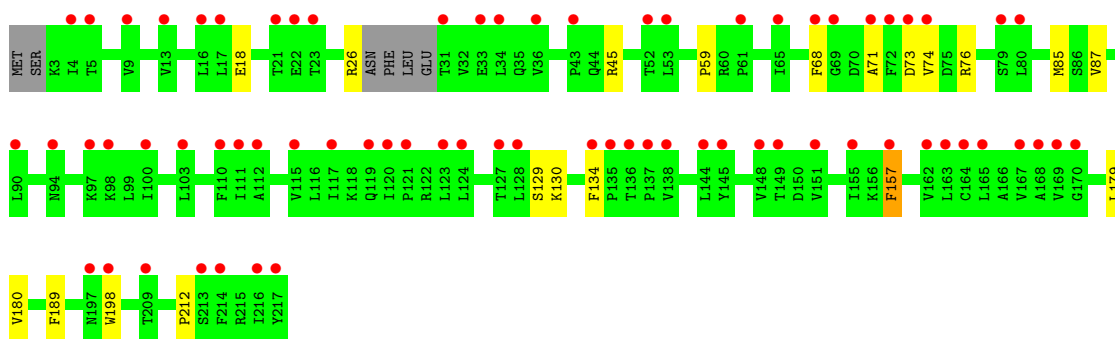
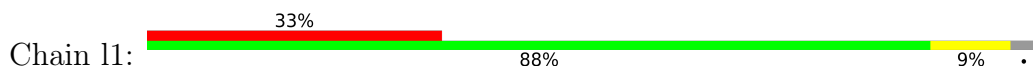
● Molecule 81: 60S ribosomal protein L12-A



• Molecule 82: Ribosomal protein



• Molecule 82: Ribosomal protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	299.77Å 294.17Å 451.17Å 90.00° 100.05° 90.00°	Depositor
Resolution (Å)	228.18 – 3.20 228.18 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (228.18-3.20) 91.7 (228.18-3.20)	Depositor EDS
$R_{merge}$	0.74	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, $R_{free}$	0.246 , 0.281 0.248 , 0.283	Depositor DCC
$R_{free}$ test set	2000 reflections (0.16%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtrriage
Anisotropy	0.105	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 40.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	408874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	94.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 i

### 5.1 Standard geometry i

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	1	0.32	0/76948	0.89	100/119959 (0.1%)
1	AS	0.31	0/77089	0.89	105/120181 (0.1%)
2	3	0.25	0/2884	0.76	0/4492
2	AT	0.26	0/2884	0.77	0/4492
3	4	0.25	0/3724	0.78	1/5798 (0.0%)
3	AU	0.26	0/3746	0.79	2/5832 (0.0%)
4	AW	0.28	0/1922	0.57	0/2581
4	j	0.27	0/1922	0.59	0/2581
5	AX	0.28	0/3145	0.58	0/4231
5	k	0.31	0/3156	0.59	0/4246
6	AY	0.26	0/2799	0.55	0/3777
6	l	0.28	0/2799	0.56	0/3777
7	AZ	0.26	0/2447	0.52	0/3294
7	m	0.27	0/2479	0.54	0/3337
8	BA	0.27	0/1231	0.55	0/1662
8	n	0.28	0/1263	0.56	0/1703
9	BB	0.27	0/1918	0.52	0/2575
9	o	0.29	0/1894	0.53	0/2542
10	BC	0.27	0/1835	0.50	0/2472
10	p	0.27	0/1869	0.51	0/2519
11	BD	0.26	0/1537	0.54	0/2067
11	q	0.28	0/1537	0.58	0/2067
12	BE	0.28	0/1724	0.57	0/2314
12	r	0.27	0/1724	0.57	0/2314
13	BF	0.27	0/1390	0.59	0/1861
13	s	0.27	0/1390	0.58	0/1861
14	BG	0.26	0/1637	0.55	0/2195
14	t	0.27	0/1637	0.57	0/2195
15	BH	0.26	0/1044	0.54	0/1407
15	u	0.27	0/1044	0.56	0/1407
16	BI	0.26	0/1753	0.60	0/2347
16	v	0.29	0/1753	0.62	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
17	BJ	0.28	0/1620	0.53	0/2167
17	w	0.28	0/1620	0.54	0/2167
18	BK	0.26	0/1429	0.58	0/1920
18	x	0.27	0/1410	0.58	0/1895
19	BL	0.27	0/1482	0.59	0/1985
19	y	0.28	0/1482	0.59	0/1985
20	BM	0.26	0/1475	0.60	0/1961
20	z	0.26	0/1475	0.60	0/1961
21	0	0.27	0/1457	0.58	0/1962
21	BN	0.27	0/1457	0.55	0/1962
22	2	0.28	0/1285	0.55	0/1723
22	BO	0.27	0/1285	0.53	0/1723
23	5	0.27	0/846	0.47	0/1140
23	BP	0.27	0/857	0.51	0/1156
24	6	0.28	0/993	0.58	0/1339
24	BQ	0.29	0/993	0.59	0/1339
25	7	0.27	0/958	0.53	0/1267
25	BR	0.26	0/814	0.55	0/1079
26	8	0.27	0/981	0.54	0/1326
26	BS	0.25	0/976	0.52	0/1319
27	9	0.26	0/999	0.54	0/1334
27	BT	0.25	0/999	0.53	0/1334
28	AA	0.27	0/1112	0.49	0/1488
28	BU	0.26	0/1112	0.49	0/1488
29	AB	0.26	0/1199	0.54	0/1607
29	BV	0.26	0/1199	0.54	0/1607
30	AC	0.25	0/483	0.60	0/642
30	BW	0.25	0/498	0.52	0/661
31	AD	0.27	0/738	0.49	0/994
31	BX	0.27	0/738	0.49	0/994
32	AE	0.26	0/907	0.57	1/1219 (0.1%)
32	BY	0.25	0/907	0.56	0/1219
33	AF	0.27	0/1021	0.54	0/1368
33	BZ	0.26	0/1025	0.56	0/1372
34	AG	0.29	0/866	0.54	0/1165
34	CA	0.28	0/866	0.54	0/1165
35	AH	0.26	0/896	0.58	0/1195
35	CB	0.25	0/896	0.58	0/1195
36	AI	0.25	0/1003	0.56	0/1336
36	CC	0.25	0/990	0.55	0/1319
37	AJ	0.26	0/741	0.56	0/984
37	CD	0.26	0/763	0.58	0/1012
38	AK	0.29	0/690	0.64	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
38	CE	0.26	0/690	0.60	0/916
39	AL	0.26	0/623	0.51	0/831
39	CF	0.30	0/623	0.57	0/831
40	AM	0.26	0/447	0.58	0/594
40	CG	0.26	0/447	0.64	0/594
41	AN	0.26	0/425	0.59	0/563
41	CH	0.32	0/417	0.65	0/553
42	AO	0.28	0/237	0.73	0/304
42	CI	0.27	0/228	0.71	0/293
43	AP	0.28	0/840	0.57	0/1110
43	CJ	0.29	0/840	0.55	0/1110
44	AQ	0.29	0/705	0.61	0/940
44	CK	0.26	0/705	0.59	0/940
45	CL	0.33	0/942	0.64	0/1258
45	i	0.30	0/942	0.66	0/1258
46	B	0.31	0/41860	0.94	87/65228 (0.1%)
46	CM	0.33	0/42081	0.94	77/65573 (0.1%)
47	C	0.25	0/1666	0.50	0/2273
47	CN	0.26	0/1666	0.51	0/2273
48	CO	0.26	0/1750	0.58	0/2354
48	D	0.25	0/1750	0.54	0/2354
49	CP	0.28	0/1657	0.53	0/2248
49	E	0.26	0/1657	0.51	0/2248
50	CQ	0.28	0/1731	0.63	2/2324 (0.1%)
50	F	0.27	0/1731	0.61	1/2324 (0.0%)
51	CR	0.27	0/2096	0.57	0/2822
51	G	0.26	0/2092	0.56	0/2817
52	CS	0.27	0/1631	0.54	0/2199
52	H	0.25	0/1631	0.56	0/2199
53	CT	0.28	0/1929	0.59	0/2571
53	I	0.26	0/1845	0.56	0/2464
54	CU	0.26	0/1499	0.56	0/2016
54	J	0.26	0/1516	0.55	0/2039
55	CV	0.27	0/1606	0.60	0/2150
55	K	0.27	0/1606	0.60	0/2150
56	CW	0.26	0/1478	0.57	0/1978
56	L	0.26	0/1478	0.56	0/1978
57	CX	0.28	0/809	0.59	0/1092
57	M	0.29	0/803	0.62	0/1083
58	CY	0.28	0/1154	0.57	0/1553
58	N	0.27	0/1175	0.56	0/1582
59	DA	0.26	0/1210	0.54	0/1631
59	P	0.24	0/1210	0.50	0/1631



Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
60	DB	0.29	0/953	0.67	0/1279
60	Q	0.31	0/953	0.66	1/1279 (0.1%)
61	DC	0.29	0/1049	0.61	0/1409
61	R	0.31	0/1038	0.62	1/1395 (0.1%)
62	DD	0.25	0/1109	0.54	0/1486
62	S	0.28	0/1109	0.55	0/1486
63	DE	0.28	0/1009	0.63	0/1354
63	T	0.28	0/1009	0.69	1/1354 (0.1%)
64	DF	0.26	0/1178	0.59	0/1579
64	U	0.27	0/1205	0.58	0/1615
65	DG	0.27	0/1120	0.57	0/1508
65	V	0.27	0/1120	0.59	1/1508 (0.1%)
66	DH	0.27	0/772	0.60	1/1045 (0.1%)
66	W	0.25	0/818	0.57	0/1106
67	DI	0.28	0/683	0.59	0/918
67	X	0.26	0/683	0.57	0/918
68	DJ	0.30	0/1049	0.57	0/1412
68	Y	0.25	0/1049	0.55	0/1412
69	DK	0.28	0/1128	0.60	0/1505
69	Z	0.27	0/1128	0.62	0/1505
70	DL	0.27	0/1086	0.58	0/1447
70	a	0.26	0/1100	0.57	0/1466
71	DM	0.26	0/577	0.56	0/778
71	b	0.26	0/585	0.52	0/789
72	DN	0.25	0/791	0.60	0/1060
72	c	0.26	0/791	0.61	0/1060
73	DO	0.27	0/624	0.56	0/843
73	d	0.26	0/624	0.52	0/843
74	DP	0.27	0/478	0.69	0/640
74	e	0.26	0/489	0.69	0/654
75	DQ	0.32	0/461	0.60	0/613
75	f	0.28	0/466	0.58	0/620
76	DR	0.35	0/469	0.70	0/626
76	g	0.29	0/482	0.60	0/642
77	DS	0.32	0/585	0.78	1/778 (0.1%)
77	h	0.29	0/585	0.71	1/778 (0.1%)
78	AR	0.24	0/2451	0.54	0/3337
78	DT	0.28	0/2451	0.60	0/3337
79	CZ	0.30	0/921	0.85	2/1240 (0.2%)
79	O	0.30	0/293	0.68	1/393 (0.3%)
80	P0	0.26	0/857	0.58	0/1148
80	p0	0.35	0/489	0.73	0/645
81	12	0.32	0/478	0.50	0/642

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
82	L1	0.27	0/1737	0.53	0/2335
82	l1	0.28	0/1685	0.57	0/2264
All	All	0.30	0/436812	0.79	386/640723 (0.1%)

There are no bond length outliers.

The worst 5 of 386 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1576	A	O4'-C1'-N9	13.13	118.70	108.20
46	B	724	G	N3-C4-C5	-10.96	123.12	128.60
1	1	1576	A	C4-N9-C1'	9.66	143.69	126.30
79	CZ	81	GLU	C-N-CD	-9.52	99.65	120.60
46	CM	656	C	N1-C2-O2	9.30	124.48	118.90

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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

## 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%)	239 (97%)	8 (3%)	0	100	100
4	j	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
5	AX	384/389 (99%)	371 (97%)	13 (3%)	0	100	100
5	k	385/389 (99%)	372 (97%)	13 (3%)	0	100	100
6	AY	359/363 (99%)	349 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	l	359/363 (99%)	348 (97%)	11 (3%)	0	100	100
7	AZ	290/298 (97%)	278 (96%)	12 (4%)	0	100	100
7	m	294/298 (99%)	282 (96%)	12 (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	232/241 (96%)	226 (97%)	5 (2%)	1 (0%)	30	64
9	o	229/241 (95%)	222 (97%)	6 (3%)	1 (0%)	30	64
10	BC	231/262 (88%)	219 (95%)	10 (4%)	2 (1%)	14	49
10	p	236/262 (90%)	227 (96%)	8 (3%)	1 (0%)	30	64
11	BD	188/191 (98%)	181 (96%)	7 (4%)	0	100	100
11	q	188/191 (98%)	184 (98%)	4 (2%)	0	100	100
12	BE	204/220 (93%)	199 (98%)	5 (2%)	0	100	100
12	r	204/220 (93%)	201 (98%)	3 (2%)	0	100	100
13	BF	169/174 (97%)	162 (96%)	7 (4%)	0	100	100
13	s	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
14	BG	198/202 (98%)	194 (98%)	4 (2%)	0	100	100
14	t	198/202 (98%)	196 (99%)	2 (1%)	0	100	100
15	BH	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
15	u	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
16	BI	201/204 (98%)	198 (98%)	3 (2%)	0	100	100
16	v	201/204 (98%)	197 (98%)	4 (2%)	0	100	100
17	BJ	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
17	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	BK	172/185 (93%)	167 (97%)	5 (3%)	0	100	100
18	x	169/185 (91%)	166 (98%)	3 (2%)	0	100	100
19	BL	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
19	y	183/186 (98%)	179 (98%)	4 (2%)	0	100	100
20	BM	177/190 (93%)	173 (98%)	4 (2%)	0	100	100
20	z	177/190 (93%)	174 (98%)	3 (2%)	0	100	100
21	0	168/172 (98%)	166 (99%)	2 (1%)	0	100	100
21	BN	168/172 (98%)	166 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	2	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
22	BO	157/160 (98%)	154 (98%)	3 (2%)	0	100	100
23	5	101/124 (82%)	95 (94%)	5 (5%)	1 (1%)	13	47
23	BP	101/124 (82%)	88 (87%)	11 (11%)	2 (2%)	6	32
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%)	102 (90%)	11 (10%)	1 (1%)	14	49
25	BR	94/155 (61%)	90 (96%)	4 (4%)	0	100	100
26	8	118/142 (83%)	116 (98%)	2 (2%)	0	100	100
26	BS	117/142 (82%)	115 (98%)	2 (2%)	0	100	100
27	9	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
27	BT	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
28	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
28	BU	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	AB	146/149 (98%)	138 (94%)	8 (6%)	0	100	100
29	BV	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
30	AC	57/63 (90%)	54 (95%)	1 (2%)	2 (4%)	3	20
30	BW	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
31	AD	94/106 (89%)	93 (99%)	1 (1%)	0	100	100
31	BX	94/106 (89%)	92 (98%)	2 (2%)	0	100	100
32	AE	108/112 (96%)	106 (98%)	2 (2%)	0	100	100
32	BY	108/112 (96%)	103 (95%)	3 (3%)	2 (2%)	6	34
33	AF	122/131 (93%)	122 (100%)	0	0	100	100
33	BZ	122/131 (93%)	122 (100%)	0	0	100	100
34	AG	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
34	CA	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
35	AH	110/122 (90%)	108 (98%)	2 (2%)	0	100	100
35	CB	110/122 (90%)	107 (97%)	3 (3%)	0	100	100
36	AI	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
36	CC	116/120 (97%)	114 (98%)	2 (2%)	0	100	100
37	AJ	93/99 (94%)	92 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	CD	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
38	AK	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
38	CE	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
39	AL	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
39	CF	75/78 (96%)	67 (89%)	8 (11%)	0	100	100
40	AM	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5	31
40	CG	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
41	AN	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
41	CH	49/52 (94%)	45 (92%)	1 (2%)	3 (6%)	1	9
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	CI	22/25 (88%)	22 (100%)	0	0	100	100
43	AP	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
43	CJ	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
44	CK	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	CL	117/267 (44%)	91 (78%)	23 (20%)	3 (3%)	4	27
45	i	117/267 (44%)	93 (80%)	20 (17%)	4 (3%)	3	21
47	C	206/261 (79%)	201 (98%)	5 (2%)	0	100	100
47	CN	206/261 (79%)	198 (96%)	8 (4%)	0	100	100
48	CO	212/256 (83%)	204 (96%)	8 (4%)	0	100	100
48	D	212/256 (83%)	207 (98%)	5 (2%)	0	100	100
49	CP	215/249 (86%)	209 (97%)	6 (3%)	0	100	100
49	E	215/249 (86%)	210 (98%)	5 (2%)	0	100	100
50	CQ	221/251 (88%)	211 (96%)	10 (4%)	0	100	100
50	F	221/251 (88%)	213 (96%)	8 (4%)	0	100	100
51	CR	258/262 (98%)	251 (97%)	7 (3%)	0	100	100
51	G	257/262 (98%)	253 (98%)	4 (2%)	0	100	100
52	CS	204/225 (91%)	197 (97%)	7 (3%)	0	100	100
52	H	204/225 (91%)	193 (95%)	11 (5%)	0	100	100
53	CT	234/236 (99%)	230 (98%)	4 (2%)	0	100	100
53	I	224/236 (95%)	220 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	CU	181/186 (97%)	171 (94%)	9 (5%)	1 (1%)	22	57
54	J	183/186 (98%)	171 (93%)	12 (7%)	0	100	100
55	CV	201/206 (98%)	199 (99%)	2 (1%)	0	100	100
55	K	201/206 (98%)	200 (100%)	1 (0%)	0	100	100
56	CW	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
56	L	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
57	CX	92/118 (78%)	86 (94%)	6 (6%)	0	100	100
57	M	90/118 (76%)	78 (87%)	12 (13%)	0	100	100
58	CY	139/155 (90%)	133 (96%)	5 (4%)	1 (1%)	19	54
58	N	142/155 (92%)	137 (96%)	5 (4%)	0	100	100
59	DA	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
59	P	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
60	DB	125/132 (95%)	120 (96%)	4 (3%)	1 (1%)	16	51
60	Q	125/132 (95%)	119 (95%)	5 (4%)	1 (1%)	16	51
61	DC	128/142 (90%)	108 (84%)	20 (16%)	0	100	100
61	R	127/142 (89%)	115 (91%)	11 (9%)	1 (1%)	16	51
62	DD	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
62	S	138/142 (97%)	133 (96%)	4 (3%)	1 (1%)	19	54
63	DE	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
63	T	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
64	DF	139/145 (96%)	132 (95%)	6 (4%)	1 (1%)	19	54
64	U	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
65	DG	139/145 (96%)	133 (96%)	5 (4%)	1 (1%)	19	54
65	V	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
66	DH	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
66	W	100/119 (84%)	97 (97%)	3 (3%)	0	100	100
67	DI	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
67	X	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	DJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
68	Y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
69	DK	141/145 (97%)	139 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
69	Z	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
70	DL	130/135 (96%)	130 (100%)	0	0	100	100
70	a	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
71	DM	69/105 (66%)	64 (93%)	5 (7%)	0	100	100
71	b	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
72	DN	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
72	c	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
73	DO	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
73	d	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
74	DP	59/67 (88%)	52 (88%)	7 (12%)	0	100	100
74	e	60/67 (90%)	57 (95%)	3 (5%)	0	100	100
75	DQ	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
75	f	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
76	DR	56/63 (89%)	50 (89%)	6 (11%)	0	100	100
76	g	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
77	DS	68/193 (35%)	57 (84%)	10 (15%)	1 (2%)	8	38
77	h	68/193 (35%)	54 (79%)	13 (19%)	1 (2%)	8	38
78	AR	309/317 (98%)	292 (94%)	16 (5%)	1 (0%)	37	69
78	DT	309/317 (98%)	284 (92%)	23 (7%)	2 (1%)	22	57
79	CZ	117/143 (82%)	89 (76%)	23 (20%)	5 (4%)	2	16
79	O	37/143 (26%)	32 (86%)	5 (14%)	0	100	100
80	P0	105/312 (34%)	81 (77%)	20 (19%)	4 (4%)	2	18
80	p0	55/312 (18%)	34 (62%)	19 (34%)	2 (4%)	3	20
81	12	60/165 (36%)	37 (62%)	23 (38%)	0	100	100
82	L1	215/217 (99%)	163 (76%)	48 (22%)	4 (2%)	6	34
82	l1	207/217 (95%)	118 (57%)	80 (39%)	9 (4%)	2	16
All	All	22661/25499 (89%)	21655 (96%)	945 (4%)	61 (0%)	37	69

5 of 61 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	p	205	ASN
30	AC	21	ILE

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Mol	Chain	Res	Type
40	AM	49	LEU
45	i	55	LYS
45	i	64	LEU

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AW	190/194 (98%)	188 (99%)	2 (1%)	70	86
4	j	190/194 (98%)	189 (100%)	1 (0%)	86	93
5	AX	325/328 (99%)	323 (99%)	2 (1%)	84	92
5	k	326/328 (99%)	325 (100%)	1 (0%)	91	96
6	AY	290/292 (99%)	287 (99%)	3 (1%)	73	87
6	l	290/292 (99%)	288 (99%)	2 (1%)	81	92
7	AZ	247/252 (98%)	244 (99%)	3 (1%)	67	85
7	m	250/252 (99%)	249 (100%)	1 (0%)	89	94
8	BA	132/154 (86%)	132 (100%)	0	100	100
8	n	136/154 (88%)	135 (99%)	1 (1%)	81	92
9	BB	198/204 (97%)	198 (100%)	0	100	100
9	o	195/204 (96%)	194 (100%)	1 (0%)	86	93
10	BC	193/216 (89%)	190 (98%)	3 (2%)	58	79
10	p	198/216 (92%)	197 (100%)	1 (0%)	86	93
11	BD	169/170 (99%)	169 (100%)	0	100	100
11	q	169/170 (99%)	168 (99%)	1 (1%)	84	92
12	BE	178/186 (96%)	177 (99%)	1 (1%)	84	92
12	r	178/186 (96%)	176 (99%)	2 (1%)	70	86
13	BF	146/149 (98%)	144 (99%)	2 (1%)	62	82
13	s	146/149 (98%)	144 (99%)	2 (1%)	62	82
14	BG	166/168 (99%)	164 (99%)	2 (1%)	67	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	t	166/168 (99%)	165 (99%)	1 (1%)	84	92
15	BH	108/109 (99%)	107 (99%)	1 (1%)	75	89
15	u	108/109 (99%)	108 (100%)	0	100	100
16	BI	177/178 (99%)	176 (99%)	1 (1%)	84	92
16	v	177/178 (99%)	176 (99%)	1 (1%)	84	92
17	BJ	166/167 (99%)	166 (100%)	0	100	100
17	w	166/167 (99%)	166 (100%)	0	100	100
18	BK	145/154 (94%)	142 (98%)	3 (2%)	48	74
18	x	144/154 (94%)	144 (100%)	0	100	100
19	BL	153/154 (99%)	153 (100%)	0	100	100
19	y	153/154 (99%)	153 (100%)	0	100	100
20	BM	146/153 (95%)	142 (97%)	4 (3%)	40	69
20	z	146/153 (95%)	146 (100%)	0	100	100
21	0	155/157 (99%)	154 (99%)	1 (1%)	84	92
21	BN	155/157 (99%)	155 (100%)	0	100	100
22	2	133/134 (99%)	133 (100%)	0	100	100
22	BO	133/134 (99%)	132 (99%)	1 (1%)	79	90
23	5	93/112 (83%)	93 (100%)	0	100	100
23	BP	94/112 (84%)	90 (96%)	4 (4%)	25	57
24	6	101/104 (97%)	101 (100%)	0	100	100
24	BQ	101/104 (97%)	101 (100%)	0	100	100
25	7	97/127 (76%)	95 (98%)	2 (2%)	48	74
25	BR	86/127 (68%)	84 (98%)	2 (2%)	45	72
26	8	107/121 (88%)	105 (98%)	2 (2%)	52	76
26	BS	107/121 (88%)	107 (100%)	0	100	100
27	9	111/112 (99%)	110 (99%)	1 (1%)	75	89
27	BT	111/112 (99%)	110 (99%)	1 (1%)	75	89
28	AA	117/118 (99%)	117 (100%)	0	100	100
28	BU	117/118 (99%)	116 (99%)	1 (1%)	75	89
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	46/49 (94%)	46 (100%)	0	100	100
30	BW	48/49 (98%)	48 (100%)	0	100	100
31	AD	81/90 (90%)	81 (100%)	0	100	100
31	BX	81/90 (90%)	81 (100%)	0	100	100
32	AE	98/100 (98%)	97 (99%)	1 (1%)	73	87
32	BY	98/100 (98%)	98 (100%)	0	100	100
33	AF	109/115 (95%)	109 (100%)	0	100	100
33	BZ	110/115 (96%)	110 (100%)	0	100	100
34	AG	91/92 (99%)	90 (99%)	1 (1%)	70	86
34	CA	91/92 (99%)	91 (100%)	0	100	100
35	AH	95/102 (93%)	93 (98%)	2 (2%)	48	74
35	CB	95/102 (93%)	95 (100%)	0	100	100
36	AI	106/106 (100%)	105 (99%)	1 (1%)	75	89
36	CC	105/106 (99%)	103 (98%)	2 (2%)	52	76
37	AJ	75/79 (95%)	75 (100%)	0	100	100
37	CD	77/79 (98%)	77 (100%)	0	100	100
38	AK	70/73 (96%)	70 (100%)	0	100	100
38	CE	70/73 (96%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	68 (100%)	0	100	100
39	CF	68/69 (99%)	68 (100%)	0	100	100
40	AM	46/47 (98%)	46 (100%)	0	100	100
40	CG	46/47 (98%)	45 (98%)	1 (2%)	47	73
41	AN	47/47 (100%)	47 (100%)	0	100	100
41	CH	46/47 (98%)	45 (98%)	1 (2%)	47	73
42	AO	24/24 (100%)	22 (92%)	2 (8%)	9	35
42	CI	23/24 (96%)	22 (96%)	1 (4%)	25	57
43	AP	88/91 (97%)	88 (100%)	0	100	100
43	CJ	88/91 (97%)	87 (99%)	1 (1%)	70	86
44	AQ	72/73 (99%)	72 (100%)	0	100	100
44	CK	72/73 (99%)	72 (100%)	0	100	100
45	CL	100/212 (47%)	99 (99%)	1 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	i	100/212 (47%)	99 (99%)	1 (1%)	73	87
47	C	176/215 (82%)	175 (99%)	1 (1%)	84	92
47	CN	176/215 (82%)	174 (99%)	2 (1%)	70	86
48	CO	194/229 (85%)	192 (99%)	2 (1%)	73	87
48	D	194/229 (85%)	193 (100%)	1 (0%)	86	93
49	CP	175/198 (88%)	173 (99%)	2 (1%)	70	86
49	E	175/198 (88%)	175 (100%)	0	100	100
50	CQ	174/196 (89%)	171 (98%)	3 (2%)	56	78
50	F	174/196 (89%)	172 (99%)	2 (1%)	70	86
51	CR	218/220 (99%)	217 (100%)	1 (0%)	86	93
51	G	218/220 (99%)	217 (100%)	1 (0%)	86	93
52	CS	178/197 (90%)	175 (98%)	3 (2%)	56	78
52	H	178/197 (90%)	176 (99%)	2 (1%)	70	86
53	CT	204/204 (100%)	202 (99%)	2 (1%)	73	87
53	I	195/204 (96%)	191 (98%)	4 (2%)	48	74
54	CU	164/167 (98%)	163 (99%)	1 (1%)	84	92
54	J	166/167 (99%)	166 (100%)	0	100	100
55	CV	157/160 (98%)	157 (100%)	0	100	100
55	K	157/160 (98%)	156 (99%)	1 (1%)	84	92
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	86/104 (83%)	86 (100%)	0	100	100
58	CY	122/134 (91%)	121 (99%)	1 (1%)	79	90
58	N	124/134 (92%)	122 (98%)	2 (2%)	58	79
59	DA	129/130 (99%)	128 (99%)	1 (1%)	79	90
59	P	129/130 (99%)	129 (100%)	0	100	100
60	DB	97/102 (95%)	97 (100%)	0	100	100
60	Q	97/102 (95%)	94 (97%)	3 (3%)	35	66
61	DC	112/121 (93%)	110 (98%)	2 (2%)	54	77
61	R	111/121 (92%)	109 (98%)	2 (2%)	54	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
62	DD	114/116 (98%)	113 (99%)	1 (1%)	75	89
62	S	114/116 (98%)	112 (98%)	2 (2%)	54	77
63	DE	112/122 (92%)	112 (100%)	0	100	100
63	T	112/122 (92%)	110 (98%)	2 (2%)	54	77
64	DF	125/129 (97%)	123 (98%)	2 (2%)	58	79
64	U	128/129 (99%)	126 (98%)	2 (2%)	58	79
65	DG	113/117 (97%)	113 (100%)	0	100	100
65	V	113/117 (97%)	113 (100%)	0	100	100
66	DH	87/105 (83%)	85 (98%)	2 (2%)	45	72
66	W	92/105 (88%)	89 (97%)	3 (3%)	33	64
67	DI	71/71 (100%)	70 (99%)	1 (1%)	62	82
67	X	71/71 (100%)	71 (100%)	0	100	100
68	DJ	112/113 (99%)	111 (99%)	1 (1%)	75	89
68	Y	112/113 (99%)	112 (100%)	0	100	100
69	DK	116/118 (98%)	114 (98%)	2 (2%)	56	78
69	Z	116/118 (98%)	116 (100%)	0	100	100
70	DL	109/112 (97%)	109 (100%)	0	100	100
70	a	111/112 (99%)	110 (99%)	1 (1%)	75	89
71	DM	63/85 (74%)	62 (98%)	1 (2%)	58	79
71	b	64/85 (75%)	64 (100%)	0	100	100
72	DN	84/102 (82%)	84 (100%)	0	100	100
72	c	84/102 (82%)	82 (98%)	2 (2%)	44	71
73	DO	72/73 (99%)	72 (100%)	0	100	100
73	d	72/73 (99%)	71 (99%)	1 (1%)	62	82
74	DP	53/58 (91%)	53 (100%)	0	100	100
74	e	54/58 (93%)	54 (100%)	0	100	100
75	DQ	47/48 (98%)	46 (98%)	1 (2%)	48	74
75	f	47/48 (98%)	46 (98%)	1 (2%)	48	74
76	DR	50/54 (93%)	47 (94%)	3 (6%)	16	48
76	g	51/54 (94%)	49 (96%)	2 (4%)	27	60
77	DS	62/175 (35%)	57 (92%)	5 (8%)	9	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	h	62/175 (35%)	60 (97%)	2 (3%)	34	65
78	AR	259/263 (98%)	258 (100%)	1 (0%)	89	94
78	DT	259/263 (98%)	255 (98%)	4 (2%)	60	81
79	CZ	101/123 (82%)	99 (98%)	2 (2%)	50	75
79	O	34/123 (28%)	34 (100%)	0	100	100
80	P0	92/247 (37%)	86 (94%)	6 (6%)	14	45
80	p0	52/247 (21%)	50 (96%)	2 (4%)	28	60
81	12	52/137 (38%)	47 (90%)	5 (10%)	7	28
82	L1	196/196 (100%)	187 (95%)	9 (5%)	23	56
82	l1	190/196 (97%)	178 (94%)	12 (6%)	15	46
All	All	19461/21471 (91%)	19272 (99%)	189 (1%)	73	87

5 of 189 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
49	CP	136	ARG
76	DR	31	GLN
51	CR	10	LYS
61	DC	36	LEU
77	DS	186	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
62	DD	138	GLN
71	DM	38	HIS
82	L1	182	GLN
62	S	39	GLN
61	R	103	ASN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3212/3359 (95%)	614 (19%)	45 (1%)
1	AS	3219/3359 (95%)	618 (19%)	50 (1%)
2	3	120/121 (99%)	9 (7%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	AT	120/121 (99%)	9 (7%)	0
3	4	156/158 (98%)	23 (14%)	3 (1%)
3	AU	157/158 (99%)	23 (14%)	3 (1%)
46	B	1753/1787 (98%)	447 (25%)	45 (2%)
46	CM	1762/1787 (98%)	454 (25%)	54 (3%)
All	All	10499/10850 (96%)	2197 (20%)	200 (1%)

5 of 2197 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 200 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AS	2090	U
3	AU	85	G
46	CM	1581	G
1	AS	2431	U
1	AS	2519	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 1676 ligands modelled in this entry, 1674 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
83	3K5	AS	3401	-	62,63,63	2.83	28 (45%)	82,95,95	1.67	12 (14%)
83	3K5	1	3401	-	62,63,63	2.85	27 (43%)	82,95,95	1.68	17 (20%)

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	-	-	11/29/121/121	0/7/7/7
83	3K5	1	3401	-	-	11/29/121/121	0/7/7/7

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
83	1	3401	3K5	C17-C22	-9.20	1.36	1.53
83	AS	3401	3K5	C17-C22	-7.96	1.38	1.53
83	1	3401	3K5	O4-C22	7.38	1.59	1.43
83	AS	3401	3K5	O4-C22	7.14	1.59	1.43
83	1	3401	3K5	C21-C22	5.98	1.63	1.52

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	AS	3401	3K5	O14-C38-C39	5.41	121.04	111.09
83	1	3401	3K5	O14-C38-C39	4.92	120.15	111.09
83	AS	3401	3K5	C2-O-C3	-4.88	110.21	113.66
83	AS	3401	3K5	O9-C30-C31	4.88	120.07	111.09
83	AS	3401	3K5	C8-C7-C6	-4.40	108.84	122.26

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	1	3401	3K5	C4-C5-O1-C6
83	1	3401	3K5	C7-C6-O1-C5
83	1	3401	3K5	C31-C30-O9-C26

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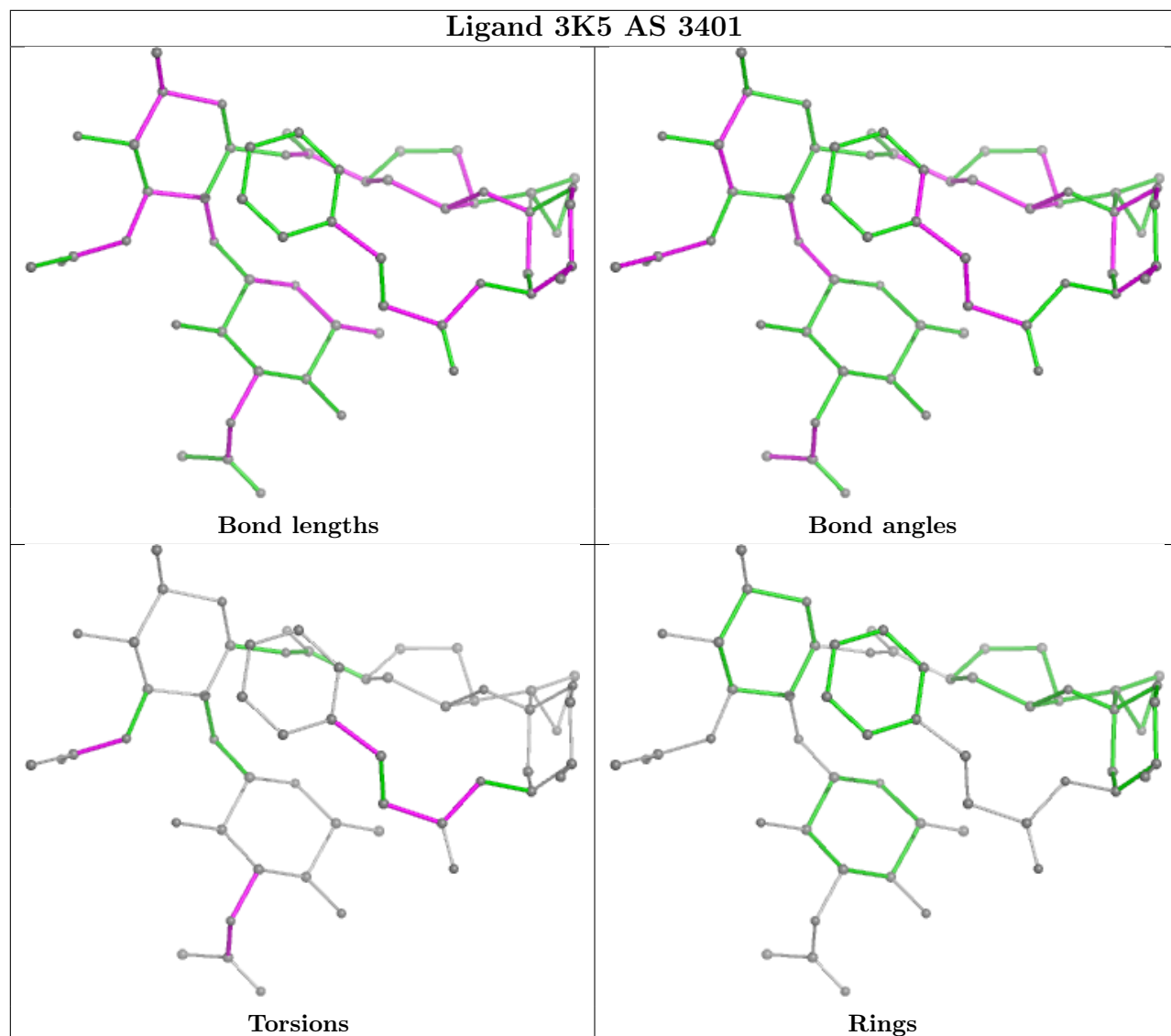
<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atoms</b>
83	AS	3401	3K5	C39-C38-O14-C34
83	AS	3401	3K5	C35-C34-O14-C38

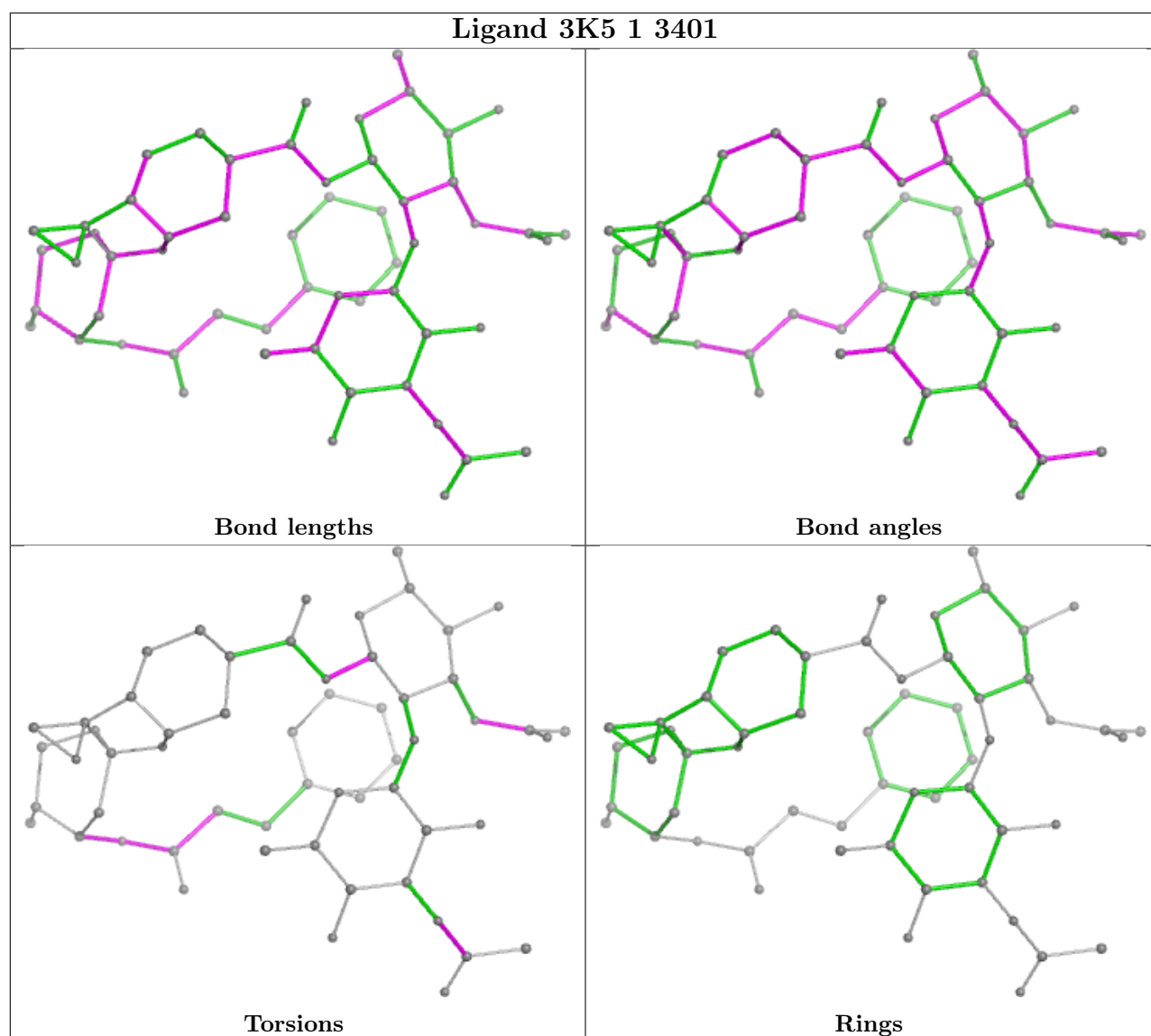
There are no ring outliers.

No monomer is involved in short contacts.

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







## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	1	3216/3359 (95%)	0.47	248 (7%) 21 14	36, 65, 187, 389	0
1	AS	3222/3359 (95%)	0.77	364 (11%) 11 8	44, 79, 214, 339	0
2	3	121/121 (100%)	0.19	1 (0%) 82 70	44, 80, 102, 135	0
2	AT	121/121 (100%)	0.63	6 (4%) 35 24	45, 79, 104, 152	0
3	4	157/158 (99%)	0.18	3 (1%) 66 50	50, 69, 125, 185	0
3	AU	158/158 (100%)	0.90	14 (8%) 17 12	65, 101, 152, 231	0
4	AW	249/254 (98%)	1.14	51 (20%) 3 3	45, 83, 111, 135	0
4	j	249/254 (98%)	0.81	24 (9%) 15 10	35, 56, 84, 174	0
5	AX	386/389 (99%)	0.71	25 (6%) 26 18	45, 69, 103, 162	0
5	k	386/389 (99%)	0.64	21 (5%) 32 22	34, 60, 83, 137	1 (0%)
6	AY	361/363 (99%)	2.05	126 (34%) 1 1	54, 85, 119, 141	0
6	l	361/363 (99%)	1.07	50 (13%) 7 5	34, 73, 112, 147	0
7	AZ	292/298 (97%)	1.92	111 (38%) 1 1	52, 105, 142, 169	0
7	m	296/298 (99%)	1.54	77 (26%) 2 2	56, 92, 128, 151	0
8	BA	153/176 (86%)	1.00	19 (12%) 9 7	60, 84, 116, 152	0
8	n	157/176 (89%)	1.03	22 (14%) 7 5	55, 80, 115, 153	0
9	BB	234/241 (97%)	0.77	23 (9%) 14 10	45, 66, 125, 183	0
9	o	231/241 (95%)	0.63	11 (4%) 36 25	44, 61, 113, 169	0
10	BC	233/262 (88%)	1.86	85 (36%) 1 1	100, 135, 171, 191	0
10	p	238/262 (90%)	1.21	48 (20%) 3 3	60, 86, 141, 178	0
11	BD	190/191 (99%)	1.31	38 (20%) 3 3	66, 88, 121, 160	0
11	q	190/191 (99%)	0.76	11 (5%) 30 20	56, 81, 111, 143	0
12	BE	208/220 (94%)	0.83	22 (10%) 13 9	40, 62, 116, 155	0
12	r	208/220 (94%)	1.07	30 (14%) 7 5	39, 64, 104, 125	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	BF	171/174 (98%)	1.56	38 (22%) 3 2	64, 95, 130, 147	0
13	s	171/174 (98%)	1.27	34 (19%) 3 3	62, 95, 119, 138	0
14	BG	200/202 (99%)	1.56	59 (29%) 1 1	51, 105, 142, 162	0
14	t	200/202 (99%)	1.05	28 (14%) 7 5	47, 79, 127, 156	0
15	BH	130/131 (99%)	0.72	14 (10%) 12 9	59, 79, 110, 133	0
15	u	130/131 (99%)	0.44	5 (3%) 44 30	54, 71, 102, 124	0
16	BI	203/204 (99%)	1.76	69 (33%) 1 1	62, 96, 118, 126	0
16	v	203/204 (99%)	0.67	14 (6%) 24 17	36, 60, 78, 92	0
17	BJ	199/200 (99%)	0.74	24 (12%) 10 7	44, 60, 105, 139	0
17	w	199/200 (99%)	0.46	9 (4%) 39 26	39, 55, 93, 122	0
18	BK	176/185 (95%)	1.17	29 (16%) 5 4	49, 73, 105, 148	0
18	x	173/185 (93%)	0.93	18 (10%) 13 9	42, 63, 105, 130	0
19	BL	185/186 (99%)	1.35	35 (18%) 4 3	57, 80, 99, 112	0
19	y	185/186 (99%)	1.06	30 (16%) 5 4	44, 67, 88, 102	0
20	BM	179/190 (94%)	1.14	27 (15%) 6 5	67, 94, 154, 187	0
20	z	179/190 (94%)	1.09	30 (16%) 5 4	55, 75, 141, 155	0
21	0	170/172 (98%)	0.46	8 (4%) 37 25	49, 61, 87, 153	0
21	BN	170/172 (98%)	0.65	11 (6%) 26 18	50, 68, 93, 127	0
22	2	159/160 (99%)	0.88	18 (11%) 11 8	47, 63, 131, 153	0
22	BO	159/160 (99%)	1.17	25 (15%) 6 4	46, 67, 128, 158	0
23	5	103/124 (83%)	1.37	27 (26%) 2 2	93, 123, 153, 170	0
23	BP	102/124 (82%)	1.66	31 (30%) 1 1	99, 143, 163, 177	1 (0%)
24	6	131/137 (95%)	0.65	12 (9%) 16 11	42, 55, 84, 103	0
24	BQ	131/137 (95%)	0.95	17 (12%) 9 6	42, 61, 98, 112	0
25	7	118/155 (76%)	0.91	16 (13%) 8 6	43, 82, 135, 146	0
25	BR	98/155 (63%)	1.29	18 (18%) 4 3	57, 83, 141, 152	0
26	8	120/142 (84%)	1.00	14 (11%) 10 8	60, 78, 103, 121	0
26	BS	119/142 (83%)	1.52	26 (21%) 3 2	76, 109, 131, 142	0
27	9	126/127 (99%)	1.32	23 (18%) 4 3	53, 82, 109, 134	0
27	BT	126/127 (99%)	1.67	35 (27%) 2 1	67, 106, 142, 162	0
28	AA	135/136 (99%)	1.46	28 (20%) 3 3	66, 96, 118, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
28	BU	135/136 (99%)	1.89	57 (42%) 1 1	103, 132, 155, 181	0
29	AB	148/149 (99%)	0.80	11 (7%) 22 16	41, 65, 100, 127	0
29	BV	148/149 (99%)	1.54	44 (29%) 1 1	52, 85, 114, 133	0
30	AC	59/63 (93%)	1.58	17 (28%) 1 1	46, 77, 125, 141	0
30	BW	61/63 (96%)	2.19	27 (44%) 1 1	47, 86, 141, 156	0
31	AD	96/106 (90%)	0.68	5 (5%) 34 23	62, 84, 109, 129	0
31	BX	96/106 (90%)	1.22	16 (16%) 5 4	87, 125, 150, 159	0
32	AE	110/112 (98%)	0.95	8 (7%) 22 16	51, 71, 124, 159	0
32	BY	110/112 (98%)	1.21	18 (16%) 5 4	56, 88, 129, 160	0
33	AF	124/131 (94%)	1.11	18 (14%) 7 5	42, 65, 86, 97	0
33	BZ	124/131 (94%)	1.61	35 (28%) 1 1	45, 75, 102, 119	0
34	AG	106/107 (99%)	0.67	6 (5%) 30 20	48, 61, 79, 95	0
34	CA	106/107 (99%)	0.63	7 (6%) 26 17	48, 64, 80, 99	0
35	AH	112/122 (91%)	1.46	28 (25%) 2 2	53, 77, 130, 148	0
35	CB	112/122 (91%)	2.03	45 (40%) 1 1	72, 111, 154, 174	0
36	AI	120/120 (100%)	1.22	18 (15%) 6 5	68, 89, 119, 150	0
36	CC	118/120 (98%)	2.06	51 (43%) 1 1	92, 117, 142, 151	0
37	AJ	95/99 (95%)	0.61	3 (3%) 50 35	60, 76, 105, 144	0
37	CD	97/99 (97%)	1.64	31 (31%) 1 1	90, 110, 148, 165	0
38	AK	86/90 (95%)	0.95	12 (13%) 7 5	44, 58, 102, 122	0
38	CE	86/90 (95%)	1.62	26 (30%) 1 1	53, 78, 122, 147	0
39	AL	77/78 (98%)	1.43	17 (22%) 3 2	86, 106, 146, 169	0
39	CF	77/78 (98%)	2.19	37 (48%) 0 1	102, 133, 167, 176	0
40	AM	50/51 (98%)	1.02	5 (10%) 14 10	53, 66, 92, 97	0
40	CG	50/51 (98%)	1.76	13 (26%) 2 2	70, 87, 104, 113	0
41	AN	52/52 (100%)	2.28	25 (48%) 0 1	104, 134, 149, 158	0
41	CH	51/52 (98%)	2.82	40 (78%) 0 0	109, 139, 156, 162	0
42	AO	25/25 (100%)	1.27	5 (20%) 3 3	60, 69, 83, 84	0
42	CI	24/25 (96%)	1.10	3 (12%) 9 7	55, 65, 79, 92	0
43	AP	103/106 (97%)	0.90	17 (16%) 5 4	36, 65, 116, 130	0
43	CJ	103/106 (97%)	1.12	19 (18%) 4 3	51, 77, 128, 139	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
44	AQ	91/92 (98%)	0.95	11 (12%) 10 7	43, 63, 102, 130	0
44	CK	91/92 (98%)	1.08	13 (14%) 7 5	58, 89, 124, 136	0
45	CL	121/267 (45%)	2.70	71 (58%) 0 1	66, 107, 141, 150	0
45	i	121/267 (45%)	2.00	51 (42%) 1 1	71, 111, 146, 151	0
46	B	1756/1787 (98%)	0.91	242 (13%) 8 5	45, 91, 186, 461	0
46	CM	1765/1787 (98%)	0.75	158 (8%) 17 11	42, 87, 190, 469	0
47	C	208/261 (79%)	1.65	61 (29%) 1 1	90, 123, 151, 168	0
47	CN	208/261 (79%)	1.43	47 (22%) 3 2	67, 109, 142, 181	0
48	CO	214/256 (83%)	1.63	55 (25%) 2 2	82, 131, 155, 182	0
48	D	214/256 (83%)	1.11	28 (13%) 8 6	72, 100, 123, 135	0
49	CP	217/249 (87%)	1.11	28 (12%) 9 6	51, 78, 111, 133	0
49	E	217/249 (87%)	1.83	67 (30%) 1 1	74, 102, 127, 150	0
50	CQ	223/251 (88%)	1.14	34 (15%) 6 5	60, 84, 150, 174	0
50	F	223/251 (88%)	1.79	70 (31%) 1 1	82, 112, 162, 180	0
51	CR	260/262 (99%)	1.49	63 (24%) 2 2	70, 95, 120, 158	0
51	G	259/262 (98%)	1.88	89 (34%) 1 1	71, 105, 131, 161	0
52	CS	206/225 (91%)	1.79	65 (31%) 1 1	82, 112, 155, 202	0
52	H	206/225 (91%)	1.38	50 (24%) 2 2	78, 107, 145, 178	0
53	CT	236/236 (100%)	1.59	62 (26%) 2 2	66, 109, 153, 171	0
53	I	226/236 (95%)	1.52	48 (21%) 3 2	63, 107, 150, 195	0
54	CU	183/186 (98%)	1.54	50 (27%) 2 2	74, 142, 181, 195	0
54	J	185/186 (99%)	1.95	69 (37%) 1 1	73, 140, 167, 181	0
55	CV	203/206 (98%)	1.75	75 (36%) 1 1	47, 79, 139, 171	0
55	K	203/206 (98%)	1.59	58 (28%) 1 1	51, 88, 132, 159	0
56	CW	178/189 (94%)	2.01	71 (39%) 1 1	73, 103, 132, 149	0
56	L	178/189 (94%)	2.47	99 (55%) 0 1	82, 115, 136, 153	0
57	CX	94/118 (79%)	1.06	15 (15%) 6 4	61, 103, 143, 162	0
57	M	94/118 (79%)	1.89	35 (37%) 1 1	86, 124, 148, 163	0
58	CY	141/155 (90%)	0.91	20 (14%) 7 5	47, 72, 107, 163	0
58	N	144/155 (92%)	1.26	25 (17%) 5 4	57, 84, 122, 155	0
59	DA	150/151 (99%)	1.12	22 (14%) 7 5	60, 99, 132, 157	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9	
59	P	150/151 (99%)	1.12	27 (18%)	4	4	62, 100, 122, 137	0
60	DB	127/132 (96%)	1.36	26 (20%)	3	3	61, 109, 139, 148	0
60	Q	127/132 (96%)	0.98	17 (13%)	8	6	56, 87, 110, 117	0
61	DC	130/142 (91%)	1.52	37 (28%)	1	1	69, 108, 136, 162	0
61	R	129/142 (90%)	1.36	30 (23%)	2	2	73, 101, 141, 161	0
62	DD	140/142 (98%)	1.63	36 (25%)	2	2	65, 109, 142, 157	0
62	S	140/142 (98%)	1.87	53 (37%)	1	1	76, 114, 150, 161	0
63	DE	124/137 (90%)	1.76	46 (37%)	1	1	71, 130, 174, 183	0
63	T	124/137 (90%)	1.90	45 (36%)	1	1	89, 132, 176, 183	0
64	DF	141/145 (97%)	1.60	38 (26%)	2	2	61, 109, 142, 171	0
64	U	144/145 (99%)	1.21	25 (17%)	5	4	69, 89, 124, 149	0
65	DG	141/145 (97%)	1.51	40 (28%)	1	1	69, 107, 138, 160	0
65	V	141/145 (97%)	1.24	26 (18%)	4	3	82, 106, 142, 164	0
66	DH	97/119 (81%)	1.28	14 (14%)	7	5	57, 109, 133, 152	0
66	W	102/119 (85%)	1.81	37 (36%)	1	1	76, 132, 155, 163	0
67	DI	87/87 (100%)	1.13	11 (12%)	9	7	72, 94, 129, 159	0
67	X	87/87 (100%)	1.17	13 (14%)	7	5	85, 113, 136, 147	0
68	DJ	129/130 (99%)	1.06	18 (13%)	7	5	57, 74, 95, 107	0
68	Y	129/130 (99%)	1.43	32 (24%)	2	2	75, 92, 115, 123	0
69	DK	143/145 (98%)	0.92	11 (7%)	21	14	47, 72, 98, 133	0
69	Z	143/145 (98%)	1.49	36 (25%)	2	2	64, 77, 96, 122	0
70	DL	132/135 (97%)	1.52	35 (26%)	2	2	89, 118, 145, 190	0
70	a	134/135 (99%)	1.84	48 (35%)	1	1	82, 121, 140, 154	0
71	DM	71/105 (67%)	1.65	22 (30%)	1	1	104, 137, 155, 161	0
71	b	72/105 (68%)	1.22	15 (20%)	3	3	93, 114, 141, 156	0
72	DN	98/119 (82%)	1.61	33 (33%)	1	1	69, 89, 146, 156	0
72	c	98/119 (82%)	1.70	25 (25%)	2	2	71, 92, 132, 153	0
73	DO	81/82 (98%)	1.52	23 (28%)	1	1	82, 112, 180, 193	0
73	d	81/82 (98%)	1.41	17 (20%)	3	3	84, 108, 165, 181	0
74	DP	61/67 (91%)	1.65	14 (22%)	2	2	90, 117, 147, 169	0
74	e	62/67 (92%)	2.09	24 (38%)	1	1	90, 117, 146, 156	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
75	DQ	54/56 (96%)	1.24	12 (22%) 3 2	54, 74, 106, 129	0
75	f	55/56 (98%)	1.27	10 (18%) 4 3	77, 92, 120, 142	0
76	DR	58/63 (92%)	1.85	19 (32%) 1 1	73, 109, 178, 188	0
76	g	60/63 (95%)	2.16	26 (43%) 1 1	82, 114, 166, 177	0
77	DS	70/193 (36%)	2.71	48 (68%) 0 0	106, 185, 202, 224	0
77	h	70/193 (36%)	2.24	36 (51%) 0 1	133, 179, 195, 202	0
78	AR	311/317 (98%)	1.80	118 (37%) 1 1	132, 165, 186, 202	0
78	DT	311/317 (98%)	2.09	154 (49%) 0 1	112, 162, 187, 201	0
79	CZ	119/143 (83%)	1.95	56 (47%) 0 1	142, 174, 188, 196	0
79	O	39/143 (27%)	2.06	20 (51%) 0 1	167, 186, 197, 206	0
80	P0	107/312 (34%)	2.35	57 (53%) 0 1	109, 124, 138, 165	0
80	p0	61/312 (19%)	3.11	45 (73%) 0 0	112, 126, 141, 145	0
81	12	62/165 (37%)	2.08	28 (45%) 1 1	103, 127, 146, 153	0
82	L1	217/217 (100%)	1.39	58 (26%) 2 2	101, 128, 165, 236	0
82	l1	211/217 (97%)	1.63	71 (33%) 1 1	111, 135, 155, 205	0
All	All	33513/36349 (92%)	1.15	6350 (18%) 4 3	34, 89, 165, 469	2 (0%)

The worst 5 of 6350 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	E	86	ARG	18.6
49	CP	86	ARG	14.3
1	AS	3319	U	13.9
6	AY	66	TRP	13.0
56	L	138	LYS	12.7

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
84	MG	1	3628	1/1	0.01	0.28	175,175,175,175	0
84	MG	1	3801	1/1	0.20	0.35	118,118,118,118	0
84	MG	B	1928	1/1	0.25	0.30	131,131,131,131	0
84	MG	AS	3649	1/1	0.46	0.26	83,83,83,83	0
84	MG	J	201	1/1	0.50	0.17	145,145,145,145	0
84	MG	AT	210	1/1	0.50	0.45	71,71,71,71	0
84	MG	B	1943	1/1	0.51	0.35	87,87,87,87	0
84	MG	1	3938	1/1	0.51	0.34	69,69,69,69	0
84	MG	AE	202	1/1	0.52	0.14	84,84,84,84	0
84	MG	AS	3590	1/1	0.53	0.40	96,96,96,96	0
84	MG	AS	3597	1/1	0.54	0.21	78,78,78,78	0
84	MG	B	1939	1/1	0.55	0.25	118,118,118,118	0
84	MG	2	201	1/1	0.56	0.39	95,95,95,95	0
84	MG	k	404	1/1	0.56	0.34	76,76,76,76	0
84	MG	AS	3586	1/1	0.57	0.36	77,77,77,77	0
84	MG	I	301	1/1	0.58	0.31	112,112,112,112	0
84	MG	B	1824	1/1	0.60	0.33	67,67,67,67	0
84	MG	AS	3662	1/1	0.61	0.30	88,88,88,88	0
84	MG	1	3593	1/1	0.61	0.35	94,94,94,94	0
85	ZN	DO	101	1/1	0.61	0.14	229,229,229,229	0
84	MG	CM	1813	1/1	0.62	0.37	57,57,57,57	0
84	MG	AS	3747	1/1	0.62	0.10	58,58,58,58	0
84	MG	1	3726	1/1	0.63	0.28	61,61,61,61	0
84	MG	AS	3628	1/1	0.63	0.19	49,49,49,49	0
84	MG	B	1836	1/1	0.63	0.21	287,287,287,287	0
84	MG	1	3808	1/1	0.63	0.32	102,102,102,102	0
84	MG	1	3874	1/1	0.64	0.29	57,57,57,57	0
84	MG	1	3513	1/1	0.65	0.34	44,44,44,44	0
84	MG	B	1946	1/1	0.66	0.32	78,78,78,78	0
84	MG	AS	3636	1/1	0.66	0.28	67,67,67,67	0
84	MG	B	1923	1/1	0.66	0.13	70,70,70,70	0
84	MG	CM	1871	1/1	0.66	0.32	89,89,89,89	0
84	MG	1	3921	1/1	0.66	0.22	80,80,80,80	0
84	MG	CM	1808	1/1	0.67	0.34	99,99,99,99	0
84	MG	AS	3634	1/1	0.67	0.36	69,69,69,69	0
84	MG	1	3826	1/1	0.67	0.17	43,43,43,43	0
85	ZN	CJ	201	1/1	0.67	0.19	255,255,255,255	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	B	1949	1/1	0.67	0.23	79,79,79,79	0
84	MG	1	3788	1/1	0.68	0.30	54,54,54,54	0
84	MG	1	3909	1/1	0.68	0.17	50,50,50,50	0
84	MG	1	3920	1/1	0.68	0.14	45,45,45,45	0
84	MG	CM	1879	1/1	0.68	0.26	63,63,63,63	0
84	MG	CM	1885	1/1	0.68	0.31	84,84,84,84	0
84	MG	w	303	1/1	0.68	0.28	86,86,86,86	0
84	MG	AS	3458	1/1	0.68	0.42	64,64,64,64	0
84	MG	1	3927	1/1	0.69	0.28	76,76,76,76	0
84	MG	3	202	1/1	0.69	0.27	83,83,83,83	0
84	MG	AS	3728	1/1	0.69	0.22	46,46,46,46	0
84	MG	B	1898	1/1	0.69	0.33	74,74,74,74	0
84	MG	1	3847	1/1	0.70	0.26	59,59,59,59	0
84	MG	BF	201	1/1	0.70	0.31	70,70,70,70	0
84	MG	1	3800	1/1	0.70	0.31	65,65,65,65	0
84	MG	B	1945	1/1	0.71	0.12	74,74,74,74	0
84	MG	AS	3661	1/1	0.71	0.47	75,75,75,75	0
84	MG	1	3584	1/1	0.71	0.28	52,52,52,52	0
84	MG	3	214	1/1	0.71	0.32	74,74,74,74	0
84	MG	B	1936	1/1	0.71	0.30	74,74,74,74	0
84	MG	1	3755	1/1	0.71	0.26	70,70,70,70	0
84	MG	B	1913	1/1	0.71	0.21	71,71,71,71	0
84	MG	AS	3501	1/1	0.72	0.45	64,64,64,64	0
84	MG	1	3754	1/1	0.72	0.31	76,76,76,76	0
84	MG	AS	3815	1/1	0.72	0.17	49,49,49,49	0
84	MG	1	4032	1/1	0.72	0.12	46,46,46,46	0
84	MG	B	1855	1/1	0.72	0.36	58,58,58,58	0
84	MG	B	1816	1/1	0.72	0.17	64,64,64,64	0
84	MG	AD	201	1/1	0.73	0.43	71,71,71,71	0
84	MG	BN	201	1/1	0.73	0.10	61,61,61,61	0
84	MG	1	3676	1/1	0.73	0.24	57,57,57,57	0
84	MG	y	202	1/1	0.73	0.14	63,63,63,63	0
84	MG	B	1907	1/1	0.73	0.11	47,47,47,47	0
84	MG	B	1941	1/1	0.73	0.27	94,94,94,94	0
84	MG	1	3728	1/1	0.73	0.31	49,49,49,49	0
84	MG	CM	1968	1/1	0.73	0.11	48,48,48,48	0
84	MG	AS	3820	1/1	0.73	0.20	50,50,50,50	0
84	MG	AS	3494	1/1	0.73	0.33	50,50,50,50	0
84	MG	B	1861	1/1	0.74	0.26	76,76,76,76	0
84	MG	AS	3506	1/1	0.74	0.23	49,49,49,49	0
84	MG	1	3758	1/1	0.74	0.44	60,60,60,60	0
84	MG	B	1903	1/1	0.74	0.24	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	1	3779	1/1	0.74	0.23	44,44,44,44	0
84	MG	1	3609	1/1	0.74	0.13	48,48,48,48	0
84	MG	B	1915	1/1	0.74	0.27	62,62,62,62	0
84	MG	1	3686	1/1	0.74	0.20	57,57,57,57	0
84	MG	CM	1837	1/1	0.74	0.39	53,53,53,53	0
84	MG	B	1924	1/1	0.74	0.19	50,50,50,50	0
84	MG	R	201	1/1	0.74	0.27	78,78,78,78	0
84	MG	1	4020	1/1	0.74	0.16	57,57,57,57	0
84	MG	AS	3666	1/1	0.74	0.23	47,47,47,47	0
84	MG	AS	3715	1/1	0.74	0.14	49,49,49,49	0
84	MG	1	3757	1/1	0.74	0.36	69,69,69,69	0
84	MG	B	1803	1/1	0.75	0.41	56,56,56,56	0
84	MG	CM	1855	1/1	0.75	0.34	65,65,65,65	0
84	MG	1	3563	1/1	0.75	0.22	70,70,70,70	0
84	MG	B	1947	1/1	0.75	0.28	83,83,83,83	0
84	MG	AS	3534	1/1	0.75	0.24	67,67,67,67	0
84	MG	BZ	203	1/1	0.75	0.25	86,86,86,86	0
84	MG	CM	1978	1/1	0.75	0.10	42,42,42,42	0
84	MG	DB	202	1/1	0.75	0.33	83,83,83,83	0
84	MG	AS	3455	1/1	0.75	0.28	64,64,64,64	0
84	MG	1	3558	1/1	0.75	0.30	61,61,61,61	0
84	MG	1	3694	1/1	0.76	0.32	29,29,29,29	0
84	MG	B	1815	1/1	0.76	0.32	68,68,68,68	0
84	MG	1	3906	1/1	0.76	0.28	65,65,65,65	0
84	MG	1	3997	1/1	0.76	0.17	58,58,58,58	0
84	MG	AS	3671	1/1	0.76	0.32	55,55,55,55	0
84	MG	CM	1828	1/1	0.76	0.54	43,43,43,43	0
84	MG	CM	1836	1/1	0.76	0.31	59,59,59,59	0
84	MG	1	3720	1/1	0.76	0.29	97,97,97,97	0
84	MG	B	1839	1/1	0.76	0.33	68,68,68,68	0
84	MG	1	4029	1/1	0.76	0.16	46,46,46,46	0
84	MG	CM	1875	1/1	0.76	0.27	63,63,63,63	0
84	MG	CM	1876	1/1	0.76	0.23	63,63,63,63	0
84	MG	AS	3749	1/1	0.76	0.20	57,57,57,57	0
84	MG	B	1860	1/1	0.76	0.25	67,67,67,67	0
84	MG	1	3722	1/1	0.76	0.11	28,28,28,28	0
84	MG	AS	3829	1/1	0.76	0.20	43,43,43,43	0
84	MG	AT	208	1/1	0.76	0.25	57,57,57,57	0
84	MG	1	3670	1/1	0.76	0.14	57,57,57,57	0
84	MG	AU	205	1/1	0.76	0.23	44,44,44,44	0
84	MG	AS	3785	1/1	0.77	0.12	43,43,43,43	0
84	MG	AS	3479	1/1	0.77	0.32	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	AS	3491	1/1	0.77	0.25	50,50,50,50	0
84	MG	1	3829	1/1	0.77	0.21	51,51,51,51	0
84	MG	1	3633	1/1	0.77	0.29	48,48,48,48	0
84	MG	1	3751	1/1	0.77	0.18	61,61,61,61	0
84	MG	AS	3533	1/1	0.77	0.40	60,60,60,60	0
84	MG	B	1901	1/1	0.77	0.38	77,77,77,77	0
84	MG	B	1831	1/1	0.77	0.34	65,65,65,65	0
84	MG	1	3663	1/1	0.77	0.40	53,53,53,53	0
84	MG	AS	3733	1/1	0.77	0.16	53,53,53,53	0
84	MG	1	3422	1/1	0.77	0.34	46,46,46,46	0
84	MG	1	4010	1/1	0.77	0.14	41,41,41,41	0
84	MG	CM	1810	1/1	0.78	0.23	39,39,39,39	0
84	MG	B	1940	1/1	0.78	0.20	78,78,78,78	0
84	MG	1	3597	1/1	0.78	0.30	68,68,68,68	0
84	MG	1	3469	1/1	0.78	0.36	45,45,45,45	0
84	MG	1	4013	1/1	0.78	0.09	41,41,41,41	0
84	MG	AS	3816	1/1	0.78	0.30	48,48,48,48	0
84	MG	1	3843	1/1	0.78	0.24	53,53,53,53	0
84	MG	1	3660	1/1	0.78	0.33	35,35,35,35	0
84	MG	AT	207	1/1	0.78	0.33	59,59,59,59	0
84	MG	1	3925	1/1	0.78	0.11	49,49,49,49	0
84	MG	B	1978	1/1	0.78	0.25	51,51,51,51	0
84	MG	CM	1906	1/1	0.78	0.17	46,46,46,46	0
84	MG	CM	1919	1/1	0.78	0.26	49,49,49,49	0
84	MG	CM	1963	1/1	0.78	0.23	45,45,45,45	0
84	MG	1	3860	1/1	0.78	0.23	65,65,65,65	0
84	MG	AS	3706	1/1	0.78	0.18	46,46,46,46	0
84	MG	AS	3535	1/1	0.78	0.28	66,66,66,66	0
84	MG	3	208	1/1	0.78	0.26	70,70,70,70	0
84	MG	1	3786	1/1	0.78	0.18	69,69,69,69	0
84	MG	CL	302	1/1	0.79	0.45	72,72,72,72	0
84	MG	B	1938	1/1	0.79	0.25	47,47,47,47	0
84	MG	1	3498	1/1	0.79	0.32	39,39,39,39	0
84	MG	1	3512	1/1	0.79	0.34	58,58,58,58	0
84	MG	CM	1821	1/1	0.79	0.18	42,42,42,42	0
84	MG	B	1875	1/1	0.79	0.40	63,63,63,63	0
84	MG	B	1886	1/1	0.79	0.27	95,95,95,95	0
84	MG	B	1891	1/1	0.79	0.29	62,62,62,62	0
84	MG	B	1893	1/1	0.79	0.37	57,57,57,57	0
84	MG	AS	3589	1/1	0.79	0.19	51,51,51,51	0
84	MG	1	3680	1/1	0.79	0.14	40,40,40,40	0
84	MG	1	3892	1/1	0.79	0.23	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	1	3942	1/1	0.79	0.17	47,47,47,47	0
84	MG	AT	206	1/1	0.79	0.36	42,42,42,42	0
84	MG	1	3982	1/1	0.79	0.19	43,43,43,43	0
84	MG	CM	1918	1/1	0.79	0.15	46,46,46,46	0
84	MG	3	215	1/1	0.79	0.23	65,65,65,65	0
84	MG	CM	1954	1/1	0.79	0.15	41,41,41,41	0
84	MG	4	201	1/1	0.79	0.31	54,54,54,54	0
84	MG	1	3586	1/1	0.79	0.43	60,60,60,60	0
84	MG	1	3688	1/1	0.79	0.25	57,57,57,57	0
84	MG	B	1849	1/1	0.79	0.15	56,56,56,56	0
84	MG	BZ	202	1/1	0.79	0.27	68,68,68,68	0
84	MG	1	3618	1/1	0.79	0.26	72,72,72,72	0
84	MG	1	3496	1/1	0.80	0.18	31,31,31,31	0
84	MG	AS	3827	1/1	0.80	0.11	44,44,44,44	0
84	MG	CM	1851	1/1	0.80	0.29	78,78,78,78	0
84	MG	AS	3503	1/1	0.80	0.40	53,53,53,53	0
84	MG	CM	1858	1/1	0.80	0.27	51,51,51,51	0
84	MG	CM	1861	1/1	0.80	0.18	51,51,51,51	0
84	MG	1	3404	1/1	0.80	0.38	38,38,38,38	0
84	MG	B	1873	1/1	0.80	0.30	62,62,62,62	0
84	MG	1	3517	1/1	0.80	0.35	60,60,60,60	0
84	MG	CM	1878	1/1	0.80	0.27	47,47,47,47	0
84	MG	a	201	1/1	0.80	0.29	86,86,86,86	0
84	MG	AS	3697	1/1	0.80	0.16	42,42,42,42	0
84	MG	CM	1889	1/1	0.80	0.36	47,47,47,47	0
84	MG	AS	3558	1/1	0.80	0.25	53,53,53,53	0
84	MG	CM	1916	1/1	0.80	0.25	48,48,48,48	0
84	MG	1	3696	1/1	0.80	0.16	200,200,200,200	0
84	MG	B	1887	1/1	0.80	0.27	76,76,76,76	0
84	MG	1	3735	1/1	0.80	0.24	53,53,53,53	0
84	MG	CM	1957	1/1	0.80	0.20	50,50,50,50	0
84	MG	AS	3742	1/1	0.80	0.24	42,42,42,42	0
84	MG	1	3876	1/1	0.80	0.16	46,46,46,46	0
84	MG	AS	3617	1/1	0.80	0.27	56,56,56,56	0
84	MG	AS	3622	1/1	0.80	0.41	68,68,68,68	0
84	MG	DJ	202	1/1	0.80	0.12	56,56,56,56	0
84	MG	1	3736	1/1	0.80	0.17	31,31,31,31	0
84	MG	AS	3499	1/1	0.80	0.25	59,59,59,59	0
84	MG	1	3583	1/1	0.81	0.13	56,56,56,56	0
84	MG	1	3963	1/1	0.81	0.22	48,48,48,48	0
84	MG	AS	3770	1/1	0.81	0.13	56,56,56,56	0
84	MG	1	4036	1/1	0.81	0.31	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3980	1/1	0.81	0.14	34,34,34,34	0
84	MG	1	3511	1/1	0.81	0.28	42,42,42,42	0
84	MG	CM	1866	1/1	0.81	0.22	73,73,73,73	0
84	MG	AS	3818	1/1	0.81	0.16	44,44,44,44	0
84	MG	B	1808	1/1	0.81	0.28	45,45,45,45	0
84	MG	3	211	1/1	0.81	0.39	58,58,58,58	0
84	MG	1	3923	1/1	0.81	0.13	56,56,56,56	0
84	MG	AS	3646	1/1	0.81	0.07	43,43,43,43	0
84	MG	1	3846	1/1	0.81	0.27	57,57,57,57	0
84	MG	AS	3658	1/1	0.81	0.25	59,59,59,59	0
84	MG	1	3444	1/1	0.81	0.39	57,57,57,57	0
84	MG	j	302	1/1	0.81	0.11	69,69,69,69	0
84	MG	B	1838	1/1	0.81	0.49	60,60,60,60	0
84	MG	1	3580	1/1	0.81	0.16	52,52,52,52	0
84	MG	BS	202	1/1	0.81	0.13	58,58,58,58	0
84	MG	B	1955	1/1	0.81	0.31	40,40,40,40	0
84	MG	B	1977	1/1	0.81	0.28	45,45,45,45	0
84	MG	1	4027	1/1	0.81	0.26	56,56,56,56	0
84	MG	AS	3725	1/1	0.81	0.21	45,45,45,45	0
84	MG	AS	3574	1/1	0.81	0.32	46,46,46,46	0
84	MG	AS	3585	1/1	0.81	0.26	52,52,52,52	0
85	ZN	AH	201	1/1	0.81	0.11	207,207,207,207	0
84	MG	AS	3741	1/1	0.81	0.09	53,53,53,53	0
84	MG	B	1851	1/1	0.81	0.22	61,61,61,61	0
84	MG	B	1956	1/1	0.82	0.31	46,46,46,46	0
84	MG	CM	1806	1/1	0.82	0.34	52,52,52,52	0
84	MG	1	3433	1/1	0.82	0.33	40,40,40,40	0
84	MG	AS	3539	1/1	0.82	0.32	54,54,54,54	0
84	MG	B	1804	1/1	0.82	0.35	61,61,61,61	0
84	MG	CM	1819	1/1	0.82	0.26	58,58,58,58	0
84	MG	AS	3732	1/1	0.82	0.28	51,51,51,51	0
84	MG	B	1864	1/1	0.82	0.30	70,70,70,70	0
84	MG	AS	3580	1/1	0.82	0.38	58,58,58,58	0
84	MG	3	217	1/1	0.82	0.12	42,42,42,42	0
84	MG	1	3914	1/1	0.82	0.32	59,59,59,59	0
84	MG	Z	201	1/1	0.82	0.20	48,48,48,48	0
84	MG	1	3523	1/1	0.82	0.45	51,51,51,51	0
84	MG	AS	3784	1/1	0.82	0.11	44,44,44,44	0
84	MG	c	202	1/1	0.82	0.19	63,63,63,63	0
84	MG	AS	3794	1/1	0.82	0.28	48,48,48,48	0
84	MG	AS	3803	1/1	0.82	0.47	52,52,52,52	0
84	MG	AS	3611	1/1	0.82	0.23	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	CM	1877	1/1	0.82	0.13	86,86,86,86	0
84	MG	AS	3419	1/1	0.82	0.65	47,47,47,47	0
84	MG	1	3979	1/1	0.82	0.19	45,45,45,45	0
84	MG	v	304	1/1	0.82	0.16	50,50,50,50	0
84	MG	AS	3825	1/1	0.82	0.17	45,45,45,45	0
84	MG	AS	3631	1/1	0.82	0.33	51,51,51,51	0
84	MG	AS	3468	1/1	0.82	0.23	51,51,51,51	0
84	MG	AT	203	1/1	0.82	0.24	63,63,63,63	0
84	MG	1	3673	1/1	0.82	0.17	46,46,46,46	0
84	MG	CM	1941	1/1	0.82	0.19	48,48,48,48	0
84	MG	1	3882	1/1	0.82	0.19	37,37,37,37	0
84	MG	1	3748	1/1	0.82	0.31	40,40,40,40	0
84	MG	AS	3498	1/1	0.82	0.30	57,57,57,57	0
84	MG	2	202	1/1	0.82	0.41	51,51,51,51	0
84	MG	AY	401	1/1	0.82	0.10	46,46,46,46	0
84	MG	DA	201	1/1	0.82	0.17	61,61,61,61	0
84	MG	1	3464	1/1	0.82	0.24	40,40,40,40	0
84	MG	DJ	201	1/1	0.82	0.15	53,53,53,53	0
84	MG	B	1912	1/1	0.82	0.34	58,58,58,58	0
84	MG	B	1954	1/1	0.82	0.15	52,52,52,52	0
85	ZN	CB	201	1/1	0.82	0.09	237,237,237,237	0
84	MG	AS	3683	1/1	0.82	0.23	43,43,43,43	0
84	MG	1	3930	1/1	0.82	0.23	59,59,59,59	0
84	MG	AS	3618	1/1	0.83	0.26	49,49,49,49	0
84	MG	AS	3751	1/1	0.83	0.13	39,39,39,39	0
84	MG	AS	3621	1/1	0.83	0.26	65,65,65,65	0
84	MG	o	306	1/1	0.83	0.18	40,40,40,40	0
84	MG	3	210	1/1	0.83	0.19	72,72,72,72	0
84	MG	AS	3789	1/1	0.83	0.16	40,40,40,40	0
84	MG	AS	3790	1/1	0.83	0.13	43,43,43,43	0
84	MG	B	1909	1/1	0.83	0.24	52,52,52,52	0
84	MG	AS	3797	1/1	0.83	0.26	49,49,49,49	0
84	MG	1	3529	1/1	0.83	0.42	53,53,53,53	0
84	MG	AS	3809	1/1	0.83	0.08	45,45,45,45	0
84	MG	1	3685	1/1	0.83	0.09	93,93,93,93	0
84	MG	CM	1873	1/1	0.83	0.20	56,56,56,56	0
84	MG	AS	3642	1/1	0.83	0.36	71,71,71,71	0
84	MG	AS	3644	1/1	0.83	0.30	56,56,56,56	0
84	MG	B	1866	1/1	0.83	0.29	66,66,66,66	0
84	MG	AS	3821	1/1	0.83	0.26	45,45,45,45	0
84	MG	B	1967	1/1	0.83	0.26	51,51,51,51	0
84	MG	B	1872	1/1	0.83	0.17	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	1	3861	1/1	0.83	0.24	65,65,65,65	0
84	MG	1	3958	1/1	0.83	0.09	40,40,40,40	0
84	MG	AT	204	1/1	0.83	0.14	86,86,86,86	0
84	MG	B	1934	1/1	0.83	0.11	87,87,87,87	0
84	MG	AS	3669	1/1	0.83	0.15	71,71,71,71	0
84	MG	CM	1928	1/1	0.83	0.15	44,44,44,44	0
84	MG	Q	201	1/1	0.83	0.12	34,34,34,34	0
84	MG	AS	3679	1/1	0.83	0.28	45,45,45,45	0
84	MG	B	1882	1/1	0.83	0.36	57,57,57,57	0
84	MG	U	201	1/1	0.83	0.15	51,51,51,51	0
84	MG	Y	202	1/1	0.83	0.25	76,76,76,76	0
84	MG	8	201	1/1	0.83	0.25	50,50,50,50	0
84	MG	CN	301	1/1	0.83	0.34	67,67,67,67	0
84	MG	1	3698	1/1	0.83	0.23	37,37,37,37	0
84	MG	BV	201	1/1	0.83	0.10	48,48,48,48	0
84	MG	3	204	1/1	0.83	0.30	56,56,56,56	0
84	MG	AH	202	1/1	0.83	0.18	72,72,72,72	0
84	MG	AS	3442	1/1	0.83	0.27	38,38,38,38	0
85	ZN	d	101	1/1	0.83	0.10	251,251,251,251	0
84	MG	AS	3452	1/1	0.83	0.38	41,41,41,41	0
84	MG	1	3816	1/1	0.83	0.25	42,42,42,42	0
84	MG	B	1854	1/1	0.83	0.28	61,61,61,61	0
84	MG	1	3482	1/1	0.84	0.31	49,49,49,49	0
84	MG	AS	3428	1/1	0.84	0.28	36,36,36,36	0
84	MG	AS	3438	1/1	0.84	0.38	54,54,54,54	0
84	MG	AG	202	1/1	0.84	0.13	57,57,57,57	0
84	MG	1	3665	1/1	0.84	0.30	43,43,43,43	0
84	MG	CM	1845	1/1	0.84	0.12	31,31,31,31	0
84	MG	1	3814	1/1	0.84	0.17	47,47,47,47	0
84	MG	1	3543	1/1	0.84	0.18	41,41,41,41	0
84	MG	B	1805	1/1	0.84	0.43	54,54,54,54	0
84	MG	1	3821	1/1	0.84	0.20	39,39,39,39	0
84	MG	CM	1862	1/1	0.84	0.12	64,64,64,64	0
84	MG	AS	3487	1/1	0.84	0.33	39,39,39,39	0
84	MG	3	218	1/1	0.84	0.12	47,47,47,47	0
84	MG	AS	3653	1/1	0.84	0.36	41,41,41,41	0
84	MG	B	1953	1/1	0.84	0.10	48,48,48,48	0
84	MG	AS	3660	1/1	0.84	0.28	66,66,66,66	0
84	MG	1	3672	1/1	0.84	0.12	52,52,52,52	0
84	MG	4	208	1/1	0.84	0.17	38,38,38,38	0
84	MG	B	1829	1/1	0.84	0.27	53,53,53,53	0
84	MG	AS	3833	1/1	0.84	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3648	1/1	0.84	0.25	69,69,69,69	0
84	MG	B	1972	1/1	0.84	0.17	54,54,54,54	0
84	MG	AS	3672	1/1	0.84	0.10	47,47,47,47	0
84	MG	1	3655	1/1	0.84	0.15	58,58,58,58	0
84	MG	1	3656	1/1	0.84	0.34	59,59,59,59	0
84	MG	AT	209	1/1	0.84	0.32	47,47,47,47	0
84	MG	AS	3690	1/1	0.84	0.15	41,41,41,41	0
84	MG	CM	1942	1/1	0.84	0.15	46,46,46,46	0
84	MG	CM	1952	1/1	0.84	0.19	48,48,48,48	0
84	MG	B	1979	1/1	0.84	0.19	49,49,49,49	0
84	MG	B	1992	1/1	0.84	0.13	45,45,45,45	0
84	MG	CM	1961	1/1	0.84	0.13	46,46,46,46	0
84	MG	CM	1962	1/1	0.84	0.22	53,53,53,53	0
84	MG	1	3784	1/1	0.84	0.11	32,32,32,32	0
84	MG	1	4030	1/1	0.84	0.10	41,41,41,41	0
84	MG	1	3853	1/1	0.84	0.22	54,54,54,54	0
84	MG	B	1852	1/1	0.84	0.32	42,42,42,42	0
84	MG	CW	202	1/1	0.84	0.11	57,57,57,57	0
84	MG	1	3682	1/1	0.84	0.28	68,68,68,68	0
84	MG	1	3413	1/1	0.84	0.32	42,42,42,42	0
84	MG	1	3873	1/1	0.84	0.39	56,56,56,56	0
84	MG	CL	303	1/1	0.84	0.20	61,61,61,61	0
84	MG	9	201	1/1	0.84	0.35	65,65,65,65	0
84	MG	1	3662	1/1	0.84	0.30	54,54,54,54	0
84	MG	AR	401	1/1	0.84	0.22	69,69,69,69	0
84	MG	CM	1811	1/1	0.84	0.21	50,50,50,50	0
84	MG	AS	3765	1/1	0.84	0.12	44,44,44,44	0
84	MG	1	3781	1/1	0.85	0.26	48,48,48,48	0
84	MG	AS	3425	1/1	0.85	0.28	46,46,46,46	0
84	MG	AE	201	1/1	0.85	0.14	79,79,79,79	0
84	MG	AS	3431	1/1	0.85	0.37	52,52,52,52	0
84	MG	1	3782	1/1	0.85	0.26	30,30,30,30	0
84	MG	AF	202	1/1	0.85	0.12	55,55,55,55	0
84	MG	CL	304	1/1	0.85	0.09	54,54,54,54	0
84	MG	CM	1801	1/1	0.85	0.17	52,52,52,52	0
84	MG	CM	1804	1/1	0.85	0.36	40,40,40,40	0
84	MG	1	3480	1/1	0.85	0.35	36,36,36,36	0
84	MG	CM	1807	1/1	0.85	0.31	48,48,48,48	0
84	MG	B	1919	1/1	0.85	0.25	61,61,61,61	0
84	MG	B	1920	1/1	0.85	0.24	48,48,48,48	0
84	MG	AS	3688	1/1	0.85	0.20	39,39,39,39	0
84	MG	1	4017	1/1	0.85	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3604	1/1	0.85	0.28	33,33,33,33	0
84	MG	1	3471	1/1	0.85	0.24	24,24,24,24	0
84	MG	AS	3712	1/1	0.85	0.21	45,45,45,45	0
84	MG	CM	1835	1/1	0.85	0.29	58,58,58,58	0
84	MG	1	3880	1/1	0.85	0.09	38,38,38,38	0
84	MG	1	3797	1/1	0.85	0.29	51,51,51,51	0
84	MG	1	3799	1/1	0.85	0.33	69,69,69,69	0
84	MG	CM	1850	1/1	0.85	0.23	44,44,44,44	0
84	MG	1	4035	1/1	0.85	0.16	53,53,53,53	0
84	MG	1	3897	1/1	0.85	0.14	72,72,72,72	0
84	MG	AS	3502	1/1	0.85	0.21	45,45,45,45	0
84	MG	1	3898	1/1	0.85	0.16	40,40,40,40	0
84	MG	1	3522	1/1	0.85	0.31	37,37,37,37	0
84	MG	1	3622	1/1	0.85	0.30	44,44,44,44	0
84	MG	1	3807	1/1	0.85	0.27	45,45,45,45	0
84	MG	AS	3753	1/1	0.85	0.07	55,55,55,55	0
84	MG	1	3745	1/1	0.85	0.31	38,38,38,38	0
84	MG	3	213	1/1	0.85	0.31	49,49,49,49	0
84	MG	AS	3775	1/1	0.85	0.25	45,45,45,45	0
84	MG	1	3809	1/1	0.85	0.28	47,47,47,47	0
84	MG	AS	3568	1/1	0.85	0.26	42,42,42,42	0
84	MG	1	3664	1/1	0.85	0.24	44,44,44,44	0
84	MG	AS	3578	1/1	0.85	0.26	45,45,45,45	0
84	MG	CM	1895	1/1	0.85	0.32	52,52,52,52	0
84	MG	3	216	1/1	0.85	0.25	65,65,65,65	0
84	MG	CM	1909	1/1	0.85	0.21	52,52,52,52	0
84	MG	CM	1911	1/1	0.85	0.24	47,47,47,47	0
84	MG	1	3690	1/1	0.85	0.17	86,86,86,86	0
84	MG	B	1958	1/1	0.85	0.10	43,43,43,43	0
84	MG	1	3926	1/1	0.85	0.47	64,64,64,64	0
84	MG	1	3475	1/1	0.85	0.21	26,26,26,26	0
84	MG	1	3822	1/1	0.85	0.18	46,46,46,46	0
84	MG	1	3933	1/1	0.85	0.36	51,51,51,51	0
84	MG	AS	3612	1/1	0.85	0.25	46,46,46,46	0
84	MG	1	3568	1/1	0.85	0.16	46,46,46,46	0
84	MG	B	1981	1/1	0.85	0.15	46,46,46,46	0
84	MG	AS	3619	1/1	0.85	0.33	57,57,57,57	0
84	MG	1	3643	1/1	0.85	0.32	34,34,34,34	0
84	MG	r	303	1/1	0.85	0.10	54,54,54,54	0
84	MG	s	201	1/1	0.85	0.24	46,46,46,46	0
84	MG	K	301	1/1	0.85	0.16	72,72,72,72	0
84	MG	1	3949	1/1	0.85	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	CW	201	1/1	0.85	0.10	41,41,41,41	0
84	MG	1	3839	1/1	0.85	0.28	40,40,40,40	0
84	MG	AS	3637	1/1	0.85	0.28	44,44,44,44	0
84	MG	1	3716	1/1	0.85	0.13	51,51,51,51	0
84	MG	1	3964	1/1	0.85	0.16	44,44,44,44	0
84	MG	AU	203	1/1	0.85	0.28	48,48,48,48	0
84	MG	1	3778	1/1	0.85	0.17	39,39,39,39	0
85	ZN	AP	201	1/1	0.85	0.11	226,226,226,226	0
84	MG	B	1899	1/1	0.85	0.22	60,60,60,60	0
84	MG	1	3594	1/1	0.85	0.16	37,37,37,37	0
84	MG	BH	201	1/1	0.85	0.17	50,50,50,50	0
84	MG	1	3780	1/1	0.85	0.19	40,40,40,40	0
84	MG	1	3750	1/1	0.86	0.13	49,49,49,49	0
84	MG	1	3432	1/1	0.86	0.12	54,54,54,54	0
84	MG	1	3753	1/1	0.86	0.18	33,33,33,33	0
84	MG	AT	213	1/1	0.86	0.28	44,44,44,44	0
84	MG	AS	3729	1/1	0.86	0.28	48,48,48,48	0
84	MG	1	3508	1/1	0.86	0.22	43,43,43,43	0
84	MG	Q	202	1/1	0.86	0.27	65,65,65,65	0
84	MG	CM	1880	1/1	0.86	0.14	44,44,44,44	0
84	MG	BB	305	1/1	0.86	0.39	64,64,64,64	0
84	MG	AS	3734	1/1	0.86	0.22	43,43,43,43	0
84	MG	AS	3627	1/1	0.86	0.17	54,54,54,54	0
84	MG	1	3704	1/1	0.86	0.48	42,42,42,42	0
84	MG	1	3886	1/1	0.86	0.12	42,42,42,42	0
84	MG	1	4016	1/1	0.86	0.10	39,39,39,39	0
84	MG	CM	1913	1/1	0.86	0.07	48,48,48,48	0
84	MG	AS	3512	1/1	0.86	0.33	64,64,64,64	0
84	MG	CM	1917	1/1	0.86	0.16	55,55,55,55	0
84	MG	AS	3528	1/1	0.86	0.30	55,55,55,55	0
84	MG	AS	3764	1/1	0.86	0.11	44,44,44,44	0
84	MG	CM	1923	1/1	0.86	0.20	53,53,53,53	0
84	MG	AS	3638	1/1	0.86	0.12	39,39,39,39	0
84	MG	CM	1929	1/1	0.86	0.08	52,52,52,52	0
84	MG	1	3928	1/1	0.86	0.09	55,55,55,55	0
84	MG	1	3582	1/1	0.86	0.23	58,58,58,58	0
84	MG	1	3487	1/1	0.86	0.12	52,52,52,52	0
84	MG	AS	3536	1/1	0.86	0.30	42,42,42,42	0
84	MG	1	3815	1/1	0.86	0.23	72,72,72,72	0
84	MG	1	3859	1/1	0.86	0.10	43,43,43,43	0
84	MG	1	3794	1/1	0.86	0.18	42,42,42,42	0
84	MG	B	1966	1/1	0.86	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	4033	1/1	0.86	0.22	42,42,42,42	0
84	MG	CM	1970	1/1	0.86	0.13	43,43,43,43	0
84	MG	CM	1974	1/1	0.86	0.09	43,43,43,43	0
84	MG	CM	1975	1/1	0.86	0.23	48,48,48,48	0
84	MG	AS	3579	1/1	0.86	0.25	53,53,53,53	0
84	MG	1	3954	1/1	0.86	0.16	43,43,43,43	0
84	MG	CQ	303	1/1	0.86	0.08	39,39,39,39	0
84	MG	1	3912	1/1	0.86	0.16	36,36,36,36	0
84	MG	1	3442	1/1	0.86	0.25	63,63,63,63	0
84	MG	1	3917	1/1	0.86	0.15	70,70,70,70	0
84	MG	DB	201	1/1	0.86	0.20	62,62,62,62	0
84	MG	AS	3682	1/1	0.86	0.22	42,42,42,42	0
84	MG	DB	203	1/1	0.86	0.30	58,58,58,58	0
84	MG	B	1884	1/1	0.86	0.12	89,89,89,89	0
84	MG	B	1990	1/1	0.86	0.12	54,54,54,54	0
84	MG	AS	3598	1/1	0.86	0.17	41,41,41,41	0
84	MG	AS	3601	1/1	0.86	0.25	49,49,49,49	0
84	MG	AS	3698	1/1	0.86	0.15	44,44,44,44	0
84	MG	AS	3702	1/1	0.86	0.47	50,50,50,50	0
84	MG	B	1828	1/1	0.86	0.20	45,45,45,45	0
84	MG	D	302	1/1	0.86	0.10	35,35,35,35	0
84	MG	AS	3551	1/1	0.87	0.28	43,43,43,43	0
84	MG	AS	3710	1/1	0.87	0.26	48,48,48,48	0
84	MG	AS	3555	1/1	0.87	0.21	38,38,38,38	0
84	MG	CM	1809	1/1	0.87	0.28	102,102,102,102	0
84	MG	B	1904	1/1	0.87	0.10	50,50,50,50	0
84	MG	AS	3718	1/1	0.87	0.17	43,43,43,43	0
84	MG	1	3530	1/1	0.87	0.27	37,37,37,37	0
84	MG	AS	3726	1/1	0.87	0.27	50,50,50,50	0
84	MG	4	202	1/1	0.87	0.31	57,57,57,57	0
84	MG	B	1910	1/1	0.87	0.15	50,50,50,50	0
84	MG	AS	3730	1/1	0.87	0.18	42,42,42,42	0
84	MG	4	205	1/1	0.87	0.63	48,48,48,48	0
84	MG	1	3924	1/1	0.87	0.12	62,62,62,62	0
84	MG	CM	1840	1/1	0.87	0.43	56,56,56,56	0
84	MG	AS	3583	1/1	0.87	0.20	46,46,46,46	0
84	MG	AS	3738	1/1	0.87	0.09	54,54,54,54	0
84	MG	4	210	1/1	0.87	0.27	38,38,38,38	0
84	MG	4	211	1/1	0.87	0.15	63,63,63,63	0
84	MG	1	3466	1/1	0.87	0.20	37,37,37,37	0
84	MG	1	3555	1/1	0.87	0.23	60,60,60,60	0
84	MG	AS	3595	1/1	0.87	0.20	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	o	305	1/1	0.87	0.15	42,42,42,42	0
84	MG	AS	3760	1/1	0.87	0.08	36,36,36,36	0
84	MG	1	3448	1/1	0.87	0.28	36,36,36,36	0
84	MG	AS	3600	1/1	0.87	0.24	50,50,50,50	0
84	MG	B	1930	1/1	0.87	0.17	64,64,64,64	0
84	MG	AS	3609	1/1	0.87	0.15	44,44,44,44	0
84	MG	g	101	1/1	0.87	0.53	87,87,87,87	0
84	MG	B	1932	1/1	0.87	0.14	36,36,36,36	0
84	MG	AS	3417	1/1	0.87	0.29	36,36,36,36	0
84	MG	CM	1883	1/1	0.87	0.26	42,42,42,42	0
84	MG	1	4024	1/1	0.87	0.25	44,44,44,44	0
84	MG	1	3652	1/1	0.87	0.30	67,67,67,67	0
84	MG	v	303	1/1	0.87	0.20	49,49,49,49	0
84	MG	CM	1900	1/1	0.87	0.26	47,47,47,47	0
84	MG	1	3445	1/1	0.87	0.33	31,31,31,31	0
84	MG	AS	3804	1/1	0.87	0.15	67,67,67,67	0
84	MG	AS	3623	1/1	0.87	0.19	51,51,51,51	0
84	MG	1	3931	1/1	0.87	0.19	61,61,61,61	0
84	MG	1	3783	1/1	0.87	0.15	59,59,59,59	0
84	MG	1	3825	1/1	0.87	0.33	48,48,48,48	0
84	MG	1	3737	1/1	0.87	0.40	24,24,24,24	0
84	MG	AS	3456	1/1	0.87	0.19	58,58,58,58	0
84	MG	B	1867	1/1	0.87	0.22	90,90,90,90	0
84	MG	AS	3826	1/1	0.87	0.15	39,39,39,39	0
84	MG	1	3525	1/1	0.87	0.13	55,55,55,55	0
84	MG	CM	1940	1/1	0.87	0.14	46,46,46,46	0
84	MG	AS	3470	1/1	0.87	0.26	46,46,46,46	0
84	MG	AS	3643	1/1	0.87	0.17	61,61,61,61	0
84	MG	CM	1950	1/1	0.87	0.06	40,40,40,40	0
84	MG	1	3657	1/1	0.87	0.27	54,54,54,54	0
84	MG	AS	3645	1/1	0.87	0.19	50,50,50,50	0
84	MG	B	1951	1/1	0.87	0.09	49,49,49,49	0
84	MG	CM	1958	1/1	0.87	0.10	59,59,59,59	0
84	MG	1	3574	1/1	0.87	0.10	41,41,41,41	0
84	MG	1	3960	1/1	0.87	0.10	43,43,43,43	0
84	MG	1	3911	1/1	0.87	0.19	36,36,36,36	0
84	MG	CM	1966	1/1	0.87	0.18	54,54,54,54	0
84	MG	1	3608	1/1	0.87	0.14	71,71,71,71	0
84	MG	1	3978	1/1	0.87	0.08	36,36,36,36	0
84	MG	1	3575	1/1	0.87	0.23	49,49,49,49	0
84	MG	AU	204	1/1	0.87	0.12	43,43,43,43	0
84	MG	B	1892	1/1	0.87	0.15	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3612	1/1	0.87	0.41	49,49,49,49	0
84	MG	AS	3511	1/1	0.87	0.24	48,48,48,48	0
84	MG	BE	303	1/1	0.87	0.24	52,52,52,52	0
84	MG	1	3528	1/1	0.87	0.19	52,52,52,52	0
84	MG	AS	3676	1/1	0.87	0.27	35,35,35,35	0
84	MG	1	3989	1/1	0.87	0.08	35,35,35,35	0
84	MG	BO	201	1/1	0.87	0.11	48,48,48,48	0
84	MG	AS	3681	1/1	0.87	0.12	33,33,33,33	0
84	MG	DG	201	1/1	0.87	0.18	77,77,77,77	0
84	MG	1	3503	1/1	0.87	0.22	49,49,49,49	0
84	MG	B	1902	1/1	0.87	0.16	63,63,63,63	0
84	MG	B	1985	1/1	0.87	0.08	54,54,54,54	0
84	MG	B	1986	1/1	0.87	0.11	44,44,44,44	0
84	MG	B	1809	1/1	0.87	0.28	42,42,42,42	0
84	MG	AS	3542	1/1	0.87	0.38	56,56,56,56	0
84	MG	AS	3548	1/1	0.87	0.26	42,42,42,42	0
84	MG	AS	3705	1/1	0.87	0.15	48,48,48,48	0
84	MG	B	1862	1/1	0.88	0.24	54,54,54,54	0
84	MG	y	203	1/1	0.88	0.25	44,44,44,44	0
84	MG	AS	3762	1/1	0.88	0.23	42,42,42,42	0
84	MG	1	3894	1/1	0.88	0.23	73,73,73,73	0
84	MG	1	3419	1/1	0.88	0.24	18,18,18,18	0
84	MG	CM	1848	1/1	0.88	0.22	39,39,39,39	0
84	MG	AS	3626	1/1	0.88	0.12	45,45,45,45	0
84	MG	B	1868	1/1	0.88	0.20	70,70,70,70	0
84	MG	1	3412	1/1	0.88	0.30	49,49,49,49	0
84	MG	AS	3630	1/1	0.88	0.12	59,59,59,59	0
84	MG	AS	3476	1/1	0.88	0.22	33,33,33,33	0
84	MG	AS	3633	1/1	0.88	0.37	84,84,84,84	0
84	MG	1	3902	1/1	0.88	0.10	57,57,57,57	0
84	MG	CM	1869	1/1	0.88	0.15	46,46,46,46	0
84	MG	AA	201	1/1	0.88	0.13	57,57,57,57	0
84	MG	B	1877	1/1	0.88	0.27	62,62,62,62	0
84	MG	AS	3492	1/1	0.88	0.39	56,56,56,56	0
84	MG	AS	3805	1/1	0.88	0.22	45,45,45,45	0
84	MG	B	1879	1/1	0.88	0.23	42,42,42,42	0
84	MG	AB	202	1/1	0.88	0.19	53,53,53,53	0
84	MG	B	1961	1/1	0.88	0.10	54,54,54,54	0
84	MG	AS	3500	1/1	0.88	0.26	50,50,50,50	0
84	MG	1	3581	1/1	0.88	0.26	45,45,45,45	0
84	MG	1	3678	1/1	0.88	0.11	55,55,55,55	0
84	MG	1	3971	1/1	0.88	0.07	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3974	1/1	0.88	0.10	43,43,43,43	0
84	MG	1	3654	1/1	0.88	0.21	52,52,52,52	0
84	MG	AS	3828	1/1	0.88	0.11	47,47,47,47	0
84	MG	1	3681	1/1	0.88	0.08	45,45,45,45	0
84	MG	AS	3832	1/1	0.88	0.15	39,39,39,39	0
84	MG	CM	1912	1/1	0.88	0.10	44,44,44,44	0
84	MG	B	1980	1/1	0.88	0.11	49,49,49,49	0
84	MG	B	1897	1/1	0.88	0.24	47,47,47,47	0
84	MG	AP	203	1/1	0.88	0.35	74,74,74,74	0
84	MG	1	3785	1/1	0.88	0.23	53,53,53,53	0
84	MG	1	3426	1/1	0.88	0.30	22,22,22,22	0
84	MG	1	3564	1/1	0.88	0.44	54,54,54,54	0
84	MG	CM	1924	1/1	0.88	0.17	53,53,53,53	0
84	MG	1	3567	1/1	0.88	0.17	41,41,41,41	0
84	MG	AS	3547	1/1	0.88	0.19	41,41,41,41	0
84	MG	E	301	1/1	0.88	0.07	48,48,48,48	0
84	MG	AS	3550	1/1	0.88	0.28	35,35,35,35	0
84	MG	1	4003	1/1	0.88	0.11	48,48,48,48	0
84	MG	CM	1949	1/1	0.88	0.10	52,52,52,52	0
84	MG	4	207	1/1	0.88	0.24	43,43,43,43	0
84	MG	AS	3694	1/1	0.88	0.13	54,54,54,54	0
84	MG	1	3795	1/1	0.88	0.15	40,40,40,40	0
84	MG	1	3687	1/1	0.88	0.17	43,43,43,43	0
84	MG	B	1826	1/1	0.88	0.26	47,47,47,47	0
84	MG	B	1827	1/1	0.88	0.20	58,58,58,58	0
84	MG	BI	301	1/1	0.88	0.09	45,45,45,45	0
84	MG	1	3585	1/1	0.88	0.10	57,57,57,57	0
84	MG	1	3689	1/1	0.88	0.12	42,42,42,42	0
84	MG	AS	3582	1/1	0.88	0.33	47,47,47,47	0
84	MG	k	401	1/1	0.88	0.14	65,65,65,65	0
84	MG	CM	1973	1/1	0.88	0.17	45,45,45,45	0
84	MG	1	4019	1/1	0.88	0.21	42,42,42,42	0
84	MG	1	3431	1/1	0.88	0.14	53,53,53,53	0
84	MG	CM	1976	1/1	0.88	0.21	55,55,55,55	0
84	MG	CL	301	1/1	0.88	0.14	49,49,49,49	0
84	MG	CM	1981	1/1	0.88	0.23	45,45,45,45	0
84	MG	1	3802	1/1	0.88	0.20	75,75,75,75	0
84	MG	B	1840	1/1	0.88	0.21	37,37,37,37	0
84	MG	1	3589	1/1	0.88	0.21	33,33,33,33	0
84	MG	1	3632	1/1	0.88	0.11	42,42,42,42	0
84	MG	u	202	1/1	0.88	0.09	47,47,47,47	0
84	MG	AS	3426	1/1	0.88	0.21	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3697	1/1	0.88	0.12	61,61,61,61	0
84	MG	1	3524	1/1	0.88	0.38	50,50,50,50	0
84	MG	AS	3437	1/1	0.88	0.42	54,54,54,54	0
84	MG	1	3640	1/1	0.88	0.12	59,59,59,59	0
84	MG	AS	3743	1/1	0.88	0.08	47,47,47,47	0
84	MG	AS	3614	1/1	0.88	0.15	46,46,46,46	0
84	MG	AS	3439	1/1	0.88	0.35	44,44,44,44	0
84	MG	1	3944	1/1	0.88	0.09	39,39,39,39	0
84	MG	CM	1823	1/1	0.88	0.17	49,49,49,49	0
84	MG	AS	3752	1/1	0.88	0.21	47,47,47,47	0
84	MG	CM	1834	1/1	0.88	0.32	43,43,43,43	0
84	MG	AS	3739	1/1	0.89	0.06	43,43,43,43	0
84	MG	AS	3599	1/1	0.89	0.20	48,48,48,48	0
84	MG	CM	1822	1/1	0.89	0.18	47,47,47,47	0
84	MG	AS	3405	1/1	0.89	0.28	34,34,34,34	0
84	MG	CM	1824	1/1	0.89	0.13	48,48,48,48	0
84	MG	1	3446	1/1	0.89	0.15	29,29,29,29	0
84	MG	AS	3745	1/1	0.89	0.08	62,62,62,62	0
84	MG	1	3934	1/1	0.89	0.10	51,51,51,51	0
84	MG	AS	3748	1/1	0.89	0.14	36,36,36,36	0
84	MG	1	3733	1/1	0.89	0.23	52,52,52,52	0
84	MG	CM	1839	1/1	0.89	0.20	42,42,42,42	0
84	MG	1	3875	1/1	0.89	0.29	52,52,52,52	0
84	MG	1	3675	1/1	0.89	0.17	54,54,54,54	0
84	MG	1	3545	1/1	0.89	0.40	46,46,46,46	0
84	MG	AS	3754	1/1	0.89	0.15	40,40,40,40	0
84	MG	1	3881	1/1	0.89	0.20	44,44,44,44	0
84	MG	CM	1853	1/1	0.89	0.11	48,48,48,48	0
84	MG	CM	1854	1/1	0.89	0.10	37,37,37,37	0
84	MG	B	1822	1/1	0.89	0.30	47,47,47,47	0
84	MG	CM	1856	1/1	0.89	0.30	54,54,54,54	0
84	MG	1	3550	1/1	0.89	0.17	51,51,51,51	0
84	MG	B	1825	1/1	0.89	0.26	47,47,47,47	0
84	MG	1	3601	1/1	0.89	0.25	51,51,51,51	0
84	MG	1	3647	1/1	0.89	0.23	48,48,48,48	0
84	MG	1	3602	1/1	0.89	0.10	53,53,53,53	0
84	MG	1	3967	1/1	0.89	0.07	51,51,51,51	0
84	MG	AS	3461	1/1	0.89	0.27	33,33,33,33	0
84	MG	AS	3463	1/1	0.89	0.13	54,54,54,54	0
84	MG	AS	3792	1/1	0.89	0.10	64,64,64,64	0
84	MG	1	3968	1/1	0.89	0.10	45,45,45,45	0
84	MG	1	3896	1/1	0.89	0.14	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	AS	3799	1/1	0.89	0.08	44,44,44,44	0
84	MG	AS	3635	1/1	0.89	0.13	36,36,36,36	0
84	MG	1	3684	1/1	0.89	0.33	78,78,78,78	0
84	MG	1	3438	1/1	0.89	0.21	34,34,34,34	0
84	MG	1	3901	1/1	0.89	0.17	51,51,51,51	0
84	MG	1	3653	1/1	0.89	0.21	48,48,48,48	0
84	MG	4	212	1/1	0.89	0.16	44,44,44,44	0
84	MG	j	301	1/1	0.89	0.16	35,35,35,35	0
84	MG	1	3607	1/1	0.89	0.23	54,54,54,54	0
84	MG	1	3984	1/1	0.89	0.27	53,53,53,53	0
84	MG	k	403	1/1	0.89	0.20	56,56,56,56	0
84	MG	1	3985	1/1	0.89	0.09	34,34,34,34	0
84	MG	AS	3655	1/1	0.89	0.12	46,46,46,46	0
84	MG	1	3987	1/1	0.89	0.24	44,44,44,44	0
84	MG	1	3908	1/1	0.89	0.20	43,43,43,43	0
84	MG	B	1962	1/1	0.89	0.10	46,46,46,46	0
84	MG	CM	1920	1/1	0.89	0.08	44,44,44,44	0
84	MG	1	3994	1/1	0.89	0.19	37,37,37,37	0
84	MG	1	3557	1/1	0.89	0.25	54,54,54,54	0
84	MG	1	4002	1/1	0.89	0.13	39,39,39,39	0
84	MG	AS	3530	1/1	0.89	0.24	38,38,38,38	0
84	MG	v	302	1/1	0.89	0.21	68,68,68,68	0
84	MG	AS	3674	1/1	0.89	0.34	65,65,65,65	0
84	MG	1	3416	1/1	0.89	0.22	46,46,46,46	0
84	MG	CM	1948	1/1	0.89	0.12	58,58,58,58	0
84	MG	1	4004	1/1	0.89	0.10	48,48,48,48	0
84	MG	AT	211	1/1	0.89	0.09	44,44,44,44	0
84	MG	1	3411	1/1	0.89	0.36	32,32,32,32	0
84	MG	1	3693	1/1	0.89	0.14	47,47,47,47	0
84	MG	B	1880	1/1	0.89	0.27	47,47,47,47	0
84	MG	AS	3685	1/1	0.89	0.14	44,44,44,44	0
84	MG	AU	208	1/1	0.89	0.09	42,42,42,42	0
84	MG	AS	3686	1/1	0.89	0.23	38,38,38,38	0
84	MG	AS	3544	1/1	0.89	0.12	48,48,48,48	0
84	MG	CM	1965	1/1	0.89	0.19	53,53,53,53	0
84	MG	BE	302	1/1	0.89	0.23	36,36,36,36	0
84	MG	1	3915	1/1	0.89	0.17	30,30,30,30	0
84	MG	z	201	1/1	0.89	0.15	74,74,74,74	0
84	MG	0	202	1/1	0.89	0.17	59,59,59,59	0
84	MG	B	1993	1/1	0.89	0.17	42,42,42,42	0
84	MG	1	3659	1/1	0.89	0.26	41,41,41,41	0
84	MG	AS	3704	1/1	0.89	0.13	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	BS	201	1/1	0.89	0.10	49,49,49,49	0
84	MG	1	3614	1/1	0.89	0.15	78,78,78,78	0
84	MG	CM	1983	1/1	0.89	0.27	51,51,51,51	0
84	MG	1	3841	1/1	0.89	0.23	42,42,42,42	0
84	MG	AS	3709	1/1	0.89	0.24	43,43,43,43	0
84	MG	1	4021	1/1	0.89	0.08	47,47,47,47	0
84	MG	1	4022	1/1	0.89	0.06	40,40,40,40	0
84	MG	1	3616	1/1	0.89	0.28	26,26,26,26	0
84	MG	1	3486	1/1	0.89	0.35	37,37,37,37	0
84	MG	AS	3719	1/1	0.89	0.17	42,42,42,42	0
84	MG	1	3467	1/1	0.89	0.34	43,43,43,43	0
84	MG	1	3624	1/1	0.89	0.19	55,55,55,55	0
84	MG	1	3669	1/1	0.89	0.27	42,42,42,42	0
84	MG	1	3427	1/1	0.89	0.28	37,37,37,37	0
84	MG	1	3629	1/1	0.89	0.26	32,32,32,32	0
84	MG	B	1908	1/1	0.89	0.39	53,53,53,53	0
84	MG	1	3862	1/1	0.89	0.17	58,58,58,58	0
84	MG	B	1802	1/1	0.89	0.35	34,34,34,34	0
84	MG	CM	1812	1/1	0.89	0.13	44,44,44,44	0
84	MG	AS	3404	1/1	0.89	0.44	34,34,34,34	0
84	MG	B	1916	1/1	0.90	0.09	58,58,58,58	0
84	MG	B	1917	1/1	0.90	0.33	53,53,53,53	0
84	MG	1	3877	1/1	0.90	0.35	63,63,63,63	0
84	MG	1	3879	1/1	0.90	0.14	41,41,41,41	0
84	MG	1	3499	1/1	0.90	0.26	37,37,37,37	0
84	MG	CM	1826	1/1	0.90	0.10	47,47,47,47	0
84	MG	CM	1827	1/1	0.90	0.21	51,51,51,51	0
84	MG	1	3729	1/1	0.90	0.33	43,43,43,43	0
84	MG	CM	1833	1/1	0.90	0.25	49,49,49,49	0
84	MG	1	3969	1/1	0.90	0.08	43,43,43,43	0
84	MG	1	3526	1/1	0.90	0.25	54,54,54,54	0
84	MG	AS	3440	1/1	0.90	0.20	28,28,28,28	0
84	MG	1	3734	1/1	0.90	0.38	54,54,54,54	0
84	MG	AS	3758	1/1	0.90	0.10	57,57,57,57	0
84	MG	AS	3446	1/1	0.90	0.23	36,36,36,36	0
84	MG	CM	1842	1/1	0.90	0.14	52,52,52,52	0
84	MG	B	1933	1/1	0.90	0.19	70,70,70,70	0
84	MG	1	3976	1/1	0.90	0.07	40,40,40,40	0
84	MG	1	3500	1/1	0.90	0.19	36,36,36,36	0
84	MG	AS	3769	1/1	0.90	0.17	47,47,47,47	0
84	MG	CM	1852	1/1	0.90	0.20	35,35,35,35	0
84	MG	B	1834	1/1	0.90	0.16	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	AS	3772	1/1	0.90	0.22	46,46,46,46	0
84	MG	1	3650	1/1	0.90	0.39	43,43,43,43	0
84	MG	AS	3778	1/1	0.90	0.09	50,50,50,50	0
84	MG	1	3606	1/1	0.90	0.21	52,52,52,52	0
84	MG	AS	3467	1/1	0.90	0.27	68,68,68,68	0
84	MG	AS	3788	1/1	0.90	0.13	49,49,49,49	0
84	MG	1	3803	1/1	0.90	0.17	40,40,40,40	0
84	MG	1	3738	1/1	0.90	0.22	35,35,35,35	0
84	MG	B	1843	1/1	0.90	0.29	58,58,58,58	0
84	MG	B	1845	1/1	0.90	0.10	49,49,49,49	0
84	MG	AS	3484	1/1	0.90	0.26	40,40,40,40	0
84	MG	1	3900	1/1	0.90	0.21	53,53,53,53	0
84	MG	1	3743	1/1	0.90	0.17	32,32,32,32	0
84	MG	o	302	1/1	0.90	0.24	34,34,34,34	0
84	MG	1	3477	1/1	0.90	0.39	42,42,42,42	0
84	MG	AS	3807	1/1	0.90	0.05	42,42,42,42	0
84	MG	AS	3808	1/1	0.90	0.07	50,50,50,50	0
84	MG	1	3993	1/1	0.90	0.12	40,40,40,40	0
84	MG	1	3434	1/1	0.90	0.25	23,23,23,23	0
84	MG	CM	1890	1/1	0.90	0.29	34,34,34,34	0
84	MG	1	3542	1/1	0.90	0.33	40,40,40,40	0
84	MG	1	3435	1/1	0.90	0.23	27,27,27,27	0
84	MG	AS	3819	1/1	0.90	0.09	36,36,36,36	0
84	MG	1	3483	1/1	0.90	0.17	37,37,37,37	0
84	MG	1	3418	1/1	0.90	0.24	31,31,31,31	0
84	MG	1	3514	1/1	0.90	0.23	26,26,26,26	0
84	MG	AS	3509	1/1	0.90	0.23	37,37,37,37	0
84	MG	CM	1915	1/1	0.90	0.30	34,34,34,34	0
84	MG	1	3756	1/1	0.90	0.19	47,47,47,47	0
84	MG	B	1870	1/1	0.90	0.21	50,50,50,50	0
84	MG	AS	3514	1/1	0.90	0.26	33,33,33,33	0
84	MG	AS	3670	1/1	0.90	0.12	42,42,42,42	0
84	MG	1	3916	1/1	0.90	0.20	75,75,75,75	0
84	MG	CM	1921	1/1	0.90	0.11	42,42,42,42	0
84	MG	1	3827	1/1	0.90	0.20	52,52,52,52	0
84	MG	AS	3673	1/1	0.90	0.13	49,49,49,49	0
84	MG	1	3918	1/1	0.90	0.06	53,53,53,53	0
84	MG	AS	3675	1/1	0.90	0.17	49,49,49,49	0
84	MG	CM	1935	1/1	0.90	0.11	44,44,44,44	0
84	MG	CM	1939	1/1	0.90	0.15	45,45,45,45	0
84	MG	0	201	1/1	0.90	0.19	41,41,41,41	0
84	MG	1	3620	1/1	0.90	0.15	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3835	1/1	0.90	0.24	35,35,35,35	0
84	MG	1	3838	1/1	0.90	0.23	67,67,67,67	0
84	MG	B	1883	1/1	0.90	0.16	37,37,37,37	0
84	MG	AS	3684	1/1	0.90	0.17	32,32,32,32	0
84	MG	AS	3543	1/1	0.90	0.23	60,60,60,60	0
84	MG	1	3415	1/1	0.90	0.29	38,38,38,38	0
84	MG	CM	1955	1/1	0.90	0.24	42,42,42,42	0
84	MG	AU	206	1/1	0.90	0.11	42,42,42,42	0
84	MG	AS	3687	1/1	0.90	0.33	44,44,44,44	0
84	MG	AS	3546	1/1	0.90	0.16	42,42,42,42	0
84	MG	BB	302	1/1	0.90	0.34	44,44,44,44	0
84	MG	1	3759	1/1	0.90	0.12	36,36,36,36	0
84	MG	B	1994	1/1	0.90	0.11	58,58,58,58	0
84	MG	1	3768	1/1	0.90	0.15	28,28,28,28	0
84	MG	1	3770	1/1	0.90	0.15	33,33,33,33	0
84	MG	1	3494	1/1	0.90	0.08	37,37,37,37	0
84	MG	1	3849	1/1	0.90	0.17	38,38,38,38	0
84	MG	AS	3559	1/1	0.90	0.24	46,46,46,46	0
84	MG	AS	3565	1/1	0.90	0.31	35,35,35,35	0
84	MG	1	4034	1/1	0.90	0.07	58,58,58,58	0
84	MG	AS	3569	1/1	0.90	0.15	37,37,37,37	0
84	MG	CM	1980	1/1	0.90	0.08	43,43,43,43	0
84	MG	1	3592	1/1	0.90	0.18	53,53,53,53	0
84	MG	1	3666	1/1	0.90	0.19	42,42,42,42	0
84	MG	1	3559	1/1	0.90	0.16	43,43,43,43	0
84	MG	AI	201	1/1	0.90	0.08	54,54,54,54	0
84	MG	1	3714	1/1	0.90	0.21	42,42,42,42	0
84	MG	1	3460	1/1	0.90	0.22	21,21,21,21	0
84	MG	AS	3727	1/1	0.90	0.17	51,51,51,51	0
84	MG	1	3867	1/1	0.90	0.14	94,94,94,94	0
84	MG	1	3462	1/1	0.90	0.30	50,50,50,50	0
84	MG	1	3638	1/1	0.90	0.16	38,38,38,38	0
84	MG	1	3955	1/1	0.90	0.11	41,41,41,41	0
84	MG	AS	3593	1/1	0.90	0.19	52,52,52,52	0
84	MG	1	3600	1/1	0.90	0.10	47,47,47,47	0
84	MG	AS	3737	1/1	0.90	0.06	36,36,36,36	0
84	MG	AS	3596	1/1	0.90	0.16	142,142,142,142	0
84	MG	B	1813	1/1	0.90	0.22	50,50,50,50	0
85	ZN	h	201	1/1	0.90	0.09	238,238,238,238	0
84	MG	1	3727	1/1	0.90	0.11	36,36,36,36	0
84	MG	CM	1815	1/1	0.90	0.24	44,44,44,44	0
84	MG	CM	1817	1/1	0.90	0.24	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3833	1/1	0.91	0.11	34,34,34,34	0
84	MG	AS	3572	1/1	0.91	0.20	36,36,36,36	0
84	MG	1	3507	1/1	0.91	0.28	32,32,32,32	0
84	MG	1	3465	1/1	0.91	0.25	38,38,38,38	0
84	MG	1	3730	1/1	0.91	0.24	32,32,32,32	0
84	MG	Y	203	1/1	0.91	0.18	85,85,85,85	0
84	MG	B	1906	1/1	0.91	0.17	39,39,39,39	0
84	MG	1	3610	1/1	0.91	0.13	28,28,28,28	0
84	MG	1	3842	1/1	0.91	0.26	50,50,50,50	0
84	MG	AS	3736	1/1	0.91	0.08	35,35,35,35	0
84	MG	1	3910	1/1	0.91	0.11	69,69,69,69	0
84	MG	CM	1820	1/1	0.91	0.36	42,42,42,42	0
84	MG	AS	3587	1/1	0.91	0.21	44,44,44,44	0
84	MG	1	3611	1/1	0.91	0.27	31,31,31,31	0
84	MG	4	203	1/1	0.91	0.25	40,40,40,40	0
84	MG	AS	3592	1/1	0.91	0.09	42,42,42,42	0
84	MG	1	3844	1/1	0.91	0.18	54,54,54,54	0
84	MG	AS	3594	1/1	0.91	0.42	43,43,43,43	0
84	MG	B	1819	1/1	0.91	0.19	40,40,40,40	0
84	MG	CM	1830	1/1	0.91	0.24	36,36,36,36	0
84	MG	1	3983	1/1	0.91	0.08	44,44,44,44	0
84	MG	AS	3423	1/1	0.91	0.23	27,27,27,27	0
83	3K5	AS	3401	57/57	0.91	0.16	47,66,88,92	0
84	MG	4	209	1/1	0.91	0.15	39,39,39,39	0
84	MG	1	3644	1/1	0.91	0.15	34,34,34,34	0
84	MG	CM	1838	1/1	0.91	0.14	53,53,53,53	0
84	MG	1	3691	1/1	0.91	0.21	43,43,43,43	0
84	MG	AS	3602	1/1	0.91	0.44	43,43,43,43	0
84	MG	AS	3759	1/1	0.91	0.18	42,42,42,42	0
84	MG	AS	3608	1/1	0.91	0.22	50,50,50,50	0
84	MG	AS	3761	1/1	0.91	0.26	42,42,42,42	0
84	MG	1	3791	1/1	0.91	0.16	31,31,31,31	0
84	MG	B	1926	1/1	0.91	0.21	56,56,56,56	0
84	MG	4	213	1/1	0.91	0.14	43,43,43,43	0
84	MG	B	1929	1/1	0.91	0.18	45,45,45,45	0
84	MG	1	3856	1/1	0.91	0.22	46,46,46,46	0
84	MG	B	1833	1/1	0.91	0.12	34,34,34,34	0
84	MG	AS	3447	1/1	0.91	0.24	43,43,43,43	0
84	MG	AS	3450	1/1	0.91	0.21	41,41,41,41	0
84	MG	AS	3782	1/1	0.91	0.11	50,50,50,50	0
84	MG	1	3667	1/1	0.91	0.13	43,43,43,43	0
84	MG	AS	3454	1/1	0.91	0.32	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	CM	1868	1/1	0.91	0.17	48,48,48,48	0
84	MG	1	3995	1/1	0.91	0.10	45,45,45,45	0
84	MG	B	1935	1/1	0.91	0.20	86,86,86,86	0
84	MG	k	402	1/1	0.91	0.10	62,62,62,62	0
84	MG	1	3645	1/1	0.91	0.13	34,34,34,34	0
84	MG	AS	3793	1/1	0.91	0.13	59,59,59,59	0
84	MG	1	3613	1/1	0.91	0.23	33,33,33,33	0
84	MG	AS	3795	1/1	0.91	0.08	41,41,41,41	0
84	MG	B	1841	1/1	0.91	0.25	28,28,28,28	0
84	MG	B	1842	1/1	0.91	0.20	35,35,35,35	0
84	MG	k	405	1/1	0.91	0.18	34,34,34,34	0
84	MG	AS	3472	1/1	0.91	0.24	40,40,40,40	0
84	MG	CM	1888	1/1	0.91	0.11	39,39,39,39	0
84	MG	1	3533	1/1	0.91	0.16	31,31,31,31	0
84	MG	1	3865	1/1	0.91	0.12	56,56,56,56	0
84	MG	CM	1893	1/1	0.91	0.18	31,31,31,31	0
84	MG	AS	3480	1/1	0.91	0.12	38,38,38,38	0
84	MG	CM	1898	1/1	0.91	0.27	44,44,44,44	0
84	MG	AS	3483	1/1	0.91	0.23	32,32,32,32	0
84	MG	CM	1901	1/1	0.91	0.08	60,60,60,60	0
84	MG	CM	1905	1/1	0.91	0.31	35,35,35,35	0
84	MG	1	3866	1/1	0.91	0.13	52,52,52,52	0
84	MG	1	3598	1/1	0.91	0.38	42,42,42,42	0
84	MG	1	3699	1/1	0.91	0.15	40,40,40,40	0
84	MG	AS	3648	1/1	0.91	0.07	44,44,44,44	0
84	MG	1	3929	1/1	0.91	0.24	52,52,52,52	0
84	MG	B	1858	1/1	0.91	0.12	36,36,36,36	0
84	MG	1	4018	1/1	0.91	0.26	39,39,39,39	0
84	MG	1	3700	1/1	0.91	0.17	28,28,28,28	0
84	MG	1	3703	1/1	0.91	0.20	53,53,53,53	0
84	MG	1	3539	1/1	0.91	0.35	48,48,48,48	0
84	MG	x	201	1/1	0.91	0.28	28,28,28,28	0
84	MG	AS	3831	1/1	0.91	0.07	44,44,44,44	0
84	MG	B	1963	1/1	0.91	0.20	59,59,59,59	0
84	MG	AS	3667	1/1	0.91	0.10	36,36,36,36	0
84	MG	AS	3834	1/1	0.91	0.25	30,30,30,30	0
84	MG	AT	202	1/1	0.91	0.30	47,47,47,47	0
84	MG	AS	3668	1/1	0.91	0.12	41,41,41,41	0
84	MG	B	1964	1/1	0.91	0.06	55,55,55,55	0
84	MG	AS	3507	1/1	0.91	0.37	48,48,48,48	0
84	MG	1	3708	1/1	0.91	0.23	40,40,40,40	0
84	MG	1	3935	1/1	0.91	0.22	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	4026	1/1	0.91	0.12	42,42,42,42	0
84	MG	AS	3513	1/1	0.91	0.20	40,40,40,40	0
84	MG	B	1976	1/1	0.91	0.11	40,40,40,40	0
84	MG	AT	212	1/1	0.91	0.20	44,44,44,44	0
84	MG	CM	1953	1/1	0.91	0.28	42,42,42,42	0
84	MG	AS	3515	1/1	0.91	0.33	46,46,46,46	0
84	MG	1	3937	1/1	0.91	0.17	70,70,70,70	0
84	MG	AS	3680	1/1	0.91	0.13	49,49,49,49	0
84	MG	1	3711	1/1	0.91	0.10	31,31,31,31	0
84	MG	1	3561	1/1	0.91	0.20	43,43,43,43	0
84	MG	1	4031	1/1	0.91	0.08	43,43,43,43	0
84	MG	AW	302	1/1	0.91	0.27	42,42,42,42	0
84	MG	CM	1964	1/1	0.91	0.11	49,49,49,49	0
84	MG	AX	1300	1/1	0.91	0.30	36,36,36,36	0
84	MG	1	3501	1/1	0.91	0.14	28,28,28,28	0
84	MG	BB	301	1/1	0.91	0.12	37,37,37,37	0
84	MG	1	3765	1/1	0.91	0.16	33,33,33,33	0
84	MG	BB	304	1/1	0.91	0.08	40,40,40,40	0
84	MG	1	3953	1/1	0.91	0.12	38,38,38,38	0
84	MG	BB	306	1/1	0.91	0.15	42,42,42,42	0
84	MG	BE	301	1/1	0.91	0.17	37,37,37,37	0
84	MG	AS	3540	1/1	0.91	0.30	47,47,47,47	0
84	MG	1	3767	1/1	0.91	0.27	61,61,61,61	0
84	MG	B	1991	1/1	0.91	0.13	38,38,38,38	0
84	MG	AC	102	1/1	0.91	0.07	42,42,42,42	0
84	MG	1	3425	1/1	0.91	0.30	27,27,27,27	0
84	MG	CQ	302	1/1	0.91	0.08	41,41,41,41	0
84	MG	BJ	303	1/1	0.91	0.24	41,41,41,41	0
84	MG	1	4037	1/1	0.91	0.42	30,30,30,30	0
84	MG	B	1995	1/1	0.91	0.07	41,41,41,41	0
84	MG	AS	3549	1/1	0.91	0.11	40,40,40,40	0
84	MG	1	3627	1/1	0.91	0.21	40,40,40,40	0
84	MG	1	3895	1/1	0.91	0.18	36,36,36,36	0
84	MG	1	3774	1/1	0.91	0.14	44,44,44,44	0
84	MG	AS	3557	1/1	0.91	0.28	46,46,46,46	0
84	MG	BZ	204	1/1	0.91	0.20	43,43,43,43	0
84	MG	CA	201	1/1	0.91	0.12	51,51,51,51	0
84	MG	CJ	202	1/1	0.91	0.21	55,55,55,55	0
84	MG	1	3544	1/1	0.91	0.12	47,47,47,47	0
84	MG	1	3505	1/1	0.91	0.23	32,32,32,32	0
84	MG	AS	3717	1/1	0.91	0.12	39,39,39,39	0
84	MG	K	302	1/1	0.91	0.15	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	AJ	101	1/1	0.91	0.14	68,68,68,68	0
84	MG	AS	3724	1/1	0.91	0.11	38,38,38,38	0
85	ZN	DS	201	1/1	0.91	0.11	208,208,208,208	0
84	MG	1	4001	1/1	0.92	0.16	43,43,43,43	0
84	MG	1	3472	1/1	0.92	0.26	27,27,27,27	0
84	MG	1	3615	1/1	0.92	0.17	40,40,40,40	0
84	MG	AS	3562	1/1	0.92	0.15	50,50,50,50	0
84	MG	w	302	1/1	0.92	0.15	53,53,53,53	0
84	MG	1	3502	1/1	0.92	0.27	46,46,46,46	0
84	MG	1	3845	1/1	0.92	0.16	44,44,44,44	0
84	MG	AS	3570	1/1	0.92	0.07	29,29,29,29	0
84	MG	AS	3571	1/1	0.92	0.15	61,61,61,61	0
84	MG	y	201	1/1	0.92	0.14	43,43,43,43	0
84	MG	1	4012	1/1	0.92	0.34	47,47,47,47	0
84	MG	AS	3576	1/1	0.92	0.12	46,46,46,46	0
84	MG	AS	3577	1/1	0.92	0.27	45,45,45,45	0
84	MG	1	3617	1/1	0.92	0.15	40,40,40,40	0
84	MG	1	3718	1/1	0.92	0.11	43,43,43,43	0
84	MG	CM	1825	1/1	0.92	0.17	34,34,34,34	0
84	MG	AS	3744	1/1	0.92	0.07	55,55,55,55	0
84	MG	1	3848	1/1	0.92	0.43	55,55,55,55	0
84	MG	1	3456	1/1	0.92	0.28	19,19,19,19	0
84	MG	1	3535	1/1	0.92	0.15	25,25,25,25	0
84	MG	1	3476	1/1	0.92	0.25	27,27,27,27	0
84	MG	Z	202	1/1	0.92	0.36	55,55,55,55	0
84	MG	1	3459	1/1	0.92	0.32	27,27,27,27	0
84	MG	AS	3588	1/1	0.92	0.13	43,43,43,43	0
84	MG	1	3478	1/1	0.92	0.28	31,31,31,31	0
84	MG	AS	3757	1/1	0.92	0.13	49,49,49,49	0
84	MG	1	3587	1/1	0.92	0.24	41,41,41,41	0
84	MG	1	4025	1/1	0.92	0.13	40,40,40,40	0
84	MG	1	3588	1/1	0.92	0.24	31,31,31,31	0
84	MG	1	3509	1/1	0.92	0.28	28,28,28,28	0
84	MG	AS	3406	1/1	0.92	0.51	32,32,32,32	0
84	MG	AS	3408	1/1	0.92	0.09	43,43,43,43	0
84	MG	AS	3410	1/1	0.92	0.35	32,32,32,32	0
84	MG	AS	3768	1/1	0.92	0.15	39,39,39,39	0
84	MG	AS	3416	1/1	0.92	0.30	22,22,22,22	0
84	MG	1	3591	1/1	0.92	0.31	54,54,54,54	0
84	MG	AS	3771	1/1	0.92	0.19	42,42,42,42	0
84	MG	1	3636	1/1	0.92	0.11	33,33,33,33	0
84	MG	AS	3773	1/1	0.92	0.12	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	CM	1859	1/1	0.92	0.11	40,40,40,40	0
84	MG	1	3936	1/1	0.92	0.17	70,70,70,70	0
84	MG	AG	201	1/1	0.92	0.10	57,57,57,57	0
84	MG	AS	3606	1/1	0.92	0.12	59,59,59,59	0
84	MG	CM	1867	1/1	0.92	0.18	74,74,74,74	0
84	MG	1	3868	1/1	0.92	0.22	40,40,40,40	0
84	MG	B	1911	1/1	0.92	0.31	49,49,49,49	0
84	MG	1	3872	1/1	0.92	0.11	54,54,54,54	0
84	MG	AS	3434	1/1	0.92	0.29	39,39,39,39	0
84	MG	1	3424	1/1	0.92	0.15	40,40,40,40	0
84	MG	1	3481	1/1	0.92	0.27	34,34,34,34	0
84	MG	AP	202	1/1	0.92	0.25	33,33,33,33	0
84	MG	1	3945	1/1	0.92	0.14	40,40,40,40	0
84	MG	1	3443	1/1	0.92	0.21	37,37,37,37	0
84	MG	1	3951	1/1	0.92	0.11	40,40,40,40	0
84	MG	1	3952	1/1	0.92	0.18	44,44,44,44	0
84	MG	AS	3448	1/1	0.92	0.31	38,38,38,38	0
84	MG	1	3739	1/1	0.92	0.32	32,32,32,32	0
84	MG	AS	3451	1/1	0.92	0.31	51,51,51,51	0
84	MG	1	3740	1/1	0.92	0.19	53,53,53,53	0
84	MG	1	3556	1/1	0.92	0.28	46,46,46,46	0
84	MG	B	1812	1/1	0.92	0.21	61,61,61,61	0
84	MG	CM	1897	1/1	0.92	0.27	31,31,31,31	0
84	MG	AS	3810	1/1	0.92	0.21	42,42,42,42	0
84	MG	AS	3812	1/1	0.92	0.08	45,45,45,45	0
84	MG	3	212	1/1	0.92	0.13	60,60,60,60	0
84	MG	B	1931	1/1	0.92	0.14	47,47,47,47	0
84	MG	1	3956	1/1	0.92	0.07	42,42,42,42	0
84	MG	1	3957	1/1	0.92	0.12	44,44,44,44	0
84	MG	AS	3464	1/1	0.92	0.24	50,50,50,50	0
84	MG	B	1817	1/1	0.92	0.28	38,38,38,38	0
84	MG	AS	3824	1/1	0.92	0.16	48,48,48,48	0
84	MG	CM	1914	1/1	0.92	0.12	54,54,54,54	0
84	MG	1	3806	1/1	0.92	0.14	43,43,43,43	0
84	MG	AS	3469	1/1	0.92	0.16	37,37,37,37	0
84	MG	1	3744	1/1	0.92	0.17	47,47,47,47	0
84	MG	B	1823	1/1	0.92	0.28	36,36,36,36	0
84	MG	1	3414	1/1	0.92	0.35	29,29,29,29	0
84	MG	1	3885	1/1	0.92	0.22	47,47,47,47	0
84	MG	3	219	1/1	0.92	0.11	46,46,46,46	0
84	MG	AS	3482	1/1	0.92	0.20	32,32,32,32	0
84	MG	1	3965	1/1	0.92	0.07	30,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3746	1/1	0.92	0.23	40,40,40,40	0
84	MG	1	3516	1/1	0.92	0.10	45,45,45,45	0
84	MG	CM	1932	1/1	0.92	0.16	49,49,49,49	0
84	MG	AS	3489	1/1	0.92	0.24	40,40,40,40	0
84	MG	AT	205	1/1	0.92	0.11	54,54,54,54	0
84	MG	AS	3665	1/1	0.92	0.36	51,51,51,51	0
84	MG	B	1830	1/1	0.92	0.26	34,34,34,34	0
84	MG	1	3436	1/1	0.92	0.28	33,33,33,33	0
84	MG	CM	1947	1/1	0.92	0.37	44,44,44,44	0
84	MG	4	206	1/1	0.92	0.20	30,30,30,30	0
84	MG	1	3970	1/1	0.92	0.25	46,46,46,46	0
84	MG	1	3649	1/1	0.92	0.13	65,65,65,65	0
84	MG	1	3819	1/1	0.92	0.07	32,32,32,32	0
84	MG	1	3430	1/1	0.92	0.27	34,34,34,34	0
84	MG	AT	214	1/1	0.92	0.14	39,39,39,39	0
84	MG	1	3977	1/1	0.92	0.14	45,45,45,45	0
84	MG	1	3562	1/1	0.92	0.20	37,37,37,37	0
84	MG	AS	3504	1/1	0.92	0.10	55,55,55,55	0
84	MG	1	3899	1/1	0.92	0.07	50,50,50,50	0
84	MG	4	215	1/1	0.92	0.16	30,30,30,30	0
84	MG	1	3823	1/1	0.92	0.10	29,29,29,29	0
84	MG	B	1965	1/1	0.92	0.17	46,46,46,46	0
84	MG	1	3447	1/1	0.92	0.25	25,25,25,25	0
84	MG	1	3468	1/1	0.92	0.27	38,38,38,38	0
84	MG	B	1969	1/1	0.92	0.08	46,46,46,46	0
84	MG	BB	303	1/1	0.92	0.07	44,44,44,44	0
84	MG	CM	1971	1/1	0.92	0.13	42,42,42,42	0
84	MG	1	3440	1/1	0.92	0.26	40,40,40,40	0
84	MG	AS	3520	1/1	0.92	0.27	51,51,51,51	0
84	MG	AS	3523	1/1	0.92	0.10	27,27,27,27	0
84	MG	B	1975	1/1	0.92	0.08	45,45,45,45	0
84	MG	1	3470	1/1	0.92	0.19	26,26,26,26	0
84	MG	1	3569	1/1	0.92	0.13	39,39,39,39	0
84	MG	1	3761	1/1	0.92	0.28	24,24,24,24	0
84	MG	o	301	1/1	0.92	0.20	38,38,38,38	0
84	MG	AS	3699	1/1	0.92	0.14	50,50,50,50	0
84	MG	AS	3700	1/1	0.92	0.07	37,37,37,37	0
84	MG	1	3992	1/1	0.92	0.11	40,40,40,40	0
84	MG	AS	3703	1/1	0.92	0.07	41,41,41,41	0
84	MG	o	303	1/1	0.92	0.20	34,34,34,34	0
84	MG	CY	201	1/1	0.92	0.15	49,49,49,49	0
84	MG	B	1982	1/1	0.92	0.12	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	B	1983	1/1	0.92	0.06	56,56,56,56	0
84	MG	AS	3708	1/1	0.92	0.06	56,56,56,56	0
84	MG	B	1984	1/1	0.92	0.09	62,62,62,62	0
84	MG	1	3836	1/1	0.92	0.17	38,38,38,38	0
84	MG	1	3573	1/1	0.92	0.13	50,50,50,50	0
84	MG	CA	202	1/1	0.92	0.07	46,46,46,46	0
84	MG	B	1987	1/1	0.92	0.07	46,46,46,46	0
84	MG	1	3527	1/1	0.92	0.22	38,38,38,38	0
84	MG	1	3996	1/1	0.92	0.24	40,40,40,40	0
84	MG	B	1869	1/1	0.92	0.18	72,72,72,72	0
84	MG	AS	3721	1/1	0.92	0.10	47,47,47,47	0
84	MG	AS	3723	1/1	0.92	0.24	47,47,47,47	0
84	MG	1	3453	1/1	0.92	0.33	26,26,26,26	0
84	MG	v	301	1/1	0.92	0.08	36,36,36,36	0
84	MG	CM	1829	1/1	0.93	0.27	35,35,35,35	0
84	MG	1	3661	1/1	0.93	0.20	39,39,39,39	0
84	MG	CM	1831	1/1	0.93	0.17	51,51,51,51	0
84	MG	AF	201	1/1	0.93	0.07	41,41,41,41	0
84	MG	AS	3781	1/1	0.93	0.12	42,42,42,42	0
84	MG	1	3732	1/1	0.93	0.16	32,32,32,32	0
84	MG	1	3603	1/1	0.93	0.08	52,52,52,52	0
84	MG	1	3551	1/1	0.93	0.28	52,52,52,52	0
84	MG	AS	3786	1/1	0.93	0.17	44,44,44,44	0
84	MG	1	3552	1/1	0.93	0.08	56,56,56,56	0
84	MG	1	3932	1/1	0.93	0.16	43,43,43,43	0
84	MG	1	3437	1/1	0.93	0.21	26,26,26,26	0
84	MG	AO	101	1/1	0.93	0.21	43,43,43,43	0
84	MG	1	3474	1/1	0.93	0.19	31,31,31,31	0
84	MG	B	1988	1/1	0.93	0.09	43,43,43,43	0
84	MG	B	1989	1/1	0.93	0.07	42,42,42,42	0
84	MG	1	3831	1/1	0.93	0.19	44,44,44,44	0
84	MG	AS	3656	1/1	0.93	0.07	35,35,35,35	0
84	MG	1	3458	1/1	0.93	0.21	35,35,35,35	0
84	MG	AS	3659	1/1	0.93	0.27	45,45,45,45	0
84	MG	B	1896	1/1	0.93	0.10	58,58,58,58	0
84	MG	AS	3806	1/1	0.93	0.08	34,34,34,34	0
83	3K5	1	3401	57/57	0.93	0.14	40,55,74,85	0
84	MG	1	3888	1/1	0.93	0.13	44,44,44,44	0
84	MG	1	3939	1/1	0.93	0.10	35,35,35,35	0
84	MG	AS	3517	1/1	0.93	0.20	34,34,34,34	0
84	MG	AS	3811	1/1	0.93	0.04	38,38,38,38	0
84	MG	B	1806	1/1	0.93	0.14	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	AS	3521	1/1	0.93	0.39	43,43,43,43	0
84	MG	1	3941	1/1	0.93	0.10	34,34,34,34	0
84	MG	1	3891	1/1	0.93	0.07	57,57,57,57	0
84	MG	B	1811	1/1	0.93	0.20	39,39,39,39	0
84	MG	1	4006	1/1	0.93	0.07	44,44,44,44	0
84	MG	4	214	1/1	0.93	0.09	45,45,45,45	0
84	MG	1	4009	1/1	0.93	0.08	43,43,43,43	0
84	MG	1	3943	1/1	0.93	0.09	36,36,36,36	0
84	MG	1	4011	1/1	0.93	0.09	37,37,37,37	0
84	MG	CM	1882	1/1	0.93	0.20	42,42,42,42	0
84	MG	1	3493	1/1	0.93	0.08	41,41,41,41	0
84	MG	B	1820	1/1	0.93	0.39	48,48,48,48	0
84	MG	1	3560	1/1	0.93	0.12	27,27,27,27	0
84	MG	1	4015	1/1	0.93	0.08	38,38,38,38	0
84	MG	1	3787	1/1	0.93	0.20	38,38,38,38	0
84	MG	1	3520	1/1	0.93	0.10	25,25,25,25	0
84	MG	1	3789	1/1	0.93	0.16	39,39,39,39	0
84	MG	1	3521	1/1	0.93	0.11	32,32,32,32	0
84	MG	1	3705	1/1	0.93	0.17	47,47,47,47	0
84	MG	1	3707	1/1	0.93	0.29	40,40,40,40	0
84	MG	1	3749	1/1	0.93	0.27	39,39,39,39	0
84	MG	CM	1902	1/1	0.93	0.32	50,50,50,50	0
84	MG	CM	1903	1/1	0.93	0.20	51,51,51,51	0
84	MG	AS	3691	1/1	0.93	0.09	47,47,47,47	0
84	MG	B	1927	1/1	0.93	0.07	48,48,48,48	0
84	MG	1	3540	1/1	0.93	0.17	35,35,35,35	0
84	MG	CM	1910	1/1	0.93	0.07	53,53,53,53	0
84	MG	1	3541	1/1	0.93	0.23	30,30,30,30	0
84	MG	AS	3411	1/1	0.93	0.05	29,29,29,29	0
84	MG	AS	3563	1/1	0.93	0.10	47,47,47,47	0
84	MG	AS	3701	1/1	0.93	0.09	42,42,42,42	0
84	MG	AS	3564	1/1	0.93	0.25	50,50,50,50	0
84	MG	u	201	1/1	0.93	0.09	37,37,37,37	0
84	MG	B	1835	1/1	0.93	0.28	43,43,43,43	0
84	MG	1	3506	1/1	0.93	0.34	43,43,43,43	0
84	MG	B	1837	1/1	0.93	0.21	38,38,38,38	0
84	MG	AS	3424	1/1	0.93	0.26	31,31,31,31	0
84	MG	1	3961	1/1	0.93	0.06	41,41,41,41	0
84	MG	CM	1922	1/1	0.93	0.07	43,43,43,43	0
84	MG	1	4028	1/1	0.93	0.09	46,46,46,46	0
84	MG	AW	303	1/1	0.93	0.23	52,52,52,52	0
84	MG	CM	1926	1/1	0.93	0.16	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	AW	304	1/1	0.93	0.09	62,62,62,62	0
84	MG	1	3962	1/1	0.93	0.09	38,38,38,38	0
84	MG	CM	1930	1/1	0.93	0.24	45,45,45,45	0
84	MG	CM	1931	1/1	0.93	0.11	43,43,43,43	0
84	MG	AS	3713	1/1	0.93	0.14	54,54,54,54	0
84	MG	CM	1933	1/1	0.93	0.09	45,45,45,45	0
84	MG	AS	3714	1/1	0.93	0.07	46,46,46,46	0
84	MG	1	3851	1/1	0.93	0.22	46,46,46,46	0
84	MG	1	3406	1/1	0.93	0.30	33,33,33,33	0
84	MG	AS	3435	1/1	0.93	0.14	33,33,33,33	0
84	MG	1	3854	1/1	0.93	0.06	29,29,29,29	0
84	MG	AS	3720	1/1	0.93	0.09	46,46,46,46	0
84	MG	1	3717	1/1	0.93	0.18	43,43,43,43	0
84	MG	B	1848	1/1	0.93	0.10	51,51,51,51	0
84	MG	B	1944	1/1	0.93	0.11	82,82,82,82	0
84	MG	1	3858	1/1	0.93	0.14	45,45,45,45	0
84	MG	AS	3445	1/1	0.93	0.33	47,47,47,47	0
84	MG	B	1850	1/1	0.93	0.19	77,77,77,77	0
84	MG	BJ	301	1/1	0.93	0.09	30,30,30,30	0
84	MG	CM	1956	1/1	0.93	0.29	47,47,47,47	0
84	MG	1	3804	1/1	0.93	0.15	48,48,48,48	0
84	MG	BK	201	1/1	0.93	0.29	36,36,36,36	0
84	MG	B	1948	1/1	0.93	0.09	61,61,61,61	0
84	MG	AS	3449	1/1	0.93	0.13	27,27,27,27	0
84	MG	1	3451	1/1	0.93	0.27	24,24,24,24	0
84	MG	1	3683	1/1	0.93	0.42	72,72,72,72	0
84	MG	B	1952	1/1	0.93	0.09	42,42,42,42	0
84	MG	1	3972	1/1	0.93	0.20	49,49,49,49	0
84	MG	3	203	1/1	0.93	0.29	45,45,45,45	0
84	MG	CM	1969	1/1	0.93	0.04	43,43,43,43	0
84	MG	1	3973	1/1	0.93	0.19	43,43,43,43	0
84	MG	AS	3457	1/1	0.93	0.29	32,32,32,32	0
84	MG	1	3463	1/1	0.93	0.11	33,33,33,33	0
84	MG	AS	3459	1/1	0.93	0.24	34,34,34,34	0
84	MG	B	1957	1/1	0.93	0.16	55,55,55,55	0
84	MG	6	202	1/1	0.93	0.08	31,31,31,31	0
84	MG	B	1959	1/1	0.93	0.22	52,52,52,52	0
84	MG	AS	3466	1/1	0.93	0.21	45,45,45,45	0
84	MG	AS	3610	1/1	0.93	0.08	41,41,41,41	0
84	MG	CM	1803	1/1	0.93	0.15	29,29,29,29	0
84	MG	B	1863	1/1	0.93	0.09	87,87,87,87	0
84	MG	CO	301	1/1	0.93	0.22	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	AS	3750	1/1	0.93	0.14	41,41,41,41	0
84	MG	3	209	1/1	0.93	0.06	43,43,43,43	0
84	MG	AS	3613	1/1	0.93	0.08	44,44,44,44	0
84	MG	B	1865	1/1	0.93	0.31	39,39,39,39	0
84	MG	1	3725	1/1	0.93	0.23	44,44,44,44	0
84	MG	AS	3471	1/1	0.93	0.17	30,30,30,30	0
84	MG	1	3547	1/1	0.93	0.25	35,35,35,35	0
84	MG	1	3626	1/1	0.93	0.12	37,37,37,37	0
84	MG	AS	3478	1/1	0.93	0.09	40,40,40,40	0
84	MG	1	3441	1/1	0.93	0.29	36,36,36,36	0
84	MG	1	3578	1/1	0.93	0.16	40,40,40,40	0
84	MG	B	1871	1/1	0.93	0.20	75,75,75,75	0
84	MG	B	1973	1/1	0.93	0.06	44,44,44,44	0
84	MG	AS	3629	1/1	0.93	0.15	41,41,41,41	0
84	MG	AD	202	1/1	0.93	0.11	50,50,50,50	0
84	MG	AS	3485	1/1	0.93	0.34	35,35,35,35	0
84	MG	AS	3632	1/1	0.93	0.16	40,40,40,40	0
84	MG	1	3820	1/1	0.93	0.23	39,39,39,39	0
84	MG	B	1874	1/1	0.93	0.21	38,38,38,38	0
84	MG	AS	3774	1/1	0.93	0.08	59,59,59,59	0
84	MG	AS	3541	1/1	0.94	0.25	37,37,37,37	0
84	MG	1	3950	1/1	0.94	0.12	49,49,49,49	0
84	MG	1	3658	1/1	0.94	0.16	27,27,27,27	0
84	MG	1	3887	1/1	0.94	0.33	44,44,44,44	0
84	MG	AS	3545	1/1	0.94	0.31	39,39,39,39	0
84	MG	1	3775	1/1	0.94	0.11	38,38,38,38	0
84	MG	AS	3813	1/1	0.94	0.06	51,51,51,51	0
84	MG	1	4023	1/1	0.94	0.19	48,48,48,48	0
84	MG	1	3776	1/1	0.94	0.14	35,35,35,35	0
84	MG	1	3537	1/1	0.94	0.17	42,42,42,42	0
84	MG	B	1937	1/1	0.94	0.15	46,46,46,46	0
84	MG	1	3828	1/1	0.94	0.19	40,40,40,40	0
84	MG	1	3510	1/1	0.94	0.23	22,22,22,22	0
84	MG	CM	1863	1/1	0.94	0.24	58,58,58,58	0
84	MG	AS	3822	1/1	0.94	0.15	47,47,47,47	0
84	MG	AS	3556	1/1	0.94	0.20	46,46,46,46	0
84	MG	w	304	1/1	0.94	0.08	40,40,40,40	0
84	MG	1	3457	1/1	0.94	0.16	26,26,26,26	0
84	MG	x	202	1/1	0.94	0.14	38,38,38,38	0
84	MG	AS	3432	1/1	0.94	0.23	32,32,32,32	0
84	MG	CM	1874	1/1	0.94	0.32	42,42,42,42	0
84	MG	1	3488	1/1	0.94	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3450	1/1	0.94	0.23	33,33,33,33	0
84	MG	B	1853	1/1	0.94	0.06	58,58,58,58	0
84	MG	AS	3566	1/1	0.94	0.36	44,44,44,44	0
84	MG	AS	3695	1/1	0.94	0.28	34,34,34,34	0
84	MG	AT	201	1/1	0.94	0.22	24,24,24,24	0
84	MG	CM	1881	1/1	0.94	0.15	43,43,43,43	0
84	MG	AS	3696	1/1	0.94	0.10	41,41,41,41	0
84	MG	AS	3567	1/1	0.94	0.19	23,23,23,23	0
84	MG	CM	1884	1/1	0.94	0.13	43,43,43,43	0
84	MG	1	3417	1/1	0.94	0.15	45,45,45,45	0
84	MG	CM	1887	1/1	0.94	0.22	74,74,74,74	0
84	MG	1	3473	1/1	0.94	0.33	19,19,19,19	0
84	MG	B	1857	1/1	0.94	0.10	47,47,47,47	0
84	MG	AS	3441	1/1	0.94	0.14	42,42,42,42	0
84	MG	1	3639	1/1	0.94	0.17	26,26,26,26	0
84	MG	AS	3573	1/1	0.94	0.07	41,41,41,41	0
84	MG	CM	1896	1/1	0.94	0.25	36,36,36,36	0
84	MG	B	1859	1/1	0.94	0.11	71,71,71,71	0
84	MG	1	3840	1/1	0.94	0.07	28,28,28,28	0
84	MG	CM	1899	1/1	0.94	0.12	33,33,33,33	0
84	MG	0	203	1/1	0.94	0.09	50,50,50,50	0
84	MG	1	3903	1/1	0.94	0.18	43,43,43,43	0
84	MG	1	3402	1/1	0.94	0.19	19,19,19,19	0
84	MG	AU	201	1/1	0.94	0.24	28,28,28,28	0
84	MG	1	3668	1/1	0.94	0.11	45,45,45,45	0
84	MG	3	201	1/1	0.94	0.21	23,23,23,23	0
84	MG	CM	1907	1/1	0.94	0.07	52,52,52,52	0
84	MG	CM	1908	1/1	0.94	0.21	49,49,49,49	0
84	MG	1	3642	1/1	0.94	0.29	33,33,33,33	0
84	MG	AS	3584	1/1	0.94	0.18	36,36,36,36	0
84	MG	1	3741	1/1	0.94	0.19	29,29,29,29	0
84	MG	1	3790	1/1	0.94	0.40	41,41,41,41	0
84	MG	AC	101	1/1	0.94	0.09	38,38,38,38	0
84	MG	3	207	1/1	0.94	0.07	39,39,39,39	0
84	MG	1	3566	1/1	0.94	0.13	22,22,22,22	0
84	MG	1	3792	1/1	0.94	0.26	34,34,34,34	0
84	MG	1	3793	1/1	0.94	0.17	33,33,33,33	0
84	MG	1	3671	1/1	0.94	0.06	44,44,44,44	0
84	MG	B	1970	1/1	0.94	0.21	47,47,47,47	0
84	MG	AS	3465	1/1	0.94	0.19	37,37,37,37	0
84	MG	1	3518	1/1	0.94	0.14	28,28,28,28	0
84	MG	1	3706	1/1	0.94	0.20	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	B	1974	1/1	0.94	0.15	56,56,56,56	0
84	MG	B	1878	1/1	0.94	0.30	38,38,38,38	0
84	MG	CM	1925	1/1	0.94	0.14	45,45,45,45	0
84	MG	1	3919	1/1	0.94	0.12	41,41,41,41	0
84	MG	1	3981	1/1	0.94	0.15	41,41,41,41	0
84	MG	B	1881	1/1	0.94	0.18	64,64,64,64	0
84	MG	AS	3605	1/1	0.94	0.13	40,40,40,40	0
84	MG	1	3590	1/1	0.94	0.23	50,50,50,50	0
84	MG	AS	3477	1/1	0.94	0.09	27,27,27,27	0
84	MG	BJ	304	1/1	0.94	0.11	50,50,50,50	0
84	MG	1	3855	1/1	0.94	0.09	39,39,39,39	0
84	MG	CM	1938	1/1	0.94	0.07	33,33,33,33	0
84	MG	1	3519	1/1	0.94	0.30	57,57,57,57	0
84	MG	B	1885	1/1	0.94	0.15	60,60,60,60	0
84	MG	BO	202	1/1	0.94	0.26	50,50,50,50	0
84	MG	AM	101	1/1	0.94	0.36	45,45,45,45	0
84	MG	CM	1946	1/1	0.94	0.07	40,40,40,40	0
84	MG	1	3709	1/1	0.94	0.16	39,39,39,39	0
84	MG	1	3710	1/1	0.94	0.10	32,32,32,32	0
84	MG	BZ	201	1/1	0.94	0.18	47,47,47,47	0
84	MG	AS	3746	1/1	0.94	0.07	40,40,40,40	0
84	MG	CM	1951	1/1	0.94	0.16	41,41,41,41	0
84	MG	AS	3616	1/1	0.94	0.29	44,44,44,44	0
84	MG	1	3531	1/1	0.94	0.28	26,26,26,26	0
84	MG	1	3990	1/1	0.94	0.27	45,45,45,45	0
84	MG	4	204	1/1	0.94	0.20	32,32,32,32	0
84	MG	1	3991	1/1	0.94	0.42	47,47,47,47	0
84	MG	1	3532	1/1	0.94	0.27	32,32,32,32	0
84	MG	1	3805	1/1	0.94	0.19	52,52,52,52	0
84	MG	CM	1960	1/1	0.94	0.08	50,50,50,50	0
84	MG	1	3679	1/1	0.94	0.23	30,30,30,30	0
84	MG	1	3554	1/1	0.94	0.09	36,36,36,36	0
84	MG	1	3595	1/1	0.94	0.23	31,31,31,31	0
84	MG	1	3719	1/1	0.94	0.08	41,41,41,41	0
84	MG	B	1996	1/1	0.94	0.06	40,40,40,40	0
84	MG	CM	1805	1/1	0.94	0.28	34,34,34,34	0
84	MG	D	301	1/1	0.94	0.15	44,44,44,44	0
84	MG	1	4000	1/1	0.94	0.11	35,35,35,35	0
84	MG	1	3870	1/1	0.94	0.16	51,51,51,51	0
84	MG	1	3810	1/1	0.94	0.13	34,34,34,34	0
84	MG	1	3812	1/1	0.94	0.15	48,48,48,48	0
84	MG	AS	3510	1/1	0.94	0.34	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	1	3813	1/1	0.94	0.09	62,62,62,62	0
84	MG	1	3454	1/1	0.94	0.06	23,23,23,23	0
84	MG	CM	1977	1/1	0.94	0.15	56,56,56,56	0
84	MG	AS	3639	1/1	0.94	0.14	49,49,49,49	0
84	MG	1	4007	1/1	0.94	0.44	38,38,38,38	0
84	MG	1	4008	1/1	0.94	0.07	47,47,47,47	0
84	MG	CM	1982	1/1	0.94	0.08	42,42,42,42	0
84	MG	B	1914	1/1	0.94	0.16	46,46,46,46	0
84	MG	1	3576	1/1	0.94	0.06	29,29,29,29	0
84	MG	AS	3518	1/1	0.94	0.26	28,28,28,28	0
84	MG	CQ	301	1/1	0.94	0.26	40,40,40,40	0
84	MG	AS	3519	1/1	0.94	0.17	38,38,38,38	0
84	MG	1	3764	1/1	0.94	0.11	51,51,51,51	0
84	MG	AS	3652	1/1	0.94	0.13	44,44,44,44	0
84	MG	1	3818	1/1	0.94	0.13	36,36,36,36	0
84	MG	AS	3654	1/1	0.94	0.13	33,33,33,33	0
84	MG	k	406	1/1	0.94	0.07	33,33,33,33	0
84	MG	1	3724	1/1	0.94	0.13	33,33,33,33	0
84	MG	Z	203	1/1	0.94	0.38	66,66,66,66	0
84	MG	AS	3531	1/1	0.94	0.15	38,38,38,38	0
84	MG	AS	3532	1/1	0.94	0.19	59,59,59,59	0
84	MG	1	3623	1/1	0.94	0.20	44,44,44,44	0
84	MG	1	3577	1/1	0.94	0.26	28,28,28,28	0
84	MG	AS	3798	1/1	0.94	0.15	37,37,37,37	0
85	ZN	AN	101	1/1	0.94	0.13	142,142,142,142	0
84	MG	AS	3663	1/1	0.94	0.06	94,94,94,94	0
84	MG	1	3883	1/1	0.94	0.17	42,42,42,42	0
84	MG	1	3948	1/1	0.94	0.10	38,38,38,38	0
84	MG	r	301	1/1	0.94	0.16	34,34,34,34	0
84	MG	1	3428	1/1	0.94	0.29	27,27,27,27	0
84	MG	CM	1843	1/1	0.94	0.25	42,42,42,42	0
84	MG	CM	1844	1/1	0.94	0.16	41,41,41,41	0
84	MG	CM	1894	1/1	0.95	0.23	43,43,43,43	0
84	MG	BN	203	1/1	0.95	0.10	39,39,39,39	0
84	MG	AS	3783	1/1	0.95	0.07	46,46,46,46	0
84	MG	1	3763	1/1	0.95	0.07	30,30,30,30	0
84	MG	1	3546	1/1	0.95	0.23	44,44,44,44	0
84	MG	AS	3689	1/1	0.95	0.24	38,38,38,38	0
84	MG	AS	3604	1/1	0.95	0.18	26,26,26,26	0
84	MG	B	1888	1/1	0.95	0.19	46,46,46,46	0
84	MG	AS	3527	1/1	0.95	0.13	63,63,63,63	0
84	MG	AS	3791	1/1	0.95	0.10	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	CM	1904	1/1	0.95	0.25	44,44,44,44	0
84	MG	AS	3607	1/1	0.95	0.20	37,37,37,37	0
84	MG	B	1889	1/1	0.95	0.22	36,36,36,36	0
84	MG	AS	3529	1/1	0.95	0.33	52,52,52,52	0
84	MG	1	3455	1/1	0.95	0.12	29,29,29,29	0
84	MG	AS	3796	1/1	0.95	0.24	43,43,43,43	0
84	MG	G	301	1/1	0.95	0.15	54,54,54,54	0
84	MG	o	304	1/1	0.95	0.16	41,41,41,41	0
84	MG	1	3766	1/1	0.95	0.20	45,45,45,45	0
84	MG	B	1894	1/1	0.95	0.19	40,40,40,40	0
84	MG	AS	3615	1/1	0.95	0.15	47,47,47,47	0
84	MG	1	4005	1/1	0.95	0.13	42,42,42,42	0
84	MG	1	3549	1/1	0.95	0.15	40,40,40,40	0
84	MG	AS	3538	1/1	0.95	0.16	42,42,42,42	0
84	MG	B	1844	1/1	0.95	0.27	41,41,41,41	0
84	MG	AS	3462	1/1	0.95	0.16	31,31,31,31	0
84	MG	1	3565	1/1	0.95	0.23	26,26,26,26	0
84	MG	1	3713	1/1	0.95	0.28	32,32,32,32	0
84	MG	AS	3625	1/1	0.95	0.12	65,65,65,65	0
84	MG	1	3966	1/1	0.95	0.06	33,33,33,33	0
84	MG	AS	3814	1/1	0.95	0.06	47,47,47,47	0
84	MG	1	3771	1/1	0.95	0.13	38,38,38,38	0
84	MG	CM	1816	1/1	0.95	0.28	31,31,31,31	0
84	MG	CM	1927	1/1	0.95	0.12	33,33,33,33	0
84	MG	1	3884	1/1	0.95	0.15	49,49,49,49	0
84	MG	CM	1818	1/1	0.95	0.18	29,29,29,29	0
84	MG	AS	3817	1/1	0.95	0.06	42,42,42,42	0
84	MG	B	1960	1/1	0.95	0.27	41,41,41,41	0
84	MG	i	301	1/1	0.95	0.06	40,40,40,40	0
84	MG	B	1801	1/1	0.95	0.21	38,38,38,38	0
84	MG	1	3772	1/1	0.95	0.06	34,34,34,34	0
84	MG	CM	1936	1/1	0.95	0.13	46,46,46,46	0
84	MG	CM	1937	1/1	0.95	0.14	49,49,49,49	0
84	MG	AS	3722	1/1	0.95	0.07	59,59,59,59	0
84	MG	1	3773	1/1	0.95	0.08	46,46,46,46	0
84	MG	AS	3475	1/1	0.95	0.14	36,36,36,36	0
84	MG	AS	3552	1/1	0.95	0.23	37,37,37,37	0
84	MG	1	3534	1/1	0.95	0.20	30,30,30,30	0
84	MG	CM	1944	1/1	0.95	0.08	55,55,55,55	0
84	MG	1	3409	1/1	0.95	0.26	22,22,22,22	0
84	MG	1	3605	1/1	0.95	0.10	44,44,44,44	0
84	MG	B	1807	1/1	0.95	0.08	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	AS	3407	1/1	0.95	0.22	23,23,23,23	0
84	MG	AS	3731	1/1	0.95	0.08	49,49,49,49	0
84	MG	AS	3560	1/1	0.95	0.10	32,32,32,32	0
84	MG	AS	3481	1/1	0.95	0.11	41,41,41,41	0
84	MG	1	3811	1/1	0.95	0.04	43,43,43,43	0
84	MG	1	3536	1/1	0.95	0.21	34,34,34,34	0
84	MG	AS	3647	1/1	0.95	0.08	37,37,37,37	0
84	MG	1	3852	1/1	0.95	0.19	43,43,43,43	0
84	MG	CM	1841	1/1	0.95	0.18	49,49,49,49	0
84	MG	1	3692	1/1	0.95	0.06	59,59,59,59	0
84	MG	AS	3486	1/1	0.95	0.12	44,44,44,44	0
84	MG	1	3515	1/1	0.95	0.23	33,33,33,33	0
84	MG	AS	3488	1/1	0.95	0.20	36,36,36,36	0
84	MG	CM	1846	1/1	0.95	0.14	46,46,46,46	0
84	MG	CM	1847	1/1	0.95	0.16	45,45,45,45	0
84	MG	AS	3418	1/1	0.95	0.11	17,17,17,17	0
84	MG	AS	3490	1/1	0.95	0.17	39,39,39,39	0
84	MG	CM	1967	1/1	0.95	0.07	60,60,60,60	0
84	MG	1	3485	1/1	0.95	0.21	37,37,37,37	0
84	MG	AS	3420	1/1	0.95	0.17	50,50,50,50	0
84	MG	AS	3493	1/1	0.95	0.22	34,34,34,34	0
84	MG	1	3497	1/1	0.95	0.25	29,29,29,29	0
84	MG	AS	3496	1/1	0.95	0.07	31,31,31,31	0
84	MG	1	3857	1/1	0.95	0.12	29,29,29,29	0
84	MG	1	3631	1/1	0.95	0.09	23,23,23,23	0
84	MG	1	3408	1/1	0.95	0.16	22,22,22,22	0
84	MG	AU	207	1/1	0.95	0.06	40,40,40,40	0
84	MG	1	3752	1/1	0.95	0.19	37,37,37,37	0
84	MG	AS	3756	1/1	0.95	0.17	35,35,35,35	0
84	MG	CM	1865	1/1	0.95	0.24	51,51,51,51	0
84	MG	AS	3430	1/1	0.95	0.28	29,29,29,29	0
84	MG	1	3904	1/1	0.95	0.24	46,46,46,46	0
84	MG	1	3677	1/1	0.95	0.15	47,47,47,47	0
84	MG	6	203	1/1	0.95	0.08	39,39,39,39	0
84	MG	CP	301	1/1	0.95	0.23	38,38,38,38	0
84	MG	1	3420	1/1	0.95	0.17	42,42,42,42	0
84	MG	CM	1872	1/1	0.95	0.23	32,32,32,32	0
84	MG	AS	3508	1/1	0.95	0.27	29,29,29,29	0
84	MG	AS	3763	1/1	0.95	0.12	41,41,41,41	0
84	MG	1	3635	1/1	0.95	0.13	26,26,26,26	0
84	MG	1	3421	1/1	0.95	0.38	26,26,26,26	0
84	MG	AB	201	1/1	0.95	0.21	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	AS	3677	1/1	0.95	0.08	31,31,31,31	0
84	MG	AS	3678	1/1	0.95	0.35	29,29,29,29	0
84	MG	1	3731	1/1	0.95	0.10	34,34,34,34	0
84	MG	1	3490	1/1	0.95	0.11	50,50,50,50	0
84	MG	1	3579	1/1	0.95	0.11	55,55,55,55	0
84	MG	AS	3443	1/1	0.95	0.09	48,48,48,48	0
84	MG	AS	3516	1/1	0.95	0.30	35,35,35,35	0
84	MG	BJ	302	1/1	0.95	0.14	53,53,53,53	0
84	MG	CM	1886	1/1	0.95	0.13	53,53,53,53	0
84	MG	1	3760	1/1	0.95	0.21	33,33,33,33	0
84	MG	AS	3779	1/1	0.95	0.24	48,48,48,48	0
84	MG	1	3491	1/1	0.95	0.11	35,35,35,35	0
84	MG	1	3762	1/1	0.95	0.13	38,38,38,38	0
84	MG	CM	1891	1/1	0.95	0.09	54,54,54,54	0
84	MG	BN	202	1/1	0.95	0.08	37,37,37,37	0
84	MG	AS	3657	1/1	0.96	0.07	47,47,47,47	0
84	MG	1	3907	1/1	0.96	0.18	30,30,30,30	0
84	MG	AS	3505	1/1	0.96	0.16	63,63,63,63	0
84	MG	1	3651	1/1	0.96	0.20	39,39,39,39	0
84	MG	B	1846	1/1	0.96	0.19	36,36,36,36	0
84	MG	B	1890	1/1	0.96	0.08	37,37,37,37	0
84	MG	B	1942	1/1	0.96	0.29	49,49,49,49	0
84	MG	B	1847	1/1	0.96	0.18	41,41,41,41	0
84	MG	1	3405	1/1	0.96	0.37	33,33,33,33	0
84	MG	1	3832	1/1	0.96	0.16	36,36,36,36	0
84	MG	B	1997	1/1	0.96	0.08	48,48,48,48	0
84	MG	1	3747	1/1	0.96	0.16	43,43,43,43	0
84	MG	B	1895	1/1	0.96	0.09	52,52,52,52	0
84	MG	1	3834	1/1	0.96	0.08	35,35,35,35	0
84	MG	B	1810	1/1	0.96	0.12	21,21,21,21	0
84	MG	AS	3755	1/1	0.96	0.18	43,43,43,43	0
84	MG	B	1950	1/1	0.96	0.16	55,55,55,55	0
84	MG	1	3452	1/1	0.96	0.08	32,32,32,32	0
84	MG	AS	3453	1/1	0.96	0.25	33,33,33,33	0
84	MG	1	3596	1/1	0.96	0.20	32,32,32,32	0
84	MG	CM	1934	1/1	0.96	0.06	53,53,53,53	0
84	MG	AS	3522	1/1	0.96	0.25	31,31,31,31	0
84	MG	B	1900	1/1	0.96	0.18	63,63,63,63	0
84	MG	AS	3524	1/1	0.96	0.14	47,47,47,47	0
84	MG	AS	3525	1/1	0.96	0.12	65,65,65,65	0
84	MG	AS	3526	1/1	0.96	0.20	40,40,40,40	0
84	MG	1	3975	1/1	0.96	0.04	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
84	MG	AS	3766	1/1	0.96	0.06	52,52,52,52	0
84	MG	AS	3767	1/1	0.96	0.10	53,53,53,53	0
84	MG	B	1856	1/1	0.96	0.13	38,38,38,38	0
84	MG	1	3641	1/1	0.96	0.25	29,29,29,29	0
84	MG	1	3946	1/1	0.96	0.12	35,35,35,35	0
84	MG	Y	201	1/1	0.96	0.06	30,30,30,30	0
84	MG	1	3889	1/1	0.96	0.13	36,36,36,36	0
84	MG	B	1818	1/1	0.96	0.19	36,36,36,36	0
84	MG	1	3890	1/1	0.96	0.06	27,27,27,27	0
84	MG	1	4014	1/1	0.96	0.10	43,43,43,43	0
84	MG	CM	1860	1/1	0.96	0.06	52,52,52,52	0
84	MG	B	1821	1/1	0.96	0.23	31,31,31,31	0
84	MG	AS	3693	1/1	0.96	0.10	52,52,52,52	0
84	MG	AS	3780	1/1	0.96	0.12	47,47,47,47	0
84	MG	AS	3537	1/1	0.96	0.11	50,50,50,50	0
84	MG	1	3712	1/1	0.96	0.18	32,32,32,32	0
84	MG	CM	1959	1/1	0.96	0.12	56,56,56,56	0
84	MG	1	3461	1/1	0.96	0.20	19,19,19,19	0
84	MG	f	102	1/1	0.96	0.09	61,61,61,61	0
84	MG	1	3893	1/1	0.96	0.18	39,39,39,39	0
84	MG	CM	1870	1/1	0.96	0.16	63,63,63,63	0
84	MG	1	3429	1/1	0.96	0.12	35,35,35,35	0
84	MG	AS	3787	1/1	0.96	0.08	55,55,55,55	0
84	MG	AS	3620	1/1	0.96	0.18	37,37,37,37	0
84	MG	AS	3403	1/1	0.96	0.23	22,22,22,22	0
84	MG	AS	3474	1/1	0.96	0.15	33,33,33,33	0
84	MG	r	302	1/1	0.96	0.22	29,29,29,29	0
84	MG	AS	3624	1/1	0.96	0.09	37,37,37,37	0
84	MG	B	1968	1/1	0.96	0.14	58,58,58,58	0
84	MG	1	3599	1/1	0.96	0.17	43,43,43,43	0
84	MG	AS	3707	1/1	0.96	0.25	33,33,33,33	0
84	MG	1	3403	1/1	0.96	0.19	46,46,46,46	0
84	MG	B	1971	1/1	0.96	0.12	46,46,46,46	0
84	MG	AS	3409	1/1	0.96	0.26	24,24,24,24	0
84	MG	B	1918	1/1	0.96	0.07	47,47,47,47	0
84	MG	AS	3800	1/1	0.96	0.06	41,41,41,41	0
84	MG	AS	3801	1/1	0.96	0.12	54,54,54,54	0
84	MG	1	3986	1/1	0.96	0.06	36,36,36,36	0
84	MG	AS	3412	1/1	0.96	0.36	47,47,47,47	0
84	MG	AS	3415	1/1	0.96	0.21	28,28,28,28	0
84	MG	1	3701	1/1	0.96	0.05	47,47,47,47	0
84	MG	1	3777	1/1	0.96	0.24	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	CM	1892	1/1	0.96	0.14	43,43,43,43	0
84	MG	B	1832	1/1	0.96	0.27	38,38,38,38	0
84	MG	1	3702	1/1	0.96	0.06	55,55,55,55	0
84	MG	B	1876	1/1	0.96	0.13	58,58,58,58	0
84	MG	1	3959	1/1	0.96	0.14	47,47,47,47	0
84	MG	AS	3640	1/1	0.96	0.15	48,48,48,48	0
84	MG	1	3619	1/1	0.96	0.05	38,38,38,38	0
84	MG	w	301	1/1	0.96	0.27	42,42,42,42	0
84	MG	1	3721	1/1	0.96	0.08	40,40,40,40	0
84	MG	AS	3427	1/1	0.96	0.20	30,30,30,30	0
84	MG	AS	3495	1/1	0.96	0.12	34,34,34,34	0
84	MG	DG	202	1/1	0.96	0.10	61,61,61,61	0
84	MG	1	3479	1/1	0.96	0.28	17,17,17,17	0
84	MG	AS	3497	1/1	0.96	0.19	36,36,36,36	0
84	MG	1	3723	1/1	0.96	0.09	30,30,30,30	0
84	MG	AS	3650	1/1	0.96	0.07	30,30,30,30	0
84	MG	CM	1814	1/1	0.96	0.29	41,41,41,41	0
84	MG	1	3621	1/1	0.96	0.06	58,58,58,58	0
84	MG	1	3905	1/1	0.96	0.06	36,36,36,36	0
84	MG	AS	3735	1/1	0.96	0.05	31,31,31,31	0
85	ZN	CH	101	1/1	0.96	0.12	150,150,150,150	0
84	MG	AS	3433	1/1	0.96	0.08	41,41,41,41	0
84	MG	1	3998	1/1	0.96	0.09	40,40,40,40	0
84	MG	1	3495	1/1	0.96	0.24	23,23,23,23	0
84	MG	AS	3664	1/1	0.97	0.06	80,80,80,80	0
84	MG	k	407	1/1	0.97	0.16	36,36,36,36	0
84	MG	AS	3716	1/1	0.97	0.09	33,33,33,33	0
84	MG	CM	1832	1/1	0.97	0.30	31,31,31,31	0
84	MG	6	201	1/1	0.97	0.12	38,38,38,38	0
84	MG	1	3504	1/1	0.97	0.07	26,26,26,26	0
84	MG	1	3940	1/1	0.97	0.13	40,40,40,40	0
84	MG	AS	3823	1/1	0.97	0.19	43,43,43,43	0
84	MG	1	3824	1/1	0.97	0.10	46,46,46,46	0
84	MG	AS	3575	1/1	0.97	0.08	40,40,40,40	0
84	MG	1	3489	1/1	0.97	0.25	23,23,23,23	0
84	MG	1	3695	1/1	0.97	0.09	39,39,39,39	0
84	MG	1	3449	1/1	0.97	0.24	44,44,44,44	0
84	MG	B	1814	1/1	0.97	0.07	45,45,45,45	0
84	MG	AS	3777	1/1	0.97	0.24	42,42,42,42	0
84	MG	1	3646	1/1	0.97	0.12	37,37,37,37	0
84	MG	AS	3581	1/1	0.97	0.09	33,33,33,33	0
84	MG	1	3999	1/1	0.97	0.03	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3742	1/1	0.97	0.17	33,33,33,33	0
84	MG	1	3947	1/1	0.97	0.07	31,31,31,31	0
84	MG	CM	1849	1/1	0.97	0.05	46,46,46,46	0
84	MG	1	3922	1/1	0.97	0.21	48,48,48,48	0
84	MG	AS	3414	1/1	0.97	0.07	58,58,58,58	0
84	MG	1	3572	1/1	0.97	0.09	34,34,34,34	0
84	MG	B	1921	1/1	0.97	0.10	78,78,78,78	0
84	MG	AS	3460	1/1	0.97	0.10	34,34,34,34	0
84	MG	B	1922	1/1	0.97	0.07	41,41,41,41	0
84	MG	AS	3591	1/1	0.97	0.22	47,47,47,47	0
84	MG	CM	1857	1/1	0.97	0.14	29,29,29,29	0
84	MG	CM	1979	1/1	0.97	0.07	55,55,55,55	0
84	MG	1	3484	1/1	0.97	0.18	30,30,30,30	0
84	MG	1	3637	1/1	0.97	0.07	40,40,40,40	0
84	MG	CM	1802	1/1	0.97	0.41	29,29,29,29	0
84	MG	AS	3740	1/1	0.97	0.05	46,46,46,46	0
84	MG	B	1925	1/1	0.97	0.12	54,54,54,54	0
84	MG	AS	3421	1/1	0.97	0.09	29,29,29,29	0
84	MG	CM	1864	1/1	0.97	0.12	43,43,43,43	0
84	MG	1	3715	1/1	0.97	0.08	30,30,30,30	0
84	MG	AU	202	1/1	0.97	0.12	55,55,55,55	0
84	MG	1	3796	1/1	0.97	0.15	50,50,50,50	0
84	MG	1	3674	1/1	0.97	0.08	34,34,34,34	0
84	MG	1	3837	1/1	0.97	0.14	68,68,68,68	0
84	MG	AS	3554	1/1	0.97	0.11	44,44,44,44	0
84	MG	1	3798	1/1	0.97	0.23	35,35,35,35	0
84	MG	1	3553	1/1	0.97	0.07	50,50,50,50	0
84	MG	AU	209	1/1	0.97	0.04	33,33,33,33	0
84	MG	AS	3603	1/1	0.97	0.11	38,38,38,38	0
84	MG	AS	3651	1/1	0.97	0.08	54,54,54,54	0
84	MG	AS	3429	1/1	0.97	0.28	27,27,27,27	0
84	MG	1	3538	1/1	0.97	0.12	36,36,36,36	0
84	MG	1	3492	1/1	0.97	0.25	22,22,22,22	0
84	MG	3	205	1/1	0.97	0.17	30,30,30,30	0
84	MG	3	206	1/1	0.97	0.08	63,63,63,63	0
84	MG	1	3863	1/1	0.97	0.05	57,57,57,57	0
84	MG	1	3864	1/1	0.97	0.11	51,51,51,51	0
84	MG	1	3988	1/1	0.97	0.10	69,69,69,69	0
84	MG	CM	1943	1/1	0.97	0.15	48,48,48,48	0
84	MG	1	3410	1/1	0.97	0.32	25,25,25,25	0
84	MG	1	3913	1/1	0.97	0.09	33,33,33,33	0
85	ZN	DN	201	1/1	0.97	0.04	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	3548	1/1	0.97	0.16	26,26,26,26	0
84	MG	B	1905	1/1	0.97	0.05	39,39,39,39	0
84	MG	AS	3553	1/1	0.98	0.10	29,29,29,29	0
84	MG	AS	3711	1/1	0.98	0.05	45,45,45,45	0
84	MG	1	3817	1/1	0.98	0.17	34,34,34,34	0
84	MG	AS	3776	1/1	0.98	0.07	40,40,40,40	0
84	MG	1	3878	1/1	0.98	0.04	35,35,35,35	0
84	MG	1	3769	1/1	0.98	0.11	27,27,27,27	0
84	MG	1	3850	1/1	0.98	0.15	28,28,28,28	0
84	MG	AS	3802	1/1	0.98	0.04	48,48,48,48	0
84	MG	1	3869	1/1	0.98	0.12	48,48,48,48	0
84	MG	AS	3473	1/1	0.98	0.15	28,28,28,28	0
84	MG	CM	1945	1/1	0.98	0.09	40,40,40,40	0
84	MG	j	303	1/1	0.98	0.11	26,26,26,26	0
84	MG	CM	1972	1/1	0.98	0.07	40,40,40,40	0
84	MG	AS	3561	1/1	0.98	0.05	29,29,29,29	0
84	MG	1	3634	1/1	0.98	0.08	33,33,33,33	0
84	MG	1	3871	1/1	0.98	0.08	47,47,47,47	0
84	MG	AS	3444	1/1	0.98	0.10	41,41,41,41	0
84	MG	AS	3641	1/1	0.98	0.06	41,41,41,41	0
85	ZN	AQ	101	1/1	0.98	0.06	84,84,84,84	0
84	MG	AW	301	1/1	0.98	0.12	37,37,37,37	0
85	ZN	f	101	1/1	0.98	0.08	75,75,75,75	0
84	MG	1	3630	1/1	0.98	0.07	44,44,44,44	0
84	MG	AS	3413	1/1	0.98	0.24	25,25,25,25	0
85	ZN	CE	101	1/1	0.98	0.04	71,71,71,71	0
84	MG	x	203	1/1	0.98	0.30	37,37,37,37	0
84	MG	1	3570	1/1	0.98	0.15	29,29,29,29	0
84	MG	1	3625	1/1	0.98	0.23	31,31,31,31	0
84	MG	1	3830	1/1	0.98	0.06	37,37,37,37	0
85	ZN	DQ	101	1/1	0.98	0.10	51,51,51,51	0
84	MG	1	3571	1/1	0.98	0.05	26,26,26,26	0
84	MG	AS	3402	1/1	0.99	0.04	39,39,39,39	0
84	MG	AS	3692	1/1	0.99	0.03	50,50,50,50	0
85	ZN	c	201	1/1	0.99	0.04	84,84,84,84	0
85	ZN	CK	101	1/1	0.99	0.03	116,116,116,116	0
84	MG	AS	3436	1/1	0.99	0.09	37,37,37,37	0
84	MG	1	3423	1/1	0.99	0.30	24,24,24,24	0
84	MG	AS	3830	1/1	0.99	0.04	49,49,49,49	0
84	MG	AS	3422	1/1	0.99	0.06	28,28,28,28	0
84	MG	1	3407	1/1	1.00	0.03	42,42,42,42	0
85	ZN	AK	101	1/1	1.00	0.04	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
84	MG	1	3439	1/1	1.00	0.07	28,28,28,28	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.