



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 4, 2024 – 02:27 am GMT

PDB ID : 8C3A
Title : Crystal structure of ailanthone bound to the Candida albicans 80S ribosome
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on : 2022-12-23
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

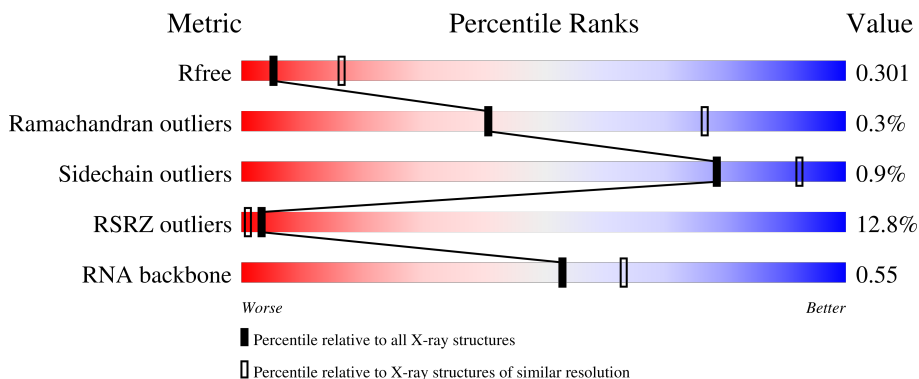
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.




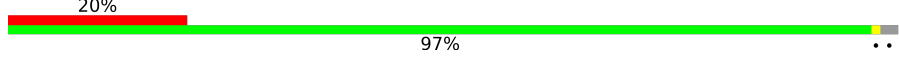
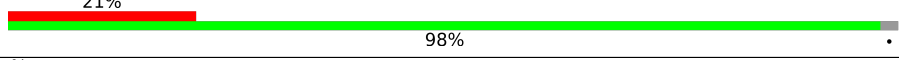
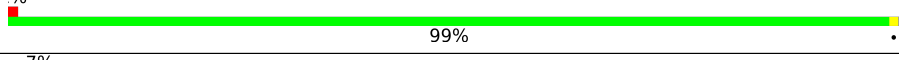
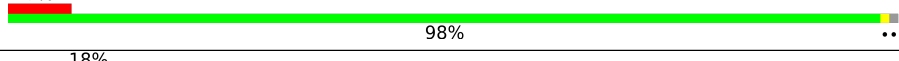
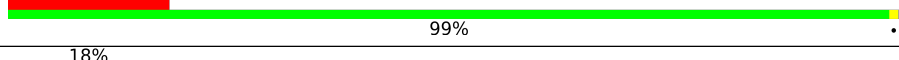
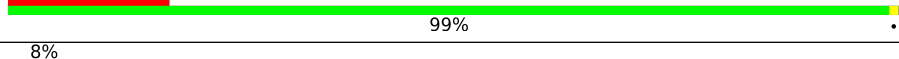
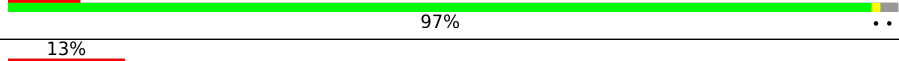
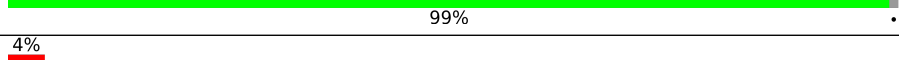
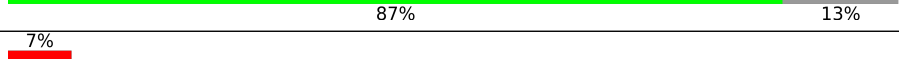
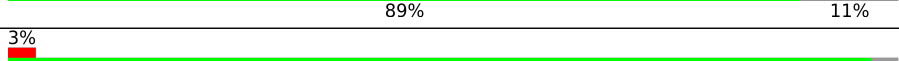
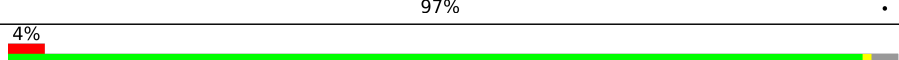
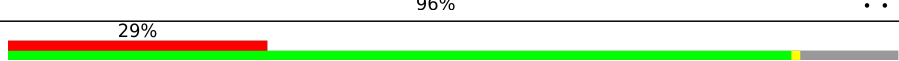
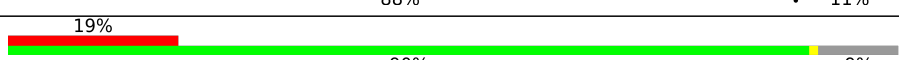
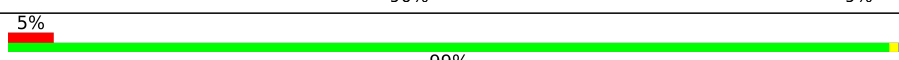
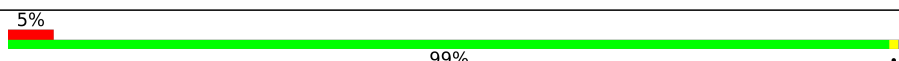
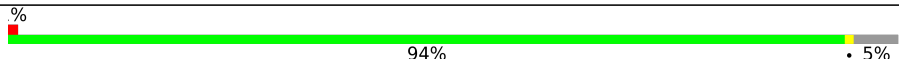
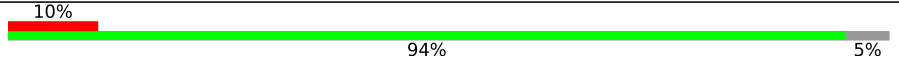
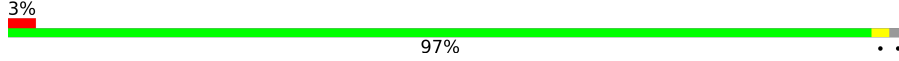
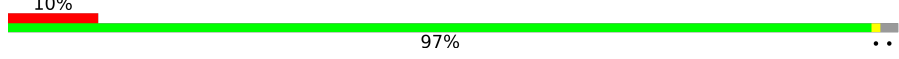
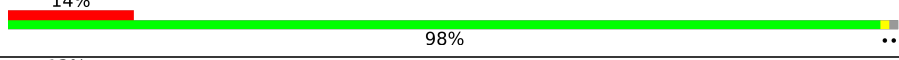
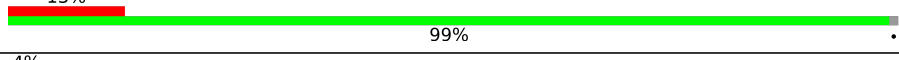
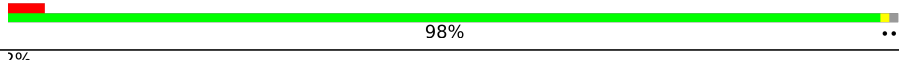
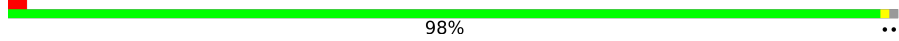

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)
RNA backbone	3102	1173 (3.30-2.70)

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

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

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Mol	Chain	Length	Quality of chain
3	AU	158	
4	AW	254	
4	j	254	
5	AX	389	
5	k	389	
6	AY	363	
6	l	363	
7	AZ	298	
7	m	298	
8	BA	176	
8	n	176	
9	BB	241	
9	o	241	
10	BC	262	
10	p	262	
11	BD	191	
11	q	191	
12	BE	220	
12	r	220	
13	BF	174	
13	s	174	
14	BG	202	
14	t	202	
15	BH	131	
15	u	131	

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Mol	Chain	Length	Quality of chain
16	BI	204	61% 100%
16	v	204	18% 99%
17	BJ	200	2% 100%
17	w	200	4% 99%
18	BK	185	15% 94% 5%
18	x	185	17% 93% 6%
19	BL	186	13% 99% .
19	y	186	19% 99% .
20	BM	190	3% 92% 6%
20	z	190	4% 94% 6%
21	0	172	3% 98% ..
21	BN	172	3% 99% .
22	2	160	19% 99% .
22	BO	160	14% 99% ..
23	5	124	11% 81% 17%
23	BP	124	12% 77% 5% 18%
24	6	137	11% 96% .
24	BQ	137	13% 94% ..
25	7	155	6% 75% 24%
25	BR	155	6% 62% 37%
26	8	142	16% 85% 15%
26	BS	142	28% 84% 16%
27	9	127	26% 98% ..
27	BT	127	24% 98% ..
28	AA	136	12% 99% .

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Mol	Chain	Length	Quality of chain
28	BU	136	21% 98%
29	AB	149	32% 99%
29	BV	149	17% 99%
30	AC	63	21% 95%
30	BW	63	24% 97%
31	AD	106	3% 91%
31	BX	106	16% 91%
32	AE	112	15% 96%
32	BY	112	13% 97%
33	AF	131	18% 95%
33	BZ	131	10% 94%
34	AG	107	6% 98%
34	CA	107	4% 99%
35	AH	122	21% 92%
35	CB	122	36% 92%
36	AI	120	18% 98%
36	CC	120	30% 97%
37	AJ	99	12% 97%
37	CD	99	22% 98%
38	AK	87	22% 99%
38	CE	87	32% 99%
39	AL	78	22% 99%
39	CF	78	42% 97%
40	AM	51	8% 96%
40	CG	51	39% 98%

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Mol	Chain	Length	Quality of chain
41	AN	52	10% 100%
41	CH	52	13% 90% 8%
42	AO	25	76% 92% 8%
42	CI	25	60% 96%
43	AP	106	9% 96%
43	CJ	106	8% 95%
44	AQ	92	18% 99%
44	CK	92	18% 99%
45	CL	267	3% 44% 55%
45	i	267	6% 44% 55%
46	B	1787	3% 71% 26%
46	CM	1787	3% 71% 26%
47	C	261	8% 79% 20%
47	CN	261	4% 79% 20%
48	CO	256	14% 84% 16%
48	D	256	7% 83% 16%
49	CP	249	6% 86% 13%
49	E	249	33% 87% 13%
50	CQ	251	8% 86% 11%
50	F	251	33% 88% 11%
51	CR	262	28% 99%
51	G	262	27% 99%
52	CS	225	20% 91% 8%
52	H	225	26% 91% 8%
53	CT	236	13% 99%

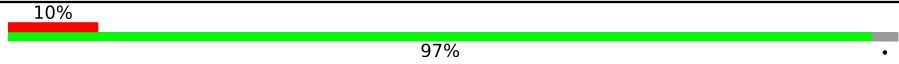
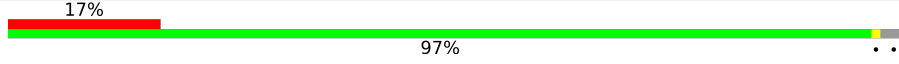
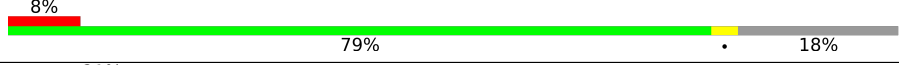

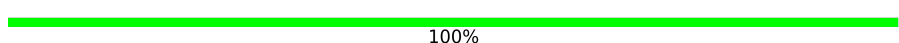
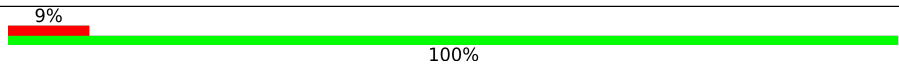
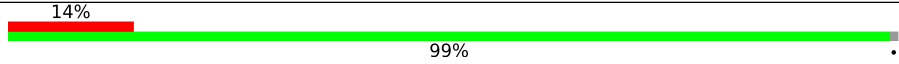
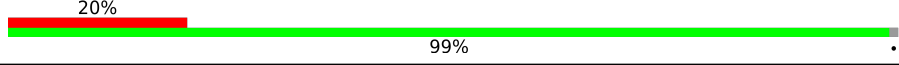
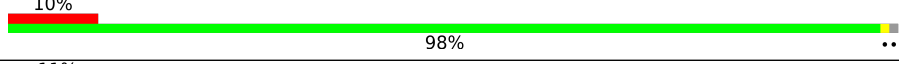
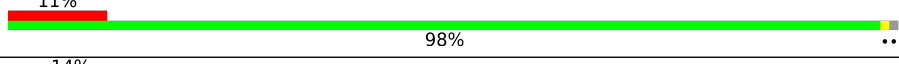
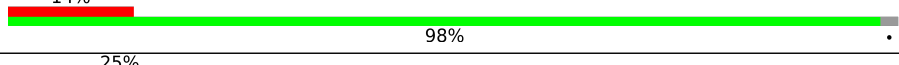
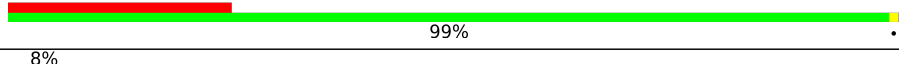
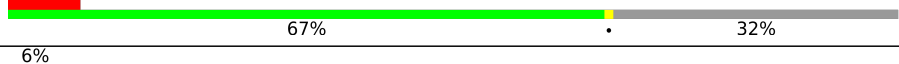



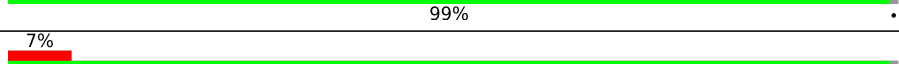
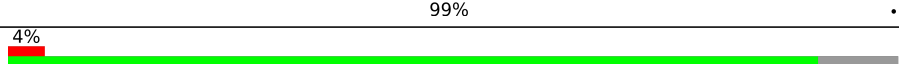
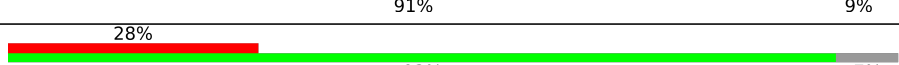
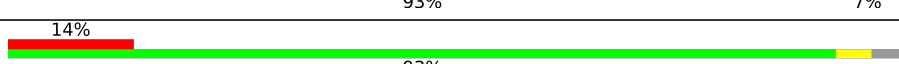
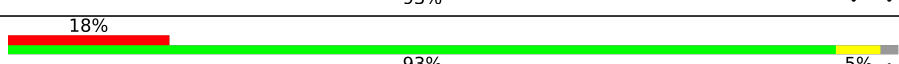
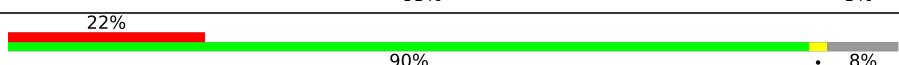
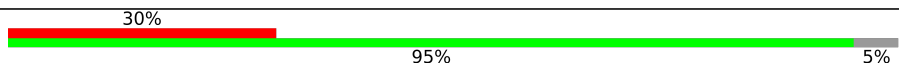
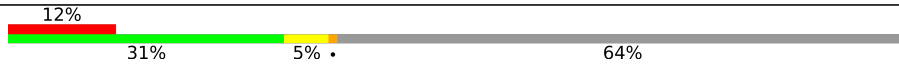

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Mol	Chain	Length	Quality of chain
53	I	236	10% 95%
54	CU	186	15% 97%
54	J	186	30% 99%
55	CV	206	13% 99%
55	K	206	11% 98%
56	CW	189	25% 94% 6%
56	L	189	48% 94% 6%
57	CX	118	7% 80% 20%
57	M	118	19% 82% 17%
58	CY	155	15% 90% 9%
58	N	155	25% 92% 7%
59	CZ	143	16% 77% 6% 17%
59	O	143	29% 75% 6% 19%
60	DA	151	22% 99%
60	P	151	14% 99%
61	DB	132	14% 95%
61	Q	132	3% 95%
62	DC	142	18% 90% 8%
62	R	142	23% 88% 9%
63	DD	142	37% 97%
63	S	142	53% 97%
64	DE	137	18% 91% 9%
64	T	137	33% 90% 9%
65	DF	145	7% 94%
65	U	145	8% 96%


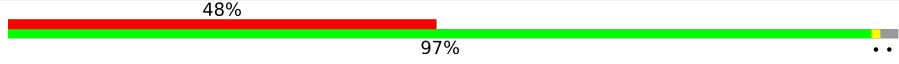
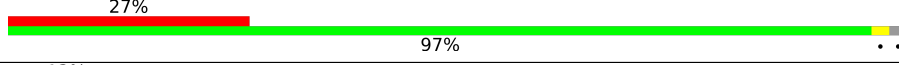

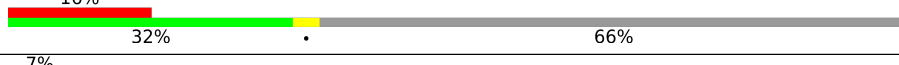

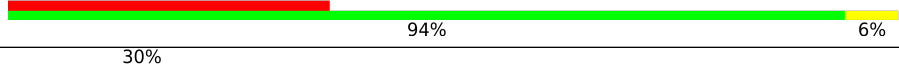
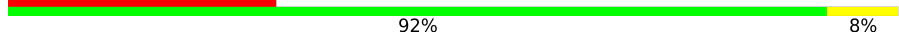
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Mol	Chain	Length	Quality of chain
66	DG	145	
66	V	145	
67	DH	119	
67	W	119	
68	DI	87	
68	X	87	
69	DJ	130	
69	Y	130	
70	DK	145	
70	Z	145	
71	DL	135	
71	a	135	
72	DM	105	
72	b	105	
73	DN	119	
73	c	119	
74	DO	82	
74	d	82	
75	DP	67	
75	e	67	
76	DQ	56	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

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Mol	Chain	Length	Quality of chain
78	h	193	
79	AR	317	
79	DT	317	
80	P0	312	
80	p0	312	
81	12	165	
82	L1	217	
82	l1	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
83	MG	0	203	-	-	-	X
83	MG	1	3419	-	-	-	X
83	MG	1	3518	-	-	-	X
83	MG	1	3548	-	-	-	X
83	MG	1	3549	-	-	-	X
83	MG	1	3582	-	-	-	X
83	MG	1	3588	-	-	-	X
83	MG	1	3604	-	-	-	X
83	MG	1	3629	-	-	-	X
83	MG	1	3642	-	-	-	X
83	MG	1	3654	-	-	-	X
83	MG	1	3679	-	-	-	X
83	MG	1	3681	-	-	-	X
83	MG	1	3691	-	-	-	X
83	MG	1	3716	-	-	-	X
83	MG	1	3722	-	-	-	X
83	MG	1	3802	-	-	-	X
83	MG	1	3866	-	-	-	X
83	MG	1	3890	-	-	-	X
83	MG	1	3918	-	-	-	X
83	MG	1	3920	-	-	-	X
83	MG	1	3947	-	-	-	X
83	MG	1	3957	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
83	MG	3	208	-	-	-	X
83	MG	4	207	-	-	-	X
83	MG	9	202	-	-	-	X
83	MG	AC	101	-	-	-	X
83	MG	AF	202	-	-	-	X
83	MG	AS	3463	-	-	-	X
83	MG	AS	3630	-	-	-	X
83	MG	AS	3634	-	-	-	X
83	MG	AS	3649	-	-	-	X
83	MG	AS	3654	-	-	-	X
83	MG	AS	3670	-	-	-	X
83	MG	AS	3701	-	-	-	X
83	MG	AS	3709	-	-	-	X
83	MG	AS	3744	-	-	-	X
83	MG	AS	3753	-	-	-	X
83	MG	AS	3757	-	-	-	X
83	MG	AS	3768	-	-	-	X
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83	MG	CM	1917	-	-	-	X
83	MG	I	301	-	-	-	X
83	MG	j	302	-	-	-	X
83	MG	k	406	-	-	-	X

2 Entry composition [i](#)

There are 87 unique types of molecules in this entry. The entry contains 410139 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	3217	Total	C	N	O	P	0	0	0
			68771	30722	12362	22470	3217			
1	AS	3229	Total	C	N	O	P	0	0	0
			69025	30835	12406	22555	3229			

- 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	1	0
			1894	1185	377	330	2			
4	AW	249	Total	C	N	O	S	0	1	0
			1894	1185	377	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	234	Total	C	N	O	S	0	0	0
			1885	1208	345	331	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	6	2	0
			843	550	138	155			

- 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	121	Total	C	N	O	S	0	0	0
			974	622	175	176	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	62	493	307	105	81		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	1	0
			998	634	196	167	1			
36	CC	118	Total	C	N	O		6	1	0
			985	626	194	165				

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
40	AM	50	Total	C	N	O	0	0	0
			438	275	97	66			
40	CG	50	Total	C	N	O	0	1	0
			446	280	100	66			

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

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

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

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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			930	563	166	201			
45	CL	121	Total	C	N	O	0	0	0
			930	563	166	201			

- Molecule 46 is a RNA chain called 18S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B	1761	Total	C	N	O	P	0	0	0
			37537	16780	6656	12340	1761			
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	98	Total	C	N	O	S	0	0	0
			817	531	135	150	1			
57	CX	94	Total	C	N	O	S	0	0	0
			791	515	131	144	1			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 67 is a protein called Ribosomal protein S10.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 82 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
82	L1	217	Total	C	N	O	S	0	0	0
			1711	1096	294	312	9			
82	11	217	Total	C	N	O	S	0	0	0
			1711	1096	294	312	9			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	1	556	Total	Mg	0	0
			556	556		
83	3	15	Total	Mg	0	0
			15	15		
83	4	11	Total	Mg	0	0
			11	11		
83	j	3	Total	Mg	0	0
			3	3		
83	k	6	Total	Mg	0	0
			6	6		
83	o	4	Total	Mg	0	0
			4	4		
83	r	2	Total	Mg	0	0
			2	2		
83	s	1	Total	Mg	0	0
			1	1		
83	u	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	v	2	Total Mg 2 2	0	0
83	w	3	Total Mg 3 3	0	0
83	x	2	Total Mg 2 2	0	0
83	0	4	Total Mg 4 4	0	0
83	2	1	Total Mg 1 1	0	0
83	6	4	Total Mg 4 4	0	0
83	8	3	Total Mg 3 3	0	0
83	9	2	Total Mg 2 2	0	0
83	AB	2	Total Mg 2 2	0	0
83	AC	1	Total Mg 1 1	0	0
83	AE	3	Total Mg 3 3	0	0
83	AF	2	Total Mg 2 2	0	0
83	AG	3	Total Mg 3 3	0	0
83	AH	2	Total Mg 2 2	0	0
83	AK	1	Total Mg 1 1	0	0
83	AP	2	Total Mg 2 2	0	0
83	i	1	Total Mg 1 1	0	0
83	B	172	Total Mg 172 172	0	0
83	D	1	Total Mg 1 1	0	0
83	G	2	Total Mg 2 2	0	0
83	I	1	Total Mg 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	J	1	Total 1	Mg 1	0	0
83	K	1	Total 1	Mg 1	0	0
83	Q	2	Total 2	Mg 2	0	0
83	R	1	Total 1	Mg 1	0	0
83	V	1	Total 1	Mg 1	0	0
83	Y	3	Total 3	Mg 3	0	0
83	Z	2	Total 2	Mg 2	0	0
83	f	1	Total 1	Mg 1	0	0
83	g	1	Total 1	Mg 1	0	0
83	AR	1	Total 1	Mg 1	0	0
83	AS	380	Total 380	Mg 380	0	0
83	AT	10	Total 10	Mg 10	0	0
83	AU	10	Total 10	Mg 10	0	0
83	AW	4	Total 4	Mg 4	0	0
83	AX	2	Total 2	Mg 2	0	0
83	AY	1	Total 1	Mg 1	0	0
83	AZ	1	Total 1	Mg 1	0	0
83	BB	4	Total 4	Mg 4	0	0
83	BE	2	Total 2	Mg 2	0	0
83	BF	1	Total 1	Mg 1	0	0
83	BH	1	Total 1	Mg 1	0	0

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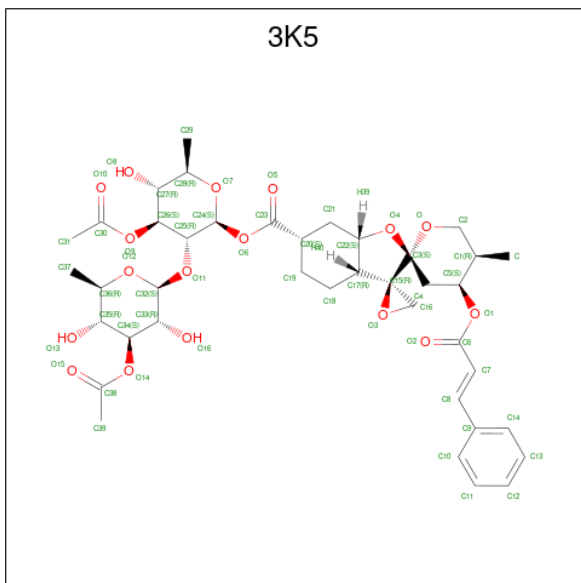
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
83	BI	1	Total Mg 1 1	0	0
83	BJ	3	Total Mg 3 3	0	0
83	BK	2	Total Mg 2 2	0	0
83	BN	1	Total Mg 1 1	0	0
83	BO	1	Total Mg 1 1	0	0
83	BS	1	Total Mg 1 1	0	0
83	BV	1	Total Mg 1 1	0	0
83	BZ	4	Total Mg 4 4	0	0
83	CA	3	Total Mg 3 3	0	0
83	CJ	1	Total Mg 1 1	0	0
83	CK	2	Total Mg 2 2	0	0
83	CL	3	Total Mg 3 3	0	0
83	CM	148	Total Mg 148 148	0	0
83	CO	1	Total Mg 1 1	0	0
83	CP	1	Total Mg 1 1	0	0
83	CQ	2	Total Mg 2 2	0	0
83	CY	1	Total Mg 1 1	0	0
83	DA	1	Total Mg 1 1	0	0
83	DB	4	Total Mg 4 4	0	0
83	DG	2	Total Mg 2 2	0	0
83	DJ	2	Total Mg 2 2	0	0

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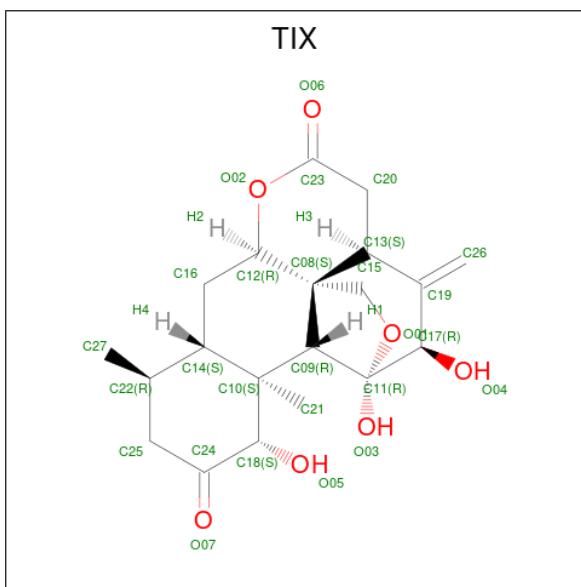
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
83	DQ	1	Total	Mg	0	0
			1	1		

- Molecule 84 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-[[[(2R,2'S,3a'R,4'S,5''R,6'S,7a'S)-5''-methyl-4''-[[[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2',2''-pyran]-6'-yl]carbonyl]-beta-D-glucopyranose (three-letter code: 3K5) (formula: C₄₀H₅₂O₁₇).



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

- Molecule 85 is aianthone (three-letter code: TIX) (formula: C₂₀H₂₆O₇).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	1	1	Total	C O	0	0
			27	20 7		
85	AS	1	Total	C O	0	0
			27	20 7		

- Molecule 86 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

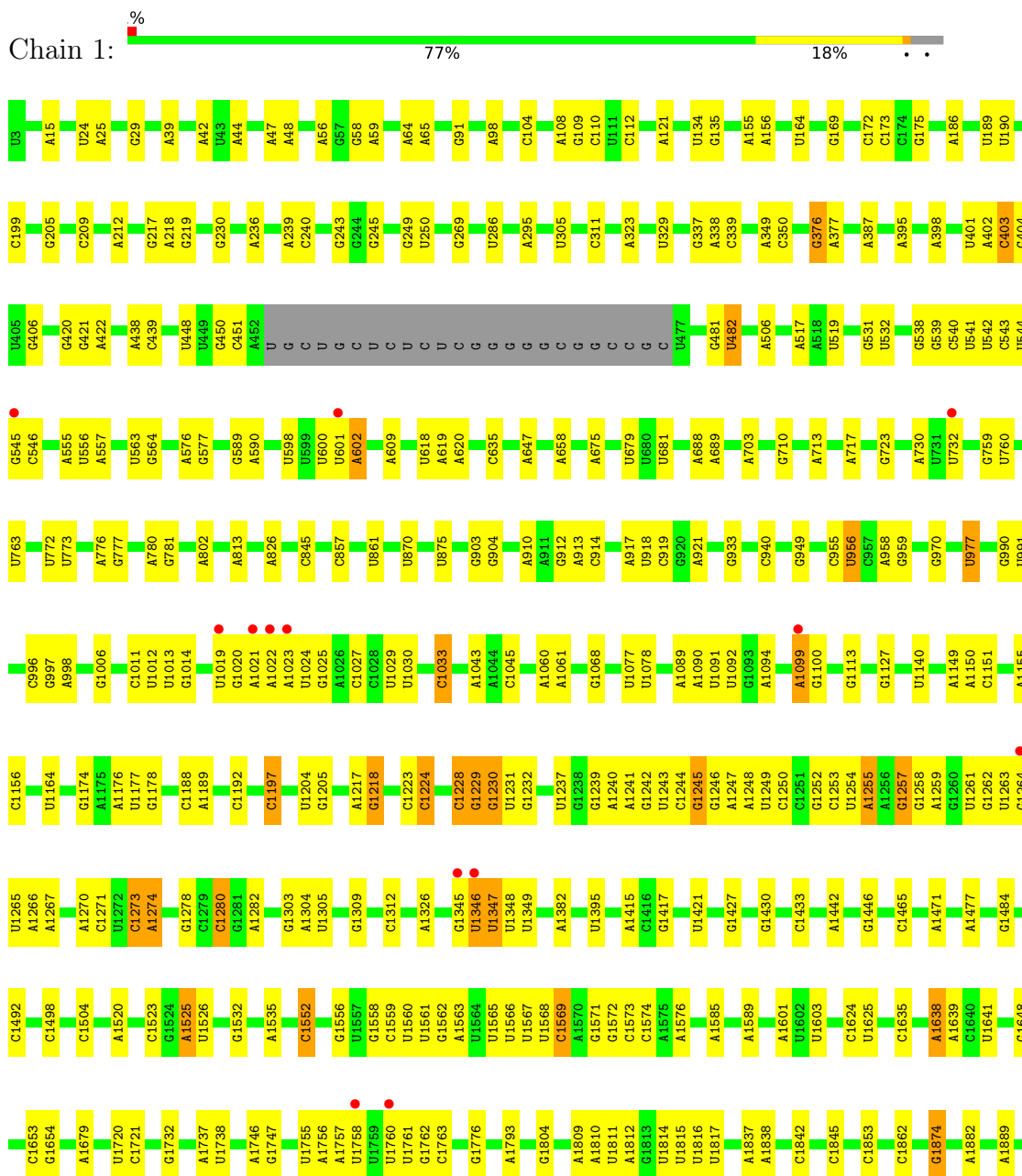
- Molecule 87 is water.

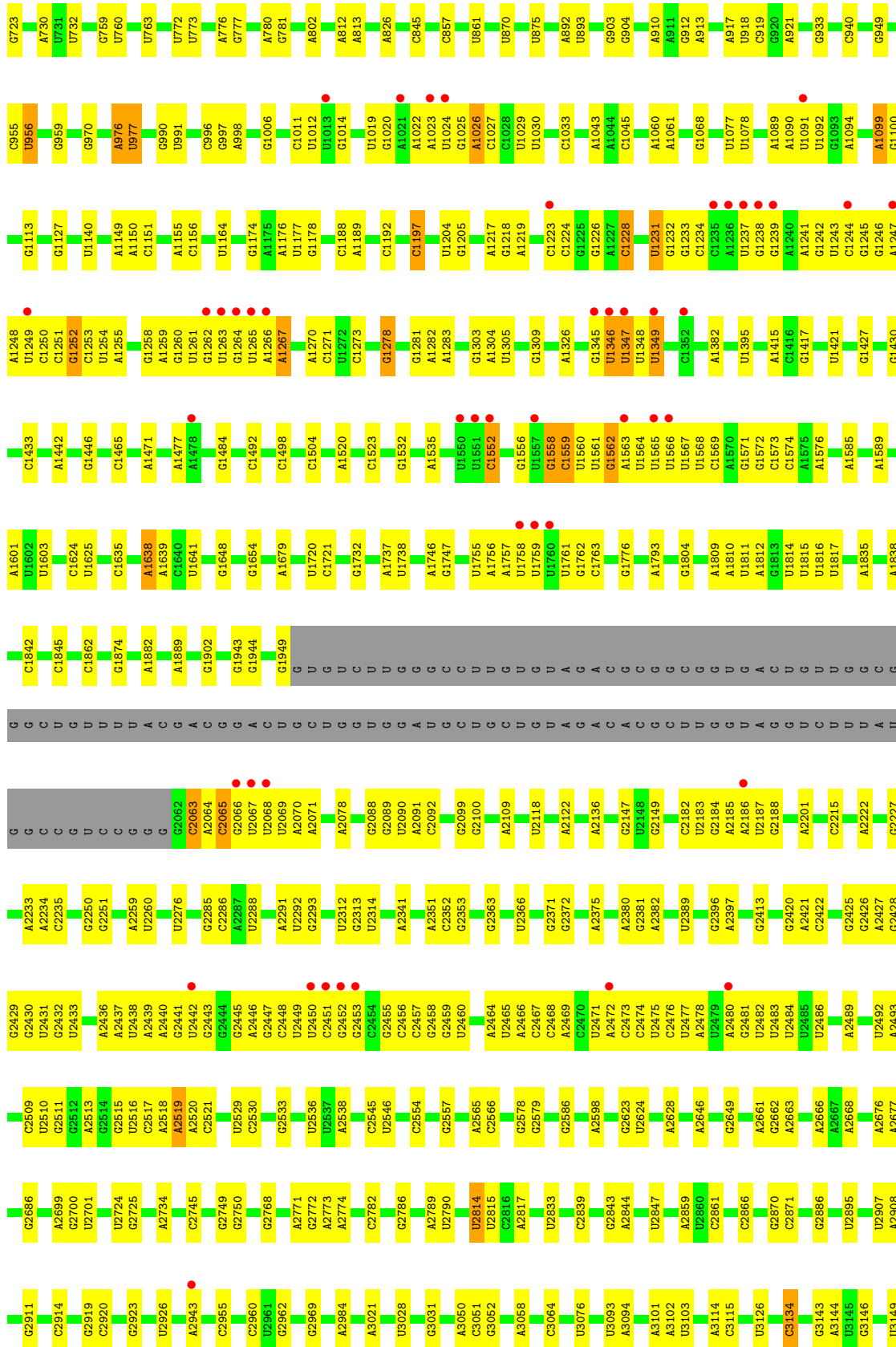
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
87	1	20	Total 20	O 20	0	0
87	4	3	Total 3	O 3	0	0
87	1	1	Total 1	O 1	0	0
87	B	12	Total 12	O 12	0	0
87	AS	26	Total 26	O 26	0	0
87	BQ	3	Total 3	O 3	0	0
87	BV	1	Total 1	O 1	0	0

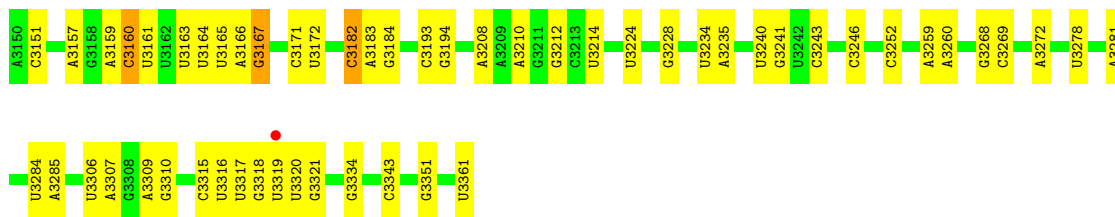
3 Residue-property plots [i](#)

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

- Molecule 1: 25S







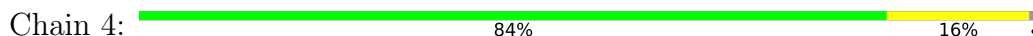
• Molecule 2: 5S



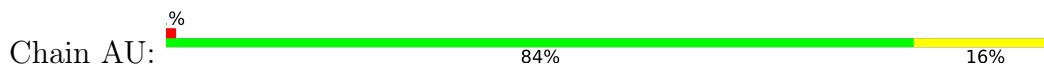
• Molecule 2: 5S



• Molecule 3: 5.8S



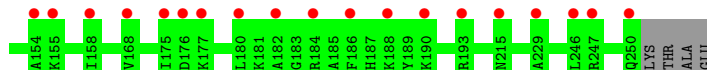
• Molecule 3: 5.8S

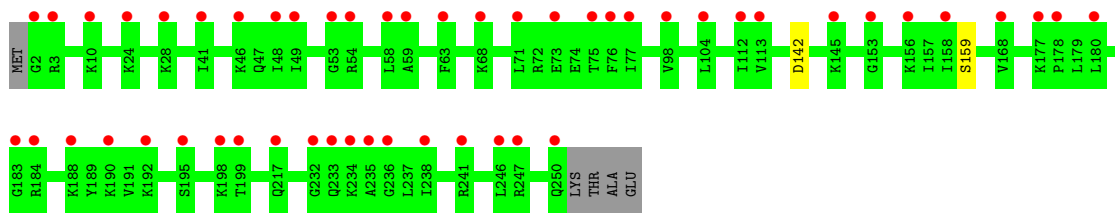


• Molecule 4: 60S ribosomal protein L2-B

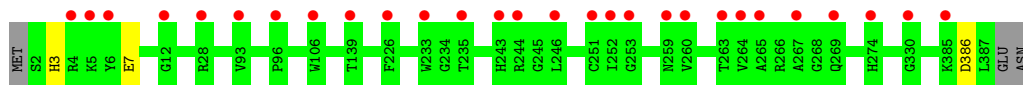


• Molecule 4: 60S ribosomal protein L2-B

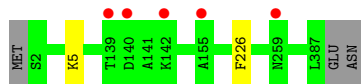




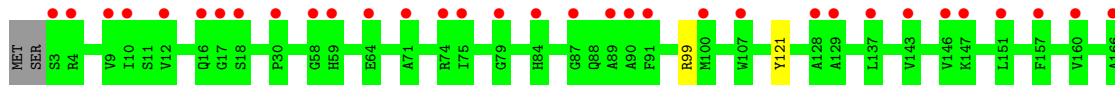
- Molecule 5: 60S ribosomal protein L3



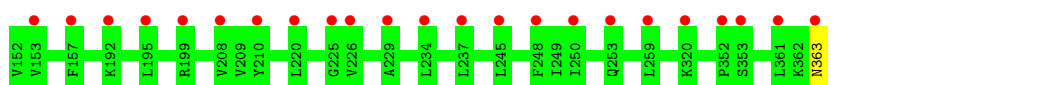
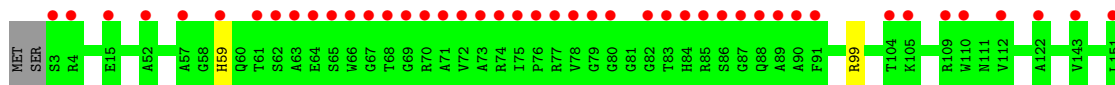
- Molecule 5: 60S ribosomal protein L3



- Molecule 6: 60S ribosomal protein L4-B

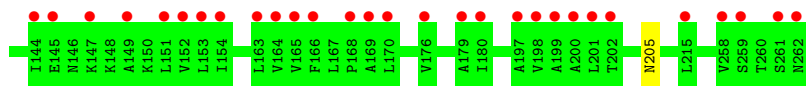


- Molecule 6: 60S ribosomal protein L4-B

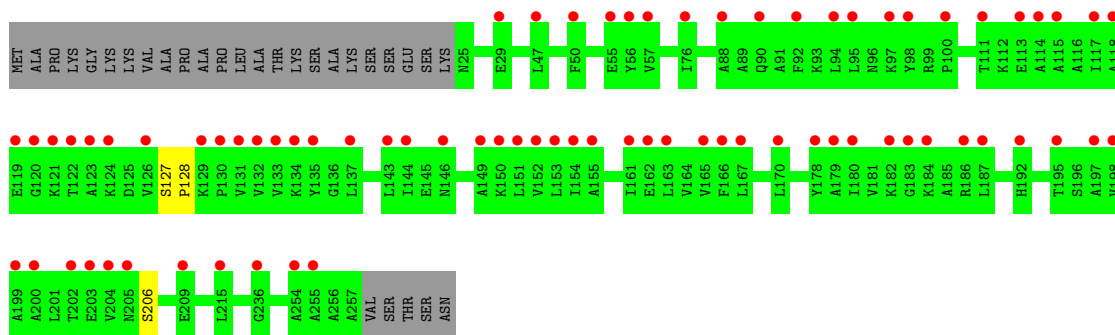
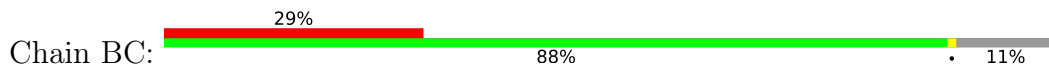


- Molecule 7: Uncharacterized protein CaJ7.0206

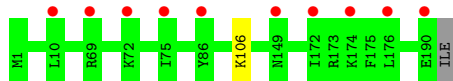




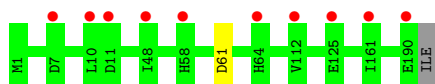
- Molecule 10: 60S ribosomal protein L8



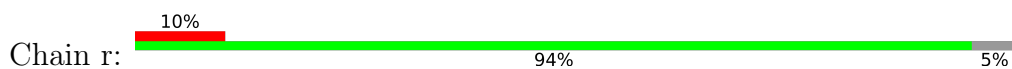
- Molecule 11: 60S ribosomal protein L9-B



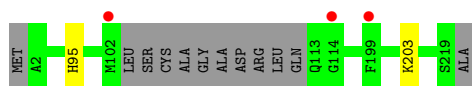
- Molecule 11: 60S ribosomal protein L9-B



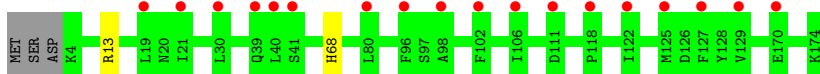
- Molecule 12: 60S ribosomal protein L10



- Molecule 12: 60S ribosomal protein L10



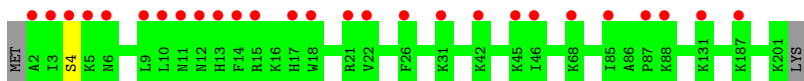
- Molecule 13: 60S ribosomal protein L11-B



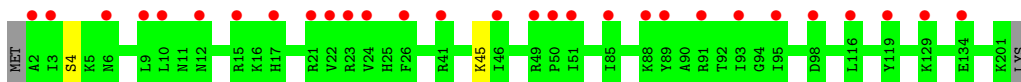
- Molecule 13: 60S ribosomal protein L11-B



- Molecule 14: 60S ribosomal protein L13



- Molecule 14: 60S ribosomal protein L13



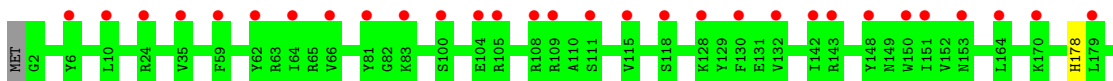
- Molecule 15: 60S ribosomal protein L14-B

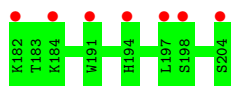


- Molecule 15: 60S ribosomal protein L14-B

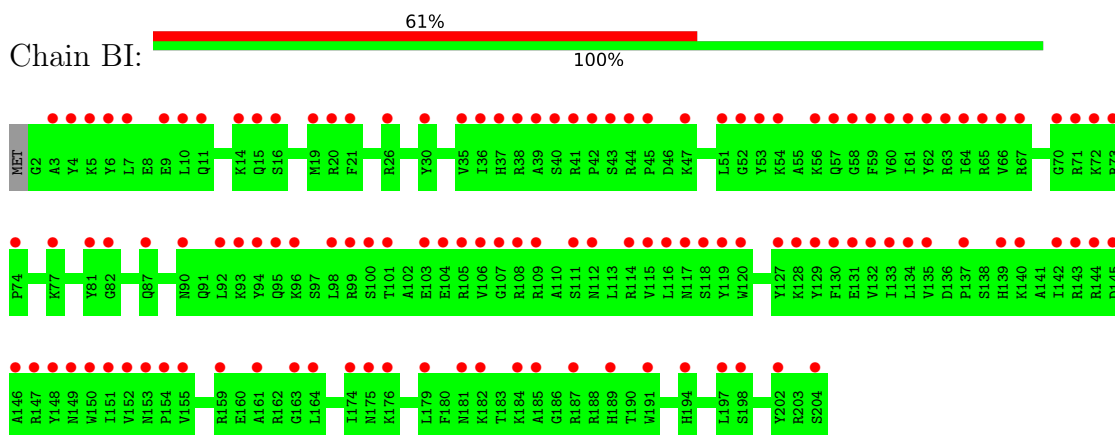


- Molecule 16: 60S ribosomal protein L15-A

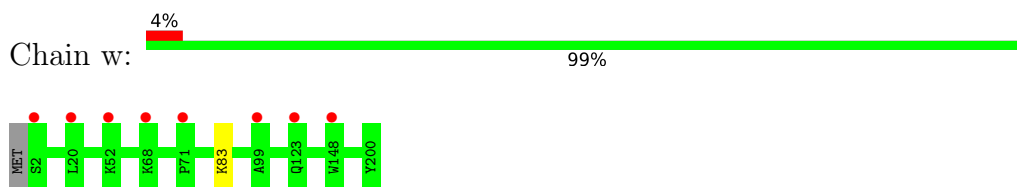




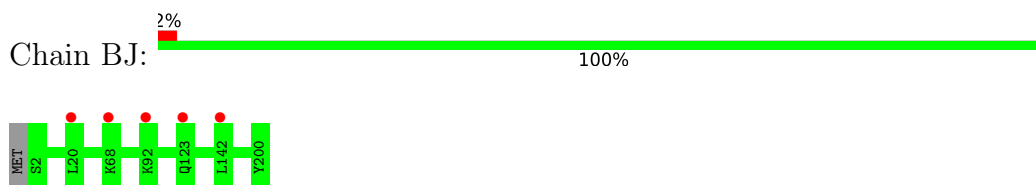
- Molecule 16: 60S ribosomal protein L15-A



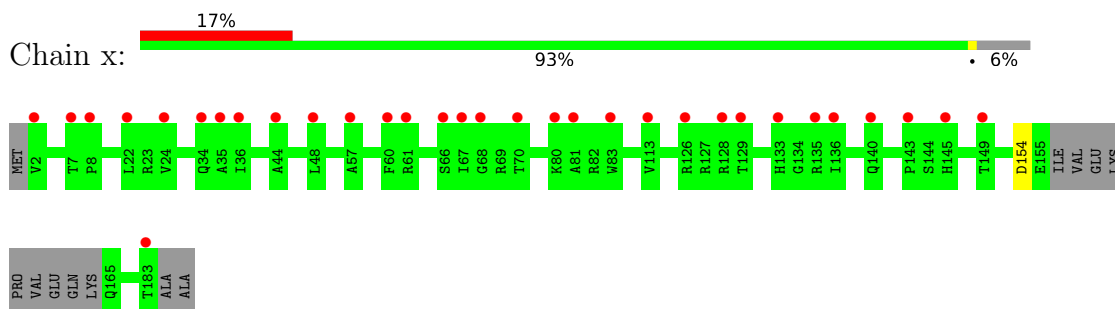
- Molecule 17: Ribosomal protein L13



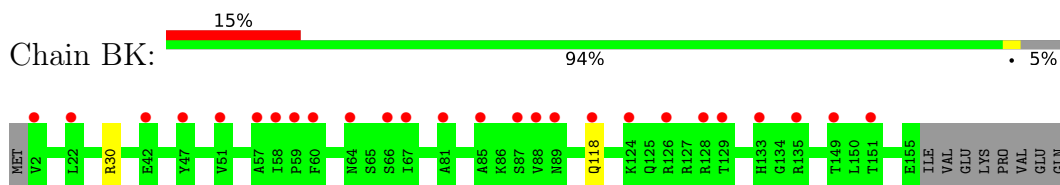
- Molecule 17: Ribosomal protein L13



- Molecule 18: Ribosomal protein L22

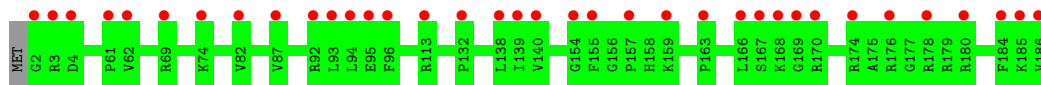


- Molecule 18: Ribosomal protein L22

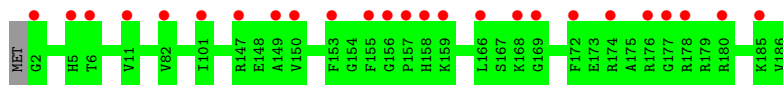




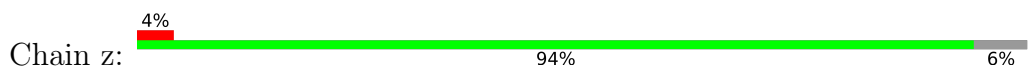
- Molecule 19: 60S ribosomal protein L18-A



- Molecule 19: 60S ribosomal protein L18-A



- Molecule 20: 60S ribosomal protein L19-A



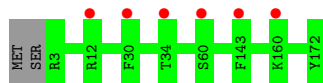
- Molecule 20: 60S ribosomal protein L19-A



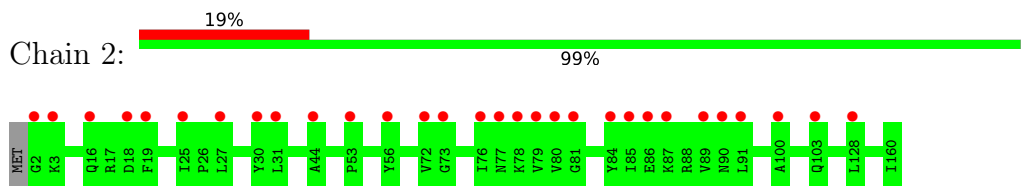
- Molecule 21: 60S ribosomal protein L20



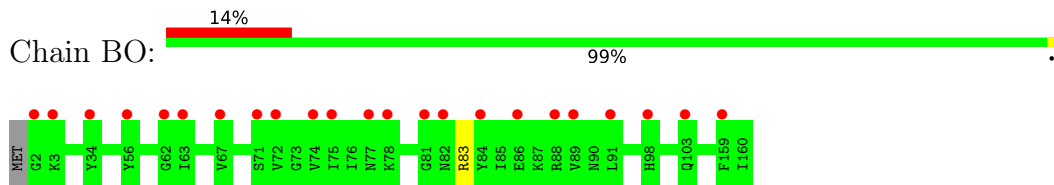
- Molecule 21: 60S ribosomal protein L20



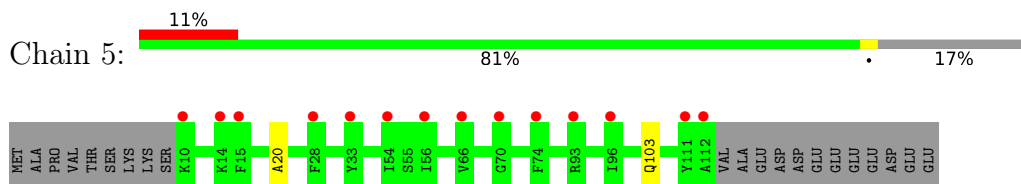
- Molecule 22: 60S ribosomal protein L21-A



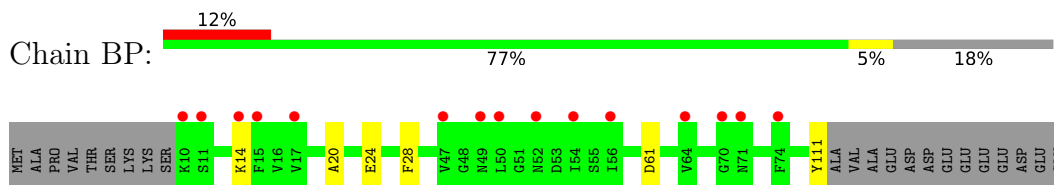
• Molecule 22: 60S ribosomal protein L21-A



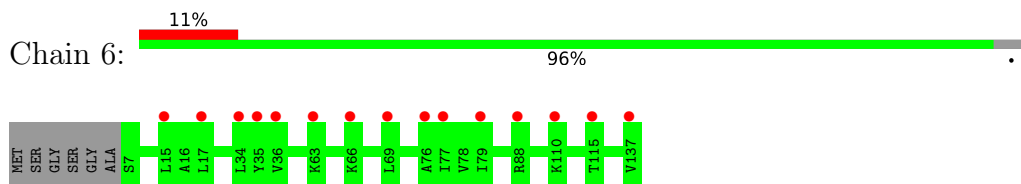
• Molecule 23: 60S ribosomal protein L22-B



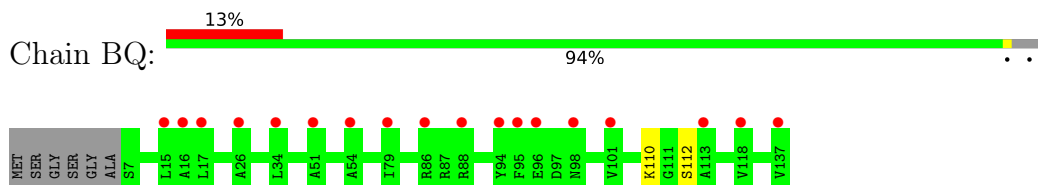
• Molecule 23: 60S ribosomal protein L22-B



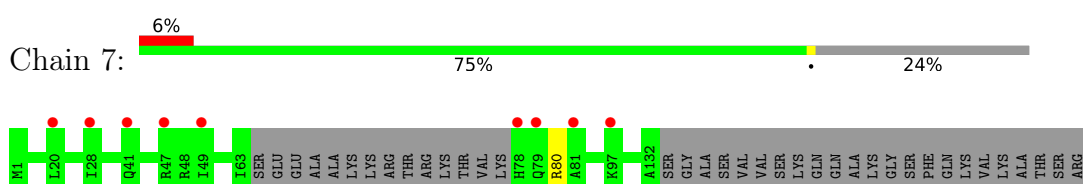
• Molecule 24: 60S ribosomal protein L23-A



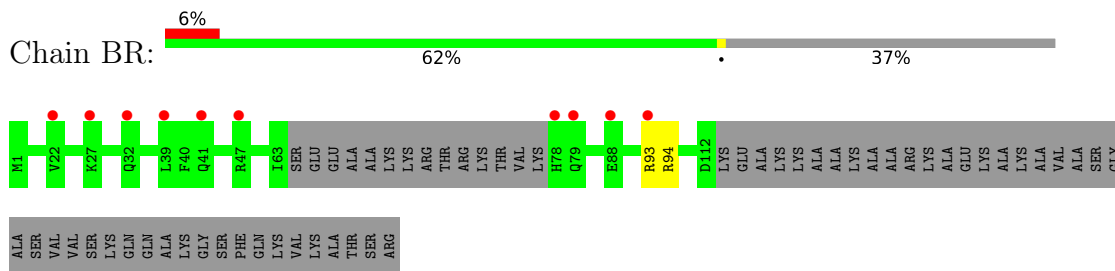
• Molecule 24: 60S ribosomal protein L23-A



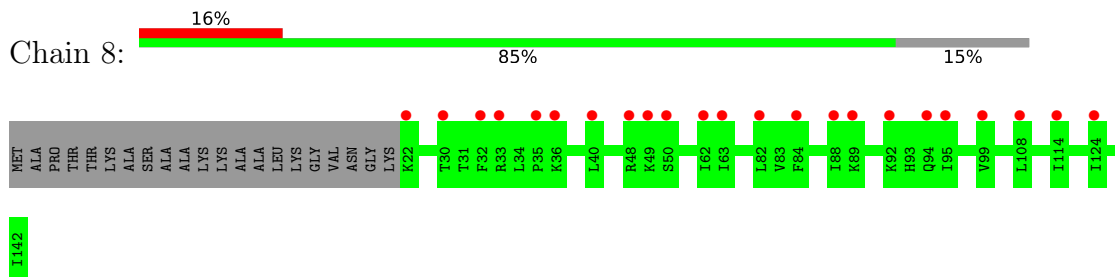
• Molecule 25: 60S ribosomal protein L24-A



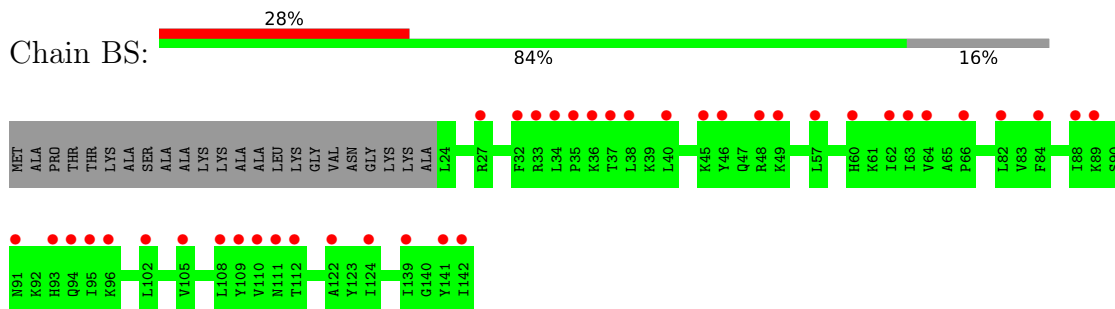
- Molecule 25: 60S ribosomal protein L24-A



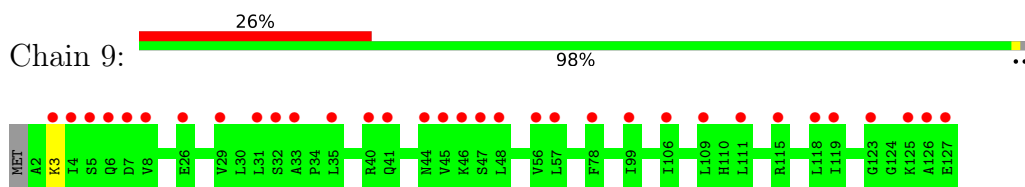
- Molecule 26: 60S ribosomal protein L25



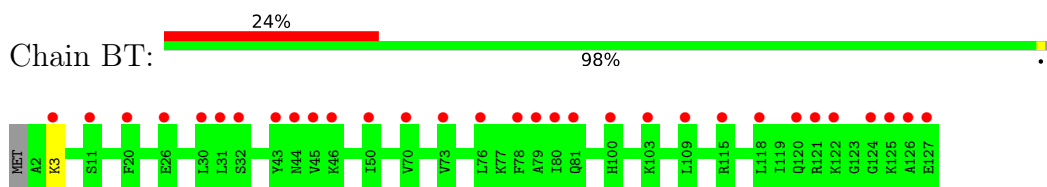
- Molecule 26: 60S ribosomal protein L25



- Molecule 27: Ribosomal protein L24

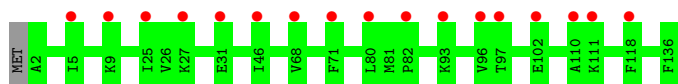


- Molecule 27: Ribosomal protein L24

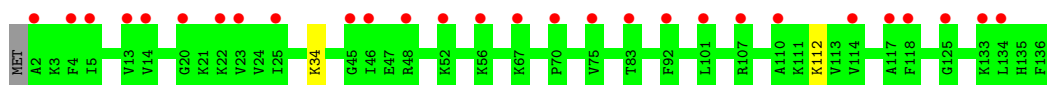


- Molecule 28: 60S ribosomal protein L27

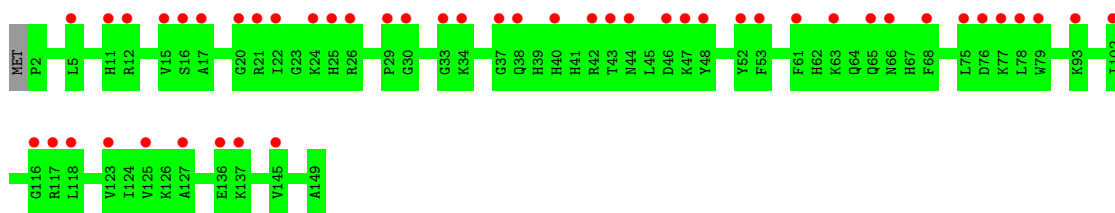




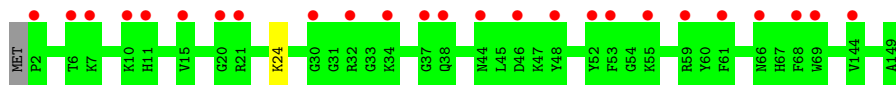
- Molecule 28: 60S ribosomal protein L27



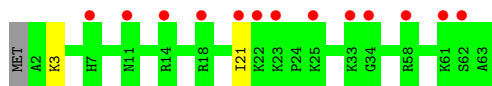
- Molecule 29: 60S ribosomal protein L28



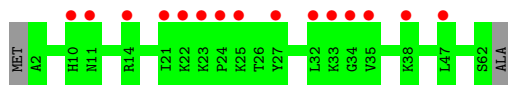
- Molecule 29: 60S ribosomal protein L28



- Molecule 30: 60S ribosomal protein L29

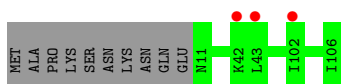


- Molecule 30: 60S ribosomal protein L29

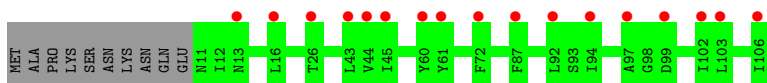


- Molecule 31: 60S ribosomal protein L30

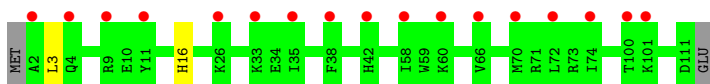




- Molecule 31: 60S ribosomal protein L30



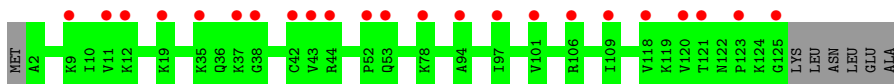
- Molecule 32: 60S ribosomal protein L31-B



- Molecule 32: 60S ribosomal protein L31-B



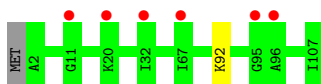
- Molecule 33: 60S ribosomal protein L32



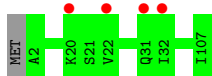
- Molecule 33: 60S ribosomal protein L32



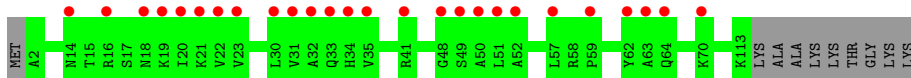
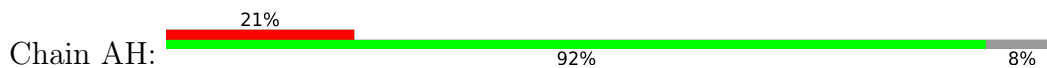
- Molecule 34: 60S ribosomal protein L33-A



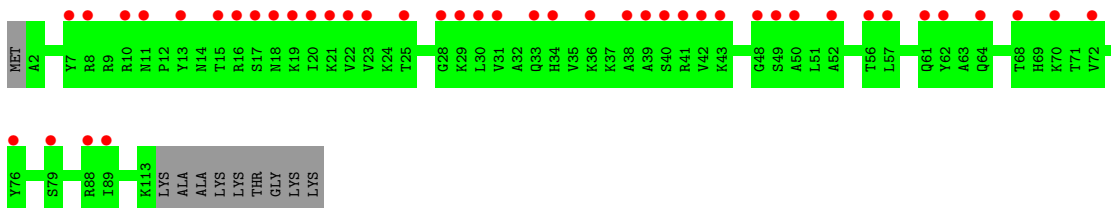
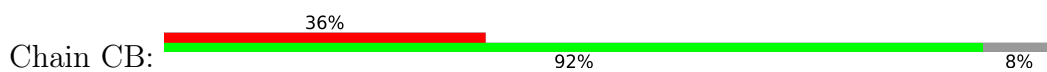
- Molecule 34: 60S ribosomal protein L33-A



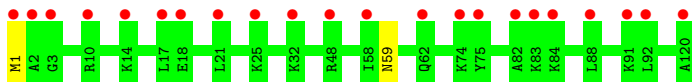
- Molecule 35: 60S ribosomal protein L34-B



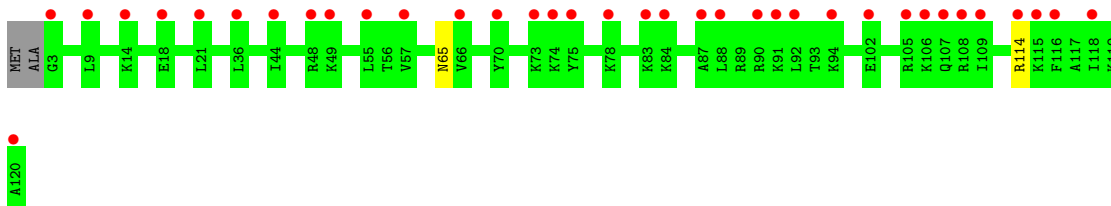
- Molecule 35: 60S ribosomal protein L34-B



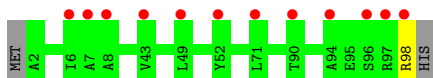
- Molecule 36: Ribosomal protein L29



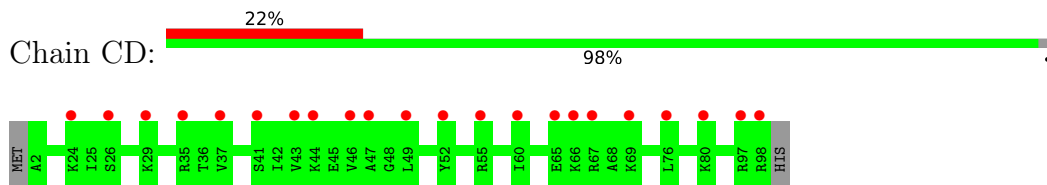
- Molecule 36: Ribosomal protein L29



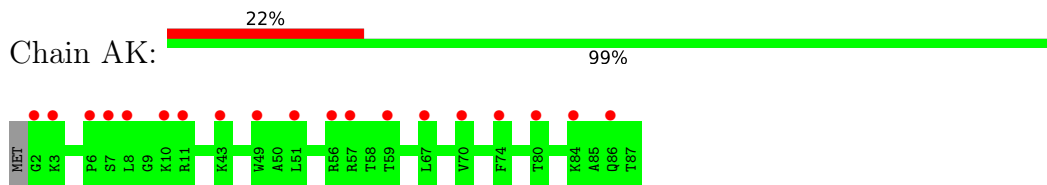
- Molecule 37: 60S ribosomal protein L36



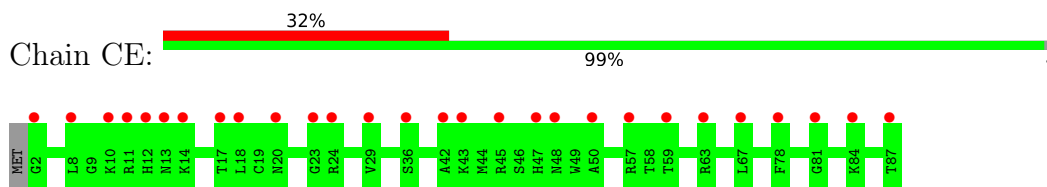
- Molecule 37: 60S ribosomal protein L36



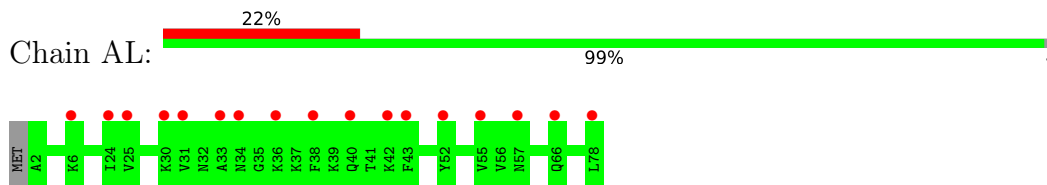
- Molecule 38: 60S ribosomal protein L37-B



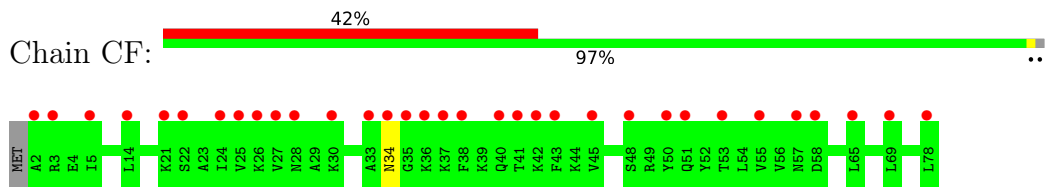
- Molecule 38: 60S ribosomal protein L37-B



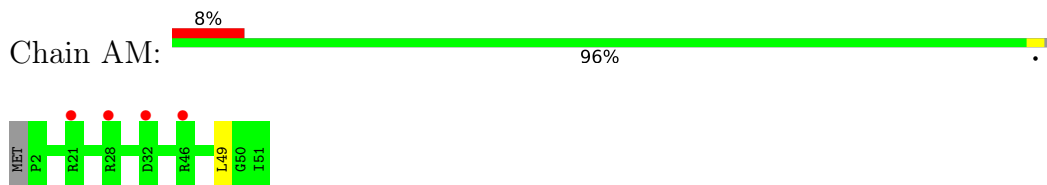
- Molecule 39: 60S ribosomal protein L38



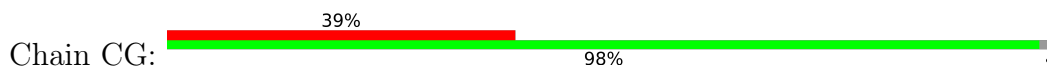
- Molecule 39: 60S ribosomal protein L38

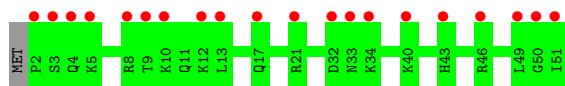


- Molecule 40: 60S ribosomal protein L39

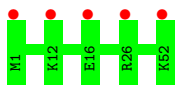


- Molecule 40: 60S ribosomal protein L39

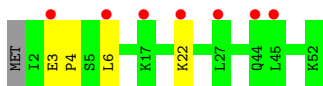
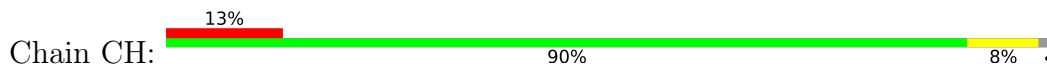




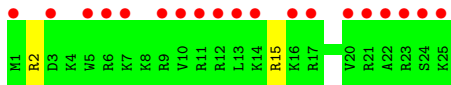
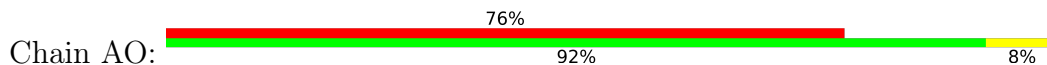
- Molecule 41: 60S ribosomal protein L40-B



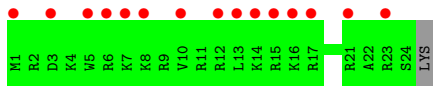
- Molecule 41: 60S ribosomal protein L40-B



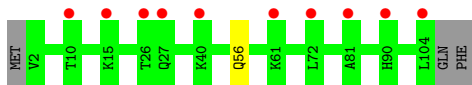
- Molecule 42: 60S ribosomal protein L41



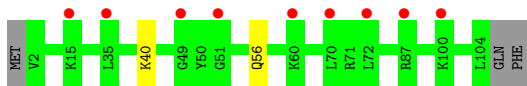
- Molecule 42: 60S ribosomal protein L41



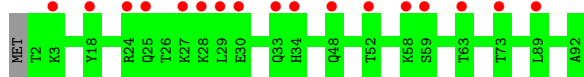
- Molecule 43: 60S ribosomal protein L42-B



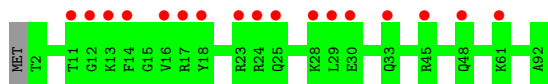
- Molecule 43: 60S ribosomal protein L42-B



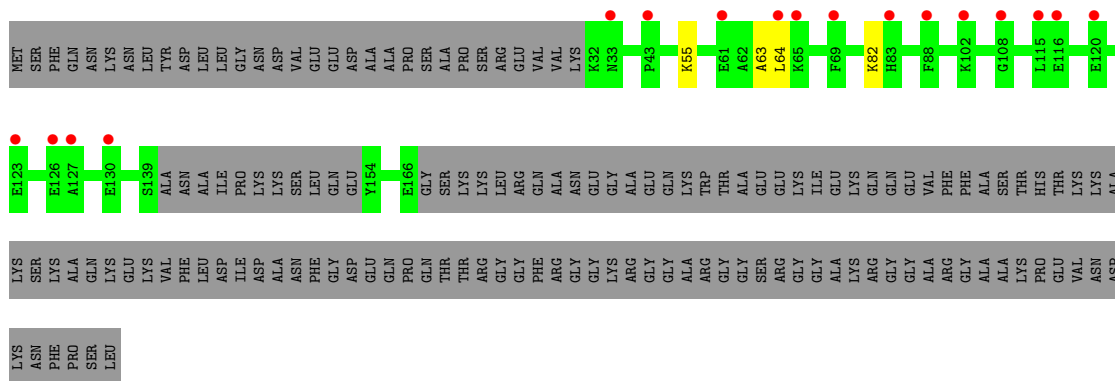
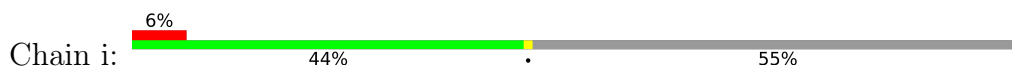
- Molecule 44: 60S ribosomal protein L43-A



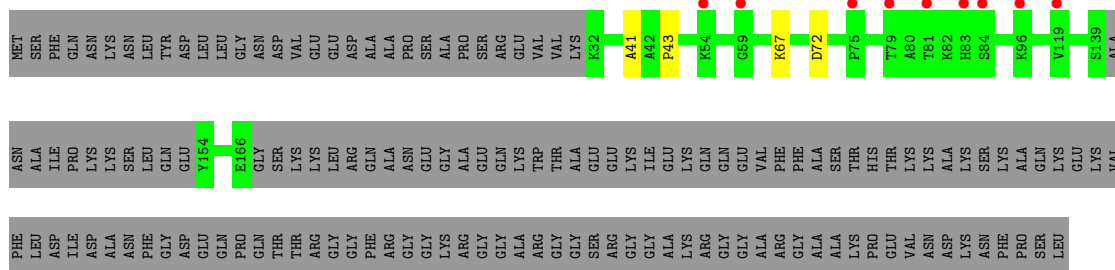
- Molecule 44: 60S ribosomal protein L43-A



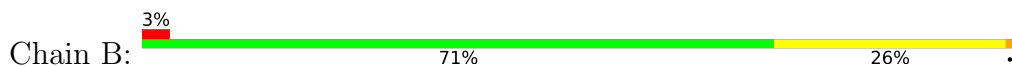
- Molecule 45: 60S ribosomal protein CAALFM_C304810CA

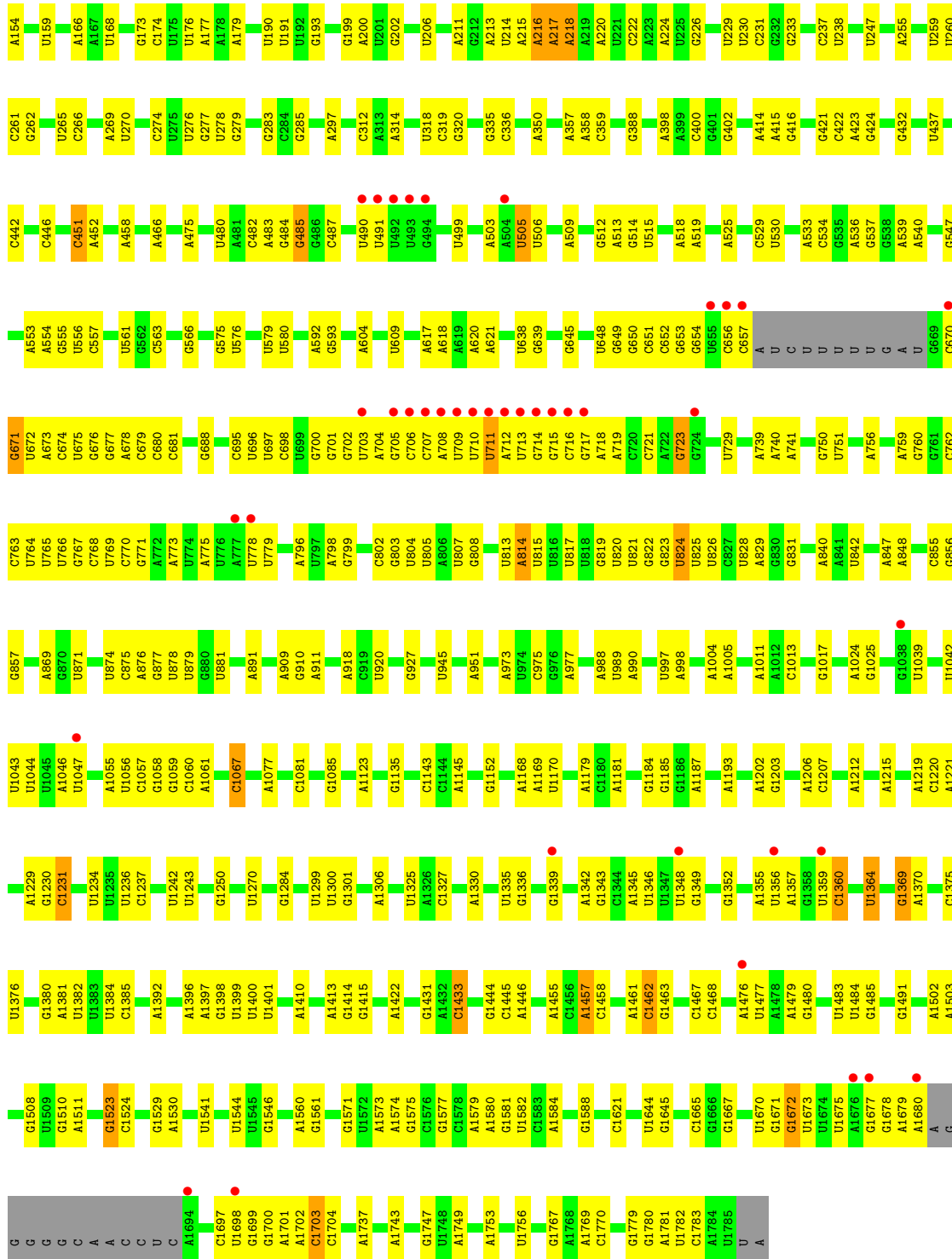


- Molecule 45: 60S ribosomal protein CAALFM_C304810CA

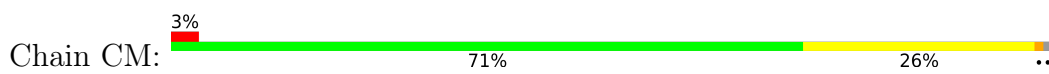


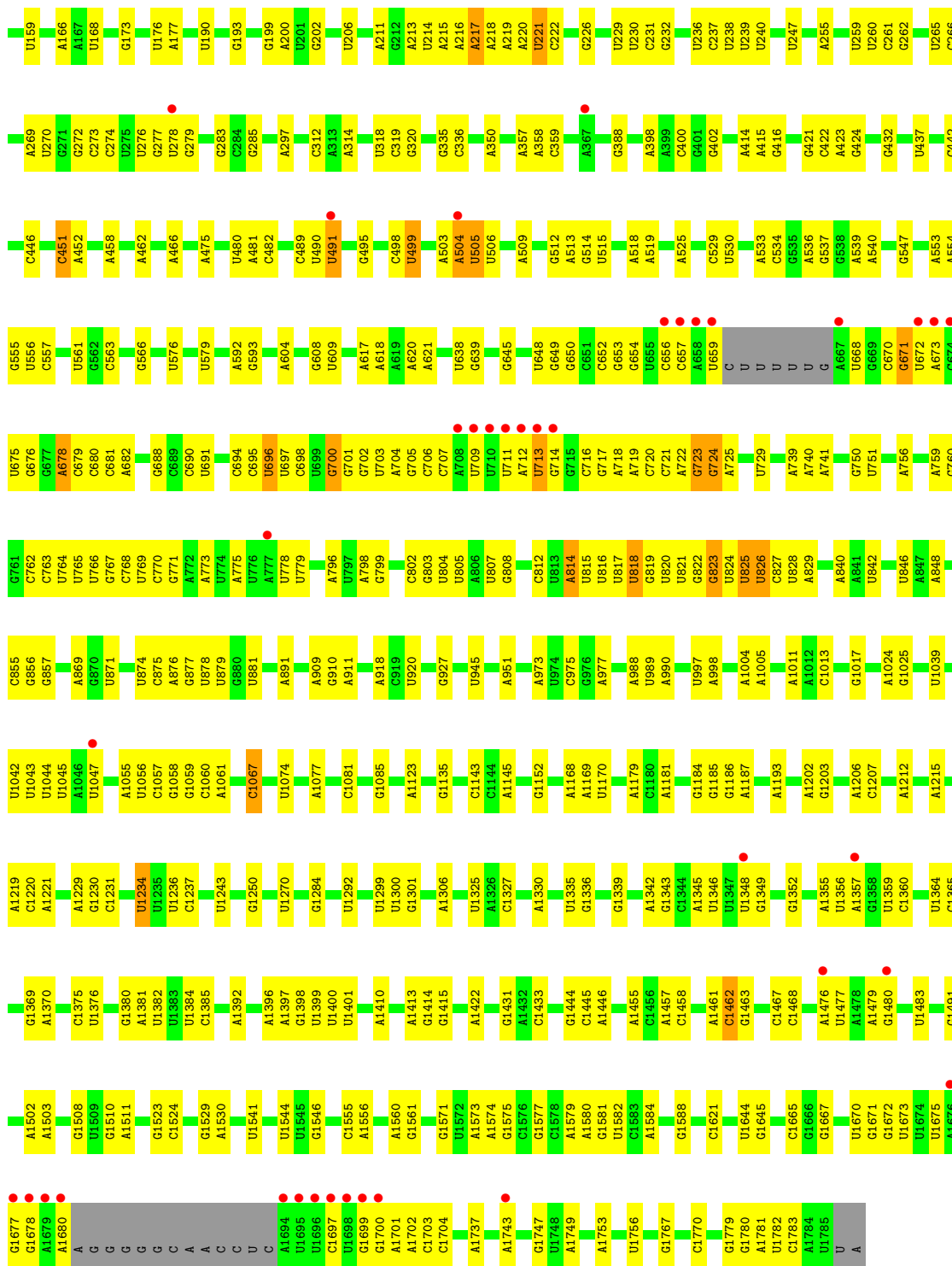
- Molecule 46: 18S



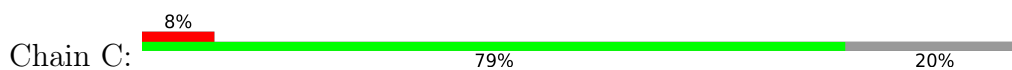


• Molecule 46: 18S



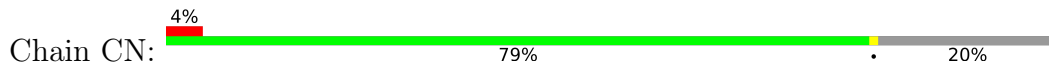


● Molecule 47: 40S ribosomal protein S0



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

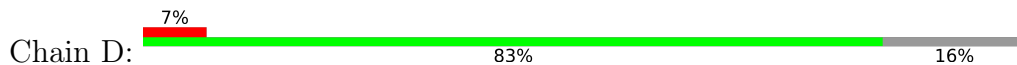
• Molecule 47: 40S ribosomal protein S0



MET S2 L16 M46 R79 L87 R127 Y185 K167 I170 I178 L184 R205 E209
ILE GLU GLN ASN ALA VAL GLU ALA LYS THR GLU VAL VAL ALA ALA ALA THR TRP THR GLU VAL ASP ASP

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

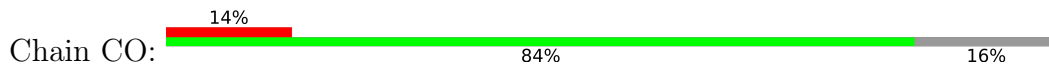
• Molecule 48: 40S ribosomal protein S1



MET
ALA
VAL
GLY
LYS
ASN
LYS
ARG
LEU
SER
SER
GLY
PHE
LYS
GLY
LYS
LYS
LYS
V20
V29
F38
L47
L54
K55
N56
A57
L61
K62
G63
E90
T98
K116
I140
Q146
A156
Q157
S158
Y176
R195
L217
G233
GLU
GLY
SER

THR
GLU
GLU
LYS
GLY
LYS
VAL
SER
SER
GLY
PHE
ASP
VAL
VAL
LEU
LEU
GLU
SER
VAL

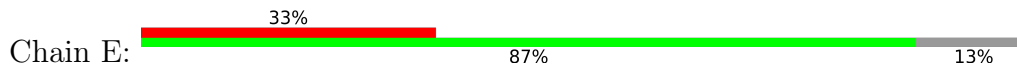
• Molecule 48: 40S ribosomal protein S1



MET
ALA
VAL
GLY
LYS
ASN
LYS
ARG
LEU
SER
SER
GLY
GLY
LYS
LYS
LYS
LYS
V20
F24
W29
F30
F38
K45
T46
L47
G53
L54
K55
B59
G60
L61
K62
G63
R64
E67
R85
E90
L95
L97
T98
H101
G102
H110
L120
V121

Y137
K152
Y155
A156
K216
L217
L218
K219
Q220
L225
H231
H232
G233
GLU
SER
THR
GLU
GLY
LYS
LYS
VAL
SER
SER
GLY
PHE
LYS
ASP
VAL
VAL
LEU
SER
VAL

• Molecule 49: Ribosomal protein S5

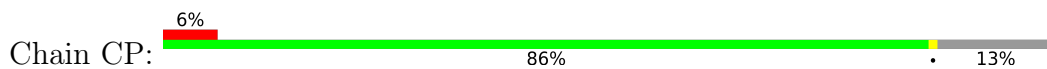


MET
SER
ALA
GLU
ALA
PRO
LYS
ARG
GLN
PHE
GLY
ASP
ARG
ARG
ARG
GLY
ARG
GLY
GLY
ARG
ARG
K28
S47
I51
L56
C151
P152
V153
T154
K155
K156
I64
D65
L66
K72
V75
M76
K77
I78
R79
S80
V81
Q82
K83
R86
A87
G88
Q89
R90
T91

R92
M93
A94
A95
V96
L108
G109
I110
K111
T112
A113
K114
E115
S118
A119
I120
I124
K128
I134
R135
L143
G144
Q145
L149
P150
C151
K152
V153
T154
G155
K156
V160
A161
V162
R163
L164
P168
K171
G172
I173
V174
A175
V178
V179
K180
Q184
L185

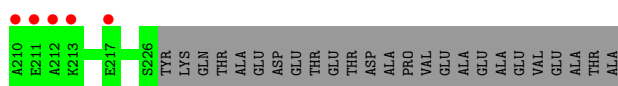
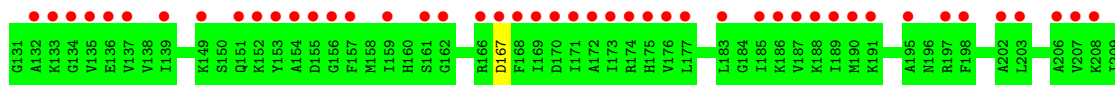
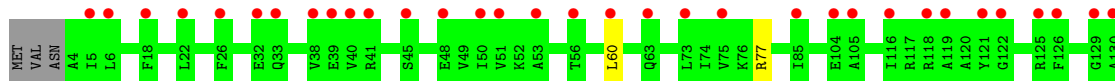
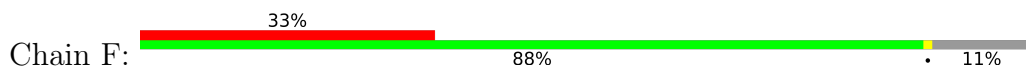
Y188
E189
Y192
T193
S194
S195
S196
G197
S198
T199
T202
E203
M204
T205
L206
A209
F210
I213
L220
F234
L235
A244
GLY
LYS
LYS
ARG
TYR

• Molecule 49: Ribosomal protein S5

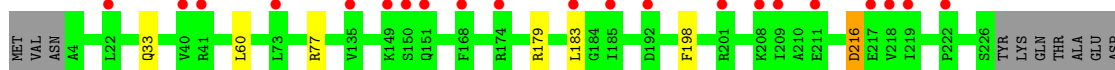
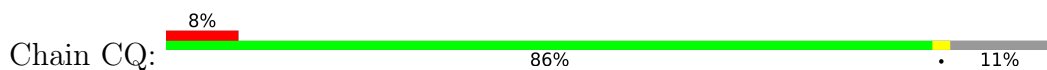


ARG
TYR

- Molecule 50: Ribosomal protein S3

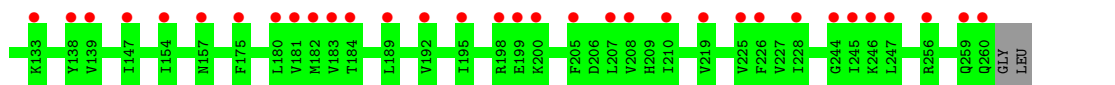
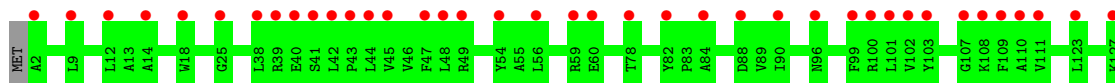


- Molecule 50: Ribosomal protein S3

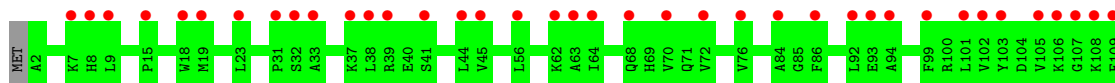


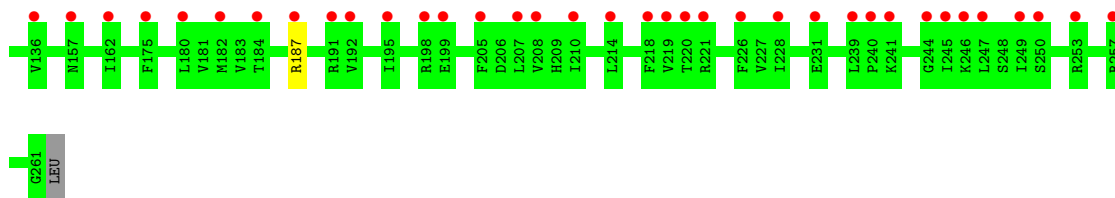
GLU
THR
THR
ASP
PRO
VAL
VAL
ALA
GLU
GLU
VAL
ALA
ALA
VAL
ALA

- Molecule 51: 40S ribosomal protein S4

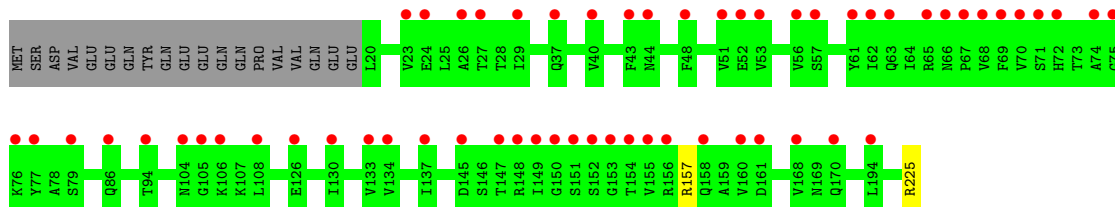
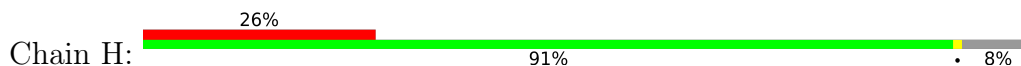


- Molecule 51: 40S ribosomal protein S4

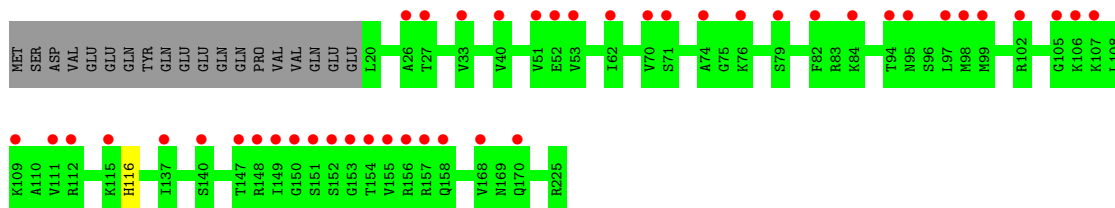




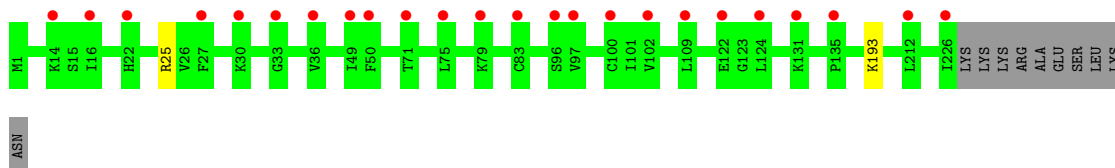
• Molecule 52: Ribosomal protein S7



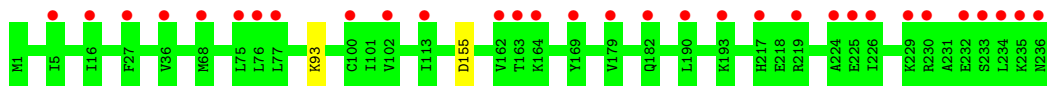
• Molecule 52: Ribosomal protein S7



• Molecule 53: 40S ribosomal protein S6

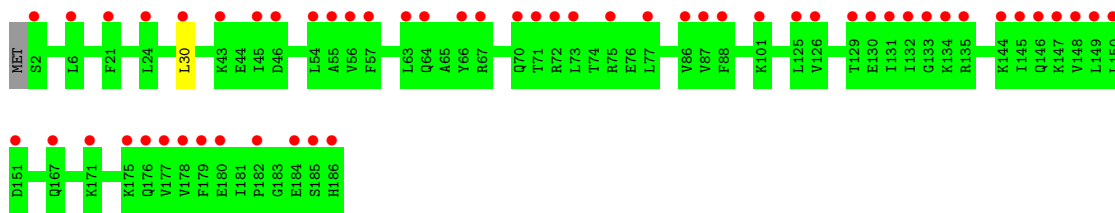


• Molecule 53: 40S ribosomal protein S6

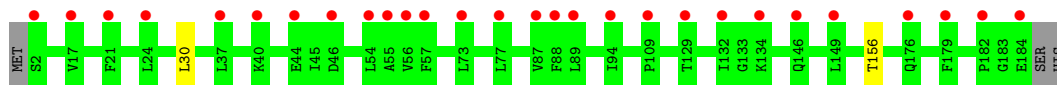


• Molecule 54: 40S ribosomal protein S7

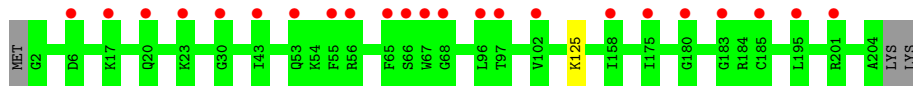




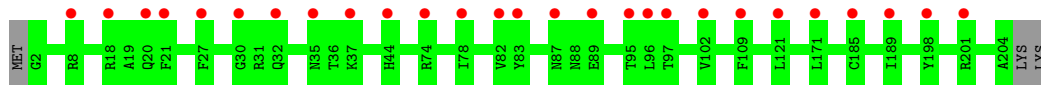
• Molecule 54: 40S ribosomal protein S7



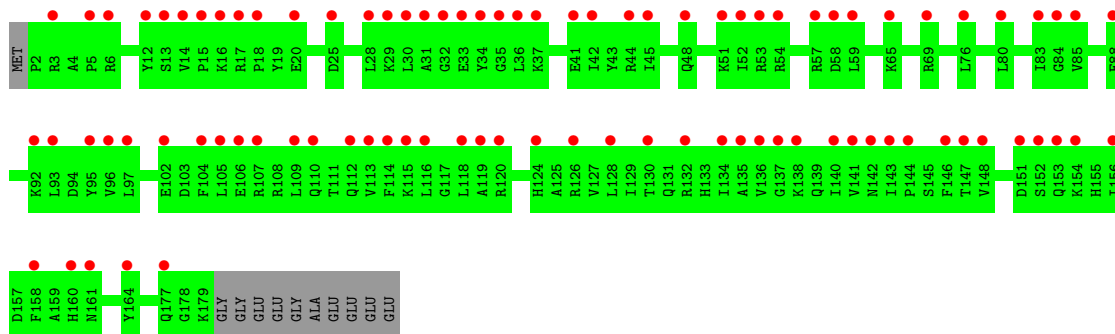
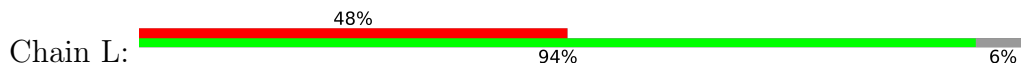
• Molecule 55: 40S ribosomal protein S8



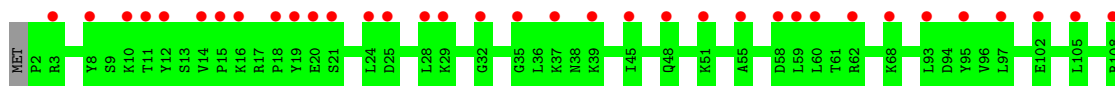
• Molecule 55: 40S ribosomal protein S8

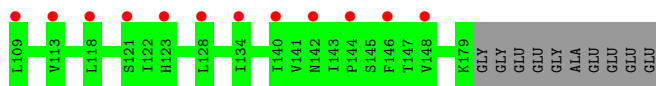


• Molecule 56: Ribosomal protein S4

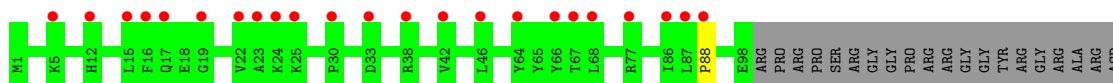
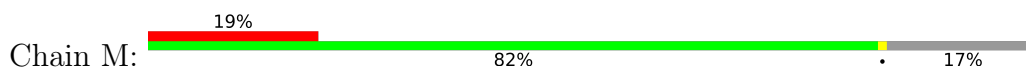


• Molecule 56: Ribosomal protein S4

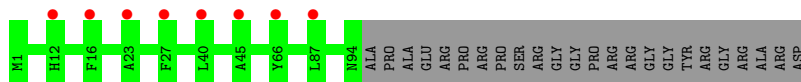
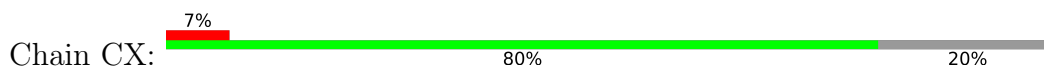




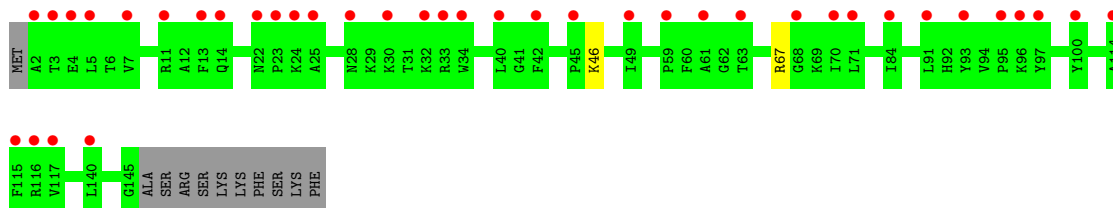
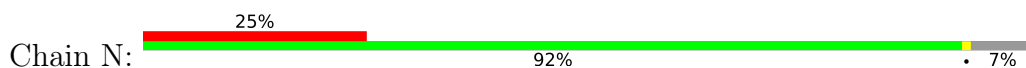
- Molecule 57: 40S ribosomal protein S10-A



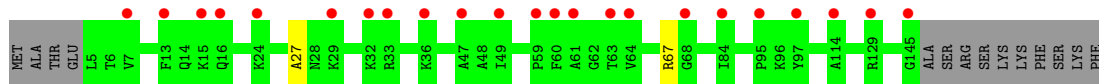
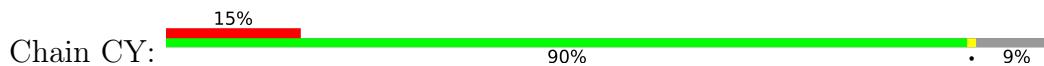
- Molecule 57: 40S ribosomal protein S10-A



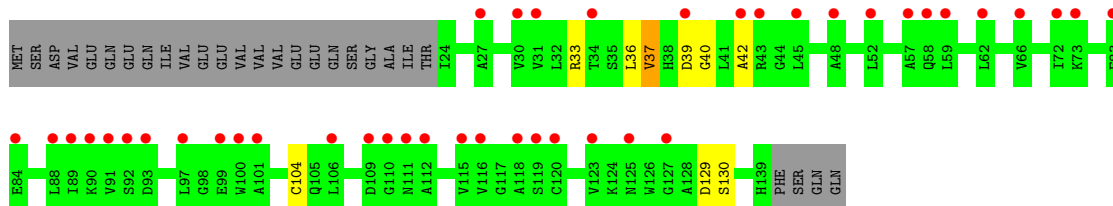
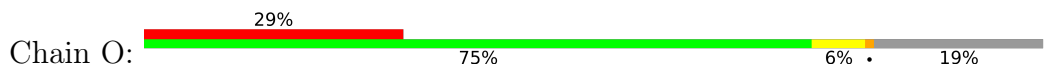
- Molecule 58: 40S ribosomal protein S11A



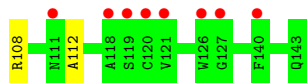
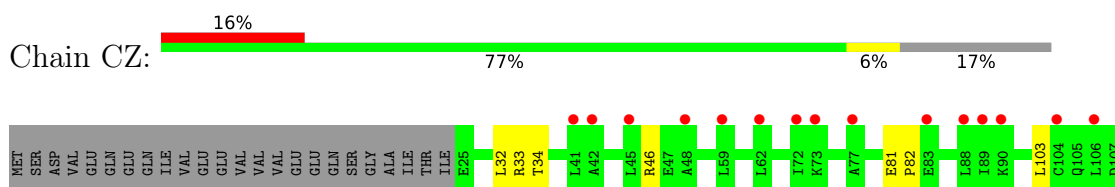
- Molecule 58: 40S ribosomal protein S11A



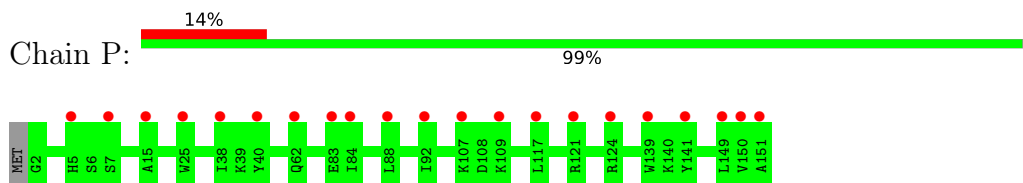
- Molecule 59: 40S ribosomal protein S12



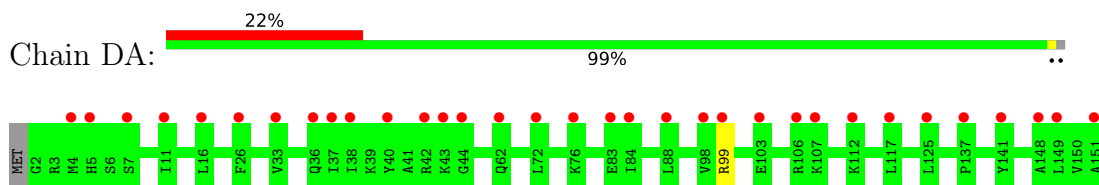
- Molecule 59: 40S ribosomal protein S12



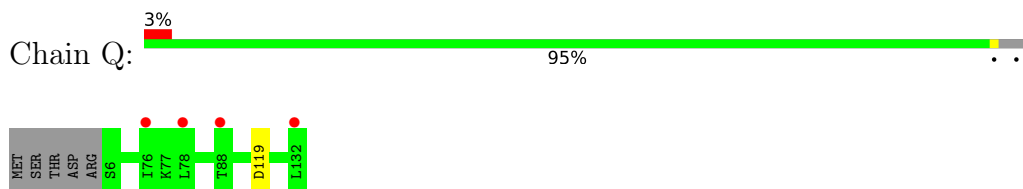
- Molecule 60: 40S ribosomal protein S13



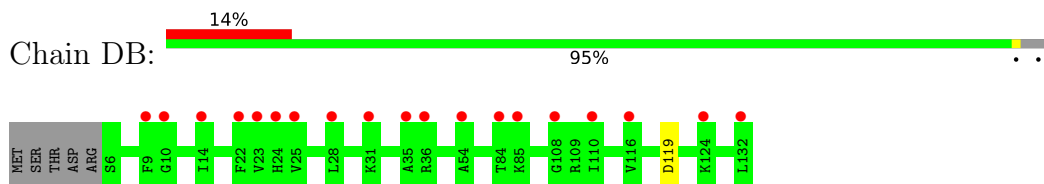
- Molecule 60: 40S ribosomal protein S13



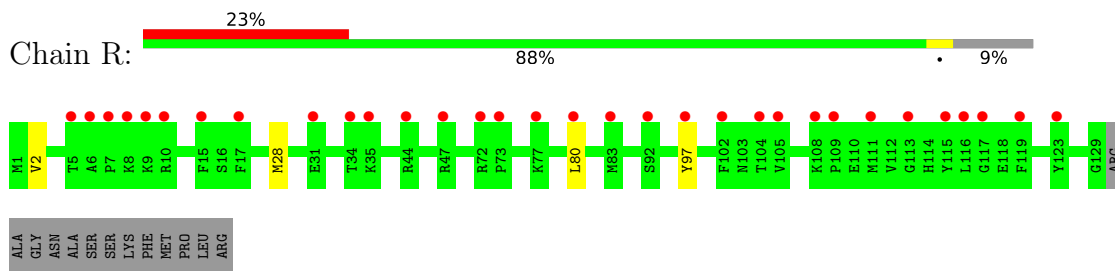
- Molecule 61: 40S ribosomal protein S14-A



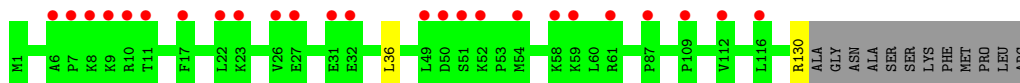
- Molecule 61: 40S ribosomal protein S14-A



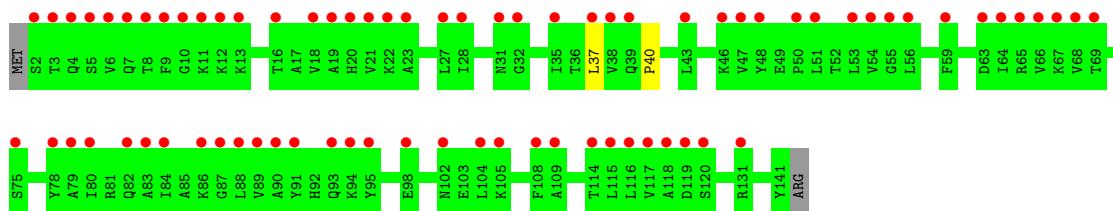
- Molecule 62: 40S ribosomal protein S15



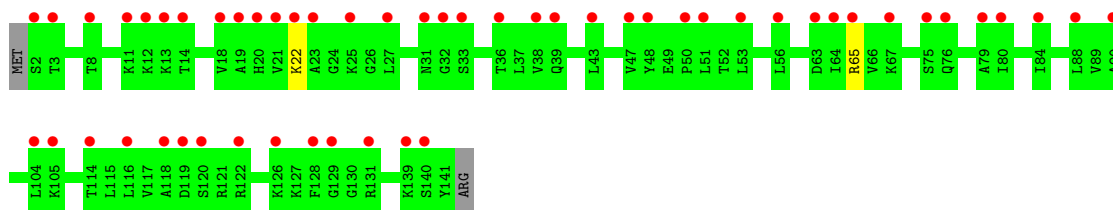
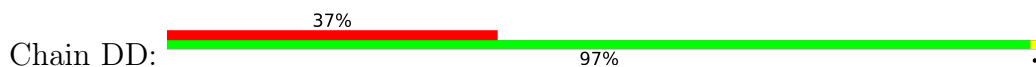
- Molecule 62: 40S ribosomal protein S15



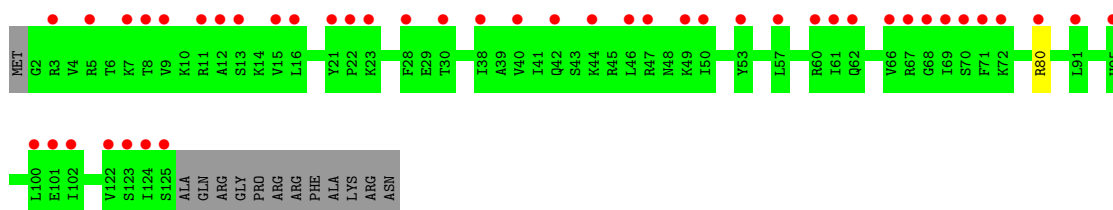
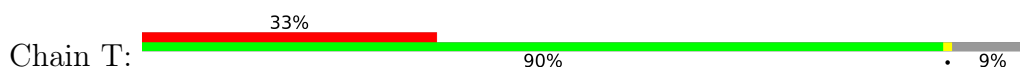
- Molecule 63: 40S ribosomal protein S16



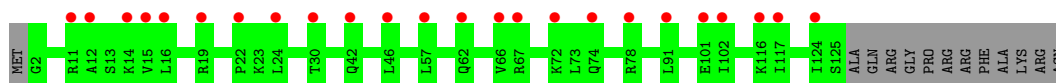
- Molecule 63: 40S ribosomal protein S16



- Molecule 64: 40S ribosomal protein S17-B



- Molecule 64: 40S ribosomal protein S17-B

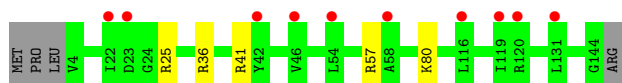


- Molecule 65: 40S ribosomal protein S18-B

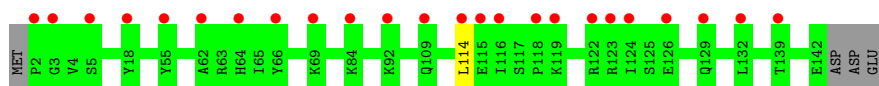




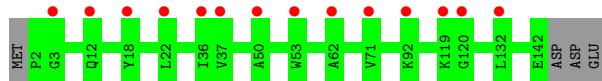
- Molecule 65: 40S ribosomal protein S18-B



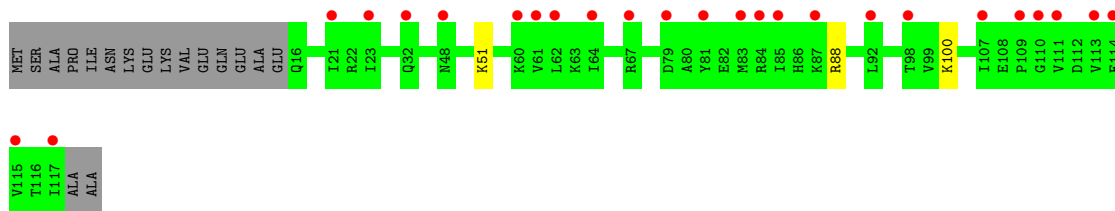
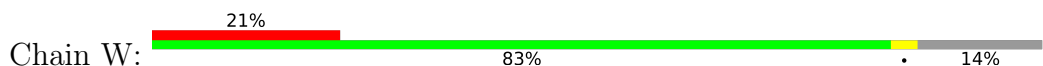
- Molecule 66: 40S ribosomal protein S19-A



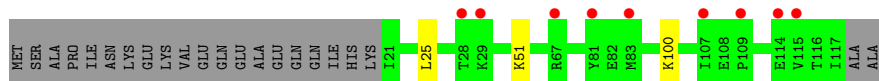
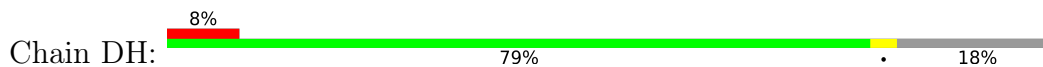
- Molecule 66: 40S ribosomal protein S19-A



- Molecule 67: Ribosomal protein S10

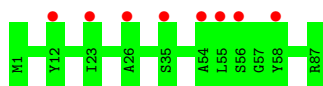


- Molecule 67: Ribosomal protein S10



- Molecule 68: 40S ribosomal protein S21



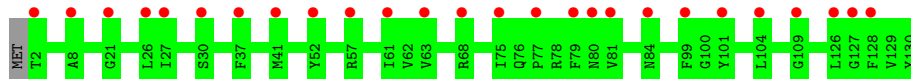


- Molecule 68: 40S ribosomal protein S21



There are no outlier residues recorded for this chain.

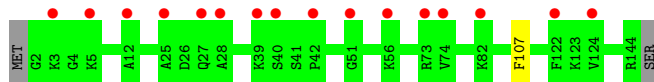
- Molecule 69: 40S ribosomal protein S22-A



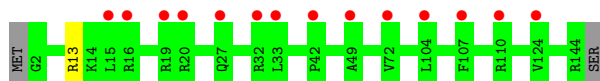
- Molecule 69: 40S ribosomal protein S22-A



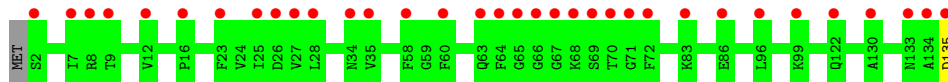
- Molecule 70: Ribosomal protein S23 (S12)



- Molecule 70: Ribosomal protein S23 (S12)



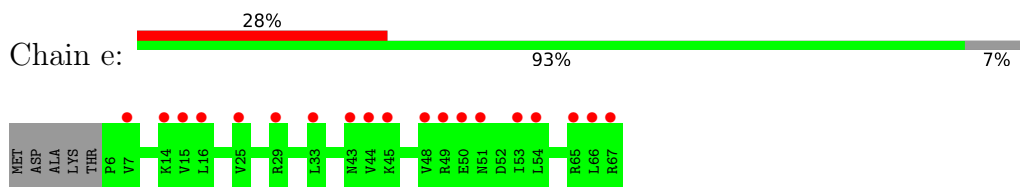
- Molecule 71: 40S ribosomal protein S24



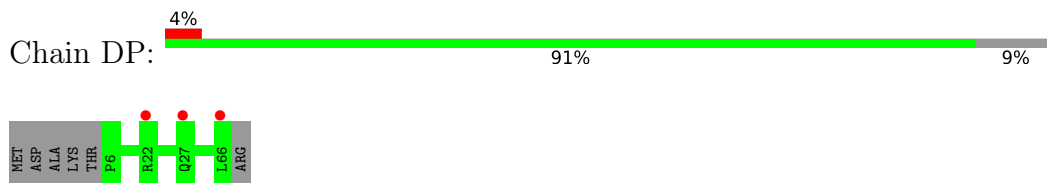
- Molecule 71: 40S ribosomal protein S24



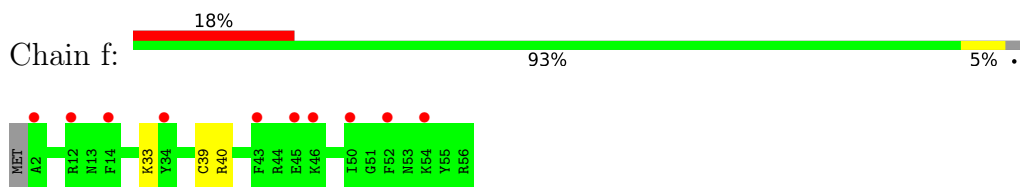
- Molecule 75: 40S ribosomal protein S28-B



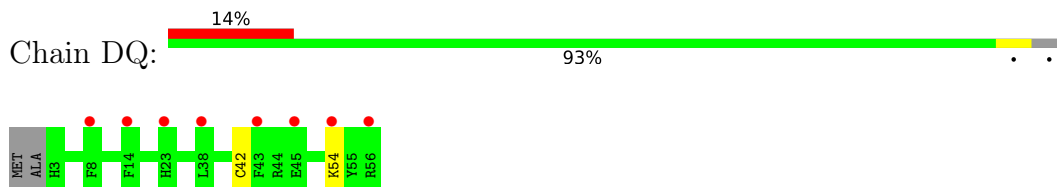
- Molecule 75: 40S ribosomal protein S28-B



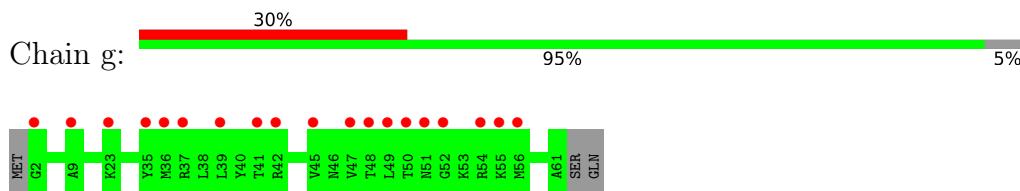
- Molecule 76: 40S ribosomal protein S29A



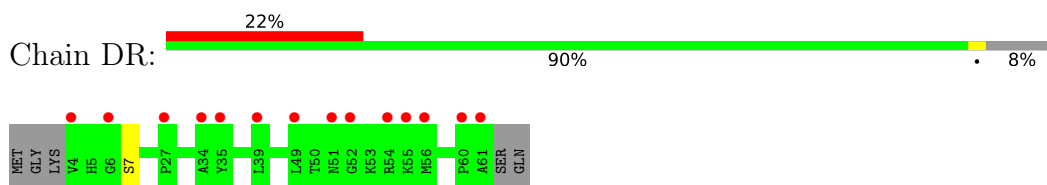
- Molecule 76: 40S ribosomal protein S29A



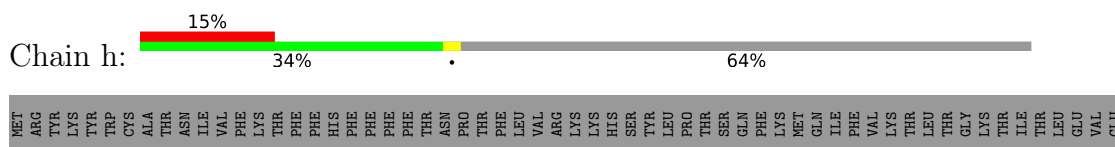
- Molecule 77: 40S ribosomal protein S30

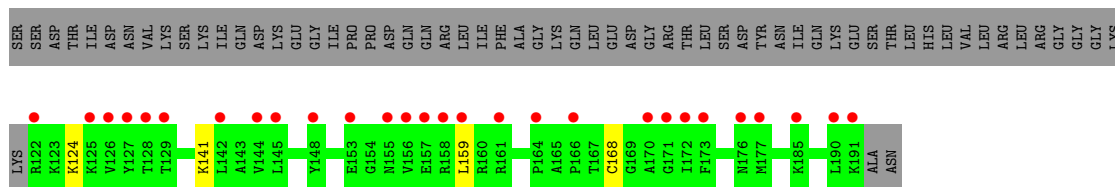


- Molecule 77: 40S ribosomal protein S30

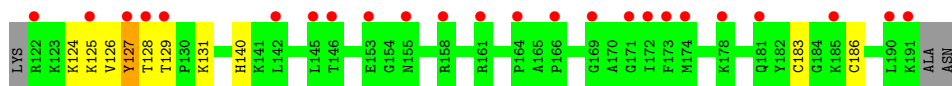
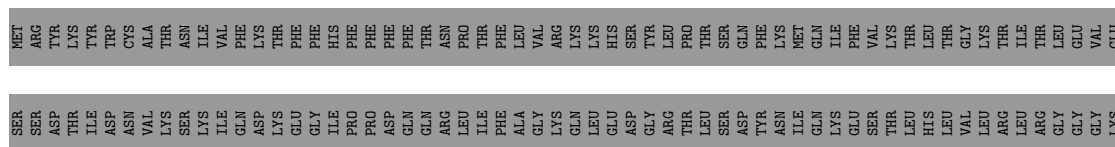


- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

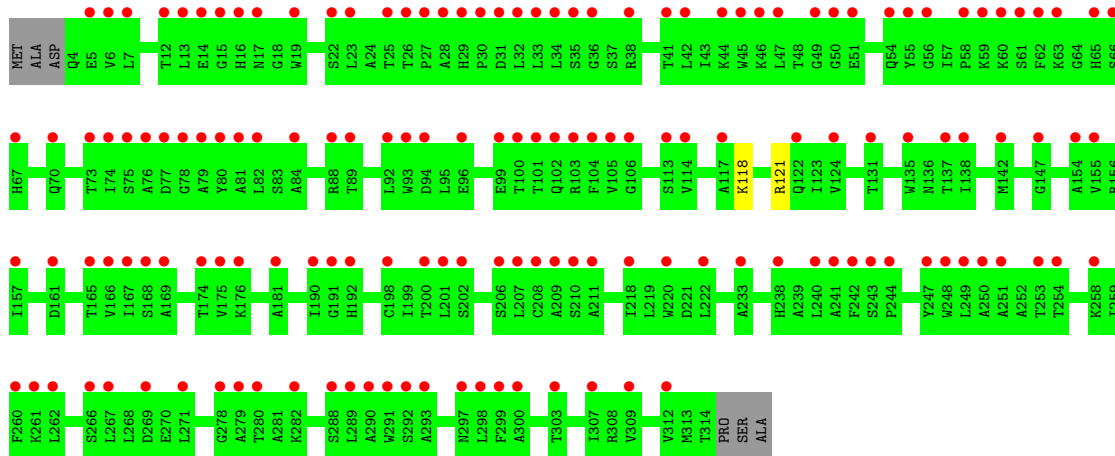




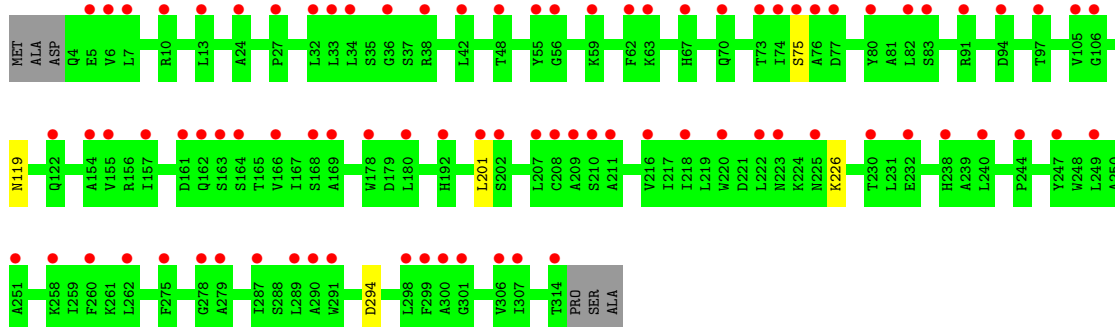
• Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein



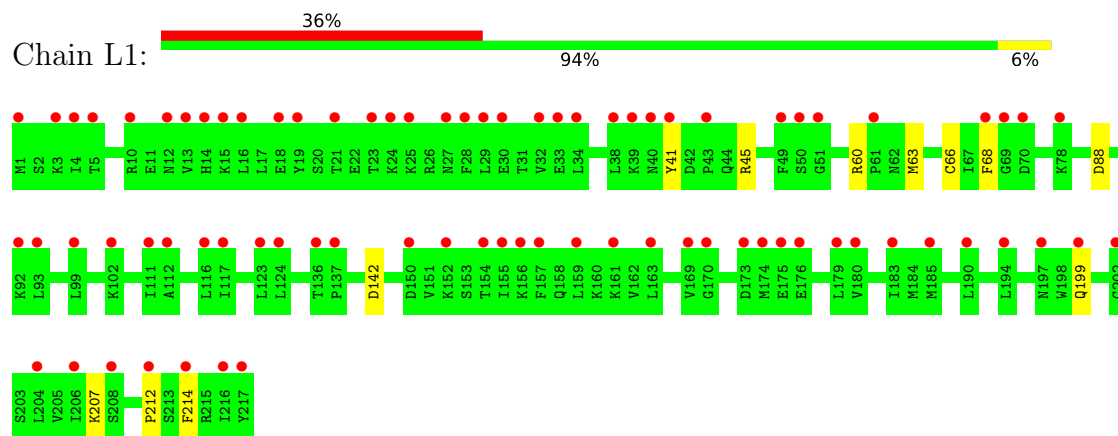
• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



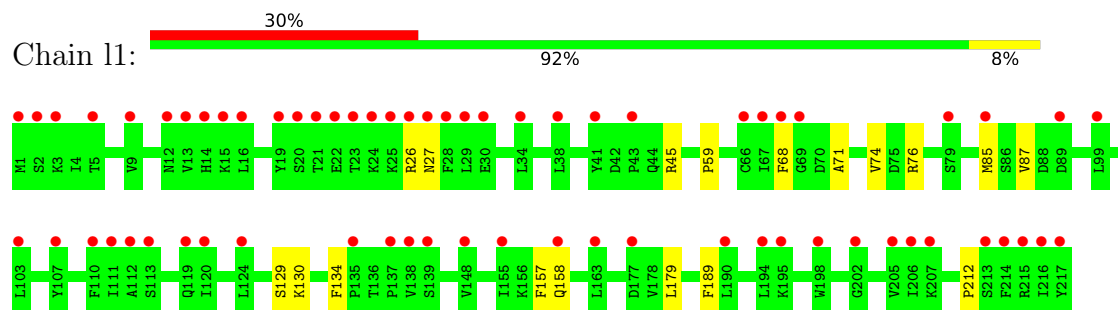
• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



- 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, α , β , γ	298.96Å 294.09Å 450.21Å 90.00° 100.12° 90.00°	Depositor
Resolution (Å)	227.46 – 3.00 267.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (227.46-3.00) 89.8 (267.82-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.01Å)	Xtrriage
Refinement program	PHENIX 19.2	Depositor
R, R_{free}	0.268 , 0.299 0.270 , 0.301	Depositor DCC
R_{free} test set	2000 reflections (0.13%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtrriage
Anisotropy	0.128	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	410139	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.40% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.30	1/76970 (0.0%)	0.90	96/119993 (0.1%)
1	AS	0.30	0/77254	0.90	94/120438 (0.1%)
2	3	0.25	0/2884	0.78	0/4492
2	AT	0.25	0/2884	0.79	0/4492
3	4	0.25	0/3724	0.81	1/5798 (0.0%)
3	AU	0.24	0/3746	0.81	2/5832 (0.0%)
4	AW	0.27	0/1931	0.57	0/2592
4	j	0.27	0/1931	0.59	0/2592
5	AX	0.27	0/3145	0.57	0/4231
5	k	0.27	0/3156	0.57	1/4246 (0.0%)
6	AY	0.26	0/2799	0.54	0/3777
6	l	0.27	0/2799	0.55	0/3777
7	AZ	0.26	0/2447	0.52	0/3294
7	m	0.26	0/2479	0.53	0/3337
8	BA	0.28	0/1231	0.55	0/1662
8	n	0.28	0/1263	0.55	0/1703
9	BB	0.27	0/1918	0.51	0/2575
9	o	0.28	0/1918	0.53	0/2575
10	BC	0.26	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	0.27	0/1724	0.57	0/2314
12	r	0.27	0/1724	0.57	0/2314
13	BF	0.26	0/1390	0.58	0/1861
13	s	0.26	0/1390	0.58	0/1861
14	BG	0.25	0/1637	0.55	0/2195
14	t	0.28	0/1637	0.57	0/2195
15	BH	0.27	0/1044	0.54	0/1407
15	u	0.26	0/1044	0.54	0/1407
16	BI	0.26	0/1753	0.60	0/2347
16	v	0.27	0/1753	0.60	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	BJ	0.27	0/1620	0.53	0/2167
17	w	0.27	0/1620	0.53	0/2167
18	BK	0.25	0/1429	0.57	0/1920
18	x	0.26	0/1410	0.58	0/1895
19	BL	0.27	0/1482	0.59	0/1985
19	y	0.27	0/1482	0.59	0/1985
20	BM	0.25	0/1475	0.59	0/1961
20	z	0.26	0/1475	0.60	0/1961
21	0	0.27	0/1457	0.57	0/1962
21	BN	0.26	0/1457	0.54	0/1962
22	2	0.26	0/1285	0.53	0/1723
22	BO	0.27	0/1285	0.54	0/1723
23	5	0.26	0/846	0.47	0/1140
23	BP	0.28	0/866	0.51	0/1168
24	6	0.28	0/993	0.57	0/1339
24	BQ	0.28	0/993	0.59	0/1339
25	7	0.26	0/958	0.53	0/1267
25	BR	0.25	0/814	0.54	0/1079
26	8	0.26	0/990	0.54	0/1337
26	BS	0.25	0/976	0.52	0/1319
27	9	0.25	0/999	0.53	0/1334
27	BT	0.26	0/999	0.54	0/1334
28	AA	0.27	0/1112	0.48	0/1488
28	BU	0.26	0/1112	0.49	0/1488
29	AB	0.26	0/1199	0.55	0/1607
29	BV	0.26	0/1199	0.54	0/1607
30	AC	0.27	0/503	0.59	0/668
30	BW	0.24	0/498	0.53	0/661
31	AD	0.26	0/738	0.48	0/994
31	BX	0.26	0/738	0.49	0/994
32	AE	0.25	0/907	0.57	1/1219 (0.1%)
32	BY	0.24	0/907	0.57	0/1219
33	AF	0.26	0/1021	0.54	0/1368
33	BZ	0.25	0/1025	0.56	0/1372
34	AG	0.28	0/866	0.55	0/1165
34	CA	0.28	0/866	0.54	0/1165
35	AH	0.25	0/896	0.59	0/1195
35	CB	0.25	0/896	0.59	0/1195
36	AI	0.26	0/1012	0.56	0/1347
36	CC	0.24	0/999	0.55	0/1330
37	AJ	0.25	0/763	0.58	0/1012
37	CD	0.26	0/763	0.58	0/1012
38	AK	0.27	0/690	0.60	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CE	0.26	0/690	0.61	0/916
39	AL	0.26	0/623	0.49	0/831
39	CF	0.27	0/623	0.58	0/831
40	AM	0.26	0/447	0.59	0/594
40	CG	0.27	0/458	0.64	0/609
41	AN	0.26	0/425	0.58	0/563
41	CH	0.29	0/417	0.59	0/553
42	AO	0.26	0/237	0.72	0/304
42	CI	0.27	0/228	0.72	0/293
43	AP	0.28	0/840	0.55	0/1110
43	CJ	0.28	0/840	0.55	0/1110
44	AQ	0.30	0/705	0.62	0/940
44	CK	0.26	0/705	0.59	0/940
45	CL	0.31	0/941	0.64	0/1257
45	i	0.28	0/941	0.67	0/1257
46	B	0.29	0/41987	0.94	70/65427 (0.1%)
46	CM	0.30	0/42081	0.94	63/65573 (0.1%)
47	C	0.25	0/1666	0.51	0/2273
47	CN	0.26	0/1666	0.52	0/2273
48	CO	0.26	0/1750	0.58	0/2354
48	D	0.25	0/1750	0.55	0/2354
49	CP	0.27	0/1657	0.54	0/2248
49	E	0.25	0/1657	0.52	0/2248
50	CQ	0.27	0/1731	0.63	3/2324 (0.1%)
50	F	0.27	0/1731	0.61	1/2324 (0.0%)
51	CR	0.26	0/2096	0.56	0/2822
51	G	0.26	0/2092	0.56	0/2817
52	CS	0.25	0/1631	0.54	0/2199
52	H	0.25	0/1631	0.56	0/2199
53	CT	0.27	0/1929	0.58	0/2571
53	I	0.25	0/1845	0.56	0/2464
54	CU	0.27	0/1499	0.56	0/2016
54	J	0.25	0/1516	0.55	0/2039
55	CV	0.27	0/1606	0.61	0/2150
55	K	0.27	0/1606	0.60	0/2150
56	CW	0.26	0/1478	0.56	0/1978
56	L	0.26	0/1478	0.57	0/1978
57	CX	0.29	0/809	0.57	0/1092
57	M	0.29	0/836	0.62	0/1130
58	CY	0.28	0/1154	0.58	0/1553
58	N	0.27	0/1175	0.58	0/1582
59	CZ	0.31	0/921	0.86	1/1240 (0.1%)
59	O	0.31	0/892	0.72	0/1203

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	DA	0.25	0/1210	0.54	0/1631
60	P	0.25	0/1210	0.51	0/1631
61	DB	0.30	0/953	0.65	0/1279
61	Q	0.30	0/953	0.64	0/1279
62	DC	0.29	0/1049	0.60	0/1409
62	R	0.30	0/1038	0.62	1/1395 (0.1%)
63	DD	0.25	0/1109	0.54	0/1486
63	S	0.27	0/1109	0.57	0/1486
64	DE	0.28	0/1009	0.63	0/1354
64	T	0.26	0/1009	0.63	0/1354
65	DF	0.26	0/1178	0.58	0/1579
65	U	0.27	0/1205	0.59	0/1615
66	DG	0.26	0/1120	0.55	0/1508
66	V	0.27	0/1120	0.59	1/1508 (0.1%)
67	DH	0.26	0/772	0.59	1/1045 (0.1%)
67	W	0.25	0/818	0.56	0/1106
68	DI	0.28	0/683	0.59	0/918
68	X	0.26	0/683	0.58	0/918
69	DJ	0.26	0/1049	0.56	0/1412
69	Y	0.25	0/1049	0.54	0/1412
70	DK	0.28	0/1128	0.59	0/1505
70	Z	0.28	0/1128	0.62	0/1505
71	DL	0.27	0/1086	0.58	0/1447
71	a	0.26	0/1100	0.56	0/1466
72	DM	0.26	0/577	0.57	0/778
72	b	0.24	0/585	0.52	0/789
73	DN	0.26	0/791	0.61	0/1060
73	c	0.27	0/791	0.62	0/1060
74	DO	0.28	0/624	0.59	0/843
74	d	0.26	0/624	0.54	0/843
75	DP	0.34	0/478	0.73	0/640
75	e	0.27	0/489	0.68	0/654
76	DQ	0.29	0/461	0.62	0/613
76	f	0.30	0/466	0.65	1/620 (0.2%)
77	DR	0.31	0/469	0.72	0/626
77	g	0.28	0/482	0.63	0/642
78	DS	0.34	0/585	0.75	0/778
78	h	0.26	0/585	0.69	1/778 (0.1%)
79	AR	0.27	0/2451	0.56	0/3337
79	DT	0.27	0/2451	0.60	0/3337
80	P0	0.26	0/857	0.56	0/1148
80	p0	0.27	0/857	0.63	1/1148 (0.1%)
81	12	0.26	0/486	0.51	0/653

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
82	L1	0.26	0/1737	0.52	0/2335
82	l1	0.27	0/1737	0.55	0/2335
All	All	0.28	1/438315 (0.0%)	0.79	339/642822 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	2482	U	C1'-N1	5.94	1.57	1.48

The worst 5 of 339 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AS	1267	A	O5'-P-OP2	-14.80	92.38	105.70
46	B	676	G	O4'-C1'-N9	11.57	117.45	108.20
1	AS	487	C	O5'-P-OP1	-11.41	95.43	105.70
59	CZ	81	GLU	C-N-CD	-11.20	95.95	120.60
1	1	1228	C	C6-N1-C2	-11.16	115.83	120.30

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	248/254 (98%)	240 (97%)	8 (3%)	0	100	100
4	j	248/254 (98%)	240 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	AX	384/389 (99%)	372 (97%)	12 (3%)	0	100	100
5	k	385/389 (99%)	371 (96%)	14 (4%)	0	100	100
6	AY	359/363 (99%)	349 (97%)	10 (3%)	0	100	100
6	l	359/363 (99%)	348 (97%)	11 (3%)	0	100	100
7	AZ	290/298 (97%)	279 (96%)	11 (4%)	0	100	100
7	m	294/298 (99%)	282 (96%)	11 (4%)	1 (0%)	41	76
8	BA	149/176 (85%)	147 (99%)	2 (1%)	0	100	100
8	n	153/176 (87%)	149 (97%)	4 (3%)	0	100	100
9	BB	232/241 (96%)	226 (97%)	5 (2%)	1 (0%)	34	72
9	o	232/241 (96%)	226 (97%)	5 (2%)	1 (0%)	34	72
10	BC	231/262 (88%)	219 (95%)	10 (4%)	2 (1%)	17	55
10	p	236/262 (90%)	227 (96%)	8 (3%)	1 (0%)	34	72
11	BD	188/191 (98%)	183 (97%)	5 (3%)	0	100	100
11	q	188/191 (98%)	183 (97%)	5 (3%)	0	100	100
12	BE	204/220 (93%)	199 (98%)	5 (2%)	0	100	100
12	r	204/220 (93%)	201 (98%)	3 (2%)	0	100	100
13	BF	169/174 (97%)	163 (96%)	6 (4%)	0	100	100
13	s	169/174 (97%)	161 (95%)	8 (5%)	0	100	100
14	BG	198/202 (98%)	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%)	197 (98%)	4 (2%)	0	100	100
16	v	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	BJ	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
17	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	BK	172/185 (93%)	168 (98%)	4 (2%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
22	2	157/160 (98%)	155 (99%)	2 (1%)	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%)	15	53
23	BP	102/124 (82%)	89 (87%)	11 (11%)	2 (2%)	7	34
24	6	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
24	BQ	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
25	7	114/155 (74%)	103 (90%)	11 (10%)	0	100	100
25	BR	94/155 (61%)	91 (97%)	3 (3%)	0	100	100
26	8	119/142 (84%)	117 (98%)	2 (2%)	0	100	100
26	BS	117/142 (82%)	115 (98%)	2 (2%)	0	100	100
27	9	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
27	BT	124/127 (98%)	123 (99%)	1 (1%)	0	100	100
28	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
28	BU	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
29	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
29	BV	146/149 (98%)	139 (95%)	6 (4%)	1 (1%)	22	60
30	AC	60/63 (95%)	56 (93%)	2 (3%)	2 (3%)	4	21
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%)	104 (96%)	3 (3%)	1 (1%)	17	55
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%)	101 (97%)	3 (3%)	0	100	100
34	CA	104/107 (97%)	101 (97%)	3 (3%)	0	100	100
35	AH	110/122 (90%)	108 (98%)	2 (2%)	0	100	100
35	CB	110/122 (90%)	107 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	AI	119/120 (99%)	114 (96%)	5 (4%)	0	100	100
36	CC	117/120 (98%)	114 (97%)	3 (3%)	0	100	100
37	AJ	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
37	CD	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
38	AK	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
38	CE	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
39	AL	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
39	CF	75/78 (96%)	69 (92%)	6 (8%)	0	100	100
40	AM	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	7	33
40	CG	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
41	AN	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
41	CH	49/52 (94%)	46 (94%)	0	3 (6%)	1	8
42	AO	23/25 (92%)	22 (96%)	1 (4%)	0	100	100
42	CI	22/25 (88%)	22 (100%)	0	0	100	100
43	AP	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
43	CJ	101/106 (95%)	99 (98%)	2 (2%)	0	100	100
44	AQ	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
44	CK	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	CL	117/267 (44%)	92 (79%)	22 (19%)	3 (3%)	5	27
45	i	117/267 (44%)	95 (81%)	19 (16%)	3 (3%)	5	27
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%)	210 (98%)	5 (2%)	0	100	100
49	E	215/249 (86%)	210 (98%)	5 (2%)	0	100	100
50	CQ	221/251 (88%)	211 (96%)	10 (4%)	0	100	100
50	F	221/251 (88%)	213 (96%)	8 (4%)	0	100	100
51	CR	258/262 (98%)	254 (98%)	4 (2%)	0	100	100
51	G	257/262 (98%)	253 (98%)	4 (2%)	0	100	100
52	CS	204/225 (91%)	197 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
54	CU	181/186 (97%)	171 (94%)	9 (5%)	1 (1%)	25	64
54	J	183/186 (98%)	174 (95%)	9 (5%)	0	100	100
55	CV	201/206 (98%)	199 (99%)	2 (1%)	0	100	100
55	K	201/206 (98%)	200 (100%)	1 (0%)	0	100	100
56	CW	176/189 (93%)	174 (99%)	2 (1%)	0	100	100
56	L	176/189 (93%)	175 (99%)	1 (1%)	0	100	100
57	CX	92/118 (78%)	85 (92%)	7 (8%)	0	100	100
57	M	96/118 (81%)	82 (85%)	13 (14%)	1 (1%)	15	53
58	CY	139/155 (90%)	133 (96%)	5 (4%)	1 (1%)	22	60
58	N	142/155 (92%)	137 (96%)	5 (4%)	0	100	100
59	CZ	117/143 (82%)	90 (77%)	21 (18%)	6 (5%)	2	12
59	O	114/143 (80%)	89 (78%)	20 (18%)	5 (4%)	2	15
60	DA	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
60	P	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
61	DB	125/132 (95%)	120 (96%)	4 (3%)	1 (1%)	19	57
61	Q	125/132 (95%)	119 (95%)	6 (5%)	0	100	100
62	DC	128/142 (90%)	111 (87%)	17 (13%)	0	100	100
62	R	127/142 (89%)	115 (91%)	11 (9%)	1 (1%)	19	57
63	DD	138/142 (97%)	134 (97%)	4 (3%)	0	100	100
63	S	138/142 (97%)	132 (96%)	5 (4%)	1 (1%)	22	60
64	DE	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
64	T	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
65	DF	139/145 (96%)	134 (96%)	3 (2%)	2 (1%)	11	43
65	U	142/145 (98%)	137 (96%)	5 (4%)	0	100	100
66	DG	139/145 (96%)	134 (96%)	5 (4%)	0	100	100
66	V	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
67	DH	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
67	W	100/119 (84%)	97 (97%)	3 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
68	DI	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	X	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
69	DJ	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
69	Y	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
70	DK	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
70	Z	141/145 (97%)	138 (98%)	3 (2%)	0	100	100
71	DL	130/135 (96%)	130 (100%)	0	0	100	100
71	a	132/135 (98%)	130 (98%)	2 (2%)	0	100	100
72	DM	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
72	b	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
73	DN	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
73	c	96/119 (81%)	94 (98%)	2 (2%)	0	100	100
74	DO	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
74	d	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
75	DP	59/67 (88%)	53 (90%)	6 (10%)	0	100	100
75	e	60/67 (90%)	57 (95%)	3 (5%)	0	100	100
76	DQ	52/56 (93%)	50 (96%)	2 (4%)	0	100	100
76	f	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
77	DR	56/63 (89%)	50 (89%)	5 (9%)	1 (2%)	8	37
77	g	58/63 (92%)	54 (93%)	4 (7%)	0	100	100
78	DS	68/193 (35%)	57 (84%)	10 (15%)	1 (2%)	10	42
78	h	68/193 (35%)	56 (82%)	10 (15%)	2 (3%)	4	24
79	AR	309/317 (98%)	292 (94%)	16 (5%)	1 (0%)	41	76
79	DT	309/317 (98%)	287 (93%)	21 (7%)	1 (0%)	41	76
80	P0	105/312 (34%)	87 (83%)	16 (15%)	2 (2%)	8	36
80	p0	105/312 (34%)	74 (70%)	28 (27%)	3 (3%)	4	24
81	12	61/165 (37%)	36 (59%)	25 (41%)	0	100	100
82	L1	215/217 (99%)	173 (80%)	40 (19%)	2 (1%)	17	55
82	l1	215/217 (99%)	132 (61%)	74 (34%)	9 (4%)	3	16
All	All	22818/25493 (90%)	21825 (96%)	929 (4%)	64 (0%)	41	76

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	AC	21	ILE
40	AM	49	LEU
45	i	55	LYS
45	i	64	LEU
59	O	130	SER

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	191/194 (98%)	189 (99%)	2 (1%)	76	91
4	j	191/194 (98%)	191 (100%)	0	100	100
5	AX	325/328 (99%)	323 (99%)	2 (1%)	86	95
5	k	326/328 (99%)	324 (99%)	2 (1%)	86	95
6	AY	290/292 (99%)	287 (99%)	3 (1%)	76	91
6	l	290/292 (99%)	288 (99%)	2 (1%)	84	94
7	AZ	247/252 (98%)	245 (99%)	2 (1%)	81	93
7	m	250/252 (99%)	250 (100%)	0	100	100
8	BA	132/154 (86%)	132 (100%)	0	100	100
8	n	136/154 (88%)	136 (100%)	0	100	100
9	BB	198/204 (97%)	198 (100%)	0	100	100
9	o	198/204 (97%)	196 (99%)	2 (1%)	76	91
10	BC	193/216 (89%)	193 (100%)	0	100	100
10	p	198/216 (92%)	197 (100%)	1 (0%)	88	96
11	BD	169/170 (99%)	168 (99%)	1 (1%)	86	95
11	q	169/170 (99%)	168 (99%)	1 (1%)	86	95
12	BE	178/186 (96%)	176 (99%)	2 (1%)	73	90
12	r	178/186 (96%)	177 (99%)	1 (1%)	86	95
13	BF	146/149 (98%)	143 (98%)	3 (2%)	53	82
13	s	146/149 (98%)	144 (99%)	2 (1%)	67	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	BG	166/168 (99%)	164 (99%)	2 (1%)	71	90
14	t	166/168 (99%)	165 (99%)	1 (1%)	86	95
15	BH	108/109 (99%)	107 (99%)	1 (1%)	78	92
15	u	108/109 (99%)	107 (99%)	1 (1%)	78	92
16	BI	177/178 (99%)	177 (100%)	0	100	100
16	v	177/178 (99%)	176 (99%)	1 (1%)	86	95
17	BJ	166/167 (99%)	166 (100%)	0	100	100
17	w	166/167 (99%)	165 (99%)	1 (1%)	86	95
18	BK	145/154 (94%)	142 (98%)	3 (2%)	53	82
18	x	144/154 (94%)	143 (99%)	1 (1%)	84	94
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%)	44	77
20	z	146/153 (95%)	146 (100%)	0	100	100
21	0	155/157 (99%)	154 (99%)	1 (1%)	86	95
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%)	81	93
23	5	93/112 (83%)	92 (99%)	1 (1%)	73	90
23	BP	95/112 (85%)	91 (96%)	4 (4%)	30	66
24	6	101/104 (97%)	101 (100%)	0	100	100
24	BQ	101/104 (97%)	99 (98%)	2 (2%)	55	83
25	7	97/127 (76%)	96 (99%)	1 (1%)	76	91
25	BR	86/127 (68%)	84 (98%)	2 (2%)	50	80
26	8	108/121 (89%)	108 (100%)	0	100	100
26	BS	107/121 (88%)	107 (100%)	0	100	100
27	9	111/112 (99%)	110 (99%)	1 (1%)	78	92
27	BT	111/112 (99%)	110 (99%)	1 (1%)	78	92
28	AA	117/118 (99%)	117 (100%)	0	100	100
28	BU	117/118 (99%)	115 (98%)	2 (2%)	60	85
29	AB	120/121 (99%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	BV	120/121 (99%)	120 (100%)	0	100	100
30	AC	48/49 (98%)	48 (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%)	76	91
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%)	109 (99%)	1 (1%)	78	92
34	AG	91/92 (99%)	90 (99%)	1 (1%)	73	90
34	CA	91/92 (99%)	91 (100%)	0	100	100
35	AH	95/102 (93%)	95 (100%)	0	100	100
35	CB	95/102 (93%)	95 (100%)	0	100	100
36	AI	107/106 (101%)	105 (98%)	2 (2%)	57	84
36	CC	106/106 (100%)	104 (98%)	2 (2%)	57	84
37	AJ	77/79 (98%)	76 (99%)	1 (1%)	69	89
37	CD	77/79 (98%)	77 (100%)	0	100	100
38	AK	70/71 (99%)	70 (100%)	0	100	100
38	CE	70/71 (99%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	68 (100%)	0	100	100
39	CF	68/69 (99%)	67 (98%)	1 (2%)	65	87
40	AM	46/47 (98%)	46 (100%)	0	100	100
40	CG	47/47 (100%)	47 (100%)	0	100	100
41	AN	47/47 (100%)	47 (100%)	0	100	100
41	CH	46/47 (98%)	45 (98%)	1 (2%)	52	81
42	AO	24/24 (100%)	22 (92%)	2 (8%)	11	39
42	CI	23/24 (96%)	23 (100%)	0	100	100
43	AP	88/91 (97%)	87 (99%)	1 (1%)	73	90
43	CJ	88/91 (97%)	86 (98%)	2 (2%)	50	80
44	AQ	72/73 (99%)	72 (100%)	0	100	100
44	CK	72/73 (99%)	72 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
45	CL	99/212 (47%)	98 (99%)	1 (1%)	76	91
45	i	99/212 (47%)	98 (99%)	1 (1%)	76	91
47	C	176/215 (82%)	175 (99%)	1 (1%)	86	95
47	CN	176/215 (82%)	174 (99%)	2 (1%)	73	90
48	CO	194/229 (85%)	194 (100%)	0	100	100
48	D	194/229 (85%)	193 (100%)	1 (0%)	88	96
49	CP	175/198 (88%)	173 (99%)	2 (1%)	73	90
49	E	175/198 (88%)	175 (100%)	0	100	100
50	CQ	174/196 (89%)	169 (97%)	5 (3%)	42	76
50	F	174/196 (89%)	172 (99%)	2 (1%)	73	90
51	CR	218/220 (99%)	217 (100%)	1 (0%)	88	96
51	G	218/220 (99%)	218 (100%)	0	100	100
52	CS	178/197 (90%)	177 (99%)	1 (1%)	86	95
52	H	178/197 (90%)	176 (99%)	2 (1%)	73	90
53	CT	204/204 (100%)	202 (99%)	2 (1%)	76	91
53	I	195/204 (96%)	193 (99%)	2 (1%)	76	91
54	CU	164/167 (98%)	163 (99%)	1 (1%)	86	95
54	J	166/167 (99%)	165 (99%)	1 (1%)	86	95
55	CV	157/160 (98%)	157 (100%)	0	100	100
55	K	157/160 (98%)	156 (99%)	1 (1%)	86	95
56	CW	153/160 (96%)	153 (100%)	0	100	100
56	L	153/160 (96%)	153 (100%)	0	100	100
57	CX	88/104 (85%)	88 (100%)	0	100	100
57	M	90/104 (86%)	90 (100%)	0	100	100
58	CY	122/134 (91%)	121 (99%)	1 (1%)	81	93
58	N	124/134 (92%)	122 (98%)	2 (2%)	62	86
59	CZ	101/123 (82%)	99 (98%)	2 (2%)	55	83
59	O	98/123 (80%)	93 (95%)	5 (5%)	24	60
60	DA	129/130 (99%)	128 (99%)	1 (1%)	81	93
60	P	129/130 (99%)	129 (100%)	0	100	100
61	DB	97/102 (95%)	97 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	Q	97/102 (95%)	96 (99%)	1 (1%)	76	91
62	DC	112/121 (93%)	110 (98%)	2 (2%)	59	85
62	R	111/121 (92%)	109 (98%)	2 (2%)	59	85
63	DD	114/116 (98%)	112 (98%)	2 (2%)	59	85
63	S	114/116 (98%)	113 (99%)	1 (1%)	78	92
64	DE	112/122 (92%)	112 (100%)	0	100	100
64	T	112/122 (92%)	111 (99%)	1 (1%)	78	92
65	DF	125/129 (97%)	122 (98%)	3 (2%)	49	79
65	U	128/129 (99%)	123 (96%)	5 (4%)	32	69
66	DG	113/117 (97%)	113 (100%)	0	100	100
66	V	113/117 (97%)	113 (100%)	0	100	100
67	DH	87/105 (83%)	85 (98%)	2 (2%)	50	80
67	W	92/105 (88%)	89 (97%)	3 (3%)	38	73
68	DI	71/71 (100%)	71 (100%)	0	100	100
68	X	71/71 (100%)	71 (100%)	0	100	100
69	DJ	112/113 (99%)	112 (100%)	0	100	100
69	Y	112/113 (99%)	112 (100%)	0	100	100
70	DK	116/118 (98%)	115 (99%)	1 (1%)	78	92
70	Z	116/118 (98%)	115 (99%)	1 (1%)	78	92
71	DL	109/112 (97%)	109 (100%)	0	100	100
71	a	111/112 (99%)	110 (99%)	1 (1%)	78	92
72	DM	63/85 (74%)	62 (98%)	1 (2%)	62	86
72	b	64/85 (75%)	64 (100%)	0	100	100
73	DN	84/102 (82%)	84 (100%)	0	100	100
73	c	84/102 (82%)	82 (98%)	2 (2%)	49	79
74	DO	72/73 (99%)	72 (100%)	0	100	100
74	d	72/73 (99%)	72 (100%)	0	100	100
75	DP	53/58 (91%)	53 (100%)	0	100	100
75	e	54/58 (93%)	54 (100%)	0	100	100
76	DQ	47/48 (98%)	45 (96%)	2 (4%)	29	66
76	f	47/48 (98%)	45 (96%)	2 (4%)	29	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
77	DR	50/54 (93%)	50 (100%)	0	100	100
77	g	51/54 (94%)	51 (100%)	0	100	100
78	DS	62/175 (35%)	52 (84%)	10 (16%)	2	12
78	h	62/175 (35%)	61 (98%)	1 (2%)	62	86
79	AR	259/263 (98%)	258 (100%)	1 (0%)	91	97
79	DT	259/263 (98%)	256 (99%)	3 (1%)	71	90
80	P0	92/247 (37%)	88 (96%)	4 (4%)	29	66
80	p0	92/247 (37%)	88 (96%)	4 (4%)	29	66
81	12	53/137 (39%)	51 (96%)	2 (4%)	33	69
82	L1	196/196 (100%)	186 (95%)	10 (5%)	24	60
82	11	196/196 (100%)	187 (95%)	9 (5%)	27	64
All	All	19588/21467 (91%)	19403 (99%)	185 (1%)	78	92

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

Mol	Chain	Res	Type
49	CP	233	SER
78	DS	124	LYS
50	CQ	198	PHE
62	DC	36	LEU
78	DS	140	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
26	BS	111	ASN
47	CN	33	ASN
79	DT	53	ASN
45	CL	33	ASN
48	CO	232	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3213/3359 (95%)	613 (19%)	43 (1%)
1	AS	3226/3359 (96%)	634 (19%)	53 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	3	120/121 (99%)	9 (7%)	0
2	AT	120/121 (99%)	9 (7%)	0
3	4	156/158 (98%)	23 (14%)	3 (1%)
3	AU	157/158 (99%)	22 (14%)	3 (1%)
46	B	1758/1787 (98%)	446 (25%)	45 (2%)
46	CM	1762/1787 (98%)	451 (25%)	52 (2%)
All	All	10512/10850 (96%)	2207 (20%)	199 (1%)

5 of 2207 RNA backbone outliers are listed below:

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

5 of 199 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AS	2183	U
1	AS	3317	U
1	AS	2442	U
1	AS	2519	A
46	CM	137	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1452 ligands modelled in this entry, 1448 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
85	TIX	1	3958	-	31,31,31	3.30	14 (45%)	36,54,54	3.04	18 (50%)
85	TIX	AS	3782	-	31,31,31	3.69	16 (51%)	36,54,54	3.01	17 (47%)
84	3K5	1	3403	-	62,63,63	2.86	26 (41%)	82,95,95	1.62	15 (18%)
84	3K5	AS	3401	-	62,63,63	0.35	0	82,95,95	0.82	4 (4%)

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
85	TIX	1	3958	-	-	-	0/6/5/5
85	TIX	AS	3782	-	-	-	0/6/5/5
84	3K5	1	3403	-	-	10/29/121/121	0/7/7/7
84	3K5	AS	3401	-	-	5/29/121/121	0/7/7/7

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	AS	3782	TIX	C15-C08	10.25	1.66	1.54
84	1	3403	3K5	C17-C22	-8.90	1.36	1.53
85	AS	3782	TIX	C08-C12	8.12	1.65	1.53
85	1	3958	TIX	C15-C08	7.89	1.63	1.54
85	1	3958	TIX	C08-C12	7.38	1.63	1.53

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	AS	3782	TIX	C15-C08-C12	7.91	125.77	112.79
85	1	3958	TIX	C15-C08-C12	6.86	124.05	112.79
85	AS	3782	TIX	C27-C22-C25	5.91	118.95	110.75
85	1	3958	TIX	O05-C18-C10	-5.57	104.67	112.34
85	1	3958	TIX	O02-C23-O06	-5.40	112.09	117.88

There are no chirality outliers.

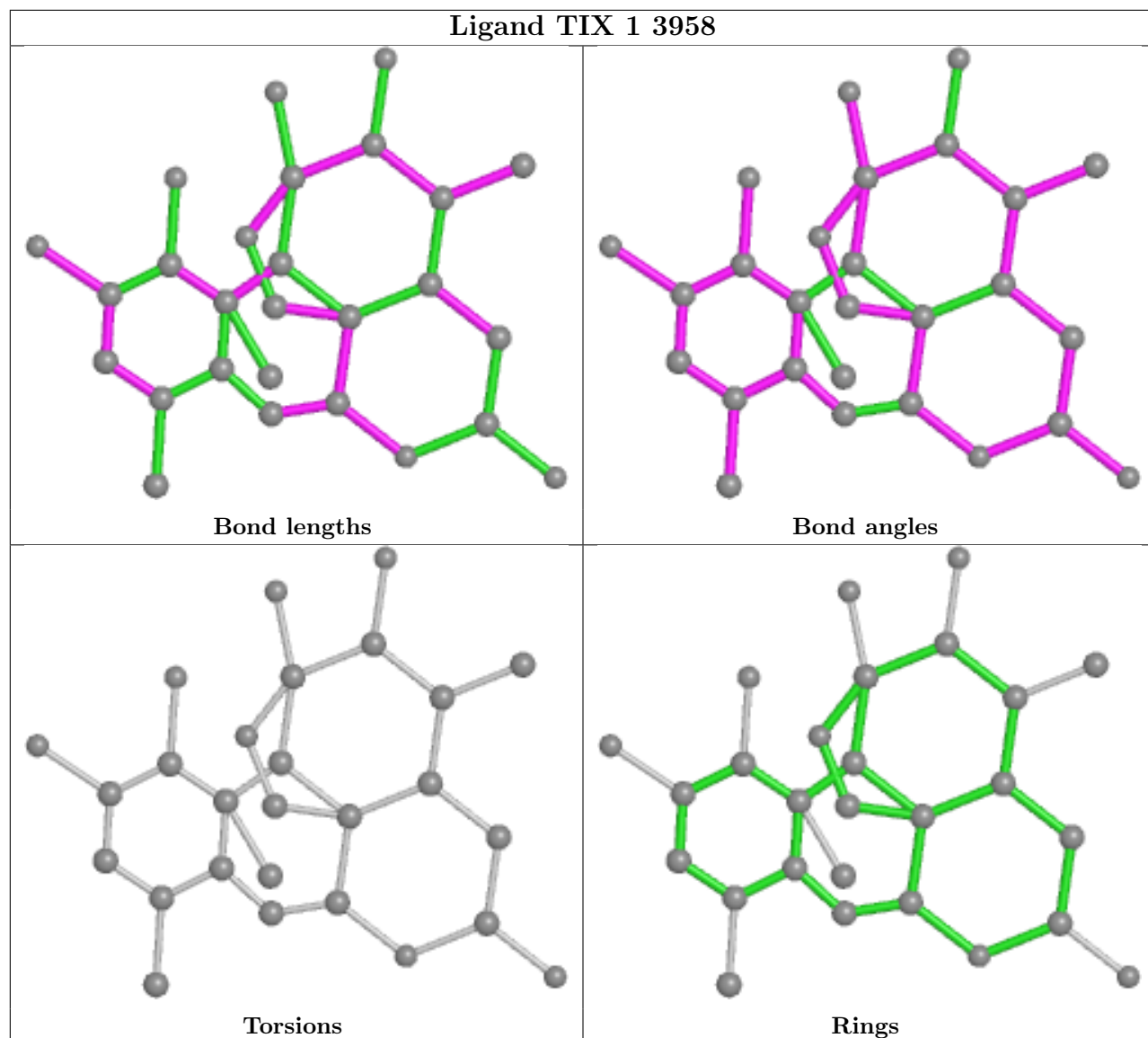
5 of 15 torsion outliers are listed below:

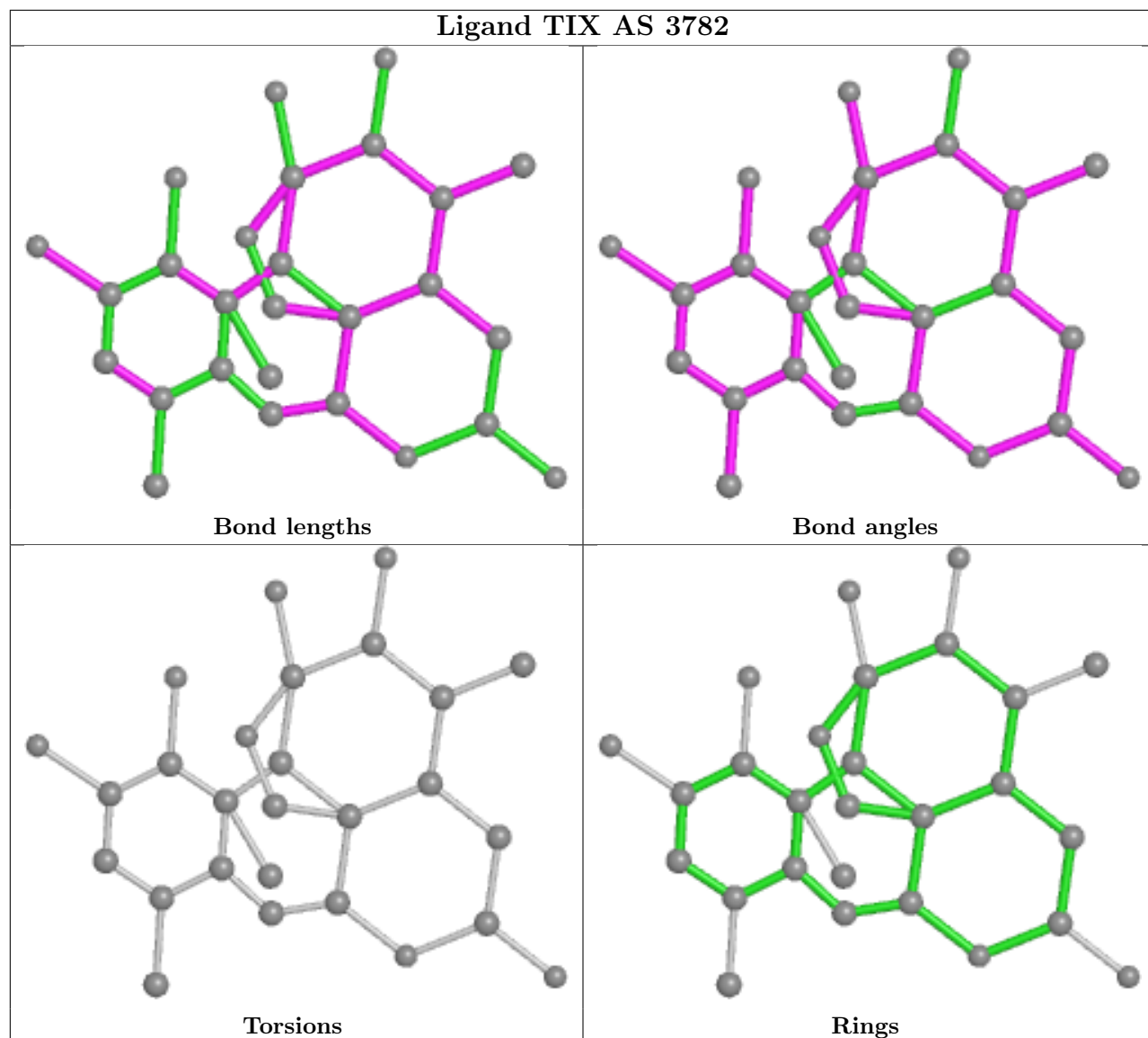
Mol	Chain	Res	Type	Atoms
84	1	3403	3K5	C4-C5-O1-C6
84	1	3403	3K5	C7-C6-O1-C5
84	1	3403	3K5	O15-C38-O14-C34
84	1	3403	3K5	C39-C38-O14-C34
84	1	3403	3K5	O7-C24-O6-C23

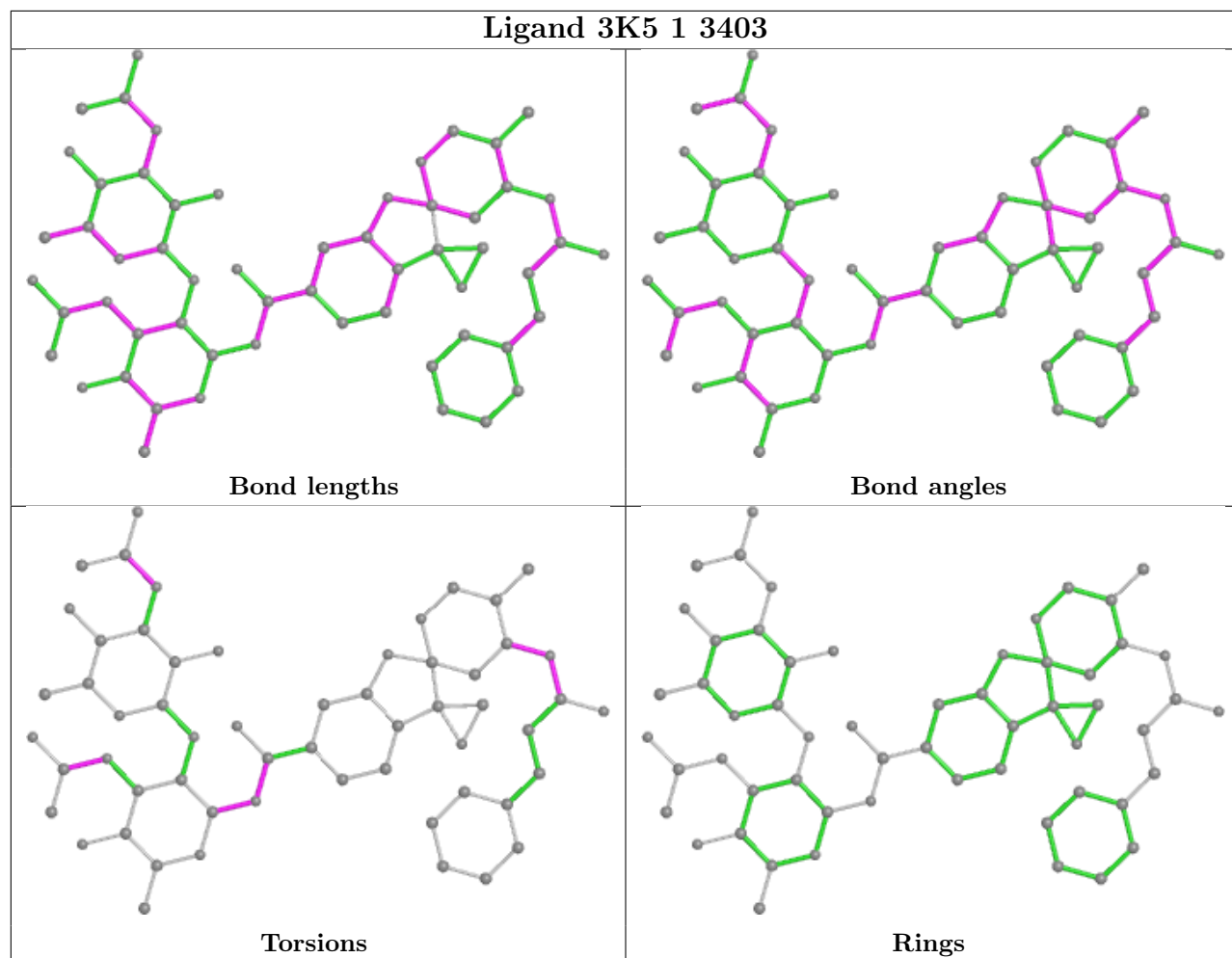
There are no ring outliers.

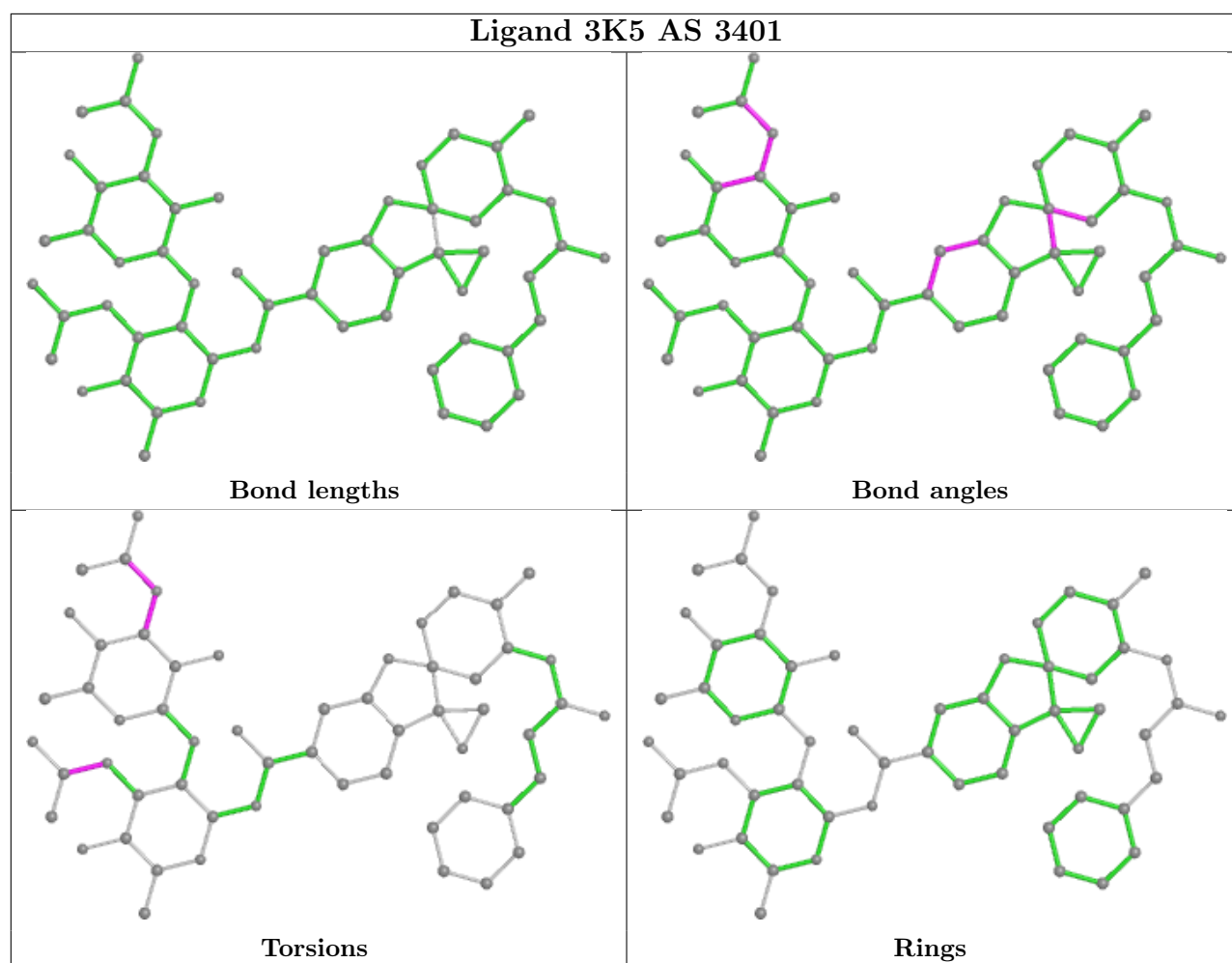
No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q < 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	3217/3359 (95%)	0.00	24 (0%) 87 69	32, 63, 177, 378	0
1	AS	3229/3359 (96%)	0.05	53 (1%) 72 44	35, 70, 206, 323	0
2	3	121/121 (100%)	-0.24	0 100 100	41, 76, 96, 129	0
2	AT	121/121 (100%)	-0.16	0 100 100	37, 71, 94, 142	0
3	4	157/158 (99%)	-0.11	0 100 100	48, 66, 113, 171	0
3	AU	158/158 (100%)	-0.11	1 (0%) 89 72	55, 92, 141, 221	0
4	AW	249/254 (98%)	1.10	51 (20%) 1 0	41, 75, 99, 109	0
4	j	249/254 (98%)	1.25	53 (21%) 0 0	27, 53, 77, 136	0
5	AX	386/389 (99%)	0.24	5 (1%) 77 51	34, 58, 89, 152	0
5	k	386/389 (99%)	0.44	28 (7%) 15 4	34, 58, 78, 128	0
6	AY	361/363 (99%)	0.96	67 (18%) 1 0	47, 75, 106, 143	0
6	l	361/363 (99%)	1.06	65 (18%) 1 0	37, 70, 104, 140	0
7	AZ	292/298 (97%)	0.63	24 (8%) 11 3	47, 93, 127, 143	0
7	m	296/298 (99%)	0.81	40 (13%) 3 1	48, 87, 119, 145	0
8	BA	153/176 (86%)	0.60	7 (4%) 32 12	47, 70, 103, 132	0
8	n	157/176 (89%)	0.65	13 (8%) 11 3	57, 77, 110, 146	0
9	BB	234/241 (97%)	0.33	8 (3%) 45 19	35, 58, 106, 166	0
9	o	234/241 (97%)	0.53	9 (3%) 40 16	35, 64, 126, 166	0
10	BC	233/262 (88%)	1.62	76 (32%) 0 0	86, 123, 162, 183	0
10	p	238/262 (90%)	1.13	49 (20%) 1 0	55, 79, 131, 167	0
11	BD	190/191 (99%)	0.65	10 (5%) 26 10	56, 75, 105, 150	0
11	q	190/191 (99%)	0.59	10 (5%) 26 10	54, 75, 97, 138	0
12	BE	208/220 (94%)	0.14	3 (1%) 75 49	34, 53, 100, 140	0
12	r	208/220 (94%)	0.83	23 (11%) 5 1	37, 61, 102, 115	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	BF	171/174 (98%)	0.48	5 (2%) 51 23	58, 83, 115, 131	0
13	s	171/174 (98%)	0.78	18 (10%) 6 2	58, 90, 113, 125	0
14	BG	200/202 (99%)	0.91	29 (14%) 2 1	49, 96, 130, 153	0
14	t	200/202 (99%)	0.65	27 (13%) 3 1	43, 76, 114, 142	0
15	BH	130/131 (99%)	0.36	5 (3%) 40 16	47, 68, 95, 124	0
15	u	130/131 (99%)	0.08	2 (1%) 73 46	53, 72, 89, 110	0
16	BI	203/204 (99%)	2.76	125 (61%) 0 0	57, 87, 109, 116	0
16	v	203/204 (99%)	1.15	37 (18%) 1 0	35, 57, 73, 83	0
17	BJ	199/200 (99%)	0.54	5 (2%) 57 29	35, 51, 89, 125	0
17	w	199/200 (99%)	0.61	8 (4%) 38 15	36, 55, 85, 113	0
18	BK	176/185 (95%)	1.07	28 (15%) 1 1	45, 65, 95, 130	0
18	x	173/185 (93%)	1.12	32 (18%) 1 0	41, 62, 96, 125	0
19	BL	185/186 (99%)	0.74	25 (13%) 3 1	47, 71, 88, 99	0
19	y	185/186 (99%)	1.09	36 (19%) 1 0	46, 66, 85, 99	0
20	BM	179/190 (94%)	0.64	6 (3%) 45 19	54, 82, 142, 169	0
20	z	179/190 (94%)	0.63	8 (4%) 33 12	52, 71, 127, 143	0
21	0	170/172 (98%)	0.26	5 (2%) 51 23	44, 63, 87, 138	0
21	BN	170/172 (98%)	0.49	6 (3%) 44 18	40, 59, 83, 113	0
22	2	159/160 (99%)	0.99	30 (18%) 1 0	43, 60, 116, 152	0
22	BO	159/160 (99%)	0.90	23 (14%) 2 1	44, 61, 116, 145	0
23	5	103/124 (83%)	0.80	14 (13%) 3 1	84, 111, 142, 162	0
23	BP	102/124 (82%)	0.94	15 (14%) 2 1	92, 129, 152, 176	0
24	6	131/137 (95%)	0.87	15 (11%) 4 1	38, 56, 78, 90	0
24	BQ	131/137 (95%)	0.97	18 (13%) 3 1	34, 54, 77, 98	0
25	7	118/155 (76%)	0.56	9 (7%) 13 4	38, 77, 126, 140	0
25	BR	98/155 (63%)	0.77	10 (10%) 6 2	42, 65, 130, 139	0
26	8	121/142 (85%)	0.98	23 (19%) 1 0	60, 73, 91, 127	0
26	BS	119/142 (83%)	1.46	40 (33%) 0 0	65, 98, 115, 129	0
27	9	126/127 (99%)	1.37	33 (26%) 0 0	58, 78, 99, 117	0
27	BT	126/127 (99%)	1.21	31 (24%) 0 0	65, 93, 131, 147	0
28	AA	135/136 (99%)	0.82	17 (12%) 3 1	64, 88, 109, 143	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BU	135/136 (99%)	1.11	28 (20%) 1 0	93, 120, 141, 167	0
29	AB	148/149 (99%)	1.49	48 (32%) 0 0	37, 62, 87, 126	0
29	BV	148/149 (99%)	0.94	25 (16%) 1 0	47, 74, 100, 114	0
30	AC	62/63 (98%)	1.13	13 (20%) 1 0	42, 75, 123, 147	0
30	BW	61/63 (96%)	1.23	15 (24%) 0 0	46, 81, 120, 140	0
31	AD	96/106 (90%)	0.30	3 (3%) 49 21	57, 76, 100, 111	0
31	BX	96/106 (90%)	1.09	17 (17%) 1 0	86, 109, 132, 149	0
32	AE	110/112 (98%)	1.06	17 (15%) 2 1	48, 67, 110, 148	0
32	BY	110/112 (98%)	0.97	15 (13%) 3 1	47, 75, 121, 151	0
33	AF	124/131 (94%)	1.17	23 (18%) 1 0	35, 66, 83, 106	0
33	BZ	124/131 (94%)	0.98	13 (10%) 6 2	34, 63, 90, 112	0
34	AG	106/107 (99%)	0.63	6 (5%) 23 8	47, 60, 76, 93	0
34	CA	106/107 (99%)	0.64	4 (3%) 40 16	40, 54, 74, 87	0
35	AH	112/122 (91%)	1.17	26 (23%) 0 0	52, 70, 118, 140	0
35	CB	112/122 (91%)	1.76	44 (39%) 0 0	62, 98, 137, 159	0
36	AI	120/120 (100%)	1.11	22 (18%) 1 0	58, 82, 110, 126	0
36	CC	118/120 (98%)	1.35	36 (30%) 0 0	81, 105, 127, 161	0
37	AJ	97/99 (97%)	0.82	12 (12%) 4 1	54, 72, 100, 168	0
37	CD	97/99 (97%)	1.03	22 (22%) 0 0	83, 99, 128, 152	0
38	AK	86/87 (98%)	1.23	19 (22%) 0 0	41, 55, 95, 111	0
38	CE	86/87 (98%)	1.63	28 (32%) 0 0	47, 74, 115, 128	0
39	AL	77/78 (98%)	1.24	17 (22%) 0 0	77, 98, 133, 165	0
39	CF	77/78 (98%)	2.33	33 (42%) 0 0	90, 118, 156, 165	0
40	AM	50/51 (98%)	1.02	4 (8%) 12 4	47, 64, 83, 92	0
40	CG	50/51 (98%)	1.79	20 (40%) 0 0	58, 80, 98, 103	0
41	AN	52/52 (100%)	1.05	5 (9%) 8 2	75, 101, 116, 132	0
41	CH	51/52 (98%)	0.95	7 (13%) 3 1	73, 105, 122, 126	0
42	AO	25/25 (100%)	3.14	19 (76%) 0 0	55, 67, 76, 85	0
42	CI	24/25 (96%)	2.39	15 (62%) 0 0	48, 60, 68, 73	0
43	AP	103/106 (97%)	0.74	10 (9%) 7 2	31, 61, 98, 121	0
43	CJ	103/106 (97%)	0.65	9 (8%) 10 3	40, 73, 115, 122	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AQ	91/92 (98%)	1.12	17 (18%) 1 0	40, 58, 101, 116	0
44	CK	91/92 (98%)	1.10	17 (18%) 1 0	48, 78, 110, 121	0
45	CL	121/267 (45%)	0.69	9 (7%) 14 4	59, 92, 127, 139	0
45	i	121/267 (45%)	0.79	17 (14%) 2 1	63, 106, 136, 143	0
46	B	1761/1787 (98%)	0.07	45 (2%) 56 27	46, 87, 178, 458	0
46	CM	1765/1787 (98%)	0.07	45 (2%) 57 29	40, 79, 182, 465	0
47	C	208/261 (79%)	0.67	21 (10%) 7 2	80, 114, 140, 154	0
47	CN	208/261 (79%)	0.46	10 (4%) 30 11	62, 101, 130, 165	0
48	CO	214/256 (83%)	0.95	37 (17%) 1 0	76, 118, 139, 166	0
48	D	214/256 (83%)	0.68	18 (8%) 11 3	67, 92, 115, 127	0
49	CP	217/249 (87%)	0.43	14 (6%) 18 5	46, 71, 98, 118	0
49	E	217/249 (87%)	1.55	82 (37%) 0 0	71, 95, 121, 144	0
50	CQ	223/251 (88%)	0.70	21 (9%) 8 3	53, 77, 136, 169	0
50	F	223/251 (88%)	1.71	84 (37%) 0 0	73, 106, 152, 173	0
51	CR	260/262 (99%)	1.38	74 (28%) 0 0	62, 87, 111, 146	0
51	G	259/262 (98%)	1.38	72 (27%) 0 0	68, 96, 119, 143	0
52	CS	206/225 (91%)	1.32	44 (21%) 0 0	68, 101, 146, 194	0
52	H	206/225 (91%)	1.49	59 (28%) 0 0	76, 102, 142, 162	0
53	CT	236/236 (100%)	0.84	31 (13%) 3 1	52, 98, 139, 158	0
53	I	226/236 (95%)	0.68	24 (10%) 6 2	60, 98, 147, 179	0
54	CU	183/186 (98%)	0.83	28 (15%) 2 1	68, 127, 165, 179	0
54	J	185/186 (99%)	1.49	55 (29%) 0 0	80, 129, 156, 164	0
55	CV	203/206 (98%)	0.88	27 (13%) 3 1	41, 71, 122, 150	0
55	K	203/206 (98%)	0.78	23 (11%) 5 1	37, 80, 124, 156	0
56	CW	178/189 (94%)	1.20	47 (26%) 0 0	65, 94, 119, 140	0
56	L	178/189 (94%)	2.20	90 (50%) 0 0	74, 108, 126, 147	0
57	CX	94/118 (79%)	0.80	8 (8%) 10 3	54, 86, 128, 142	0
57	M	98/118 (83%)	1.24	23 (23%) 0 0	83, 117, 143, 161	0
58	CY	141/155 (90%)	1.02	23 (16%) 1 0	45, 67, 93, 145	0
58	N	144/155 (92%)	1.33	39 (27%) 0 0	45, 78, 114, 156	0
59	CZ	119/143 (83%)	1.12	23 (19%) 1 0	130, 159, 176, 180	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	O	116/143 (81%)	2.01	42 (36%) 0 0	151, 178, 195, 200	0
60	DA	150/151 (99%)	1.20	33 (22%) 0 0	58, 92, 121, 136	0
60	P	150/151 (99%)	1.02	21 (14%) 2 1	55, 92, 112, 120	0
61	DB	127/132 (96%)	0.90	19 (14%) 2 1	55, 99, 125, 132	0
61	Q	127/132 (96%)	0.39	4 (3%) 49 21	51, 79, 98, 111	0
62	DC	130/142 (91%)	1.19	25 (19%) 1 0	58, 91, 128, 145	0
62	R	129/142 (90%)	1.28	32 (24%) 0 0	63, 98, 136, 151	0
63	DD	140/142 (98%)	1.61	53 (37%) 0 0	61, 98, 133, 145	0
63	S	140/142 (98%)	3.09	75 (53%) 0 0	70, 110, 145, 155	0
64	DE	124/137 (90%)	1.10	24 (19%) 1 0	62, 112, 160, 169	0
64	T	124/137 (90%)	1.83	45 (36%) 0 0	87, 122, 167, 171	0
65	DF	141/145 (97%)	0.72	10 (7%) 16 5	59, 93, 124, 154	0
65	U	144/145 (99%)	0.62	11 (7%) 13 4	60, 86, 114, 150	0
66	DG	141/145 (97%)	0.72	14 (9%) 7 2	58, 93, 117, 153	0
66	V	141/145 (97%)	0.86	24 (17%) 1 0	79, 101, 135, 147	0
67	DH	97/119 (81%)	0.67	9 (9%) 8 3	46, 96, 125, 144	0
67	W	102/119 (85%)	1.30	25 (24%) 0 0	72, 122, 147, 157	0
68	DI	87/87 (100%)	0.12	0 100 100	61, 86, 120, 144	0
68	X	87/87 (100%)	0.52	8 (9%) 9 3	83, 102, 123, 127	0
69	DJ	129/130 (99%)	0.82	18 (13%) 2 1	49, 67, 87, 93	0
69	Y	129/130 (99%)	1.23	26 (20%) 1 0	67, 84, 103, 121	0
70	DK	143/145 (98%)	0.87	14 (9%) 7 2	43, 64, 88, 113	0
70	Z	143/145 (98%)	0.78	16 (11%) 5 1	52, 73, 92, 106	0
71	DL	132/135 (97%)	0.73	19 (14%) 2 1	77, 112, 132, 174	0
71	a	134/135 (99%)	1.20	34 (25%) 0 0	74, 113, 126, 156	0
72	DM	71/105 (67%)	0.75	8 (11%) 5 1	93, 124, 143, 149	0
72	b	72/105 (68%)	0.30	6 (8%) 11 3	87, 109, 132, 143	0
73	DN	98/119 (82%)	1.06	23 (23%) 0 0	56, 77, 136, 143	0
73	c	98/119 (82%)	1.21	23 (23%) 0 0	60, 83, 128, 139	0
74	DO	81/82 (98%)	0.86	15 (18%) 1 0	71, 105, 166, 173	0
74	d	81/82 (98%)	0.67	6 (7%) 14 4	80, 101, 155, 169	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	DP	61/67 (91%)	0.65	3 (4%) 29 11	78, 108, 132, 152	0
75	e	62/67 (92%)	1.53	19 (30%) 0 0	90, 110, 134, 143	0
76	DQ	54/56 (96%)	1.02	8 (14%) 2 1	49, 67, 89, 109	0
76	f	55/56 (98%)	0.99	10 (18%) 1 0	71, 89, 114, 136	0
77	DR	58/63 (92%)	1.41	14 (24%) 0 0	69, 99, 156, 178	0
77	g	60/63 (95%)	1.40	19 (31%) 0 0	76, 105, 151, 167	0
78	DS	70/193 (36%)	1.50	24 (34%) 0 0	92, 164, 183, 195	0
78	h	70/193 (36%)	2.02	28 (40%) 0 0	117, 163, 189, 191	0
79	AR	311/317 (98%)	2.50	152 (48%) 0 0	118, 156, 178, 192	0
79	DT	311/317 (98%)	1.43	86 (27%) 0 0	107, 150, 175, 192	0
80	P0	107/312 (34%)	1.82	41 (38%) 0 0	113, 127, 146, 154	0
80	p0	107/312 (34%)	2.99	50 (46%) 0 0	116, 139, 156, 164	0
81	12	63/165 (38%)	0.98	12 (19%) 1 0	111, 130, 149, 158	0
82	L1	217/217 (100%)	1.61	79 (36%) 0 0	99, 128, 165, 231	0
82	l1	217/217 (100%)	1.66	65 (29%) 0 0	110, 137, 163, 196	0
All	All	33669/36343 (92%)	0.71	4298 (12%) 3 1	27, 81, 155, 465	0

The worst 5 of 4298 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
80	p0	28	VAL	30.9
82	l1	1	MET	23.2
52	CS	152	SER	18.6
46	CM	1680	A	16.3
63	S	65	ARG	15.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	AS	3757	1/1	-0.22	0.71	80,80,80,80	0
83	MG	AS	3451	1/1	0.11	0.33	67,67,67,67	0
83	MG	B	1929	1/1	0.15	0.27	112,112,112,112	0
83	MG	B	1844	1/1	0.18	0.29	72,72,72,72	0
86	ZN	DO	101	1/1	0.26	0.21	225,225,225,225	0
83	MG	AS	3724	1/1	0.36	0.28	69,69,69,69	0
83	MG	1	3883	1/1	0.40	0.18	76,76,76,76	0
83	MG	B	1837	1/1	0.40	0.14	321,321,321,321	0
83	MG	1	3629	1/1	0.42	0.41	156,156,156,156	0
83	MG	B	1889	1/1	0.43	0.22	73,73,73,73	0
83	MG	1	3518	1/1	0.43	0.68	79,79,79,79	0
86	ZN	h	201	1/1	0.45	0.14	216,216,216,216	0
83	MG	1	3691	1/1	0.46	0.58	80,80,80,80	0
83	MG	B	1814	1/1	0.47	0.20	57,57,57,57	0
83	MG	AS	3649	1/1	0.48	0.97	66,66,66,66	0
83	MG	AS	3776	1/1	0.48	0.31	72,72,72,72	0
83	MG	AS	3764	1/1	0.49	0.23	76,76,76,76	0
83	MG	1	3604	1/1	0.50	0.48	70,70,70,70	0
83	MG	1	3890	1/1	0.51	0.53	76,76,76,76	0
83	MG	CM	1945	1/1	0.51	0.16	61,61,61,61	0
83	MG	0	203	1/1	0.52	0.51	63,63,63,63	0
83	MG	B	1923	1/1	0.52	0.20	62,62,62,62	0
83	MG	1	3862	1/1	0.53	0.15	72,72,72,72	0
83	MG	B	1817	1/1	0.54	0.20	82,82,82,82	0
83	MG	AS	3598	1/1	0.54	0.16	129,129,129,129	0
83	MG	9	202	1/1	0.54	2.34	72,72,72,72	0
83	MG	1	3588	1/1	0.54	0.82	73,73,73,73	0
83	MG	B	1936	1/1	0.54	0.98	98,98,98,98	0
83	MG	CM	1926	1/1	0.55	0.31	58,58,58,58	0
83	MG	1	3657	1/1	0.56	0.22	62,62,62,62	0
83	MG	1	3934	1/1	0.57	0.18	89,89,89,89	0
83	MG	AS	3670	1/1	0.57	0.44	73,73,73,73	0
86	ZN	d	101	1/1	0.57	0.35	273,273,273,273	0
83	MG	BS	201	1/1	0.57	1.14	76,76,76,76	0
83	MG	CM	1836	1/1	0.57	0.23	76,76,76,76	0
83	MG	k	404	1/1	0.58	0.20	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	B	1914	1/1	0.58	0.42	87,87,87,87	0
83	MG	AS	3758	1/1	0.58	0.33	61,61,61,61	0
83	MG	AF	202	1/1	0.58	0.68	71,71,71,71	0
83	MG	CM	1948	1/1	0.59	0.29	76,76,76,76	0
83	MG	AS	3463	1/1	0.60	0.84	65,65,65,65	0
83	MG	1	3566	1/1	0.60	0.14	61,61,61,61	0
83	MG	DJ	202	1/1	0.60	0.18	74,74,74,74	0
83	MG	B	1960	1/1	0.61	0.17	75,75,75,75	0
83	MG	AS	3775	1/1	0.61	0.46	66,66,66,66	0
83	MG	1	3836	1/1	0.61	0.20	56,56,56,56	0
83	MG	B	1959	1/1	0.61	0.20	73,73,73,73	0
83	MG	AS	3634	1/1	0.62	0.41	79,79,79,79	0
83	MG	1	3670	1/1	0.62	0.28	52,52,52,52	0
83	MG	R	201	1/1	0.63	0.21	78,78,78,78	0
83	MG	AS	3630	1/1	0.63	0.51	87,87,87,87	0
83	MG	1	3722	1/1	0.63	0.41	51,51,51,51	0
83	MG	u	201	1/1	0.63	0.22	56,56,56,56	0
83	MG	1	3940	1/1	0.64	0.30	77,77,77,77	0
83	MG	1	3419	1/1	0.64	1.10	69,69,69,69	0
83	MG	1	3910	1/1	0.65	0.20	24,24,24,24	0
83	MG	AU	209	1/1	0.65	0.83	72,72,72,72	0
83	MG	AS	3636	1/1	0.65	0.22	71,71,71,71	0
83	MG	AS	3643	1/1	0.65	0.24	56,56,56,56	0
83	MG	1	3919	1/1	0.65	0.14	69,69,69,69	0
83	MG	1	3840	1/1	0.65	0.18	60,60,60,60	0
83	MG	AS	3459	1/1	0.65	0.22	47,47,47,47	0
83	MG	1	3466	1/1	0.65	0.18	37,37,37,37	0
83	MG	AS	3507	1/1	0.65	0.15	63,63,63,63	0
83	MG	B	1956	1/1	0.65	0.15	74,74,74,74	0
83	MG	4	207	1/1	0.65	0.72	52,52,52,52	0
83	MG	AS	3744	1/1	0.66	0.42	68,68,68,68	0
83	MG	1	3547	1/1	0.66	0.20	49,49,49,49	0
83	MG	1	3798	1/1	0.66	0.22	96,96,96,96	0
83	MG	1	3541	1/1	0.66	0.23	60,60,60,60	0
83	MG	4	201	1/1	0.67	0.11	72,72,72,72	0
83	MG	1	3929	1/1	0.67	0.24	77,77,77,77	0
83	MG	1	3654	1/1	0.68	0.86	70,70,70,70	0
83	MG	B	1919	1/1	0.68	0.33	83,83,83,83	0
83	MG	1	3650	1/1	0.68	0.37	82,82,82,82	0
83	MG	DB	204	1/1	0.68	0.20	57,57,57,57	0
83	MG	1	3936	1/1	0.69	0.16	61,61,61,61	0
83	MG	1	3519	1/1	0.69	0.21	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AS	3654	1/1	0.69	1.27	66,66,66,66	0
83	MG	B	1893	1/1	0.69	0.19	58,58,58,58	0
83	MG	1	3897	1/1	0.69	0.34	66,66,66,66	0
83	MG	BB	303	1/1	0.69	0.22	48,48,48,48	0
83	MG	B	1942	1/1	0.69	0.21	75,75,75,75	0
83	MG	B	1943	1/1	0.69	0.14	94,94,94,94	0
83	MG	AS	3768	1/1	0.70	0.46	74,74,74,74	0
83	MG	AS	3753	1/1	0.70	1.53	75,75,75,75	0
83	MG	1	3700	1/1	0.70	0.23	44,44,44,44	0
83	MG	1	3716	1/1	0.70	1.72	70,70,70,70	0
83	MG	j	302	1/1	0.70	0.55	59,59,59,59	0
83	MG	Z	202	1/1	0.71	0.24	67,67,67,67	0
83	MG	B	1941	1/1	0.71	0.18	75,75,75,75	0
83	MG	1	3508	1/1	0.71	0.11	42,42,42,42	0
83	MG	BI	301	1/1	0.71	0.77	61,61,61,61	0
83	MG	AS	3701	1/1	0.71	1.48	97,97,97,97	0
83	MG	B	1972	1/1	0.71	0.19	84,84,84,84	0
83	MG	B	1958	1/1	0.71	0.89	76,76,76,76	0
83	MG	CM	1879	1/1	0.72	0.17	61,61,61,61	0
83	MG	CM	1882	1/1	0.72	0.11	49,49,49,49	0
83	MG	B	1841	1/1	0.72	0.24	46,46,46,46	0
83	MG	AS	3709	1/1	0.72	0.42	60,60,60,60	0
83	MG	1	3925	1/1	0.72	0.12	75,75,75,75	0
83	MG	AH	202	1/1	0.72	0.14	58,58,58,58	0
83	MG	1	3779	1/1	0.72	0.12	51,51,51,51	0
83	MG	1	3432	1/1	0.72	0.27	65,65,65,65	0
83	MG	AS	3529	1/1	0.72	0.16	60,60,60,60	0
83	MG	1	3841	1/1	0.72	0.22	72,72,72,72	0
83	MG	1	3814	1/1	0.73	0.37	56,56,56,56	0
83	MG	AS	3747	1/1	0.73	0.10	69,69,69,69	0
83	MG	AS	3528	1/1	0.73	0.25	64,64,64,64	0
83	MG	CO	301	1/1	0.73	0.21	46,46,46,46	0
83	MG	1	3665	1/1	0.73	0.25	54,54,54,54	0
83	MG	AC	101	1/1	0.73	1.18	57,57,57,57	0
83	MG	1	3788	1/1	0.73	0.22	56,56,56,56	0
83	MG	1	3706	1/1	0.73	0.19	47,47,47,47	0
83	MG	1	3802	1/1	0.73	0.51	49,49,49,49	0
83	MG	AS	3777	1/1	0.74	0.28	38,38,38,38	0
83	MG	1	3784	1/1	0.74	0.11	63,63,63,63	0
83	MG	1	3918	1/1	0.74	0.45	59,59,59,59	0
83	MG	1	3952	1/1	0.74	0.16	59,59,59,59	0
83	MG	k	406	1/1	0.74	1.81	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3953	1/1	0.74	0.19	62,62,62,62	0
83	MG	1	3806	1/1	0.74	0.20	54,54,54,54	0
83	MG	I	301	1/1	0.74	0.48	113,113,113,113	0
83	MG	CM	1917	1/1	0.74	0.45	59,59,59,59	0
83	MG	1	3835	1/1	0.75	0.14	66,66,66,66	0
83	MG	1	3866	1/1	0.75	2.24	86,86,86,86	0
83	MG	CM	1934	1/1	0.75	0.16	40,40,40,40	0
83	MG	AS	3714	1/1	0.75	0.14	35,35,35,35	0
83	MG	AS	3539	1/1	0.75	0.15	50,50,50,50	0
83	MG	CM	1822	1/1	0.75	0.39	64,64,64,64	0
83	MG	AS	3556	1/1	0.75	0.16	56,56,56,56	0
83	MG	CM	1870	1/1	0.75	0.17	54,54,54,54	0
83	MG	1	3684	1/1	0.75	0.21	69,69,69,69	0
83	MG	x	202	1/1	0.75	0.19	32,32,32,32	0
83	MG	CM	1897	1/1	0.75	0.47	69,69,69,69	0
83	MG	w	302	1/1	0.76	0.38	40,40,40,40	0
83	MG	B	1920	1/1	0.76	0.13	62,62,62,62	0
83	MG	1	3914	1/1	0.76	0.18	75,75,75,75	0
83	MG	1	3451	1/1	0.76	0.20	41,41,41,41	0
83	MG	CM	1821	1/1	0.76	0.19	57,57,57,57	0
83	MG	1	3904	1/1	0.76	0.29	61,61,61,61	0
83	MG	AS	3478	1/1	0.76	0.15	73,73,73,73	0
83	MG	B	1899	1/1	0.76	0.20	73,73,73,73	0
83	MG	AS	3727	1/1	0.76	0.16	69,69,69,69	0
83	MG	1	3514	1/1	0.76	0.22	79,79,79,79	0
83	MG	AT	204	1/1	0.76	0.29	74,74,74,74	0
83	MG	AW	301	1/1	0.77	0.12	38,38,38,38	0
83	MG	CM	1907	1/1	0.77	0.22	59,59,59,59	0
83	MG	AX	401	1/1	0.77	0.21	59,59,59,59	0
83	MG	1	3810	1/1	0.77	0.23	54,54,54,54	0
83	MG	1	3548	1/1	0.77	0.49	48,48,48,48	0
83	MG	CM	1937	1/1	0.77	0.12	50,50,50,50	0
83	MG	B	1951	1/1	0.77	0.16	79,79,79,79	0
83	MG	1	3933	1/1	0.77	0.22	62,62,62,62	0
83	MG	1	3582	1/1	0.77	0.96	52,52,52,52	0
83	MG	1	3679	1/1	0.77	0.66	66,66,66,66	0
83	MG	B	1852	1/1	0.77	0.29	65,65,65,65	0
83	MG	w	303	1/1	0.77	0.19	73,73,73,73	0
83	MG	i	301	1/1	0.77	0.27	69,69,69,69	0
83	MG	CM	1896	1/1	0.77	0.30	42,42,42,42	0
83	MG	1	3756	1/1	0.78	0.23	57,57,57,57	0
83	MG	1	3905	1/1	0.78	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	B	1802	1/1	0.78	0.24	71,71,71,71	0
83	MG	B	1805	1/1	0.78	0.30	91,91,91,91	0
83	MG	1	3589	1/1	0.78	0.36	49,49,49,49	0
83	MG	AS	3780	1/1	0.78	0.13	59,59,59,59	0
83	MG	1	3427	1/1	0.78	0.21	26,26,26,26	0
83	MG	B	1822	1/1	0.78	0.11	45,45,45,45	0
83	MG	1	3872	1/1	0.78	0.17	58,58,58,58	0
83	MG	AS	3719	1/1	0.78	0.30	74,74,74,74	0
83	MG	1	3433	1/1	0.78	0.13	80,80,80,80	0
83	MG	1	3957	1/1	0.78	0.79	59,59,59,59	0
83	MG	1	3920	1/1	0.78	1.01	69,69,69,69	0
83	MG	1	3683	1/1	0.78	0.13	67,67,67,67	0
83	MG	1	3663	1/1	0.78	0.28	61,61,61,61	0
83	MG	B	1898	1/1	0.78	0.14	49,49,49,49	0
83	MG	AH	201	1/1	0.78	0.31	60,60,60,60	0
83	MG	AU	208	1/1	0.79	0.22	74,74,74,74	0
83	MG	CM	1900	1/1	0.79	0.13	54,54,54,54	0
83	MG	1	3879	1/1	0.79	0.20	62,62,62,62	0
83	MG	CM	1915	1/1	0.79	0.20	62,62,62,62	0
83	MG	AS	3673	1/1	0.79	0.28	65,65,65,65	0
83	MG	1	3405	1/1	0.79	0.19	59,59,59,59	0
83	MG	B	1835	1/1	0.79	0.24	62,62,62,62	0
83	MG	AS	3765	1/1	0.79	0.20	65,65,65,65	0
83	MG	1	3681	1/1	0.79	0.67	30,30,30,30	0
83	MG	3	208	1/1	0.79	0.49	64,64,64,64	0
83	MG	1	3896	1/1	0.79	0.35	64,64,64,64	0
83	MG	CQ	302	1/1	0.79	0.29	67,67,67,67	0
83	MG	4	202	1/1	0.79	0.20	43,43,43,43	0
83	MG	1	3549	1/1	0.79	0.44	59,59,59,59	0
83	MG	1	3753	1/1	0.79	0.30	52,52,52,52	0
83	MG	AT	210	1/1	0.79	0.17	50,50,50,50	0
83	MG	AU	203	1/1	0.79	0.10	54,54,54,54	0
83	MG	1	3642	1/1	0.80	0.46	41,41,41,41	0
83	MG	AS	3732	1/1	0.80	0.25	56,56,56,56	0
83	MG	B	1864	1/1	0.80	0.19	68,68,68,68	0
83	MG	AS	3542	1/1	0.80	0.11	66,66,66,66	0
83	MG	CM	1852	1/1	0.80	0.22	85,85,85,85	0
83	MG	1	3446	1/1	0.80	0.13	82,82,82,82	0
83	MG	CM	1873	1/1	0.80	0.30	80,80,80,80	0
83	MG	AS	3561	1/1	0.80	0.18	45,45,45,45	0
83	MG	AS	3575	1/1	0.80	0.30	58,58,58,58	0
83	MG	1	3490	1/1	0.80	0.16	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	AS	3599	1/1	0.80	0.26	79,79,79,79	0
83	MG	1	3600	1/1	0.80	0.69	81,81,81,81	0
83	MG	AS	3769	1/1	0.80	0.25	70,70,70,70	0
83	MG	1	3527	1/1	0.80	0.67	48,48,48,48	0
83	MG	D	301	1/1	0.80	0.19	60,60,60,60	0
83	MG	B	1804	1/1	0.80	0.26	70,70,70,70	0
83	MG	1	3947	1/1	0.80	0.78	55,55,55,55	0
83	MG	1	3917	1/1	0.80	0.25	64,64,64,64	0
83	MG	1	3884	1/1	0.80	0.22	53,53,53,53	0
83	MG	1	3586	1/1	0.80	0.16	35,35,35,35	0
83	MG	1	3891	1/1	0.80	0.61	65,65,65,65	0
83	MG	AS	3467	1/1	0.80	0.12	73,73,73,73	0
83	MG	DA	201	1/1	0.80	0.20	62,62,62,62	0
83	MG	AS	3711	1/1	0.80	0.14	50,50,50,50	0
83	MG	AW	303	1/1	0.80	0.24	46,46,46,46	0
83	MG	3	209	1/1	0.80	0.13	60,60,60,60	0
83	MG	AB	202	1/1	0.80	0.74	54,54,54,54	0
83	MG	1	3859	1/1	0.80	0.26	67,67,67,67	0
83	MG	1	3534	1/1	0.81	0.20	37,37,37,37	0
83	MG	AU	204	1/1	0.81	0.39	70,70,70,70	0
83	MG	1	3781	1/1	0.81	0.79	78,78,78,78	0
83	MG	1	3922	1/1	0.81	0.79	75,75,75,75	0
83	MG	AS	3756	1/1	0.81	0.56	59,59,59,59	0
83	MG	CM	1909	1/1	0.81	0.14	74,74,74,74	0
83	MG	CM	1914	1/1	0.81	0.16	55,55,55,55	0
83	MG	1	3782	1/1	0.81	0.38	58,58,58,58	0
83	MG	AW	304	1/1	0.81	1.57	67,67,67,67	0
83	MG	1	3640	1/1	0.81	0.41	49,49,49,49	0
83	MG	1	3607	1/1	0.81	0.21	42,42,42,42	0
83	MG	AS	3535	1/1	0.81	0.20	58,58,58,58	0
83	MG	CM	1942	1/1	0.81	0.84	62,62,62,62	0
83	MG	1	3901	1/1	0.81	0.41	49,49,49,49	0
83	MG	1	3643	1/1	0.81	0.20	46,46,46,46	0
83	MG	1	3863	1/1	0.81	0.20	67,67,67,67	0
83	MG	CM	1825	1/1	0.81	0.11	39,39,39,39	0
83	MG	1	3909	1/1	0.81	0.18	45,45,45,45	0
83	MG	1	3742	1/1	0.81	0.18	36,36,36,36	0
83	MG	CM	1864	1/1	0.81	0.16	68,68,68,68	0
83	MG	1	3748	1/1	0.81	0.19	51,51,51,51	0
83	MG	1	3685	1/1	0.81	0.55	76,76,76,76	0
83	MG	1	3619	1/1	0.81	0.50	50,50,50,50	0
83	MG	1	3668	1/1	0.82	0.15	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	3	215	1/1	0.82	0.11	65,65,65,65	0
83	MG	1	3686	1/1	0.82	0.13	88,88,88,88	0
83	MG	AS	3638	1/1	0.82	1.16	56,56,56,56	0
83	MG	1	3603	1/1	0.82	0.56	52,52,52,52	0
83	MG	AS	3530	1/1	0.82	0.20	29,29,29,29	0
83	MG	AS	3534	1/1	0.82	0.11	64,64,64,64	0
83	MG	AY	401	1/1	0.82	0.15	62,62,62,62	0
83	MG	AS	3669	1/1	0.82	0.83	64,64,64,64	0
83	MG	Q	201	1/1	0.82	0.15	60,60,60,60	0
83	MG	AS	3672	1/1	0.82	0.32	42,42,42,42	0
83	MG	1	3926	1/1	0.82	0.31	63,63,63,63	0
83	MG	AS	3700	1/1	0.82	0.16	46,46,46,46	0
83	MG	1	3719	1/1	0.82	0.20	90,90,90,90	0
83	MG	1	3826	1/1	0.82	0.31	57,57,57,57	0
83	MG	3	206	1/1	0.82	0.61	57,57,57,57	0
83	MG	CM	1863	1/1	0.82	0.12	64,64,64,64	0
83	MG	AS	3779	1/1	0.82	0.40	59,59,59,59	0
83	MG	o	302	1/1	0.82	0.13	37,37,37,37	0
83	MG	AS	3715	1/1	0.82	0.22	66,66,66,66	0
83	MG	1	3697	1/1	0.82	0.76	38,38,38,38	0
83	MG	AS	3468	1/1	0.82	0.24	58,58,58,58	0
83	MG	o	301	1/1	0.83	0.19	33,33,33,33	0
83	MG	1	3730	1/1	0.83	0.15	34,34,34,34	0
83	MG	B	1946	1/1	0.83	0.19	59,59,59,59	0
83	MG	1	3733	1/1	0.83	0.10	61,61,61,61	0
83	MG	AS	3639	1/1	0.83	0.09	40,40,40,40	0
83	MG	1	3935	1/1	0.83	0.20	76,76,76,76	0
83	MG	B	1894	1/1	0.83	0.20	61,61,61,61	0
83	MG	1	3873	1/1	0.83	0.14	46,46,46,46	0
83	MG	1	3596	1/1	0.83	0.23	56,56,56,56	0
83	MG	CM	1916	1/1	0.83	0.28	57,57,57,57	0
83	MG	1	3857	1/1	0.83	0.30	64,64,64,64	0
83	MG	1	3950	1/1	0.83	0.27	39,39,39,39	0
83	MG	CL	302	1/1	0.83	0.27	77,77,77,77	0
83	MG	CM	1802	1/1	0.83	0.17	34,34,34,34	0
83	MG	G	302	1/1	0.83	0.74	62,62,62,62	0
83	MG	1	3535	1/1	0.83	0.19	34,34,34,34	0
83	MG	J	201	1/1	0.83	0.10	121,121,121,121	0
83	MG	1	3674	1/1	0.83	0.55	49,49,49,49	0
83	MG	1	3418	1/1	0.83	0.31	46,46,46,46	0
83	MG	CM	1853	1/1	0.83	0.18	57,57,57,57	0
83	MG	AS	3564	1/1	0.83	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AG	201	1/1	0.83	0.16	67,67,67,67	0
83	MG	CM	1865	1/1	0.83	0.18	38,38,38,38	0
83	MG	AS	3419	1/1	0.83	0.14	38,38,38,38	0
83	MG	AG	202	1/1	0.83	0.39	43,43,43,43	0
83	MG	k	402	1/1	0.84	0.26	57,57,57,57	0
83	MG	1	3470	1/1	0.84	0.16	34,34,34,34	0
83	MG	V	201	1/1	0.84	0.17	46,46,46,46	0
83	MG	1	3931	1/1	0.84	0.13	62,62,62,62	0
83	MG	g	101	1/1	0.84	0.16	78,78,78,78	0
83	MG	AR	401	1/1	0.84	0.24	60,60,60,60	0
83	MG	AS	3685	1/1	0.84	0.27	41,41,41,41	0
83	MG	CM	1801	1/1	0.84	0.16	51,51,51,51	0
83	MG	B	1913	1/1	0.84	0.16	58,58,58,58	0
83	MG	1	3652	1/1	0.84	0.23	44,44,44,44	0
83	MG	AS	3704	1/1	0.84	0.17	56,56,56,56	0
83	MG	AS	3707	1/1	0.84	0.21	70,70,70,70	0
83	MG	AS	3455	1/1	0.84	0.12	65,65,65,65	0
83	MG	AS	3583	1/1	0.84	0.15	45,45,45,45	0
83	MG	1	3725	1/1	0.84	0.13	33,33,33,33	0
83	MG	1	3800	1/1	0.84	0.18	44,44,44,44	0
83	MG	B	1965	1/1	0.84	1.22	61,61,61,61	0
83	MG	1	3766	1/1	0.84	0.14	34,34,34,34	0
83	MG	1	3510	1/1	0.84	0.15	24,24,24,24	0
83	MG	CM	1872	1/1	0.84	0.20	65,65,65,65	0
83	MG	1	3597	1/1	0.84	0.18	61,61,61,61	0
83	MG	1	3717	1/1	0.84	0.17	51,51,51,51	0
83	MG	1	3928	1/1	0.84	0.20	74,74,74,74	0
83	MG	AS	3624	1/1	0.85	0.15	42,42,42,42	0
83	MG	1	3877	1/1	0.85	0.60	49,49,49,49	0
83	MG	AS	3487	1/1	0.85	1.05	70,70,70,70	0
83	MG	CM	1874	1/1	0.85	0.14	49,49,49,49	0
83	MG	1	3536	1/1	0.85	0.16	17,17,17,17	0
83	MG	AW	302	1/1	0.85	0.12	35,35,35,35	0
83	MG	AS	3521	1/1	0.85	0.14	45,45,45,45	0
83	MG	1	3844	1/1	0.85	0.13	70,70,70,70	0
83	MG	B	1944	1/1	0.85	0.15	67,67,67,67	0
83	MG	AS	3646	1/1	0.85	0.30	65,65,65,65	0
83	MG	B	1945	1/1	0.85	0.20	71,71,71,71	0
83	MG	Z	201	1/1	0.85	1.23	72,72,72,72	0
83	MG	BN	201	1/1	0.85	0.11	56,56,56,56	0
83	MG	AS	3667	1/1	0.85	0.18	54,54,54,54	0
83	MG	CK	101	1/1	0.85	0.19	67,67,67,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	CM	1918	1/1	0.85	0.13	51,51,51,51	0
83	MG	B	1809	1/1	0.85	0.14	46,46,46,46	0
83	MG	1	3554	1/1	0.85	0.22	51,51,51,51	0
83	MG	1	3701	1/1	0.85	0.15	51,51,51,51	0
83	MG	CM	1814	1/1	0.85	0.29	39,39,39,39	0
83	MG	1	3560	1/1	0.85	0.60	79,79,79,79	0
83	MG	B	1833	1/1	0.85	0.20	45,45,45,45	0
83	MG	1	3609	1/1	0.85	0.99	72,72,72,72	0
83	MG	AS	3571	1/1	0.85	0.09	60,60,60,60	0
83	MG	CY	201	1/1	0.85	0.69	71,71,71,71	0
83	MG	CM	1838	1/1	0.85	0.19	44,44,44,44	0
83	MG	r	302	1/1	0.85	0.67	56,56,56,56	0
83	MG	1	3690	1/1	0.85	0.34	57,57,57,57	0
83	MG	1	3565	1/1	0.85	0.26	51,51,51,51	0
83	MG	1	3721	1/1	0.85	0.21	26,26,26,26	0
83	MG	AS	3602	1/1	0.85	0.22	44,44,44,44	0
83	MG	B	1862	1/1	0.86	0.14	67,67,67,67	0
83	MG	CM	1818	1/1	0.86	0.10	43,43,43,43	0
83	MG	0	204	1/1	0.86	0.12	59,59,59,59	0
83	MG	B	1876	1/1	0.86	0.26	50,50,50,50	0
83	MG	1	3816	1/1	0.86	0.13	51,51,51,51	0
83	MG	AS	3574	1/1	0.86	0.10	47,47,47,47	0
83	MG	AS	3749	1/1	0.86	0.10	44,44,44,44	0
83	MG	1	3773	1/1	0.86	0.34	38,38,38,38	0
83	MG	1	3724	1/1	0.86	0.13	35,35,35,35	0
83	MG	1	3608	1/1	0.86	0.46	57,57,57,57	0
83	MG	1	3838	1/1	0.86	0.14	54,54,54,54	0
83	MG	AS	3600	1/1	0.86	0.18	50,50,50,50	0
83	MG	B	1912	1/1	0.86	0.15	55,55,55,55	0
83	MG	AS	3622	1/1	0.86	0.13	62,62,62,62	0
83	MG	1	3728	1/1	0.86	0.16	46,46,46,46	0
83	MG	1	3495	1/1	0.86	0.28	54,54,54,54	0
83	MG	B	1917	1/1	0.86	0.14	54,54,54,54	0
83	MG	1	3843	1/1	0.86	0.17	27,27,27,27	0
83	MG	AS	3402	1/1	0.86	0.11	42,42,42,42	0
83	MG	4	209	1/1	0.86	0.24	29,29,29,29	0
83	MG	1	3930	1/1	0.86	0.20	51,51,51,51	0
83	MG	B	1924	1/1	0.86	0.47	74,74,74,74	0
83	MG	1	3618	1/1	0.86	0.25	37,37,37,37	0
83	MG	B	1931	1/1	0.86	0.13	44,44,44,44	0
83	MG	1	3898	1/1	0.86	0.84	66,66,66,66	0
83	MG	1	3852	1/1	0.86	0.20	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AU	210	1/1	0.86	0.35	33,33,33,33	0
83	MG	1	3467	1/1	0.86	0.22	37,37,37,37	0
83	MG	AS	3480	1/1	0.86	0.15	45,45,45,45	0
83	MG	1	3746	1/1	0.86	0.13	42,42,42,42	0
83	MG	1	3718	1/1	0.86	0.56	39,39,39,39	0
83	MG	CM	1941	1/1	0.86	0.11	59,59,59,59	0
83	MG	AS	3693	1/1	0.86	0.77	43,43,43,43	0
83	MG	1	3942	1/1	0.86	0.56	54,54,54,54	0
83	MG	v	302	1/1	0.86	0.14	69,69,69,69	0
83	MG	BF	201	1/1	0.86	0.09	58,58,58,58	0
83	MG	1	3625	1/1	0.86	0.39	57,57,57,57	0
83	MG	1	3913	1/1	0.86	0.18	28,28,28,28	0
83	MG	1	3544	1/1	0.86	0.25	57,57,57,57	0
83	MG	CA	203	1/1	0.86	0.41	68,68,68,68	0
83	MG	1	3468	1/1	0.86	0.16	55,55,55,55	0
83	MG	B	1860	1/1	0.86	0.15	36,36,36,36	0
83	MG	B	1961	1/1	0.86	0.20	74,74,74,74	0
83	MG	AS	3548	1/1	0.86	0.21	40,40,40,40	0
83	MG	B	1874	1/1	0.87	0.24	53,53,53,53	0
83	MG	AS	3691	1/1	0.87	0.41	70,70,70,70	0
83	MG	AT	202	1/1	0.87	0.25	34,34,34,34	0
83	MG	AS	3446	1/1	0.87	0.11	45,45,45,45	0
83	MG	AS	3447	1/1	0.87	0.18	41,41,41,41	0
83	MG	AU	202	1/1	0.87	0.18	46,46,46,46	0
83	MG	4	203	1/1	0.87	0.25	56,56,56,56	0
83	MG	AS	3580	1/1	0.87	0.12	33,33,33,33	0
83	MG	1	3581	1/1	0.87	0.34	37,37,37,37	0
83	MG	B	1807	1/1	0.87	0.15	43,43,43,43	0
83	MG	CM	1887	1/1	0.87	0.11	38,38,38,38	0
83	MG	0	201	1/1	0.87	0.28	49,49,49,49	0
83	MG	1	3673	1/1	0.87	0.30	37,37,37,37	0
83	MG	B	1815	1/1	0.87	0.11	86,86,86,86	0
83	MG	1	3885	1/1	0.87	0.47	42,42,42,42	0
83	MG	1	3464	1/1	0.87	0.80	58,58,58,58	0
83	MG	1	3871	1/1	0.87	0.45	66,66,66,66	0
83	MG	1	3622	1/1	0.87	0.70	52,52,52,52	0
83	MG	AS	3733	1/1	0.87	0.11	79,79,79,79	0
83	MG	1	3602	1/1	0.87	0.17	51,51,51,51	0
83	MG	AS	3746	1/1	0.87	0.19	62,62,62,62	0
83	MG	1	3876	1/1	0.87	0.17	61,61,61,61	0
83	MG	o	304	1/1	0.87	0.20	56,56,56,56	0
83	MG	BZ	204	1/1	0.87	0.42	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	B	1845	1/1	0.87	0.21	42,42,42,42	0
83	MG	AS	3531	1/1	0.87	0.13	29,29,29,29	0
83	MG	1	3667	1/1	0.87	0.09	37,37,37,37	0
83	MG	B	1856	1/1	0.87	0.16	84,84,84,84	0
83	MG	AS	3761	1/1	0.87	0.19	53,53,53,53	0
83	MG	AS	3656	1/1	0.87	0.14	44,44,44,44	0
83	MG	AS	3660	1/1	0.87	0.16	70,70,70,70	0
83	MG	B	1857	1/1	0.87	0.43	57,57,57,57	0
83	MG	1	3477	1/1	0.87	0.13	25,25,25,25	0
83	MG	DG	202	1/1	0.87	0.13	45,45,45,45	0
83	MG	AS	3772	1/1	0.87	0.23	45,45,45,45	0
86	ZN	AP	203	1/1	0.87	0.14	147,147,147,147	0
83	MG	B	1861	1/1	0.87	0.32	86,86,86,86	0
83	MG	1	3939	1/1	0.87	0.38	52,52,52,52	0
83	MG	1	3924	1/1	0.87	0.15	36,36,36,36	0
83	MG	1	3849	1/1	0.88	0.07	59,59,59,59	0
83	MG	AS	3540	1/1	0.88	0.17	41,41,41,41	0
83	MG	1	3479	1/1	0.88	0.15	42,42,42,42	0
83	MG	1	3546	1/1	0.88	0.07	56,56,56,56	0
83	MG	1	3749	1/1	0.88	0.24	59,59,59,59	0
83	MG	B	1887	1/1	0.88	0.15	91,91,91,91	0
83	MG	CM	1866	1/1	0.88	0.14	74,74,74,74	0
83	MG	AS	3436	1/1	0.88	0.08	50,50,50,50	0
83	MG	1	3860	1/1	0.88	0.12	51,51,51,51	0
83	MG	AS	3694	1/1	0.88	0.10	39,39,39,39	0
83	MG	1	3808	1/1	0.88	0.20	70,70,70,70	0
83	MG	B	1953	1/1	0.88	0.10	57,57,57,57	0
83	MG	AU	206	1/1	0.88	0.15	45,45,45,45	0
83	MG	AU	207	1/1	0.88	0.40	73,73,73,73	0
83	MG	1	3561	1/1	0.88	0.31	62,62,62,62	0
83	MG	1	3687	1/1	0.88	0.14	68,68,68,68	0
83	MG	AS	3591	1/1	0.88	0.12	41,41,41,41	0
83	MG	1	3562	1/1	0.88	0.09	51,51,51,51	0
83	MG	1	3771	1/1	0.88	0.12	39,39,39,39	0
83	MG	1	3615	1/1	0.88	0.41	62,62,62,62	0
83	MG	1	3692	1/1	0.88	0.18	38,38,38,38	0
83	MG	AS	3612	1/1	0.88	0.13	40,40,40,40	0
83	MG	AS	3621	1/1	0.88	0.14	72,72,72,72	0
83	MG	1	3485	1/1	0.88	0.19	36,36,36,36	0
83	MG	1	3941	1/1	0.88	0.10	46,46,46,46	0
83	MG	AS	3625	1/1	0.88	0.45	52,52,52,52	0
83	MG	AS	3488	1/1	0.88	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	k	405	1/1	0.88	1.08	54,54,54,54	0
83	MG	BZ	202	1/1	0.88	1.08	71,71,71,71	0
83	MG	AS	3514	1/1	0.88	0.11	36,36,36,36	0
83	MG	AS	3752	1/1	0.88	0.17	62,62,62,62	0
83	MG	AS	3515	1/1	0.88	0.12	33,33,33,33	0
83	MG	B	1855	1/1	0.88	0.20	49,49,49,49	0
83	MG	1	3526	1/1	0.88	0.17	43,43,43,43	0
83	MG	AS	3645	1/1	0.88	0.39	47,47,47,47	0
83	MG	DB	202	1/1	0.88	0.14	67,67,67,67	0
83	MG	CM	1806	1/1	0.88	0.14	52,52,52,52	0
83	MG	1	3507	1/1	0.88	0.16	45,45,45,45	0
83	MG	1	3550	1/1	0.88	0.16	33,33,33,33	0
83	MG	1	3715	1/1	0.88	0.53	38,38,38,38	0
83	MG	Y	203	1/1	0.88	0.22	61,61,61,61	0
83	MG	B	1939	1/1	0.88	0.24	77,77,77,77	0
83	MG	AS	3665	1/1	0.88	0.11	29,29,29,29	0
83	MG	j	303	1/1	0.89	0.15	22,22,22,22	0
83	MG	k	401	1/1	0.89	0.27	63,63,63,63	0
83	MG	f	102	1/1	0.89	0.20	59,59,59,59	0
83	MG	CL	303	1/1	0.89	0.14	41,41,41,41	0
83	MG	1	3726	1/1	0.89	0.17	47,47,47,47	0
83	MG	1	3452	1/1	0.89	0.18	23,23,23,23	0
83	MG	1	3861	1/1	0.89	0.43	85,85,85,85	0
83	MG	AS	3728	1/1	0.89	0.13	57,57,57,57	0
83	MG	AS	3588	1/1	0.89	0.14	74,74,74,74	0
83	MG	AS	3415	1/1	0.89	0.25	46,46,46,46	0
83	MG	AS	3593	1/1	0.89	0.10	48,48,48,48	0
83	MG	1	3676	1/1	0.89	0.15	67,67,67,67	0
83	MG	1	3818	1/1	0.89	0.10	40,40,40,40	0
83	MG	AS	3443	1/1	0.89	0.11	49,49,49,49	0
83	MG	AS	3751	1/1	0.89	0.16	74,74,74,74	0
83	MG	1	3865	1/1	0.89	0.30	77,77,77,77	0
83	MG	CM	1859	1/1	0.89	0.18	59,59,59,59	0
83	MG	AS	3608	1/1	0.89	0.13	40,40,40,40	0
83	MG	AS	3609	1/1	0.89	0.28	45,45,45,45	0
83	MG	B	1828	1/1	0.89	0.17	47,47,47,47	0
83	MG	AS	3616	1/1	0.89	0.21	48,48,48,48	0
83	MG	AS	3617	1/1	0.89	0.14	44,44,44,44	0
83	MG	1	3732	1/1	0.89	0.65	58,58,58,58	0
83	MG	1	3943	1/1	0.89	0.39	40,40,40,40	0
83	MG	AS	3458	1/1	0.89	0.30	40,40,40,40	0
83	MG	CM	1875	1/1	0.89	0.10	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3539	1/1	0.89	0.41	73,73,73,73	0
83	MG	CM	1881	1/1	0.89	0.21	72,72,72,72	0
83	MG	1	3737	1/1	0.89	0.13	41,41,41,41	0
83	MG	1	3951	1/1	0.89	0.14	48,48,48,48	0
83	MG	1	3783	1/1	0.89	0.27	49,49,49,49	0
83	MG	AS	3471	1/1	0.89	0.21	43,43,43,43	0
83	MG	CM	1899	1/1	0.89	0.15	50,50,50,50	0
83	MG	AS	3477	1/1	0.89	0.12	46,46,46,46	0
83	MG	AS	3642	1/1	0.89	0.19	58,58,58,58	0
83	MG	1	3874	1/1	0.89	0.12	49,49,49,49	0
83	MG	CM	1912	1/1	0.89	0.18	58,58,58,58	0
83	MG	1	3409	1/1	0.89	0.09	61,61,61,61	0
83	MG	1	3694	1/1	0.89	0.24	26,26,26,26	0
83	MG	3	207	1/1	0.89	0.49	66,66,66,66	0
83	MG	B	1955	1/1	0.89	0.12	60,60,60,60	0
83	MG	1	3576	1/1	0.89	0.14	50,50,50,50	0
83	MG	1	3882	1/1	0.89	1.02	61,61,61,61	0
83	MG	CM	1933	1/1	0.89	0.31	53,53,53,53	0
83	MG	1	3669	1/1	0.89	0.34	45,45,45,45	0
83	MG	AE	201	1/1	0.89	0.26	33,33,33,33	0
83	MG	B	1869	1/1	0.89	0.14	71,71,71,71	0
83	MG	AE	203	1/1	0.89	0.21	84,84,84,84	0
83	MG	1	3846	1/1	0.89	0.21	64,64,64,64	0
83	MG	AS	3532	1/1	0.89	0.09	55,55,55,55	0
83	MG	1	3634	1/1	0.89	0.31	68,68,68,68	0
83	MG	CQ	301	1/1	0.89	0.13	42,42,42,42	0
83	MG	1	3434	1/1	0.89	0.19	42,42,42,42	0
83	MG	AS	3538	1/1	0.89	0.25	37,37,37,37	0
83	MG	4	204	1/1	0.89	0.14	32,32,32,32	0
83	MG	1	3762	1/1	0.89	0.14	52,52,52,52	0
83	MG	AP	202	1/1	0.89	1.32	85,85,85,85	0
83	MG	DG	201	1/1	0.89	0.24	48,48,48,48	0
83	MG	1	3895	1/1	0.89	0.23	71,71,71,71	0
83	MG	B	1900	1/1	0.89	0.12	56,56,56,56	0
83	MG	BO	201	1/1	0.89	0.17	57,57,57,57	0
83	MG	AS	3708	1/1	0.89	0.17	44,44,44,44	0
83	MG	1	3858	1/1	0.89	0.14	41,41,41,41	0
83	MG	AS	3710	1/1	0.89	0.16	47,47,47,47	0
83	MG	1	3442	1/1	0.90	0.23	50,50,50,50	0
83	MG	AS	3705	1/1	0.90	0.10	51,51,51,51	0
83	MG	1	3738	1/1	0.90	0.12	46,46,46,46	0
83	MG	1	3740	1/1	0.90	0.21	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	CK	102	1/1	0.90	0.39	48,48,48,48	0
83	MG	CL	301	1/1	0.90	0.18	41,41,41,41	0
83	MG	1	3839	1/1	0.90	0.17	39,39,39,39	0
83	MG	B	1902	1/1	0.90	0.16	74,74,74,74	0
83	MG	1	3587	1/1	0.90	0.08	49,49,49,49	0
83	MG	B	1816	1/1	0.90	0.22	52,52,52,52	0
83	MG	1	3559	1/1	0.90	0.10	51,51,51,51	0
83	MG	AS	3717	1/1	0.90	0.18	52,52,52,52	0
83	MG	AS	3581	1/1	0.90	0.09	36,36,36,36	0
83	MG	CM	1820	1/1	0.90	0.23	33,33,33,33	0
83	MG	AS	3722	1/1	0.90	0.18	69,69,69,69	0
83	MG	1	3955	1/1	0.90	0.08	32,32,32,32	0
83	MG	AS	3585	1/1	0.90	0.27	49,49,49,49	0
83	MG	CM	1835	1/1	0.90	0.23	49,49,49,49	0
83	MG	1	3792	1/1	0.90	0.10	51,51,51,51	0
83	MG	AS	3589	1/1	0.90	0.12	33,33,33,33	0
83	MG	AS	3413	1/1	0.90	0.21	55,55,55,55	0
83	MG	B	1832	1/1	0.90	0.22	46,46,46,46	0
83	MG	AS	3745	1/1	0.90	0.11	63,63,63,63	0
83	MG	3	202	1/1	0.90	0.10	57,57,57,57	0
83	MG	AS	3421	1/1	0.90	0.13	28,28,28,28	0
83	MG	B	1834	1/1	0.90	0.26	35,35,35,35	0
83	MG	AS	3750	1/1	0.90	0.12	43,43,43,43	0
83	MG	1	3796	1/1	0.90	0.11	67,67,67,67	0
83	MG	1	3651	1/1	0.90	0.34	55,55,55,55	0
83	MG	B	1934	1/1	0.90	0.10	86,86,86,86	0
83	MG	1	3848	1/1	0.90	0.14	45,45,45,45	0
83	MG	AS	3614	1/1	0.90	0.10	57,57,57,57	0
83	MG	CM	1878	1/1	0.90	0.17	34,34,34,34	0
83	MG	B	1937	1/1	0.90	0.48	52,52,52,52	0
83	MG	AS	3456	1/1	0.90	0.12	55,55,55,55	0
83	MG	1	3402	1/1	0.90	0.22	20,20,20,20	0
83	MG	3	211	1/1	0.90	0.13	52,52,52,52	0
83	MG	AS	3767	1/1	0.90	0.11	30,30,30,30	0
83	MG	1	3707	1/1	0.90	0.10	31,31,31,31	0
83	MG	1	3524	1/1	0.90	0.19	43,43,43,43	0
83	MG	1	3757	1/1	0.90	0.26	50,50,50,50	0
83	MG	AS	3633	1/1	0.90	0.50	80,80,80,80	0
83	MG	1	3729	1/1	0.90	0.15	50,50,50,50	0
83	MG	1	3417	1/1	0.90	0.14	30,30,30,30	0
83	MG	B	1948	1/1	0.90	0.22	69,69,69,69	0
83	MG	1	3658	1/1	0.90	0.15	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	B	1952	1/1	0.90	0.11	49,49,49,49	0
83	MG	1	3583	1/1	0.90	0.32	38,38,38,38	0
83	MG	AS	3491	1/1	0.90	0.18	42,42,42,42	0
83	MG	CM	1924	1/1	0.90	0.14	43,43,43,43	0
83	MG	1	3902	1/1	0.90	0.12	60,60,60,60	0
83	MG	CM	1927	1/1	0.90	0.33	56,56,56,56	0
83	MG	AS	3647	1/1	0.90	0.09	76,76,76,76	0
83	MG	AS	3511	1/1	0.90	0.09	39,39,39,39	0
83	MG	B	1865	1/1	0.90	0.18	61,61,61,61	0
83	MG	1	3938	1/1	0.90	0.45	25,25,25,25	0
83	MG	B	1871	1/1	0.90	0.22	53,53,53,53	0
83	MG	CM	1944	1/1	0.90	0.41	75,75,75,75	0
83	MG	1	3903	1/1	0.90	0.21	48,48,48,48	0
83	MG	1	3735	1/1	0.90	0.19	25,25,25,25	0
83	MG	B	1962	1/1	0.90	0.18	65,65,65,65	0
83	MG	CP	301	1/1	0.90	0.21	36,36,36,36	0
83	MG	B	1881	1/1	0.90	0.18	40,40,40,40	0
83	MG	B	1967	1/1	0.90	0.12	70,70,70,70	0
83	MG	B	1969	1/1	0.90	0.14	28,28,28,28	0
83	MG	B	1882	1/1	0.90	0.21	63,63,63,63	0
83	MG	AS	3688	1/1	0.90	0.10	29,29,29,29	0
83	MG	AS	3690	1/1	0.90	0.98	68,68,68,68	0
83	MG	B	1801	1/1	0.90	0.25	38,38,38,38	0
83	MG	BH	201	1/1	0.90	0.13	35,35,35,35	0
83	MG	1	3830	1/1	0.90	0.29	48,48,48,48	0
84	3K5	AS	3401	57/57	0.90	0.36	42,64,91,93	0
85	TIX	1	3958	27/27	0.90	0.33	51,60,85,184	0
83	MG	B	1890	1/1	0.90	0.14	38,38,38,38	0
83	MG	1	3831	1/1	0.90	0.35	42,42,42,42	0
83	MG	AS	3544	1/1	0.90	0.10	46,46,46,46	0
83	MG	BV	201	1/1	0.90	0.15	45,45,45,45	0
83	MG	1	3497	1/1	0.91	0.15	39,39,39,39	0
83	MG	AS	3457	1/1	0.91	0.20	31,31,31,31	0
83	MG	B	1949	1/1	0.91	0.11	61,61,61,61	0
83	MG	CM	1803	1/1	0.91	0.14	31,31,31,31	0
83	MG	AS	3730	1/1	0.91	0.28	49,49,49,49	0
83	MG	CM	1808	1/1	0.91	0.33	81,81,81,81	0
83	MG	1	3502	1/1	0.91	0.13	39,39,39,39	0
83	MG	CM	1816	1/1	0.91	0.24	25,25,25,25	0
83	MG	AS	3606	1/1	0.91	0.23	41,41,41,41	0
83	MG	AS	3741	1/1	0.91	0.15	46,46,46,46	0
83	MG	1	3593	1/1	0.91	0.32	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	1	3637	1/1	0.91	0.29	47,47,47,47	0
83	MG	CM	1824	1/1	0.91	0.09	28,28,28,28	0
83	MG	B	1954	1/1	0.91	0.13	34,34,34,34	0
83	MG	B	1808	1/1	0.91	0.13	75,75,75,75	0
83	MG	1	3428	1/1	0.91	0.15	25,25,25,25	0
83	MG	o	303	1/1	0.91	0.15	41,41,41,41	0
83	MG	CM	1841	1/1	0.91	0.21	38,38,38,38	0
83	MG	CM	1848	1/1	0.91	0.14	62,62,62,62	0
83	MG	1	3750	1/1	0.91	0.11	56,56,56,56	0
83	MG	AS	3486	1/1	0.91	0.10	43,43,43,43	0
83	MG	1	3751	1/1	0.91	0.14	37,37,37,37	0
83	MG	AS	3755	1/1	0.91	0.41	63,63,63,63	0
83	MG	1	3915	1/1	0.91	0.18	71,71,71,71	0
83	MG	AS	3489	1/1	0.91	0.19	32,32,32,32	0
83	MG	AS	3632	1/1	0.91	1.00	51,51,51,51	0
83	MG	CM	1868	1/1	0.91	0.31	73,73,73,73	0
83	MG	CM	1869	1/1	0.91	0.18	40,40,40,40	0
83	MG	1	3709	1/1	0.91	0.33	41,41,41,41	0
83	MG	AS	3493	1/1	0.91	0.20	49,49,49,49	0
83	MG	AS	3504	1/1	0.91	0.11	38,38,38,38	0
83	MG	AS	3766	1/1	0.91	0.71	53,53,53,53	0
83	MG	B	1826	1/1	0.91	0.23	49,49,49,49	0
83	MG	B	1827	1/1	0.91	0.17	30,30,30,30	0
83	MG	1	3585	1/1	0.91	0.10	38,38,38,38	0
83	MG	B	1904	1/1	0.91	0.17	90,90,90,90	0
83	MG	AS	3773	1/1	0.91	0.26	53,53,53,53	0
83	MG	B	1909	1/1	0.91	0.18	30,30,30,30	0
83	MG	B	1911	1/1	0.91	0.34	61,61,61,61	0
83	MG	1	3799	1/1	0.91	0.13	65,65,65,65	0
83	MG	1	3880	1/1	0.91	0.14	46,46,46,46	0
83	MG	1	3598	1/1	0.91	0.08	33,33,33,33	0
83	MG	1	3801	1/1	0.91	0.11	62,62,62,62	0
83	MG	CM	1908	1/1	0.91	0.18	45,45,45,45	0
83	MG	AS	3533	1/1	0.91	0.25	60,60,60,60	0
83	MG	AT	205	1/1	0.91	0.11	57,57,57,57	0
83	MG	CM	1913	1/1	0.91	0.74	70,70,70,70	0
83	MG	1	3515	1/1	0.91	0.11	41,41,41,41	0
83	MG	1	3763	1/1	0.91	0.62	60,60,60,60	0
83	MG	AS	3668	1/1	0.91	0.18	64,64,64,64	0
83	MG	1	3888	1/1	0.91	0.55	43,43,43,43	0
83	MG	AU	205	1/1	0.91	0.11	40,40,40,40	0
83	MG	1	3889	1/1	0.91	0.40	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	B	1928	1/1	0.91	0.24	39,39,39,39	0
83	MG	B	1850	1/1	0.91	0.28	53,53,53,53	0
83	MG	AS	3675	1/1	0.91	0.18	20,20,20,20	0
83	MG	AS	3682	1/1	0.91	0.18	43,43,43,43	0
83	MG	1	3601	1/1	0.91	0.55	56,56,56,56	0
83	MG	1	3856	1/1	0.91	0.37	36,36,36,36	0
83	MG	AS	3553	1/1	0.91	0.17	21,21,21,21	0
83	MG	AS	3408	1/1	0.91	0.11	45,45,45,45	0
83	MG	AS	3412	1/1	0.91	0.09	29,29,29,29	0
83	MG	AS	3563	1/1	0.91	0.15	38,38,38,38	0
83	MG	AS	3698	1/1	0.91	0.62	41,41,41,41	0
83	MG	BB	304	1/1	0.91	1.43	63,63,63,63	0
83	MG	1	3893	1/1	0.91	0.14	55,55,55,55	0
83	MG	1	3621	1/1	0.91	0.22	40,40,40,40	0
83	MG	B	1858	1/1	0.91	0.08	38,38,38,38	0
83	MG	BJ	303	1/1	0.91	0.12	24,24,24,24	0
83	MG	B	1940	1/1	0.91	0.27	73,73,73,73	0
83	MG	AS	3424	1/1	0.91	0.13	45,45,45,45	0
83	MG	AS	3431	1/1	0.91	0.18	42,42,42,42	0
83	MG	1	3811	1/1	0.91	0.12	50,50,50,50	0
83	MG	4	210	1/1	0.91	0.31	58,58,58,58	0
83	MG	DQ	101	1/1	0.91	0.24	63,63,63,63	0
83	MG	1	3579	1/1	0.91	0.12	32,32,32,32	0
83	MG	1	3774	1/1	0.91	0.21	26,26,26,26	0
83	MG	1	3817	1/1	0.91	0.11	31,31,31,31	0
83	MG	1	3776	1/1	0.91	0.83	51,51,51,51	0
83	MG	AS	3594	1/1	0.91	0.13	35,35,35,35	0
83	MG	AS	3597	1/1	0.91	0.17	54,54,54,54	0
83	MG	AF	201	1/1	0.92	0.11	54,54,54,54	0
83	MG	CM	1840	1/1	0.92	0.16	51,51,51,51	0
83	MG	1	3815	1/1	0.92	0.09	42,42,42,42	0
83	MG	B	1859	1/1	0.92	0.16	59,59,59,59	0
83	MG	1	3509	1/1	0.92	0.12	44,44,44,44	0
83	MG	AS	3559	1/1	0.92	0.20	41,41,41,41	0
83	MG	CM	1854	1/1	0.92	0.10	29,29,29,29	0
83	MG	AS	3560	1/1	0.92	0.16	34,34,34,34	0
83	MG	CM	1861	1/1	0.92	0.12	43,43,43,43	0
83	MG	AS	3428	1/1	0.92	0.14	35,35,35,35	0
83	MG	AT	201	1/1	0.92	0.23	17,17,17,17	0
83	MG	AS	3679	1/1	0.92	0.18	37,37,37,37	0
83	MG	1	3567	1/1	0.92	0.12	64,64,64,64	0
83	MG	AS	3435	1/1	0.92	0.14	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AT	208	1/1	0.92	0.20	44,44,44,44	0
83	MG	AS	3569	1/1	0.92	0.08	37,37,37,37	0
83	MG	1	3780	1/1	0.92	0.21	29,29,29,29	0
83	MG	B	1863	1/1	0.92	0.17	59,59,59,59	0
83	MG	1	3680	1/1	0.92	0.25	30,30,30,30	0
83	MG	AK	101	1/1	0.92	0.24	32,32,32,32	0
83	MG	CM	1876	1/1	0.92	0.32	50,50,50,50	0
83	MG	CM	1877	1/1	0.92	0.11	42,42,42,42	0
83	MG	4	211	1/1	0.92	0.07	51,51,51,51	0
83	MG	1	3444	1/1	0.92	0.19	40,40,40,40	0
83	MG	B	1872	1/1	0.92	0.19	56,56,56,56	0
83	MG	1	3578	1/1	0.92	0.06	50,50,50,50	0
83	MG	B	1875	1/1	0.92	0.24	47,47,47,47	0
83	MG	CM	1889	1/1	0.92	0.16	39,39,39,39	0
83	MG	1	3833	1/1	0.92	0.16	32,32,32,32	0
83	MG	B	1880	1/1	0.92	0.26	52,52,52,52	0
83	MG	1	3556	1/1	0.92	0.20	42,42,42,42	0
83	MG	k	403	1/1	0.92	0.22	60,60,60,60	0
83	MG	AS	3470	1/1	0.92	0.16	44,44,44,44	0
83	MG	1	3557	1/1	0.92	0.37	35,35,35,35	0
83	MG	BB	301	1/1	0.92	0.08	29,29,29,29	0
83	MG	1	3946	1/1	0.92	0.77	41,41,41,41	0
83	MG	1	3599	1/1	0.92	0.09	60,60,60,60	0
83	MG	B	1891	1/1	0.92	0.09	49,49,49,49	0
83	MG	AS	3482	1/1	0.92	0.13	29,29,29,29	0
83	MG	1	3720	1/1	0.92	0.46	42,42,42,42	0
83	MG	BJ	301	1/1	0.92	0.64	64,64,64,64	0
83	MG	1	3426	1/1	0.92	0.09	38,38,38,38	0
83	MG	1	3628	1/1	0.92	0.20	61,61,61,61	0
83	MG	1	3533	1/1	0.92	0.14	22,22,22,22	0
83	MG	1	3633	1/1	0.92	0.34	41,41,41,41	0
83	MG	1	3693	1/1	0.92	0.17	51,51,51,51	0
83	MG	AS	3736	1/1	0.92	0.13	48,48,48,48	0
83	MG	CM	1936	1/1	0.92	0.21	67,67,67,67	0
83	MG	1	3847	1/1	0.92	0.14	37,37,37,37	0
83	MG	w	301	1/1	0.92	0.16	29,29,29,29	0
83	MG	AS	3510	1/1	0.92	0.18	23,23,23,23	0
83	MG	3	203	1/1	0.92	0.26	47,47,47,47	0
83	MG	3	204	1/1	0.92	0.23	58,58,58,58	0
83	MG	CM	1947	1/1	0.92	0.19	44,44,44,44	0
83	MG	1	3803	1/1	0.92	0.11	32,32,32,32	0
83	MG	1	3584	1/1	0.92	0.14	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	AS	3523	1/1	0.92	0.15	33,33,33,33	0
83	MG	1	3483	1/1	0.92	0.16	56,56,56,56	0
83	MG	1	3854	1/1	0.92	0.10	32,32,32,32	0
83	MG	CM	1804	1/1	0.92	0.09	42,42,42,42	0
83	MG	8	202	1/1	0.92	1.17	59,59,59,59	0
83	MG	DB	201	1/1	0.92	0.20	38,38,38,38	0
83	MG	1	3462	1/1	0.92	0.25	18,18,18,18	0
83	MG	DB	203	1/1	0.92	0.18	61,61,61,61	0
83	MG	3	213	1/1	0.92	0.13	62,62,62,62	0
83	MG	1	3450	1/1	0.92	0.13	33,33,33,33	0
83	MG	B	1853	1/1	0.92	0.10	32,32,32,32	0
83	MG	AS	3763	1/1	0.92	0.08	41,41,41,41	0
83	MG	AS	3407	1/1	0.92	0.11	23,23,23,23	0
84	3K5	1	3403	57/57	0.92	0.29	36,53,77,93	0
83	MG	1	3702	1/1	0.92	0.19	46,46,46,46	0
83	MG	AS	3655	1/1	0.92	0.12	48,48,48,48	0
85	TIX	AS	3782	27/27	0.92	0.38	48,60,73,150	0
83	MG	AS	3409	1/1	0.92	0.20	20,20,20,20	0
83	MG	CM	1829	1/1	0.92	0.29	33,33,33,33	0
83	MG	B	1933	1/1	0.92	0.16	60,60,60,60	0
86	ZN	CB	201	1/1	0.92	0.17	180,180,180,180	0
83	MG	1	3932	1/1	0.92	0.23	35,35,35,35	0
83	MG	1	3423	1/1	0.93	0.12	38,38,38,38	0
83	MG	1	3487	1/1	0.93	0.16	38,38,38,38	0
83	MG	AS	3737	1/1	0.93	0.23	18,18,18,18	0
83	MG	B	1838	1/1	0.93	0.22	35,35,35,35	0
83	MG	AS	3742	1/1	0.93	0.10	57,57,57,57	0
83	MG	1	3864	1/1	0.93	0.55	49,49,49,49	0
83	MG	1	3537	1/1	0.93	0.61	43,43,43,43	0
83	MG	1	3454	1/1	0.93	0.09	42,42,42,42	0
83	MG	1	3867	1/1	0.93	0.18	28,28,28,28	0
83	MG	AS	3607	1/1	0.93	0.13	37,37,37,37	0
83	MG	B	1851	1/1	0.93	0.17	63,63,63,63	0
83	MG	1	3804	1/1	0.93	0.10	31,31,31,31	0
83	MG	AS	3611	1/1	0.93	0.14	50,50,50,50	0
83	MG	1	3644	1/1	0.93	0.22	24,24,24,24	0
83	MG	CM	1845	1/1	0.93	0.19	28,28,28,28	0
83	MG	AS	3754	1/1	0.93	0.17	35,35,35,35	0
83	MG	B	1947	1/1	0.93	0.08	55,55,55,55	0
83	MG	1	3647	1/1	0.93	0.13	26,26,26,26	0
83	MG	u	202	1/1	0.93	0.08	30,30,30,30	0
83	MG	1	3491	1/1	0.93	0.08	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AS	3759	1/1	0.93	0.28	50,50,50,50	0
83	MG	1	3695	1/1	0.93	0.24	184,184,184,184	0
83	MG	1	3812	1/1	0.93	0.30	69,69,69,69	0
83	MG	1	3696	1/1	0.93	0.18	45,45,45,45	0
83	MG	AS	3628	1/1	0.93	0.13	61,61,61,61	0
83	MG	1	3457	1/1	0.93	0.15	28,28,28,28	0
83	MG	AS	3631	1/1	0.93	0.15	54,54,54,54	0
83	MG	1	3414	1/1	0.93	0.30	56,56,56,56	0
83	MG	1	3605	1/1	0.93	0.22	34,34,34,34	0
83	MG	AS	3503	1/1	0.93	0.12	45,45,45,45	0
83	MG	1	3944	1/1	0.93	0.43	47,47,47,47	0
83	MG	8	201	1/1	0.93	0.12	52,52,52,52	0
83	MG	1	3945	1/1	0.93	0.24	28,28,28,28	0
83	MG	8	203	1/1	0.93	0.43	38,38,38,38	0
83	MG	1	3521	1/1	0.93	0.14	52,52,52,52	0
83	MG	1	3820	1/1	0.93	0.32	34,34,34,34	0
83	MG	CM	1880	1/1	0.93	0.38	33,33,33,33	0
83	MG	AS	3517	1/1	0.93	0.21	24,24,24,24	0
83	MG	1	3498	1/1	0.93	0.12	26,26,26,26	0
83	MG	AS	3522	1/1	0.93	0.40	40,40,40,40	0
83	MG	1	3412	1/1	0.93	0.25	25,25,25,25	0
83	MG	AT	207	1/1	0.93	0.23	49,49,49,49	0
83	MG	1	3758	1/1	0.93	0.30	41,41,41,41	0
83	MG	1	3708	1/1	0.93	0.16	36,36,36,36	0
83	MG	1	3954	1/1	0.93	0.44	51,51,51,51	0
83	MG	CM	1905	1/1	0.93	0.19	82,82,82,82	0
83	MG	CM	1906	1/1	0.93	0.07	64,64,64,64	0
83	MG	1	3610	1/1	0.93	0.13	57,57,57,57	0
83	MG	1	3765	1/1	0.93	0.11	43,43,43,43	0
83	MG	1	3714	1/1	0.93	0.37	25,25,25,25	0
83	MG	CM	1910	1/1	0.93	0.17	65,65,65,65	0
83	MG	1	3770	1/1	0.93	0.09	31,31,31,31	0
83	MG	1	3503	1/1	0.93	0.11	44,44,44,44	0
83	MG	1	3553	1/1	0.93	0.16	47,47,47,47	0
83	MG	1	3842	1/1	0.93	0.27	54,54,54,54	0
83	MG	1	3528	1/1	0.93	0.12	39,39,39,39	0
83	MG	AS	3678	1/1	0.93	0.27	43,43,43,43	0
83	MG	1	3529	1/1	0.93	0.07	40,40,40,40	0
83	MG	CM	1919	1/1	0.93	0.31	52,52,52,52	0
83	MG	AS	3681	1/1	0.93	0.21	53,53,53,53	0
83	MG	1	3845	1/1	0.93	0.17	78,78,78,78	0
83	MG	AS	3547	1/1	0.93	0.18	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
83	MG	AS	3687	1/1	0.93	0.20	31,31,31,31	0
83	MG	1	3907	1/1	0.93	0.11	39,39,39,39	0
83	MG	BB	302	1/1	0.93	0.20	32,32,32,32	0
83	MG	1	3908	1/1	0.93	0.19	70,70,70,70	0
83	MG	1	3777	1/1	0.93	0.18	32,32,32,32	0
83	MG	BE	302	1/1	0.93	0.50	45,45,45,45	0
83	MG	AS	3558	1/1	0.93	0.09	34,34,34,34	0
83	MG	1	3530	1/1	0.93	0.11	58,58,58,58	0
83	MG	CM	1946	1/1	0.93	0.09	43,43,43,43	0
83	MG	1	3558	1/1	0.93	0.28	49,49,49,49	0
83	MG	1	3627	1/1	0.93	0.55	66,66,66,66	0
83	MG	1	3590	1/1	0.93	0.19	46,46,46,46	0
83	MG	BK	202	1/1	0.93	0.16	30,30,30,30	0
83	MG	1	3723	1/1	0.93	0.09	36,36,36,36	0
83	MG	1	3531	1/1	0.93	0.09	37,37,37,37	0
83	MG	AS	3570	1/1	0.93	0.17	33,33,33,33	0
83	MG	B	1825	1/1	0.93	0.09	58,58,58,58	0
83	MG	AS	3573	1/1	0.93	0.09	39,39,39,39	0
83	MG	AS	3425	1/1	0.93	0.13	49,49,49,49	0
83	MG	CA	202	1/1	0.93	0.12	53,53,53,53	0
83	MG	1	3631	1/1	0.93	0.71	42,42,42,42	0
83	MG	CJ	201	1/1	0.93	0.21	49,49,49,49	0
83	MG	AS	3712	1/1	0.93	0.16	32,32,32,32	0
83	MG	AS	3577	1/1	0.93	0.23	40,40,40,40	0
83	MG	B	1927	1/1	0.93	0.28	49,49,49,49	0
83	MG	1	3682	1/1	0.93	0.12	47,47,47,47	0
83	MG	AS	3582	1/1	0.93	0.07	51,51,51,51	0
83	MG	1	3921	1/1	0.93	0.28	69,69,69,69	0
83	MG	1	3421	1/1	0.93	0.22	12,12,12,12	0
83	MG	1	3484	1/1	0.93	0.11	39,39,39,39	0
86	ZN	AQ	101	1/1	0.93	0.20	65,65,65,65	0
83	MG	1	3635	1/1	0.93	0.24	36,36,36,36	0
83	MG	B	1935	1/1	0.93	0.10	71,71,71,71	0
83	MG	AS	3453	1/1	0.93	0.17	39,39,39,39	0
83	MG	CM	1811	1/1	0.93	0.10	42,42,42,42	0
83	MG	AS	3706	1/1	0.94	0.23	44,44,44,44	0
83	MG	1	3671	1/1	0.94	0.97	73,73,73,73	0
83	MG	B	1821	1/1	0.94	0.33	37,37,37,37	0
83	MG	1	3698	1/1	0.94	0.19	41,41,41,41	0
83	MG	1	3413	1/1	0.94	0.17	21,21,21,21	0
83	MG	1	3469	1/1	0.94	0.15	42,42,42,42	0
83	MG	CM	1805	1/1	0.94	0.18	31,31,31,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3675	1/1	0.94	0.14	39,39,39,39	0
83	MG	AS	3427	1/1	0.94	0.27	32,32,32,32	0
83	MG	CM	1809	1/1	0.94	0.35	86,86,86,86	0
83	MG	1	3456	1/1	0.94	0.10	7,7,7,7	0
83	MG	B	1925	1/1	0.94	0.19	54,54,54,54	0
83	MG	AS	3432	1/1	0.94	0.18	23,23,23,23	0
83	MG	AS	3720	1/1	0.94	0.09	43,43,43,43	0
83	MG	AS	3721	1/1	0.94	0.28	64,64,64,64	0
83	MG	B	1830	1/1	0.94	0.26	42,42,42,42	0
83	MG	1	3739	1/1	0.94	0.22	19,19,19,19	0
83	MG	AS	3438	1/1	0.94	0.14	43,43,43,43	0
83	MG	AS	3440	1/1	0.94	0.12	28,28,28,28	0
83	MG	1	3677	1/1	0.94	0.21	55,55,55,55	0
83	MG	CM	1831	1/1	0.94	0.20	25,25,25,25	0
83	MG	CM	1833	1/1	0.94	0.32	36,36,36,36	0
83	MG	AS	3587	1/1	0.94	0.21	38,38,38,38	0
83	MG	AS	3445	1/1	0.94	0.28	39,39,39,39	0
83	MG	CM	1837	1/1	0.94	0.09	29,29,29,29	0
83	MG	AS	3734	1/1	0.94	0.11	40,40,40,40	0
83	MG	CM	1839	1/1	0.94	0.08	40,40,40,40	0
83	MG	AS	3735	1/1	0.94	0.12	44,44,44,44	0
83	MG	1	3538	1/1	0.94	0.18	43,43,43,43	0
83	MG	CM	1842	1/1	0.94	0.11	36,36,36,36	0
83	MG	AS	3590	1/1	0.94	0.32	38,38,38,38	0
83	MG	AS	3738	1/1	0.94	0.08	62,62,62,62	0
83	MG	AS	3739	1/1	0.94	0.10	54,54,54,54	0
83	MG	s	201	1/1	0.94	0.19	35,35,35,35	0
83	MG	AS	3450	1/1	0.94	0.15	35,35,35,35	0
83	MG	CM	1857	1/1	0.94	0.09	44,44,44,44	0
83	MG	CM	1858	1/1	0.94	0.11	55,55,55,55	0
83	MG	1	3790	1/1	0.94	0.12	31,31,31,31	0
83	MG	1	3892	1/1	0.94	0.10	39,39,39,39	0
83	MG	1	3493	1/1	0.94	0.14	33,33,33,33	0
83	MG	1	3894	1/1	0.94	0.09	45,45,45,45	0
83	MG	1	3648	1/1	0.94	0.56	35,35,35,35	0
83	MG	B	1848	1/1	0.94	0.22	33,33,33,33	0
83	MG	1	3797	1/1	0.94	0.20	58,58,58,58	0
83	MG	1	3948	1/1	0.94	0.18	40,40,40,40	0
83	MG	AS	3466	1/1	0.94	0.07	44,44,44,44	0
83	MG	1	3624	1/1	0.94	0.26	56,56,56,56	0
83	MG	AS	3610	1/1	0.94	0.31	34,34,34,34	0
83	MG	0	202	1/1	0.94	0.43	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3445	1/1	0.94	0.28	36,36,36,36	0
83	MG	1	3900	1/1	0.94	0.83	56,56,56,56	0
83	MG	6	203	1/1	0.94	0.11	43,43,43,43	0
83	MG	1	3626	1/1	0.94	0.18	30,30,30,30	0
83	MG	AS	3620	1/1	0.94	0.40	44,44,44,44	0
83	MG	1	3424	1/1	0.94	0.95	45,45,45,45	0
83	MG	1	3850	1/1	0.94	0.10	51,51,51,51	0
83	MG	AS	3623	1/1	0.94	0.21	62,62,62,62	0
83	MG	CM	1883	1/1	0.94	0.12	65,65,65,65	0
83	MG	CM	1884	1/1	0.94	0.10	44,44,44,44	0
83	MG	CM	1886	1/1	0.94	0.21	36,36,36,36	0
83	MG	AS	3485	1/1	0.94	0.09	42,42,42,42	0
83	MG	1	3655	1/1	0.94	0.18	47,47,47,47	0
83	MG	CM	1894	1/1	0.94	0.18	40,40,40,40	0
83	MG	CM	1895	1/1	0.94	0.07	32,32,32,32	0
83	MG	AS	3627	1/1	0.94	0.11	55,55,55,55	0
83	MG	1	3438	1/1	0.94	0.30	28,28,28,28	0
83	MG	CM	1898	1/1	0.94	0.10	38,38,38,38	0
83	MG	1	3688	1/1	0.94	0.09	33,33,33,33	0
83	MG	1	3805	1/1	0.94	0.21	85,85,85,85	0
83	MG	CM	1903	1/1	0.94	0.30	43,43,43,43	0
83	MG	AE	202	1/1	0.94	0.12	87,87,87,87	0
83	MG	B	1957	1/1	0.94	0.19	82,82,82,82	0
83	MG	AS	3495	1/1	0.94	0.13	37,37,37,37	0
83	MG	AS	3496	1/1	0.94	0.19	20,20,20,20	0
83	MG	AS	3637	1/1	0.94	0.15	51,51,51,51	0
83	MG	B	1866	1/1	0.94	0.28	47,47,47,47	0
83	MG	AT	203	1/1	0.94	0.23	52,52,52,52	0
83	MG	B	1867	1/1	0.94	0.21	56,56,56,56	0
83	MG	1	3759	1/1	0.94	0.26	37,37,37,37	0
83	MG	1	3807	1/1	0.94	0.08	32,32,32,32	0
83	MG	AS	3644	1/1	0.94	0.10	27,27,27,27	0
83	MG	1	3761	1/1	0.94	0.14	27,27,27,27	0
83	MG	B	1963	1/1	0.94	0.38	55,55,55,55	0
83	MG	1	3606	1/1	0.94	0.48	47,47,47,47	0
83	MG	CM	1921	1/1	0.94	0.14	28,28,28,28	0
83	MG	CM	1923	1/1	0.94	0.08	39,39,39,39	0
83	MG	1	3594	1/1	0.94	0.12	55,55,55,55	0
83	MG	AS	3519	1/1	0.94	0.21	26,26,26,26	0
83	MG	AS	3520	1/1	0.94	0.15	44,44,44,44	0
83	MG	CM	1932	1/1	0.94	0.13	52,52,52,52	0
83	MG	B	1968	1/1	0.94	0.21	61,61,61,61	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3764	1/1	0.94	0.11	34,34,34,34	0
83	MG	AS	3663	1/1	0.94	0.08	56,56,56,56	0
83	MG	AS	3664	1/1	0.94	0.12	23,23,23,23	0
83	MG	1	3632	1/1	0.94	0.21	42,42,42,42	0
83	MG	1	3595	1/1	0.94	0.10	42,42,42,42	0
83	MG	1	3441	1/1	0.94	0.15	33,33,33,33	0
83	MG	B	1885	1/1	0.94	0.19	78,78,78,78	0
83	MG	1	3727	1/1	0.94	0.18	40,40,40,40	0
83	MG	1	3868	1/1	0.94	0.13	41,41,41,41	0
83	MG	Q	202	1/1	0.94	0.26	52,52,52,52	0
83	MG	1	3923	1/1	0.94	0.10	59,59,59,59	0
83	MG	1	3869	1/1	0.94	0.09	58,58,58,58	0
83	MG	AS	3537	1/1	0.94	0.17	39,39,39,39	0
83	MG	1	3772	1/1	0.94	0.23	35,35,35,35	0
83	MG	1	3401	1/1	0.94	0.16	20,20,20,20	0
83	MG	AS	3683	1/1	0.94	0.16	47,47,47,47	0
83	MG	j	301	1/1	0.94	0.14	19,19,19,19	0
83	MG	1	3823	1/1	0.94	0.08	36,36,36,36	0
83	MG	BJ	302	1/1	0.94	0.10	37,37,37,37	0
83	MG	B	1810	1/1	0.94	0.19	43,43,43,43	0
83	MG	AS	3545	1/1	0.94	0.12	29,29,29,29	0
83	MG	B	1812	1/1	0.94	0.27	33,33,33,33	0
83	MG	B	1813	1/1	0.94	0.26	46,46,46,46	0
83	MG	AS	3549	1/1	0.94	0.28	41,41,41,41	0
83	MG	AS	3695	1/1	0.94	0.12	46,46,46,46	0
83	MG	AS	3697	1/1	0.94	0.35	32,32,32,32	0
83	MG	AS	3405	1/1	0.94	0.19	26,26,26,26	0
83	MG	CA	201	1/1	0.94	0.08	40,40,40,40	0
83	MG	AS	3699	1/1	0.94	0.90	71,71,71,71	0
83	MG	1	3825	1/1	0.94	0.21	31,31,31,31	0
83	MG	B	1910	1/1	0.94	0.24	37,37,37,37	0
83	MG	AS	3703	1/1	0.94	0.20	18,18,18,18	0
83	MG	1	3613	1/1	0.94	0.15	32,32,32,32	0
86	ZN	CJ	202	1/1	0.94	0.17	173,173,173,173	0
83	MG	1	3828	1/1	0.94	0.19	35,35,35,35	0
83	MG	1	3710	1/1	0.95	0.08	21,21,21,21	0
83	MG	B	1831	1/1	0.95	0.08	39,39,39,39	0
83	MG	B	1926	1/1	0.95	0.18	46,46,46,46	0
83	MG	1	3435	1/1	0.95	0.10	23,23,23,23	0
83	MG	CM	1826	1/1	0.95	0.14	48,48,48,48	0
83	MG	1	3819	1/1	0.95	0.20	63,63,63,63	0
83	MG	CM	1830	1/1	0.95	0.20	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3672	1/1	0.95	0.08	33,33,33,33	0
83	MG	AS	3448	1/1	0.95	0.09	34,34,34,34	0
83	MG	AS	3595	1/1	0.95	0.13	52,52,52,52	0
83	MG	B	1930	1/1	0.95	0.14	48,48,48,48	0
83	MG	1	3580	1/1	0.95	0.11	32,32,32,32	0
83	MG	1	3824	1/1	0.95	0.11	47,47,47,47	0
83	MG	1	3437	1/1	0.95	0.21	19,19,19,19	0
83	MG	B	1839	1/1	0.95	0.22	55,55,55,55	0
83	MG	B	1840	1/1	0.95	0.20	59,59,59,59	0
83	MG	v	301	1/1	0.95	0.31	31,31,31,31	0
83	MG	CM	1843	1/1	0.95	0.24	34,34,34,34	0
83	MG	B	1938	1/1	0.95	0.14	35,35,35,35	0
83	MG	CM	1846	1/1	0.95	0.30	53,53,53,53	0
83	MG	B	1843	1/1	0.95	0.23	37,37,37,37	0
83	MG	CM	1849	1/1	0.95	0.14	41,41,41,41	0
83	MG	AS	3464	1/1	0.95	0.29	47,47,47,47	0
83	MG	1	3768	1/1	0.95	0.12	36,36,36,36	0
83	MG	1	3458	1/1	0.95	0.12	18,18,18,18	0
83	MG	AS	3613	1/1	0.95	0.21	37,37,37,37	0
83	MG	B	1847	1/1	0.95	0.12	41,41,41,41	0
83	MG	AS	3615	1/1	0.95	0.15	35,35,35,35	0
83	MG	AS	3469	1/1	0.95	0.21	26,26,26,26	0
83	MG	1	3886	1/1	0.95	0.22	29,29,29,29	0
83	MG	1	3555	1/1	0.95	0.33	41,41,41,41	0
83	MG	AS	3475	1/1	0.95	0.13	29,29,29,29	0
83	MG	AS	3476	1/1	0.95	0.16	20,20,20,20	0
83	MG	1	3511	1/1	0.95	0.18	16,16,16,16	0
83	MG	1	3678	1/1	0.95	0.10	32,32,32,32	0
83	MG	1	3834	1/1	0.95	0.13	65,65,65,65	0
83	MG	1	3459	1/1	0.95	0.13	27,27,27,27	0
83	MG	AS	3483	1/1	0.95	0.20	22,22,22,22	0
83	MG	AS	3629	1/1	0.95	0.06	38,38,38,38	0
83	MG	1	3641	1/1	0.95	0.12	21,21,21,21	0
83	MG	1	3475	1/1	0.95	0.20	9,9,9,9	0
83	MG	AS	3771	1/1	0.95	0.15	47,47,47,47	0
83	MG	6	204	1/1	0.95	0.17	20,20,20,20	0
83	MG	1	3778	1/1	0.95	0.23	43,43,43,43	0
83	MG	1	3476	1/1	0.95	0.19	59,59,59,59	0
83	MG	1	3496	1/1	0.95	0.44	55,55,55,55	0
83	MG	9	201	1/1	0.95	0.12	45,45,45,45	0
83	MG	1	3645	1/1	0.95	0.11	30,30,30,30	0
83	MG	1	3956	1/1	0.95	0.15	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	CM	1885	1/1	0.95	0.23	47,47,47,47	0
83	MG	AS	3501	1/1	0.95	0.20	55,55,55,55	0
83	MG	AS	3502	1/1	0.95	0.10	28,28,28,28	0
83	MG	1	3611	1/1	0.95	0.17	23,23,23,23	0
83	MG	CM	1891	1/1	0.95	0.24	27,27,27,27	0
83	MG	1	3612	1/1	0.95	0.20	34,34,34,34	0
83	MG	1	3430	1/1	0.95	0.22	30,30,30,30	0
83	MG	1	3786	1/1	0.95	0.08	43,43,43,43	0
83	MG	AS	3648	1/1	0.95	0.29	22,22,22,22	0
83	MG	1	3453	1/1	0.95	0.13	23,23,23,23	0
83	MG	AS	3650	1/1	0.95	0.15	27,27,27,27	0
83	MG	AS	3653	1/1	0.95	0.11	40,40,40,40	0
83	MG	AS	3512	1/1	0.95	0.19	60,60,60,60	0
83	MG	AS	3513	1/1	0.95	0.15	26,26,26,26	0
83	MG	1	3789	1/1	0.95	0.22	41,41,41,41	0
83	MG	AS	3659	1/1	0.95	0.14	69,69,69,69	0
83	MG	B	1966	1/1	0.95	0.08	41,41,41,41	0
83	MG	1	3616	1/1	0.95	0.26	34,34,34,34	0
83	MG	1	3653	1/1	0.95	0.19	34,34,34,34	0
83	MG	3	210	1/1	0.95	0.30	48,48,48,48	0
83	MG	1	3736	1/1	0.95	0.19	25,25,25,25	0
83	MG	3	212	1/1	0.95	0.28	41,41,41,41	0
83	MG	1	3853	1/1	0.95	0.30	49,49,49,49	0
83	MG	3	214	1/1	0.95	0.15	61,61,61,61	0
83	MG	B	1886	1/1	0.95	0.20	61,61,61,61	0
83	MG	1	3912	1/1	0.95	0.16	56,56,56,56	0
83	MG	AS	3674	1/1	0.95	0.20	27,27,27,27	0
83	MG	1	3591	1/1	0.95	0.17	23,23,23,23	0
83	MG	CM	1922	1/1	0.95	0.08	43,43,43,43	0
83	MG	1	3592	1/1	0.95	0.15	29,29,29,29	0
83	MG	1	3656	1/1	0.95	0.32	60,60,60,60	0
83	MG	CM	1925	1/1	0.95	0.16	47,47,47,47	0
83	MG	Y	201	1/1	0.95	0.09	39,39,39,39	0
83	MG	B	1806	1/1	0.95	0.36	53,53,53,53	0
83	MG	CM	1931	1/1	0.95	0.10	42,42,42,42	0
83	MG	1	3564	1/1	0.95	0.13	39,39,39,39	0
83	MG	B	1896	1/1	0.95	0.12	54,54,54,54	0
83	MG	4	205	1/1	0.95	0.33	40,40,40,40	0
83	MG	CM	1935	1/1	0.95	0.19	48,48,48,48	0
83	MG	1	3525	1/1	0.95	0.19	53,53,53,53	0
83	MG	1	3743	1/1	0.95	0.19	29,29,29,29	0
83	MG	B	1901	1/1	0.95	0.09	69,69,69,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AS	3692	1/1	0.95	0.26	25,25,25,25	0
83	MG	1	3659	1/1	0.95	0.11	23,23,23,23	0
83	MG	1	3660	1/1	0.95	0.26	31,31,31,31	0
83	MG	B	1905	1/1	0.95	0.19	46,46,46,46	0
83	MG	BZ	203	1/1	0.95	0.23	74,74,74,74	0
83	MG	B	1907	1/1	0.95	0.07	29,29,29,29	0
83	MG	AS	3410	1/1	0.95	0.10	54,54,54,54	0
83	MG	AS	3554	1/1	0.95	0.28	45,45,45,45	0
83	MG	AS	3411	1/1	0.95	0.26	29,29,29,29	0
83	MG	B	1908	1/1	0.95	0.29	49,49,49,49	0
83	MG	1	3699	1/1	0.95	0.18	23,23,23,23	0
83	MG	1	3480	1/1	0.95	0.15	21,21,21,21	0
83	MG	AS	3417	1/1	0.95	0.24	22,22,22,22	0
83	MG	1	3664	1/1	0.95	0.12	53,53,53,53	0
83	MG	1	3465	1/1	0.95	0.10	24,24,24,24	0
83	MG	AS	3565	1/1	0.95	0.11	22,22,22,22	0
83	MG	AS	3422	1/1	0.95	0.10	55,55,55,55	0
83	MG	AS	3423	1/1	0.95	0.19	22,22,22,22	0
83	MG	1	3754	1/1	0.95	0.07	67,67,67,67	0
83	MG	1	3705	1/1	0.95	0.16	47,47,47,47	0
83	MG	AS	3426	1/1	0.95	0.13	20,20,20,20	0
83	MG	B	1916	1/1	0.95	0.20	37,37,37,37	0
83	MG	1	3570	1/1	0.95	0.56	48,48,48,48	0
83	MG	CM	1810	1/1	0.95	0.12	43,43,43,43	0
86	ZN	AH	203	1/1	0.95	0.25	122,122,122,122	0
83	MG	AS	3430	1/1	0.95	0.16	26,26,26,26	0
83	MG	CM	1813	1/1	0.95	0.40	46,46,46,46	0
83	MG	1	3505	1/1	0.95	0.09	41,41,41,41	0
83	MG	1	3577	1/1	0.95	0.14	53,53,53,53	0
83	MG	B	1921	1/1	0.95	0.15	55,55,55,55	0
83	MG	CM	1819	1/1	0.95	0.44	56,56,56,56	0
83	MG	1	3422	1/1	0.95	0.08	43,43,43,43	0
86	ZN	DS	201	1/1	0.95	0.19	134,134,134,134	0
83	MG	AS	3568	1/1	0.96	0.09	24,24,24,24	0
83	MG	AS	3666	1/1	0.96	0.48	39,39,39,39	0
83	MG	AS	3774	1/1	0.96	0.25	50,50,50,50	0
83	MG	1	3532	1/1	0.96	0.13	31,31,31,31	0
83	MG	r	301	1/1	0.96	0.23	23,23,23,23	0
83	MG	1	3744	1/1	0.96	0.18	40,40,40,40	0
83	MG	AS	3572	1/1	0.96	0.16	35,35,35,35	0
83	MG	AS	3671	1/1	0.96	0.25	38,38,38,38	0
83	MG	AS	3781	1/1	0.96	0.09	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3878	1/1	0.96	0.28	57,57,57,57	0
83	MG	1	3745	1/1	0.96	0.15	31,31,31,31	0
83	MG	1	3775	1/1	0.96	0.12	38,38,38,38	0
83	MG	1	3474	1/1	0.96	0.14	29,29,29,29	0
83	MG	AS	3677	1/1	0.96	0.09	27,27,27,27	0
83	MG	AT	206	1/1	0.96	0.28	39,39,39,39	0
83	MG	3	205	1/1	0.96	0.17	46,46,46,46	0
83	MG	1	3639	1/1	0.96	0.09	34,34,34,34	0
83	MG	AS	3484	1/1	0.96	0.17	23,23,23,23	0
83	MG	1	3520	1/1	0.96	0.14	41,41,41,41	0
83	MG	B	1870	1/1	0.96	0.32	42,42,42,42	0
83	MG	AS	3684	1/1	0.96	0.18	36,36,36,36	0
83	MG	1	3448	1/1	0.96	0.14	23,23,23,23	0
83	MG	AS	3686	1/1	0.96	0.15	36,36,36,36	0
83	MG	1	3813	1/1	0.96	0.07	44,44,44,44	0
83	MG	1	3927	1/1	0.96	0.08	55,55,55,55	0
83	MG	AS	3490	1/1	0.96	0.13	39,39,39,39	0
83	MG	B	1820	1/1	0.96	0.11	38,38,38,38	0
83	MG	AS	3592	1/1	0.96	0.19	71,71,71,71	0
83	MG	1	3571	1/1	0.96	0.32	37,37,37,37	0
83	MG	AS	3494	1/1	0.96	0.06	45,45,45,45	0
83	MG	B	1877	1/1	0.96	0.21	53,53,53,53	0
83	MG	AS	3696	1/1	0.96	0.35	38,38,38,38	0
83	MG	AS	3596	1/1	0.96	0.11	29,29,29,29	0
83	MG	AZ	301	1/1	0.96	0.27	27,27,27,27	0
83	MG	1	3752	1/1	0.96	0.08	29,29,29,29	0
83	MG	AS	3499	1/1	0.96	0.24	39,39,39,39	0
83	MG	B	1823	1/1	0.96	0.23	31,31,31,31	0
83	MG	AS	3416	1/1	0.96	0.26	25,25,25,25	0
83	MG	1	3851	1/1	0.96	0.16	63,63,63,63	0
83	MG	AS	3605	1/1	0.96	0.09	21,21,21,21	0
83	MG	AS	3418	1/1	0.96	0.07	30,30,30,30	0
83	MG	2	201	1/1	0.96	0.34	43,43,43,43	0
83	MG	AS	3420	1/1	0.96	0.10	42,42,42,42	0
83	MG	1	3661	1/1	0.96	0.21	25,25,25,25	0
83	MG	1	3575	1/1	0.96	0.26	26,26,26,26	0
83	MG	1	3755	1/1	0.96	0.19	35,35,35,35	0
83	MG	1	3703	1/1	0.96	0.73	43,43,43,43	0
83	MG	1	3787	1/1	0.96	0.14	34,34,34,34	0
83	MG	B	1892	1/1	0.96	0.12	46,46,46,46	0
83	MG	1	3821	1/1	0.96	0.16	63,63,63,63	0
83	MG	AS	3716	1/1	0.96	0.12	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3937	1/1	0.96	0.15	53,53,53,53	0
83	MG	AS	3718	1/1	0.96	0.08	76,76,76,76	0
83	MG	AB	201	1/1	0.96	0.14	37,37,37,37	0
83	MG	1	3822	1/1	0.96	0.11	32,32,32,32	0
83	MG	1	3522	1/1	0.96	0.13	32,32,32,32	0
83	MG	AS	3525	1/1	0.96	0.08	60,60,60,60	0
83	MG	AS	3526	1/1	0.96	0.13	30,30,30,30	0
83	MG	AS	3725	1/1	0.96	0.12	55,55,55,55	0
83	MG	AS	3527	1/1	0.96	0.23	55,55,55,55	0
83	MG	AS	3433	1/1	0.96	0.07	38,38,38,38	0
83	MG	AS	3626	1/1	0.96	0.17	50,50,50,50	0
83	MG	1	3416	1/1	0.96	0.16	27,27,27,27	0
83	MG	CM	1929	1/1	0.96	0.15	32,32,32,32	0
83	MG	CM	1930	1/1	0.96	0.15	35,35,35,35	0
83	MG	1	3666	1/1	0.96	0.19	45,45,45,45	0
83	MG	1	3646	1/1	0.96	0.10	33,33,33,33	0
83	MG	AS	3439	1/1	0.96	0.18	29,29,29,29	0
83	MG	1	3793	1/1	0.96	0.13	57,57,57,57	0
83	MG	1	3486	1/1	0.96	0.21	29,29,29,29	0
83	MG	B	1906	1/1	0.96	0.18	29,29,29,29	0
83	MG	1	3429	1/1	0.96	0.15	45,45,45,45	0
83	MG	AS	3635	1/1	0.96	0.14	37,37,37,37	0
83	MG	B	1846	1/1	0.96	0.10	58,58,58,58	0
83	MG	CM	1943	1/1	0.96	0.14	38,38,38,38	0
83	MG	CM	1812	1/1	0.96	0.09	42,42,42,42	0
83	MG	B	1964	1/1	0.96	0.14	57,57,57,57	0
83	MG	1	3832	1/1	0.96	0.07	34,34,34,34	0
83	MG	1	3711	1/1	0.96	0.21	27,27,27,27	0
83	MG	AS	3641	1/1	0.96	0.13	38,38,38,38	0
83	MG	AS	3748	1/1	0.96	0.08	33,33,33,33	0
83	MG	1	3499	1/1	0.96	0.10	24,24,24,24	0
83	MG	AS	3454	1/1	0.96	0.12	22,22,22,22	0
83	MG	1	3870	1/1	0.96	0.29	46,46,46,46	0
83	MG	AP	201	1/1	0.96	0.08	31,31,31,31	0
83	MG	B	1971	1/1	0.96	0.24	63,63,63,63	0
83	MG	AS	3550	1/1	0.96	0.31	37,37,37,37	0
83	MG	CM	1827	1/1	0.96	0.30	38,38,38,38	0
83	MG	CM	1828	1/1	0.96	0.13	50,50,50,50	0
83	MG	1	3513	1/1	0.96	0.16	32,32,32,32	0
83	MG	B	1915	1/1	0.96	0.10	46,46,46,46	0
83	MG	AS	3460	1/1	0.96	0.16	24,24,24,24	0
83	MG	DJ	201	1/1	0.96	0.15	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	CM	1832	1/1	0.96	0.22	32,32,32,32	0
83	MG	AS	3651	1/1	0.96	0.12	28,28,28,28	0
83	MG	CM	1834	1/1	0.96	0.28	54,54,54,54	0
83	MG	AS	3461	1/1	0.96	0.21	23,23,23,23	0
83	MG	AS	3760	1/1	0.96	0.76	70,70,70,70	0
83	MG	G	301	1/1	0.96	0.16	82,82,82,82	0
83	MG	1	3500	1/1	0.96	0.14	36,36,36,36	0
83	MG	1	3455	1/1	0.96	0.21	26,26,26,26	0
83	MG	AS	3657	1/1	0.96	0.09	30,30,30,30	0
86	ZN	c	201	1/1	0.96	0.15	71,71,71,71	0
83	MG	AS	3658	1/1	0.96	0.28	37,37,37,37	0
83	MG	B	1918	1/1	0.96	0.17	32,32,32,32	0
83	MG	1	3472	1/1	0.96	0.05	23,23,23,23	0
86	ZN	CE	101	1/1	0.96	0.10	66,66,66,66	0
83	MG	B	1803	1/1	0.96	0.25	39,39,39,39	0
86	ZN	DN	201	1/1	0.96	0.15	69,69,69,69	0
83	MG	AS	3567	1/1	0.96	0.30	22,22,22,22	0
83	MG	CM	1847	1/1	0.96	0.31	44,44,44,44	0
83	MG	AS	3509	1/1	0.97	0.19	32,32,32,32	0
83	MG	CM	1860	1/1	0.97	0.12	31,31,31,31	0
83	MG	AS	3689	1/1	0.97	0.29	59,59,59,59	0
83	MG	CM	1862	1/1	0.97	0.24	62,62,62,62	0
83	MG	AS	3429	1/1	0.97	0.15	23,23,23,23	0
83	MG	AT	209	1/1	0.97	0.28	53,53,53,53	0
83	MG	1	3829	1/1	0.97	0.22	44,44,44,44	0
83	MG	1	3747	1/1	0.97	0.07	26,26,26,26	0
83	MG	CM	1867	1/1	0.97	0.15	60,60,60,60	0
83	MG	AS	3603	1/1	0.97	0.44	49,49,49,49	0
83	MG	AS	3604	1/1	0.97	0.07	37,37,37,37	0
83	MG	1	3489	1/1	0.97	0.18	44,44,44,44	0
83	MG	B	1842	1/1	0.97	0.09	29,29,29,29	0
83	MG	1	3713	1/1	0.97	0.10	39,39,39,39	0
83	MG	1	3439	1/1	0.97	0.09	28,28,28,28	0
83	MG	4	206	1/1	0.97	0.03	27,27,27,27	0
83	MG	1	3420	1/1	0.97	0.14	33,33,33,33	0
83	MG	1	3408	1/1	0.97	0.20	33,33,33,33	0
83	MG	AS	3702	1/1	0.97	0.17	31,31,31,31	0
83	MG	AS	3442	1/1	0.97	0.23	32,32,32,32	0
83	MG	1	3443	1/1	0.97	0.14	50,50,50,50	0
83	MG	AS	3444	1/1	0.97	0.21	34,34,34,34	0
83	MG	B	1849	1/1	0.97	0.22	43,43,43,43	0
83	MG	1	3837	1/1	0.97	0.26	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3794	1/1	0.97	0.08	32,32,32,32	0
83	MG	AS	3619	1/1	0.97	0.07	42,42,42,42	0
83	MG	B	1970	1/1	0.97	0.15	59,59,59,59	0
83	MG	1	3795	1/1	0.97	0.38	39,39,39,39	0
83	MG	1	3887	1/1	0.97	0.18	46,46,46,46	0
83	MG	CM	1890	1/1	0.97	0.16	30,30,30,30	0
83	MG	AS	3713	1/1	0.97	0.15	28,28,28,28	0
83	MG	CM	1892	1/1	0.97	0.18	28,28,28,28	0
83	MG	AS	3452	1/1	0.97	0.24	28,28,28,28	0
83	MG	1	3478	1/1	0.97	0.23	22,22,22,22	0
83	MG	1	3516	1/1	0.97	0.31	33,33,33,33	0
83	MG	1	3406	1/1	0.97	0.29	32,32,32,32	0
83	MG	AS	3536	1/1	0.97	0.20	31,31,31,31	0
83	MG	1	3411	1/1	0.97	0.26	24,24,24,24	0
83	MG	1	3481	1/1	0.97	0.12	31,31,31,31	0
83	MG	CM	1902	1/1	0.97	0.09	33,33,33,33	0
83	MG	1	3689	1/1	0.97	0.51	63,63,63,63	0
83	MG	CM	1904	1/1	0.97	0.10	34,34,34,34	0
83	MG	1	3760	1/1	0.97	0.17	37,37,37,37	0
83	MG	1	3540	1/1	0.97	0.39	37,37,37,37	0
83	MG	1	3436	1/1	0.97	0.23	28,28,28,28	0
83	MG	AS	3726	1/1	0.97	0.23	56,56,56,56	0
83	MG	AS	3462	1/1	0.97	0.13	34,34,34,34	0
83	MG	1	3568	1/1	0.97	0.07	24,24,24,24	0
83	MG	Y	202	1/1	0.97	0.47	66,66,66,66	0
83	MG	AS	3731	1/1	0.97	0.33	35,35,35,35	0
83	MG	1	3569	1/1	0.97	0.15	27,27,27,27	0
83	MG	1	3630	1/1	0.97	0.19	23,23,23,23	0
83	MG	AS	3551	1/1	0.97	0.23	32,32,32,32	0
83	MG	AS	3640	1/1	0.97	0.08	48,48,48,48	0
83	MG	AS	3552	1/1	0.97	0.18	20,20,20,20	0
83	MG	B	1811	1/1	0.97	0.13	24,24,24,24	0
83	MG	CM	1920	1/1	0.97	0.09	45,45,45,45	0
83	MG	1	3415	1/1	0.97	0.24	36,36,36,36	0
83	MG	AS	3555	1/1	0.97	0.10	36,36,36,36	0
83	MG	AS	3740	1/1	0.97	0.07	69,69,69,69	0
83	MG	1	3809	1/1	0.97	0.18	37,37,37,37	0
83	MG	B	1932	1/1	0.97	0.08	24,24,24,24	0
83	MG	AS	3743	1/1	0.97	0.06	40,40,40,40	0
83	MG	CM	1807	1/1	0.97	0.20	35,35,35,35	0
83	MG	1	3767	1/1	0.97	0.17	24,24,24,24	0
83	MG	1	3545	1/1	0.97	0.27	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AS	3406	1/1	0.97	0.18	34,34,34,34	0
83	MG	1	3769	1/1	0.97	0.17	22,22,22,22	0
83	MG	AS	3479	1/1	0.97	0.08	21,21,21,21	0
83	MG	AS	3652	1/1	0.97	0.10	31,31,31,31	0
83	MG	1	3731	1/1	0.97	0.18	20,20,20,20	0
83	MG	AS	3566	1/1	0.97	0.08	32,32,32,32	0
83	MG	AS	3481	1/1	0.97	0.17	25,25,25,25	0
83	MG	CM	1938	1/1	0.97	0.19	44,44,44,44	0
83	MG	CM	1939	1/1	0.97	0.91	64,64,64,64	0
83	MG	B	1818	1/1	0.97	0.29	24,24,24,24	0
83	MG	1	3572	1/1	0.97	0.68	52,52,52,52	0
83	MG	B	1879	1/1	0.97	0.16	27,27,27,27	0
83	MG	1	3573	1/1	0.97	0.26	27,27,27,27	0
83	MG	CM	1823	1/1	0.97	0.39	37,37,37,37	0
83	MG	1	3734	1/1	0.97	0.11	28,28,28,28	0
83	MG	AS	3661	1/1	0.97	0.12	87,87,87,87	0
83	MG	AS	3662	1/1	0.97	0.10	76,76,76,76	0
83	MG	AS	3414	1/1	0.97	0.35	28,28,28,28	0
83	MG	1	3911	1/1	0.97	0.56	39,39,39,39	0
83	MG	AS	3762	1/1	0.97	0.06	38,38,38,38	0
83	MG	B	1883	1/1	0.97	0.30	39,39,39,39	0
83	MG	AS	3576	1/1	0.97	0.13	44,44,44,44	0
83	MG	1	3574	1/1	0.97	0.40	36,36,36,36	0
83	MG	AS	3578	1/1	0.97	0.12	31,31,31,31	0
83	MG	1	3523	1/1	0.97	0.37	31,31,31,31	0
83	MG	AS	3492	1/1	0.97	0.12	30,30,30,30	0
83	MG	1	3638	1/1	0.97	0.18	32,32,32,32	0
83	MG	AS	3770	1/1	0.97	0.10	31,31,31,31	0
83	MG	1	3471	1/1	0.97	0.12	39,39,39,39	0
83	MG	AS	3584	1/1	0.97	0.14	42,42,42,42	0
83	MG	1	3504	1/1	0.97	0.07	22,22,22,22	0
83	MG	1	3431	1/1	0.97	0.08	31,31,31,31	0
83	MG	1	3506	1/1	0.97	0.10	22,22,22,22	0
83	MG	AS	3500	1/1	0.97	0.21	31,31,31,31	0
83	MG	CM	1844	1/1	0.97	0.19	32,32,32,32	0
83	MG	1	3551	1/1	0.97	0.18	22,22,22,22	0
83	MG	AS	3778	1/1	0.97	0.09	32,32,32,32	0
83	MG	AS	3680	1/1	0.97	0.19	33,33,33,33	0
83	MG	1	3552	1/1	0.97	0.13	45,45,45,45	0
83	MG	1	3473	1/1	0.97	0.19	23,23,23,23	0
83	MG	CM	1850	1/1	0.97	0.17	42,42,42,42	0
83	MG	1	3827	1/1	0.97	0.14	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	AS	3505	1/1	0.97	0.08	41,41,41,41	0
83	MG	AS	3506	1/1	0.97	0.08	39,39,39,39	0
83	MG	CM	1855	1/1	0.97	0.19	41,41,41,41	0
86	ZN	CK	103	1/1	0.97	0.13	87,87,87,87	0
83	MG	CM	1856	1/1	0.97	0.15	25,25,25,25	0
83	MG	1	3488	1/1	0.97	0.20	26,26,26,26	0
86	ZN	DQ	102	1/1	0.97	0.26	55,55,55,55	0
83	MG	AS	3508	1/1	0.97	0.19	25,25,25,25	0
83	MG	AG	203	1/1	0.98	0.07	39,39,39,39	0
83	MG	AS	3601	1/1	0.98	0.08	55,55,55,55	0
83	MG	1	3482	1/1	0.98	0.23	28,28,28,28	0
83	MG	1	3617	1/1	0.98	0.22	25,25,25,25	0
83	MG	1	3636	1/1	0.98	0.16	38,38,38,38	0
83	MG	1	3449	1/1	0.98	0.27	24,24,24,24	0
83	MG	AS	3543	1/1	0.98	0.10	54,54,54,54	0
83	MG	B	1878	1/1	0.98	0.17	64,64,64,64	0
83	MG	1	3741	1/1	0.98	0.16	28,28,28,28	0
83	MG	AS	3546	1/1	0.98	0.24	21,21,21,21	0
83	MG	1	3447	1/1	0.98	0.20	21,21,21,21	0
83	MG	1	3916	1/1	0.98	0.12	73,73,73,73	0
83	MG	AS	3676	1/1	0.98	0.17	15,15,15,15	0
83	MG	1	3501	1/1	0.98	0.26	31,31,31,31	0
83	MG	x	201	1/1	0.98	0.16	23,23,23,23	0
83	MG	B	1884	1/1	0.98	0.24	41,41,41,41	0
83	MG	AS	3437	1/1	0.98	0.07	61,61,61,61	0
83	MG	BE	301	1/1	0.98	0.22	25,25,25,25	0
83	MG	1	3791	1/1	0.98	0.14	28,28,28,28	0
83	MG	K	301	1/1	0.98	0.14	52,52,52,52	0
83	MG	1	3563	1/1	0.98	0.07	29,29,29,29	0
83	MG	AS	3441	1/1	0.98	0.10	28,28,28,28	0
83	MG	AS	3557	1/1	0.98	0.16	29,29,29,29	0
83	MG	CM	1928	1/1	0.98	0.08	52,52,52,52	0
83	MG	CM	1851	1/1	0.98	0.12	27,27,27,27	0
83	MG	1	3623	1/1	0.98	0.30	51,51,51,51	0
83	MG	AS	3497	1/1	0.98	0.20	26,26,26,26	0
83	MG	BK	201	1/1	0.98	0.11	22,22,22,22	0
83	MG	AS	3498	1/1	0.98	0.22	36,36,36,36	0
83	MG	B	1888	1/1	0.98	0.27	53,53,53,53	0
83	MG	AS	3562	1/1	0.98	0.07	35,35,35,35	0
83	MG	1	3949	1/1	0.98	0.17	49,49,49,49	0
83	MG	4	208	1/1	0.98	0.07	27,27,27,27	0
83	MG	BZ	201	1/1	0.98	0.08	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3512	1/1	0.98	0.14	33,33,33,33	0
83	MG	CM	1940	1/1	0.98	0.08	59,59,59,59	0
83	MG	6	201	1/1	0.98	0.11	37,37,37,37	0
83	MG	6	202	1/1	0.98	0.12	40,40,40,40	0
83	MG	AS	3449	1/1	0.98	0.09	12,12,12,12	0
83	MG	1	3662	1/1	0.98	0.14	32,32,32,32	0
83	MG	B	1895	1/1	0.98	0.23	40,40,40,40	0
83	MG	1	3492	1/1	0.98	0.14	47,47,47,47	0
83	MG	B	1897	1/1	0.98	0.16	52,52,52,52	0
83	MG	1	3704	1/1	0.98	0.16	34,34,34,34	0
83	MG	AS	3403	1/1	0.98	0.19	17,17,17,17	0
83	MG	CM	1871	1/1	0.98	0.20	45,45,45,45	0
83	MG	B	1854	1/1	0.98	0.14	29,29,29,29	0
83	MG	1	3460	1/1	0.98	0.12	39,39,39,39	0
83	MG	1	3494	1/1	0.98	0.17	24,24,24,24	0
83	MG	1	3899	1/1	0.98	0.13	33,33,33,33	0
83	MG	AS	3579	1/1	0.98	0.08	46,46,46,46	0
83	MG	B	1903	1/1	0.98	0.38	82,82,82,82	0
83	MG	AS	3518	1/1	0.98	0.08	26,26,26,26	0
83	MG	1	3461	1/1	0.98	0.13	28,28,28,28	0
83	MG	B	1819	1/1	0.98	0.06	44,44,44,44	0
83	MG	3	201	1/1	0.98	0.14	21,21,21,21	0
83	MG	1	3517	1/1	0.98	0.13	36,36,36,36	0
83	MG	AS	3586	1/1	0.98	0.21	20,20,20,20	0
83	MG	AS	3465	1/1	0.98	0.18	22,22,22,22	0
83	MG	1	3543	1/1	0.98	0.26	32,32,32,32	0
83	MG	1	3649	1/1	0.98	0.12	41,41,41,41	0
83	MG	1	3410	1/1	0.98	0.04	18,18,18,18	0
83	MG	CM	1888	1/1	0.98	0.18	51,51,51,51	0
83	MG	CM	1815	1/1	0.98	0.12	32,32,32,32	0
86	ZN	AK	102	1/1	0.98	0.15	53,53,53,53	0
86	ZN	AN	101	1/1	0.98	0.19	71,71,71,71	0
83	MG	1	3712	1/1	0.98	0.14	23,23,23,23	0
83	MG	CM	1817	1/1	0.98	0.22	42,42,42,42	0
83	MG	1	3906	1/1	0.98	0.09	38,38,38,38	0
83	MG	1	3614	1/1	0.98	0.27	31,31,31,31	0
86	ZN	f	101	1/1	0.98	0.24	80,80,80,80	0
83	MG	AS	3472	1/1	0.98	0.29	31,31,31,31	0
83	MG	AS	3474	1/1	0.98	0.12	29,29,29,29	0
83	MG	B	1868	1/1	0.98	0.31	68,68,68,68	0
83	MG	B	1829	1/1	0.98	0.12	56,56,56,56	0
83	MG	AU	201	1/1	0.98	0.06	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
83	MG	1	3881	1/1	0.98	0.08	26,26,26,26	0
83	MG	CM	1901	1/1	0.98	0.14	14,14,14,14	0
83	MG	1	3463	1/1	0.98	0.09	22,22,22,22	0
83	MG	AS	3729	1/1	0.98	0.17	32,32,32,32	0
83	MG	AS	3434	1/1	0.99	0.07	55,55,55,55	0
83	MG	CM	1911	1/1	0.99	0.19	30,30,30,30	0
83	MG	AS	3723	1/1	0.99	0.14	23,23,23,23	0
83	MG	AS	3618	1/1	0.99	0.15	35,35,35,35	0
83	MG	AS	3404	1/1	0.99	0.25	26,26,26,26	0
83	MG	1	3425	1/1	0.99	0.18	19,19,19,19	0
83	MG	1	3855	1/1	0.99	0.17	32,32,32,32	0
83	MG	AS	3541	1/1	0.99	0.26	25,25,25,25	0
83	MG	CM	1893	1/1	0.99	0.22	30,30,30,30	0
83	MG	1	3785	1/1	0.99	0.22	32,32,32,32	0
83	MG	1	3542	1/1	0.99	0.10	39,39,39,39	0
83	MG	AS	3524	1/1	0.99	0.16	50,50,50,50	0
83	MG	B	1824	1/1	0.99	0.09	30,30,30,30	0
83	MG	AS	3473	1/1	0.99	0.09	25,25,25,25	0
83	MG	1	3407	1/1	0.99	0.23	35,35,35,35	0
83	MG	B	1836	1/1	0.99	0.12	27,27,27,27	0
83	MG	1	3875	1/1	0.99	0.08	33,33,33,33	0
83	MG	1	3404	1/1	0.99	0.18	28,28,28,28	0
83	MG	1	3620	1/1	0.99	0.35	27,27,27,27	0
86	ZN	CH	101	1/1	0.99	0.20	63,63,63,63	0
83	MG	B	1873	1/1	0.99	0.26	44,44,44,44	0
83	MG	B	1922	1/1	0.99	0.05	38,38,38,38	0
83	MG	AX	402	1/1	0.99	0.20	25,25,25,25	0
83	MG	1	3440	1/1	0.99	0.11	32,32,32,32	0
83	MG	AS	3516	1/1	0.99	0.15	27,27,27,27	0
83	MG	B	1950	1/1	0.99	0.19	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.