



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 26, 2026 – 09:04 PM UTC

PDB ID : 8OEQ / pdb_00008oeq
Title : Crystal structure of the Candida albicans 80S ribosome in complex with Paromomycin (250uM)
Authors : Kolosova, O.; Zgadzay, Y.; Yusupov, M.
Deposited on : 2023-03-12
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

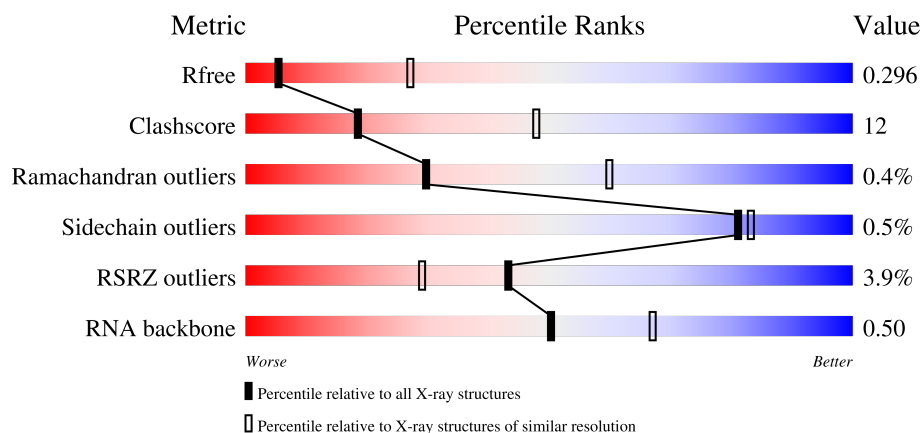
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

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



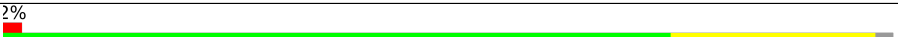
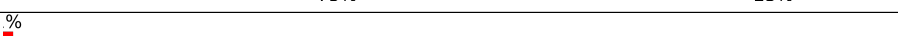
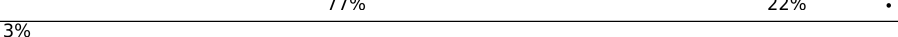
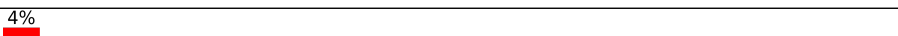
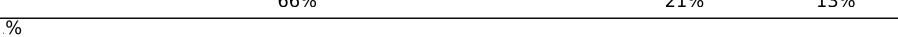
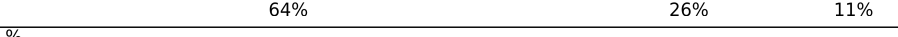
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)
RNA backbone	3983	1048 (3.60-3.00)

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

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

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

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Mol	Chain	Length	Quality of chain
15	u	131	
16	BI	204	
16	v	204	
17	BJ	200	
17	w	200	
18	BK	185	
18	x	185	
19	BL	186	
19	y	186	
20	BM	190	
20	z	190	
21	0	172	
21	BN	172	
22	2	160	
22	BO	160	
23	5	124	
23	BP	124	
24	6	137	
24	BQ	137	
25	7	155	
25	BR	155	
26	8	142	
26	BS	142	
27	9	127	
27	BT	127	

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Mol	Chain	Length	Quality of chain
28	AA	136	
28	BU	136	
29	AB	149	
29	BV	149	
30	AC	63	
30	BW	63	
31	AD	106	
31	BX	106	
32	AE	112	
32	BY	112	
33	AF	131	
33	BZ	131	
34	AG	107	
34	CA	107	
35	AH	113	
35	CB	113	
36	AI	120	
36	CC	120	
37	AJ	99	
37	CD	99	
38	AK	90	
38	CE	90	
39	AL	78	
39	CF	78	
40	AM	51	

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Mol	Chain	Length	Quality of chain
40	CG	51	
41	AN	52	
41	CH	52	
42	AO	25	
42	CI	25	
43	AP	106	
43	CJ	106	
44	AQ	92	
44	CK	92	
45	CL	267	
45	i	267	
46	B	1787	
46	CM	1787	
47	C	261	
47	CN	261	
48	CO	256	
48	D	256	
49	CP	249	
49	E	249	
50	CQ	251	
50	F	251	
51	CR	262	
51	G	262	
52	CS	225	
52	H	225	

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

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Mol	Chain	Length	Quality of chain
65	U	145	
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	

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Mol	Chain	Length	Quality of chain
78	DS	193	
78	h	193	
79	AR	317	
79	DT	317	
80	L1	217	
80	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
81	MG	1	3597	-	-	-	X
81	MG	AS	3729	-	-	-	X

2 Entry composition [i](#)

There are 85 unique types of molecules in this entry. The entry contains 405513 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	3217	Total	C	N	O	P	0	0	0
			68774	30723	12366	22468	3217			
1	AS	3199	Total	C	N	O	P	0	0	0
			68387	30550	12293	22345	3199			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	4	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
4	j	249	Total	C	N	O	S	0	0	0
			1888	1180	376	330	2			
4	AW	249	Total	C	N	O	S	0	0	0
			1888	1180	376	330	2			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 17 is a protein called Ribosomal protein L13.

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

- Molecule 18 is a protein called Ribosomal protein L22.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	5	103	Total	C	N	O		0	0	0
			831	539	138	154				
23	BP	102	Total	C	N	O		0	0	0
			826	536	137	153				

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	8	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
26	BS	119	Total	C	N	O	S	0	0	0
			960	613	172	174	1			

- Molecule 27 is a protein called Ribosomal protein L24.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	AC	62	Total	C	N	O		0	0	0
			493	307	105	81				
30	BW	63	Total	C	N	O	S	0	1	0
			509	317	109	82	1			

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

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

- 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	108	Total	C	N	O	S	0	0	0
			881	556	166	157	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	AF	124	Total	C	N	O	S	0	0	0
			1000	638	194	167	1			
33	BZ	125	Total	C	N	O	S	0	1	0
			1015	649	197	168	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	3	0
			867	558	166	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	111	Total	C	N	O	S	0	4	0
			904	561	186	153	4			

- Molecule 36 is a protein called Ribosomal protein L29.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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	1	0
			764	476	157	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	1	0
			623	398	116	109				

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	AN	52	Total	C	N	O	S	0	0	0
			419	260	86	67	6			
41	CH	52	Total	C	N	O	S	0	1	0
			427	265	89	67	6			

- 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	2	0
			841	531	168	137	5			

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	B	1712	Total	C	N	O	P	0	0	0
			36504	16318	6483	11991	1712			
46	CM	1726	Total	C	N	O	P	0	0	0
			36805	16452	6537	12090	1726			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	D	214	Total	C	N	O	S	0	0	0
			1724	1094	313	313	4			
48	CO	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
49	E	217	Total	C	N	O	S	0	0	0
			1629	1039	289	296	5			
49	CP	216	Total	C	N	O	S	0	0	0
			1620	1033	287	295	5			

- Molecule 50 is a protein called Ribosomal protein S3.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	G	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
52	H	206	Total	C	N	O	S	0	0	0
			1614	1008	301	301	4			
52	CS	195	Total	C	N	O	S	0	0	0
			1530	960	280	286	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	226	Total	C	N	O	S	0	0	0
			1820	1133	351	330	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	182	Total	C	N	O	S	0	0	0
			1466	939	264	263				

- 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	93	Total	C	N	O	S	0	0	0
			783	511	129	142	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	116	Total	C	N	O	S	0	0	0
			885	550	158	172	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	129	Total	C	N	O	S	0	0	0
			1018	649	185	177	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	125	Total	C	N	O	S	0	0	0
			1002	631	184	186	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	142	Total	C	N	O	S	0	0	0
			1169	733	228	205	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	100	Total	C	N	O	S	0	0	0
			790	499	146	143	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	97	Total	C	N	O	S	0	0	0
			770	477	161	126	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
74	DO	81	Total	C	N	O	S	0	0	0
			614	383	110	114	7			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
75	e	62	Total	C	N	O	S	0	0	0
			487	299	98	88	2			
75	DP	59	Total	C	N	O	S	0	0	0
			457	281	89	85	2			

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
77	g	60	Total	C	N	O	S	0	0	0
			474	297	96	79	2			
77	DR	56	Total	C	N	O	S	0	0	0
			444	278	89	75	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
78	h	63	Total	C	N	O	S	0	0	0
			510	320	100	84	6			
78	DS	70	Total	C	N	O	S	0	0	0
			574	362	113	93	6			

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

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

- Molecule 80 is a protein called Ribosomal protein.

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

- Molecule 81 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	1	565	Total	Mg	0	0
			565	565		
81	3	14	Total	Mg	0	0
			14	14		
81	4	16	Total	Mg	0	0
			16	16		
81	j	4	Total	Mg	0	0
			4	4		
81	k	5	Total	Mg	0	0
			5	5		
81	l	2	Total	Mg	0	0
			2	2		
81	m	1	Total	Mg	0	0
			1	1		
81	o	4	Total	Mg	0	0
			4	4		
81	r	3	Total	Mg	0	0
			3	3		
81	s	1	Total	Mg	0	0
			1	1		
81	u	2	Total	Mg	0	0
			2	2		
81	v	2	Total	Mg	0	0
			2	2		
81	w	3	Total	Mg	0	0
			3	3		
81	x	5	Total	Mg	0	0
			5	5		
81	y	2	Total	Mg	0	0
			2	2		
81	z	1	Total	Mg	0	0
			1	1		
81	0	3	Total	Mg	0	0
			3	3		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	2	1	Total 1	Mg 1	0	0
81	5	1	Total 1	Mg 1	0	0
81	6	2	Total 2	Mg 2	0	0
81	8	2	Total 2	Mg 2	0	0
81	9	2	Total 2	Mg 2	0	0
81	AB	1	Total 1	Mg 1	0	0
81	AC	1	Total 1	Mg 1	0	0
81	AD	2	Total 2	Mg 2	0	0
81	AF	4	Total 4	Mg 4	0	0
81	AG	2	Total 2	Mg 2	0	0
81	AH	2	Total 2	Mg 2	0	0
81	AI	1	Total 1	Mg 1	0	0
81	AP	3	Total 3	Mg 3	0	0
81	AQ	1	Total 1	Mg 1	0	0
81	i	1	Total 1	Mg 1	0	0
81	B	169	Total 169	Mg 169	0	0
81	D	1	Total 1	Mg 1	0	0
81	E	2	Total 2	Mg 2	0	0
81	F	1	Total 1	Mg 1	0	0
81	G	1	Total 1	Mg 1	0	0
81	H	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	I	1	Total 1	Mg 1	0	0
81	K	1	Total 1	Mg 1	0	0
81	Q	2	Total 2	Mg 2	0	0
81	V	1	Total 1	Mg 1	0	0
81	Y	1	Total 1	Mg 1	0	0
81	Z	3	Total 3	Mg 3	0	0
81	c	1	Total 1	Mg 1	0	0
81	f	1	Total 1	Mg 1	0	0
81	g	1	Total 1	Mg 1	0	0
81	AR	1	Total 1	Mg 1	0	0
81	AS	387	Total 387	Mg 387	0	0
81	AT	13	Total 13	Mg 13	0	0
81	AU	7	Total 7	Mg 7	0	0
81	AW	3	Total 3	Mg 3	0	0
81	AX	2	Total 2	Mg 2	0	0
81	AY	1	Total 1	Mg 1	0	0
81	BB	3	Total 3	Mg 3	0	0
81	BE	2	Total 2	Mg 2	0	0
81	BF	1	Total 1	Mg 1	0	0
81	BG	2	Total 2	Mg 2	0	0
81	BH	1	Total 1	Mg 1	0	0

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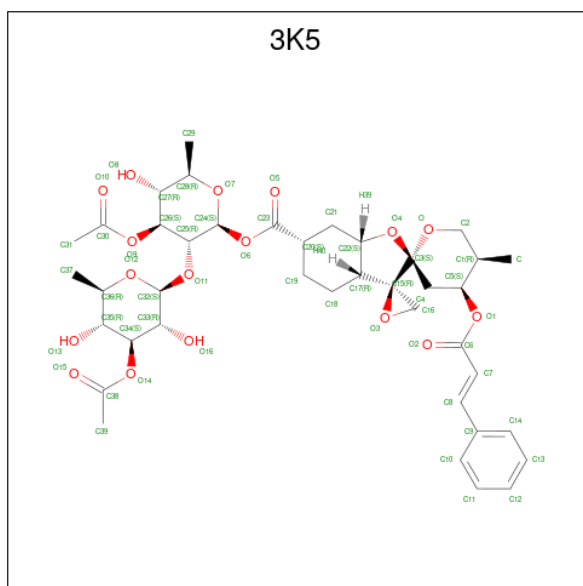
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	BI	1	Total 1	Mg 1	0	0
81	BJ	4	Total 4	Mg 4	0	0
81	BK	2	Total 2	Mg 2	0	0
81	BN	2	Total 2	Mg 2	0	0
81	BO	1	Total 1	Mg 1	0	0
81	BS	1	Total 1	Mg 1	0	0
81	BV	1	Total 1	Mg 1	0	0
81	BZ	4	Total 4	Mg 4	0	0
81	CA	1	Total 1	Mg 1	0	0
81	CJ	1	Total 1	Mg 1	0	0
81	CK	1	Total 1	Mg 1	0	0
81	CM	145	Total 145	Mg 145	0	0
81	CN	1	Total 1	Mg 1	0	0
81	CP	2	Total 2	Mg 2	0	0
81	CQ	4	Total 4	Mg 4	0	0
81	CW	1	Total 1	Mg 1	0	0
81	DA	2	Total 2	Mg 2	0	0
81	DB	4	Total 4	Mg 4	0	0
81	DC	1	Total 1	Mg 1	0	0
81	DG	1	Total 1	Mg 1	0	0
81	DJ	2	Total 2	Mg 2	0	0

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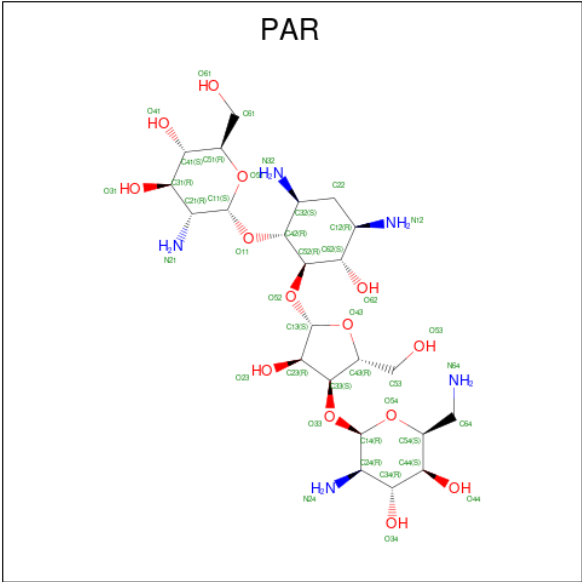
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
81	DQ	1	Total	Mg	0	0
			1	1		
81	CL	3	Total	Mg	0	0
			3	3		

- Molecule 82 is 3-O-acetyl-2-O-(3-O-acetyl-6-deoxy-beta-D-glucopyranosyl)-6-deoxy-1-O-{[(2R,2'S,3a'R,4''S,5''R,6'S,7a'S)-5''-methyl-4''-{[(2E)-3-phenylprop-2-enoyl]oxy}decahydrodispiro[oxirane-2,3'-[1]benzofuran-2'',2''-pyran]-6'-yl]carbonyl}-beta-D-glucopyranose (CCD ID: 3K5) (formula: C₄₀H₅₂O₁₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
82	1	1	Total	C	O	0	0
			57	40	17		
82	CJ	1	Total	C	O	0	0
			57	40	17		

- Molecule 83 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	1	1	Total	C	N	O	0	0
			42	23	5	14		
83	B	1	Total	C	N	O	0	0
			42	23	5	14		
83	AS	1	Total	C	N	O	0	0
			42	23	5	14		
83	AS	1	Total	C	N	O	0	0
			42	23	5	14		
83	AS	1	Total	C	N	O	0	0
			42	23	5	14		
83	CM	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 84 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	AH	1	Total	Zn	0	0
			1	1		
84	AK	1	Total	Zn	0	0
			1	1		
84	AN	1	Total	Zn	0	0
			1	1		
84	AP	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
84	AQ	1	Total 1	Zn 1	0	0
84	c	1	Total 1	Zn 1	0	0
84	f	1	Total 1	Zn 1	0	0
84	CB	1	Total 1	Zn 1	0	0
84	CE	1	Total 1	Zn 1	0	0
84	CK	1	Total 1	Zn 1	0	0
84	DQ	1	Total 1	Zn 1	0	0

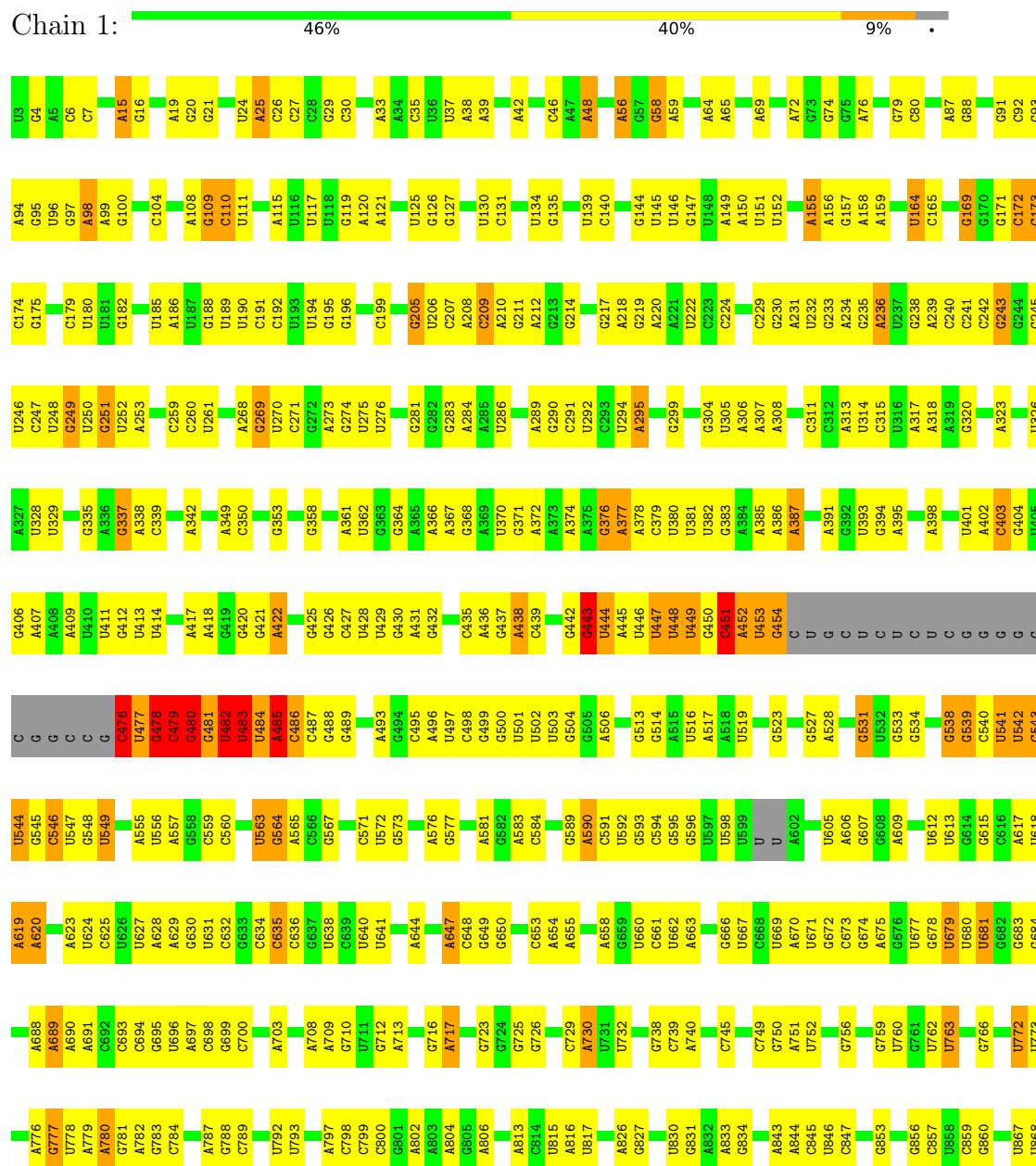
- Molecule 85 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
85	1	9	Total 9	O 9	0	0
85	4	3	Total 3	O 3	0	0
85	B	11	Total 11	O 11	0	0
85	G	1	Total 1	O 1	0	0
85	AS	20	Total 20	O 20	0	0
85	BQ	3	Total 3	O 3	0	0
85	BV	1	Total 1	O 1	0	0

3 Residue-property plots

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

• Molecule 1: 25S ribosomal RNA



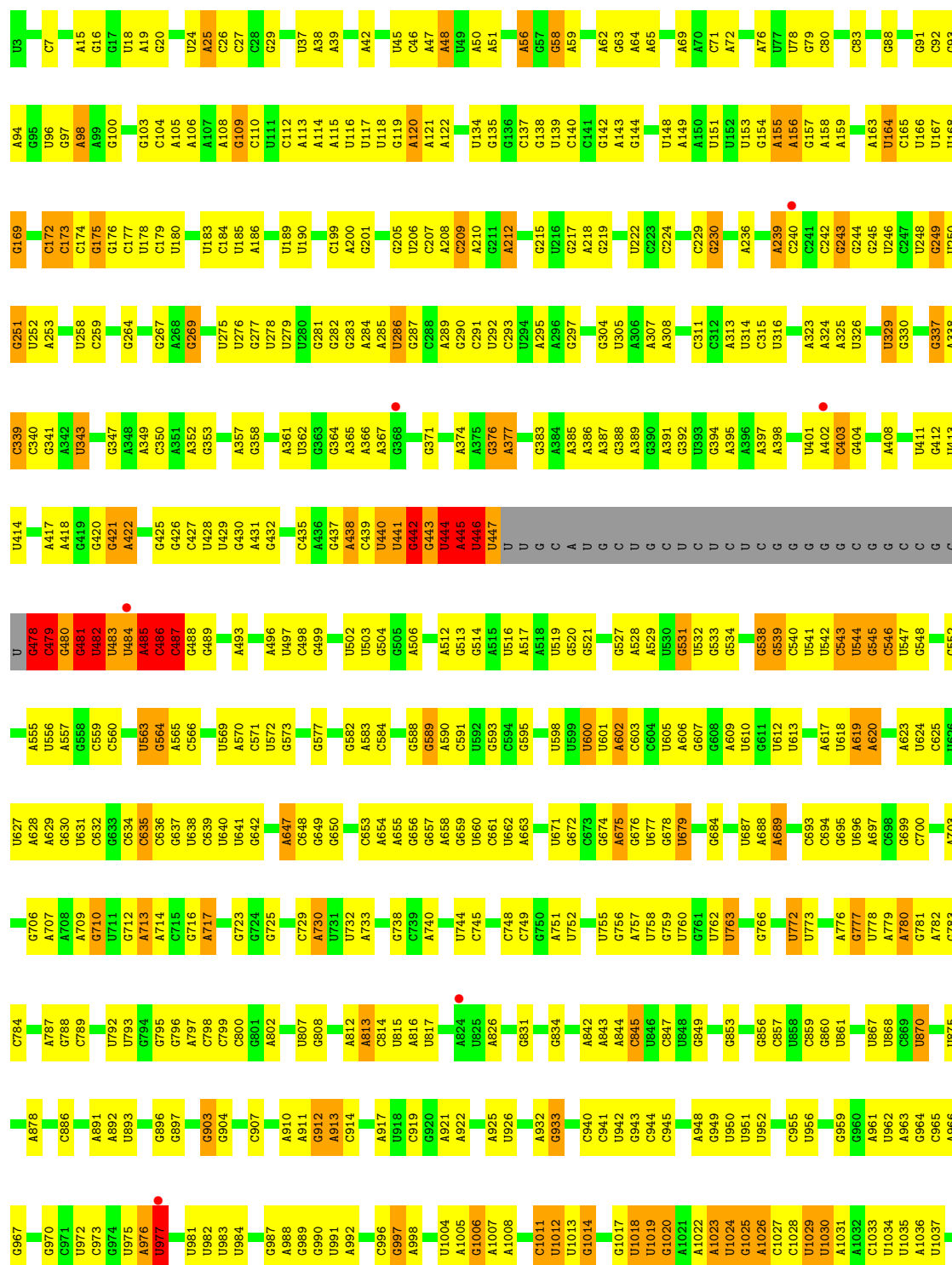




U3320
G3321
A3327
G3331
C3332
U3333
G3334
A3335
G3336
A3337
U3338
G3343
U3344
G3351
U3352
C3353
U3361

• Molecule 1: 25S ribosomal RNA

Chain AS:  %

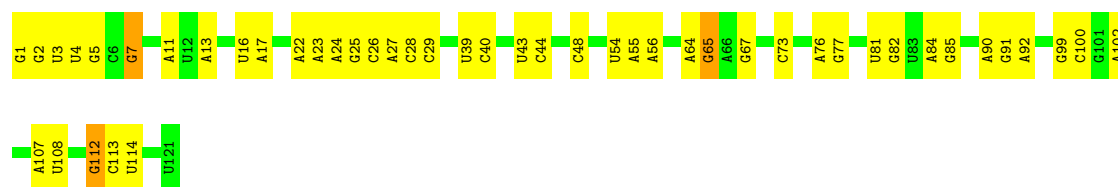


G2143	G2147	G2148	G2149	G2155	A2158	C2159	G2163	G2164	G2165	A2166	U2167	U2171	G2172	C2173	C2174	C2182	U2183	G2184	A2185	A2186	U2187	G2188	A2191	A2192	A2193	G2194	U2195	G2196	A2197	A2198	G2199	A2200	A2201	A2202	A2206	A2207	A2210	A2211	G2216	A2222	G2227	U2232	A2233	C2234	U2235	U2236							
G	G	G	G	A2064	C2065	G2066	U2067	U2068	U2069	A2070	A2071	A2078	C2079	U2080	A2084	A2085	C2086	U2087	G2088	G2089	U2090	A2091	C2092	G2093	G2099	G2100	U2107	G2108	A2109	U2115	A2116	A2117	U2118	U2119	A2120	A2121	A2122	U2126	A2127	G2128	C2129	A2130	U2131	U2134	G2135	A2136	U2137	G2138	U2139	U2236			
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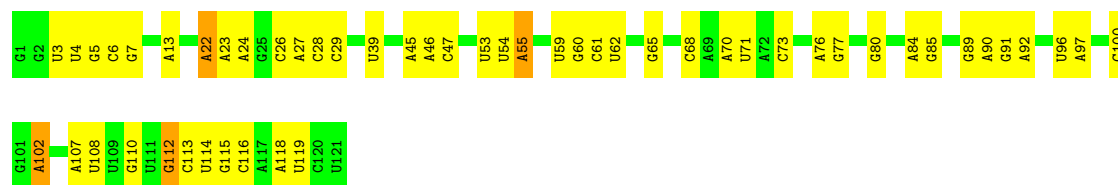
• Molecule 2: 5S ribosomal RNA

Chain 3:  61% 36% .



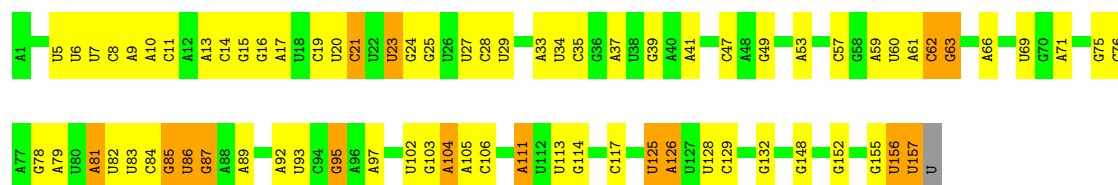
• Molecule 2: 5S ribosomal RNA

Chain AT:  57% 40% .



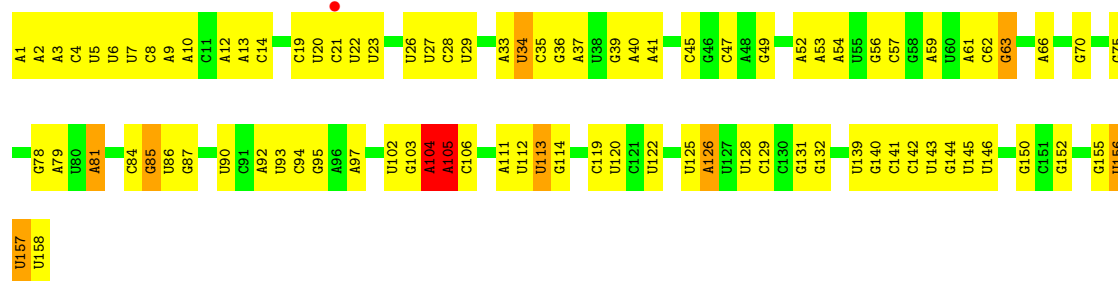
• Molecule 3: 5.8S ribosomal RNA

Chain 4:  53% 37% 9% .



• Molecule 3: 5.8S ribosomal RNA

Chain AU:  43% 51% 5% .



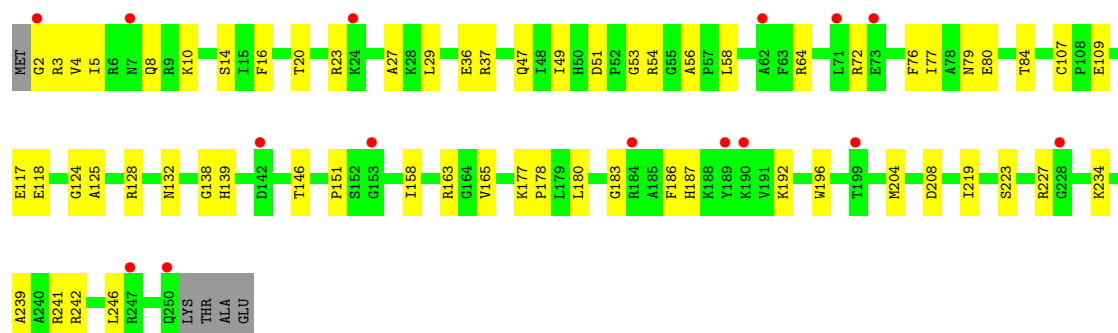
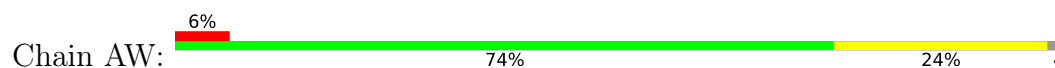
• Molecule 4: 60S ribosomal protein L2-B

Chain j:  75% 23% .

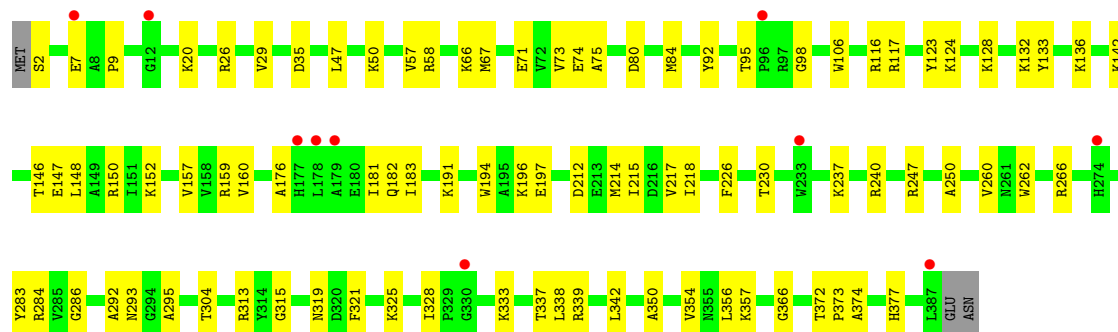
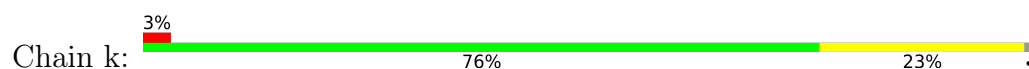




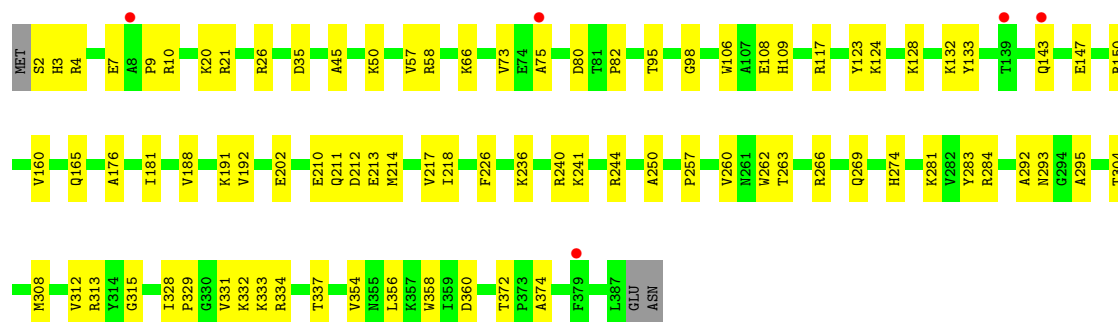
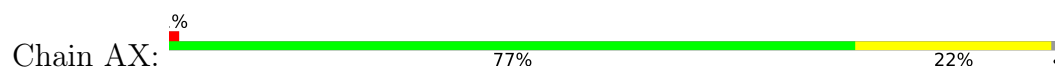
• Molecule 4: 60S ribosomal protein L2-B



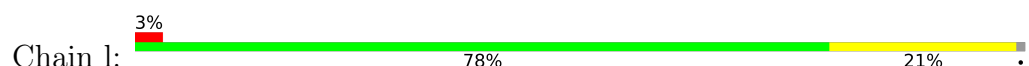
• Molecule 5: 60S ribosomal protein L3

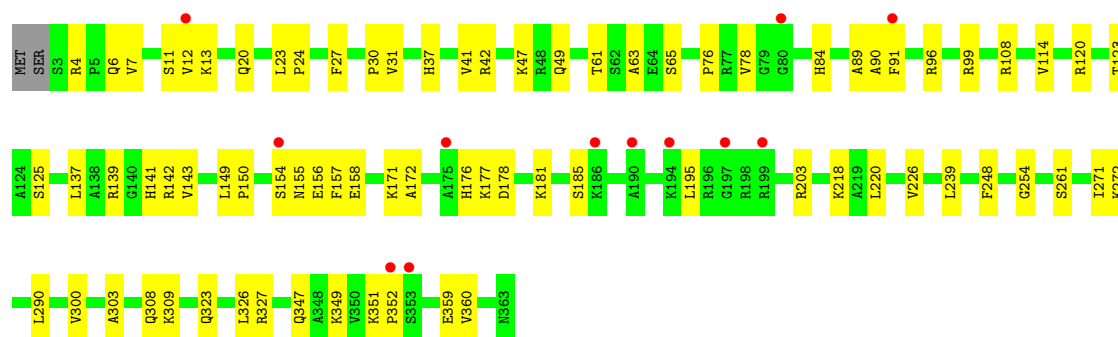


• Molecule 5: 60S ribosomal protein L3

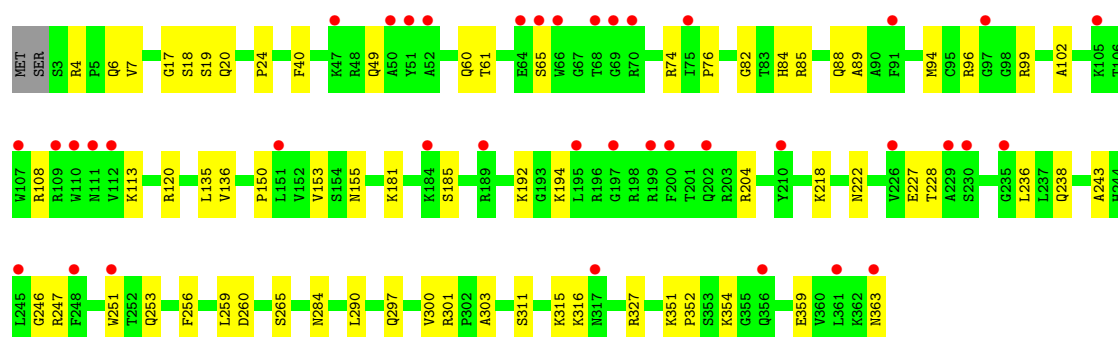
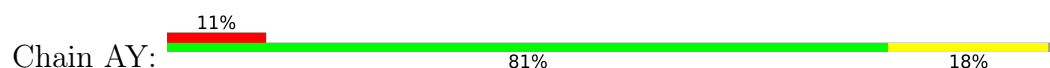


• Molecule 6: 60S ribosomal protein L4-B

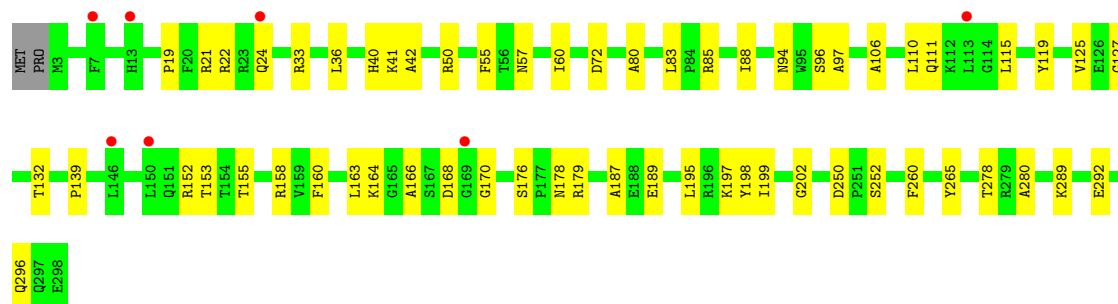
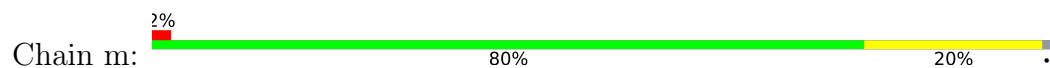




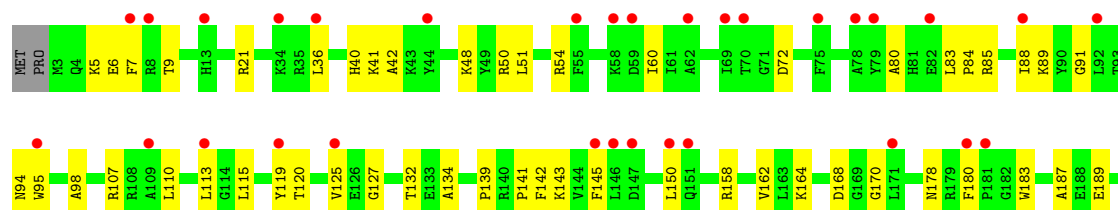
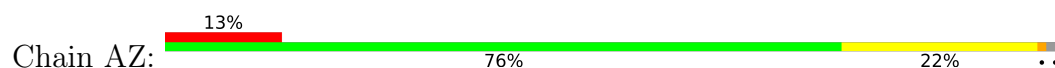
• Molecule 6: 60S ribosomal protein L4-B



• Molecule 7: Uncharacterized protein CaJ7.0206



• Molecule 7: Uncharacterized protein CaJ7.0206





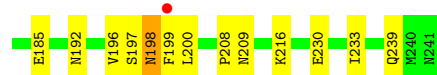
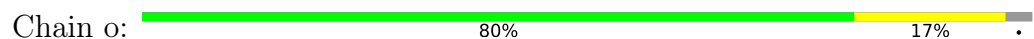
• Molecule 8: 60S ribosomal protein L6



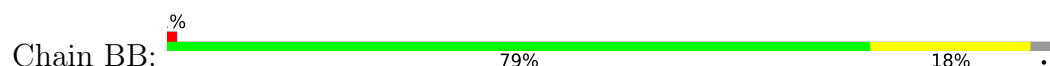
• Molecule 8: 60S ribosomal protein L6



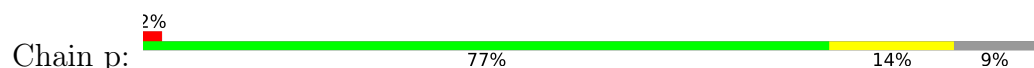
• Molecule 9: 60S ribosomal protein L7-A

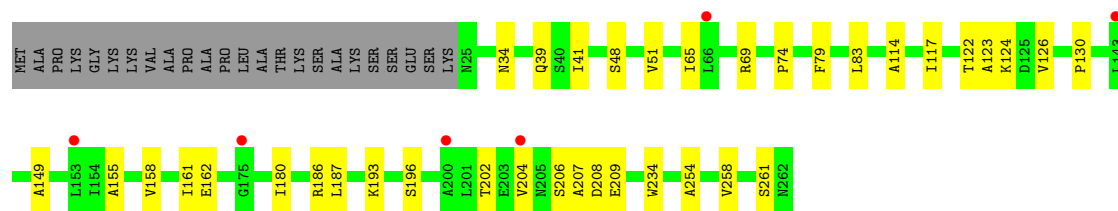


• Molecule 9: 60S ribosomal protein L7-A

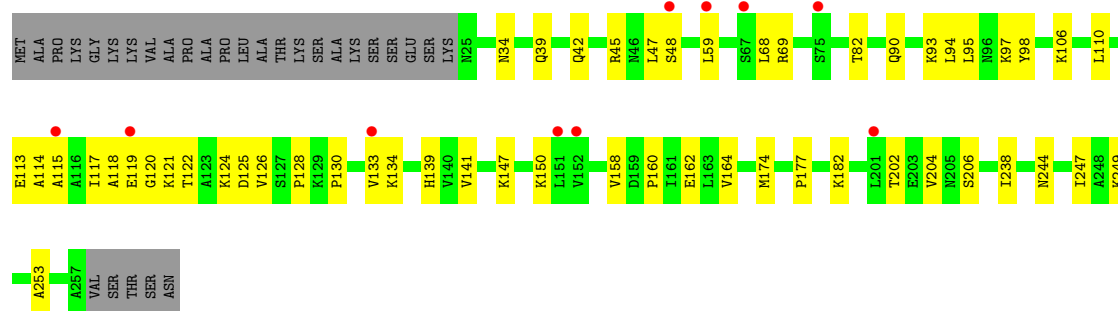
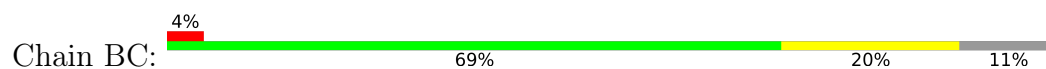


• Molecule 10: 60S ribosomal protein L8

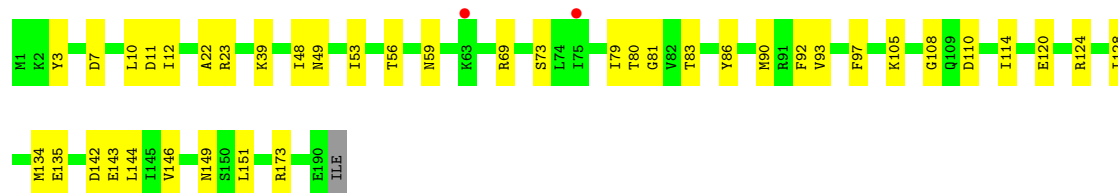
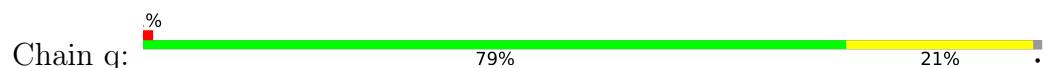




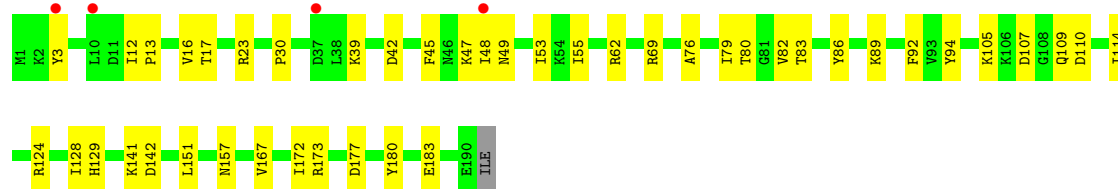
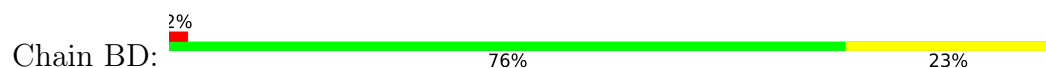
• Molecule 10: 60S ribosomal protein L8



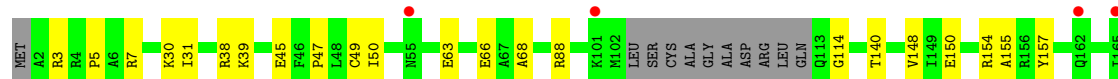
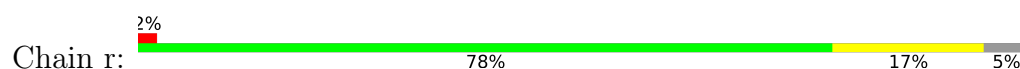
• Molecule 11: 60S ribosomal protein L9-B



• Molecule 11: 60S ribosomal protein L9-B

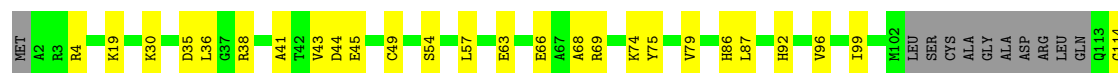


• Molecule 12: 60S ribosomal protein L10

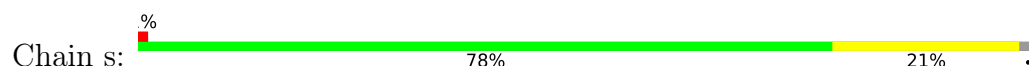




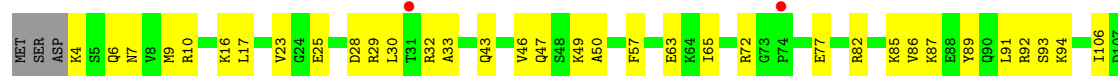
- Molecule 12: 60S ribosomal protein L10



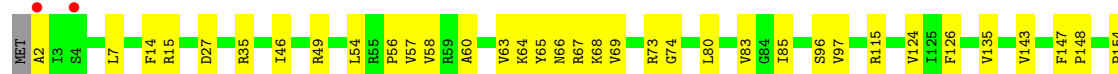
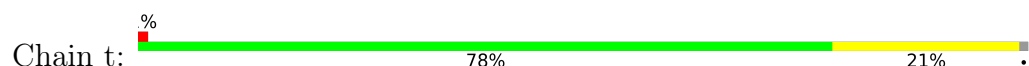
- Molecule 13: 60S ribosomal protein L11-B



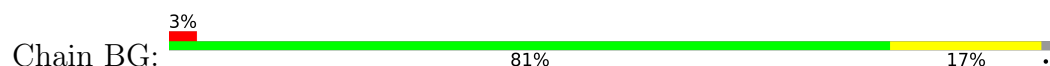
- Molecule 13: 60S ribosomal protein L11-B

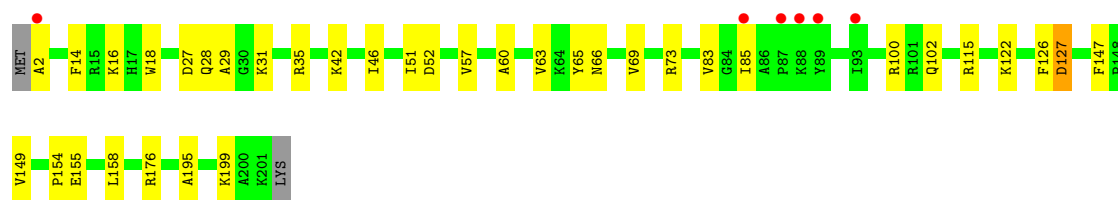


- Molecule 14: 60S ribosomal protein L13

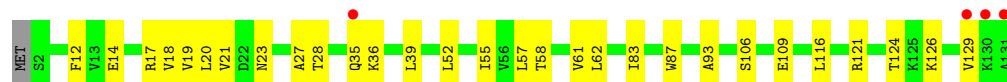
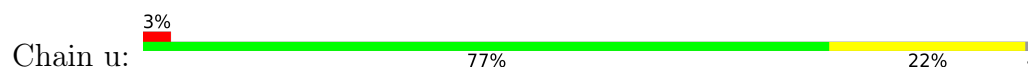


- Molecule 14: 60S ribosomal protein L13

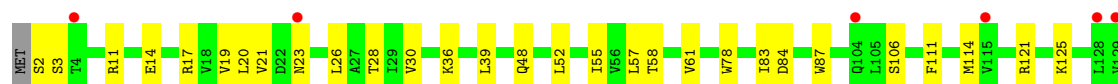
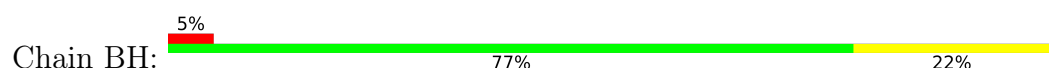




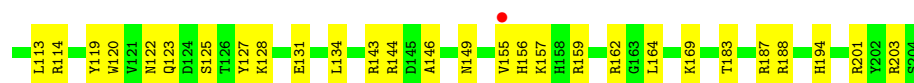
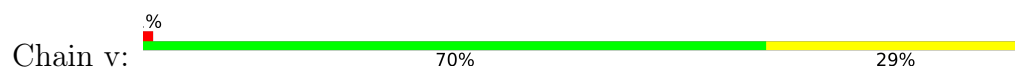
- Molecule 15: 60S ribosomal protein L14-B



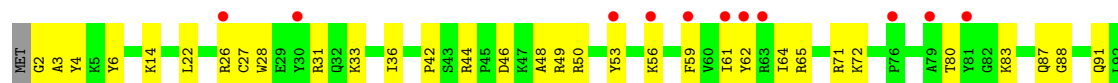
- Molecule 15: 60S ribosomal protein L14-B



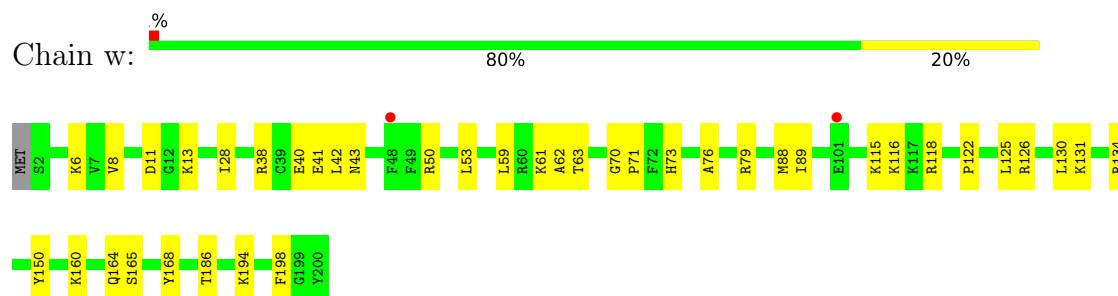
- Molecule 16: 60S ribosomal protein L15-A



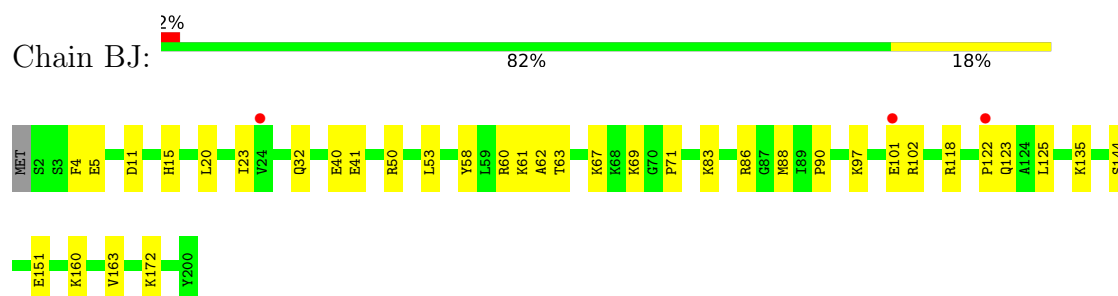
- Molecule 16: 60S ribosomal protein L15-A



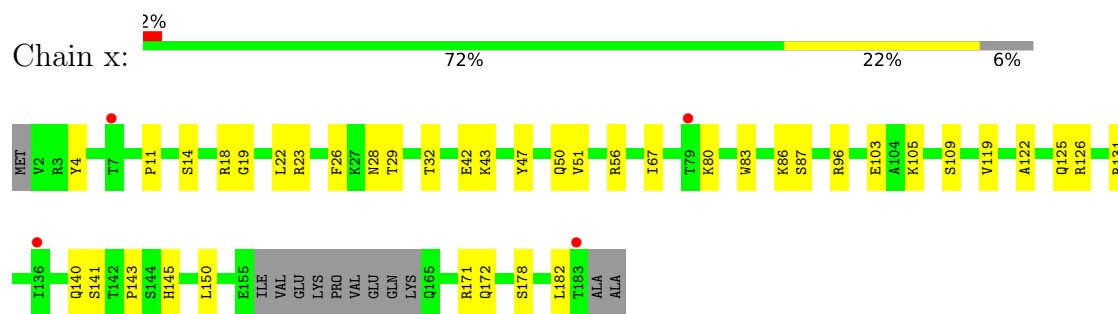
- Molecule 17: Ribosomal protein L13



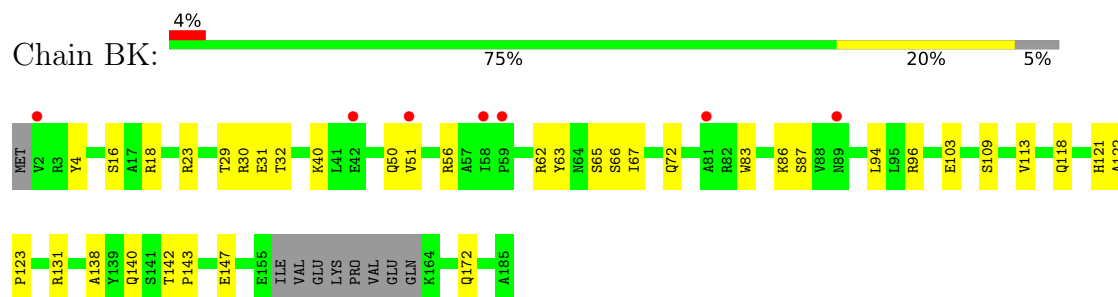
- Molecule 17: Ribosomal protein L13



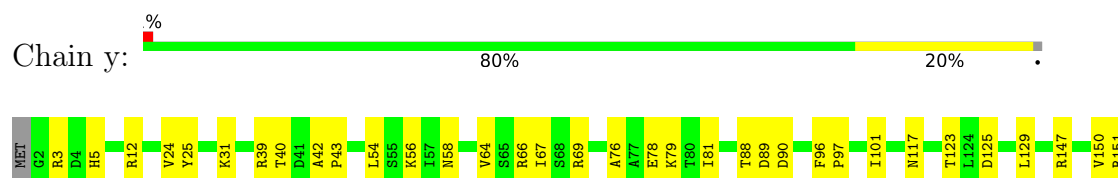
- Molecule 18: Ribosomal protein L22



- Molecule 18: Ribosomal protein L22

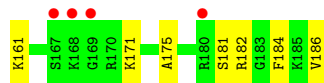
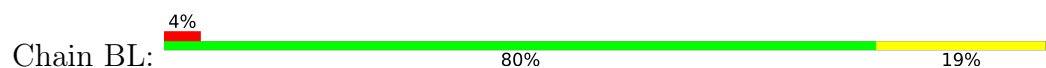


- Molecule 19: 60S ribosomal protein L18-A

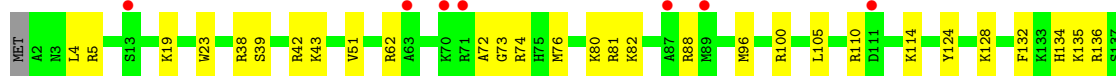
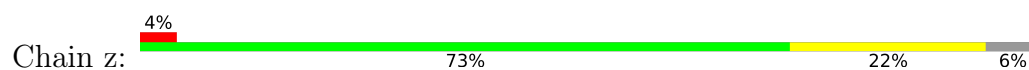




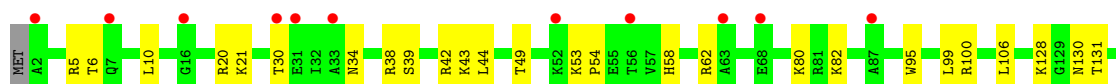
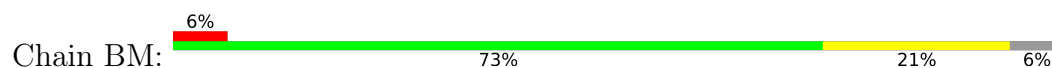
- Molecule 19: 60S ribosomal protein L18-A



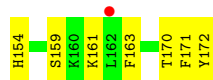
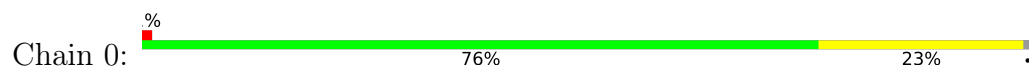
- Molecule 20: 60S ribosomal protein L19-A



- Molecule 20: 60S ribosomal protein L19-A

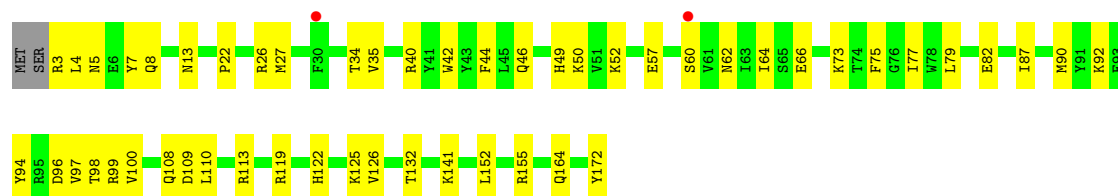


- Molecule 21: 60S ribosomal protein L20

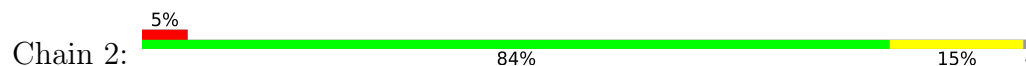


- Molecule 21: 60S ribosomal protein L20

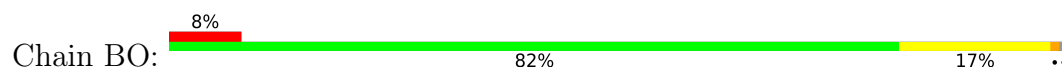




- Molecule 22: 60S ribosomal protein L21-A



- Molecule 22: 60S ribosomal protein L21-A



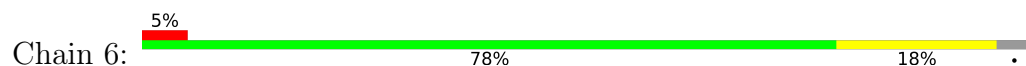
- Molecule 23: 60S ribosomal protein L22-B

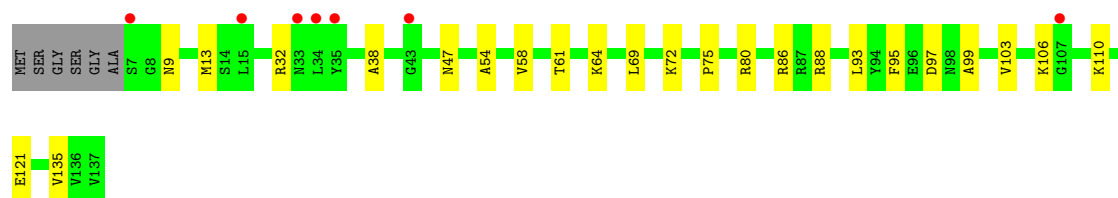


- Molecule 23: 60S ribosomal protein L22-B

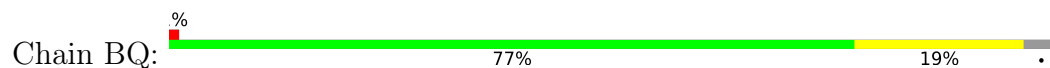


- Molecule 24: 60S ribosomal protein L23-A

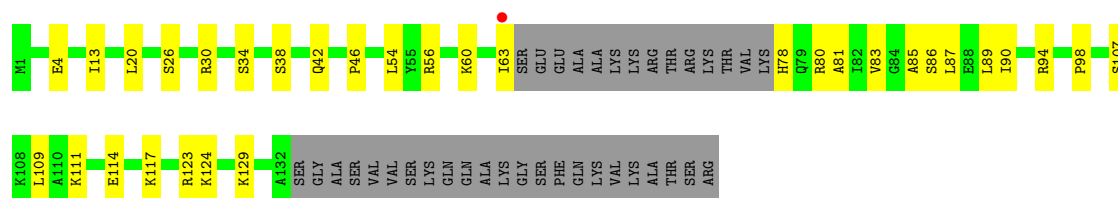




- Molecule 24: 60S ribosomal protein L23-A



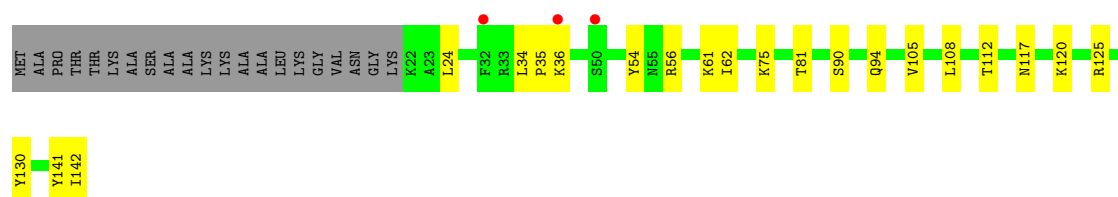
- Molecule 25: 60S ribosomal protein L24-A



- Molecule 25: 60S ribosomal protein L24-A

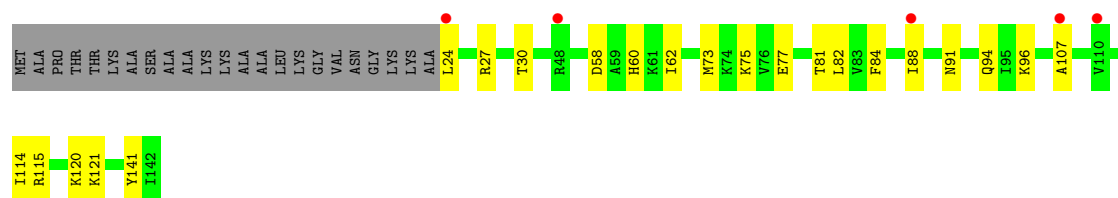


- Molecule 26: 60S ribosomal protein L25

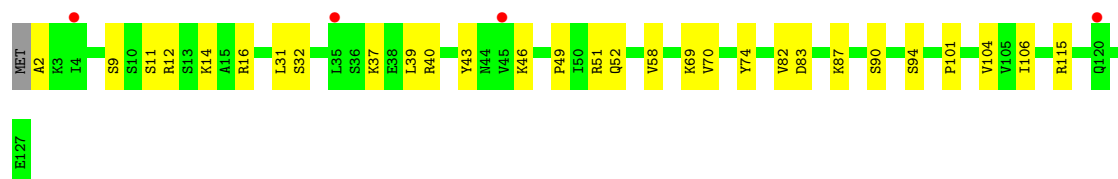
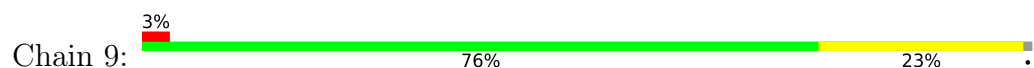


- Molecule 26: 60S ribosomal protein L25

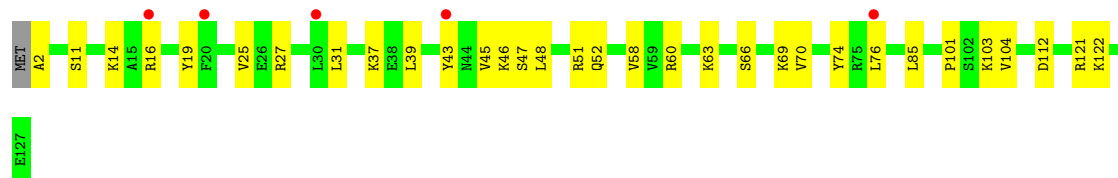
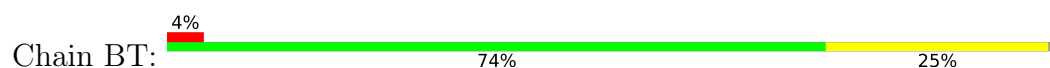




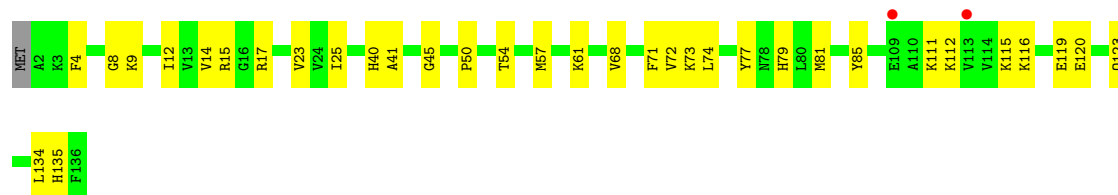
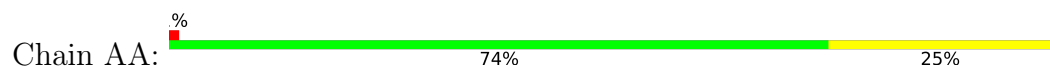
- Molecule 27: Ribosomal protein L24



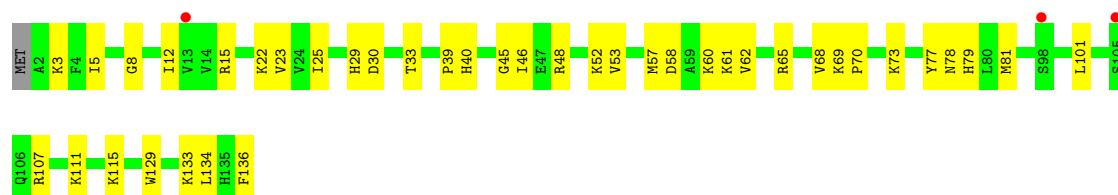
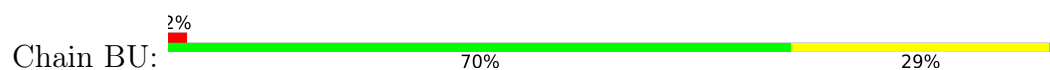
- Molecule 27: Ribosomal protein L24



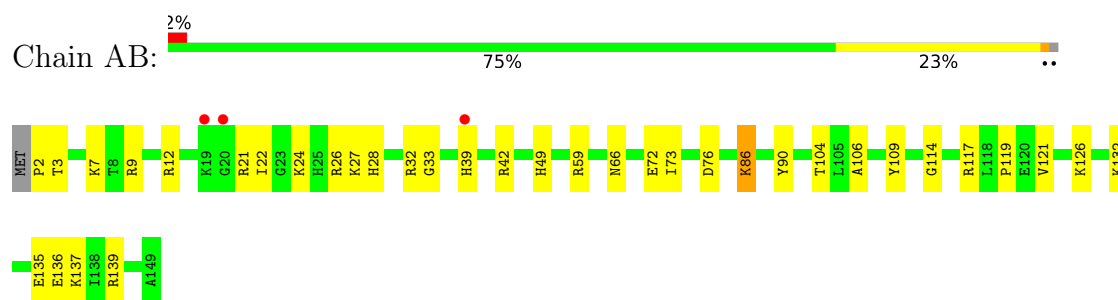
- Molecule 28: 60S ribosomal protein L27



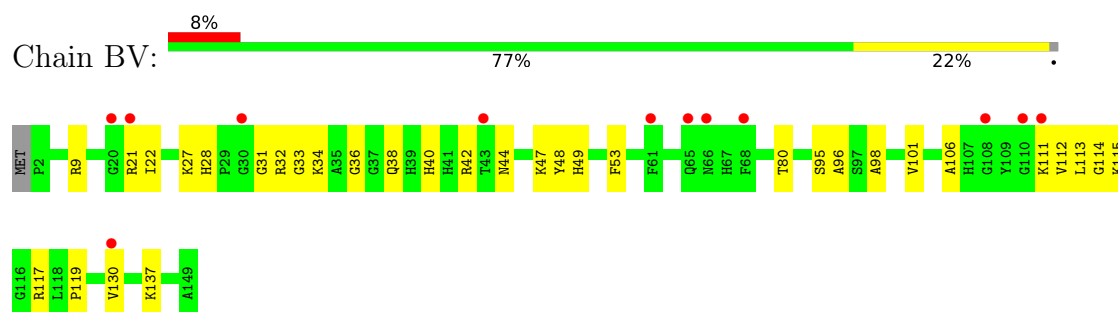
- Molecule 28: 60S ribosomal protein L27



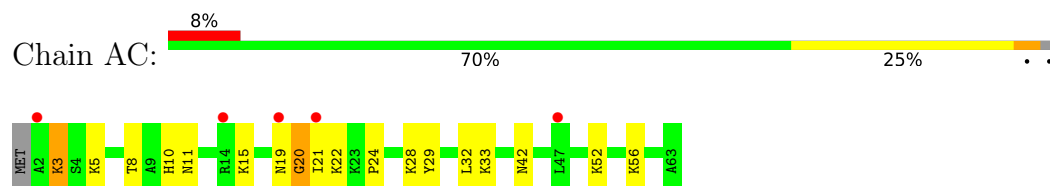
- Molecule 29: 60S ribosomal protein L28



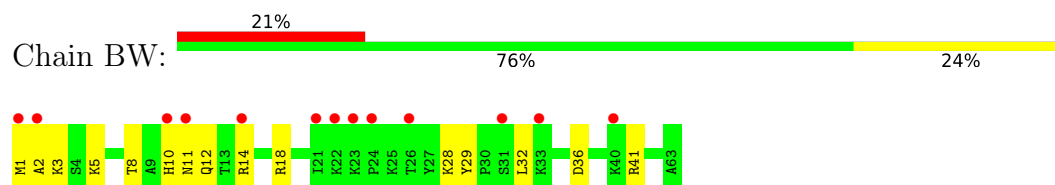
- Molecule 29: 60S ribosomal protein L28



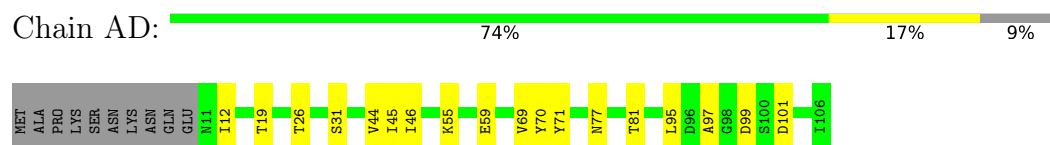
- Molecule 30: 60S ribosomal protein L29



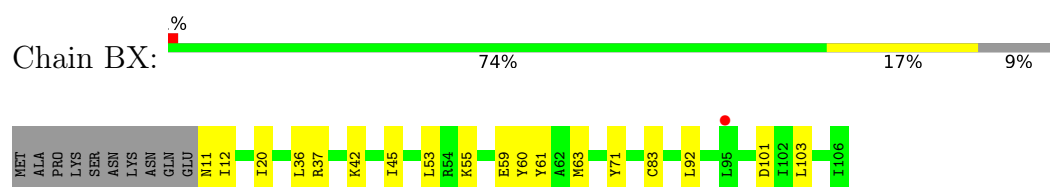
- Molecule 30: 60S ribosomal protein L29



- Molecule 31: 60S ribosomal protein L30

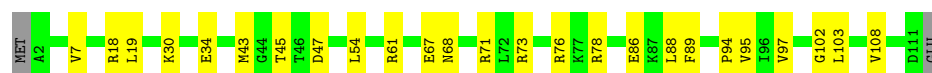


- Molecule 31: 60S ribosomal protein L30



- Molecule 32: 60S ribosomal protein L31-B

Chain AE:  76% 22% .



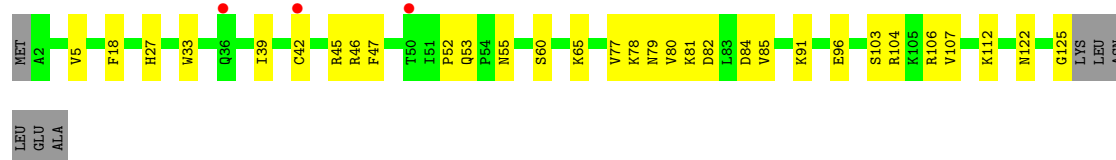
- Molecule 32: 60S ribosomal protein L31-B

Chain BY:  3% 76% 21% .



- Molecule 33: 60S ribosomal protein L32

Chain AF:  2% 71% 24% 5%



- Molecule 33: 60S ribosomal protein L32

Chain BZ:  5% 70% 25% 5%



- Molecule 34: 60S ribosomal protein L33-A

Chain AG:  % 77% 22% .

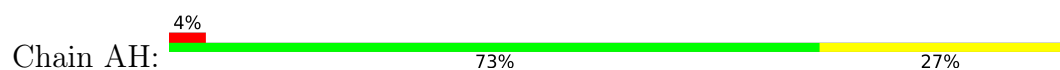


- Molecule 34: 60S ribosomal protein L33-A

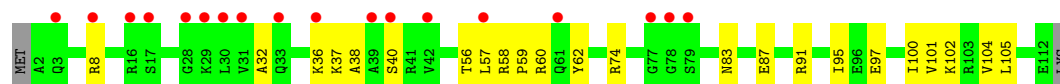
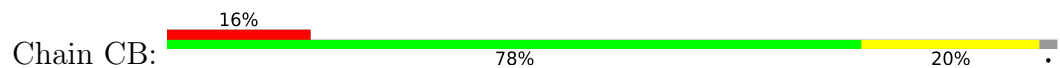
Chain CA:  3% 81% 18% .



- Molecule 35: 60S ribosomal protein L34-B



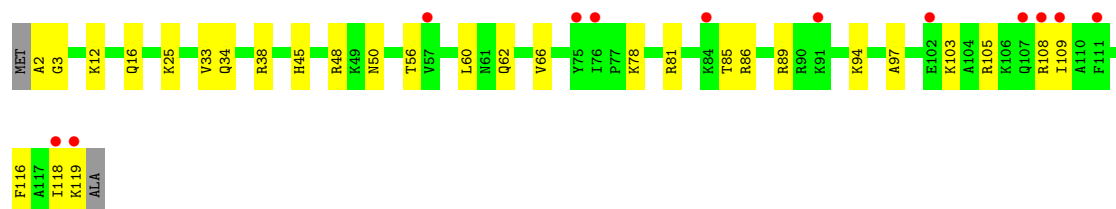
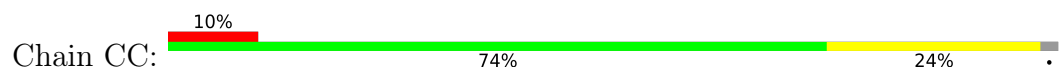
- Molecule 35: 60S ribosomal protein L34-B



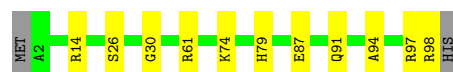
- Molecule 36: Ribosomal protein L29



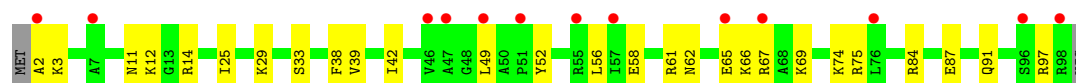
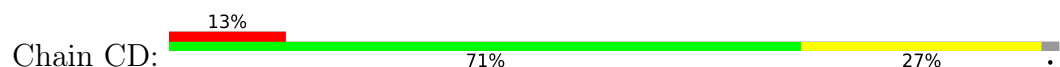
- Molecule 36: Ribosomal protein L29



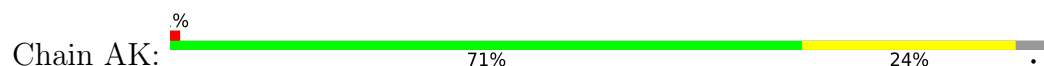
- Molecule 37: 60S ribosomal protein L36



- Molecule 37: 60S ribosomal protein L36

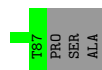


- Molecule 38: 60S ribosomal protein L37-B

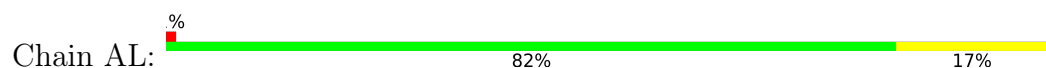




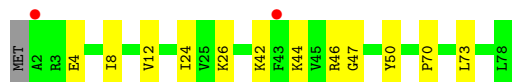
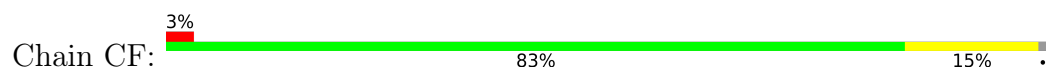
- Molecule 38: 60S ribosomal protein L37-B



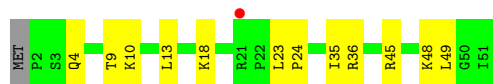
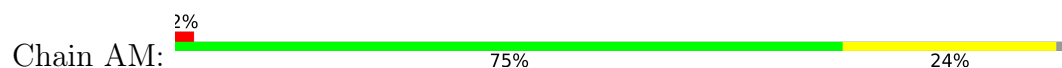
- Molecule 39: 60S ribosomal protein L38



- Molecule 39: 60S ribosomal protein L38



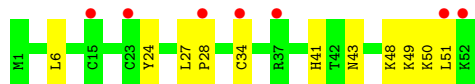
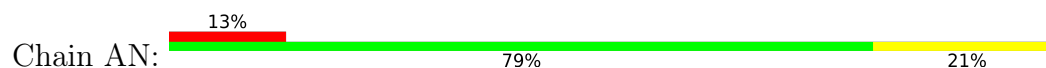
- Molecule 40: 60S ribosomal protein L39



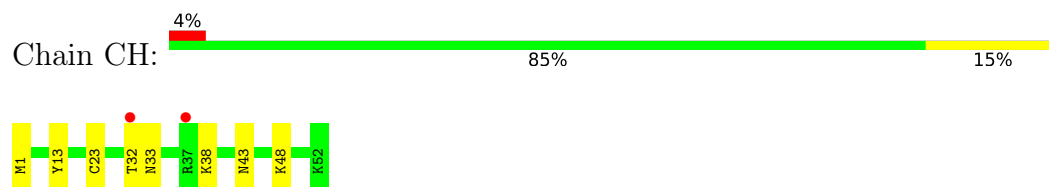
- Molecule 40: 60S ribosomal protein L39



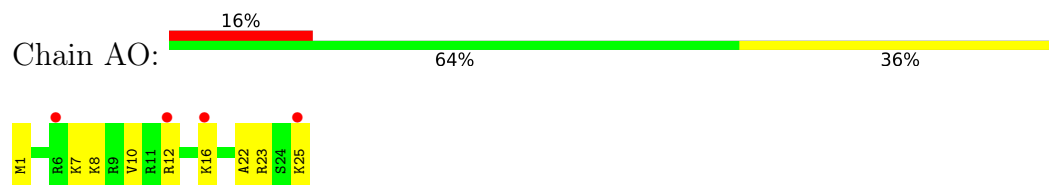
- Molecule 41: 60S ribosomal protein L40-B



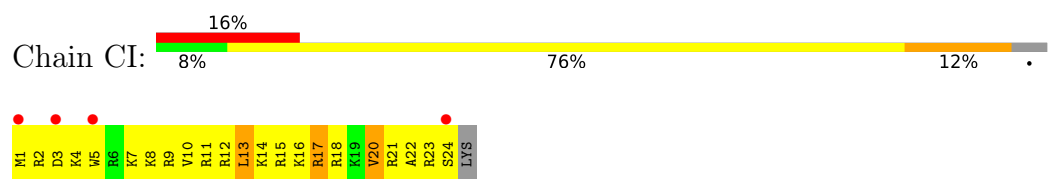
- Molecule 41: 60S ribosomal protein L40-B



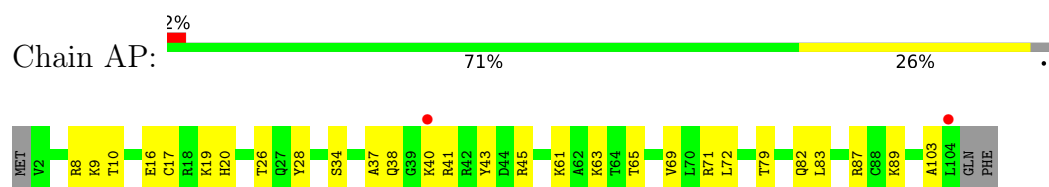
- Molecule 42: 60S ribosomal protein L41



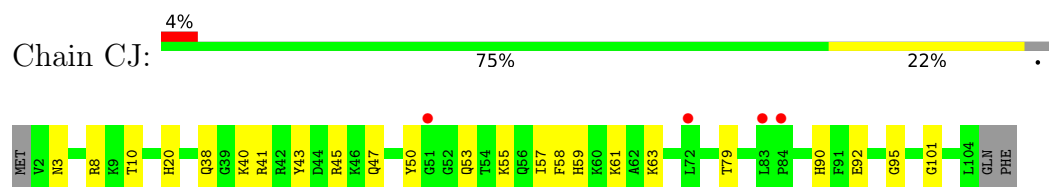
- Molecule 42: 60S ribosomal protein L41



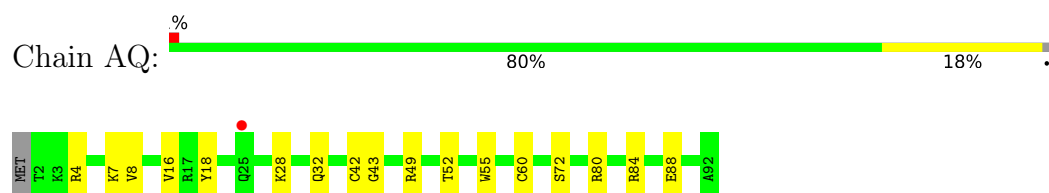
- Molecule 43: 60S ribosomal protein L42-B



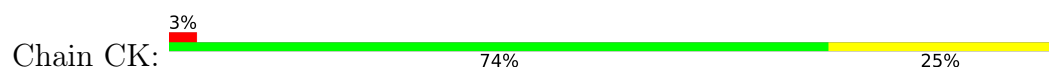
- Molecule 43: 60S ribosomal protein L42-B

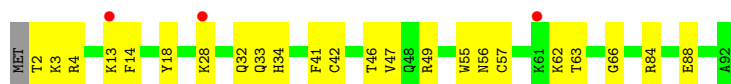


- Molecule 44: 60S ribosomal protein L43-A

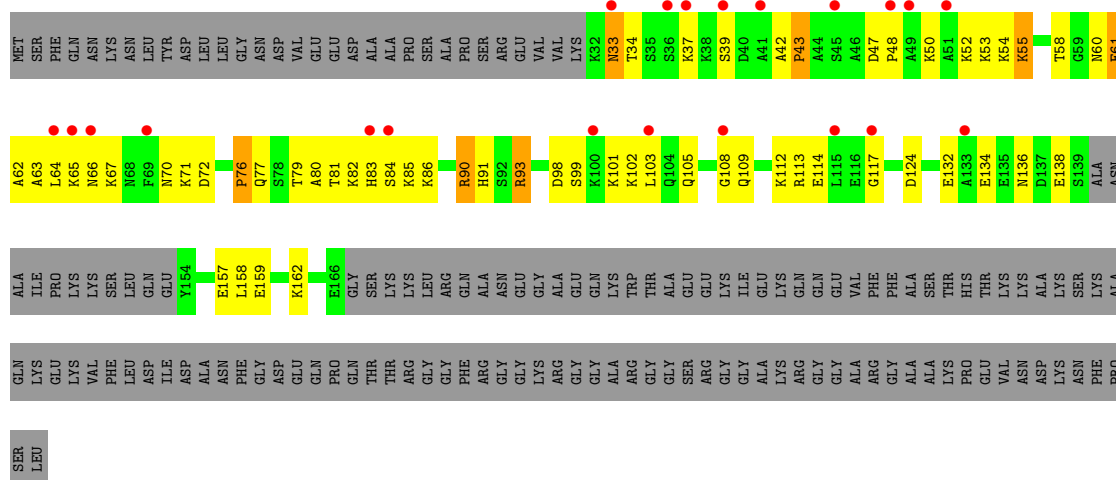


- Molecule 44: 60S ribosomal protein L43-A

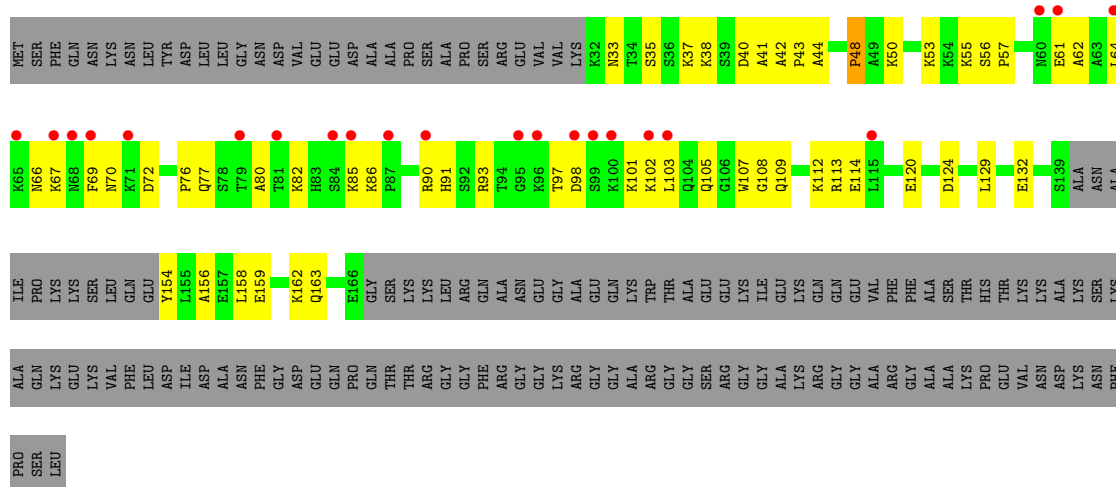
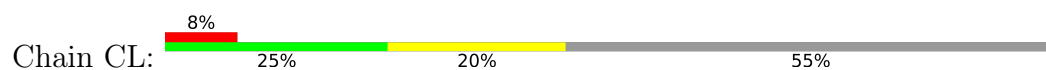




- Molecule 45: 60S ribosomal protein CAALFM_C304810CA



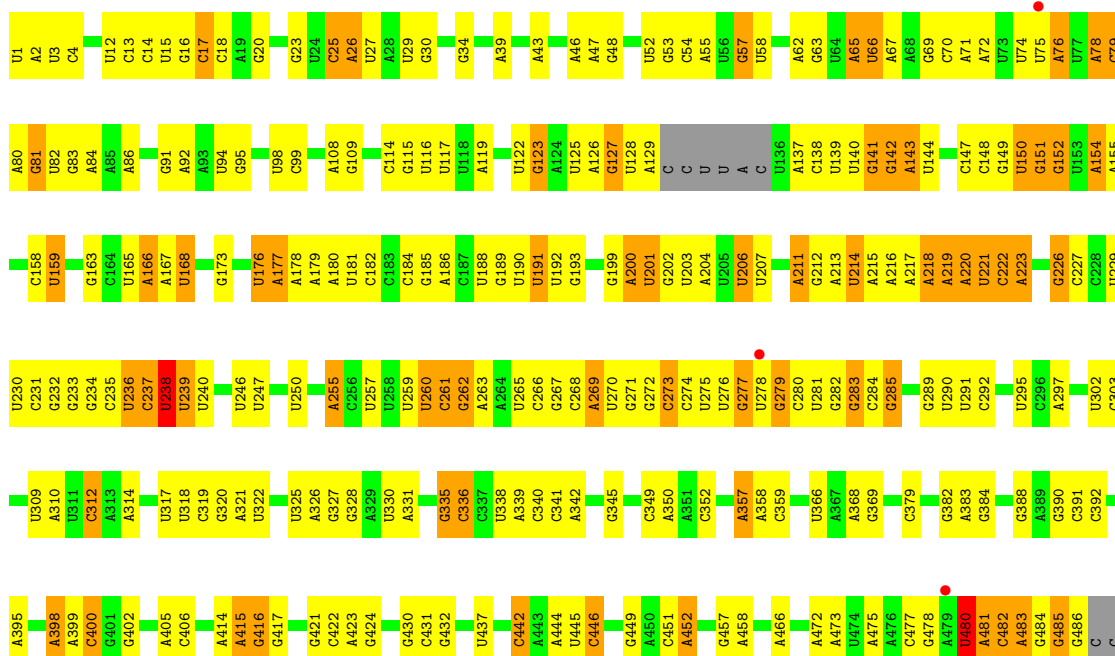
- Molecule 45: 60S ribosomal protein CAALFM_C304810CA



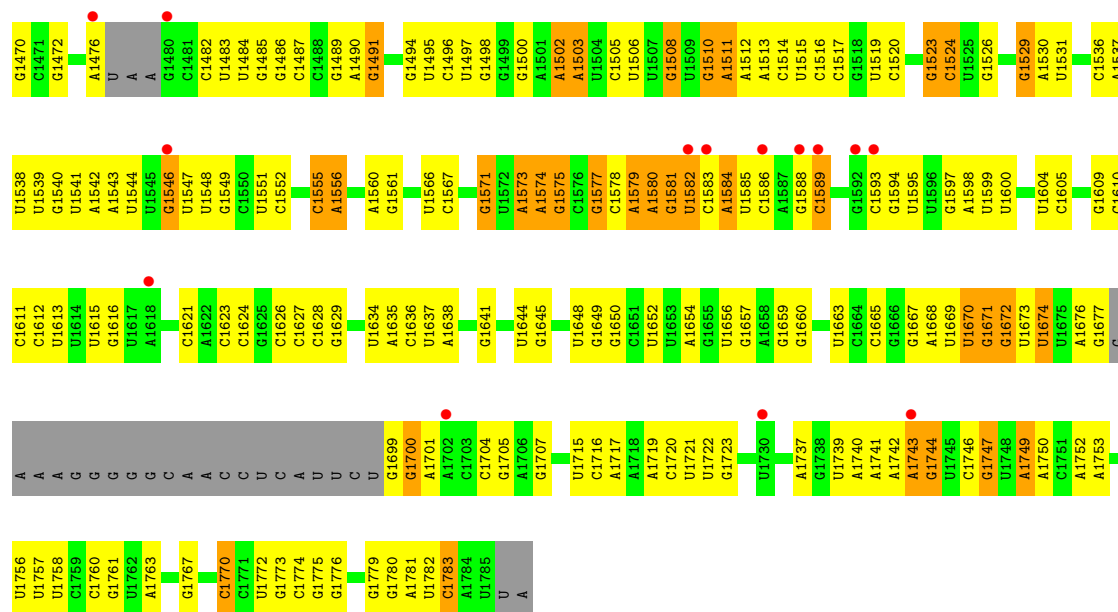
- Molecule 46: 18S ribosomal RNA



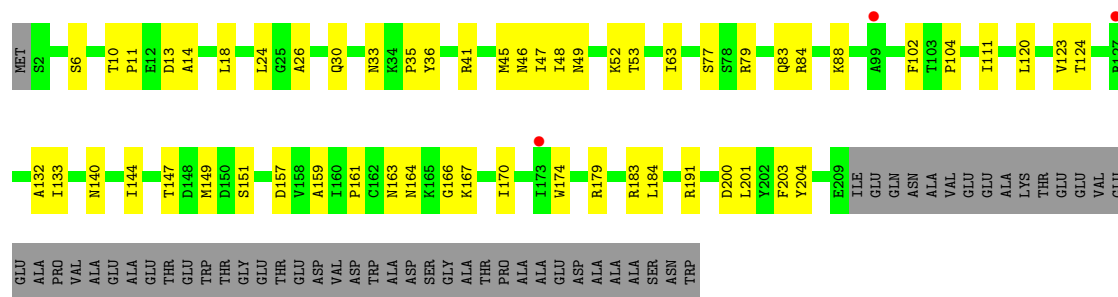
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A1156	A1073	U1003	U917	U639	A773	C	6639	G555	C	G402	A314	U229	U153	G83
C1157	A1074	A1004	A918	A940	U774	A	U644	U556	C	A405	U317	U230	A154	A84
C1158	A1075	A1005	A919	A841	A775	U	U645	C557	C	C406	U318	G231	A155	A85
C1159	A1076	U1006	U920	U842	U776	U	U646	U558	U	C407	C319	G232	U156	A86
U1160	A1077	A1007	G921	G843	U777	U	U647	G559	U	C408	G320	G233	U157	C87
G1161	A1078	U1008	G922	A844	U778	A	U648	G560	U	C409	A321	G234	C158	
	U1079	A1011	A924	U845	U779	U	U649	U561	U	C410		U235	U159	A92
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C1165	C1081	C1013	A926	A847	G781	G	U651	C563	G	G412	A326	G237	G161	U94
U1166	A1082	U1014	A927	A848	U782	C	U652	C564	G	G413	G327	U238	G96	G95
U1167	U1083	U1015	U932	G853	U783	G	U653	A565	U	A414	G328	G241	U165	C97
G1168	G1085	G1017	A933	A854	G784	A	U654	G566	C	G415	A329		A166	U96
A1169	G1086	C1018	C934	G855	G785		U655	G567	U	G416	U330	U247	A167	C99
U1170	G1087	U1019	C935	G856	G786	A	U656	U568	U	A417	U331	U248	U168	
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G1180	G1096	U1023	A938	U859	G789		U659	G575	U	C420	U334	U251	A105	A106
A1181	U1100	A1024	U939	U860	G790		U660	U576	U	C421	U335	U252	U176	
C1182	A1101	G1025	A940	G861	A791		U661	U577	U	G422	U336	U253	U177	A108
G1183	U1102	G1026	U943	G862	A792		U662	U578	U	C423	U337	U254	A178	G109
G1184	G1103	G1027	U944	G863	U793		U663	U579	U	C424	U338	U255	U110	U111
G1185	G1104	A1028	U945	U864	A794		U664	U580	U	C425	U339	U256	A179	A180
U1186	U1105	U1029	U946	A869	G795		U665	U581	U	C426	U340	U257	G114	G115
A1187	C1106	C1030	C947	G870	G796		U666	U582	U	C427	U341	U258	U181	U116
		G1031		U871	U733		U667	A583	U	C428	U342	U259	G189	U117
G1192	G1115	U1032	A951	A872	U734		U668	G584	U	C429	U343	U260	U190	U118
A1193	A1118	G1033	A952	U873	U735		U669	C585	U	C430	U344	U261	U191	A119
		U1034	U953	U874	A737		U670	U586	U	C431	U345	U262	U192	
G1198		G1035	C954	C875	A738		U671	C587	U	C432	U346	U263	G193	U122
U1121	U1121	U1036	A958	A876	A739		U672	C588	U	C433	U347	U264	G123	G124
A1122	A1123	U1041	A959	G877	A740		U673	U589	U	C434	U348	U265	A124	A125
G1203	U1203	U1042	C960	U878	A741		U674	A590	U	C435	U349	U266	U201	U202
A1204	A1127	U1043	G961	U879	U744		U675	A591	U	C436	U350	U267	G126	G127
C1205	U1128	U1044	A962	U880	A745		U676	A592	U	C437	U351	U268	U203	U204
A1206	U1129	U1045	A963	C882	G746		U677	C593	U	C438	U352	U269	U205	A129
C1207	U1130	U1046	A964	A883	A747		U678	A597	U	C439	U353	U270	U206	C130
A1208	U1131	U1047	G965	G884	G748		U679	U598	U	C440	U354	U271	U207	
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A1211	G1134	A1050	C975	G887	U751		U682	A604	U	C443	U357	U274	U213	A137
A1212	G1135	C1051	C976	U888	U752		U683	G605	U	C444	U358	U275	U214	C138
G1213			G976	U889	U753		U684	U609	U	C445	U359	U276	A215	U139
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A1215	G1138	U1055	A978	U892	U755		U686	U612	U	C447	U361	U278	A217	G141
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A1227	A1148	A1066	G832	U910	U765		U696	U622	U	C457	U371	U288	A227	
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A1229	G1150	G1068	C834	C912	G767		U698	U624	U	C459	U373	U290	A229	
G1230	A1151	U1069	A835	U913	U768		U699	U625	U	C460	U374	U291	A230	
C1231	G1152	A1071	U836	U914	U769		U700	U626	U	C461	U375	U292	A231	
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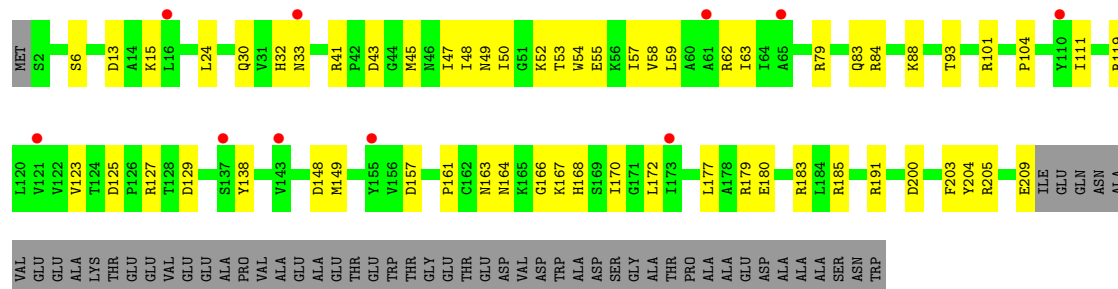
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C1427	U1353	G1284	U1216	A1151	A1078	C1007	A924	G853	U785	G714	C652	C582	G507
U1428	A1355	A1285	U1217	G1152	G1079	G1007	A925	A854	G786	G715	G653	A583	G508
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A1444	G1371	C1303	C1233	G1164	G1094	G1026	U945	A872	U805	U728	A	A597	A525
C1445	G1372	A1304	U1234	U1166	G1097	G1027	U946	U874	A806	U729	U	U598	U526
U1446	U1373	U1305	U1235	C1167	A1098	U1028	U947	C875	U807	U733	G	U599	A527
C1447	A1374	A1306	U1236	A1168	G1099	U1029	C947	A876	C808	U734	U	U600	C528
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G1451	C1378	A1310	G1240	A1173	U1032	G1025	A951	U879	U815	A738	U675	C674	C534
C1452	C1379	C1311	A1241	A1174	U1033	G1027	A952	C880	U816	A739	U676	G677	G536
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C1455	U1382	A1314	U1244	A1179	U1039	U1042	A955	A883	G819	U744	C679	G612	A539
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A1457	U1384	A1316	G1246	A1181	G1115	U1044	A963	U885	G822	G746	C681	U610	G541
C1458	C1385	C1317	U1247	C1182	A1116	U1045	A964	C887	G823	A747	A678	A617	A542
U1459	A1386	U1318	G1248	G1183	A1117	U1046	G965	U888	U824	G748	C685	A618	A543
G1460	U1387	U1319	C1249	G1184	A1118	U1047	U966	U889	U825	U749	G686	A619	U544
A1461	G1388	A1322	G1250	G1185	C1119	A1048	G972	A891	U826	U750	C687	A620	U545
C1462	A1392	C1323	G1253	G1186	U1120	U1049	A973	C899	U827	U751	A687	A621	G546
G1463	U1393	C1324	U1254	A1187	U1121	U1048	A974	U900	U828	U752	G688	G622	U547
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A1465	C1395	A1326	U1256	G1189	U1124	G1052	G976	U901	G830	A759	U692	A624	A553
C1466	U1396	C1327	U1257	U1191	A1127	G1055	G977	U902	G831	A760	U693	A628	A554
U1467	A1397	G1258	G1258	C1192	U1128	A1056	A977	U903	A832	C833	C694	G555	U556
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• Molecule 47: 40S ribosomal protein S0



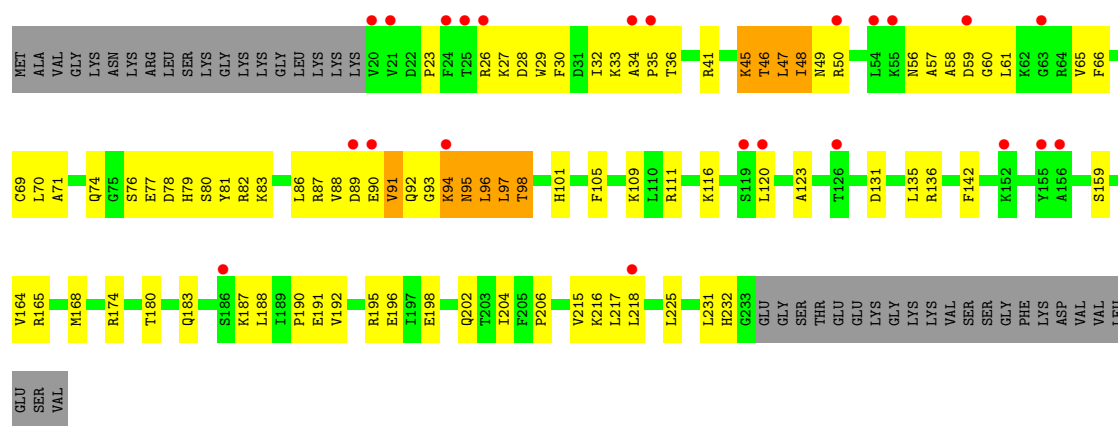
• Molecule 47: 40S ribosomal protein S0



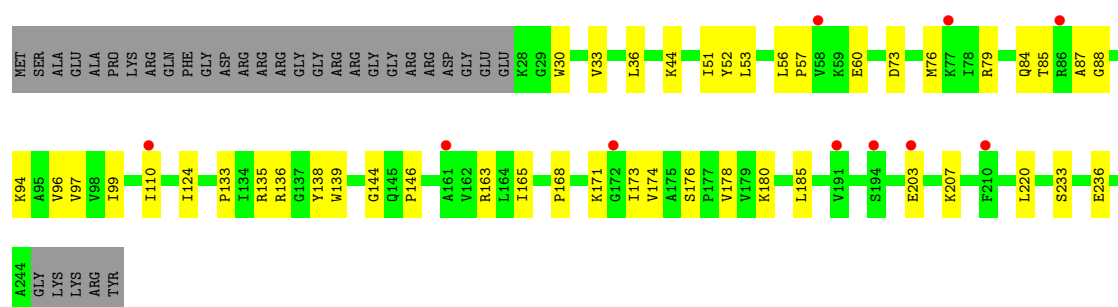
• Molecule 48: 40S ribosomal protein S1



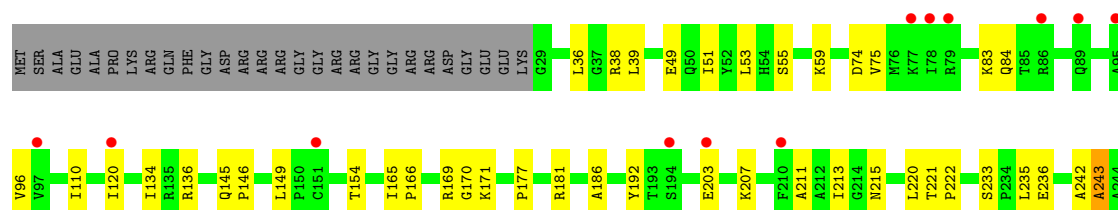
- Molecule 48: 40S ribosomal protein S1



- Molecule 49: Ribosomal protein S5



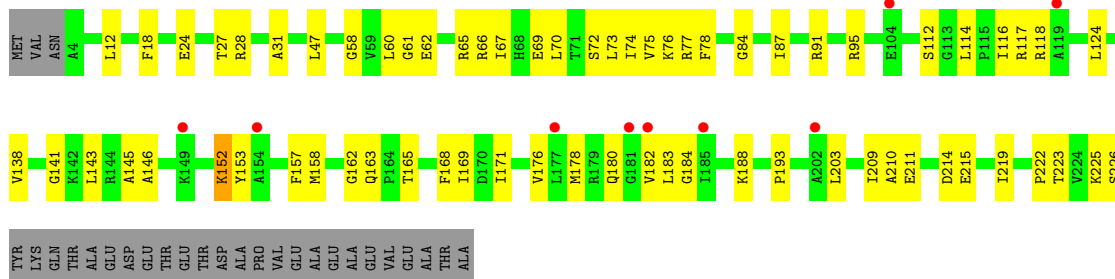
- Molecule 49: Ribosomal protein S5



GLY
LYS
LYS
ARG
TYR

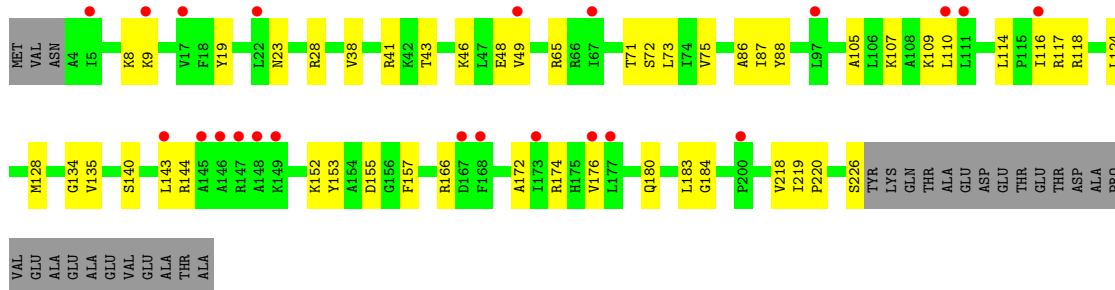
• Molecule 50: Ribosomal protein S3

Chain F: 



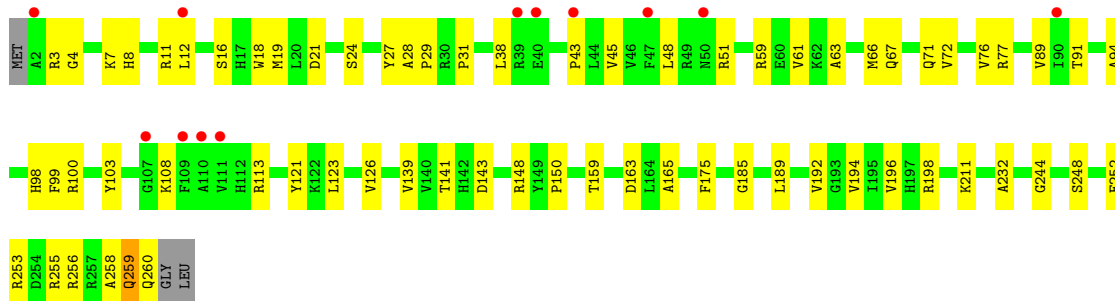
• Molecule 50: Ribosomal protein S3

Chain CQ: 



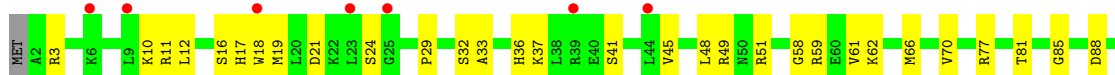
• Molecule 51: 40S ribosomal protein S4

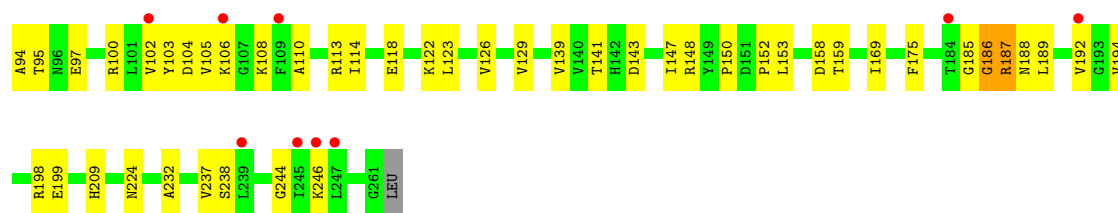
Chain G: 



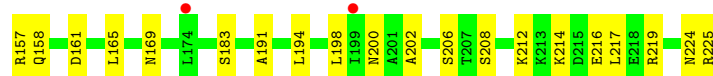
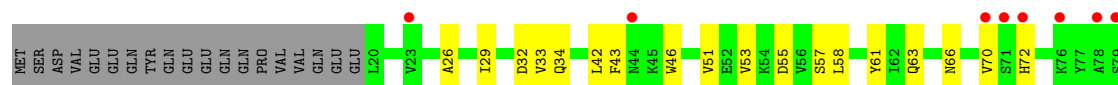
• Molecule 51: 40S ribosomal protein S4

Chain CR: 

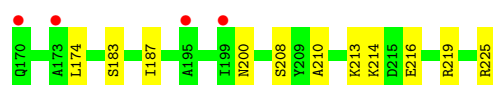
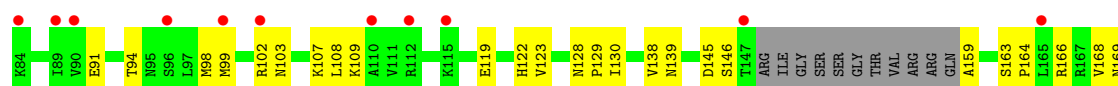




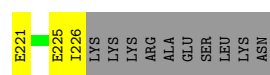
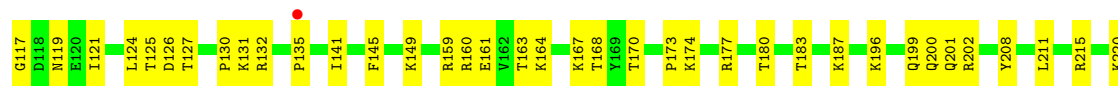
• Molecule 52: Ribosomal protein S7



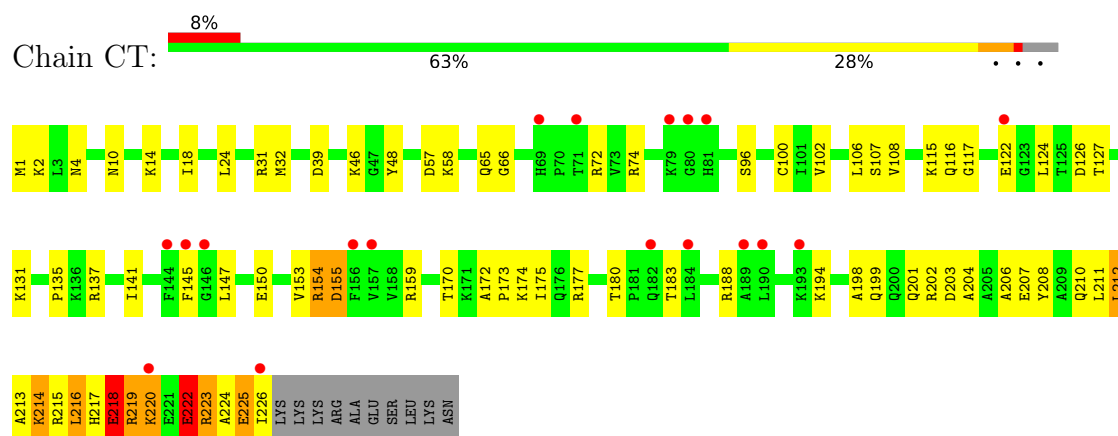
• Molecule 52: Ribosomal protein S7



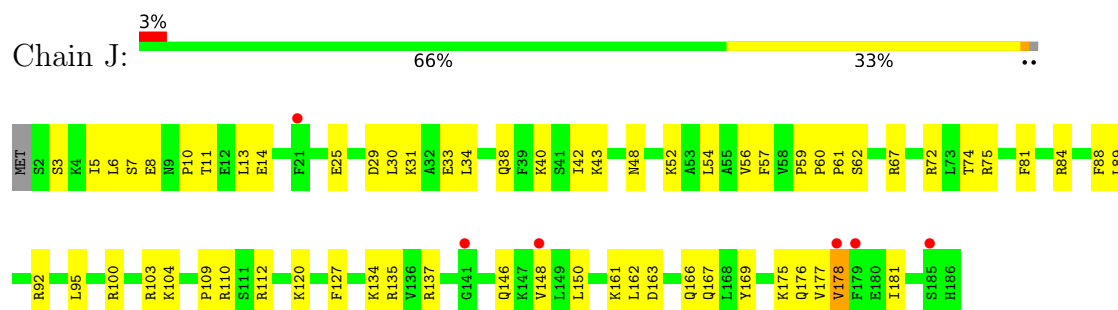
• Molecule 53: 40S ribosomal protein S6



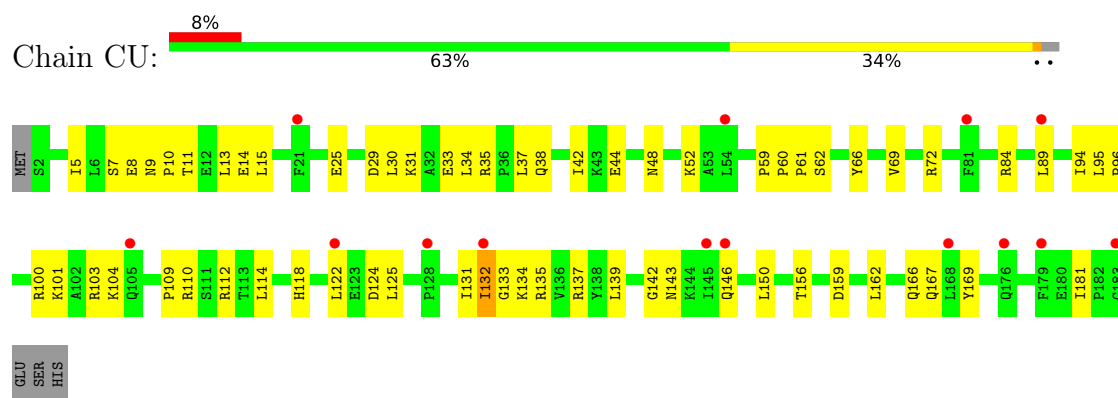
- Molecule 53: 40S ribosomal protein S6



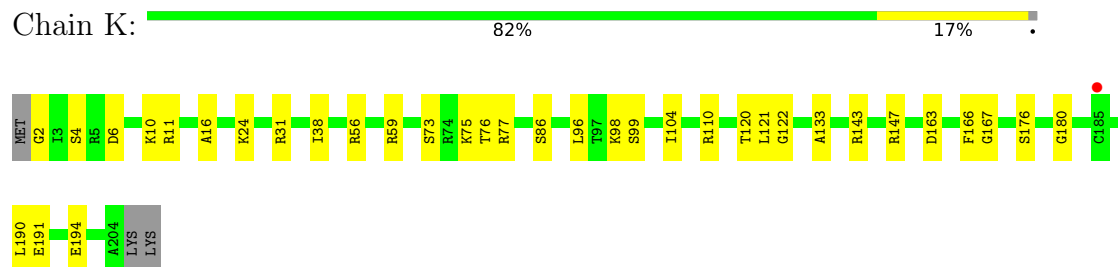
- Molecule 54: 40S ribosomal protein S7



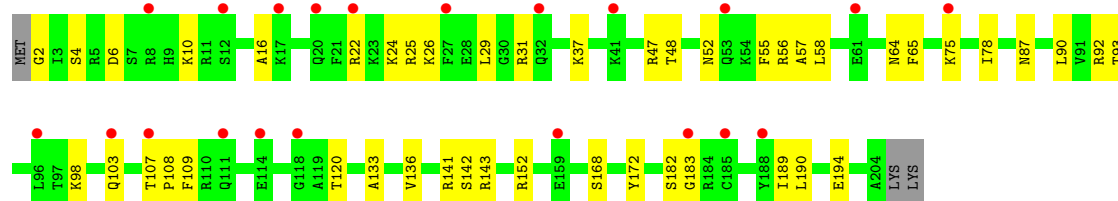
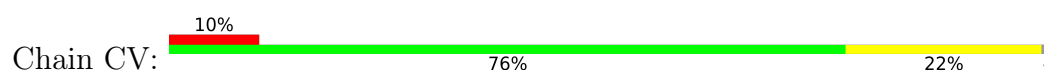
- Molecule 54: 40S ribosomal protein S7



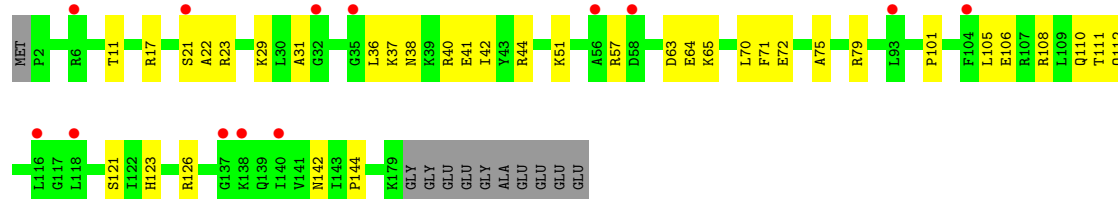
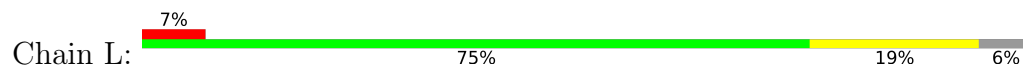
- Molecule 55: 40S ribosomal protein S8



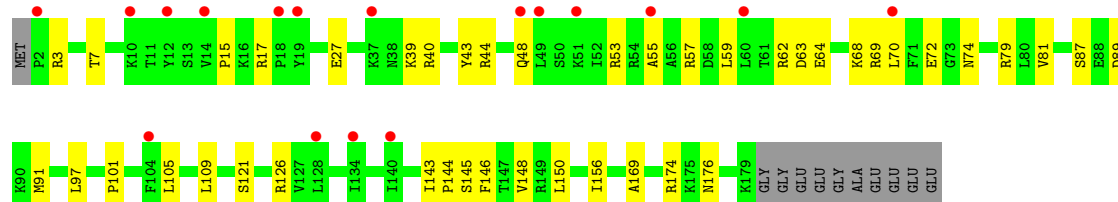
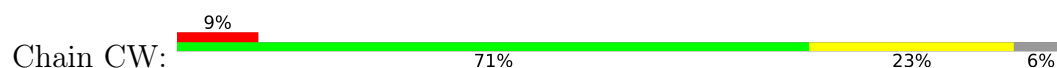
- Molecule 55: 40S ribosomal protein S8



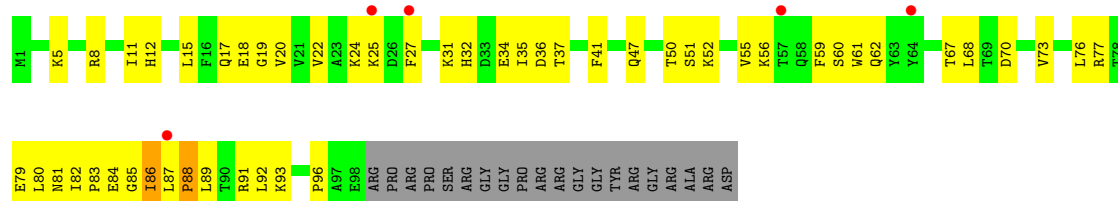
• Molecule 56: Ribosomal protein S4



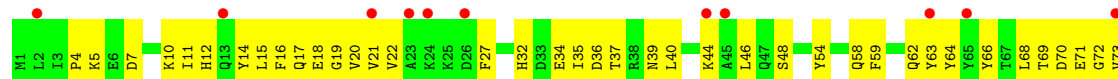
• Molecule 56: Ribosomal protein S4

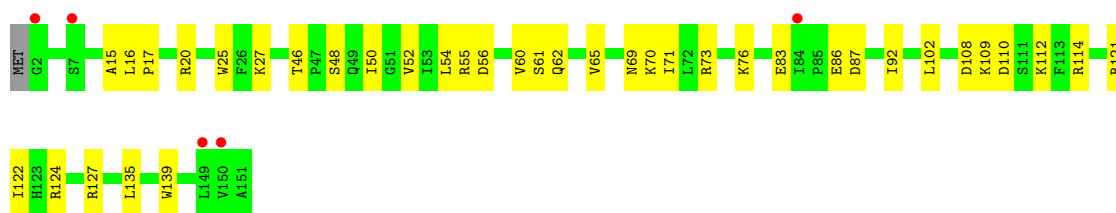


• Molecule 57: 40S ribosomal protein S10-A

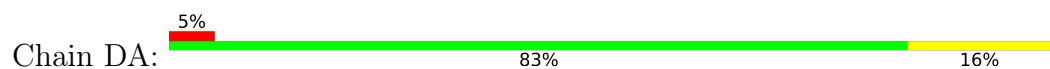


• Molecule 57: 40S ribosomal protein S10-A





- Molecule 60: 40S ribosomal protein S13



- Molecule 61: 40S ribosomal protein S14-A



- Molecule 61: 40S ribosomal protein S14-A

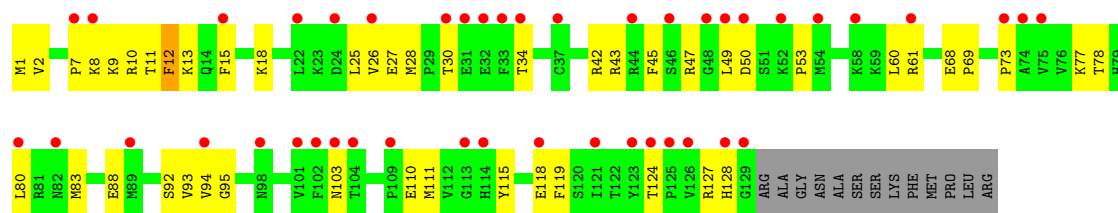


- Molecule 62: 40S ribosomal protein S15

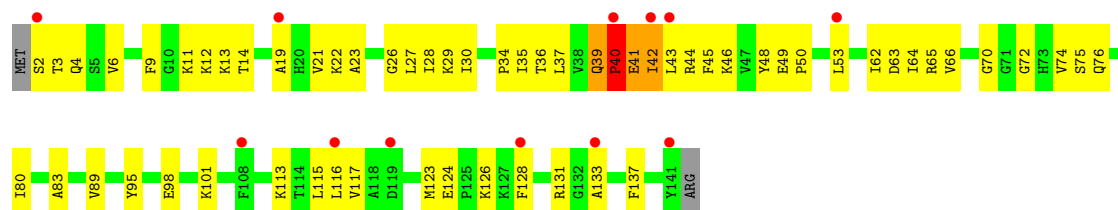


- Molecule 62: 40S ribosomal protein S15

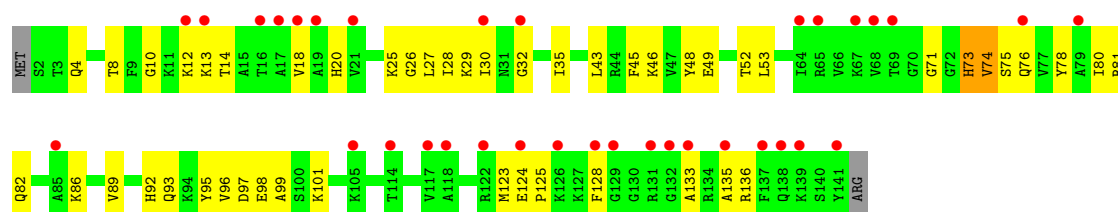




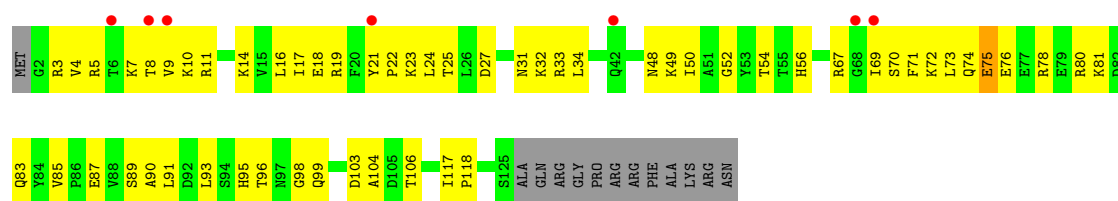
• Molecule 63: 40S ribosomal protein S16



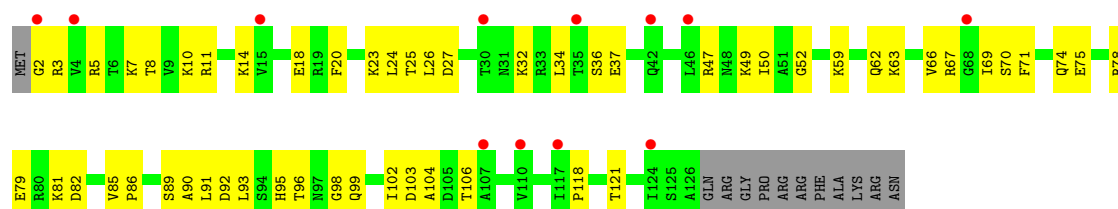
• Molecule 63: 40S ribosomal protein S16



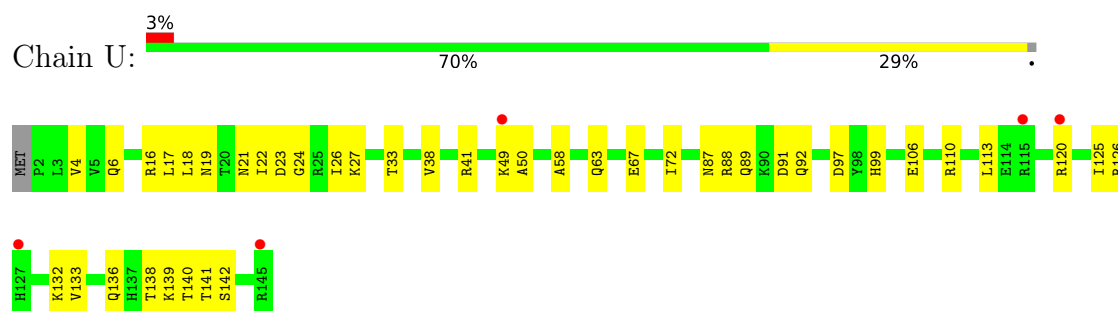
• Molecule 64: 40S ribosomal protein S17-B



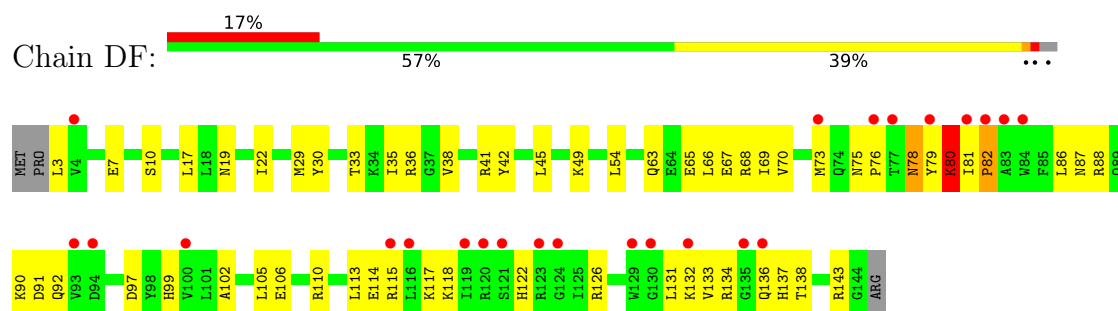
• Molecule 64: 40S ribosomal protein S17-B



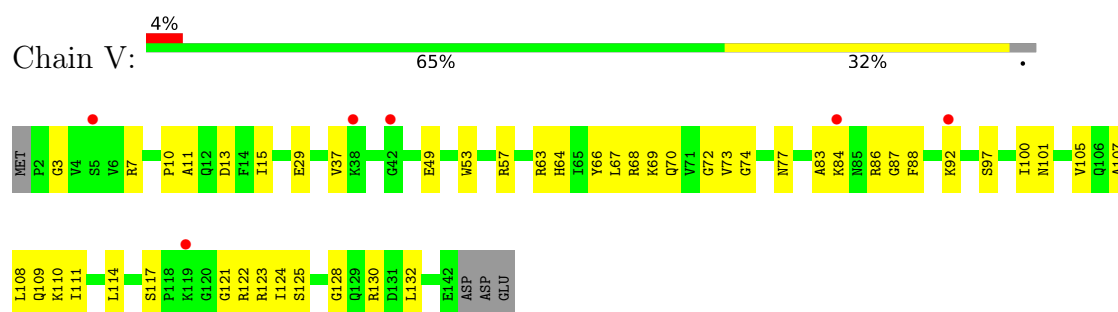
- Molecule 65: 40S ribosomal protein S18-B



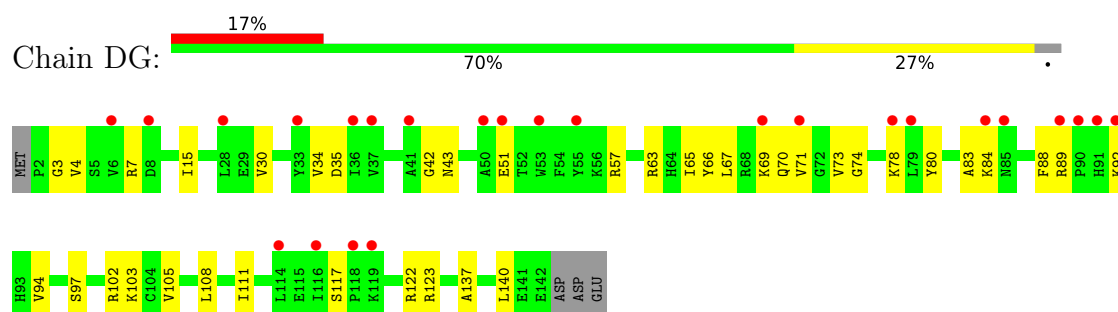
- Molecule 65: 40S ribosomal protein S18-B



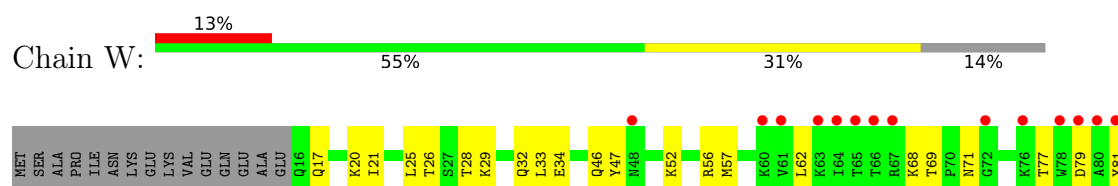
- Molecule 66: 40S ribosomal protein S19-A



- Molecule 66: 40S ribosomal protein S19-A



- Molecule 67: Ribosomal protein S10





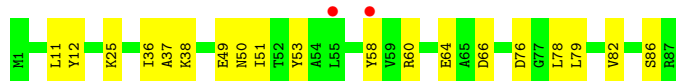
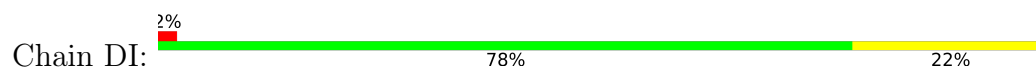
- Molecule 67: Ribosomal protein S10



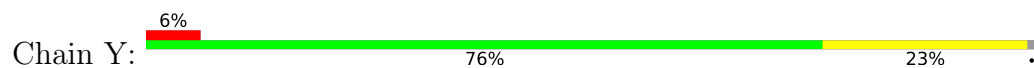
- Molecule 68: 40S ribosomal protein S21



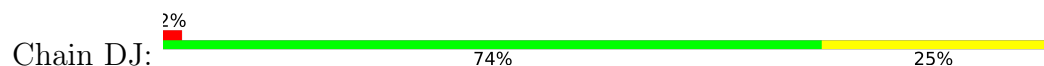
- Molecule 68: 40S ribosomal protein S21



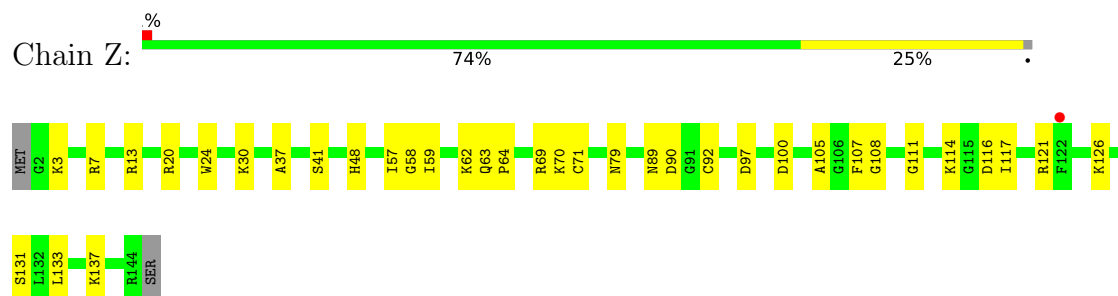
- Molecule 69: 40S ribosomal protein S22-A



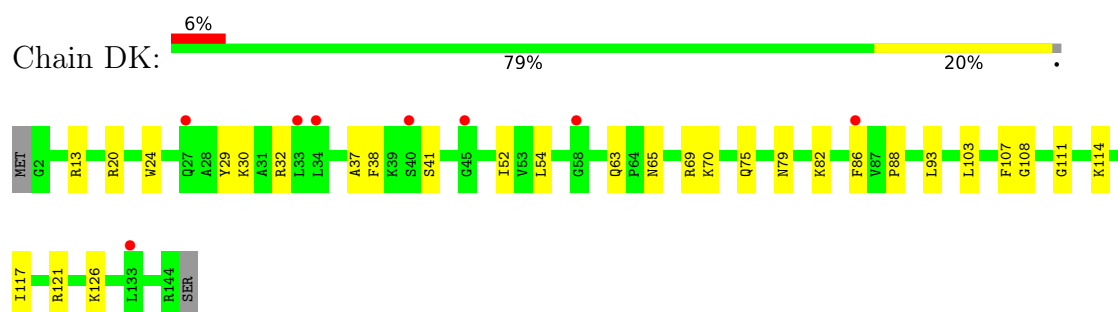
- Molecule 69: 40S ribosomal protein S22-A



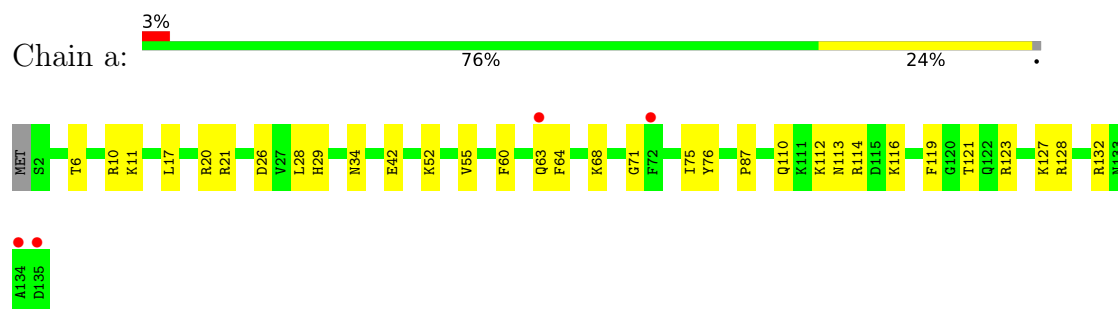
• Molecule 70: Ribosomal protein S23 (S12)



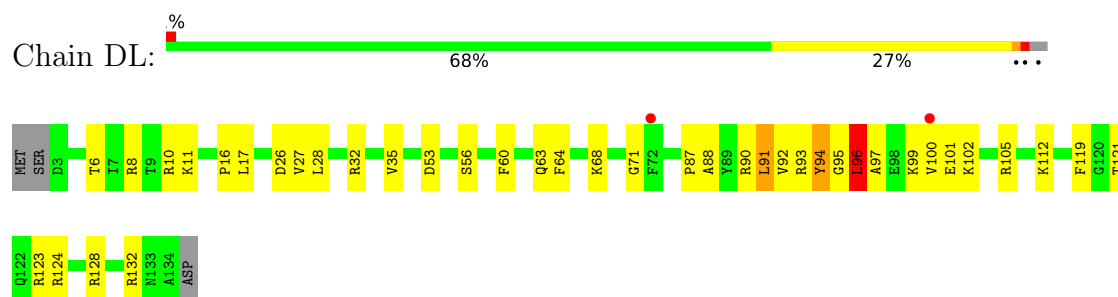
• Molecule 70: Ribosomal protein S23 (S12)



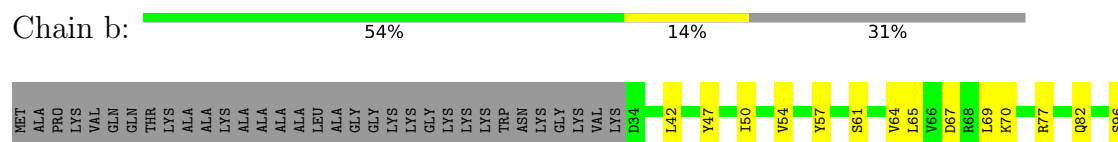
• Molecule 71: 40S ribosomal protein S24



• Molecule 71: 40S ribosomal protein S24

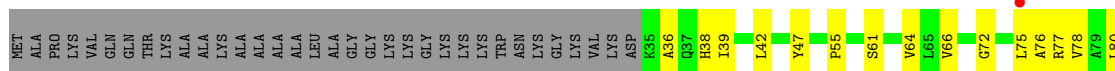


• Molecule 72: 40S ribosomal protein S25

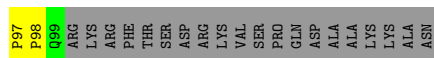




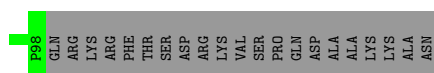
- Molecule 72: 40S ribosomal protein S25



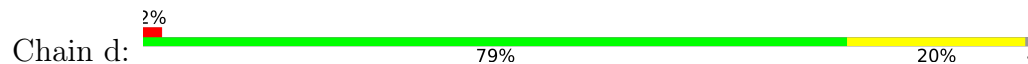
- Molecule 73: 40S ribosomal protein S26



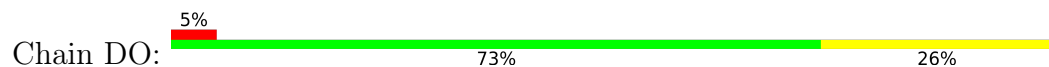
- Molecule 73: 40S ribosomal protein S26



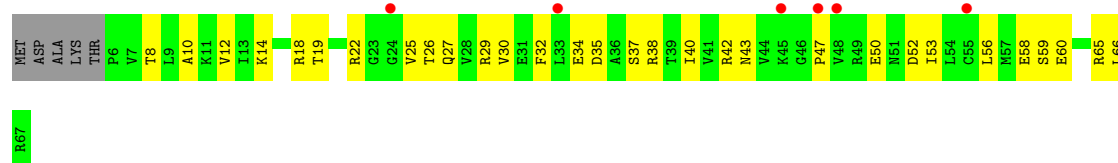
- Molecule 74: 40S ribosomal protein S27



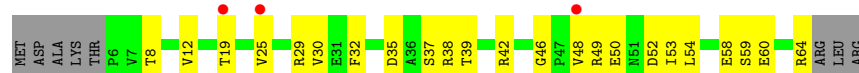
- Molecule 74: 40S ribosomal protein S27



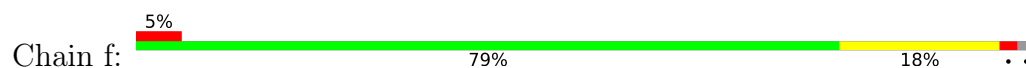
- Molecule 75: 40S ribosomal protein S28-B



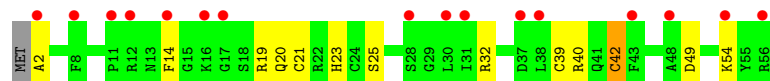
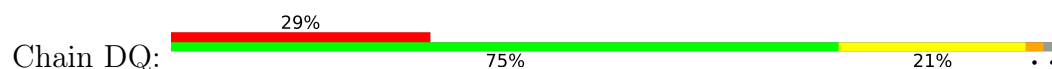
- Molecule 75: 40S ribosomal protein S28-B



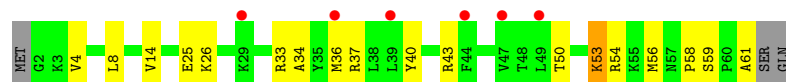
- Molecule 76: 40S ribosomal protein S29A



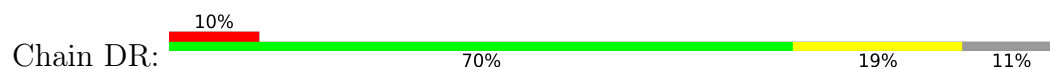
- Molecule 76: 40S ribosomal protein S29A



- Molecule 77: 40S ribosomal protein S30

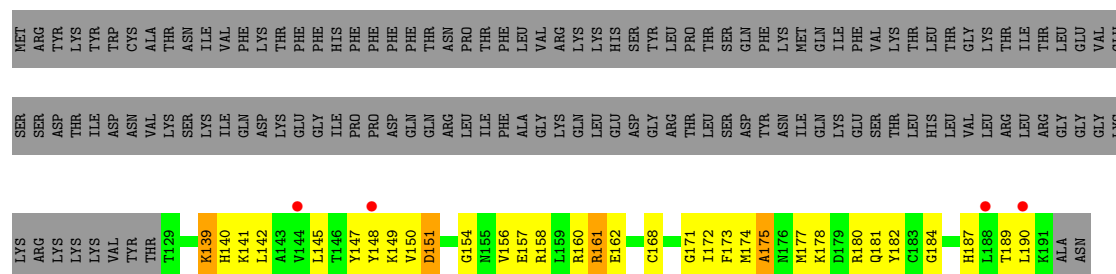


- Molecule 77: 40S ribosomal protein S30

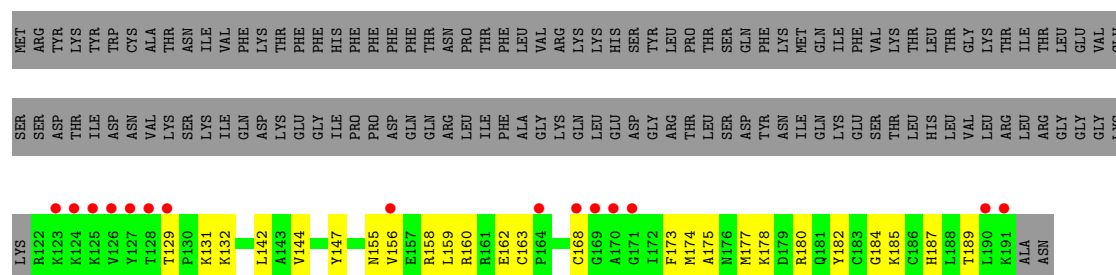


- Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

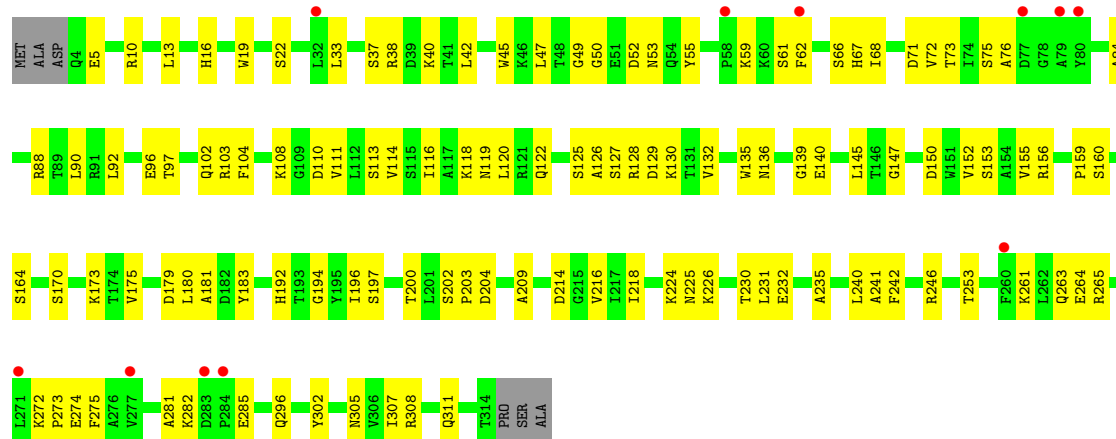




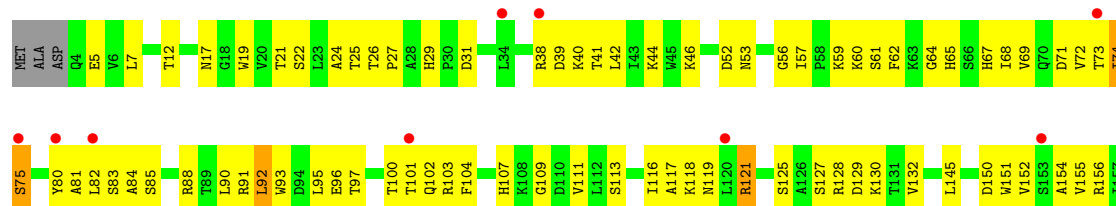
• Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

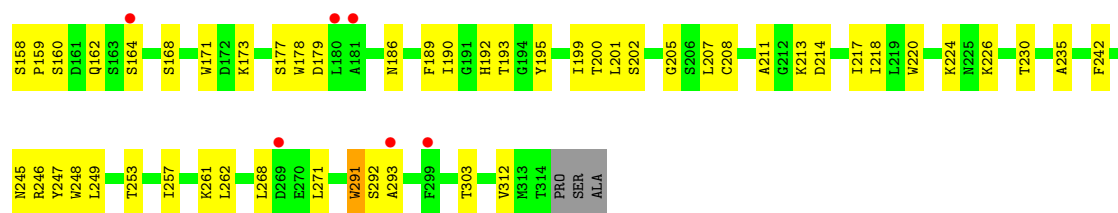


• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

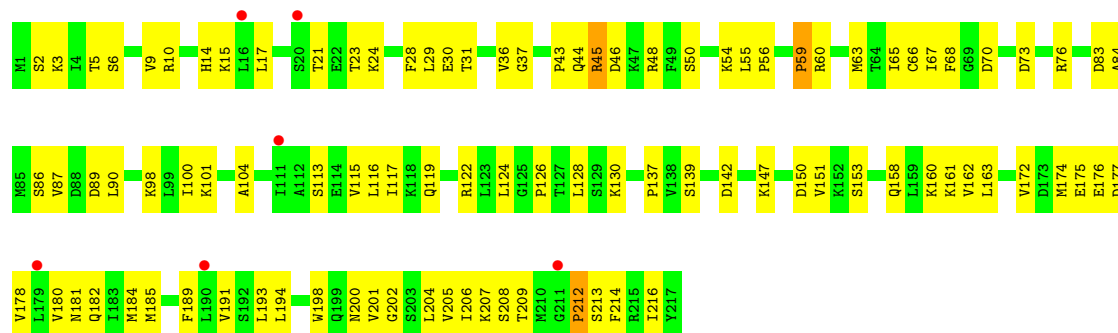


• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

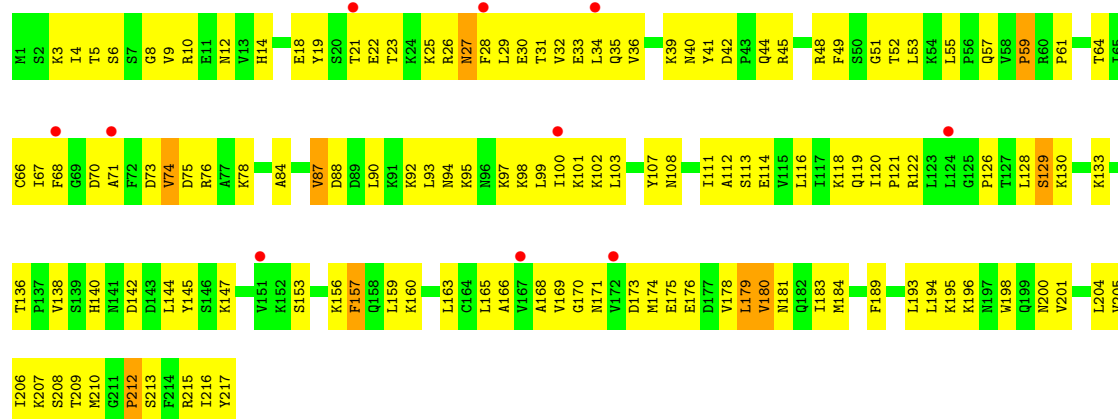




● Molecule 80: Ribosomal protein



● Molecule 80: 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	298.32Å 293.37Å 451.08Å 90.00° 100.16° 90.00°	Depositor
Resolution (Å)	177.03 – 3.30 177.03 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (177.03-3.30) 88.6 (177.03-3.30)	Depositor EDS
R_{merge}	0.69	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.254 , 0.297 0.254 , 0.296	Depositor DCC
R_{free} test set	2000 reflections (0.16%)	wwPDB-VP
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	405513	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.33% 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, PAR, 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	0.25	0/76973	0.53	37/119996 (0.0%)
1	AS	0.24	0/76539	0.52	36/119319 (0.0%)
2	3	0.20	0/2884	0.40	0/4492
2	AT	0.22	0/2884	0.41	0/4492
3	4	0.21	0/3724	0.48	2/5798 (0.0%)
3	AU	0.21	0/3746	0.49	3/5832 (0.1%)
4	AW	0.20	0/1922	0.48	0/2581
4	j	0.25	0/1922	0.53	0/2581
5	AX	0.23	0/3145	0.56	0/4231
5	k	0.23	0/3145	0.56	0/4231
6	AY	0.20	0/2799	0.56	0/3777
6	l	0.24	0/2799	0.62	0/3777
7	AZ	0.21	0/2447	0.62	0/3294
7	m	0.22	0/2479	0.58	0/3337
8	BA	0.21	0/1231	0.55	0/1662
8	n	0.22	0/1263	0.61	0/1703
9	BB	0.23	0/1918	0.55	0/2575
9	o	0.26	0/1918	0.56	0/2575
10	BC	0.22	0/1835	0.66	0/2472
10	p	0.24	0/1869	0.57	0/2519
11	BD	0.22	0/1537	0.55	0/2067
11	q	0.22	0/1537	0.56	0/2067
12	BE	0.22	0/1724	0.56	0/2314
12	r	0.21	0/1724	0.55	0/2314
13	BF	0.22	0/1390	0.64	0/1861
13	s	0.22	0/1390	0.61	0/1861
14	BG	0.20	0/1637	0.60	0/2195
14	t	0.22	0/1637	0.54	0/2195
15	BH	0.27	0/1044	0.58	0/1407
15	u	0.23	0/1044	0.55	0/1407
16	BI	0.19	0/1753	0.54	0/2347
16	v	0.24	0/1753	0.55	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	BJ	0.22	0/1620	0.58	0/2167
17	w	0.23	0/1620	0.57	0/2167
18	BK	0.21	0/1429	0.53	0/1920
18	x	0.22	0/1410	0.58	0/1895
19	BL	0.19	0/1482	0.49	0/1985
19	y	0.21	0/1482	0.52	0/1985
20	BM	0.21	0/1475	0.59	0/1961
20	z	0.21	0/1475	0.57	0/1961
21	0	0.22	0/1457	0.53	0/1962
21	BN	0.21	0/1457	0.51	0/1962
22	2	0.21	0/1285	0.56	0/1723
22	BO	0.20	0/1285	0.56	1/1723 (0.1%)
23	5	0.20	0/846	0.58	0/1140
23	BP	0.28	0/841	0.78	0/1133
24	6	0.21	0/993	0.52	0/1339
24	BQ	0.20	0/993	0.52	0/1339
25	7	0.21	0/958	0.41	0/1267
25	BR	0.21	0/814	0.40	0/1079
26	8	0.21	0/990	0.55	0/1337
26	BS	0.19	0/976	0.54	0/1319
27	9	0.20	0/999	0.51	0/1334
27	BT	0.20	0/999	0.58	0/1334
28	AA	0.19	0/1112	0.54	0/1488
28	BU	0.18	0/1112	0.56	0/1488
29	AB	0.23	0/1199	0.54	0/1607
29	BV	0.20	0/1199	0.54	0/1607
30	AC	0.21	0/503	0.79	3/668 (0.4%)
30	BW	0.23	0/522	0.69	0/692
31	AD	0.19	0/738	0.51	0/994
31	BX	0.19	0/738	0.56	0/994
32	AE	0.22	0/907	0.60	0/1219
32	BY	0.21	0/894	0.57	0/1201
33	AF	0.21	0/1021	0.57	0/1368
33	BZ	0.23	0/1039	0.60	0/1390
34	AG	0.21	0/866	0.50	0/1165
34	CA	0.24	0/895	0.52	0/1201
35	AH	0.22	0/896	0.58	0/1195
35	CB	0.20	0/925	0.55	0/1231
36	AI	0.20	0/1003	0.54	0/1336
36	CC	0.18	0/990	0.59	0/1319
37	AJ	0.21	0/763	0.55	0/1012
37	CD	0.21	0/772	0.60	0/1023
38	AK	0.27	0/690	0.62	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	CE	0.20	0/690	0.55	0/916
39	AL	0.20	0/623	0.62	0/831
39	CF	0.18	0/632	0.61	0/842
40	AM	0.23	0/447	0.55	0/594
40	CG	0.23	0/447	0.63	0/594
41	AN	0.21	0/425	0.62	0/563
41	CH	0.30	0/436	0.62	0/577
42	AO	0.23	0/237	0.57	0/304
42	CI	0.70	0/228	1.04	0/293
43	AP	0.23	0/840	0.59	0/1110
43	CJ	0.25	0/860	0.59	0/1136
44	AQ	0.25	0/705	0.55	0/940
44	CK	0.23	0/705	0.56	0/940
45	CL	0.30	0/942	0.83	0/1258
45	i	0.38	0/942	1.08	3/1258 (0.2%)
46	B	0.23	0/40832	0.53	10/63622 (0.0%)
46	CM	0.24	0/41169	0.52	5/64148 (0.0%)
47	C	0.18	0/1666	0.50	0/2273
47	CN	0.20	0/1666	0.59	0/2273
48	CO	0.34	0/1750	0.72	1/2354 (0.0%)
48	D	0.20	0/1750	0.53	0/2354
49	CP	0.22	0/1648	0.51	0/2237
49	E	0.20	0/1657	0.57	0/2248
50	CQ	0.24	0/1731	0.64	0/2324
50	F	0.26	0/1731	0.72	0/2324
51	CR	0.26	0/2096	0.60	1/2822 (0.0%)
51	G	0.20	0/2092	0.54	0/2817
52	CS	0.25	0/1546	0.60	0/2085
52	H	0.25	0/1631	0.57	0/2199
53	CT	0.35	0/1845	0.68	0/2464
53	I	0.20	0/1845	0.64	0/2464
54	CU	0.27	0/1490	0.64	1/2004 (0.0%)
54	J	0.27	0/1516	0.65	0/2039
55	CV	0.22	0/1606	0.59	0/2150
55	K	0.20	0/1606	0.55	0/2150
56	CW	0.19	0/1478	0.55	0/1978
56	L	0.21	0/1478	0.58	0/1978
57	CX	0.27	0/801	0.65	0/1081
57	M	0.30	0/836	0.82	3/1130 (0.3%)
58	CY	0.20	0/1154	0.53	0/1553
58	N	0.27	0/1175	0.66	2/1582 (0.1%)
59	CZ	0.24	0/892	0.77	0/1203
59	O	0.47	0/892	1.21	3/1203 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
60	DA	0.19	0/1210	0.55	0/1631
60	P	0.20	0/1210	0.53	0/1631
61	DB	0.23	0/953	0.70	0/1279
61	Q	0.22	0/953	0.63	0/1279
62	DC	0.28	0/1038	0.69	0/1395
62	R	0.32	0/1038	0.74	0/1395
63	DD	0.25	0/1109	0.57	0/1486
63	S	0.28	0/1109	0.64	0/1486
64	DE	0.21	0/1014	0.62	0/1361
64	T	0.25	0/1009	0.74	2/1354 (0.1%)
65	DF	0.29	0/1186	0.81	2/1590 (0.1%)
65	U	0.21	0/1205	0.58	0/1615
66	DG	0.21	0/1120	0.59	0/1508
66	V	0.24	0/1120	0.73	0/1508
67	DH	0.24	0/800	0.63	0/1082
67	W	0.23	0/818	0.70	0/1106
68	DI	0.22	0/683	0.55	0/918
68	X	0.22	0/683	0.60	0/918
69	DJ	0.22	0/1049	0.56	0/1412
69	Y	0.20	0/1049	0.54	0/1412
70	DK	0.23	0/1128	0.63	0/1505
70	Z	0.20	0/1128	0.63	0/1505
71	DL	0.32	0/1086	0.62	0/1447
71	a	0.24	0/1100	0.63	0/1466
72	DM	0.22	0/577	0.72	0/778
72	b	0.20	0/585	0.54	0/789
73	DN	0.29	0/782	0.72	0/1048
73	c	0.60	0/791	1.15	9/1060 (0.8%)
74	DO	0.21	0/624	0.62	0/843
74	d	0.22	0/624	0.63	0/843
75	DP	0.23	0/459	0.70	0/615
75	e	0.23	0/489	0.65	0/654
76	DQ	0.27	0/466	0.74	2/620 (0.3%)
76	f	0.34	0/466	0.75	1/620 (0.2%)
77	DR	0.27	0/451	0.78	0/601
77	g	0.32	0/482	0.86	1/642 (0.2%)
78	DS	0.24	0/585	0.70	0/778
78	h	0.32	0/520	1.02	2/693 (0.3%)
79	AR	0.23	0/2451	0.63	0/3337
79	DT	0.29	0/2451	0.75	2/3337 (0.1%)
80	L1	0.18	0/1737	0.39	0/2335
80	l1	0.23	0/1737	0.52	0/2335
All	All	0.24	0/433095	0.56	132/635204 (0.0%)

There are no bond length outliers.

The worst 5 of 132 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
46	B	823	G	OP1-P-O3'	-12.00	72.01	108.00
73	c	77	CYS	CB-CA-C	-10.39	94.39	110.92
1	AS	3160	C	P-O3'-C3'	-9.73	105.61	120.20
77	g	53	LYS	CA-CB-CG	9.18	132.45	114.10
1	AS	484	U	P-O3'-C3'	-9.15	106.48	120.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	68774	0	34561	1290	0
1	AS	68387	0	34366	1368	0
2	3	2579	0	1304	40	0
2	AT	2579	0	1304	46	0
3	4	3333	0	1684	61	0
3	AU	3353	0	1694	80	0
4	AW	1888	0	1962	50	0
4	j	1888	0	1962	52	0
5	AX	3077	0	3166	69	0
5	k	3077	0	3166	76	0
6	AY	2751	0	2879	62	0
6	l	2751	0	2879	74	0
7	AZ	2394	0	2362	52	0
7	m	2426	0	2389	41	0
8	BA	1210	0	1285	28	0
8	n	1242	0	1321	39	0
9	BB	1885	0	1977	33	0
9	o	1885	0	1977	36	0
10	BC	1805	0	1925	49	0
10	p	1839	0	1957	28	0
11	BD	1519	0	1588	35	0
11	q	1519	0	1588	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	BE	1689	0	1730	37	0
12	r	1689	0	1731	28	0
13	BF	1371	0	1410	41	0
13	s	1371	0	1410	32	0
14	BG	1610	0	1686	34	0
14	t	1610	0	1686	35	0
15	BH	1029	0	1116	33	0
15	u	1029	0	1116	34	0
16	BI	1713	0	1764	61	0
16	v	1713	0	1764	44	0
17	BJ	1590	0	1705	31	0
17	w	1590	0	1705	31	0
18	BK	1406	0	1431	29	0
18	x	1387	0	1408	33	0
19	BL	1458	0	1556	33	0
19	y	1458	0	1556	37	0
20	BM	1457	0	1564	41	0
20	z	1457	0	1564	41	0
21	0	1423	0	1480	33	0
21	BN	1423	0	1480	39	0
22	2	1262	0	1314	19	0
22	BO	1262	0	1314	25	0
23	5	831	0	848	24	0
23	BP	826	0	843	38	0
24	6	977	0	1026	20	0
24	BQ	977	0	1026	19	0
25	7	945	0	1010	25	0
25	BR	801	0	840	18	0
26	8	974	0	1032	17	0
26	BS	960	0	1014	19	0
27	9	989	0	1063	21	0
27	BT	989	0	1064	31	0
28	AA	1087	0	1154	27	0
28	BU	1087	0	1154	25	0
29	AB	1170	0	1203	32	0
29	BV	1170	0	1203	37	0
30	AC	493	0	520	17	0
30	BW	509	0	545	17	0
31	AD	729	0	775	13	0
31	BX	729	0	775	14	0
32	AE	894	0	941	25	0
32	BY	881	0	925	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	AF	1000	0	1069	29	0
33	BZ	1015	0	1095	25	0
34	AG	847	0	893	23	0
34	CA	867	0	932	20	0
35	AH	887	0	947	26	0
35	CB	904	0	986	23	0
36	AI	992	0	1093	27	0
36	CC	979	0	1076	27	0
37	AJ	758	0	838	15	0
37	CD	764	0	851	23	0
38	AK	677	0	697	20	0
38	CE	677	0	696	24	0
39	AL	617	0	675	8	0
39	CF	623	0	688	12	0
40	AM	438	0	475	9	0
40	CG	438	0	475	15	0
41	AN	419	0	460	12	0
41	CH	427	0	477	8	0
42	AO	236	0	285	7	0
42	CI	227	0	272	21	0
43	AP	828	0	893	27	0
43	CJ	841	0	917	25	0
44	AQ	698	0	734	13	0
44	CK	698	0	734	16	0
45	CL	931	0	908	57	0
45	i	931	0	908	89	0
46	B	36504	0	18363	867	0
46	CM	36805	0	18515	943	0
47	C	1627	0	1644	49	0
47	CN	1627	0	1644	49	0
48	CO	1724	0	1805	75	0
48	D	1724	0	1805	34	0
49	CP	1620	0	1715	35	0
49	E	1629	0	1728	36	0
50	CQ	1707	0	1807	46	0
50	F	1707	0	1807	72	0
51	CR	2055	0	2137	59	0
51	G	2051	0	2134	53	0
52	CS	1530	0	1597	43	0
52	H	1614	0	1688	59	0
53	CT	1820	0	1896	77	0
53	I	1820	0	1896	57	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	CU	1466	0	1561	51	0
54	J	1491	0	1579	43	0
55	CV	1579	0	1602	36	0
55	K	1579	0	1602	32	0
56	CW	1453	0	1532	31	0
56	L	1453	0	1532	32	0
57	CX	783	0	799	46	0
57	M	817	0	828	57	0
58	CY	1129	0	1183	27	0
58	N	1150	0	1201	19	0
59	CZ	885	0	915	37	0
59	O	885	0	915	105	0
60	DA	1187	0	1249	18	0
60	P	1187	0	1249	33	0
61	DB	942	0	981	41	0
61	Q	942	0	981	27	0
62	DC	1018	0	1065	49	0
62	R	1018	0	1065	52	0
63	DD	1091	0	1155	47	0
63	S	1091	0	1155	51	0
64	DE	1002	0	1058	51	0
64	T	997	0	1053	56	0
65	DF	1169	0	1216	61	0
65	U	1187	0	1237	39	0
66	DG	1100	0	1114	34	0
66	V	1100	0	1114	40	0
67	DH	790	0	855	29	0
67	W	808	0	871	35	0
68	DI	676	0	677	22	0
68	X	676	0	677	22	0
69	DJ	1032	0	1066	30	0
69	Y	1032	0	1066	24	0
70	DK	1110	0	1182	27	0
70	Z	1110	0	1182	28	0
71	DL	1072	0	1123	37	0
71	a	1086	0	1132	27	0
72	DM	570	0	609	16	0
72	b	578	0	613	12	0
73	DN	770	0	828	32	0
73	c	779	0	832	29	0
74	DO	614	0	630	17	0
74	d	614	0	630	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
75	DP	457	0	486	23	0
75	e	487	0	523	28	0
76	DQ	454	0	431	14	0
76	f	454	0	432	12	0
77	DR	444	0	483	12	0
77	g	474	0	515	20	0
78	DS	574	0	610	25	0
78	h	510	0	533	34	0
79	AR	2398	0	2373	90	0
79	DT	2398	0	2374	115	0
80	L1	1711	0	1817	70	0
80	l1	1711	0	1817	128	0
81	0	3	0	0	0	0
81	1	565	0	0	0	0
81	2	1	0	0	0	0
81	3	14	0	0	0	0
81	4	16	0	0	0	0
81	5	1	0	0	0	0
81	6	2	0	0	0	0
81	8	2	0	0	0	0
81	9	2	0	0	0	0
81	AB	1	0	0	0	0
81	AC	1	0	0	0	0
81	AD	2	0	0	0	0
81	AF	4	0	0	0	0
81	AG	2	0	0	0	0
81	AH	2	0	0	0	0
81	AI	1	0	0	0	0
81	AP	3	0	0	0	0
81	AQ	1	0	0	0	0
81	AR	1	0	0	0	0
81	AS	387	0	0	0	0
81	AT	13	0	0	0	0
81	AU	7	0	0	0	0
81	AW	3	0	0	0	0
81	AX	2	0	0	0	0
81	AY	1	0	0	0	0
81	B	169	0	0	0	0
81	BB	3	0	0	0	0
81	BE	2	0	0	0	0
81	BF	1	0	0	0	0
81	BG	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	BH	1	0	0	0	0
81	BI	1	0	0	0	0
81	BJ	4	0	0	0	0
81	BK	2	0	0	0	0
81	BN	2	0	0	0	0
81	BO	1	0	0	0	0
81	BS	1	0	0	0	0
81	BV	1	0	0	0	0
81	BZ	4	0	0	0	0
81	CA	1	0	0	0	0
81	CJ	1	0	0	0	0
81	CK	1	0	0	0	0
81	CL	3	0	0	0	0
81	CM	145	0	0	0	0
81	CN	1	0	0	0	0
81	CP	2	0	0	0	0
81	CQ	4	0	0	0	0
81	CW	1	0	0	0	0
81	D	1	0	0	0	0
81	DA	2	0	0	0	0
81	DB	4	0	0	0	0
81	DC	1	0	0	0	0
81	DG	1	0	0	0	0
81	DJ	2	0	0	0	0
81	DQ	1	0	0	0	0
81	E	2	0	0	0	0
81	F	1	0	0	0	0
81	G	1	0	0	0	0
81	H	1	0	0	0	0
81	I	1	0	0	0	0
81	K	1	0	0	0	0
81	Q	2	0	0	0	0
81	V	1	0	0	0	0
81	Y	1	0	0	0	0
81	Z	3	0	0	0	0
81	c	1	0	0	0	0
81	f	1	0	0	0	0
81	g	1	0	0	0	0
81	i	1	0	0	0	0
81	j	4	0	0	0	0
81	k	5	0	0	0	0
81	l	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
81	m	1	0	0	0	0
81	o	4	0	0	0	0
81	r	3	0	0	0	0
81	s	1	0	0	0	0
81	u	2	0	0	0	0
81	v	2	0	0	0	0
81	w	3	0	0	0	0
81	x	5	0	0	0	0
81	y	2	0	0	0	0
81	z	1	0	0	0	0
82	1	57	0	52	7	0
82	CJ	57	0	52	7	0
83	1	126	0	135	9	0
83	AS	126	0	135	20	0
83	B	42	0	45	18	0
83	CM	42	0	45	0	0
84	AH	1	0	0	0	0
84	AK	1	0	0	0	0
84	AN	1	0	0	0	0
84	AP	1	0	0	0	0
84	AQ	1	0	0	0	0
84	CB	1	0	0	0	0
84	CE	1	0	0	0	0
84	CK	1	0	0	0	0
84	DQ	1	0	0	0	0
84	c	1	0	0	0	0
84	f	1	0	0	0	0
85	1	9	0	0	2	0
85	4	3	0	0	1	0
85	AS	20	0	0	3	0
85	B	11	0	0	1	0
85	BQ	3	0	0	1	0
85	BV	1	0	0	0	0
85	G	1	0	0	0	0
All	All	405513	0	301774	8356	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

The worst 5 of 8356 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:AR:16:HIS:CE1	79:AR:37:SER:HB2	1.48	1.47
73:DN:23:CYS:SG	73:DN:74:CYS:HB3	1.56	1.46
73:DN:23:CYS:SG	73:DN:74:CYS:CB	2.32	1.17
79:AR:16:HIS:CE1	79:AR:37:SER:CB	2.26	1.17
46:B:1410:A:H2'	49:E:87:ALA:HB3	1.30	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AW	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
4	j	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
5	AX	384/389 (99%)	373 (97%)	11 (3%)	0	100	100
5	k	384/389 (99%)	372 (97%)	12 (3%)	0	100	100
6	AY	359/363 (99%)	348 (97%)	11 (3%)	0	100	100
6	l	359/363 (99%)	346 (96%)	13 (4%)	0	100	100
7	AZ	290/298 (97%)	275 (95%)	12 (4%)	3 (1%)	12	40
7	m	294/298 (99%)	281 (96%)	13 (4%)	0	100	100
8	BA	149/176 (85%)	146 (98%)	3 (2%)	0	100	100
8	n	153/176 (87%)	149 (97%)	4 (3%)	0	100	100
9	BB	232/241 (96%)	225 (97%)	6 (3%)	1 (0%)	30	60
9	o	232/241 (96%)	223 (96%)	8 (3%)	1 (0%)	30	60
10	BC	231/262 (88%)	220 (95%)	9 (4%)	2 (1%)	14	43
10	p	236/262 (90%)	224 (95%)	9 (4%)	3 (1%)	9	35
11	BD	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
11	q	188/191 (98%)	184 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	3 (2%)	1 (0%)	24	55
14	t	198/202 (98%)	196 (99%)	2 (1%)	0	100	100
15	BH	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
15	u	128/131 (98%)	125 (98%)	3 (2%)	0	100	100
16	BI	201/204 (98%)	195 (97%)	6 (3%)	0	100	100
16	v	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
17	BJ	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
17	w	197/200 (98%)	195 (99%)	2 (1%)	0	100	100
18	BK	172/185 (93%)	167 (97%)	5 (3%)	0	100	100
18	x	169/185 (91%)	166 (98%)	3 (2%)	0	100	100
19	BL	183/186 (98%)	178 (97%)	5 (3%)	0	100	100
19	y	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
20	BM	177/190 (93%)	171 (97%)	6 (3%)	0	100	100
20	z	177/190 (93%)	174 (98%)	3 (2%)	0	100	100
21	0	168/172 (98%)	165 (98%)	3 (2%)	0	100	100
21	BN	168/172 (98%)	166 (99%)	2 (1%)	0	100	100
22	2	157/160 (98%)	153 (98%)	4 (2%)	0	100	100
22	BO	157/160 (98%)	151 (96%)	6 (4%)	0	100	100
23	5	101/124 (82%)	95 (94%)	5 (5%)	1 (1%)	12	40
23	BP	100/124 (81%)	85 (85%)	13 (13%)	2 (2%)	6	27
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%)	100 (88%)	13 (11%)	1 (1%)	14	43
25	BR	94/155 (61%)	90 (96%)	4 (4%)	0	100	100
26	8	119/142 (84%)	117 (98%)	2 (2%)	0	100	100
26	BS	117/142 (82%)	114 (97%)	3 (3%)	0	100	100
27	9	124/127 (98%)	123 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	BT	124/127 (98%)	124 (100%)	0	0	100	100
28	AA	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
28	BU	133/136 (98%)	132 (99%)	1 (1%)	0	100	100
29	AB	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
29	BV	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
30	AC	60/63 (95%)	57 (95%)	1 (2%)	2 (3%)	3	19
30	BW	62/63 (98%)	60 (97%)	1 (2%)	1 (2%)	7	31
31	AD	94/106 (89%)	91 (97%)	2 (2%)	1 (1%)	11	39
31	BX	94/106 (89%)	92 (98%)	2 (2%)	0	100	100
32	AE	108/112 (96%)	104 (96%)	4 (4%)	0	100	100
32	BY	106/112 (95%)	105 (99%)	1 (1%)	0	100	100
33	AF	122/131 (93%)	121 (99%)	1 (1%)	0	100	100
33	BZ	124/131 (95%)	122 (98%)	2 (2%)	0	100	100
34	AG	104/107 (97%)	102 (98%)	2 (2%)	0	100	100
34	CA	107/107 (100%)	103 (96%)	4 (4%)	0	100	100
35	AH	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
35	CB	113/113 (100%)	109 (96%)	4 (4%)	0	100	100
36	AI	118/120 (98%)	114 (97%)	4 (3%)	0	100	100
36	CC	116/120 (97%)	114 (98%)	2 (2%)	0	100	100
37	AJ	95/99 (96%)	94 (99%)	1 (1%)	0	100	100
37	CD	96/99 (97%)	95 (99%)	1 (1%)	0	100	100
38	AK	84/90 (93%)	82 (98%)	2 (2%)	0	100	100
38	CE	84/90 (93%)	81 (96%)	3 (4%)	0	100	100
39	AL	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
39	CF	76/78 (97%)	73 (96%)	3 (4%)	0	100	100
40	AM	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5	26
40	CG	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
41	AN	50/52 (96%)	49 (98%)	1 (2%)	0	100	100
41	CH	51/52 (98%)	49 (96%)	2 (4%)	0	100	100
42	AO	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
42	CI	22/25 (88%)	7 (32%)	13 (59%)	2 (9%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	AP	101/106 (95%)	100 (99%)	1 (1%)	0	100	100
43	CJ	103/106 (97%)	101 (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%)	21 (18%)	4 (3%)	3	18
45	i	117/267 (44%)	89 (76%)	25 (21%)	3 (3%)	4	23
47	C	206/261 (79%)	200 (97%)	6 (3%)	0	100	100
47	CN	206/261 (79%)	200 (97%)	6 (3%)	0	100	100
48	CO	212/256 (83%)	198 (93%)	14 (7%)	0	100	100
48	D	212/256 (83%)	208 (98%)	4 (2%)	0	100	100
49	CP	214/249 (86%)	205 (96%)	8 (4%)	1 (0%)	24	55
49	E	215/249 (86%)	210 (98%)	5 (2%)	0	100	100
50	CQ	221/251 (88%)	215 (97%)	6 (3%)	0	100	100
50	F	221/251 (88%)	214 (97%)	7 (3%)	0	100	100
51	CR	258/262 (98%)	246 (95%)	12 (5%)	0	100	100
51	G	257/262 (98%)	251 (98%)	5 (2%)	1 (0%)	30	60
52	CS	191/225 (85%)	180 (94%)	11 (6%)	0	100	100
52	H	204/225 (91%)	187 (92%)	15 (7%)	2 (1%)	12	40
53	CT	224/236 (95%)	208 (93%)	11 (5%)	5 (2%)	5	26
53	I	224/236 (95%)	218 (97%)	6 (3%)	0	100	100
54	CU	180/186 (97%)	168 (93%)	10 (6%)	2 (1%)	11	39
54	J	183/186 (98%)	171 (93%)	11 (6%)	1 (0%)	24	55
55	CV	201/206 (98%)	200 (100%)	1 (0%)	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%)	173 (98%)	2 (1%)	1 (1%)	21	52
57	CX	91/118 (77%)	84 (92%)	7 (8%)	0	100	100
57	M	96/118 (81%)	83 (86%)	11 (12%)	2 (2%)	5	26
58	CY	139/155 (90%)	136 (98%)	3 (2%)	0	100	100
58	N	142/155 (92%)	132 (93%)	9 (6%)	1 (1%)	18	49
59	CZ	114/143 (80%)	98 (86%)	16 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	O	114/143 (80%)	82 (72%)	26 (23%)	6 (5%)	1	10
60	DA	148/151 (98%)	143 (97%)	5 (3%)	0	100	100
60	P	148/151 (98%)	146 (99%)	2 (1%)	0	100	100
61	DB	125/132 (95%)	118 (94%)	6 (5%)	1 (1%)	16	45
61	Q	125/132 (95%)	122 (98%)	2 (2%)	1 (1%)	16	45
62	DC	127/142 (89%)	110 (87%)	16 (13%)	1 (1%)	16	45
62	R	127/142 (89%)	110 (87%)	16 (13%)	1 (1%)	16	45
63	DD	138/142 (97%)	131 (95%)	5 (4%)	2 (1%)	9	33
63	S	138/142 (97%)	131 (95%)	5 (4%)	2 (1%)	9	33
64	DE	123/137 (90%)	118 (96%)	5 (4%)	0	100	100
64	T	122/137 (89%)	116 (95%)	6 (5%)	0	100	100
65	DF	140/145 (97%)	132 (94%)	6 (4%)	2 (1%)	9	33
65	U	142/145 (98%)	133 (94%)	9 (6%)	0	100	100
66	DG	139/145 (96%)	135 (97%)	4 (3%)	0	100	100
66	V	139/145 (96%)	136 (98%)	3 (2%)	0	100	100
67	DH	98/119 (82%)	95 (97%)	3 (3%)	0	100	100
67	W	100/119 (84%)	95 (95%)	5 (5%)	0	100	100
68	DI	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
68	X	85/87 (98%)	83 (98%)	2 (2%)	0	100	100
69	DJ	127/130 (98%)	126 (99%)	1 (1%)	0	100	100
69	Y	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
70	DK	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
70	Z	141/145 (97%)	137 (97%)	4 (3%)	0	100	100
71	DL	130/135 (96%)	125 (96%)	3 (2%)	2 (2%)	8	32
71	a	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
72	DM	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
72	b	70/105 (67%)	69 (99%)	1 (1%)	0	100	100
73	DN	95/119 (80%)	93 (98%)	2 (2%)	0	100	100
73	c	96/119 (81%)	87 (91%)	8 (8%)	1 (1%)	12	40
74	DO	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
74	d	79/82 (96%)	74 (94%)	5 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
75	DP	57/67 (85%)	51 (90%)	6 (10%)	0	100	100
75	e	60/67 (90%)	56 (93%)	4 (7%)	0	100	100
76	DQ	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
76	f	53/56 (95%)	51 (96%)	2 (4%)	0	100	100
77	DR	54/63 (86%)	51 (94%)	3 (6%)	0	100	100
77	g	58/63 (92%)	52 (90%)	6 (10%)	0	100	100
78	DS	68/193 (35%)	60 (88%)	8 (12%)	0	100	100
78	h	61/193 (32%)	49 (80%)	9 (15%)	3 (5%)	1	12
79	AR	309/317 (98%)	281 (91%)	25 (8%)	3 (1%)	12	40
79	DT	309/317 (98%)	285 (92%)	22 (7%)	2 (1%)	21	52
80	L1	215/217 (99%)	166 (77%)	45 (21%)	4 (2%)	6	28
80	l1	215/217 (99%)	124 (58%)	81 (38%)	10 (5%)	2	12
All	All	22518/24692 (91%)	21437 (95%)	995 (4%)	86 (0%)	30	60

5 of 86 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	p	208	ASP
45	i	43	PRO
45	i	55	LYS
52	H	151	SER
54	J	162	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	AW	190/194 (98%)	190 (100%)	0	100	100
4	j	190/194 (98%)	190 (100%)	0	100	100
5	AX	325/328 (99%)	325 (100%)	0	100	100
5	k	325/328 (99%)	324 (100%)	1 (0%)	86	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AY	290/292 (99%)	290 (100%)	0	100	100
6	l	290/292 (99%)	290 (100%)	0	100	100
7	AZ	247/252 (98%)	247 (100%)	0	100	100
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%)	68	76
10	BC	193/216 (89%)	192 (100%)	1 (0%)	81	83
10	p	198/216 (92%)	198 (100%)	0	100	100
11	BD	169/170 (99%)	169 (100%)	0	100	100
11	q	169/170 (99%)	169 (100%)	0	100	100
12	BE	178/186 (96%)	178 (100%)	0	100	100
12	r	178/186 (96%)	178 (100%)	0	100	100
13	BF	146/149 (98%)	146 (100%)	0	100	100
13	s	146/149 (98%)	146 (100%)	0	100	100
14	BG	166/168 (99%)	166 (100%)	0	100	100
14	t	166/168 (99%)	166 (100%)	0	100	100
15	BH	108/109 (99%)	108 (100%)	0	100	100
15	u	108/109 (99%)	108 (100%)	0	100	100
16	BI	177/178 (99%)	177 (100%)	0	100	100
16	v	177/178 (99%)	177 (100%)	0	100	100
17	BJ	166/167 (99%)	166 (100%)	0	100	100
17	w	166/167 (99%)	166 (100%)	0	100	100
18	BK	145/154 (94%)	145 (100%)	0	100	100
18	x	144/154 (94%)	144 (100%)	0	100	100
19	BL	153/154 (99%)	153 (100%)	0	100	100
19	y	153/154 (99%)	153 (100%)	0	100	100
20	BM	146/153 (95%)	144 (99%)	2 (1%)	59	73
20	z	146/153 (95%)	146 (100%)	0	100	100
21	0	155/157 (99%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	133 (100%)	0	100	100
23	5	93/112 (83%)	93 (100%)	0	100	100
23	BP	93/112 (83%)	93 (100%)	0	100	100
24	6	101/104 (97%)	101 (100%)	0	100	100
24	BQ	101/104 (97%)	101 (100%)	0	100	100
25	7	97/127 (76%)	97 (100%)	0	100	100
25	BR	86/127 (68%)	86 (100%)	0	100	100
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%)	111 (100%)	0	100	100
27	BT	111/112 (99%)	111 (100%)	0	100	100
28	AA	117/118 (99%)	117 (100%)	0	100	100
28	BU	117/118 (99%)	117 (100%)	0	100	100
29	AB	120/121 (99%)	119 (99%)	1 (1%)	73	79
29	BV	120/121 (99%)	120 (100%)	0	100	100
30	AC	48/49 (98%)	48 (100%)	0	100	100
30	BW	50/49 (102%)	50 (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%)	98 (100%)	0	100	100
32	BY	97/100 (97%)	97 (100%)	0	100	100
33	AF	109/115 (95%)	109 (100%)	0	100	100
33	BZ	111/115 (96%)	109 (98%)	2 (2%)	51	70
34	AG	91/92 (99%)	91 (100%)	0	100	100
34	CA	94/92 (102%)	94 (100%)	0	100	100
35	AH	95/96 (99%)	95 (100%)	0	100	100
35	CB	98/96 (102%)	98 (100%)	0	100	100
36	AI	106/106 (100%)	106 (100%)	0	100	100
36	CC	105/106 (99%)	105 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	AJ	77/79 (98%)	77 (100%)	0	100	100
37	CD	78/79 (99%)	78 (100%)	0	100	100
38	AK	70/73 (96%)	70 (100%)	0	100	100
38	CE	70/73 (96%)	70 (100%)	0	100	100
39	AL	68/69 (99%)	68 (100%)	0	100	100
39	CF	69/69 (100%)	69 (100%)	0	100	100
40	AM	46/47 (98%)	46 (100%)	0	100	100
40	CG	46/47 (98%)	46 (100%)	0	100	100
41	AN	47/47 (100%)	47 (100%)	0	100	100
41	CH	48/47 (102%)	47 (98%)	1 (2%)	47	67
42	AO	24/24 (100%)	24 (100%)	0	100	100
42	CI	23/24 (96%)	20 (87%)	3 (13%)	4	17
43	AP	88/91 (97%)	88 (100%)	0	100	100
43	CJ	90/91 (99%)	90 (100%)	0	100	100
44	AQ	72/73 (99%)	71 (99%)	1 (1%)	59	73
44	CK	72/73 (99%)	72 (100%)	0	100	100
45	CL	100/212 (47%)	98 (98%)	2 (2%)	48	68
45	i	100/212 (47%)	94 (94%)	6 (6%)	17	46
47	C	176/215 (82%)	176 (100%)	0	100	100
47	CN	176/215 (82%)	176 (100%)	0	100	100
48	CO	194/229 (85%)	183 (94%)	11 (6%)	18	47
48	D	194/229 (85%)	194 (100%)	0	100	100
49	CP	174/198 (88%)	174 (100%)	0	100	100
49	E	175/198 (88%)	175 (100%)	0	100	100
50	CQ	174/196 (89%)	174 (100%)	0	100	100
50	F	174/196 (89%)	173 (99%)	1 (1%)	78	81
51	CR	218/220 (99%)	217 (100%)	1 (0%)	81	83
51	G	218/220 (99%)	218 (100%)	0	100	100
52	CS	169/197 (86%)	168 (99%)	1 (1%)	78	81
52	H	178/197 (90%)	177 (99%)	1 (1%)	78	81
53	CT	195/204 (96%)	184 (94%)	11 (6%)	19	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
53	I	195/204 (96%)	195 (100%)	0	100	100
54	CU	163/167 (98%)	162 (99%)	1 (1%)	78	81
54	J	166/167 (99%)	164 (99%)	2 (1%)	63	75
55	CV	157/160 (98%)	157 (100%)	0	100	100
55	K	157/160 (98%)	157 (100%)	0	100	100
56	CW	153/160 (96%)	153 (100%)	0	100	100
56	L	153/160 (96%)	153 (100%)	0	100	100
57	CX	87/104 (84%)	87 (100%)	0	100	100
57	M	90/104 (86%)	89 (99%)	1 (1%)	65	76
58	CY	122/134 (91%)	122 (100%)	0	100	100
58	N	124/134 (92%)	121 (98%)	3 (2%)	43	65
59	CZ	98/123 (80%)	98 (100%)	0	100	100
59	O	98/123 (80%)	91 (93%)	7 (7%)	13	40
60	DA	129/130 (99%)	129 (100%)	0	100	100
60	P	129/130 (99%)	129 (100%)	0	100	100
61	DB	97/102 (95%)	97 (100%)	0	100	100
61	Q	97/102 (95%)	97 (100%)	0	100	100
62	DC	111/121 (92%)	111 (100%)	0	100	100
62	R	111/121 (92%)	106 (96%)	5 (4%)	24	53
63	DD	114/116 (98%)	114 (100%)	0	100	100
63	S	114/116 (98%)	111 (97%)	3 (3%)	40	64
64	DE	112/122 (92%)	112 (100%)	0	100	100
64	T	112/122 (92%)	112 (100%)	0	100	100
65	DF	126/129 (98%)	126 (100%)	0	100	100
65	U	128/129 (99%)	128 (100%)	0	100	100
66	DG	113/117 (97%)	113 (100%)	0	100	100
66	V	113/117 (97%)	113 (100%)	0	100	100
67	DH	90/105 (86%)	90 (100%)	0	100	100
67	W	92/105 (88%)	92 (100%)	0	100	100
68	DI	71/71 (100%)	71 (100%)	0	100	100
68	X	71/71 (100%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
69	DJ	112/113 (99%)	112 (100%)	0	100	100
69	Y	112/113 (99%)	112 (100%)	0	100	100
70	DK	116/118 (98%)	116 (100%)	0	100	100
70	Z	116/118 (98%)	116 (100%)	0	100	100
71	DL	109/112 (97%)	103 (94%)	6 (6%)	19	48
71	a	111/112 (99%)	111 (100%)	0	100	100
72	DM	63/85 (74%)	63 (100%)	0	100	100
72	b	64/85 (75%)	64 (100%)	0	100	100
73	DN	83/102 (81%)	81 (98%)	2 (2%)	43	65
73	c	84/102 (82%)	76 (90%)	8 (10%)	8	29
74	DO	72/73 (99%)	72 (100%)	0	100	100
74	d	72/73 (99%)	72 (100%)	0	100	100
75	DP	51/58 (88%)	51 (100%)	0	100	100
75	e	54/58 (93%)	54 (100%)	0	100	100
76	DQ	47/48 (98%)	47 (100%)	0	100	100
76	f	47/48 (98%)	46 (98%)	1 (2%)	47	67
77	DR	48/54 (89%)	48 (100%)	0	100	100
77	g	51/54 (94%)	51 (100%)	0	100	100
78	DS	62/175 (35%)	62 (100%)	0	100	100
78	h	55/175 (31%)	55 (100%)	0	100	100
79	AR	259/263 (98%)	259 (100%)	0	100	100
79	DT	259/263 (98%)	257 (99%)	2 (1%)	73	79
80	L1	196/196 (100%)	196 (100%)	0	100	100
80	l1	196/196 (100%)	196 (100%)	0	100	100
All	All	19326/20828 (93%)	19237 (100%)	89 (0%)	81	83

5 of 89 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	CO	92	GLN
53	CT	220	LYS
48	CO	95	ASN
53	CT	153	VAL
53	CT	226	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 178 such sidechains are listed below:

Mol	Chain	Res	Type
17	BJ	193	GLN
47	CN	33	ASN
19	BL	158	HIS
26	BS	137	ASN
53	CT	182	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3213/3359 (95%)	608 (18%)	43 (1%)
1	AS	3195/3359 (95%)	618 (19%)	51 (1%)
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%)	23 (14%)	3 (1%)
46	B	1706/1787 (95%)	407 (23%)	46 (2%)
46	CM	1720/1787 (96%)	434 (25%)	51 (2%)
All	All	10387/10850 (95%)	2131 (20%)	197 (1%)

5 of 2131 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 197 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	AS	2182	C
3	AU	85	G
1	AS	2434	A
1	AS	2545	C
46	CM	151	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1476 ligands modelled in this entry, 1466 are monoatomic - leaving 10 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
82	3K5	CJ	202	-	63,63,63	0.32	0	84,95,95	0.61	2 (2%)
83	PAR	B	1970	-	44,45,45	0.57	0	63,67,67	1.76	13 (20%)
83	PAR	CM	1946	-	44,45,45	0.44	0	63,67,67	0.77	2 (3%)
83	PAR	1	3967	-	44,45,45	0.49	0	63,67,67	1.19	5 (7%)
82	3K5	1	3406	-	63,63,63	2.89	33 (52%)	84,95,95	2.00	22 (26%)
83	PAR	AS	3788	-	44,45,45	0.61	1 (2%)	63,67,67	1.10	3 (4%)
83	PAR	AS	3790	-	44,45,45	0.54	0	63,67,67	1.29	5 (7%)
83	PAR	1	3969	-	44,45,45	0.68	1 (2%)	63,67,67	1.72	12 (19%)
83	PAR	1	3968	-	44,45,45	0.53	0	63,67,67	1.12	5 (7%)
83	PAR	AS	3789	-	44,45,45	0.50	0	63,67,67	0.74	1 (1%)

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
82	3K5	CJ	202	-	-	13/29/121/121	0/7/7/7
83	PAR	B	1970	-	-	13/18/94/94	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PAR	CM	1946	-	-	4/18/94/94	0/4/4/4
83	PAR	1	3967	-	-	9/18/94/94	0/4/4/4
82	3K5	1	3406	-	-	6/29/121/121	0/7/7/7
83	PAR	AS	3788	-	-	6/18/94/94	0/4/4/4
83	PAR	AS	3790	-	-	8/18/94/94	1/4/4/4
83	PAR	1	3969	-	-	10/18/94/94	0/4/4/4
83	PAR	1	3968	-	-	7/18/94/94	1/4/4/4
83	PAR	AS	3789	-	-	10/18/94/94	0/4/4/4

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	3406	3K5	C17-C22	-8.62	1.35	1.53
82	1	3406	3K5	O4-C22	7.55	1.60	1.43
82	1	3406	3K5	C21-C22	5.72	1.62	1.52
82	1	3406	3K5	C37-C36	-4.89	1.39	1.51
82	1	3406	3K5	O6-C23	4.70	1.45	1.34

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
83	B	1970	PAR	C13-C23-C33	-8.07	92.40	102.10
82	1	3406	3K5	O14-C38-C39	6.75	123.12	111.09
82	1	3406	3K5	C9-C8-C7	-6.64	112.41	126.92
83	AS	3788	PAR	O11-C11-C21	5.81	117.58	108.08
83	1	3969	PAR	C52-C42-C32	-5.67	100.80	111.31

There are no chirality outliers.

5 of 86 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
82	1	3406	3K5	O15-C38-O14-C34
82	CJ	202	3K5	C39-C38-O14-C34
82	CJ	202	3K5	C35-C34-O14-C38
82	CJ	202	3K5	C31-C30-O9-C26
82	CJ	202	3K5	C6-C7-C8-C9

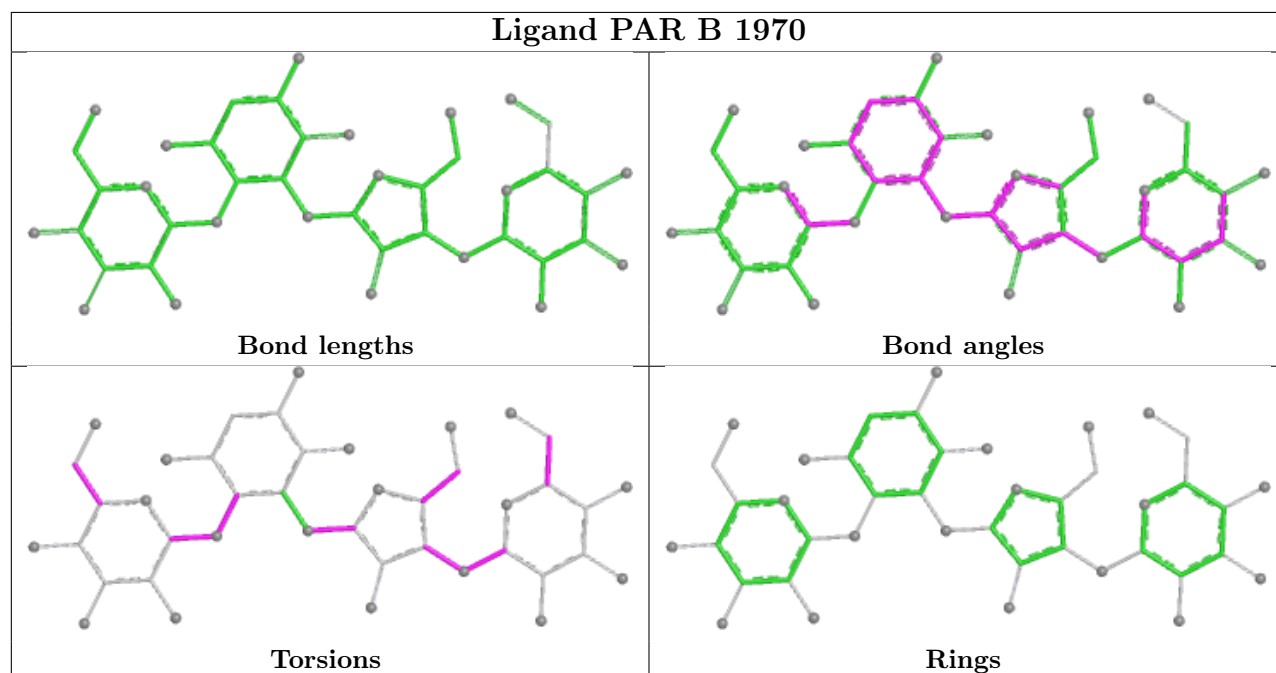
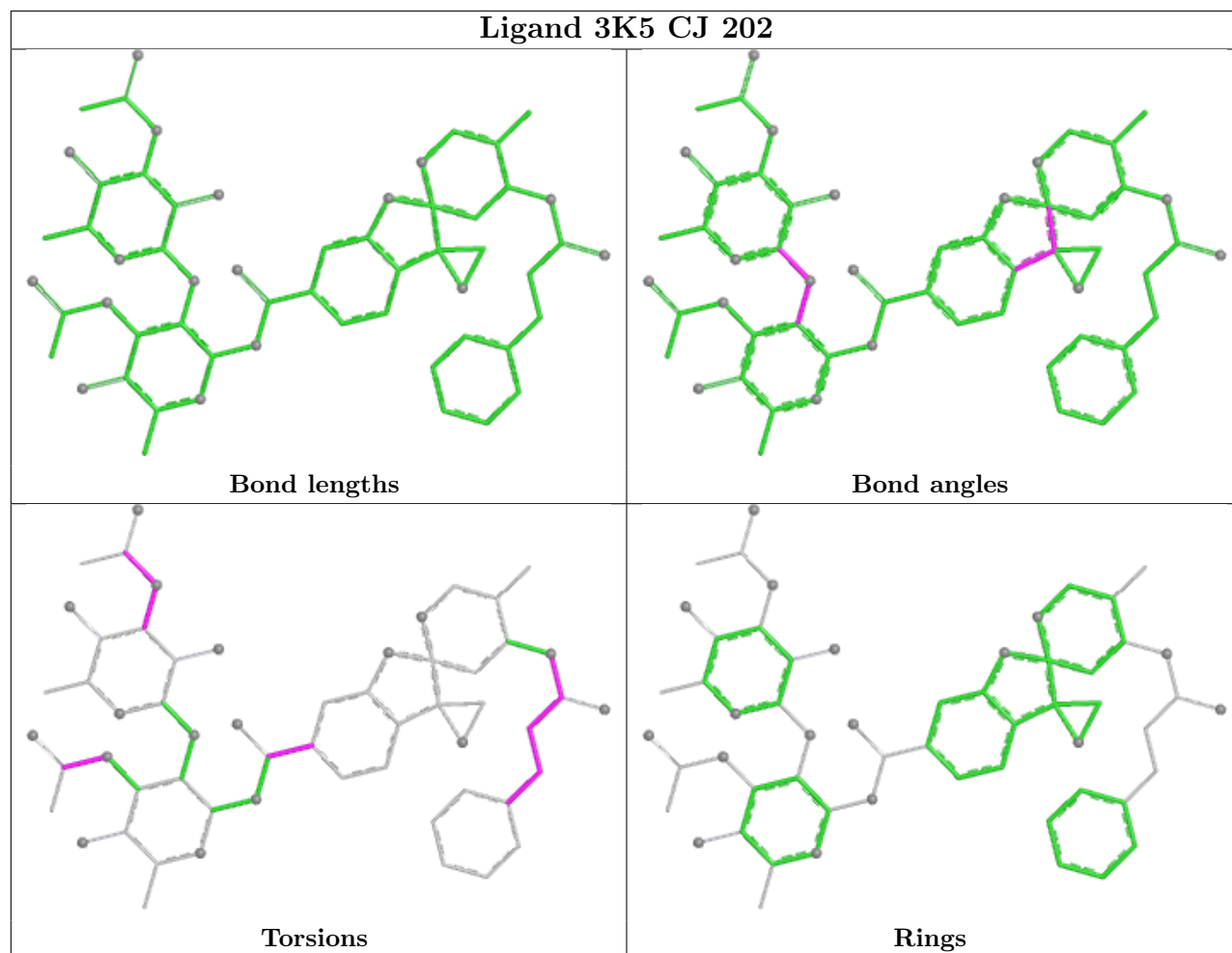
All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
83	1	3968	PAR	C12-C22-C32-C42-C52-C62
83	AS	3790	PAR	C12-C22-C32-C42-C52-C62

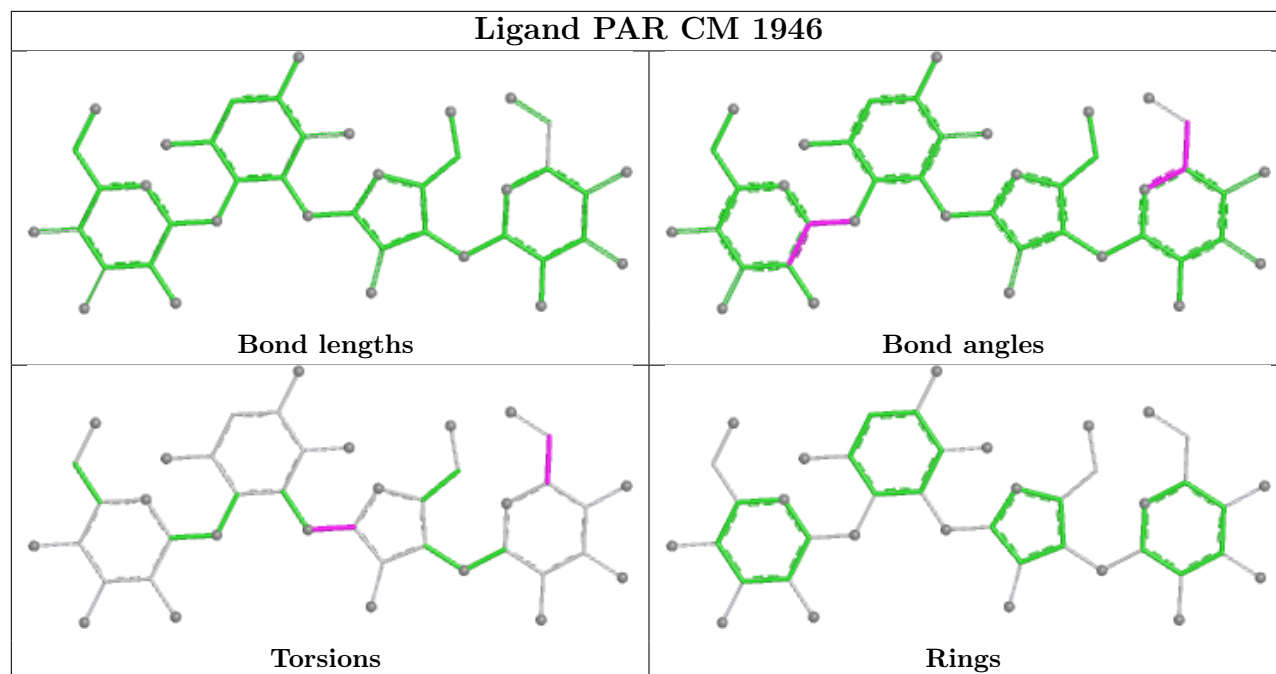
9 monomers are involved in 61 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
82	CJ	202	3K5	7	0
83	B	1970	PAR	18	0
83	1	3967	PAR	1	0
82	1	3406	3K5	7	0
83	AS	3788	PAR	2	0
83	AS	3790	PAR	5	0
83	1	3969	PAR	5	0
83	1	3968	PAR	3	0
83	AS	3789	PAR	13	0

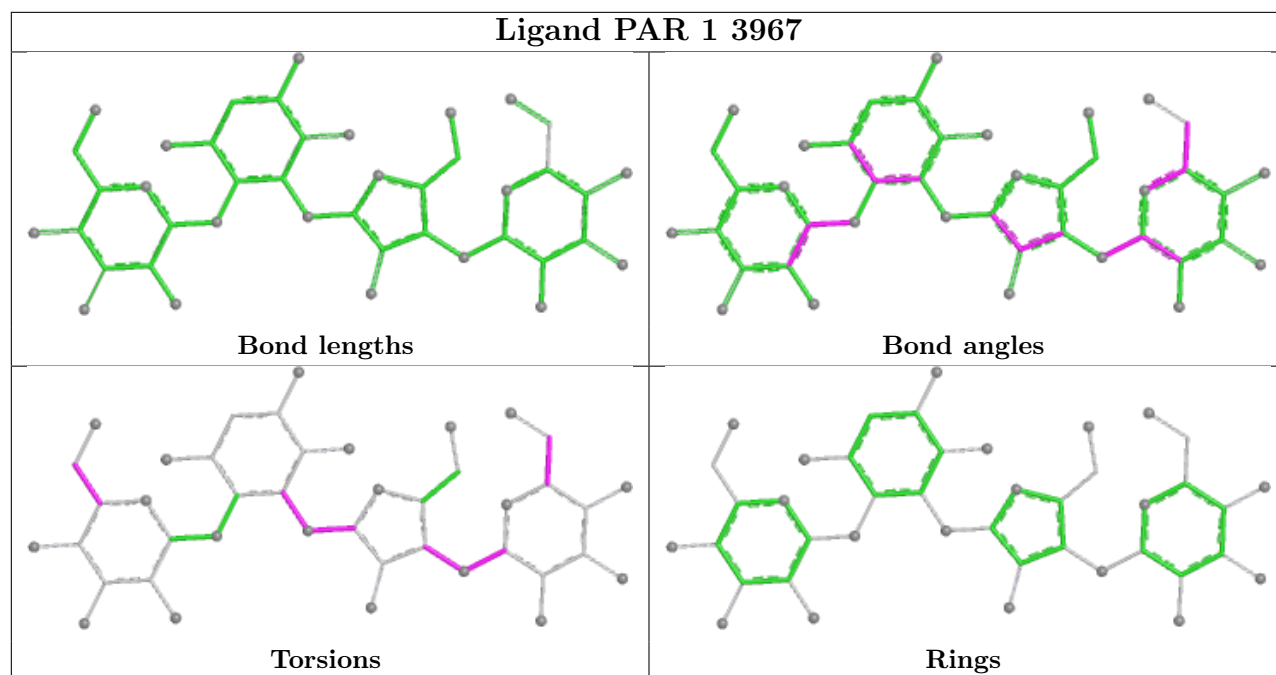
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



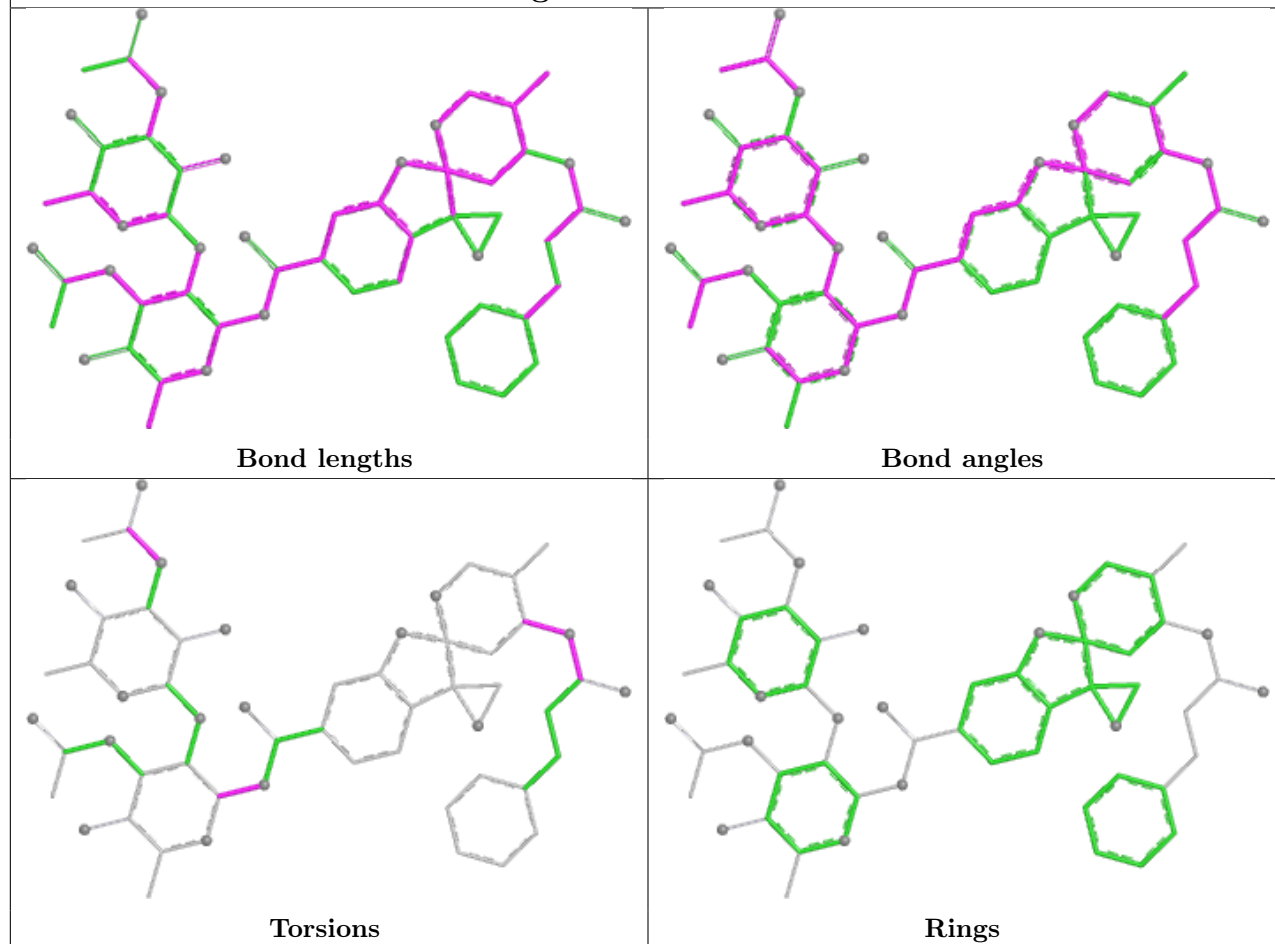
Ligand PAR CM 1946



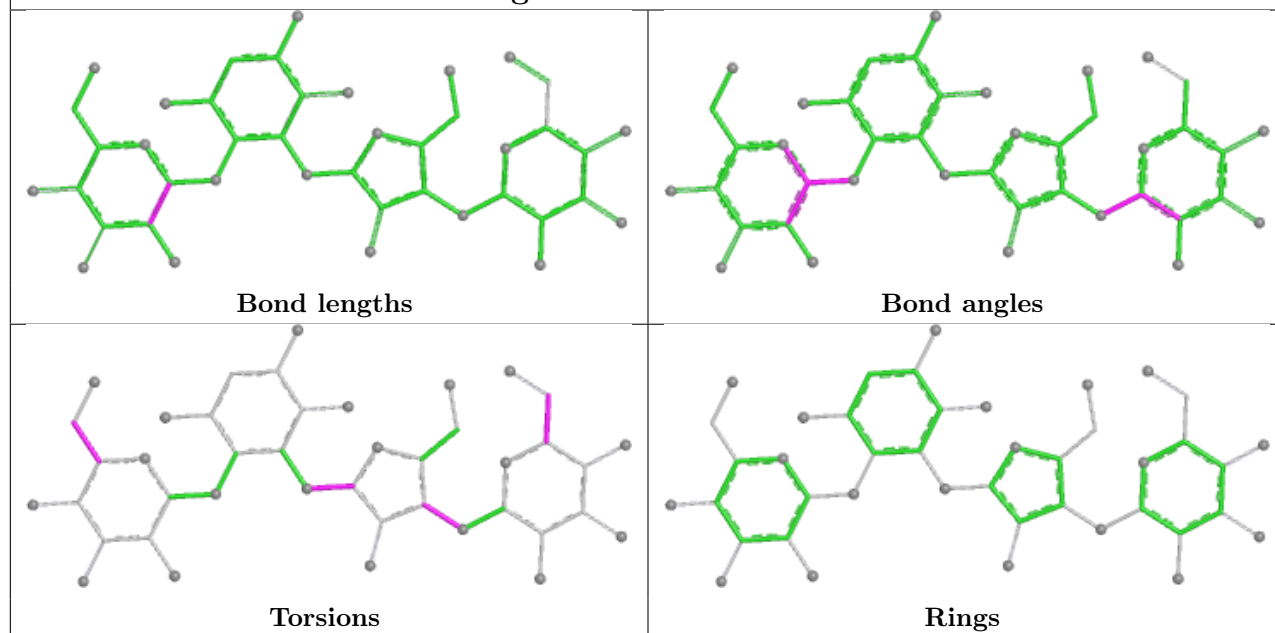
Ligand PAR 1 3967



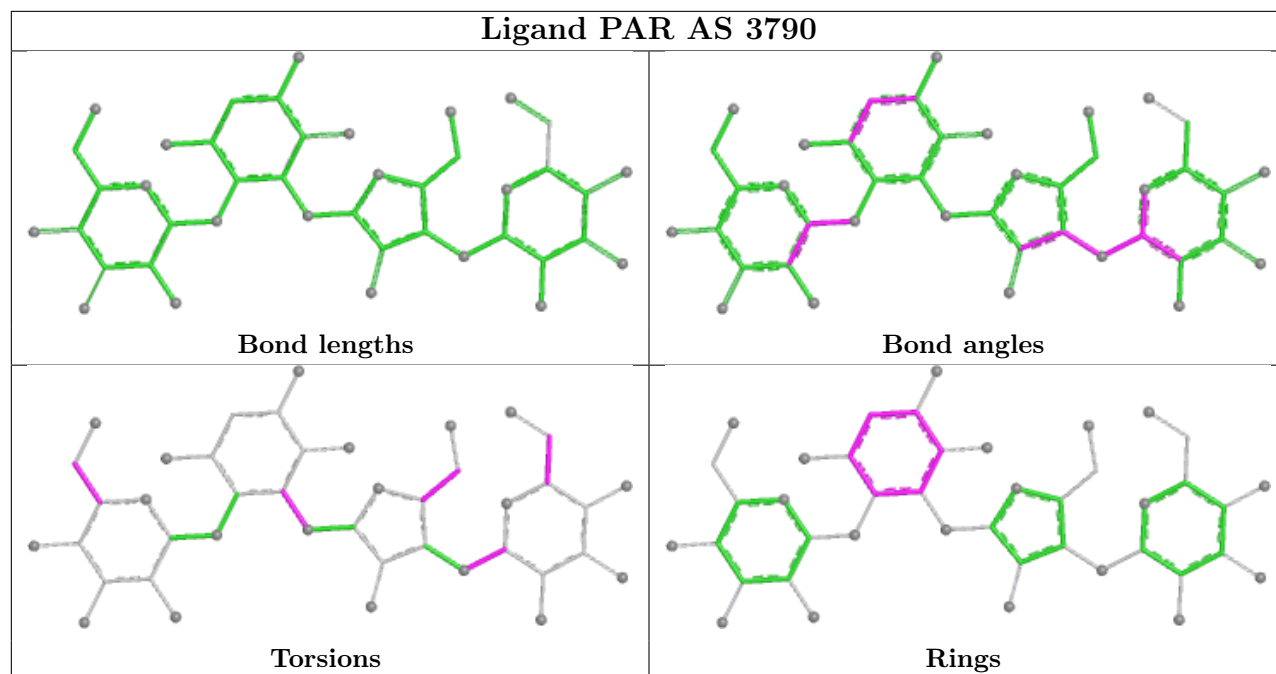
Ligand 3K5 1 3406



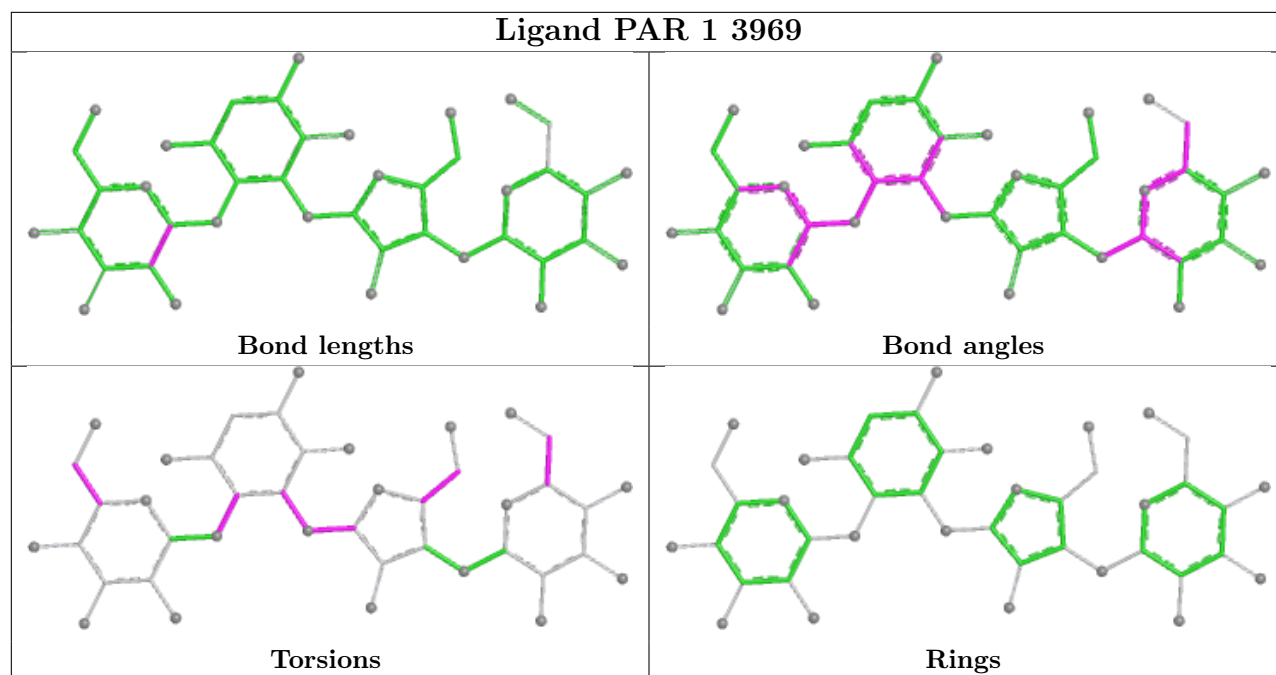
Ligand PAR AS 3788

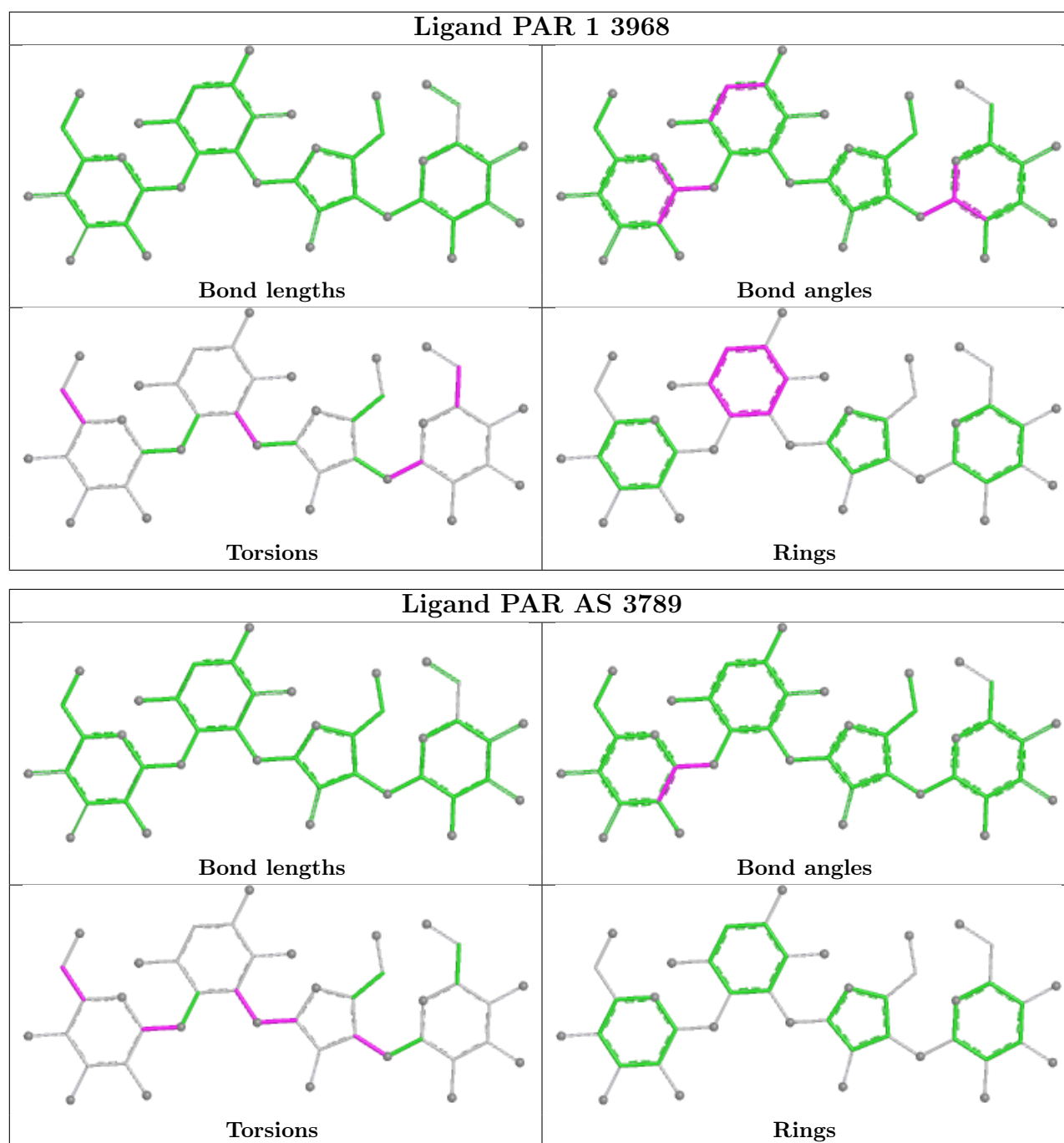


Ligand PAR AS 3790



Ligand PAR 1 3969





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	3217/3359 (95%)	-0.43	12 (0%) 88 79	33, 71, 185, 393	0
1	AS	3199/3359 (95%)	-0.21	36 (1%) 78 60	49, 89, 219, 337	0
2	3	121/121 (100%)	-0.54	0 100 100	53, 92, 111, 143	0
2	AT	121/121 (100%)	-0.24	0 100 100	53, 98, 122, 145	0
3	4	157/158 (99%)	-0.57	0 100 100	48, 71, 125, 166	0
3	AU	158/158 (100%)	-0.21	1 (0%) 85 73	68, 108, 154, 217	0
4	AW	249/254 (98%)	0.50	15 (6%) 27 19	50, 91, 113, 132	0
4	j	249/254 (98%)	0.17	5 (2%) 65 46	26, 53, 80, 240	0
5	AX	386/389 (99%)	0.16	5 (1%) 75 56	47, 76, 110, 158	0
5	k	386/389 (99%)	0.22	10 (2%) 57 38	40, 67, 91, 136	0
6	AY	361/363 (99%)	0.87	39 (10%) 11 9	63, 95, 129, 159	0
6	l	361/363 (99%)	0.24	12 (3%) 49 33	38, 79, 114, 146	0
7	AZ	292/298 (97%)	1.00	40 (13%) 6 5	63, 120, 153, 172	0
7	m	296/298 (99%)	0.34	7 (2%) 59 40	64, 100, 125, 148	0
8	BA	153/176 (86%)	0.55	7 (4%) 37 25	66, 99, 128, 152	0
8	n	157/176 (89%)	0.21	1 (0%) 85 73	69, 92, 119, 145	0
9	BB	234/241 (97%)	0.33	3 (1%) 75 56	49, 79, 140, 187	0
9	o	234/241 (97%)	0.11	1 (0%) 88 79	48, 74, 120, 164	0
10	BC	233/262 (88%)	0.60	10 (4%) 40 25	100, 128, 169, 189	0
10	p	238/262 (90%)	0.09	6 (2%) 58 39	54, 81, 127, 159	0
11	BD	190/191 (99%)	0.45	4 (2%) 63 44	71, 101, 131, 160	0
11	q	190/191 (99%)	0.31	2 (1%) 78 60	69, 90, 115, 139	0
12	BE	208/220 (94%)	0.13	2 (0%) 79 63	50, 79, 129, 163	0
12	r	208/220 (94%)	0.29	5 (2%) 59 40	46, 79, 114, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	BF	171/174 (98%)	0.65	3 (1%) 67 49	85, 125, 151, 166	0
13	s	171/174 (98%)	0.35	2 (1%) 76 58	68, 103, 125, 135	0
14	BG	200/202 (99%)	0.55	6 (3%) 52 35	60, 112, 148, 175	0
14	t	200/202 (99%)	0.06	2 (1%) 79 63	48, 85, 119, 152	0
15	BH	130/131 (99%)	0.38	7 (5%) 31 21	62, 93, 126, 146	0
15	u	130/131 (99%)	0.08	4 (3%) 51 35	67, 86, 106, 121	0
16	BI	203/204 (99%)	1.06	23 (11%) 10 8	64, 101, 120, 130	0
16	v	203/204 (99%)	0.29	3 (1%) 72 53	41, 60, 77, 96	0
17	BJ	199/200 (99%)	0.25	3 (1%) 72 53	49, 72, 111, 148	0
17	w	199/200 (99%)	0.26	2 (1%) 79 63	44, 68, 101, 129	0
18	BK	176/185 (95%)	0.63	7 (3%) 42 28	51, 84, 115, 143	0
18	x	173/185 (93%)	0.33	4 (2%) 61 42	41, 68, 111, 132	0
19	BL	185/186 (99%)	0.51	8 (4%) 40 25	63, 90, 111, 128	0
19	y	185/186 (99%)	0.40	2 (1%) 78 60	50, 75, 97, 121	0
20	BM	179/190 (94%)	0.61	12 (6%) 24 16	68, 98, 166, 190	0
20	z	179/190 (94%)	0.32	7 (3%) 43 29	49, 75, 130, 160	0
21	0	170/172 (98%)	0.08	1 (0%) 85 73	56, 76, 97, 141	0
21	BN	170/172 (98%)	0.38	2 (1%) 76 58	54, 78, 109, 127	0
22	2	159/160 (99%)	0.34	8 (5%) 34 23	49, 74, 119, 141	0
22	BO	159/160 (99%)	0.74	13 (8%) 17 13	57, 84, 139, 157	0
23	5	103/124 (83%)	0.31	0 100 100	82, 112, 136, 152	0
23	BP	102/124 (82%)	0.28	1 (0%) 79 63	101, 139, 160, 183	0
24	6	131/137 (95%)	0.36	7 (5%) 32 22	40, 65, 90, 106	0
24	BQ	131/137 (95%)	0.48	2 (1%) 72 53	49, 70, 99, 123	0
25	7	118/155 (76%)	0.23	1 (0%) 82 68	44, 91, 134, 145	0
25	BR	98/155 (63%)	0.69	6 (6%) 27 18	62, 93, 145, 155	0
26	8	121/142 (85%)	0.29	3 (2%) 58 39	56, 76, 94, 135	0
26	BS	119/142 (83%)	0.73	5 (4%) 40 26	84, 109, 128, 137	0
27	9	126/127 (99%)	0.42	4 (3%) 50 34	60, 86, 110, 122	0
27	BT	126/127 (99%)	0.51	5 (3%) 42 28	71, 109, 138, 164	0
28	AA	135/136 (99%)	0.33	2 (1%) 72 53	55, 91, 112, 144	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	BU	135/136 (99%)	0.53	3 (2%) 62 43	98, 127, 145, 166	0
29	AB	148/149 (99%)	0.27	3 (2%) 65 46	37, 70, 95, 125	0
29	BV	148/149 (99%)	0.79	12 (8%) 18 13	53, 95, 123, 144	0
30	AC	62/63 (98%)	0.80	5 (8%) 18 13	55, 87, 122, 137	0
30	BW	63/63 (100%)	1.27	13 (20%) 2 2	53, 105, 146, 167	1 (1%)
31	AD	96/106 (90%)	-0.13	0 100 100	52, 79, 107, 130	0
31	BX	96/106 (90%)	0.46	1 (1%) 79 63	90, 116, 148, 155	0
32	AE	110/112 (98%)	0.10	0 100 100	53, 74, 122, 137	0
32	BY	108/112 (96%)	0.56	3 (2%) 55 36	63, 96, 138, 172	0
33	AF	124/131 (94%)	0.42	3 (2%) 59 40	51, 75, 95, 108	0
33	BZ	125/131 (95%)	0.65	7 (5%) 30 20	52, 84, 111, 128	1 (0%)
34	AG	106/107 (99%)	0.17	1 (0%) 81 65	51, 72, 97, 109	0
34	CA	106/107 (99%)	0.38	3 (2%) 55 36	44, 73, 98, 118	3 (2%)
35	AH	112/113 (99%)	0.47	4 (3%) 46 31	51, 72, 119, 139	0
35	CB	111/113 (98%)	0.99	18 (16%) 4 4	71, 109, 145, 171	4 (3%)
36	AI	120/120 (100%)	0.30	2 (1%) 69 50	62, 86, 116, 137	0
36	CC	118/120 (98%)	0.86	12 (10%) 12 10	87, 116, 139, 160	0
37	AJ	97/99 (97%)	0.12	0 100 100	52, 78, 109, 153	0
37	CD	97/99 (97%)	1.08	13 (13%) 7 6	90, 120, 159, 176	1 (1%)
38	AK	86/90 (95%)	0.32	1 (1%) 76 58	33, 56, 93, 130	0
38	CE	86/90 (95%)	0.68	10 (11%) 9 8	63, 88, 128, 161	0
39	AL	77/78 (98%)	0.31	1 (1%) 75 56	75, 97, 121, 146	0
39	CF	77/78 (98%)	0.54	2 (2%) 57 38	93, 129, 166, 184	1 (1%)
40	AM	50/51 (98%)	0.25	1 (2%) 65 46	44, 65, 96, 97	0
40	CG	50/51 (98%)	1.08	6 (12%) 9 7	78, 95, 117, 129	0
41	AN	52/52 (100%)	0.94	7 (13%) 7 6	90, 109, 125, 140	0
41	CH	52/52 (100%)	0.71	2 (3%) 44 30	81, 121, 140, 160	1 (1%)
42	AO	25/25 (100%)	1.16	4 (16%) 5 4	69, 80, 96, 100	0
42	CI	24/25 (96%)	0.90	4 (16%) 4 4	72, 81, 96, 109	0
43	AP	103/106 (97%)	0.08	2 (1%) 66 48	39, 71, 108, 129	0
43	CJ	103/106 (97%)	0.59	4 (3%) 43 29	63, 100, 134, 159	2 (1%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	AQ	91/92 (98%)	0.16	1 (1%) 78 60	37, 59, 101, 127	0
44	CK	91/92 (98%)	0.41	3 (3%) 49 33	60, 93, 141, 151	0
45	CL	121/267 (45%)	1.12	22 (18%) 3 3	79, 119, 153, 163	0
45	i	121/267 (45%)	1.12	21 (17%) 4 4	88, 117, 147, 157	0
46	B	1712/1787 (95%)	-0.24	3 (0%) 91 86	52, 102, 183, 234	0
46	CM	1726/1787 (96%)	0.15	37 (2%) 63 44	60, 114, 210, 260	0
47	C	208/261 (79%)	0.40	3 (1%) 73 55	86, 116, 138, 150	0
47	CN	208/261 (79%)	0.61	10 (4%) 35 24	85, 128, 158, 190	0
48	CO	214/256 (83%)	0.76	23 (10%) 11 9	99, 136, 168, 188	0
48	D	214/256 (83%)	0.15	1 (0%) 87 76	69, 96, 117, 128	0
49	CP	216/249 (86%)	0.39	12 (5%) 30 20	52, 98, 135, 160	0
49	E	217/249 (87%)	0.45	10 (4%) 37 25	74, 100, 128, 146	0
50	CQ	223/251 (88%)	0.88	22 (9%) 13 10	99, 123, 165, 199	0
50	F	223/251 (88%)	0.53	9 (4%) 42 28	85, 116, 144, 157	0
51	CR	260/262 (99%)	0.68	16 (6%) 26 18	69, 108, 134, 170	0
51	G	259/262 (98%)	0.54	12 (4%) 37 25	76, 101, 118, 127	0
52	CS	195/225 (86%)	0.81	21 (10%) 11 9	108, 135, 155, 164	0
52	H	206/225 (91%)	0.54	17 (8%) 17 13	89, 111, 140, 166	0
53	CT	226/236 (95%)	0.67	18 (7%) 18 14	74, 121, 172, 204	0
53	I	226/236 (95%)	0.39	7 (3%) 51 35	65, 109, 141, 157	0
54	CU	182/186 (97%)	0.56	14 (7%) 19 14	81, 142, 173, 184	0
54	J	185/186 (99%)	0.49	6 (3%) 50 34	85, 119, 141, 156	0
55	CV	203/206 (98%)	0.98	21 (10%) 12 10	65, 100, 153, 194	0
55	K	203/206 (98%)	0.22	1 (0%) 87 76	46, 86, 131, 146	0
56	CW	178/189 (94%)	0.86	17 (9%) 13 11	81, 116, 146, 160	0
56	L	178/189 (94%)	0.90	13 (7%) 21 15	78, 110, 129, 140	0
57	CX	93/118 (78%)	0.97	14 (15%) 5 5	103, 137, 163, 177	0
57	M	98/118 (83%)	0.55	5 (5%) 33 22	94, 123, 141, 148	0
58	CY	141/155 (90%)	0.83	14 (9%) 13 10	68, 93, 131, 177	0
58	N	144/155 (92%)	0.43	3 (2%) 63 44	60, 85, 116, 178	0
59	CZ	116/143 (81%)	0.61	4 (3%) 48 32	165, 183, 200, 209	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
59	O	116/143 (81%)	0.76	12 (10%) 12 10	132, 157, 173, 175	0
60	DA	150/151 (99%)	0.82	8 (5%) 32 22	79, 113, 136, 154	0
60	P	150/151 (99%)	0.36	5 (3%) 49 33	58, 89, 115, 122	0
61	DB	127/132 (96%)	0.57	8 (6%) 26 17	84, 125, 146, 153	0
61	Q	127/132 (96%)	0.05	1 (0%) 82 68	59, 85, 104, 117	0
62	DC	129/142 (90%)	1.70	44 (34%) 1 1	113, 139, 164, 181	0
62	R	129/142 (90%)	0.63	8 (6%) 26 18	83, 113, 146, 157	0
63	DD	140/142 (98%)	1.48	34 (24%) 2 1	112, 140, 160, 173	0
63	S	140/142 (98%)	0.95	12 (8%) 16 12	90, 118, 138, 151	0
64	DE	125/137 (91%)	0.91	12 (9%) 13 11	102, 141, 182, 190	0
64	T	124/137 (90%)	0.67	7 (5%) 30 20	98, 122, 152, 158	0
65	DF	142/145 (97%)	1.24	24 (16%) 4 4	104, 136, 161, 196	0
65	U	144/145 (99%)	0.42	5 (3%) 47 31	85, 104, 126, 153	0
66	DG	141/145 (97%)	1.12	25 (17%) 4 3	105, 135, 160, 186	0
66	V	141/145 (97%)	0.57	6 (4%) 40 25	99, 118, 138, 163	0
67	DH	100/119 (84%)	1.12	15 (15%) 5 5	91, 136, 168, 175	0
67	W	102/119 (85%)	0.85	15 (14%) 6 5	86, 125, 141, 156	0
68	DI	87/87 (100%)	0.32	2 (2%) 61 42	83, 112, 147, 169	0
68	X	87/87 (100%)	0.38	3 (3%) 48 32	76, 104, 128, 144	0
69	DJ	129/130 (99%)	0.57	2 (1%) 70 52	70, 93, 113, 121	0
69	Y	129/130 (99%)	0.57	8 (6%) 26 18	71, 88, 108, 117	0
70	DK	143/145 (98%)	0.90	8 (5%) 30 20	64, 88, 115, 142	0
70	Z	143/145 (98%)	0.19	1 (0%) 84 70	65, 86, 108, 128	0
71	DL	132/135 (97%)	0.34	2 (1%) 72 53	98, 127, 151, 176	0
71	a	134/135 (99%)	0.49	4 (2%) 52 35	84, 114, 131, 142	0
72	DM	71/105 (67%)	0.35	2 (2%) 55 36	125, 148, 169, 177	0
72	b	72/105 (68%)	0.06	0 100 100	94, 122, 140, 143	0
73	DN	97/119 (81%)	0.92	14 (14%) 6 5	85, 105, 154, 166	0
73	c	98/119 (82%)	0.65	8 (8%) 17 13	71, 91, 127, 138	0
74	DO	81/82 (98%)	0.64	4 (4%) 35 23	92, 128, 173, 190	0
74	d	81/82 (98%)	0.37	2 (2%) 58 39	74, 101, 144, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
75	DP	59/67 (88%)	0.51	3 (5%) 33 22	112, 139, 163, 178	0
75	e	62/67 (92%)	0.57	6 (9%) 13 11	100, 120, 139, 145	0
76	DQ	55/56 (98%)	1.56	16 (29%) 1 1	99, 119, 163, 182	0
76	f	55/56 (98%)	0.92	3 (5%) 30 21	88, 104, 133, 144	0
77	DR	56/63 (88%)	1.11	6 (10%) 11 9	91, 125, 176, 199	0
77	g	60/63 (95%)	0.61	6 (10%) 12 10	89, 116, 141, 158	0
78	DS	70/193 (36%)	1.35	15 (21%) 2 2	166, 184, 197, 204	0
78	h	63/193 (32%)	0.77	4 (6%) 26 17	132, 154, 164, 169	0
79	AR	311/317 (98%)	0.57	11 (3%) 47 31	112, 141, 163, 176	0
79	DT	311/317 (98%)	0.67	15 (4%) 35 24	131, 161, 184, 208	0
80	L1	217/217 (100%)	0.60	6 (2%) 55 36	116, 148, 185, 242	0
80	l1	217/217 (100%)	0.73	10 (4%) 37 25	132, 158, 182, 217	0
All	All	33241/35542 (93%)	0.29	1307 (3%) 43 29	26, 98, 166, 393	14 (0%)

The worst 5 of 1307 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
63	DD	131	ARG	9.2
51	G	110	ALA	8.5
48	CO	55	LYS	6.6
6	AY	363	ASN	6.3
46	CM	1480	G	6.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
81	MG	B	1855	1/1	0.23	0.20	106,106,106,106	0
81	MG	B	1834	1/1	0.30	0.23	241,241,241,241	0
81	MG	B	1848	1/1	0.40	0.14	57,57,57,57	0
81	MG	1	3470	1/1	0.42	0.26	48,48,48,48	0
81	MG	CM	1811	1/1	0.44	0.33	73,73,73,73	0
81	MG	8	201	1/1	0.46	0.14	55,55,55,55	0
81	MG	B	1932	1/1	0.49	0.25	81,81,81,81	0
81	MG	B	1805	1/1	0.49	0.32	82,82,82,82	0
81	MG	g	101	1/1	0.51	0.28	66,66,66,66	0
81	MG	AS	3588	1/1	0.51	0.30	79,79,79,79	0
81	MG	B	1960	1/1	0.51	0.17	41,41,41,41	0
81	MG	AS	3581	1/1	0.52	0.09	66,66,66,66	0
81	MG	AS	3647	1/1	0.53	0.20	62,62,62,62	0
81	MG	AS	3484	1/1	0.53	0.16	43,43,43,43	0
81	MG	1	3694	1/1	0.54	0.16	120,120,120,120	0
81	MG	1	3800	1/1	0.54	0.23	95,95,95,95	0
81	MG	1	3603	1/1	0.54	0.23	64,64,64,64	0
81	MG	1	3783	1/1	0.55	0.14	36,36,36,36	0
81	MG	B	1919	1/1	0.55	0.14	110,110,110,110	0
81	MG	CM	1833	1/1	0.55	0.32	69,69,69,69	0
81	MG	1	3677	1/1	0.56	0.12	55,55,55,55	0
81	MG	B	1966	1/1	0.56	0.15	99,99,99,99	0
81	MG	AS	3595	1/1	0.56	0.19	47,47,47,47	0
81	MG	CM	1871	1/1	0.56	0.17	99,99,99,99	0
81	MG	CM	1925	1/1	0.56	0.27	61,61,61,61	0
81	MG	1	3457	1/1	0.57	0.18	44,44,44,44	0
81	MG	1	3869	1/1	0.57	0.23	61,61,61,61	0
81	MG	B	1854	1/1	0.57	0.15	96,96,96,96	0
81	MG	AS	3632	1/1	0.58	0.15	91,91,91,91	0
81	MG	1	3879	1/1	0.59	0.19	63,63,63,63	0
81	MG	1	3755	1/1	0.59	0.13	51,51,51,51	0
81	MG	k	403	1/1	0.60	0.28	78,78,78,78	0
81	MG	AS	3497	1/1	0.62	0.23	75,75,75,75	0
81	MG	CM	1883	1/1	0.62	0.17	65,65,65,65	0
81	MG	B	1836	1/1	0.62	0.32	78,78,78,78	0
81	MG	B	1801	1/1	0.63	0.18	54,54,54,54	0
81	MG	4	212	1/1	0.63	0.13	81,81,81,81	0
81	MG	AS	3737	1/1	0.63	0.28	60,60,60,60	0
81	MG	AS	3528	1/1	0.63	0.15	97,97,97,97	0
84	ZN	AP	201	1/1	0.63	0.26	234,234,234,234	0
81	MG	B	1843	1/1	0.64	0.09	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	B	1925	1/1	0.64	0.12	76,76,76,76	0
81	MG	1	3433	1/1	0.64	0.31	72,72,72,72	0
81	MG	1	3844	1/1	0.64	0.17	75,75,75,75	0
81	MG	1	3857	1/1	0.64	0.14	49,49,49,49	0
81	MG	CL	302	1/1	0.64	0.30	43,43,43,43	0
81	MG	AS	3762	1/1	0.64	0.09	57,57,57,57	0
81	MG	AS	3550	1/1	0.65	0.23	48,48,48,48	0
81	MG	B	1931	1/1	0.65	0.23	72,72,72,72	0
81	MG	B	1871	1/1	0.65	0.21	64,64,64,64	0
81	MG	CM	1822	1/1	0.65	0.19	81,81,81,81	0
81	MG	AS	3671	1/1	0.65	0.20	46,46,46,46	0
81	MG	1	3802	1/1	0.66	0.08	89,89,89,89	0
81	MG	3	211	1/1	0.66	0.16	64,64,64,64	0
81	MG	1	3415	1/1	0.66	0.26	23,23,23,23	0
81	MG	AT	203	1/1	0.66	0.27	71,71,71,71	0
81	MG	1	3423	1/1	0.67	0.20	55,55,55,55	0
81	MG	CM	1897	1/1	0.67	0.22	105,105,105,105	0
81	MG	B	1893	1/1	0.67	0.14	69,69,69,69	0
81	MG	CM	1940	1/1	0.67	0.26	59,59,59,59	0
81	MG	DB	201	1/1	0.67	0.18	67,67,67,67	0
81	MG	1	3668	1/1	0.67	0.21	57,57,57,57	0
81	MG	B	1956	1/1	0.67	0.11	67,67,67,67	0
81	MG	DC	201	1/1	0.68	0.29	42,42,42,42	0
81	MG	BH	201	1/1	0.68	0.09	54,54,54,54	0
81	MG	B	1889	1/1	0.68	0.21	71,71,71,71	0
81	MG	B	1923	1/1	0.69	0.14	92,92,92,92	0
81	MG	AS	3729	1/1	0.69	0.42	79,79,79,79	0
81	MG	D	301	1/1	0.69	0.29	69,69,69,69	0
81	MG	1	3584	1/1	0.69	0.21	61,61,61,61	0
81	MG	AS	3765	1/1	0.69	0.15	44,44,44,44	0
81	MG	AS	3649	1/1	0.69	0.10	54,54,54,54	0
81	MG	CM	1890	1/1	0.69	0.13	57,57,57,57	0
81	MG	B	1922	1/1	0.70	0.14	65,65,65,65	0
81	MG	CM	1857	1/1	0.70	0.17	99,99,99,99	0
81	MG	AS	3464	1/1	0.70	0.20	81,81,81,81	0
83	PAR	AS	3789	42/42	0.70	0.14	69,100,118,123	42
81	MG	AU	203	1/1	0.70	0.14	100,100,100,100	0
81	MG	1	3894	1/1	0.71	0.20	52,52,52,52	0
81	MG	1	3904	1/1	0.71	0.13	57,57,57,57	0
81	MG	B	1915	1/1	0.71	0.18	76,76,76,76	0
81	MG	B	1967	1/1	0.71	0.07	71,71,71,71	0
81	MG	1	3754	1/1	0.71	0.12	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	4	208	1/1	0.71	0.15	57,57,57,57	0
81	MG	1	3852	1/1	0.71	0.30	62,62,62,62	0
81	MG	1	3789	1/1	0.71	0.27	46,46,46,46	0
81	MG	1	3748	1/1	0.71	0.13	27,27,27,27	0
81	MG	1	3766	1/1	0.71	0.12	63,63,63,63	0
81	MG	F	301	1/1	0.72	0.18	69,69,69,69	0
81	MG	1	3890	1/1	0.72	0.08	45,45,45,45	0
81	MG	CM	1912	1/1	0.72	0.20	62,62,62,62	0
81	MG	CM	1801	1/1	0.72	0.20	36,36,36,36	0
81	MG	AS	3704	1/1	0.72	0.20	49,49,49,49	0
81	MG	AR	401	1/1	0.72	0.15	83,83,83,83	0
81	MG	1	3597	1/1	0.72	0.41	78,78,78,78	0
81	MG	1	3464	1/1	0.72	0.25	34,34,34,34	0
81	MG	3	207	1/1	0.72	0.21	87,87,87,87	0
81	MG	AS	3507	1/1	0.72	0.26	72,72,72,72	0
84	ZN	CB	201	1/1	0.72	0.23	255,255,255,255	0
81	MG	1	3864	1/1	0.73	0.09	62,62,62,62	0
81	MG	1	3931	1/1	0.73	0.09	58,58,58,58	0
81	MG	CM	1862	1/1	0.73	0.22	64,64,64,64	0
81	MG	DB	203	1/1	0.73	0.17	117,117,117,117	0
81	MG	B	1945	1/1	0.73	0.13	61,61,61,61	0
81	MG	1	3502	1/1	0.73	0.16	55,55,55,55	0
81	MG	1	3788	1/1	0.73	0.15	57,57,57,57	0
83	PAR	AS	3790	42/42	0.73	0.16	81,107,127,140	0
81	MG	1	3555	1/1	0.73	0.14	53,53,53,53	0
81	MG	1	3490	1/1	0.73	0.13	45,45,45,45	0
81	MG	CM	1915	1/1	0.74	0.20	66,66,66,66	0
81	MG	AS	3535	1/1	0.74	0.16	88,88,88,88	0
81	MG	1	3635	1/1	0.74	0.14	61,61,61,61	0
81	MG	AS	3457	1/1	0.74	0.26	37,37,37,37	0
81	MG	1	3420	1/1	0.74	0.10	38,38,38,38	0
81	MG	B	1911	1/1	0.74	0.17	58,58,58,58	0
81	MG	AS	3598	1/1	0.74	0.16	69,69,69,69	0
83	PAR	B	1970	42/42	0.74	0.15	82,119,132,143	0
81	MG	AS	3615	1/1	0.74	0.17	50,50,50,50	0
81	MG	1	3769	1/1	0.74	0.17	37,37,37,37	0
81	MG	1	3425	1/1	0.74	0.26	40,40,40,40	0
81	MG	1	3839	1/1	0.74	0.12	50,50,50,50	0
81	MG	AS	3585	1/1	0.75	0.29	58,58,58,58	0
81	MG	1	3509	1/1	0.75	0.14	30,30,30,30	0
81	MG	1	3842	1/1	0.75	0.10	27,27,27,27	0
81	MG	1	3649	1/1	0.75	0.10	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	y	202	1/1	0.75	0.11	45,45,45,45	0
81	MG	1	3798	1/1	0.75	0.18	50,50,50,50	0
81	MG	B	1874	1/1	0.75	0.21	51,51,51,51	0
81	MG	B	1946	1/1	0.75	0.09	72,72,72,72	0
81	MG	DJ	202	1/1	0.75	0.09	53,53,53,53	0
81	MG	AP	203	1/1	0.75	0.16	32,32,32,32	0
81	MG	1	3909	1/1	0.75	0.11	44,44,44,44	0
81	MG	CM	1864	1/1	0.75	0.19	54,54,54,54	0
81	MG	1	3667	1/1	0.75	0.10	50,50,50,50	0
84	ZN	AH	201	1/1	0.75	0.13	213,213,213,213	0
81	MG	1	3535	1/1	0.75	0.21	84,84,84,84	0
81	MG	1	3811	1/1	0.75	0.12	38,38,38,38	0
81	MG	CM	1945	1/1	0.76	0.16	49,49,49,49	0
81	MG	AT	208	1/1	0.76	0.27	49,49,49,49	0
81	MG	j	304	1/1	0.76	0.16	42,42,42,42	0
81	MG	CM	1873	1/1	0.76	0.30	40,40,40,40	0
81	MG	AS	3516	1/1	0.76	0.32	48,48,48,48	0
81	MG	1	3471	1/1	0.76	0.15	41,41,41,41	0
83	PAR	1	3969	42/42	0.76	0.13	47,103,124,126	0
81	MG	1	3585	1/1	0.76	0.10	53,53,53,53	0
81	MG	1	3843	1/1	0.76	0.21	63,63,63,63	0
81	MG	4	213	1/1	0.76	0.12	49,49,49,49	0
81	MG	CM	1917	1/1	0.76	0.13	86,86,86,86	0
81	MG	AS	3781	1/1	0.76	0.11	49,49,49,49	0
81	MG	B	1879	1/1	0.76	0.11	94,94,94,94	0
81	MG	1	3552	1/1	0.77	0.17	75,75,75,75	0
81	MG	B	1957	1/1	0.77	0.08	31,31,31,31	0
81	MG	AS	3618	1/1	0.77	0.14	58,58,58,58	0
81	MG	AS	3424	1/1	0.77	0.18	52,52,52,52	0
81	MG	1	3888	1/1	0.77	0.12	55,55,55,55	0
81	MG	1	3560	1/1	0.77	0.21	73,73,73,73	0
81	MG	AS	3583	1/1	0.77	0.15	61,61,61,61	0
81	MG	AS	3682	1/1	0.77	0.22	77,77,77,77	0
83	PAR	AS	3788	42/42	0.77	0.13	84,114,125,131	0
81	MG	B	1901	1/1	0.77	0.11	74,74,74,74	0
81	MG	CM	1818	1/1	0.77	0.17	40,40,40,40	0
81	MG	B	1909	1/1	0.77	0.07	62,62,62,62	0
81	MG	CM	1830	1/1	0.77	0.21	81,81,81,81	0
81	MG	B	1949	1/1	0.77	0.15	75,75,75,75	0
81	MG	AS	3743	1/1	0.78	0.14	41,41,41,41	0
81	MG	1	3823	1/1	0.78	0.15	48,48,48,48	0
81	MG	4	215	1/1	0.78	0.12	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3779	1/1	0.78	0.20	57,57,57,57	0
81	MG	V	201	1/1	0.78	0.11	75,75,75,75	0
81	MG	AS	3782	1/1	0.78	0.10	37,37,37,37	0
81	MG	AT	202	1/1	0.78	0.23	43,43,43,43	0
81	MG	Y	201	1/1	0.78	0.17	69,69,69,69	0
81	MG	1	3556	1/1	0.78	0.14	66,66,66,66	0
81	MG	CQ	304	1/1	0.78	0.09	71,71,71,71	0
81	MG	1	3771	1/1	0.78	0.15	109,109,109,109	0
81	MG	1	3558	1/1	0.78	0.12	65,65,65,65	0
81	MG	1	3532	1/1	0.78	0.24	37,37,37,37	0
81	MG	1	3611	1/1	0.78	0.13	50,50,50,50	0
81	MG	1	3561	1/1	0.78	0.23	53,53,53,53	0
83	PAR	1	3968	42/42	0.78	0.14	56,91,119,122	0
81	MG	1	3578	1/1	0.78	0.11	41,41,41,41	0
81	MG	B	1815	1/1	0.78	0.28	59,59,59,59	0
81	MG	B	1903	1/1	0.78	0.16	61,61,61,61	0
81	MG	B	1819	1/1	0.78	0.17	30,30,30,30	0
81	MG	AS	3707	1/1	0.78	0.08	27,27,27,27	0
81	MG	AS	3721	1/1	0.78	0.11	64,64,64,64	0
81	MG	1	3764	1/1	0.78	0.30	63,63,63,63	0
81	MG	1	3484	1/1	0.78	0.17	60,60,60,60	0
81	MG	CM	1891	1/1	0.79	0.11	48,48,48,48	0
81	MG	1	3590	1/1	0.79	0.08	36,36,36,36	0
81	MG	AS	3469	1/1	0.79	0.17	55,55,55,55	0
81	MG	B	1959	1/1	0.79	0.22	44,44,44,44	0
81	MG	w	303	1/1	0.79	0.39	64,64,64,64	0
81	MG	1	3960	1/1	0.79	0.16	35,35,35,35	0
81	MG	AS	3667	1/1	0.79	0.14	28,28,28,28	0
81	MG	1	3961	1/1	0.79	0.15	85,85,85,85	0
81	MG	1	3870	1/1	0.79	0.12	54,54,54,54	0
81	MG	DA	202	1/1	0.79	0.18	70,70,70,70	0
81	MG	CM	1810	1/1	0.79	0.23	45,45,45,45	0
81	MG	1	3574	1/1	0.79	0.20	53,53,53,53	0
81	MG	I	301	1/1	0.79	0.15	85,85,85,85	0
81	MG	AS	3709	1/1	0.79	0.07	52,52,52,52	0
81	MG	1	3644	1/1	0.79	0.11	56,56,56,56	0
81	MG	CM	1832	1/1	0.79	0.14	63,63,63,63	0
81	MG	AS	3727	1/1	0.79	0.23	73,73,73,73	0
81	MG	B	1813	1/1	0.79	0.16	42,42,42,42	0
81	MG	1	3466	1/1	0.79	0.32	47,47,47,47	0
81	MG	1	3715	1/1	0.79	0.22	51,51,51,51	0
81	MG	AS	3746	1/1	0.79	0.20	71,71,71,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3730	1/1	0.79	0.18	48,48,48,48	0
81	MG	1	3660	1/1	0.79	0.11	58,58,58,58	0
81	MG	AS	3612	1/1	0.79	0.16	52,52,52,52	0
81	MG	1	3866	1/1	0.80	0.13	81,81,81,81	0
81	MG	1	3416	1/1	0.80	0.21	30,30,30,30	0
81	MG	CM	1907	1/1	0.80	0.12	103,103,103,103	0
81	MG	AT	212	1/1	0.80	0.11	41,41,41,41	0
81	MG	1	3926	1/1	0.80	0.09	37,37,37,37	0
81	MG	1	3477	1/1	0.80	0.15	18,18,18,18	0
81	MG	1	3707	1/1	0.80	0.08	82,82,82,82	0
81	MG	1	3860	1/1	0.80	0.12	70,70,70,70	0
81	MG	AS	3717	1/1	0.80	0.21	64,64,64,64	0
81	MG	CM	1816	1/1	0.80	0.20	45,45,45,45	0
81	MG	1	3863	1/1	0.80	0.13	85,85,85,85	0
81	MG	AS	3603	1/1	0.80	0.18	44,44,44,44	0
81	MG	AS	3605	1/1	0.80	0.11	72,72,72,72	0
81	MG	CM	1831	1/1	0.80	0.20	36,36,36,36	0
81	MG	AS	3609	1/1	0.80	0.21	55,55,55,55	0
81	MG	AS	3495	1/1	0.80	0.24	51,51,51,51	0
81	MG	B	1880	1/1	0.80	0.12	49,49,49,49	0
81	MG	CM	1858	1/1	0.80	0.15	113,113,113,113	0
81	MG	B	1883	1/1	0.80	0.24	82,82,82,82	0
81	MG	AS	3620	1/1	0.80	0.10	110,110,110,110	0
81	MG	1	3796	1/1	0.80	0.11	62,62,62,62	0
81	MG	AS	3636	1/1	0.80	0.16	69,69,69,69	0
81	MG	5	201	1/1	0.80	0.13	65,65,65,65	0
81	MG	CM	1885	1/1	0.80	0.20	57,57,57,57	0
81	MG	B	1841	1/1	0.80	0.15	55,55,55,55	0
81	MG	AS	3774	1/1	0.81	0.17	49,49,49,49	0
81	MG	AS	3775	1/1	0.81	0.14	47,47,47,47	0
81	MG	1	3838	1/1	0.81	0.12	35,35,35,35	0
81	MG	1	3699	1/1	0.81	0.12	43,43,43,43	0
81	MG	AS	3436	1/1	0.81	0.17	65,65,65,65	0
81	MG	B	1924	1/1	0.81	0.06	89,89,89,89	0
81	MG	B	1862	1/1	0.81	0.09	80,80,80,80	0
81	MG	AT	204	1/1	0.81	0.13	85,85,85,85	0
81	MG	B	1863	1/1	0.81	0.08	103,103,103,103	0
81	MG	B	1869	1/1	0.81	0.23	59,59,59,59	0
81	MG	AS	3492	1/1	0.81	0.08	24,24,24,24	0
81	MG	AI	201	1/1	0.81	0.11	66,66,66,66	0
81	MG	1	3898	1/1	0.81	0.21	52,52,52,52	0
81	MG	1	3758	1/1	0.81	0.14	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3677	1/1	0.81	0.08	65,65,65,65	0
81	MG	1	3777	1/1	0.81	0.15	52,52,52,52	0
81	MG	DB	204	1/1	0.81	0.13	26,26,26,26	0
81	MG	AS	3522	1/1	0.81	0.21	36,36,36,36	0
81	MG	B	1809	1/1	0.81	0.12	37,37,37,37	0
81	MG	1	3760	1/1	0.81	0.15	43,43,43,43	0
81	MG	B	1890	1/1	0.81	0.14	87,87,87,87	0
81	MG	1	3545	1/1	0.81	0.14	34,34,34,34	0
81	MG	1	3856	1/1	0.81	0.13	54,54,54,54	0
81	MG	o	304	1/1	0.81	0.16	47,47,47,47	0
81	MG	B	1906	1/1	0.81	0.21	43,43,43,43	0
81	MG	1	3623	1/1	0.81	0.10	44,44,44,44	0
81	MG	x	202	1/1	0.81	0.08	25,25,25,25	0
81	MG	3	206	1/1	0.81	0.17	55,55,55,55	0
81	MG	0	202	1/1	0.81	0.29	87,87,87,87	0
81	MG	1	3772	1/1	0.82	0.20	49,49,49,49	0
81	MG	AS	3783	1/1	0.82	0.11	65,65,65,65	0
81	MG	AS	3784	1/1	0.82	0.12	54,54,54,54	0
81	MG	1	3750	1/1	0.82	0.21	46,46,46,46	0
81	MG	1	3782	1/1	0.82	0.16	66,66,66,66	0
81	MG	AS	3702	1/1	0.82	0.10	72,72,72,72	0
81	MG	1	3918	1/1	0.82	0.07	43,43,43,43	0
81	MG	AS	3410	1/1	0.82	0.29	25,25,25,25	0
81	MG	AS	3513	1/1	0.82	0.20	36,36,36,36	0
81	MG	AW	303	1/1	0.82	0.10	82,82,82,82	0
81	MG	AX	401	1/1	0.82	0.09	43,43,43,43	0
81	MG	1	3544	1/1	0.82	0.28	47,47,47,47	0
81	MG	CM	1942	1/1	0.82	0.10	42,42,42,42	0
81	MG	BS	201	1/1	0.82	0.13	83,83,83,83	0
81	MG	1	3892	1/1	0.82	0.07	71,71,71,71	0
81	MG	CM	1808	1/1	0.82	0.24	63,63,63,63	0
81	MG	AS	3437	1/1	0.82	0.20	36,36,36,36	0
81	MG	B	1882	1/1	0.82	0.09	56,56,56,56	0
81	MG	AS	3731	1/1	0.82	0.10	49,49,49,49	0
81	MG	AS	3735	1/1	0.82	0.15	56,56,56,56	0
81	MG	AS	3548	1/1	0.82	0.15	49,49,49,49	0
81	MG	AS	3742	1/1	0.82	0.09	72,72,72,72	0
81	MG	1	3893	1/1	0.82	0.10	34,34,34,34	0
81	MG	AS	3554	1/1	0.82	0.14	44,44,44,44	0
81	MG	AS	3641	1/1	0.82	0.13	80,80,80,80	0
81	MG	CM	1855	1/1	0.82	0.07	131,131,131,131	0
81	MG	AS	3561	1/1	0.82	0.12	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3483	1/1	0.82	0.17	30,30,30,30	0
81	MG	AS	3651	1/1	0.82	0.10	22,22,22,22	0
81	MG	AS	3483	1/1	0.82	0.23	31,31,31,31	0
81	MG	AS	3670	1/1	0.82	0.12	63,63,63,63	0
81	MG	AS	3506	1/1	0.83	0.18	40,40,40,40	0
81	MG	B	1884	1/1	0.83	0.15	107,107,107,107	0
81	MG	4	216	1/1	0.83	0.10	42,42,42,42	0
81	MG	AS	3733	1/1	0.83	0.10	89,89,89,89	0
81	MG	Z	202	1/1	0.83	0.29	69,69,69,69	0
81	MG	Z	203	1/1	0.83	0.17	62,62,62,62	0
81	MG	1	3572	1/1	0.83	0.10	44,44,44,44	0
81	MG	CM	1939	1/1	0.83	0.18	82,82,82,82	0
81	MG	B	1936	1/1	0.83	0.11	59,59,59,59	0
81	MG	1	3503	1/1	0.83	0.06	62,62,62,62	0
81	MG	B	1899	1/1	0.83	0.18	38,38,38,38	0
81	MG	1	3840	1/1	0.83	0.17	52,52,52,52	0
81	MG	w	301	1/1	0.83	0.28	39,39,39,39	0
81	MG	AS	3576	1/1	0.83	0.28	84,84,84,84	0
81	MG	1	3403	1/1	0.83	0.31	31,31,31,31	0
81	MG	3	212	1/1	0.83	0.19	46,46,46,46	0
81	MG	CM	1849	1/1	0.83	0.23	53,53,53,53	0
81	MG	DG	201	1/1	0.83	0.18	49,49,49,49	0
81	MG	CM	1854	1/1	0.83	0.17	90,90,90,90	0
81	MG	1	3925	1/1	0.83	0.12	39,39,39,39	0
81	MG	AS	3698	1/1	0.83	0.18	48,48,48,48	0
81	MG	AS	3700	1/1	0.83	0.14	59,59,59,59	0
81	MG	AS	3787	1/1	0.83	0.16	66,66,66,66	0
81	MG	B	1829	1/1	0.83	0.29	28,28,28,28	0
81	MG	1	3434	1/1	0.83	0.23	25,25,25,25	0
81	MG	1	3563	1/1	0.83	0.29	46,46,46,46	0
81	MG	B	1837	1/1	0.83	0.12	78,78,78,78	0
81	MG	1	3711	1/1	0.83	0.15	54,54,54,54	0
81	MG	AS	3498	1/1	0.83	0.23	33,33,33,33	0
81	MG	1	3805	1/1	0.84	0.10	28,28,28,28	0
81	MG	AS	3596	1/1	0.84	0.19	43,43,43,43	0
81	MG	1	3737	1/1	0.84	0.20	43,43,43,43	0
81	MG	1	3813	1/1	0.84	0.12	71,71,71,71	0
81	MG	AT	207	1/1	0.84	0.11	80,80,80,80	0
81	MG	1	3648	1/1	0.84	0.12	51,51,51,51	0
81	MG	AS	3608	1/1	0.84	0.20	65,65,65,65	0
81	MG	CM	1903	1/1	0.84	0.13	38,38,38,38	0
81	MG	1	3911	1/1	0.84	0.10	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	CM	1911	1/1	0.84	0.08	63,63,63,63	0
81	MG	1	3827	1/1	0.84	0.07	36,36,36,36	0
81	MG	Z	201	1/1	0.84	0.18	61,61,61,61	0
81	MG	AS	3728	1/1	0.84	0.12	21,21,21,21	0
81	MG	1	3830	1/1	0.84	0.13	28,28,28,28	0
81	MG	B	1926	1/1	0.84	0.15	70,70,70,70	0
81	MG	AS	3628	1/1	0.84	0.22	73,73,73,73	0
81	MG	AS	3734	1/1	0.84	0.13	37,37,37,37	0
81	MG	o	302	1/1	0.84	0.17	37,37,37,37	0
81	MG	CN	301	1/1	0.84	0.13	54,54,54,54	0
81	MG	1	3765	1/1	0.84	0.15	49,49,49,49	0
81	MG	AS	3639	1/1	0.84	0.15	59,59,59,59	0
81	MG	1	3598	1/1	0.84	0.08	44,44,44,44	0
81	MG	AS	3643	1/1	0.84	0.23	37,37,37,37	0
81	MG	1	3877	1/1	0.84	0.29	36,36,36,36	0
81	MG	1	3768	1/1	0.84	0.12	38,38,38,38	0
81	MG	1	3965	1/1	0.84	0.09	42,42,42,42	0
81	MG	CM	1848	1/1	0.84	0.22	61,61,61,61	0
81	MG	AS	3653	1/1	0.84	0.08	47,47,47,47	0
81	MG	AS	3778	1/1	0.84	0.07	38,38,38,38	0
81	MG	1	3579	1/1	0.84	0.22	47,47,47,47	0
81	MG	1	3693	1/1	0.84	0.11	36,36,36,36	0
81	MG	1	3661	1/1	0.84	0.18	63,63,63,63	0
81	MG	B	1907	1/1	0.84	0.15	54,54,54,54	0
81	MG	CM	1863	1/1	0.84	0.14	15,15,15,15	0
81	MG	1	3774	1/1	0.84	0.13	46,46,46,46	0
81	MG	CM	1869	1/1	0.84	0.11	55,55,55,55	0
81	MG	CM	1870	1/1	0.84	0.11	73,73,73,73	0
81	MG	1	3853	1/1	0.85	0.12	63,63,63,63	0
81	MG	CM	1841	1/1	0.85	0.08	118,118,118,118	0
81	MG	1	3524	1/1	0.85	0.09	58,58,58,58	0
81	MG	1	3923	1/1	0.85	0.14	36,36,36,36	0
81	MG	CM	1850	1/1	0.85	0.19	55,55,55,55	0
81	MG	1	3411	1/1	0.85	0.21	24,24,24,24	0
81	MG	1	3807	1/1	0.85	0.05	39,39,39,39	0
81	MG	1	3629	1/1	0.85	0.29	60,60,60,60	0
81	MG	B	1887	1/1	0.85	0.08	51,51,51,51	0
81	MG	1	3950	1/1	0.85	0.42	50,50,50,50	0
81	MG	1	3959	1/1	0.85	0.10	48,48,48,48	0
81	MG	i	301	1/1	0.85	0.19	59,59,59,59	0
81	MG	1	3812	1/1	0.85	0.21	58,58,58,58	0
81	MG	AS	3747	1/1	0.85	0.20	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3748	1/1	0.85	0.16	60,60,60,60	0
81	MG	B	1803	1/1	0.85	0.21	50,50,50,50	0
81	MG	c	202	1/1	0.85	0.10	60,60,60,60	0
81	MG	CM	1884	1/1	0.85	0.12	31,31,31,31	0
81	MG	1	3595	1/1	0.85	0.10	52,52,52,52	0
81	MG	1	3674	1/1	0.85	0.16	53,53,53,53	0
81	MG	1	3550	1/1	0.85	0.13	35,35,35,35	0
81	MG	1	3678	1/1	0.85	0.15	38,38,38,38	0
81	MG	CM	1901	1/1	0.85	0.09	53,53,53,53	0
81	MG	CM	1902	1/1	0.85	0.09	63,63,63,63	0
81	MG	B	1910	1/1	0.85	0.14	76,76,76,76	0
81	MG	1	3831	1/1	0.85	0.15	38,38,38,38	0
81	MG	AS	3442	1/1	0.85	0.17	41,41,41,41	0
81	MG	B	1914	1/1	0.85	0.15	62,62,62,62	0
81	MG	B	1820	1/1	0.85	0.21	38,38,38,38	0
81	MG	1	3880	1/1	0.85	0.11	30,30,30,30	0
81	MG	CM	1922	1/1	0.85	0.17	49,49,49,49	0
81	MG	AS	3476	1/1	0.85	0.18	37,37,37,37	0
81	MG	CM	1936	1/1	0.85	0.09	62,62,62,62	0
81	MG	1	3882	1/1	0.85	0.10	31,31,31,31	0
81	MG	B	1835	1/1	0.85	0.13	52,52,52,52	0
81	MG	1	3837	1/1	0.85	0.07	59,59,59,59	0
81	MG	1	3682	1/1	0.85	0.24	60,60,60,60	0
81	MG	1	3787	1/1	0.85	0.16	43,43,43,43	0
81	MG	1	3690	1/1	0.85	0.20	45,45,45,45	0
81	MG	1	3512	1/1	0.85	0.19	45,45,45,45	0
81	MG	AX	402	1/1	0.85	0.22	34,34,34,34	0
81	MG	1	3543	1/1	0.85	0.12	39,39,39,39	0
81	MG	l	402	1/1	0.85	0.10	51,51,51,51	0
81	MG	BZ	201	1/1	0.85	0.26	67,67,67,67	0
81	MG	AS	3687	1/1	0.85	0.14	44,44,44,44	0
81	MG	CM	1804	1/1	0.85	0.29	48,48,48,48	0
81	MG	CM	1806	1/1	0.85	0.20	68,68,68,68	0
81	MG	1	3901	1/1	0.85	0.05	39,39,39,39	0
81	MG	1	3650	1/1	0.85	0.09	30,30,30,30	0
81	MG	AS	3523	1/1	0.85	0.29	49,49,49,49	0
81	MG	B	1952	1/1	0.85	0.18	64,64,64,64	0
81	MG	AS	3531	1/1	0.85	0.16	51,51,51,51	0
81	MG	B	1955	1/1	0.85	0.21	45,45,45,45	0
81	MG	AS	3712	1/1	0.85	0.14	45,45,45,45	0
81	MG	s	201	1/1	0.85	0.15	49,49,49,49	0
81	MG	1	3653	1/1	0.85	0.09	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3914	1/1	0.86	0.14	31,31,31,31	0
81	MG	AS	3776	1/1	0.86	0.10	52,52,52,52	0
81	MG	1	3829	1/1	0.86	0.19	61,61,61,61	0
81	MG	B	1902	1/1	0.86	0.19	51,51,51,51	0
81	MG	B	1968	1/1	0.86	0.06	48,48,48,48	0
81	MG	1	3419	1/1	0.86	0.15	19,19,19,19	0
81	MG	AS	3526	1/1	0.86	0.14	50,50,50,50	0
81	MG	AS	3654	1/1	0.86	0.22	34,34,34,34	0
81	MG	1	3553	1/1	0.86	0.10	43,43,43,43	0
81	MG	AS	3668	1/1	0.86	0.15	78,78,78,78	0
81	MG	1	3832	1/1	0.86	0.07	46,46,46,46	0
81	MG	1	3795	1/1	0.86	0.13	60,60,60,60	0
81	MG	AS	3672	1/1	0.86	0.18	58,58,58,58	0
81	MG	u	202	1/1	0.86	0.07	55,55,55,55	0
81	MG	AT	209	1/1	0.86	0.06	24,24,24,24	0
81	MG	1	3946	1/1	0.86	0.05	40,40,40,40	0
81	MG	1	3460	1/1	0.86	0.15	23,23,23,23	0
81	MG	B	1846	1/1	0.86	0.18	56,56,56,56	0
81	MG	1	3953	1/1	0.86	0.19	57,57,57,57	0
81	MG	x	203	1/1	0.86	0.18	70,70,70,70	0
81	MG	1	3722	1/1	0.86	0.09	45,45,45,45	0
81	MG	BJ	302	1/1	0.86	0.09	42,42,42,42	0
81	MG	1	3728	1/1	0.86	0.12	53,53,53,53	0
81	MG	CM	1933	1/1	0.86	0.18	69,69,69,69	0
81	MG	1	3841	1/1	0.86	0.14	55,55,55,55	0
81	MG	1	3624	1/1	0.86	0.24	32,32,32,32	0
81	MG	B	1929	1/1	0.86	0.20	70,70,70,70	0
81	MG	1	3803	1/1	0.86	0.15	24,24,24,24	0
81	MG	1	3402	1/1	0.86	0.24	16,16,16,16	0
81	MG	CM	1809	1/1	0.86	0.22	34,34,34,34	0
81	MG	AQ	102	1/1	0.86	0.11	27,27,27,27	0
81	MG	1	3745	1/1	0.86	0.13	42,42,42,42	0
81	MG	1	3685	1/1	0.86	0.23	38,38,38,38	0
81	MG	AS	3611	1/1	0.86	0.07	29,29,29,29	0
81	MG	CM	1820	1/1	0.86	0.12	34,34,34,34	0
81	MG	B	1948	1/1	0.86	0.12	44,44,44,44	0
81	MG	B	1802	1/1	0.86	0.22	33,33,33,33	0
81	MG	AS	3617	1/1	0.86	0.12	62,62,62,62	0
81	MG	1	3654	1/1	0.86	0.10	49,49,49,49	0
81	MG	AS	3494	1/1	0.86	0.16	63,63,63,63	0
81	MG	AS	3621	1/1	0.86	0.14	60,60,60,60	0
81	MG	1	3566	1/1	0.86	0.09	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3630	1/1	0.86	0.12	41,41,41,41	0
81	MG	AS	3751	1/1	0.86	0.11	70,70,70,70	0
81	MG	AS	3760	1/1	0.86	0.10	146,146,146,146	0
81	MG	1	3636	1/1	0.86	0.10	34,34,34,34	0
81	MG	1	3910	1/1	0.86	0.09	50,50,50,50	0
81	MG	1	3638	1/1	0.86	0.23	48,48,48,48	0
81	MG	1	3847	1/1	0.87	0.24	50,50,50,50	0
81	MG	1	3630	1/1	0.87	0.14	34,34,34,34	0
81	MG	1	3907	1/1	0.87	0.17	77,77,77,77	0
81	MG	1	3665	1/1	0.87	0.21	25,25,25,25	0
81	MG	1	3721	1/1	0.87	0.14	42,42,42,42	0
81	MG	1	3528	1/1	0.87	0.08	45,45,45,45	0
81	MG	AS	3412	1/1	0.87	0.27	41,41,41,41	0
81	MG	o	303	1/1	0.87	0.14	52,52,52,52	0
81	MG	1	3858	1/1	0.87	0.13	62,62,62,62	0
81	MG	1	3859	1/1	0.87	0.20	43,43,43,43	0
81	MG	1	3723	1/1	0.87	0.14	51,51,51,51	0
81	MG	B	1847	1/1	0.87	0.09	28,28,28,28	0
81	MG	1	3565	1/1	0.87	0.20	31,31,31,31	0
81	MG	AS	3468	1/1	0.87	0.19	44,44,44,44	0
81	MG	B	1851	1/1	0.87	0.08	64,64,64,64	0
81	MG	1	3467	1/1	0.87	0.22	37,37,37,37	0
81	MG	AS	3764	1/1	0.87	0.14	72,72,72,72	0
81	MG	1	3776	1/1	0.87	0.12	63,63,63,63	0
81	MG	1	3943	1/1	0.87	0.09	61,61,61,61	0
81	MG	1	3867	1/1	0.87	0.12	45,45,45,45	0
81	MG	B	1865	1/1	0.87	0.14	95,95,95,95	0
81	MG	1	3570	1/1	0.87	0.17	61,61,61,61	0
81	MG	1	3952	1/1	0.87	0.19	33,33,33,33	0
81	MG	CM	1894	1/1	0.87	0.32	49,49,49,49	0
81	MG	CM	1896	1/1	0.87	0.11	32,32,32,32	0
81	MG	1	3738	1/1	0.87	0.10	22,22,22,22	0
81	MG	AF	201	1/1	0.87	0.17	82,82,82,82	0
81	MG	AS	3645	1/1	0.87	0.12	45,45,45,45	0
81	MG	AF	204	1/1	0.87	0.10	55,55,55,55	0
81	MG	1	3873	1/1	0.87	0.05	57,57,57,57	0
81	MG	1	3646	1/1	0.87	0.09	73,73,73,73	0
81	MG	AS	3517	1/1	0.87	0.21	34,34,34,34	0
81	MG	1	3747	1/1	0.87	0.16	34,34,34,34	0
81	MG	AS	3655	1/1	0.87	0.07	33,33,33,33	0
81	MG	B	1886	1/1	0.87	0.12	52,52,52,52	0
81	MG	1	3409	1/1	0.87	0.28	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3427	1/1	0.87	0.23	36,36,36,36	0
81	MG	AT	213	1/1	0.87	0.07	51,51,51,51	0
81	MG	1	3794	1/1	0.87	0.15	30,30,30,30	0
81	MG	AU	207	1/1	0.87	0.10	49,49,49,49	0
81	MG	1	3577	1/1	0.87	0.26	53,53,53,53	0
81	MG	AS	3540	1/1	0.87	0.25	55,55,55,55	0
81	MG	AS	3544	1/1	0.87	0.15	34,34,34,34	0
81	MG	AS	3683	1/1	0.87	0.20	49,49,49,49	0
81	MG	AS	3686	1/1	0.87	0.11	50,50,50,50	0
81	MG	BO	201	1/1	0.87	0.15	65,65,65,65	0
81	MG	B	1898	1/1	0.87	0.08	50,50,50,50	0
81	MG	AS	3549	1/1	0.87	0.19	34,34,34,34	0
81	MG	G	301	1/1	0.87	0.11	49,49,49,49	0
81	MG	CM	1802	1/1	0.87	0.27	18,18,18,18	0
81	MG	AS	3701	1/1	0.87	0.12	43,43,43,43	0
81	MG	1	3485	1/1	0.87	0.16	54,54,54,54	0
83	PAR	1	3967	42/42	0.87	0.15	62,83,103,110	0
81	MG	1	3514	1/1	0.87	0.14	22,22,22,22	0
81	MG	AS	3705	1/1	0.87	0.24	58,58,58,58	0
81	MG	AS	3566	1/1	0.87	0.24	37,37,37,37	0
81	MG	AS	3574	1/1	0.87	0.12	48,48,48,48	0
81	MG	AS	3711	1/1	0.87	0.17	51,51,51,51	0
81	MG	AS	3575	1/1	0.87	0.38	30,30,30,30	0
83	PAR	CM	1946	42/42	0.87	0.26	80,100,118,130	42
81	MG	1	3655	1/1	0.87	0.08	40,40,40,40	0
81	MG	AS	3719	1/1	0.87	0.07	48,48,48,48	0
81	MG	1	3473	1/1	0.87	0.26	18,18,18,18	0
81	MG	AS	3502	1/1	0.88	0.17	41,41,41,41	0
81	MG	CM	1845	1/1	0.88	0.20	60,60,60,60	0
81	MG	1	3917	1/1	0.88	0.17	27,27,27,27	0
81	MG	AS	3634	1/1	0.88	0.19	19,19,19,19	0
81	MG	1	3643	1/1	0.88	0.11	50,50,50,50	0
81	MG	AS	3755	1/1	0.88	0.05	45,45,45,45	0
81	MG	j	302	1/1	0.88	0.08	35,35,35,35	0
81	MG	AS	3761	1/1	0.88	0.10	54,54,54,54	0
81	MG	AS	3640	1/1	0.88	0.16	59,59,59,59	0
81	MG	B	1962	1/1	0.88	0.11	29,29,29,29	0
81	MG	1	3548	1/1	0.88	0.11	54,54,54,54	0
81	MG	AS	3766	1/1	0.88	0.05	29,29,29,29	0
81	MG	AS	3519	1/1	0.88	0.09	73,73,73,73	0
81	MG	1	3810	1/1	0.88	0.14	32,32,32,32	0
81	MG	AS	3648	1/1	0.88	0.08	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3777	1/1	0.88	0.12	82,82,82,82	0
81	MG	1	3604	1/1	0.88	0.11	46,46,46,46	0
81	MG	B	1969	1/1	0.88	0.12	50,50,50,50	0
81	MG	B	1823	1/1	0.88	0.16	32,32,32,32	0
81	MG	1	3929	1/1	0.88	0.07	87,87,87,87	0
81	MG	1	3438	1/1	0.88	0.17	30,30,30,30	0
81	MG	1	3933	1/1	0.88	0.07	35,35,35,35	0
81	MG	CM	1895	1/1	0.88	0.06	30,30,30,30	0
81	MG	1	3447	1/1	0.88	0.16	96,96,96,96	0
81	MG	1	3849	1/1	0.88	0.34	50,50,50,50	0
81	MG	CM	1899	1/1	0.88	0.15	65,65,65,65	0
81	MG	1	3818	1/1	0.88	0.10	75,75,75,75	0
81	MG	1	3410	1/1	0.88	0.33	42,42,42,42	0
81	MG	1	3826	1/1	0.88	0.13	53,53,53,53	0
81	MG	1	3495	1/1	0.88	0.10	50,50,50,50	0
81	MG	f	102	1/1	0.88	0.07	53,53,53,53	0
81	MG	1	3895	1/1	0.88	0.13	54,54,54,54	0
81	MG	z	201	1/1	0.88	0.07	51,51,51,51	0
81	MG	B	1920	1/1	0.88	0.20	50,50,50,50	0
81	MG	AS	3699	1/1	0.88	0.06	46,46,46,46	0
81	MG	1	3896	1/1	0.88	0.06	36,36,36,36	0
81	MG	CM	1932	1/1	0.88	0.14	78,78,78,78	0
81	MG	AS	3582	1/1	0.88	0.15	49,49,49,49	0
81	MG	1	3594	1/1	0.88	0.13	46,46,46,46	0
81	MG	B	1860	1/1	0.88	0.18	42,42,42,42	0
81	MG	3	201	1/1	0.88	0.14	62,62,62,62	0
81	MG	AC	101	1/1	0.88	0.10	43,43,43,43	0
81	MG	1	3691	1/1	0.88	0.06	35,35,35,35	0
81	MG	AS	3461	1/1	0.88	0.10	38,38,38,38	0
81	MG	BZ	203	1/1	0.88	0.18	83,83,83,83	0
81	MG	CK	102	1/1	0.88	0.14	50,50,50,50	0
81	MG	B	1867	1/1	0.88	0.18	65,65,65,65	0
81	MG	AS	3714	1/1	0.88	0.07	81,81,81,81	0
81	MG	AS	3604	1/1	0.88	0.12	61,61,61,61	0
81	MG	1	3632	1/1	0.88	0.07	45,45,45,45	0
81	MG	1	3429	1/1	0.88	0.24	13,13,13,13	0
81	MG	AS	3725	1/1	0.88	0.05	38,38,38,38	0
81	MG	B	1938	1/1	0.88	0.05	51,51,51,51	0
81	MG	AS	3481	1/1	0.88	0.34	38,38,38,38	0
81	MG	1	3833	1/1	0.88	0.12	47,47,47,47	0
81	MG	AS	3614	1/1	0.88	0.14	32,32,32,32	0
81	MG	3	214	1/1	0.88	0.16	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	4	205	1/1	0.88	0.11	76,76,76,76	0
81	MG	CM	1824	1/1	0.88	0.19	35,35,35,35	0
81	MG	CM	1829	1/1	0.88	0.14	76,76,76,76	0
81	MG	B	1881	1/1	0.88	0.21	53,53,53,53	0
81	MG	1	3525	1/1	0.88	0.17	46,46,46,46	0
81	MG	1	3546	1/1	0.88	0.21	54,54,54,54	0
81	MG	1	3804	1/1	0.88	0.16	26,26,26,26	0
81	MG	x	201	1/1	0.89	0.19	11,11,11,11	0
81	MG	CM	1840	1/1	0.89	0.18	35,35,35,35	0
81	MG	AS	3480	1/1	0.89	0.14	23,23,23,23	0
81	MG	CM	1842	1/1	0.89	0.22	41,41,41,41	0
81	MG	B	1856	1/1	0.89	0.10	65,65,65,65	0
81	MG	1	3734	1/1	0.89	0.10	44,44,44,44	0
81	MG	1	3510	1/1	0.89	0.13	14,14,14,14	0
81	MG	AS	3487	1/1	0.89	0.09	48,48,48,48	0
81	MG	AS	3623	1/1	0.89	0.14	89,89,89,89	0
81	MG	AS	3488	1/1	0.89	0.18	35,35,35,35	0
81	MG	1	3689	1/1	0.89	0.13	33,33,33,33	0
81	MG	1	3955	1/1	0.89	0.24	61,61,61,61	0
81	MG	AS	3763	1/1	0.89	0.05	38,38,38,38	0
81	MG	1	3743	1/1	0.89	0.20	34,34,34,34	0
81	MG	B	1951	1/1	0.89	0.10	67,67,67,67	0
81	MG	0	203	1/1	0.89	0.13	57,57,57,57	0
81	MG	AS	3501	1/1	0.89	0.13	60,60,60,60	0
81	MG	1	3814	1/1	0.89	0.14	41,41,41,41	0
81	MG	1	3421	1/1	0.89	0.22	17,17,17,17	0
81	MG	CM	1881	1/1	0.89	0.18	34,34,34,34	0
81	MG	1	3659	1/1	0.89	0.08	40,40,40,40	0
81	MG	1	3583	1/1	0.89	0.15	30,30,30,30	0
81	MG	AS	3515	1/1	0.89	0.26	55,55,55,55	0
81	MG	AS	3780	1/1	0.89	0.12	22,22,22,22	0
81	MG	AF	203	1/1	0.89	0.16	43,43,43,43	0
81	MG	3	202	1/1	0.89	0.21	50,50,50,50	0
81	MG	B	1964	1/1	0.89	0.10	39,39,39,39	0
81	MG	1	3906	1/1	0.89	0.06	69,69,69,69	0
81	MG	AP	202	1/1	0.89	0.17	37,37,37,37	0
81	MG	AS	3658	1/1	0.89	0.07	49,49,49,49	0
81	MG	CM	1900	1/1	0.89	0.10	86,86,86,86	0
81	MG	1	3500	1/1	0.89	0.16	37,37,37,37	0
81	MG	1	3908	1/1	0.89	0.16	47,47,47,47	0
81	MG	1	3501	1/1	0.89	0.19	33,33,33,33	0
81	MG	AS	3532	1/1	0.89	0.11	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3612	1/1	0.89	0.12	21,21,21,21	0
81	MG	4	204	1/1	0.89	0.06	37,37,37,37	0
81	MG	AS	3680	1/1	0.89	0.14	31,31,31,31	0
81	MG	AS	3541	1/1	0.89	0.11	60,60,60,60	0
81	MG	CM	1918	1/1	0.89	0.09	86,86,86,86	0
81	MG	1	3757	1/1	0.89	0.16	38,38,38,38	0
81	MG	AS	3547	1/1	0.89	0.11	36,36,36,36	0
81	MG	1	3621	1/1	0.89	0.08	35,35,35,35	0
81	MG	AS	3696	1/1	0.89	0.20	66,66,66,66	0
81	MG	4	209	1/1	0.89	0.18	45,45,45,45	0
81	MG	1	3454	1/1	0.89	0.16	29,29,29,29	0
81	MG	BN	201	1/1	0.89	0.07	33,33,33,33	0
81	MG	1	3591	1/1	0.89	0.09	35,35,35,35	0
81	MG	CM	1943	1/1	0.89	0.06	38,38,38,38	0
81	MG	AS	3557	1/1	0.89	0.09	28,28,28,28	0
81	MG	1	3922	1/1	0.89	0.33	52,52,52,52	0
81	MG	1	3487	1/1	0.89	0.14	44,44,44,44	0
81	MG	CW	201	1/1	0.89	0.16	83,83,83,83	0
81	MG	CJ	203	1/1	0.89	0.18	51,51,51,51	0
81	MG	1	3875	1/1	0.89	0.07	32,32,32,32	0
81	MG	1	3681	1/1	0.89	0.09	20,20,20,20	0
81	MG	B	1832	1/1	0.89	0.12	63,63,63,63	0
81	MG	AS	3404	1/1	0.89	0.28	33,33,33,33	0
81	MG	AS	3407	1/1	0.89	0.10	37,37,37,37	0
81	MG	1	3724	1/1	0.89	0.20	44,44,44,44	0
81	MG	1	3408	1/1	0.89	0.20	39,39,39,39	0
81	MG	1	3684	1/1	0.89	0.09	35,35,35,35	0
81	MG	AS	3430	1/1	0.89	0.18	39,39,39,39	0
81	MG	1	3934	1/1	0.89	0.10	20,20,20,20	0
81	MG	1	3936	1/1	0.89	0.23	43,43,43,43	0
81	MG	1	3941	1/1	0.89	0.19	50,50,50,50	0
81	MG	1	3808	1/1	0.89	0.26	42,42,42,42	0
81	MG	v	301	1/1	0.89	0.16	21,21,21,21	0
81	MG	v	302	1/1	0.89	0.15	54,54,54,54	0
81	MG	AS	3466	1/1	0.89	0.18	46,46,46,46	0
81	MG	1	3944	1/1	0.89	0.08	52,52,52,52	0
81	MG	1	3809	1/1	0.89	0.07	56,56,56,56	0
81	MG	B	1833	1/1	0.90	0.23	25,25,25,25	0
81	MG	B	1900	1/1	0.90	0.21	42,42,42,42	0
81	MG	AS	3754	1/1	0.90	0.10	51,51,51,51	0
81	MG	1	3942	1/1	0.90	0.13	44,44,44,44	0
81	MG	CM	1851	1/1	0.90	0.19	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3468	1/1	0.90	0.17	28,28,28,28	0
81	MG	1	3582	1/1	0.90	0.10	40,40,40,40	0
81	MG	2	201	1/1	0.90	0.24	49,49,49,49	0
81	MG	1	3478	1/1	0.90	0.14	25,25,25,25	0
81	MG	6	201	1/1	0.90	0.22	38,38,38,38	0
81	MG	1	3947	1/1	0.90	0.25	83,83,83,83	0
81	MG	1	3948	1/1	0.90	0.09	35,35,35,35	0
81	MG	AS	3527	1/1	0.90	0.19	64,64,64,64	0
81	MG	1	3497	1/1	0.90	0.24	15,15,15,15	0
81	MG	1	3518	1/1	0.90	0.14	26,26,26,26	0
81	MG	B	1917	1/1	0.90	0.10	28,28,28,28	0
81	MG	CM	1877	1/1	0.90	0.14	35,35,35,35	0
81	MG	AS	3533	1/1	0.90	0.22	19,19,19,19	0
81	MG	CM	1882	1/1	0.90	0.07	36,36,36,36	0
81	MG	B	1918	1/1	0.90	0.13	111,111,111,111	0
81	MG	AS	3536	1/1	0.90	0.09	27,27,27,27	0
81	MG	B	1853	1/1	0.90	0.19	37,37,37,37	0
81	MG	1	3883	1/1	0.90	0.17	35,35,35,35	0
81	MG	AS	3403	1/1	0.90	0.26	18,18,18,18	0
81	MG	B	1921	1/1	0.90	0.10	84,84,84,84	0
81	MG	1	3886	1/1	0.90	0.14	57,57,57,57	0
81	MG	k	404	1/1	0.90	0.13	49,49,49,49	0
81	MG	AS	3673	1/1	0.90	0.07	10,10,10,10	0
81	MG	CM	1898	1/1	0.90	0.16	60,60,60,60	0
81	MG	B	1857	1/1	0.90	0.11	51,51,51,51	0
81	MG	AS	3553	1/1	0.90	0.08	23,23,23,23	0
81	MG	1	3956	1/1	0.90	0.13	55,55,55,55	0
81	MG	AS	3425	1/1	0.90	0.14	24,24,24,24	0
81	MG	1	3587	1/1	0.90	0.17	37,37,37,37	0
81	MG	1	3920	1/1	0.90	0.07	53,53,53,53	0
81	MG	AS	3688	1/1	0.90	0.06	37,37,37,37	0
81	MG	AS	3695	1/1	0.90	0.16	36,36,36,36	0
81	MG	AS	3570	1/1	0.90	0.22	37,37,37,37	0
81	MG	AS	3697	1/1	0.90	0.15	49,49,49,49	0
81	MG	1	3537	1/1	0.90	0.26	52,52,52,52	0
81	MG	BB	301	1/1	0.90	0.14	25,25,25,25	0
81	MG	r	302	1/1	0.90	0.07	64,64,64,64	0
81	MG	AS	3444	1/1	0.90	0.06	5,5,5,5	0
81	MG	AS	3579	1/1	0.90	0.16	77,77,77,77	0
81	MG	AS	3451	1/1	0.90	0.15	35,35,35,35	0
81	MG	CM	1937	1/1	0.90	0.07	33,33,33,33	0
81	MG	1	3538	1/1	0.90	0.18	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	B	1804	1/1	0.90	0.17	55,55,55,55	0
81	MG	AS	3706	1/1	0.90	0.05	29,29,29,29	0
81	MG	B	1939	1/1	0.90	0.15	87,87,87,87	0
81	MG	B	1943	1/1	0.90	0.09	65,65,65,65	0
81	MG	AS	3594	1/1	0.90	0.13	46,46,46,46	0
81	MG	1	3539	1/1	0.90	0.19	28,28,28,28	0
81	MG	1	3573	1/1	0.90	0.20	40,40,40,40	0
81	MG	1	3596	1/1	0.90	0.09	31,31,31,31	0
81	MG	1	3522	1/1	0.90	0.20	44,44,44,44	0
81	MG	B	1818	1/1	0.90	0.17	36,36,36,36	0
81	MG	1	3430	1/1	0.90	0.22	34,34,34,34	0
81	MG	AS	3606	1/1	0.90	0.22	38,38,38,38	0
81	MG	B	1953	1/1	0.90	0.08	37,37,37,37	0
81	MG	1	3600	1/1	0.90	0.20	20,20,20,20	0
81	MG	AS	3730	1/1	0.90	0.23	44,44,44,44	0
82	3K5	CJ	202	57/57	0.90	0.13	51,79,102,115	0
81	MG	B	1822	1/1	0.90	0.17	34,34,34,34	0
81	MG	3	213	1/1	0.90	0.07	26,26,26,26	0
81	MG	B	1827	1/1	0.90	0.23	32,32,32,32	0
81	MG	1	3645	1/1	0.90	0.13	56,56,56,56	0
81	MG	B	1961	1/1	0.90	0.06	48,48,48,48	0
81	MG	AS	3739	1/1	0.90	0.20	17,17,17,17	0
81	MG	B	1891	1/1	0.90	0.25	26,26,26,26	0
81	MG	CM	1838	1/1	0.90	0.14	32,32,32,32	0
81	MG	B	1830	1/1	0.90	0.18	39,39,39,39	0
81	MG	1	3559	1/1	0.90	0.17	39,39,39,39	0
81	MG	AS	3504	1/1	0.90	0.15	44,44,44,44	0
81	MG	1	3536	1/1	0.91	0.13	48,48,48,48	0
81	MG	1	3452	1/1	0.91	0.22	22,22,22,22	0
81	MG	4	211	1/1	0.91	0.09	59,59,59,59	0
81	MG	1	3779	1/1	0.91	0.06	40,40,40,40	0
81	MG	AF	202	1/1	0.91	0.15	26,26,26,26	0
81	MG	AS	3757	1/1	0.91	0.08	29,29,29,29	0
81	MG	1	3639	1/1	0.91	0.24	28,28,28,28	0
81	MG	AS	3644	1/1	0.91	0.08	22,22,22,22	0
81	MG	4	214	1/1	0.91	0.07	25,25,25,25	0
81	MG	CM	1861	1/1	0.91	0.09	57,57,57,57	0
81	MG	AS	3401	1/1	0.91	0.23	10,10,10,10	0
81	MG	AH	202	1/1	0.91	0.07	59,59,59,59	0
81	MG	1	3854	1/1	0.91	0.10	88,88,88,88	0
81	MG	B	1858	1/1	0.91	0.07	77,77,77,77	0
81	MG	1	3698	1/1	0.91	0.13	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3822	1/1	0.91	0.14	42,42,42,42	0
81	MG	AS	3416	1/1	0.91	0.28	16,16,16,16	0
81	MG	AS	3419	1/1	0.91	0.23	26,26,26,26	0
81	MG	AS	3664	1/1	0.91	0.13	31,31,31,31	0
81	MG	AS	3665	1/1	0.91	0.11	24,24,24,24	0
81	MG	1	3426	1/1	0.91	0.34	31,31,31,31	0
81	MG	B	1930	1/1	0.91	0.14	60,60,60,60	0
81	MG	AS	3669	1/1	0.91	0.16	12,12,12,12	0
81	MG	AS	3427	1/1	0.91	0.17	22,22,22,22	0
81	MG	1	3704	1/1	0.91	0.11	79,79,79,79	0
81	MG	1	3418	1/1	0.91	0.18	18,18,18,18	0
81	MG	B	1933	1/1	0.91	0.17	50,50,50,50	0
81	MG	AS	3439	1/1	0.91	0.17	22,22,22,22	0
81	MG	AS	3562	1/1	0.91	0.07	33,33,33,33	0
81	MG	AS	3681	1/1	0.91	0.17	64,64,64,64	0
81	MG	l	401	1/1	0.91	0.07	31,31,31,31	0
81	MG	B	1870	1/1	0.91	0.09	106,106,106,106	0
81	MG	AS	3685	1/1	0.91	0.11	25,25,25,25	0
81	MG	AS	3572	1/1	0.91	0.14	58,58,58,58	0
81	MG	AU	201	1/1	0.91	0.16	34,34,34,34	0
81	MG	1	3494	1/1	0.91	0.19	20,20,20,20	0
81	MG	1	3401	1/1	0.91	0.30	24,24,24,24	0
81	MG	B	1878	1/1	0.91	0.08	86,86,86,86	0
81	MG	CM	1913	1/1	0.91	0.16	60,60,60,60	0
81	MG	1	3954	1/1	0.91	0.10	17,17,17,17	0
81	MG	B	1806	1/1	0.91	0.15	42,42,42,42	0
81	MG	1	3720	1/1	0.91	0.10	47,47,47,47	0
81	MG	BG	302	1/1	0.91	0.07	28,28,28,28	0
81	MG	CM	1924	1/1	0.91	0.18	40,40,40,40	0
81	MG	1	3496	1/1	0.91	0.07	31,31,31,31	0
81	MG	r	303	1/1	0.91	0.10	42,42,42,42	0
81	MG	B	1817	1/1	0.91	0.21	19,19,19,19	0
81	MG	B	1954	1/1	0.91	0.10	63,63,63,63	0
81	MG	1	3461	1/1	0.91	0.22	14,14,14,14	0
81	MG	1	3836	1/1	0.91	0.07	49,49,49,49	0
81	MG	AS	3485	1/1	0.91	0.14	47,47,47,47	0
81	MG	AS	3600	1/1	0.91	0.06	43,43,43,43	0
81	MG	AS	3602	1/1	0.91	0.23	49,49,49,49	0
81	MG	CM	1944	1/1	0.91	0.12	60,60,60,60	0
81	MG	1	3871	1/1	0.91	0.07	93,93,93,93	0
81	MG	1	3962	1/1	0.91	0.08	24,24,24,24	0
81	MG	CP	301	1/1	0.91	0.17	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3442	1/1	0.91	0.23	33,33,33,33	0
81	MG	B	1892	1/1	0.91	0.17	55,55,55,55	0
81	MG	AS	3607	1/1	0.91	0.10	63,63,63,63	0
81	MG	1	3874	1/1	0.91	0.12	48,48,48,48	0
81	MG	1	3481	1/1	0.91	0.19	44,44,44,44	0
81	MG	AS	3610	1/1	0.91	0.14	64,64,64,64	0
81	MG	1	3726	1/1	0.91	0.21	59,59,59,59	0
81	MG	AS	3499	1/1	0.91	0.19	42,42,42,42	0
81	MG	B	1831	1/1	0.91	0.16	37,37,37,37	0
81	MG	1	3878	1/1	0.91	0.06	40,40,40,40	0
81	MG	1	3529	1/1	0.91	0.12	10,10,10,10	0
81	MG	CM	1826	1/1	0.91	0.09	87,87,87,87	0
81	MG	1	3729	1/1	0.91	0.20	30,30,30,30	0
81	MG	0	201	1/1	0.91	0.27	59,59,59,59	0
81	MG	AS	3508	1/1	0.91	0.10	62,62,62,62	0
81	MG	1	3445	1/1	0.91	0.20	35,35,35,35	0
81	MG	AS	3740	1/1	0.91	0.09	33,33,33,33	0
81	MG	CM	1835	1/1	0.91	0.13	15,15,15,15	0
81	MG	1	3930	1/1	0.91	0.14	79,79,79,79	0
81	MG	1	3732	1/1	0.91	0.12	24,24,24,24	0
81	MG	AS	3745	1/1	0.91	0.07	41,41,41,41	0
84	ZN	c	201	1/1	0.91	0.08	91,91,91,91	0
81	MG	1	3413	1/1	0.91	0.17	9,9,9,9	0
81	MG	AS	3545	1/1	0.92	0.19	22,22,22,22	0
81	MG	AS	3546	1/1	0.92	0.08	45,45,45,45	0
81	MG	AS	3693	1/1	0.92	0.09	77,77,77,77	0
81	MG	1	3708	1/1	0.92	0.11	10,10,10,10	0
81	MG	CM	1813	1/1	0.92	0.16	22,22,22,22	0
81	MG	1	3963	1/1	0.92	0.09	35,35,35,35	0
81	MG	1	3479	1/1	0.92	0.17	21,21,21,21	0
81	MG	1	3966	1/1	0.92	0.07	63,63,63,63	0
81	MG	1	3713	1/1	0.92	0.21	29,29,29,29	0
81	MG	CM	1823	1/1	0.92	0.20	33,33,33,33	0
81	MG	1	3517	1/1	0.92	0.07	66,66,66,66	0
81	MG	3	204	1/1	0.92	0.12	39,39,39,39	0
81	MG	CM	1828	1/1	0.92	0.18	41,41,41,41	0
81	MG	1	3540	1/1	0.92	0.09	33,33,33,33	0
81	MG	AS	3703	1/1	0.92	0.15	32,32,32,32	0
81	MG	1	3662	1/1	0.92	0.14	71,71,71,71	0
81	MG	3	208	1/1	0.92	0.14	35,35,35,35	0
81	MG	AS	3568	1/1	0.92	0.08	61,61,61,61	0
81	MG	1	3663	1/1	0.92	0.04	83,83,83,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3905	1/1	0.92	0.04	39,39,39,39	0
81	MG	CM	1839	1/1	0.92	0.17	46,46,46,46	0
81	MG	1	3627	1/1	0.92	0.19	25,25,25,25	0
81	MG	AS	3406	1/1	0.92	0.23	16,16,16,16	0
81	MG	1	3456	1/1	0.92	0.10	6,6,6,6	0
81	MG	1	3448	1/1	0.92	0.26	20,20,20,20	0
81	MG	CM	1847	1/1	0.92	0.08	32,32,32,32	0
81	MG	1	3671	1/1	0.92	0.14	9,9,9,9	0
81	MG	AS	3413	1/1	0.92	0.18	18,18,18,18	0
81	MG	B	1904	1/1	0.92	0.08	72,72,72,72	0
81	MG	AS	3418	1/1	0.92	0.18	25,25,25,25	0
81	MG	CM	1853	1/1	0.92	0.12	79,79,79,79	0
81	MG	AS	3586	1/1	0.92	0.11	11,11,11,11	0
81	MG	1	3848	1/1	0.92	0.21	29,29,29,29	0
81	MG	1	3673	1/1	0.92	0.10	55,55,55,55	0
81	MG	B	1908	1/1	0.92	0.10	35,35,35,35	0
81	MG	B	1816	1/1	0.92	0.16	49,49,49,49	0
81	MG	4	210	1/1	0.92	0.08	49,49,49,49	0
81	MG	AS	3432	1/1	0.92	0.10	24,24,24,24	0
81	MG	1	3913	1/1	0.92	0.14	43,43,43,43	0
81	MG	CM	1865	1/1	0.92	0.09	32,32,32,32	0
81	MG	1	3450	1/1	0.92	0.15	82,82,82,82	0
81	MG	1	3916	1/1	0.92	0.14	29,29,29,29	0
81	MG	1	3797	1/1	0.92	0.24	23,23,23,23	0
81	MG	1	3731	1/1	0.92	0.42	30,30,30,30	0
81	MG	1	3675	1/1	0.92	0.10	69,69,69,69	0
81	MG	AS	3453	1/1	0.92	0.15	82,82,82,82	0
81	MG	1	3405	1/1	0.92	0.19	16,16,16,16	0
81	MG	1	3569	1/1	0.92	0.11	46,46,46,46	0
81	MG	1	3637	1/1	0.92	0.14	45,45,45,45	0
81	MG	1	3463	1/1	0.92	0.19	12,12,12,12	0
81	MG	CM	1886	1/1	0.92	0.07	25,25,25,25	0
81	MG	1	3928	1/1	0.92	0.14	43,43,43,43	0
81	MG	AS	3756	1/1	0.92	0.05	47,47,47,47	0
81	MG	1	3862	1/1	0.92	0.14	23,23,23,23	0
81	MG	1	3505	1/1	0.92	0.14	24,24,24,24	0
81	MG	B	1927	1/1	0.92	0.16	39,39,39,39	0
81	MG	1	3551	1/1	0.92	0.07	57,57,57,57	0
81	MG	1	3686	1/1	0.92	0.11	36,36,36,36	0
81	MG	B	1838	1/1	0.92	0.18	68,68,68,68	0
81	MG	AS	3624	1/1	0.92	0.11	67,67,67,67	0
81	MG	AS	3627	1/1	0.92	0.07	17,17,17,17	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3769	1/1	0.92	0.10	45,45,45,45	0
81	MG	AS	3772	1/1	0.92	0.10	65,65,65,65	0
81	MG	AS	3773	1/1	0.92	0.07	29,29,29,29	0
81	MG	1	3506	1/1	0.92	0.16	13,13,13,13	0
81	MG	1	3935	1/1	0.92	0.04	31,31,31,31	0
81	MG	B	1934	1/1	0.92	0.07	69,69,69,69	0
81	MG	AS	3633	1/1	0.92	0.04	15,15,15,15	0
81	MG	CM	1916	1/1	0.92	0.19	37,37,37,37	0
81	MG	B	1935	1/1	0.92	0.19	56,56,56,56	0
81	MG	1	3576	1/1	0.92	0.18	29,29,29,29	0
81	MG	AS	3637	1/1	0.92	0.07	61,61,61,61	0
81	MG	CM	1923	1/1	0.92	0.12	71,71,71,71	0
81	MG	1	3938	1/1	0.92	0.13	30,30,30,30	0
81	MG	1	3940	1/1	0.92	0.10	44,44,44,44	0
81	MG	CM	1929	1/1	0.92	0.09	61,61,61,61	0
81	MG	1	3476	1/1	0.92	0.17	49,49,49,49	0
81	MG	B	1944	1/1	0.92	0.23	51,51,51,51	0
81	MG	1	3692	1/1	0.92	0.06	35,35,35,35	0
81	MG	1	3417	1/1	0.92	0.17	15,15,15,15	0
81	MG	1	3816	1/1	0.92	0.13	51,51,51,51	0
81	MG	1	3945	1/1	0.92	0.12	30,30,30,30	0
81	MG	1	3606	1/1	0.92	0.16	35,35,35,35	0
81	MG	AS	3650	1/1	0.92	0.06	40,40,40,40	0
81	MG	y	201	1/1	0.92	0.10	32,32,32,32	0
81	MG	B	1859	1/1	0.92	0.20	45,45,45,45	0
81	MG	AS	3514	1/1	0.92	0.14	18,18,18,18	0
81	MG	1	3821	1/1	0.92	0.06	56,56,56,56	0
81	MG	CQ	302	1/1	0.92	0.07	99,99,99,99	0
81	MG	1	3763	1/1	0.92	0.19	40,40,40,40	0
81	MG	AU	206	1/1	0.92	0.12	30,30,30,30	0
81	MG	AS	3659	1/1	0.92	0.08	25,25,25,25	0
81	MG	AW	302	1/1	0.92	0.11	23,23,23,23	0
81	MG	AS	3660	1/1	0.92	0.14	34,34,34,34	0
81	MG	AS	3663	1/1	0.92	0.17	31,31,31,31	0
81	MG	1	3697	1/1	0.92	0.08	35,35,35,35	0
81	MG	1	3455	1/1	0.92	0.20	22,22,22,22	0
81	MG	B	1958	1/1	0.92	0.11	29,29,29,29	0
81	MG	CL	301	1/1	0.92	0.05	22,22,22,22	0
81	MG	1	3580	1/1	0.92	0.14	44,44,44,44	0
82	3K5	1	3406	57/57	0.92	0.14	46,67,95,99	0
81	MG	B	1868	1/1	0.92	0.12	39,39,39,39	0
81	MG	BJ	304	1/1	0.92	0.08	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3828	1/1	0.92	0.05	19,19,19,19	0
81	MG	1	3767	1/1	0.92	0.22	51,51,51,51	0
81	MG	1	3887	1/1	0.92	0.06	18,18,18,18	0
81	MG	B	1873	1/1	0.92	0.16	50,50,50,50	0
81	MG	6	202	1/1	0.92	0.07	8,8,8,8	0
81	MG	AS	3534	1/1	0.92	0.15	30,30,30,30	0
81	MG	B	1876	1/1	0.92	0.13	33,33,33,33	0
81	MG	1	3616	1/1	0.92	0.10	44,44,44,44	0
84	ZN	AK	101	1/1	0.92	0.17	42,42,42,42	0
81	MG	9	202	1/1	0.92	0.20	93,93,93,93	0
81	MG	1	3705	1/1	0.92	0.08	37,37,37,37	0
81	MG	1	3617	1/1	0.92	0.16	29,29,29,29	0
81	MG	1	3414	1/1	0.93	0.21	12,12,12,12	0
81	MG	AS	3694	1/1	0.93	0.14	62,62,62,62	0
81	MG	1	3751	1/1	0.93	0.11	28,28,28,28	0
81	MG	AS	3405	1/1	0.93	0.31	18,18,18,18	0
81	MG	1	3702	1/1	0.93	0.12	34,34,34,34	0
81	MG	1	3586	1/1	0.93	0.08	54,54,54,54	0
81	MG	k	401	1/1	0.93	0.10	41,41,41,41	0
81	MG	AS	3411	1/1	0.93	0.07	12,12,12,12	0
81	MG	CM	1827	1/1	0.93	0.17	20,20,20,20	0
81	MG	1	3625	1/1	0.93	0.17	20,20,20,20	0
81	MG	B	1828	1/1	0.93	0.17	41,41,41,41	0
81	MG	1	3474	1/1	0.93	0.21	16,16,16,16	0
81	MG	AS	3417	1/1	0.93	0.19	24,24,24,24	0
81	MG	1	3932	1/1	0.93	0.07	27,27,27,27	0
81	MG	B	1916	1/1	0.93	0.11	44,44,44,44	0
81	MG	AS	3420	1/1	0.93	0.13	18,18,18,18	0
81	MG	CM	1836	1/1	0.93	0.13	41,41,41,41	0
81	MG	1	3759	1/1	0.93	0.35	28,28,28,28	0
81	MG	m	301	1/1	0.93	0.09	60,60,60,60	0
81	MG	AS	3426	1/1	0.93	0.15	16,16,16,16	0
81	MG	o	301	1/1	0.93	0.12	29,29,29,29	0
81	MG	AS	3716	1/1	0.93	0.08	85,85,85,85	0
81	MG	AS	3584	1/1	0.93	0.05	37,37,37,37	0
81	MG	1	3588	1/1	0.93	0.12	31,31,31,31	0
81	MG	AS	3720	1/1	0.93	0.06	41,41,41,41	0
81	MG	1	3761	1/1	0.93	0.10	33,33,33,33	0
81	MG	AS	3723	1/1	0.93	0.18	50,50,50,50	0
81	MG	AS	3587	1/1	0.93	0.12	37,37,37,37	0
81	MG	AS	3726	1/1	0.93	0.16	39,39,39,39	0
81	MG	AS	3434	1/1	0.93	0.08	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3592	1/1	0.93	0.06	29,29,29,29	0
81	MG	AS	3593	1/1	0.93	0.16	61,61,61,61	0
81	MG	1	3709	1/1	0.93	0.27	12,12,12,12	0
81	MG	CM	1859	1/1	0.93	0.11	34,34,34,34	0
81	MG	CM	1860	1/1	0.93	0.15	45,45,45,45	0
81	MG	1	3819	1/1	0.93	0.06	34,34,34,34	0
81	MG	1	3876	1/1	0.93	0.14	40,40,40,40	0
81	MG	AS	3597	1/1	0.93	0.14	37,37,37,37	0
81	MG	1	3475	1/1	0.93	0.21	16,16,16,16	0
81	MG	AS	3599	1/1	0.93	0.06	40,40,40,40	0
81	MG	1	3523	1/1	0.93	0.09	28,28,28,28	0
81	MG	AS	3450	1/1	0.93	0.16	9,9,9,9	0
81	MG	B	1845	1/1	0.93	0.18	30,30,30,30	0
81	MG	1	3714	1/1	0.93	0.16	21,21,21,21	0
81	MG	1	3825	1/1	0.93	0.04	31,31,31,31	0
81	MG	1	3881	1/1	0.93	0.10	39,39,39,39	0
81	MG	1	3633	1/1	0.93	0.16	33,33,33,33	0
81	MG	1	3716	1/1	0.93	0.17	25,25,25,25	0
81	MG	1	3884	1/1	0.93	0.09	43,43,43,43	0
81	MG	1	3486	1/1	0.93	0.14	29,29,29,29	0
81	MG	AS	3472	1/1	0.93	0.13	16,16,16,16	0
81	MG	CM	1888	1/1	0.93	0.14	35,35,35,35	0
81	MG	AS	3473	1/1	0.93	0.14	33,33,33,33	0
81	MG	AS	3613	1/1	0.93	0.06	46,46,46,46	0
81	MG	CM	1893	1/1	0.93	0.22	32,32,32,32	0
81	MG	x	204	1/1	0.93	0.09	32,32,32,32	0
81	MG	AS	3478	1/1	0.93	0.15	28,28,28,28	0
81	MG	1	3571	1/1	0.93	0.11	38,38,38,38	0
81	MG	1	3412	1/1	0.93	0.25	26,26,26,26	0
81	MG	B	1940	1/1	0.93	0.07	61,61,61,61	0
81	MG	B	1942	1/1	0.93	0.12	49,49,49,49	0
81	MG	1	3526	1/1	0.93	0.16	34,34,34,34	0
81	MG	1	3488	1/1	0.93	0.22	10,10,10,10	0
81	MG	AS	3625	1/1	0.93	0.07	51,51,51,51	0
81	MG	AS	3626	1/1	0.93	0.16	51,51,51,51	0
81	MG	CM	1904	1/1	0.93	0.06	28,28,28,28	0
81	MG	CM	1906	1/1	0.93	0.13	48,48,48,48	0
81	MG	1	3641	1/1	0.93	0.13	31,31,31,31	0
81	MG	1	3778	1/1	0.93	0.09	49,49,49,49	0
81	MG	1	3575	1/1	0.93	0.08	25,25,25,25	0
81	MG	AS	3631	1/1	0.93	0.30	65,65,65,65	0
81	MG	1	3781	1/1	0.93	0.05	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3897	1/1	0.93	0.16	29,29,29,29	0
81	MG	1	3601	1/1	0.93	0.27	39,39,39,39	0
81	MG	1	3899	1/1	0.93	0.12	48,48,48,48	0
81	MG	9	201	1/1	0.93	0.26	36,36,36,36	0
81	MG	1	3489	1/1	0.93	0.11	41,41,41,41	0
81	MG	AS	3503	1/1	0.93	0.17	10,10,10,10	0
81	MG	1	3903	1/1	0.93	0.37	67,67,67,67	0
81	MG	AS	3505	1/1	0.93	0.16	23,23,23,23	0
81	MG	1	3784	1/1	0.93	0.10	45,45,45,45	0
81	MG	3	203	1/1	0.93	0.17	31,31,31,31	0
81	MG	1	3507	1/1	0.93	0.12	17,17,17,17	0
81	MG	AS	3510	1/1	0.93	0.20	26,26,26,26	0
81	MG	CM	1938	1/1	0.93	0.08	20,20,20,20	0
81	MG	3	205	1/1	0.93	0.10	42,42,42,42	0
81	MG	AT	211	1/1	0.93	0.18	41,41,41,41	0
81	MG	1	3647	1/1	0.93	0.15	50,50,50,50	0
81	MG	1	3534	1/1	0.93	0.08	30,30,30,30	0
81	MG	1	3735	1/1	0.93	0.07	28,28,28,28	0
81	MG	1	3609	1/1	0.93	0.13	63,63,63,63	0
81	MG	AU	205	1/1	0.93	0.15	50,50,50,50	0
81	MG	AS	3518	1/1	0.93	0.05	27,27,27,27	0
81	MG	1	3458	1/1	0.93	0.14	10,10,10,10	0
81	MG	CQ	303	1/1	0.93	0.07	12,12,12,12	0
81	MG	AS	3520	1/1	0.93	0.17	29,29,29,29	0
81	MG	1	3739	1/1	0.93	0.14	22,22,22,22	0
81	MG	B	1888	1/1	0.93	0.11	52,52,52,52	0
81	MG	1	3740	1/1	0.93	0.09	28,28,28,28	0
81	MG	4	203	1/1	0.93	0.12	29,29,29,29	0
81	MG	BE	302	1/1	0.93	0.15	45,45,45,45	0
81	MG	1	3443	1/1	0.93	0.15	53,53,53,53	0
81	MG	1	3855	1/1	0.93	0.05	96,96,96,96	0
81	MG	K	301	1/1	0.93	0.05	35,35,35,35	0
81	MG	Q	201	1/1	0.93	0.03	10,10,10,10	0
81	MG	1	3436	1/1	0.93	0.11	20,20,20,20	0
81	MG	B	1895	1/1	0.93	0.04	5,5,5,5	0
81	MG	B	1896	1/1	0.93	0.13	23,23,23,23	0
81	MG	AS	3537	1/1	0.93	0.10	38,38,38,38	0
81	MG	AS	3538	1/1	0.93	0.16	27,27,27,27	0
81	MG	BZ	204	1/1	0.93	0.09	57,57,57,57	0
81	MG	B	1897	1/1	0.93	0.14	35,35,35,35	0
81	MG	1	3746	1/1	0.93	0.23	34,34,34,34	0
81	MG	1	3919	1/1	0.93	0.16	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3684	1/1	0.93	0.07	57,57,57,57	0
81	MG	1	3437	1/1	0.93	0.16	13,13,13,13	0
81	MG	1	3516	1/1	0.93	0.18	34,34,34,34	0
81	MG	1	3806	1/1	0.93	0.09	28,28,28,28	0
81	MG	1	3924	1/1	0.93	0.06	24,24,24,24	0
81	MG	AS	3689	1/1	0.93	0.08	52,52,52,52	0
81	MG	AS	3690	1/1	0.93	0.09	33,33,33,33	0
81	MG	CM	1846	1/1	0.94	0.16	29,29,29,29	0
81	MG	B	1963	1/1	0.94	0.08	33,33,33,33	0
81	MG	AS	3569	1/1	0.94	0.17	29,29,29,29	0
81	MG	AS	3661	1/1	0.94	0.16	27,27,27,27	0
81	MG	AS	3662	1/1	0.94	0.12	39,39,39,39	0
81	MG	1	3688	1/1	0.94	0.11	14,14,14,14	0
81	MG	CM	1852	1/1	0.94	0.10	47,47,47,47	0
81	MG	1	3562	1/1	0.94	0.19	12,12,12,12	0
81	MG	AS	3767	1/1	0.94	0.06	56,56,56,56	0
81	MG	AS	3768	1/1	0.94	0.10	38,38,38,38	0
81	MG	4	202	1/1	0.94	0.08	29,29,29,29	0
81	MG	AS	3771	1/1	0.94	0.09	37,37,37,37	0
81	MG	AS	3474	1/1	0.94	0.12	29,29,29,29	0
81	MG	1	3610	1/1	0.94	0.19	34,34,34,34	0
81	MG	1	3435	1/1	0.94	0.16	10,10,10,10	0
81	MG	1	3727	1/1	0.94	0.13	39,39,39,39	0
81	MG	E	302	1/1	0.94	0.13	22,22,22,22	0
81	MG	1	3541	1/1	0.94	0.20	15,15,15,15	0
81	MG	B	1912	1/1	0.94	0.08	59,59,59,59	0
81	MG	CM	1866	1/1	0.94	0.06	24,24,24,24	0
81	MG	AS	3675	1/1	0.94	0.11	54,54,54,54	0
81	MG	AS	3676	1/1	0.94	0.05	43,43,43,43	0
81	MG	B	1913	1/1	0.94	0.09	37,37,37,37	0
81	MG	AS	3679	1/1	0.94	0.07	62,62,62,62	0
81	MG	CM	1874	1/1	0.94	0.09	48,48,48,48	0
81	MG	CM	1875	1/1	0.94	0.17	48,48,48,48	0
81	MG	1	3615	1/1	0.94	0.07	10,10,10,10	0
81	MG	CM	1880	1/1	0.94	0.15	13,13,13,13	0
81	MG	1	3845	1/1	0.94	0.13	34,34,34,34	0
81	MG	AS	3490	1/1	0.94	0.14	27,27,27,27	0
81	MG	1	3846	1/1	0.94	0.06	27,27,27,27	0
81	MG	1	3891	1/1	0.94	0.16	48,48,48,48	0
81	MG	1	3542	1/1	0.94	0.13	42,42,42,42	0
81	MG	AS	3496	1/1	0.94	0.20	21,21,21,21	0
81	MG	CM	1887	1/1	0.94	0.19	8,8,8,8	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3666	1/1	0.94	0.16	41,41,41,41	0
81	MG	1	3567	1/1	0.94	0.14	42,42,42,42	0
81	MG	1	3850	1/1	0.94	0.06	28,28,28,28	0
81	MG	1	3851	1/1	0.94	0.12	25,25,25,25	0
81	MG	1	3568	1/1	0.94	0.19	29,29,29,29	0
81	MG	AS	3601	1/1	0.94	0.08	82,82,82,82	0
81	MG	AU	202	1/1	0.94	0.12	47,47,47,47	0
81	MG	1	3701	1/1	0.94	0.09	25,25,25,25	0
81	MG	1	3581	1/1	0.94	0.12	12,12,12,12	0
81	MG	1	3703	1/1	0.94	0.07	49,49,49,49	0
81	MG	1	3815	1/1	0.94	0.09	38,38,38,38	0
81	MG	1	3951	1/1	0.94	0.16	32,32,32,32	0
81	MG	1	3480	1/1	0.94	0.20	15,15,15,15	0
81	MG	1	3439	1/1	0.94	0.24	25,25,25,25	0
81	MG	AS	3511	1/1	0.94	0.11	28,28,28,28	0
81	MG	AY	401	1/1	0.94	0.08	45,45,45,45	0
81	MG	B	1811	1/1	0.94	0.17	42,42,42,42	0
81	MG	BB	302	1/1	0.94	0.05	36,36,36,36	0
81	MG	B	1877	1/1	0.94	0.17	30,30,30,30	0
81	MG	BF	201	1/1	0.94	0.11	49,49,49,49	0
81	MG	CM	1914	1/1	0.94	0.17	49,49,49,49	0
81	MG	1	3742	1/1	0.94	0.06	29,29,29,29	0
81	MG	1	3706	1/1	0.94	0.43	77,77,77,77	0
81	MG	BI	301	1/1	0.94	0.09	53,53,53,53	0
81	MG	BJ	301	1/1	0.94	0.10	47,47,47,47	0
81	MG	CM	1919	1/1	0.94	0.06	16,16,16,16	0
81	MG	CM	1920	1/1	0.94	0.10	58,58,58,58	0
81	MG	AS	3415	1/1	0.94	0.20	17,17,17,17	0
81	MG	1	3626	1/1	0.94	0.18	27,27,27,27	0
81	MG	BK	202	1/1	0.94	0.06	45,45,45,45	0
81	MG	AS	3616	1/1	0.94	0.08	52,52,52,52	0
81	MG	CM	1927	1/1	0.94	0.08	41,41,41,41	0
81	MG	CM	1928	1/1	0.94	0.11	78,78,78,78	0
81	MG	1	3958	1/1	0.94	0.14	24,24,24,24	0
81	MG	1	3491	1/1	0.94	0.22	37,37,37,37	0
81	MG	BV	201	1/1	0.94	0.12	51,51,51,51	0
81	MG	1	3824	1/1	0.94	0.05	29,29,29,29	0
81	MG	1	3602	1/1	0.94	0.19	20,20,20,20	0
81	MG	AS	3422	1/1	0.94	0.17	13,13,13,13	0
81	MG	B	1885	1/1	0.94	0.09	34,34,34,34	0
81	MG	B	1821	1/1	0.94	0.18	30,30,30,30	0
81	MG	AS	3529	1/1	0.94	0.06	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3724	1/1	0.94	0.07	43,43,43,43	0
81	MG	1	3785	1/1	0.94	0.10	15,15,15,15	0
81	MG	CM	1805	1/1	0.94	0.11	16,16,16,16	0
81	MG	1	3786	1/1	0.94	0.23	33,33,33,33	0
81	MG	AS	3428	1/1	0.94	0.17	23,23,23,23	0
81	MG	AS	3429	1/1	0.94	0.23	30,30,30,30	0
81	MG	B	1947	1/1	0.94	0.12	62,62,62,62	0
81	MG	1	3915	1/1	0.94	0.10	43,43,43,43	0
81	MG	1	3680	1/1	0.94	0.13	26,26,26,26	0
81	MG	1	3652	1/1	0.94	0.04	38,38,38,38	0
81	MG	CM	1817	1/1	0.94	0.18	48,48,48,48	0
81	MG	1	3872	1/1	0.94	0.05	42,42,42,42	0
81	MG	1	3493	1/1	0.94	0.06	22,22,22,22	0
81	MG	AS	3736	1/1	0.94	0.06	35,35,35,35	0
81	MG	1	3753	1/1	0.94	0.14	44,44,44,44	0
81	MG	AS	3738	1/1	0.94	0.09	17,17,17,17	0
81	MG	1	3451	1/1	0.94	0.07	12,12,12,12	0
81	MG	1	3530	1/1	0.94	0.14	19,19,19,19	0
81	MG	1	3834	1/1	0.94	0.10	18,18,18,18	0
81	MG	AS	3452	1/1	0.94	0.13	8,8,8,8	0
81	MG	AS	3646	1/1	0.94	0.12	36,36,36,36	0
81	MG	1	3656	1/1	0.94	0.10	64,64,64,64	0
81	MG	AS	3454	1/1	0.94	0.07	48,48,48,48	0
81	MG	AS	3551	1/1	0.94	0.19	42,42,42,42	0
81	MG	AS	3750	1/1	0.94	0.05	21,21,21,21	0
81	MG	AS	3456	1/1	0.94	0.17	13,13,13,13	0
81	MG	3	210	1/1	0.94	0.13	38,38,38,38	0
81	MG	AS	3460	1/1	0.94	0.11	26,26,26,26	0
81	MG	1	3687	1/1	0.94	0.14	32,32,32,32	0
81	MG	B	1840	1/1	0.94	0.11	34,34,34,34	0
81	MG	AS	3758	1/1	0.94	0.08	22,22,22,22	0
81	MG	CM	1843	1/1	0.94	0.09	41,41,41,41	0
81	MG	1	3927	1/1	0.94	0.12	45,45,45,45	0
84	ZN	CE	101	1/1	0.94	0.07	119,119,119,119	0
81	MG	1	3889	1/1	0.95	0.12	35,35,35,35	0
81	MG	1	3631	1/1	0.95	0.08	37,37,37,37	0
81	MG	AS	3638	1/1	0.95	0.17	14,14,14,14	0
81	MG	AS	3560	1/1	0.95	0.11	34,34,34,34	0
81	MG	1	3472	1/1	0.95	0.12	29,29,29,29	0
81	MG	CM	1876	1/1	0.95	0.18	19,19,19,19	0
81	MG	1	3664	1/1	0.95	0.12	54,54,54,54	0
81	MG	BB	303	1/1	0.95	0.20	28,28,28,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	BE	301	1/1	0.95	0.15	34,34,34,34	0
81	MG	AS	3563	1/1	0.95	0.15	53,53,53,53	0
81	MG	1	3790	1/1	0.95	0.07	33,33,33,33	0
81	MG	AS	3567	1/1	0.95	0.14	9,9,9,9	0
81	MG	1	3792	1/1	0.95	0.08	20,20,20,20	0
81	MG	1	3733	1/1	0.95	0.05	33,33,33,33	0
81	MG	1	3422	1/1	0.95	0.18	1,1,1,1	0
81	MG	AS	3571	1/1	0.95	0.14	35,35,35,35	0
81	MG	B	1937	1/1	0.95	0.07	70,70,70,70	0
81	MG	BK	201	1/1	0.95	0.14	27,27,27,27	0
81	MG	CM	1892	1/1	0.95	0.09	50,50,50,50	0
81	MG	AS	3408	1/1	0.95	0.18	1,1,1,1	0
81	MG	AS	3652	1/1	0.95	0.12	57,57,57,57	0
81	MG	BN	202	1/1	0.95	0.06	31,31,31,31	0
81	MG	B	1826	1/1	0.95	0.09	54,54,54,54	0
81	MG	1	3634	1/1	0.95	0.15	27,27,27,27	0
81	MG	1	3861	1/1	0.95	0.05	54,54,54,54	0
81	MG	AS	3657	1/1	0.95	0.13	19,19,19,19	0
81	MG	4	201	1/1	0.95	0.06	29,29,29,29	0
81	MG	AS	3741	1/1	0.95	0.16	43,43,43,43	0
81	MG	1	3939	1/1	0.95	0.13	22,22,22,22	0
81	MG	AS	3500	1/1	0.95	0.03	42,42,42,42	0
81	MG	1	3736	1/1	0.95	0.13	42,42,42,42	0
81	MG	1	3900	1/1	0.95	0.08	45,45,45,45	0
81	MG	CM	1803	1/1	0.95	0.12	19,19,19,19	0
81	MG	1	3441	1/1	0.95	0.12	20,20,20,20	0
81	MG	4	206	1/1	0.95	0.07	32,32,32,32	0
81	MG	1	3651	1/1	0.95	0.21	29,29,29,29	0
81	MG	AS	3666	1/1	0.95	0.18	17,17,17,17	0
81	MG	AS	3752	1/1	0.95	0.07	33,33,33,33	0
81	MG	AS	3589	1/1	0.95	0.15	37,37,37,37	0
81	MG	1	3801	1/1	0.95	0.06	19,19,19,19	0
81	MG	CM	1812	1/1	0.95	0.12	47,47,47,47	0
81	MG	1	3669	1/1	0.95	0.13	48,48,48,48	0
81	MG	CM	1814	1/1	0.95	0.18	22,22,22,22	0
81	MG	CM	1921	1/1	0.95	0.12	38,38,38,38	0
81	MG	1	3868	1/1	0.95	0.08	67,67,67,67	0
81	MG	AS	3509	1/1	0.95	0.09	33,33,33,33	0
81	MG	B	1839	1/1	0.95	0.13	24,24,24,24	0
81	MG	CM	1819	1/1	0.95	0.08	20,20,20,20	0
81	MG	1	3482	1/1	0.95	0.18	26,26,26,26	0
81	MG	1	3835	1/1	0.95	0.08	44,44,44,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	B	1842	1/1	0.95	0.10	25,25,25,25	0
81	MG	CM	1931	1/1	0.95	0.10	58,58,58,58	0
81	MG	AD	201	1/1	0.95	0.10	88,88,88,88	0
81	MG	CM	1825	1/1	0.95	0.18	37,37,37,37	0
81	MG	1	3949	1/1	0.95	0.06	42,42,42,42	0
81	MG	1	3770	1/1	0.95	0.15	25,25,25,25	0
81	MG	1	3513	1/1	0.95	0.11	36,36,36,36	0
81	MG	1	3717	1/1	0.95	0.12	37,37,37,37	0
81	MG	AG	201	1/1	0.95	0.09	59,59,59,59	0
81	MG	AS	3770	1/1	0.95	0.06	40,40,40,40	0
81	MG	1	3773	1/1	0.95	0.07	40,40,40,40	0
81	MG	1	3744	1/1	0.95	0.08	45,45,45,45	0
81	MG	AS	3446	1/1	0.95	0.18	36,36,36,36	0
81	MG	1	3719	1/1	0.95	0.15	15,15,15,15	0
81	MG	1	3407	1/1	0.95	0.15	14,14,14,14	0
81	MG	k	405	1/1	0.95	0.16	61,61,61,61	0
81	MG	1	3696	1/1	0.95	0.09	50,50,50,50	0
81	MG	AS	3692	1/1	0.95	0.08	47,47,47,47	0
81	MG	1	3608	1/1	0.95	0.08	24,24,24,24	0
81	MG	DA	201	1/1	0.95	0.14	38,38,38,38	0
81	MG	1	3431	1/1	0.95	0.18	20,20,20,20	0
81	MG	1	3658	1/1	0.95	0.14	20,20,20,20	0
81	MG	AS	3459	1/1	0.95	0.19	6,6,6,6	0
81	MG	1	3921	1/1	0.95	0.11	33,33,33,33	0
81	MG	1	3432	1/1	0.95	0.23	21,21,21,21	0
81	MG	B	1866	1/1	0.95	0.07	63,63,63,63	0
81	MG	AS	3465	1/1	0.95	0.07	41,41,41,41	0
81	MG	1	3564	1/1	0.95	0.10	15,15,15,15	0
81	MG	AS	3543	1/1	0.95	0.15	17,17,17,17	0
81	MG	Q	202	1/1	0.95	0.07	62,62,62,62	0
81	MG	B	1808	1/1	0.95	0.17	54,54,54,54	0
81	MG	1	3817	1/1	0.95	0.07	87,87,87,87	0
81	MG	CM	1856	1/1	0.95	0.08	36,36,36,36	0
81	MG	AT	210	1/1	0.95	0.12	27,27,27,27	0
81	MG	B	1810	1/1	0.95	0.08	11,11,11,11	0
81	MG	AS	3629	1/1	0.95	0.07	41,41,41,41	0
81	MG	1	3424	1/1	0.95	0.20	7,7,7,7	0
81	MG	AS	3710	1/1	0.95	0.09	27,27,27,27	0
81	MG	1	3683	1/1	0.95	0.11	28,28,28,28	0
81	MG	AS	3477	1/1	0.95	0.11	16,16,16,16	0
81	MG	AS	3713	1/1	0.95	0.10	36,36,36,36	0
81	MG	1	3820	1/1	0.95	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3715	1/1	0.95	0.06	73,73,73,73	0
81	MG	CM	1867	1/1	0.95	0.15	35,35,35,35	0
81	MG	AS	3479	1/1	0.95	0.14	25,25,25,25	0
81	MG	1	3620	1/1	0.96	0.04	27,27,27,27	0
81	MG	AS	3759	1/1	0.96	0.04	39,39,39,39	0
81	MG	w	302	1/1	0.96	0.10	60,60,60,60	0
81	MG	1	3670	1/1	0.96	0.20	25,25,25,25	0
81	MG	1	3521	1/1	0.96	0.15	32,32,32,32	0
81	MG	AS	3423	1/1	0.96	0.15	10,10,10,10	0
81	MG	1	3672	1/1	0.96	0.05	8,8,8,8	0
81	MG	AS	3691	1/1	0.96	0.07	51,51,51,51	0
81	MG	CM	1807	1/1	0.96	0.12	28,28,28,28	0
81	MG	AS	3486	1/1	0.96	0.12	32,32,32,32	0
81	MG	1	3622	1/1	0.96	0.15	8,8,8,8	0
81	MG	1	3718	1/1	0.96	0.11	42,42,42,42	0
81	MG	x	205	1/1	0.96	0.17	30,30,30,30	0
81	MG	AS	3558	1/1	0.96	0.14	25,25,25,25	0
81	MG	1	3492	1/1	0.96	0.08	43,43,43,43	0
81	MG	1	3741	1/1	0.96	0.06	42,42,42,42	0
81	MG	CM	1815	1/1	0.96	0.13	19,19,19,19	0
81	MG	1	3912	1/1	0.96	0.06	24,24,24,24	0
81	MG	AS	3431	1/1	0.96	0.18	16,16,16,16	0
81	MG	AS	3564	1/1	0.96	0.13	47,47,47,47	0
81	MG	B	1849	1/1	0.96	0.16	28,28,28,28	0
81	MG	CM	1909	1/1	0.96	0.10	56,56,56,56	0
81	MG	CM	1910	1/1	0.96	0.09	46,46,46,46	0
81	MG	AS	3635	1/1	0.96	0.17	13,13,13,13	0
81	MG	CM	1821	1/1	0.96	0.09	16,16,16,16	0
81	MG	1	3469	1/1	0.96	0.22	33,33,33,33	0
81	MG	AS	3435	1/1	0.96	0.06	73,73,73,73	0
81	MG	B	1852	1/1	0.96	0.10	27,27,27,27	0
81	MG	1	3657	1/1	0.96	0.07	20,20,20,20	0
81	MG	AS	3438	1/1	0.96	0.14	15,15,15,15	0
81	MG	B	1894	1/1	0.96	0.05	21,21,21,21	0
81	MG	1	3640	1/1	0.96	0.16	37,37,37,37	0
81	MG	AS	3443	1/1	0.96	0.06	36,36,36,36	0
81	MG	AT	201	1/1	0.96	0.17	13,13,13,13	0
81	MG	1	3865	1/1	0.96	0.07	53,53,53,53	0
81	MG	AS	3578	1/1	0.96	0.14	74,74,74,74	0
81	MG	AS	3445	1/1	0.96	0.22	54,54,54,54	0
81	MG	CM	1834	1/1	0.96	0.05	38,38,38,38	0
81	MG	1	3504	1/1	0.96	0.14	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3449	1/1	0.96	0.14	28,28,28,28	0
81	MG	CM	1837	1/1	0.96	0.07	12,12,12,12	0
81	MG	1	3508	1/1	0.96	0.11	27,27,27,27	0
81	MG	1	3599	1/1	0.96	0.09	19,19,19,19	0
81	MG	3	209	1/1	0.96	0.12	25,25,25,25	0
81	MG	AS	3722	1/1	0.96	0.09	43,43,43,43	0
81	MG	1	3799	1/1	0.96	0.08	15,15,15,15	0
81	MG	B	1861	1/1	0.96	0.10	62,62,62,62	0
81	MG	AS	3455	1/1	0.96	0.16	26,26,26,26	0
81	MG	AS	3656	1/1	0.96	0.31	19,19,19,19	0
81	MG	1	3628	1/1	0.96	0.07	17,17,17,17	0
81	MG	AS	3591	1/1	0.96	0.05	28,28,28,28	0
81	MG	AB	201	1/1	0.96	0.16	64,64,64,64	0
81	MG	AW	301	1/1	0.96	0.06	41,41,41,41	0
81	MG	AS	3458	1/1	0.96	0.12	11,11,11,11	0
81	MG	AS	3402	1/1	0.96	0.25	16,16,16,16	0
81	MG	CP	302	1/1	0.96	0.09	54,54,54,54	0
81	MG	B	1824	1/1	0.96	0.04	32,32,32,32	0
81	MG	1	3519	1/1	0.96	0.26	45,45,45,45	0
81	MG	AS	3524	1/1	0.96	0.09	38,38,38,38	0
81	MG	AS	3462	1/1	0.96	0.17	40,40,40,40	0
81	MG	AS	3463	1/1	0.96	0.18	25,25,25,25	0
81	MG	1	3614	1/1	0.96	0.13	49,49,49,49	0
81	MG	1	3520	1/1	0.96	0.05	14,14,14,14	0
81	MG	DB	202	1/1	0.96	0.09	35,35,35,35	0
81	MG	AS	3530	1/1	0.96	0.10	52,52,52,52	0
81	MG	r	301	1/1	0.96	0.13	41,41,41,41	0
81	MG	BG	301	1/1	0.96	0.07	56,56,56,56	0
81	MG	AS	3467	1/1	0.96	0.11	19,19,19,19	0
81	MG	1	3592	1/1	0.96	0.08	68,68,68,68	0
81	MG	DQ	101	1/1	0.96	0.08	61,61,61,61	0
81	MG	AS	3744	1/1	0.96	0.10	49,49,49,49	0
81	MG	1	3593	1/1	0.96	0.13	14,14,14,14	0
81	MG	CL	303	1/1	0.96	0.07	66,66,66,66	0
81	MG	AS	3674	1/1	0.96	0.07	22,22,22,22	0
81	MG	BJ	303	1/1	0.96	0.11	20,20,20,20	0
81	MG	AS	3470	1/1	0.96	0.16	18,18,18,18	0
81	MG	AS	3471	1/1	0.96	0.13	9,9,9,9	0
81	MG	CM	1872	1/1	0.96	0.04	26,26,26,26	0
81	MG	AS	3749	1/1	0.96	0.06	51,51,51,51	0
81	MG	B	1872	1/1	0.96	0.06	12,12,12,12	0
81	MG	1	3756	1/1	0.96	0.10	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3539	1/1	0.96	0.09	57,57,57,57	0
81	MG	AS	3753	1/1	0.96	0.09	27,27,27,27	0
81	MG	CM	1879	1/1	0.96	0.14	18,18,18,18	0
81	MG	u	201	1/1	0.96	0.05	42,42,42,42	0
81	MG	1	3902	1/1	0.96	0.04	32,32,32,32	0
81	MG	BZ	202	1/1	0.96	0.15	102,102,102,102	0
84	ZN	f	101	1/1	0.96	0.09	123,123,123,123	0
81	MG	1	3619	1/1	0.96	0.10	39,39,39,39	0
81	MG	1	3957	1/1	0.96	0.20	46,46,46,46	0
81	MG	1	3557	1/1	0.97	0.11	33,33,33,33	0
81	MG	AS	3475	1/1	0.97	0.10	10,10,10,10	0
81	MG	CM	1905	1/1	0.97	0.12	29,29,29,29	0
81	MG	1	3499	1/1	0.97	0.13	11,11,11,11	0
81	MG	AS	3732	1/1	0.97	0.09	74,74,74,74	0
81	MG	AU	204	1/1	0.97	0.06	39,39,39,39	0
81	MG	AD	202	1/1	0.97	0.12	17,17,17,17	0
81	MG	1	3444	1/1	0.97	0.12	18,18,18,18	0
81	MG	1	3459	1/1	0.97	0.15	16,16,16,16	0
81	MG	B	1965	1/1	0.97	0.11	35,35,35,35	0
81	MG	1	3642	1/1	0.97	0.14	18,18,18,18	0
81	MG	AS	3482	1/1	0.97	0.07	54,54,54,54	0
81	MG	AS	3542	1/1	0.97	0.17	15,15,15,15	0
81	MG	1	3885	1/1	0.97	0.06	33,33,33,33	0
81	MG	1	3589	1/1	0.97	0.08	44,44,44,44	0
81	MG	1	3710	1/1	0.97	0.13	26,26,26,26	0
81	MG	CM	1844	1/1	0.97	0.09	34,34,34,34	0
81	MG	1	3605	1/1	0.97	0.13	17,17,17,17	0
81	MG	AS	3433	1/1	0.97	0.16	12,12,12,12	0
81	MG	AS	3678	1/1	0.97	0.20	16,16,16,16	0
81	MG	E	301	1/1	0.97	0.06	63,63,63,63	0
81	MG	1	3712	1/1	0.97	0.15	20,20,20,20	0
81	MG	AS	3491	1/1	0.97	0.06	28,28,28,28	0
81	MG	1	3547	1/1	0.97	0.14	24,24,24,24	0
81	MG	AS	3552	1/1	0.97	0.08	39,39,39,39	0
81	MG	CM	1930	1/1	0.97	0.04	29,29,29,29	0
81	MG	1	3607	1/1	0.97	0.04	13,13,13,13	0
81	MG	H	1001	1/1	0.97	0.04	79,79,79,79	0
81	MG	AS	3622	1/1	0.97	0.04	22,22,22,22	0
81	MG	CM	1935	1/1	0.97	0.07	109,109,109,109	0
81	MG	B	1928	1/1	0.97	0.03	17,17,17,17	0
81	MG	AS	3440	1/1	0.97	0.05	21,21,21,21	0
81	MG	AS	3441	1/1	0.97	0.17	22,22,22,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	1	3465	1/1	0.97	0.11	17,17,17,17	0
81	MG	1	3549	1/1	0.97	0.13	43,43,43,43	0
81	MG	CM	1941	1/1	0.97	0.05	29,29,29,29	0
81	MG	4	207	1/1	0.97	0.07	35,35,35,35	0
81	MG	B	1844	1/1	0.97	0.10	15,15,15,15	0
81	MG	1	3527	1/1	0.97	0.19	33,33,33,33	0
81	MG	AS	3447	1/1	0.97	0.12	16,16,16,16	0
81	MG	1	3453	1/1	0.97	0.10	6,6,6,6	0
81	MG	1	3511	1/1	0.97	0.17	16,16,16,16	0
81	MG	1	3613	1/1	0.97	0.10	22,22,22,22	0
81	MG	CQ	301	1/1	0.97	0.10	16,16,16,16	0
81	MG	B	1807	1/1	0.97	0.06	101,101,101,101	0
81	MG	CA	201	1/1	0.97	0.07	46,46,46,46	0
81	MG	1	3695	1/1	0.97	0.09	29,29,29,29	0
81	MG	AS	3573	1/1	0.97	0.22	16,16,16,16	0
81	MG	1	3780	1/1	0.97	0.10	33,33,33,33	0
81	MG	1	3446	1/1	0.97	0.09	5,5,5,5	0
81	MG	AS	3512	1/1	0.97	0.14	17,17,17,17	0
81	MG	AS	3577	1/1	0.97	0.11	20,20,20,20	0
81	MG	AS	3642	1/1	0.97	0.04	99,99,99,99	0
81	MG	CM	1878	1/1	0.97	0.08	13,13,13,13	0
81	MG	1	3554	1/1	0.97	0.09	36,36,36,36	0
81	MG	AS	3708	1/1	0.97	0.17	43,43,43,43	0
81	MG	DJ	201	1/1	0.97	0.12	17,17,17,17	0
81	MG	B	1812	1/1	0.97	0.12	24,24,24,24	0
81	MG	1	3752	1/1	0.97	0.18	47,47,47,47	0
81	MG	B	1814	1/1	0.97	0.06	79,79,79,79	0
81	MG	j	301	1/1	0.97	0.06	11,11,11,11	0
81	MG	1	3531	1/1	0.97	0.04	25,25,25,25	0
81	MG	j	303	1/1	0.97	0.08	13,13,13,13	0
81	MG	1	3725	1/1	0.97	0.08	6,6,6,6	0
81	MG	B	1950	1/1	0.97	0.06	54,54,54,54	0
81	MG	CM	1889	1/1	0.97	0.07	62,62,62,62	0
81	MG	1	3676	1/1	0.97	0.09	12,12,12,12	0
81	MG	AS	3718	1/1	0.97	0.04	7,7,7,7	0
81	MG	k	402	1/1	0.97	0.07	55,55,55,55	0
81	MG	AS	3590	1/1	0.97	0.06	55,55,55,55	0
81	MG	AS	3525	1/1	0.97	0.13	25,25,25,25	0
81	MG	B	1864	1/1	0.97	0.12	49,49,49,49	0
81	MG	AT	205	1/1	0.97	0.09	13,13,13,13	0
81	MG	1	3700	1/1	0.97	0.07	41,41,41,41	0
81	MG	1	3937	1/1	0.97	0.06	64,64,64,64	0

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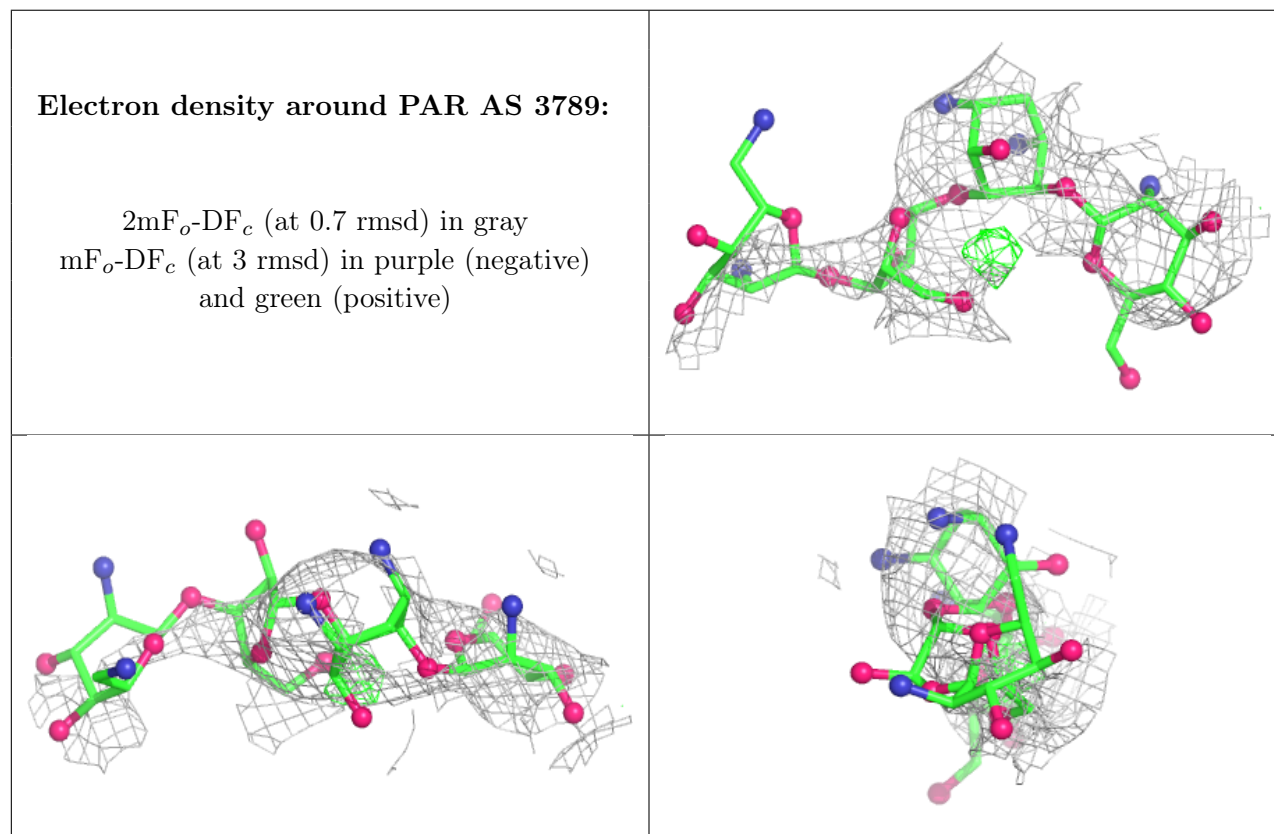
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
84	ZN	AQ	101	1/1	0.97	0.05	95,95,95,95	0
81	MG	8	202	1/1	0.97	0.11	34,34,34,34	0
81	MG	1	3498	1/1	0.97	0.10	73,73,73,73	0
81	MG	1	3618	1/1	0.97	0.10	11,11,11,11	0
81	MG	1	3679	1/1	0.97	0.23	21,21,21,21	0
81	MG	AS	3619	1/1	0.98	0.07	47,47,47,47	0
81	MG	AS	3414	1/1	0.98	0.06	71,71,71,71	0
81	MG	1	3449	1/1	0.98	0.20	14,14,14,14	0
81	MG	1	3462	1/1	0.98	0.11	13,13,13,13	0
81	MG	AT	206	1/1	0.98	0.11	50,50,50,50	0
81	MG	1	3791	1/1	0.98	0.10	22,22,22,22	0
81	MG	CM	1934	1/1	0.98	0.05	49,49,49,49	0
81	MG	AS	3555	1/1	0.98	0.08	39,39,39,39	0
81	MG	AS	3556	1/1	0.98	0.06	38,38,38,38	0
81	MG	CM	1908	1/1	0.98	0.06	23,23,23,23	0
81	MG	AG	202	1/1	0.98	0.03	43,43,43,43	0
81	MG	AS	3580	1/1	0.98	0.05	42,42,42,42	0
81	MG	1	3749	1/1	0.98	0.11	24,24,24,24	0
81	MG	AS	3559	1/1	0.98	0.11	17,17,17,17	0
81	MG	AS	3521	1/1	0.98	0.08	59,59,59,59	0
81	MG	AH	203	1/1	0.98	0.06	79,79,79,79	0
81	MG	B	1825	1/1	0.98	0.12	22,22,22,22	0
81	MG	1	3428	1/1	0.98	0.29	16,16,16,16	0
81	MG	AS	3489	1/1	0.98	0.06	23,23,23,23	0
81	MG	AS	3565	1/1	0.98	0.09	19,19,19,19	0
81	MG	1	3404	1/1	0.98	0.14	13,13,13,13	0
81	MG	B	1850	1/1	0.98	0.05	44,44,44,44	0
81	MG	CM	1868	1/1	0.98	0.12	37,37,37,37	0
84	ZN	AN	101	1/1	0.98	0.08	149,149,149,149	0
81	MG	AS	3409	1/1	0.98	0.05	91,91,91,91	0
81	MG	B	1941	1/1	0.98	0.03	48,48,48,48	0
81	MG	B	1875	1/1	0.98	0.05	103,103,103,103	0
81	MG	1	3964	1/1	0.98	0.06	76,76,76,76	0
81	MG	CM	1926	1/1	0.98	0.05	36,36,36,36	0
81	MG	AP	204	1/1	0.98	0.04	49,49,49,49	0
84	ZN	CK	101	1/1	0.98	0.05	137,137,137,137	0
84	ZN	DQ	102	1/1	0.98	0.04	47,47,47,47	0
81	MG	1	3775	1/1	0.99	0.04	31,31,31,31	0
81	MG	1	3515	1/1	0.99	0.12	11,11,11,11	0
81	MG	AS	3421	1/1	0.99	0.03	63,63,63,63	0
81	MG	1	3440	1/1	0.99	0.09	50,50,50,50	0
81	MG	B	1905	1/1	0.99	0.05	93,93,93,93	0

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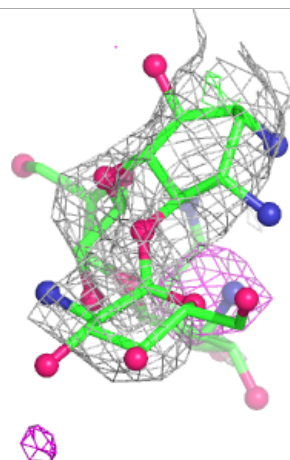
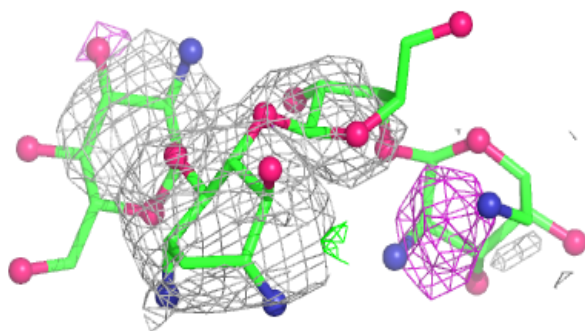
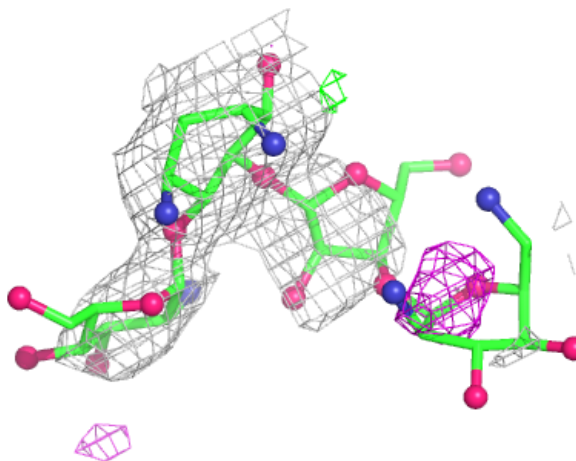
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
81	MG	AS	3493	1/1	0.99	0.06	7,7,7,7	0
81	MG	AS	3448	1/1	0.99	0.05	6,6,6,6	0
81	MG	AS	3785	1/1	0.99	0.06	13,13,13,13	0
81	MG	AS	3786	1/1	0.99	0.03	31,31,31,31	0
81	MG	1	3793	1/1	0.99	0.03	26,26,26,26	0
81	MG	1	3533	1/1	0.99	0.11	15,15,15,15	0
81	MG	1	3762	1/1	0.99	0.04	50,50,50,50	0

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



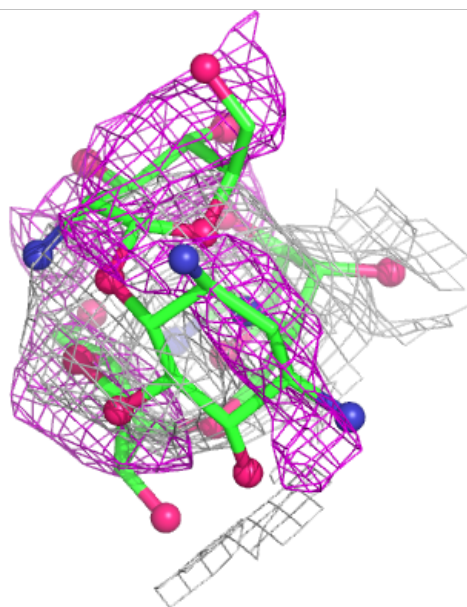
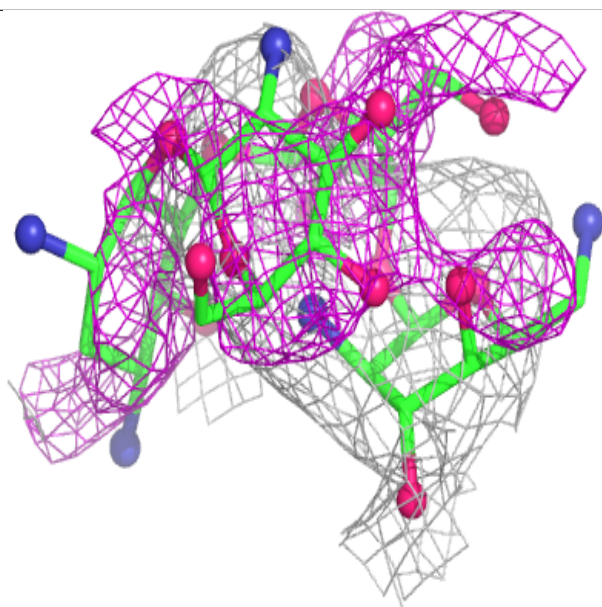
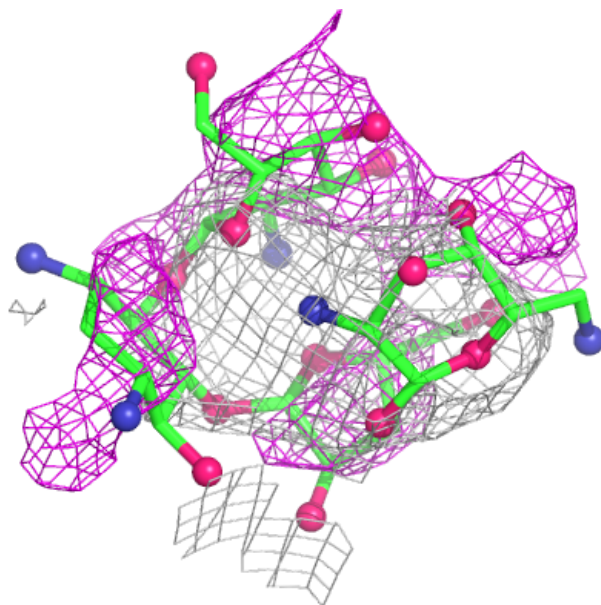
Electron density around PAR AS 3790:

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



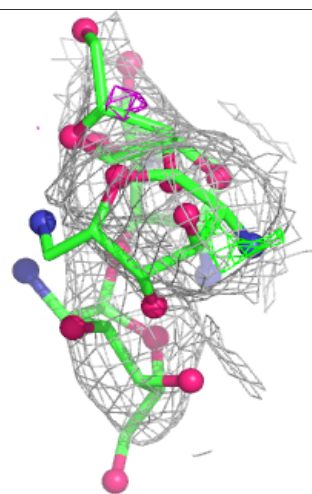
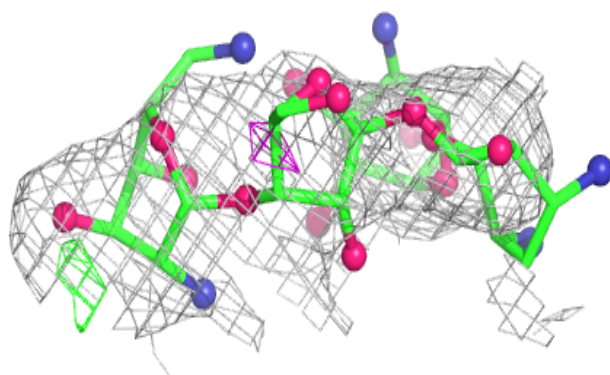
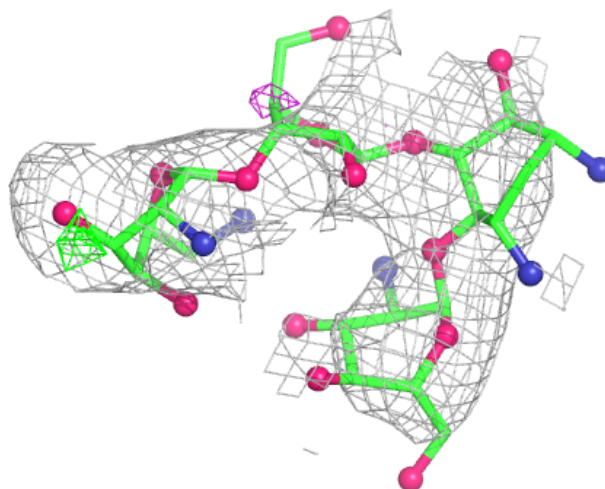
Electron density around PAR B 1970:

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



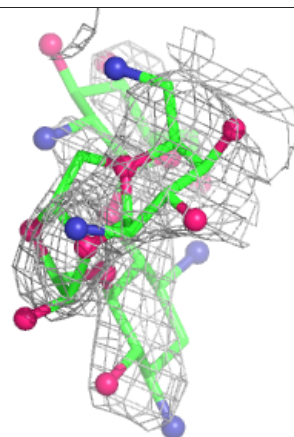
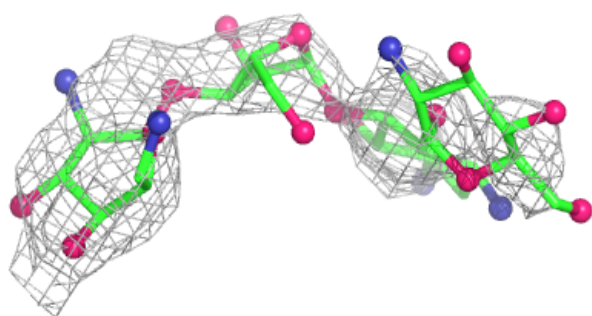
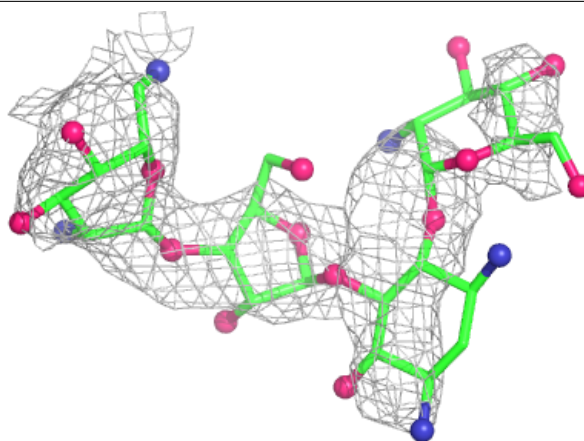
Electron density around PAR 1 3969:

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

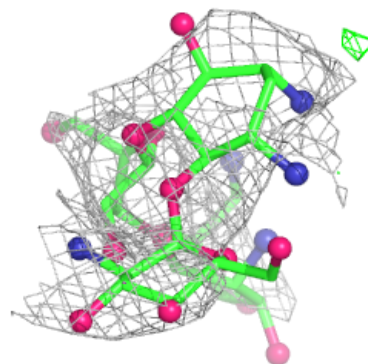
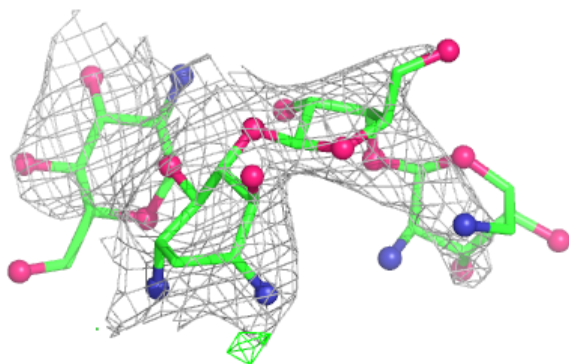
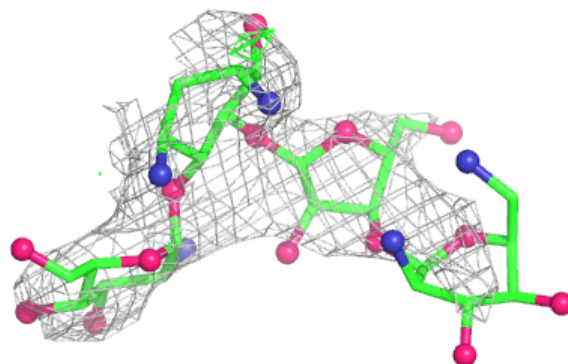


Electron density around PAR AS 3788:

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

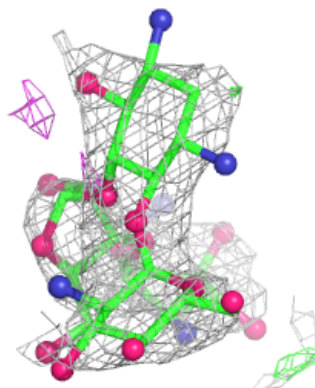
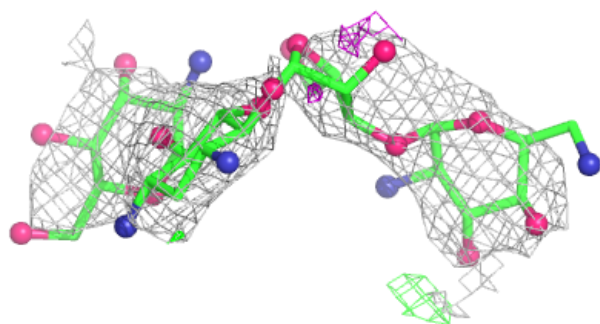
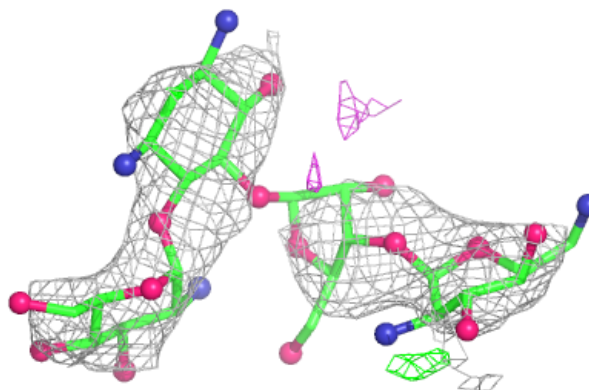
**Electron density around PAR 1 3968:**

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

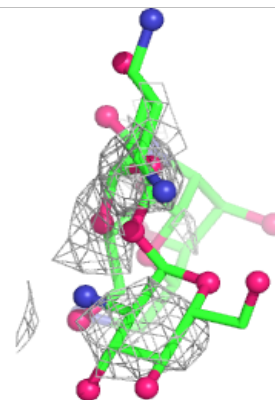
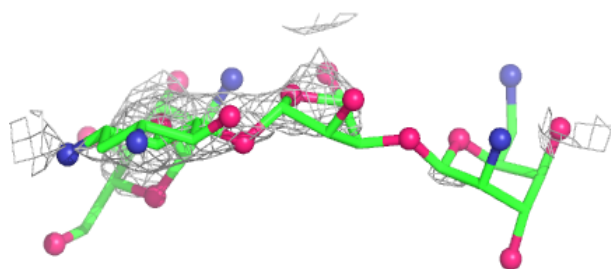
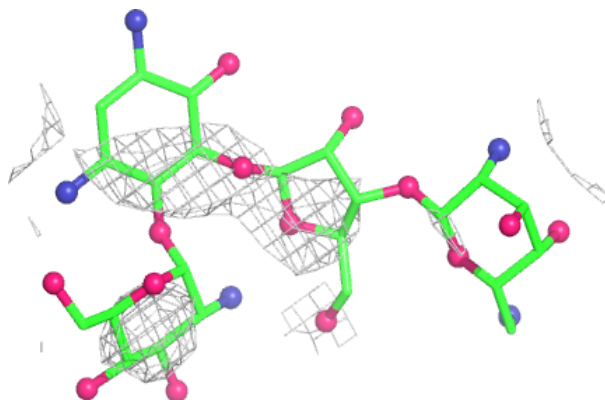


Electron density around PAR 1 3967:

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

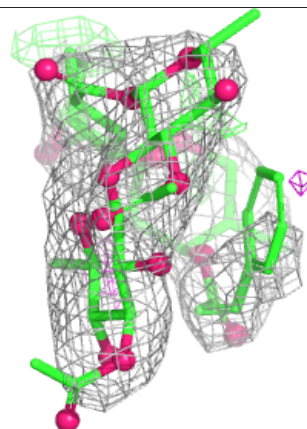
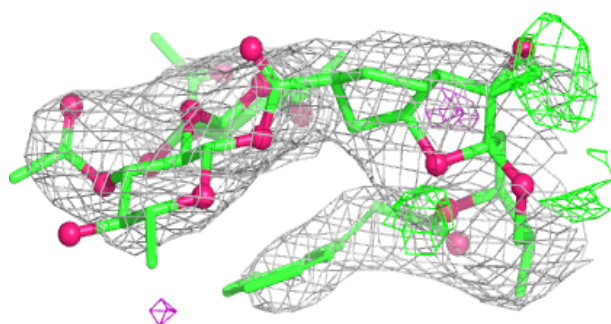
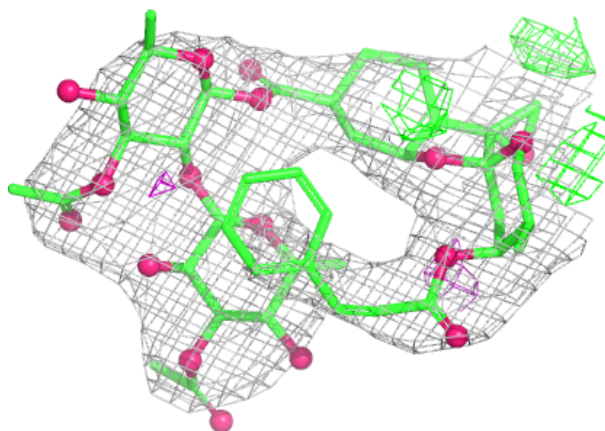
**Electron density around PAR CM 1946:**

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



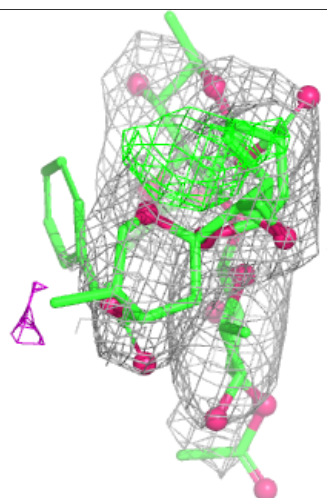
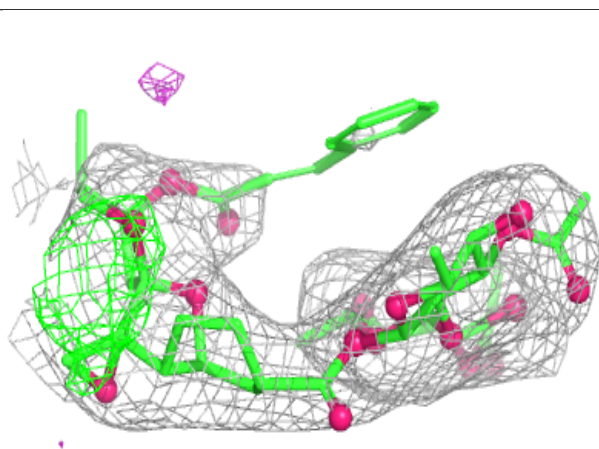
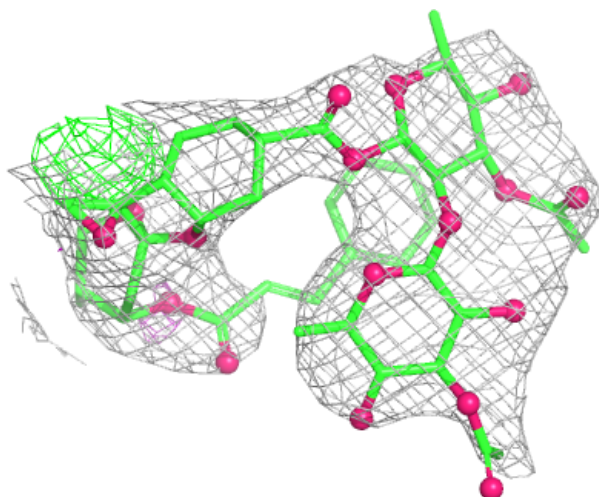
Electron density around 3K5 CJ 202:

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



Electron density around 3K5 1 3406:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.