wwPDB X-ray Structure Validation Summary Report (i)

Sep 16, 2024 – 10:21 pm BST

PDB ID	:	8OEQ
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 (i) 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 (i)) were used in the production of this report:

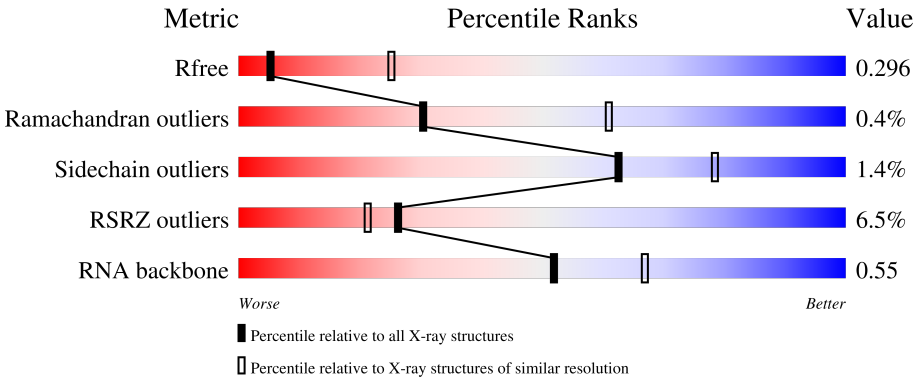
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.002 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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}	164625	1085 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)
RNA backbone	3690	1014 (3.64-2.96)

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

Mol	Chain	Length	Quality of chain
1	1	3359	75% 19%
1	AS	3359	2% 75% 18% 5%
2	3	121	92% 8%
2	AT	121	93% 7%
3	4	158	83% 15%

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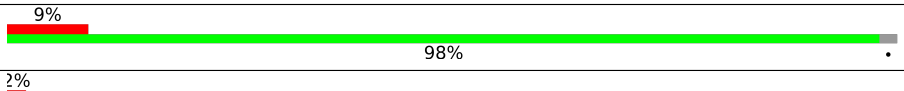
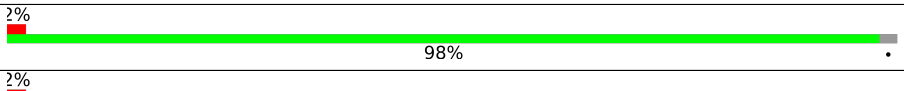
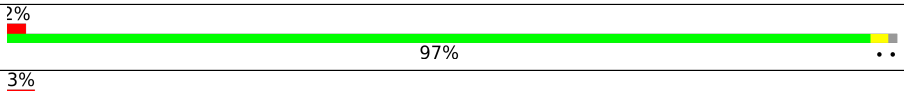
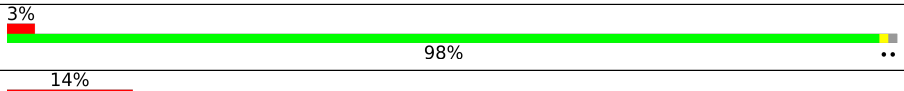
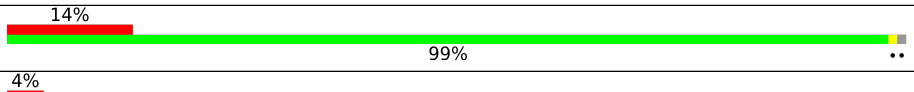
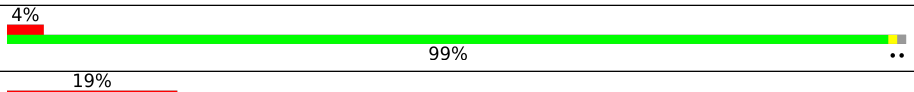
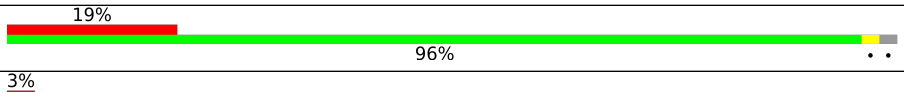
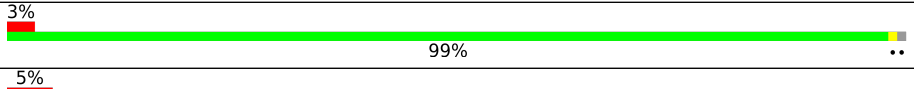
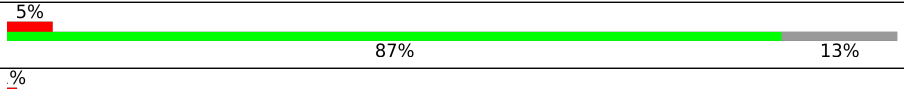
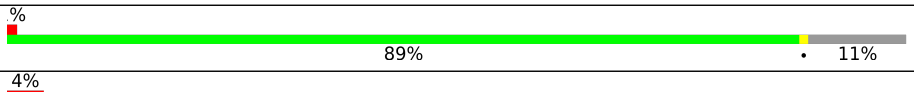
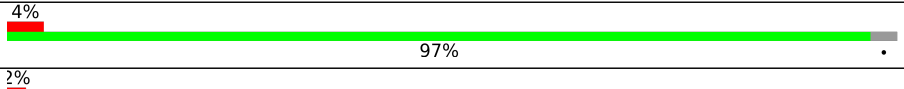
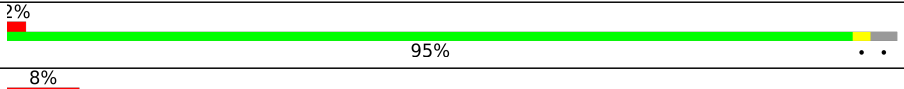
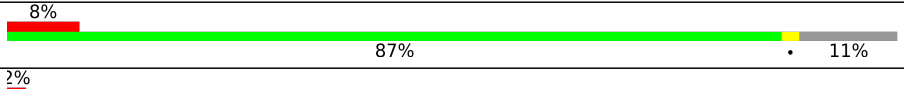
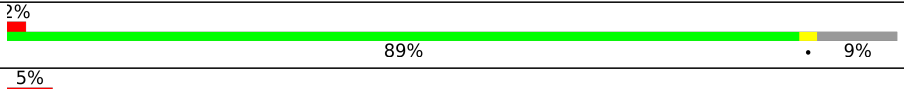
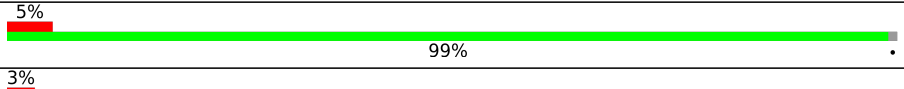
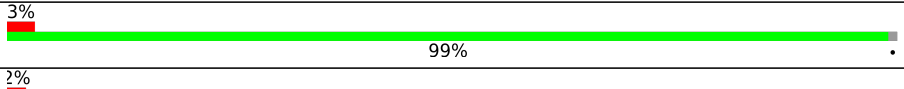
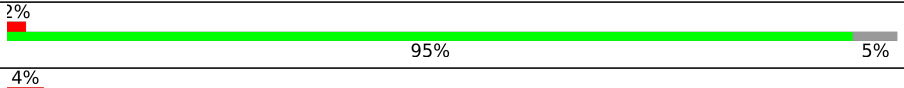
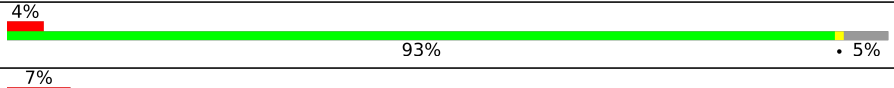
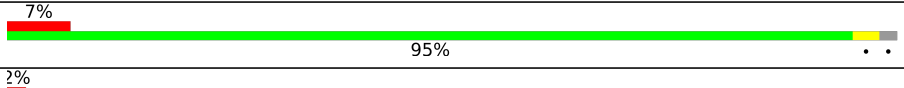
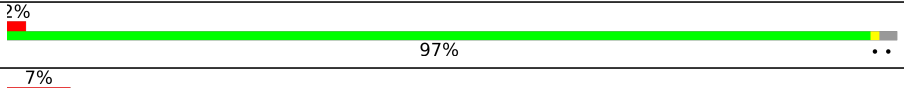
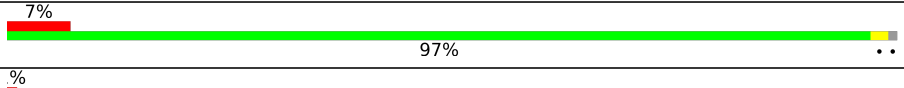
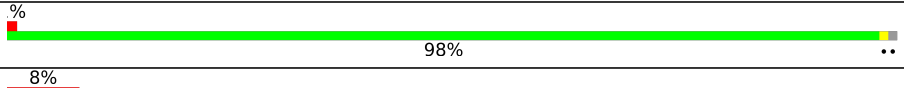
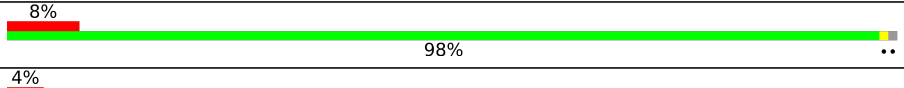
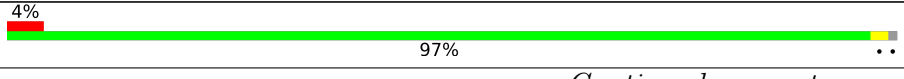
Mol	Chain	Length	Quality of chain
3	AU	158	
4	AW	254	
4	j	254	
5	AX	389	
5	k	389	
6	AY	363	
6	l	363	
7	AZ	298	
7	m	298	
8	BA	176	
8	n	176	
9	BB	241	
9	o	241	
10	BC	262	
10	p	262	
11	BD	191	
11	q	191	
12	BE	220	
12	r	220	
13	BF	174	
13	s	174	
14	BG	202	
14	t	202	
15	BH	131	
15	u	131	

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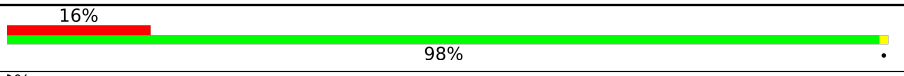
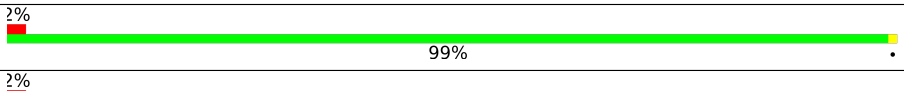
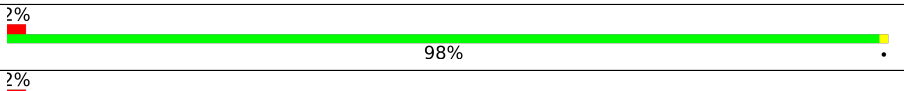
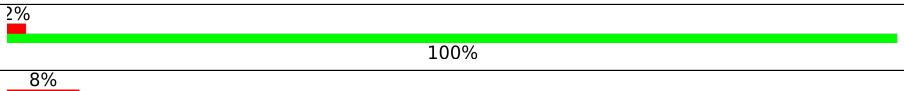
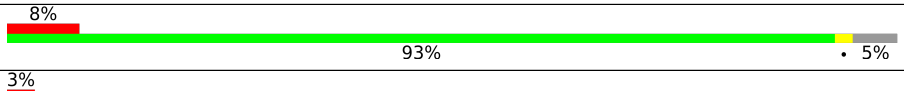
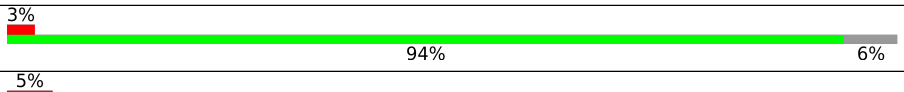
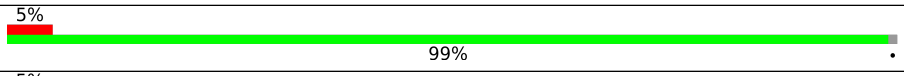
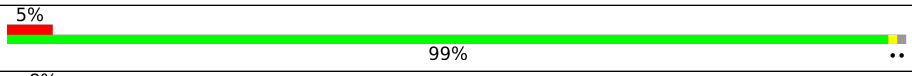
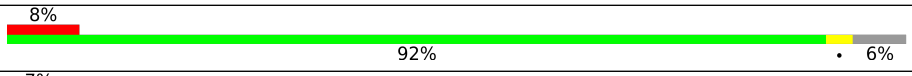
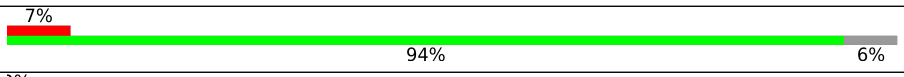
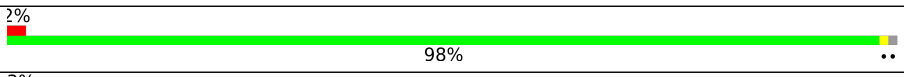
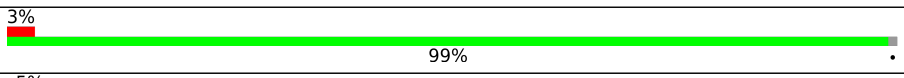
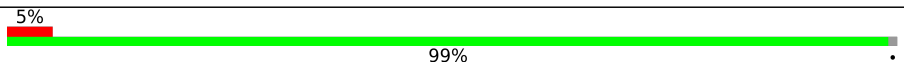
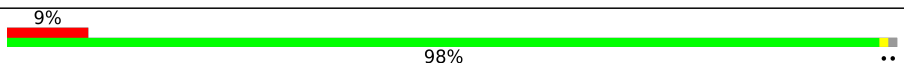
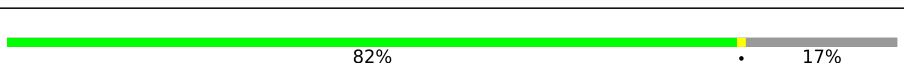
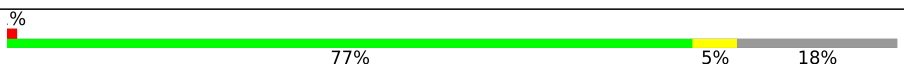
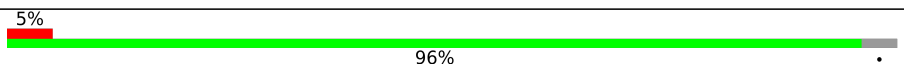
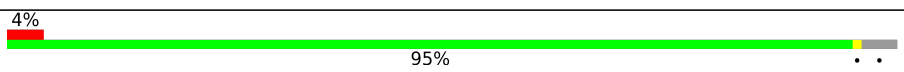
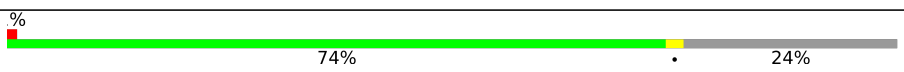
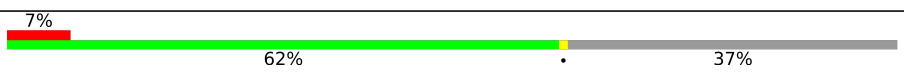
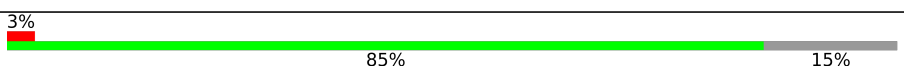
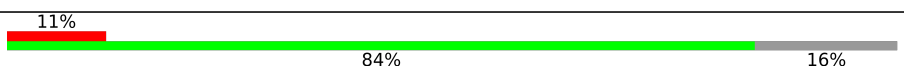
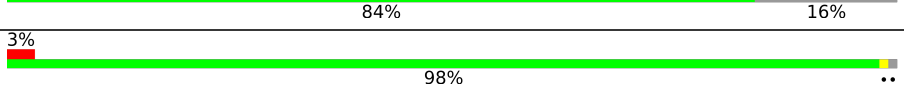
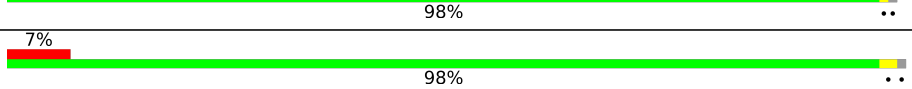
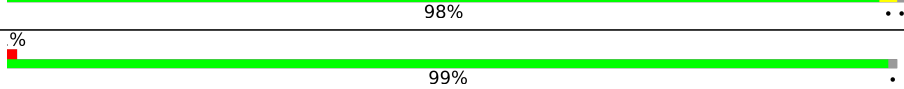
Mol	Chain	Length	Quality of chain
16	BI	204	
16	v	204	
17	BJ	200	
17	w	200	
18	BK	185	
18	x	185	
19	BL	186	
19	y	186	
20	BM	190	
20	z	190	
21	0	172	
21	BN	172	
22	2	160	
22	BO	160	
23	5	124	
23	BP	124	
24	6	137	
24	BQ	137	
25	7	155	
25	BR	155	
26	8	142	
26	BS	142	
27	9	127	
27	BT	127	
28	AA	136	

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Mol	Chain	Length	Quality of chain
28	BU	136	5% 99%
29	AB	149	4% 99%
29	BV	149	12% 99%
30	AC	63	13% 95%
30	BW	63	25% 98%
31	AD	106	2% 90% 9%
31	BX	106	5% 91% 9%
32	AE	112	96%
32	BY	112	4% 96%
33	AF	131	3% 94% 5%
33	BZ	131	8% 95% 5%
34	AG	107	2% 98%
34	CA	107	5% 99%
35	AH	113	5% 99%
35	CB	113	20% 98%
36	AI	120	2% 100%
36	CC	120	14% 98%
37	AJ	99	97%
37	CD	99	18% 97%
38	AK	90	2% 96%
38	CE	90	13% 96%
39	AL	78	4% 99%
39	CF	78	8% 99%
40	AM	51	4% 96%
40	CG	51	20% 98%

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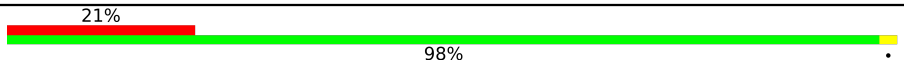
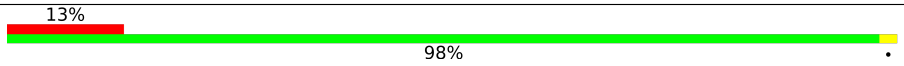
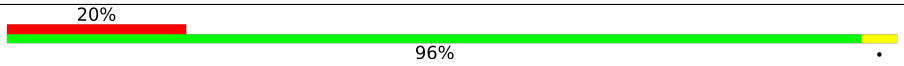
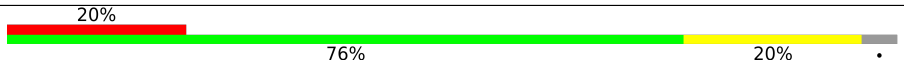
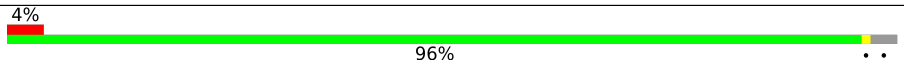
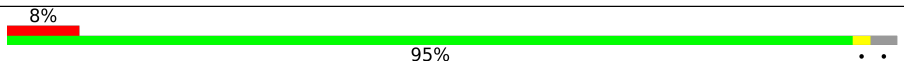
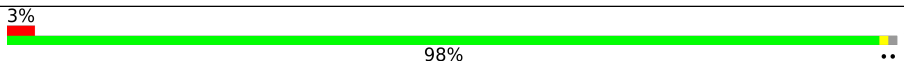
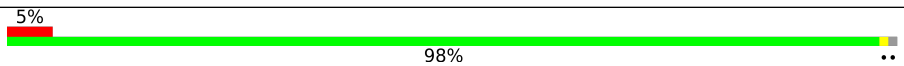
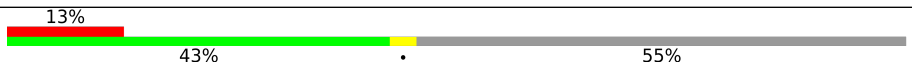
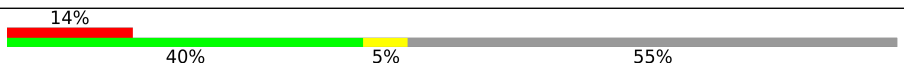
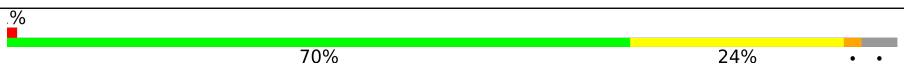
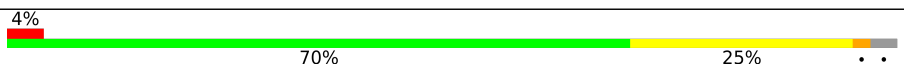
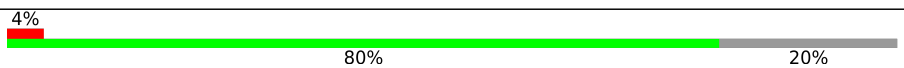
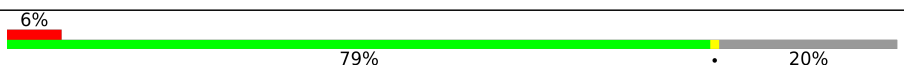
Mol	Chain	Length	Quality of chain
41	AN	52	
41	CH	52	
42	AO	25	
42	CI	25	
43	AP	106	
43	CJ	106	
44	AQ	92	
44	CK	92	
45	CL	267	
45	i	267	
46	B	1787	
46	CM	1787	
47	C	261	
47	CN	261	
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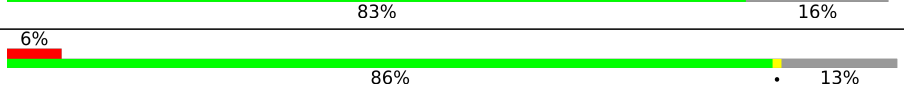
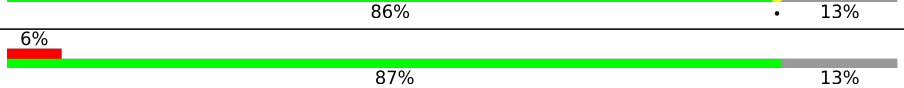
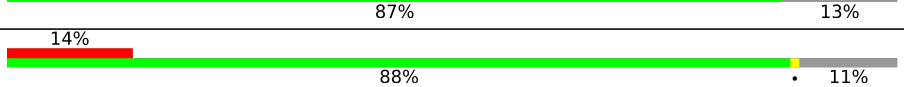
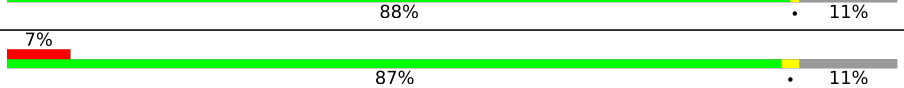
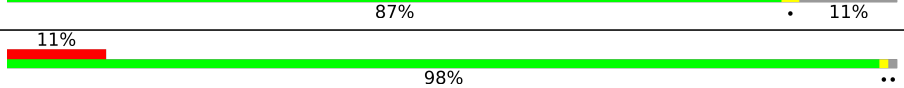
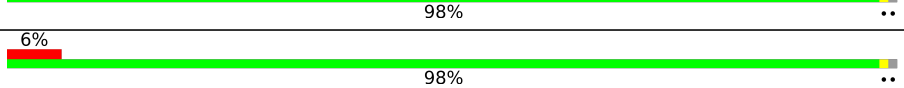
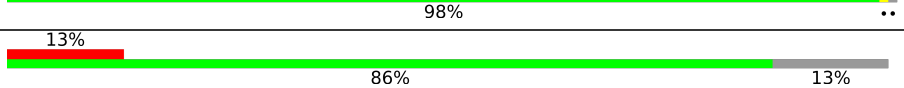
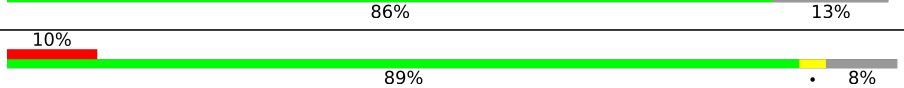
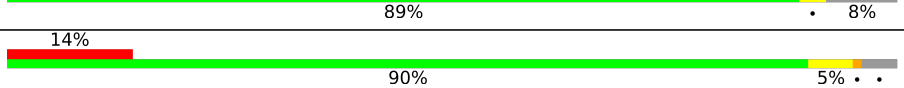
48	D	256	
49	CP	249	
49	E	249	
50	CQ	251	
50	F	251	
51	CR	262	
51	G	262	
52	CS	225	
52	H	225	
53	CT	236	

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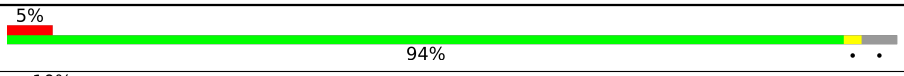
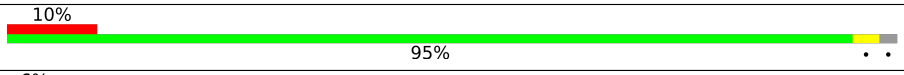
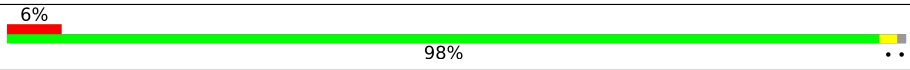
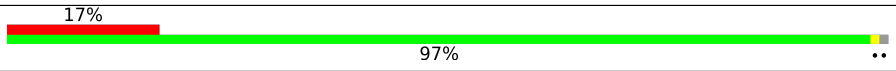
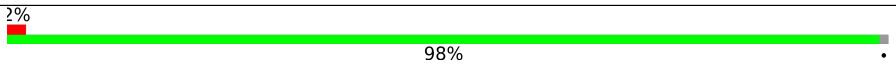
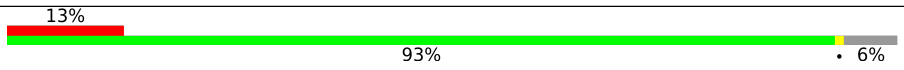
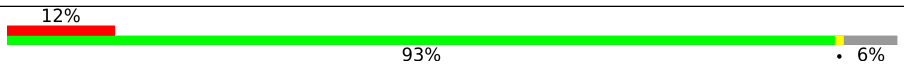
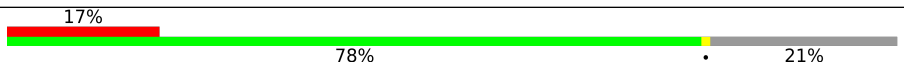
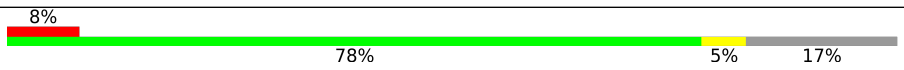
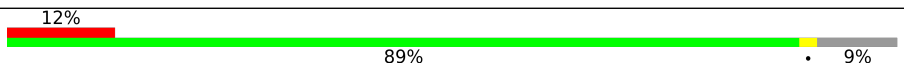
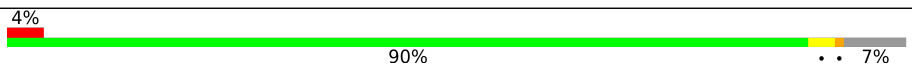
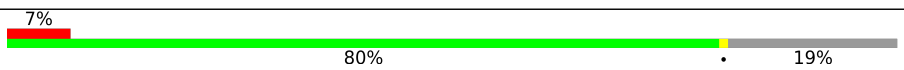
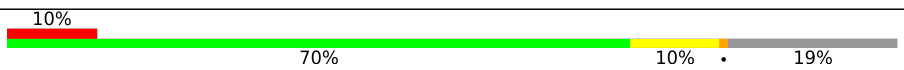
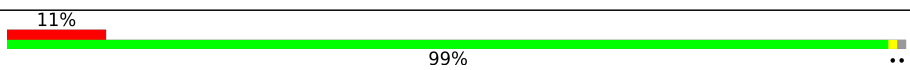
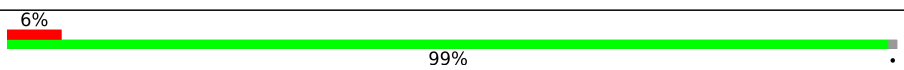
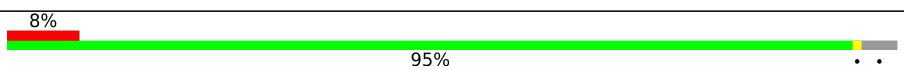
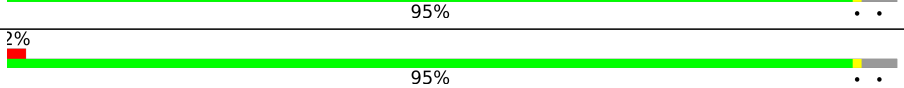
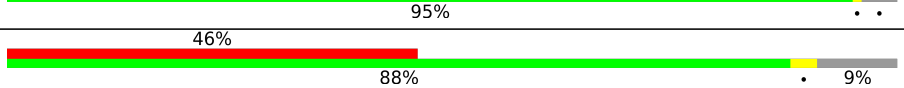
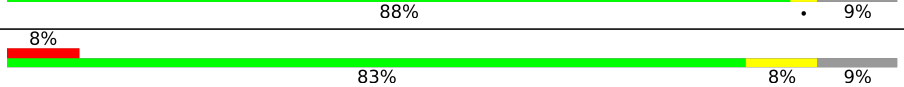
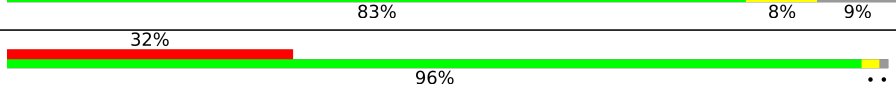
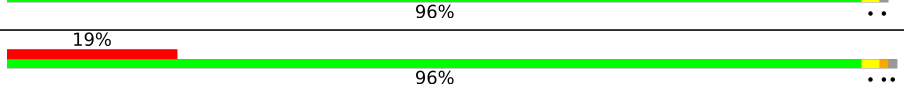
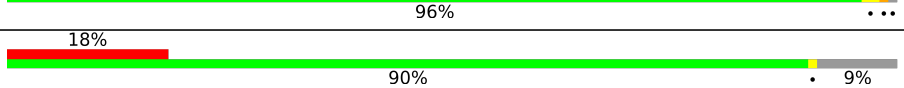
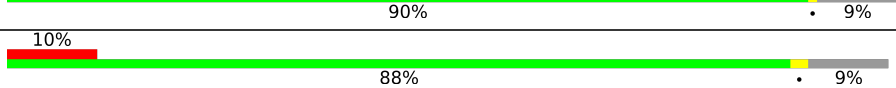
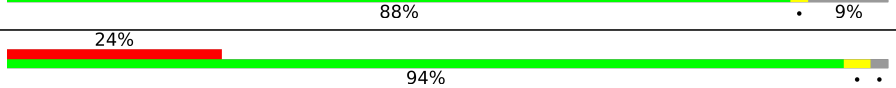
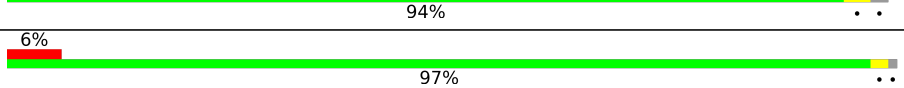
Mol	Chain	Length	Quality of chain
53	I	236	
54	CU	186	
54	J	186	
55	CV	206	
55	K	206	
56	CW	189	
56	L	189	
57	CX	118	
57	M	118	
58	CY	155	
58	N	155	
59	CZ	143	
59	O	143	
60	DA	151	
60	P	151	
61	DB	132	
61	Q	132	
62	DC	142	
62	R	142	
63	DD	142	
63	S	142	
64	DE	137	
64	T	137	
65	DF	145	
65	U	145	

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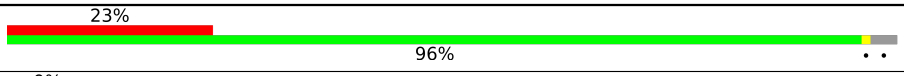
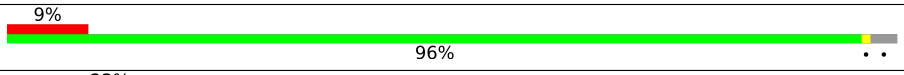
Mol	Chain	Length	Quality of chain
66	DG	145	
66	V	145	
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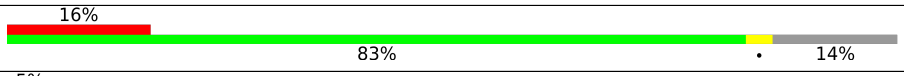
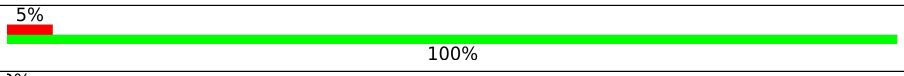
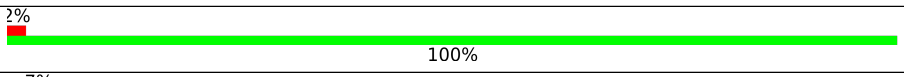
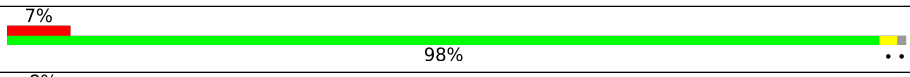
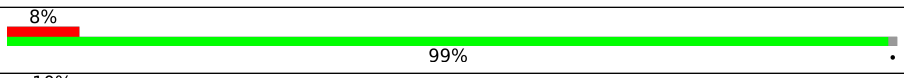
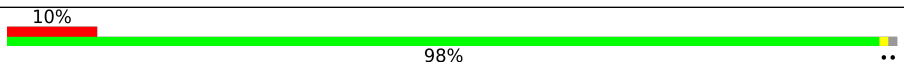
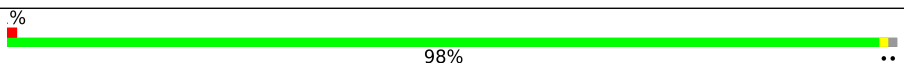
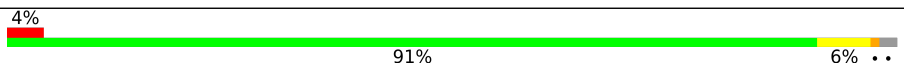
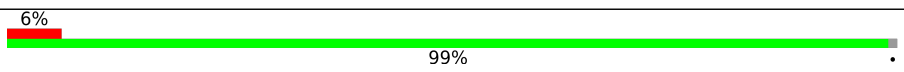
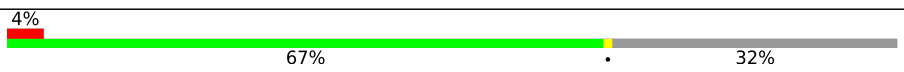
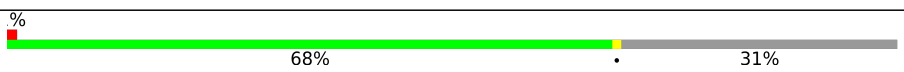
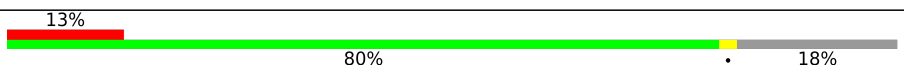
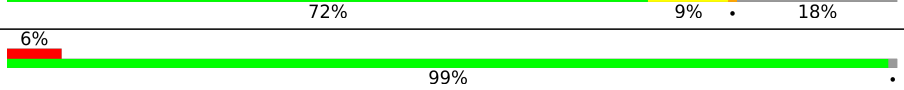
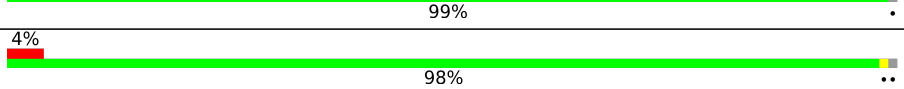
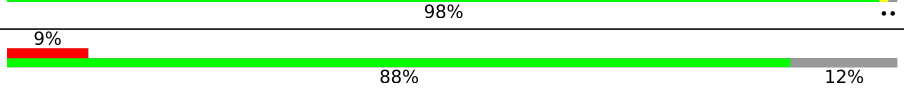
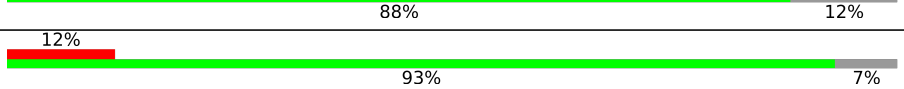
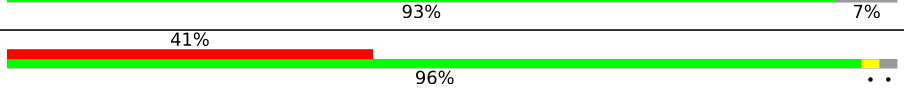
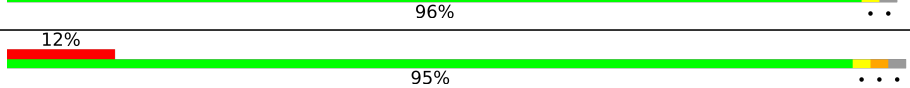
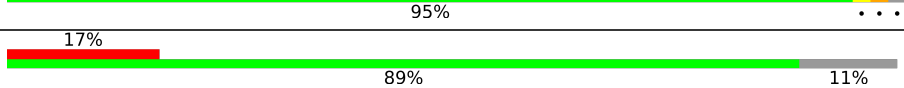
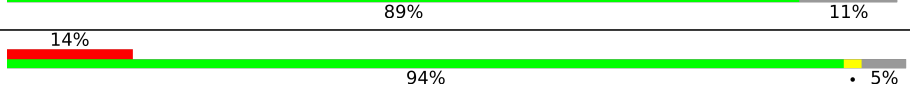
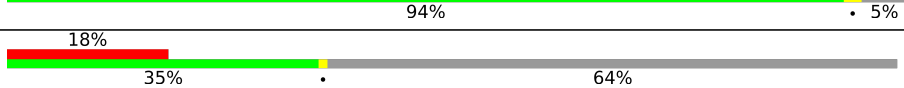
67	W	119	
68	DI	87	
68	X	87	
69	DJ	130	
69	Y	130	
70	DK	145	
70	Z	145	
71	DL	135	
71	a	135	
72	DM	105	
72	b	105	
73	DN	119	
73	c	119	
74	DO	82	
74	d	82	
75	DP	67	
75	e	67	
76	DQ	56	
76	f	56	
77	DR	63	
77	g	63	
78	DS	193	

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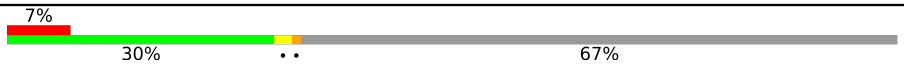
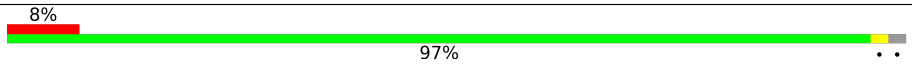
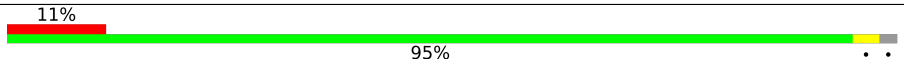
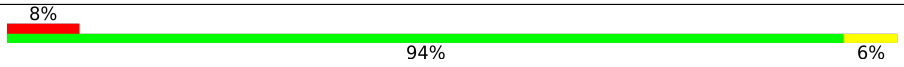
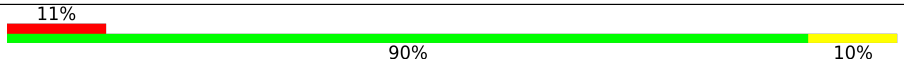
Mol	Chain	Length	Quality of chain
78	h	193	
79	AR	317	
79	DT	317	
80	L1	217	
80	l1	217	

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	0	0	0
			1491	953	269	269			
54	CU	182	Total	C	N	O	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 1711	C 1096	N 294	O 312	S 9	0	0	0
80	l1	217	Total 1711	C 1096	N 294	O 312	S 9	0	0	0

- Molecule 81 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

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

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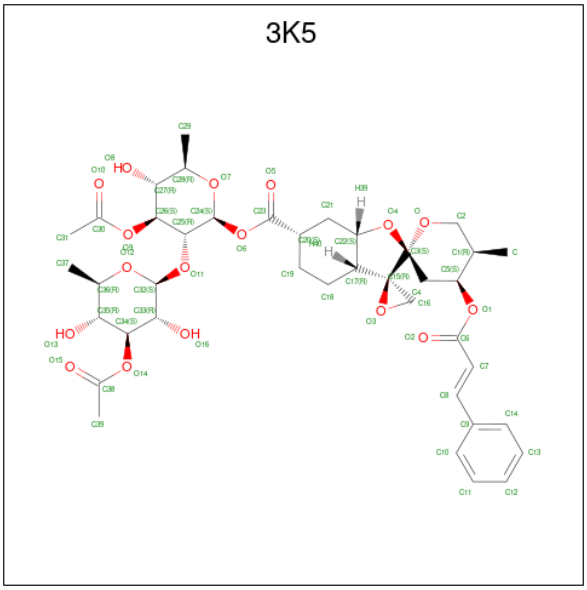
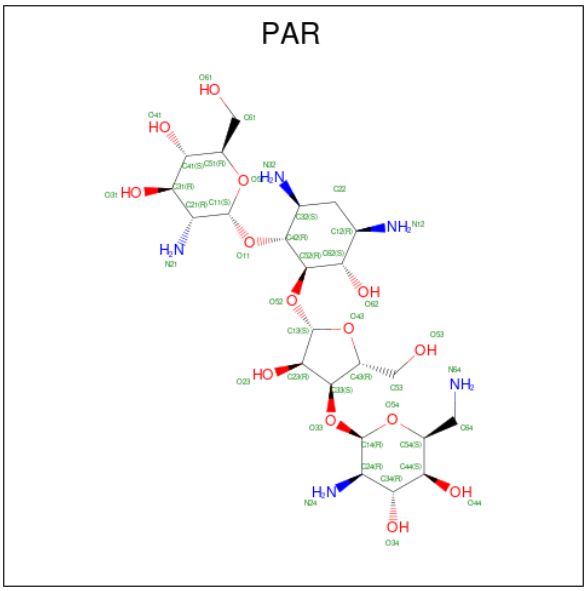
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
81	DQ	1	Total Mg 1 1	0	0
81	CL	3	Total Mg 3 3	0	0

- 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 (three-letter code: 3K5) (formula: $C_{40}H_{52}O_{17}$).



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

- Molecule 83 is PAROMOMYCIN (three-letter code: PAR) (formula: $C_{23}H_{45}N_5O_{14}$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 84 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

- Molecule 85 is water.

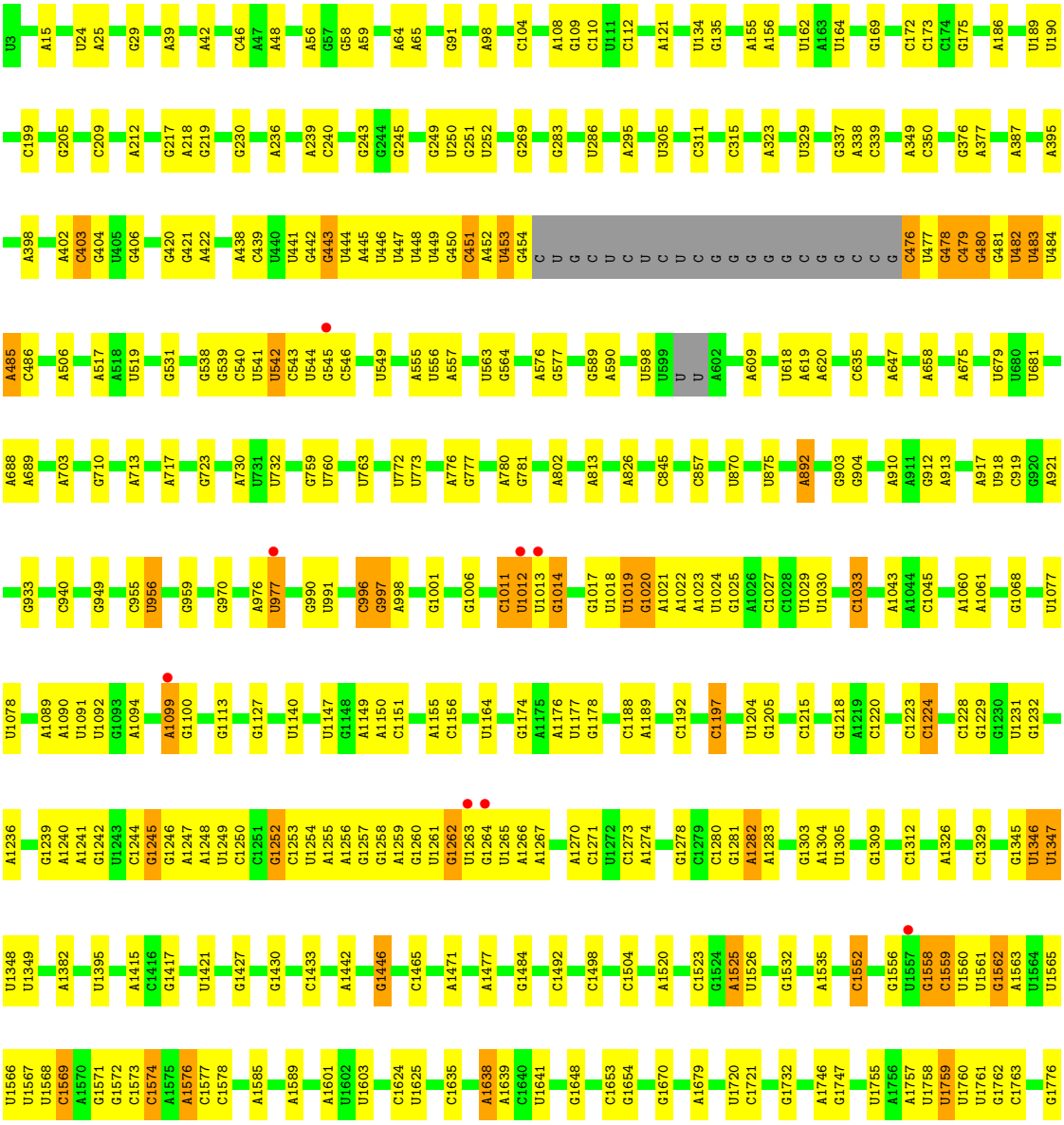
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
85	1	9	Total O 9 9	0	0
85	4	3	Total O 3 3	0	0
85	B	11	Total O 11 11	0	0
85	G	1	Total O 1 1	0	0
85	AS	20	Total O 20 20	0	0
85	BQ	3	Total O 3 3	0	0
85	BV	1	Total O 1 1	0	0

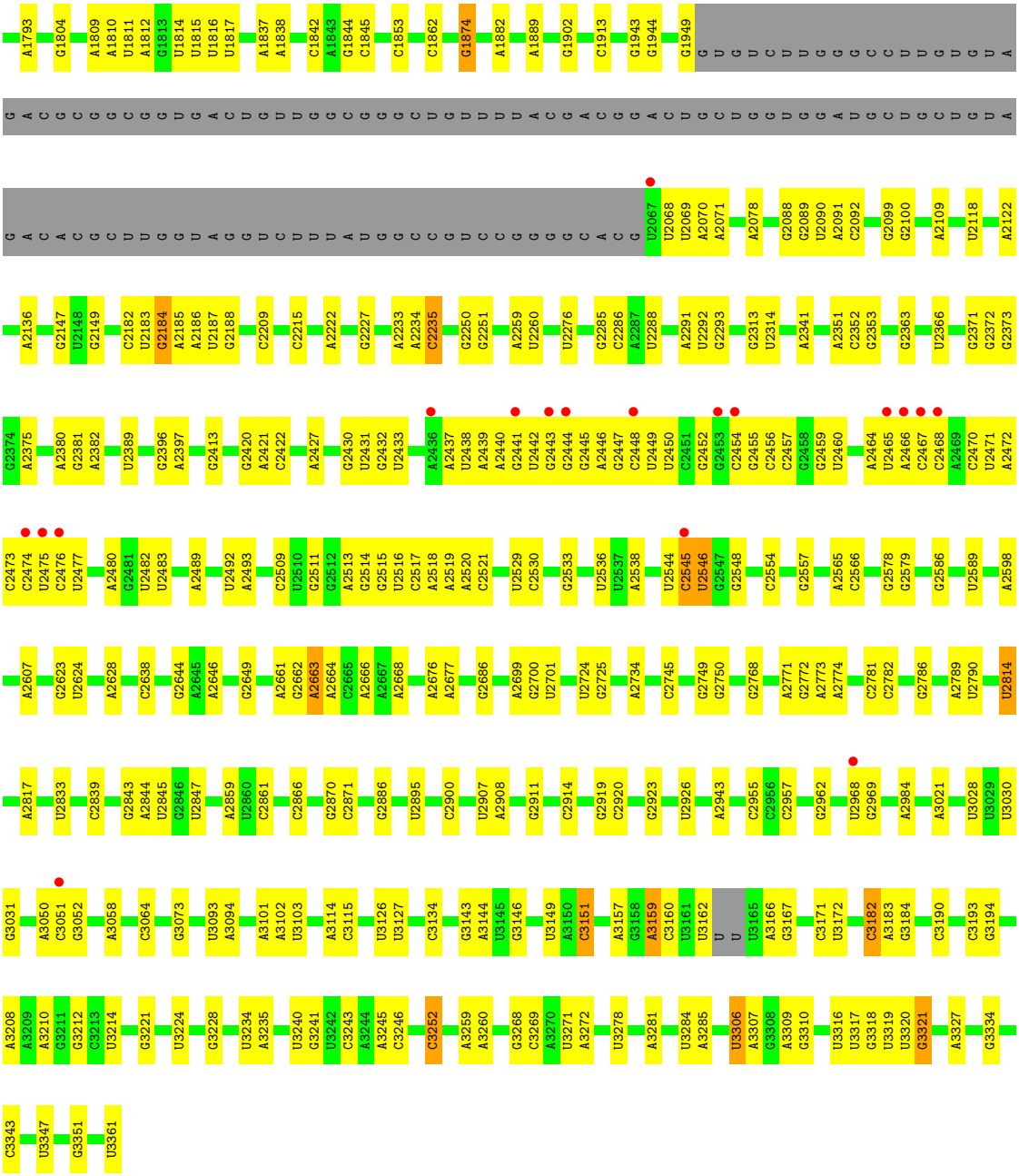
3 Residue-property plots (i)

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

- Molecule 1: 25S ribosomal RNA

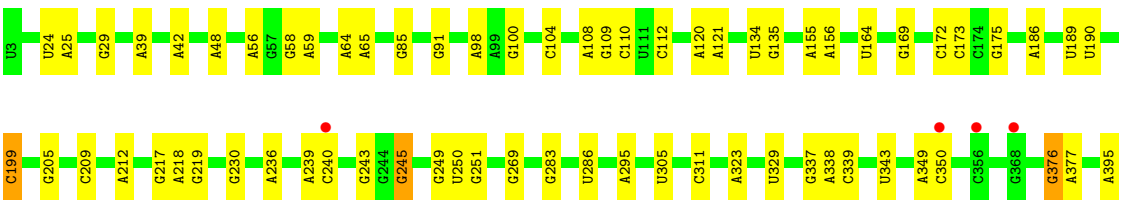
Chain 1:

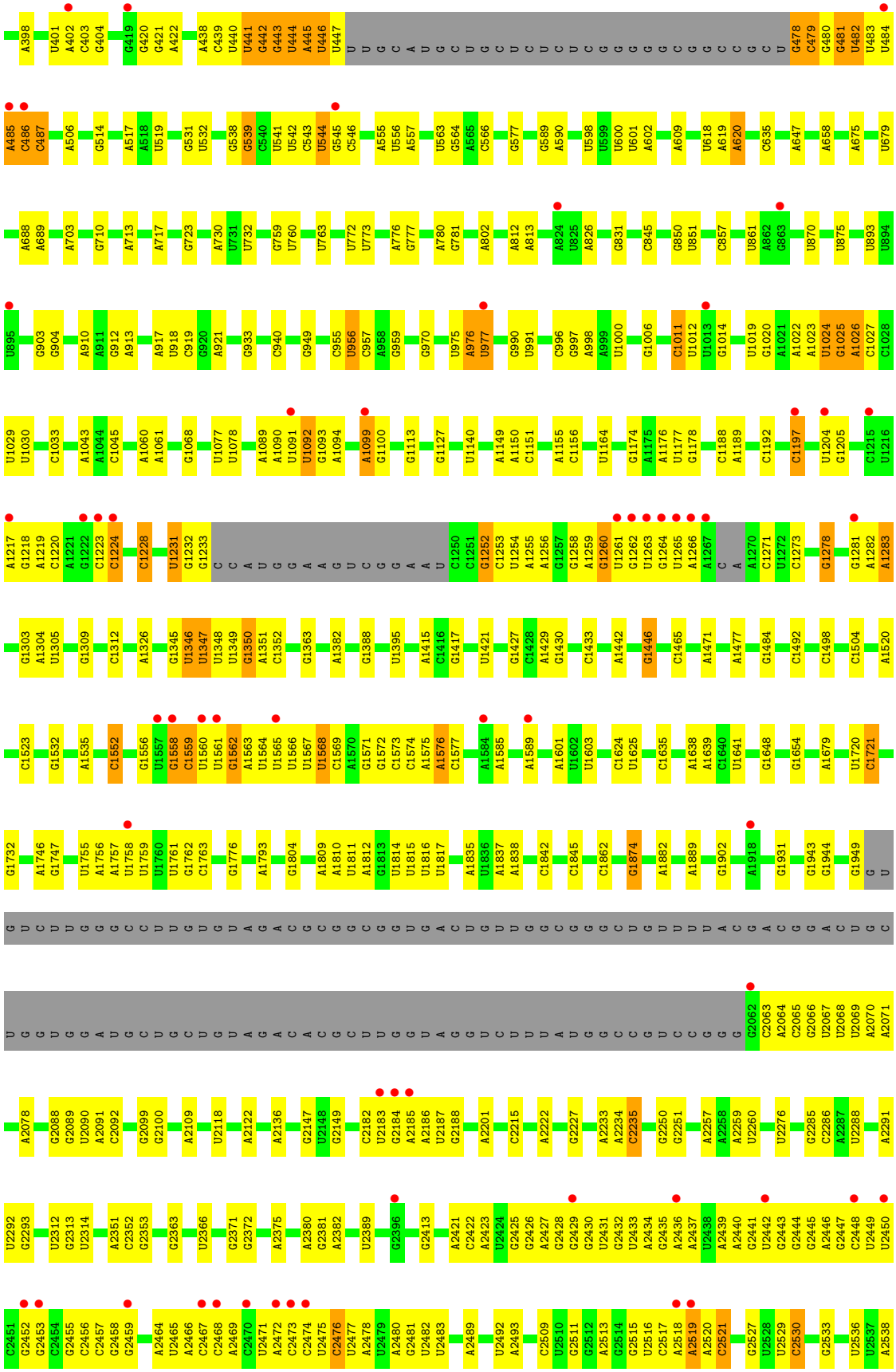


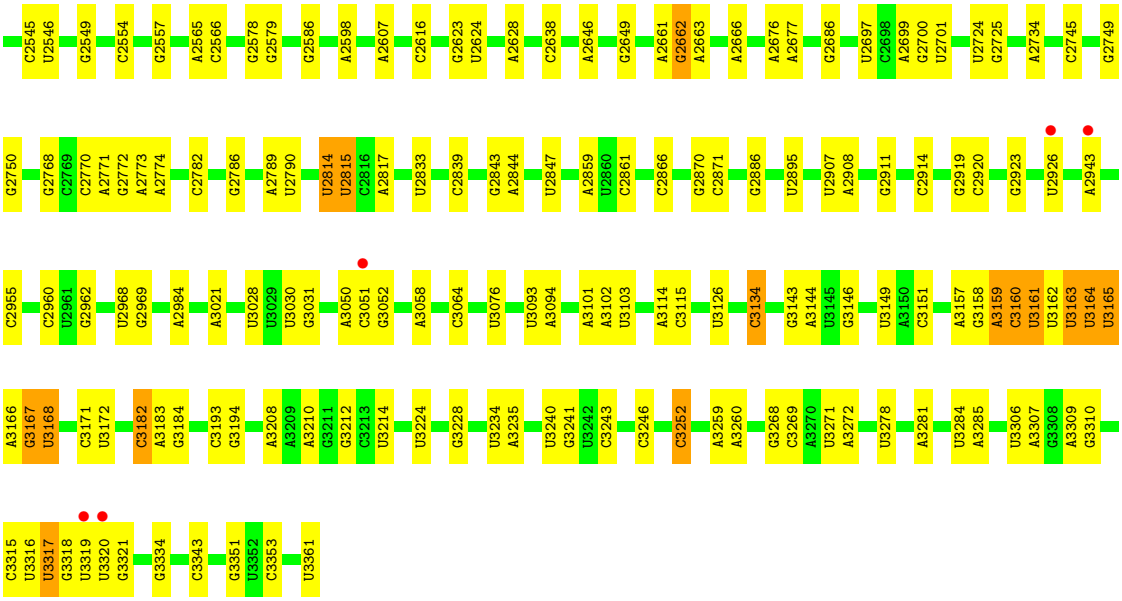


• Molecule 1: 25S ribosomal RNA

Chain AS:





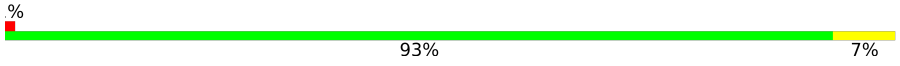


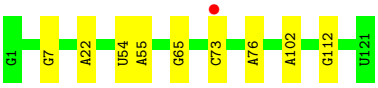
• Molecule 2: 5S ribosomal RNA

Chain 3:

• Molecule 2: 5S ribosomal RNA

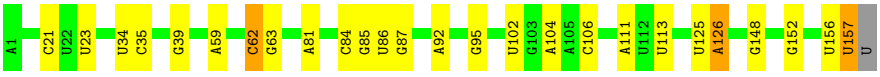
Chain AT:





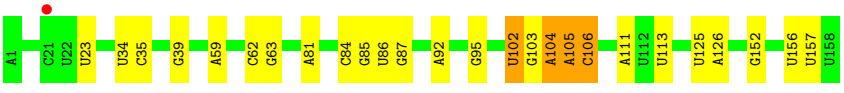
• Molecule 3: 5.8S ribosomal RNA

Chain 4:



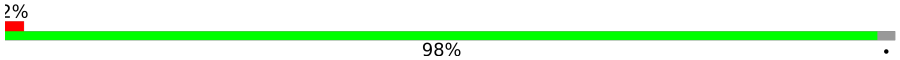
• Molecule 3: 5.8S ribosomal RNA

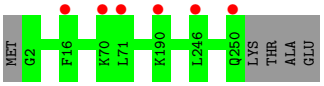
Chain AU:



• Molecule 4: 60S ribosomal protein L2-B

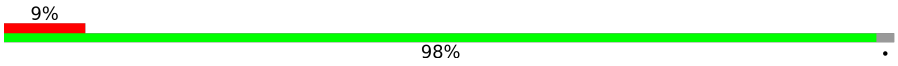
Chain j:

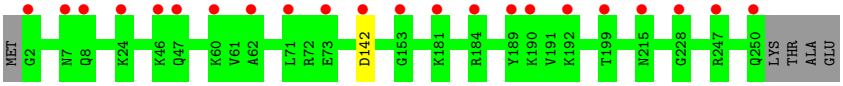




• Molecule 4: 60S ribosomal protein L2-B

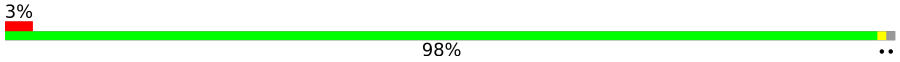
Chain AW:

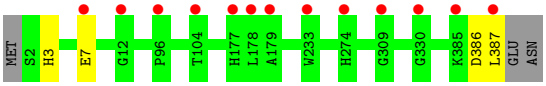




• Molecule 5: 60S ribosomal protein L3

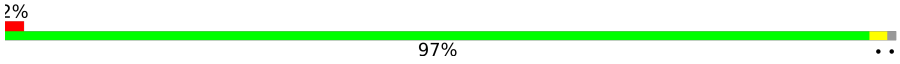
Chain k:

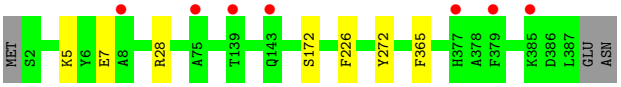




• Molecule 5: 60S ribosomal protein L3

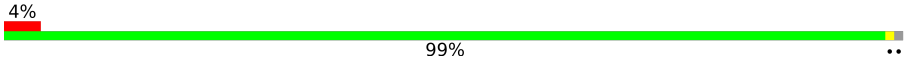
Chain AX:

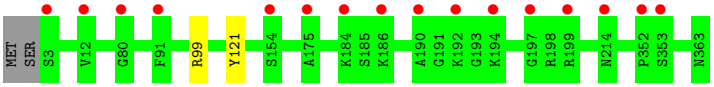




• Molecule 6: 60S ribosomal protein L4-B

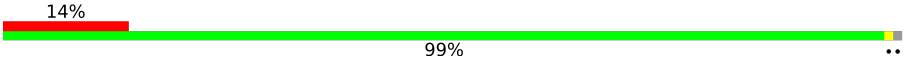
Chain l:

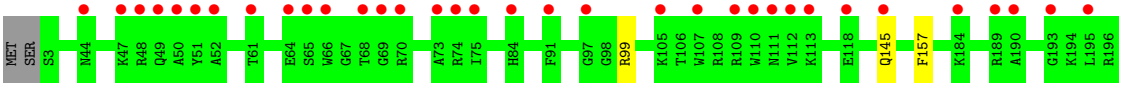


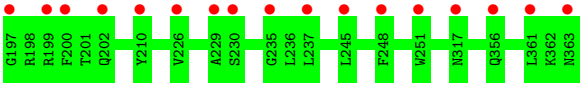


• Molecule 6: 60S ribosomal protein L4-B

Chain AY:

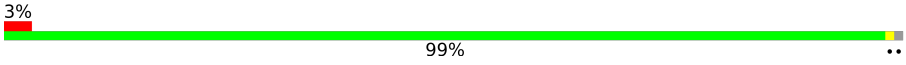


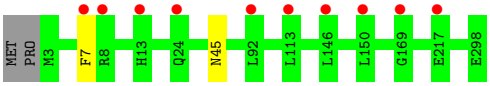




• Molecule 7: Uncharacterized protein CaJ7.0206

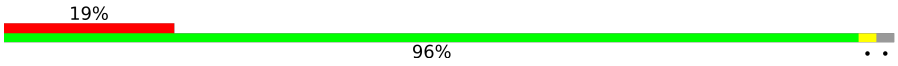
Chain m:

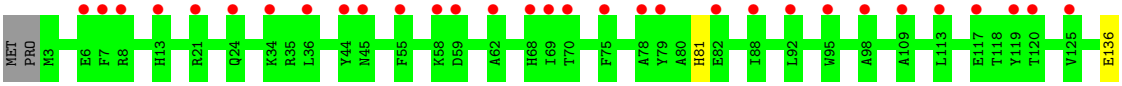


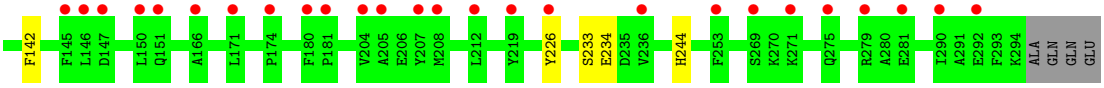


• Molecule 7: Uncharacterized protein CaJ7.0206

Chain AZ:

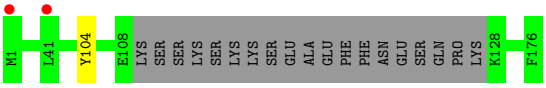






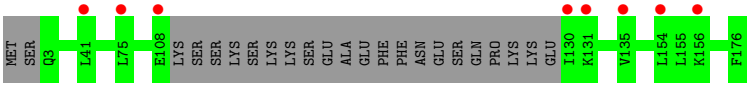
• Molecule 8: 60S ribosomal protein L6

Chain n:



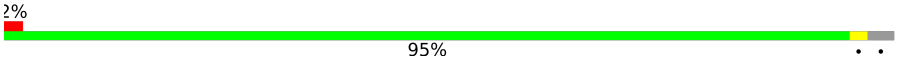
• Molecule 8: 60S ribosomal protein L6

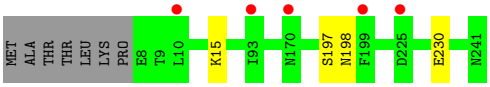
Chain BA:



• Molecule 9: 60S ribosomal protein L7-A

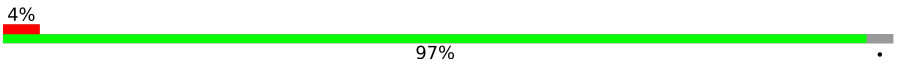
Chain o:

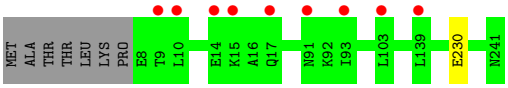




• Molecule 9: 60S ribosomal protein L7-A

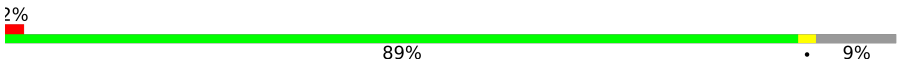
Chain BB:

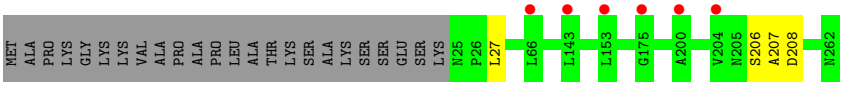




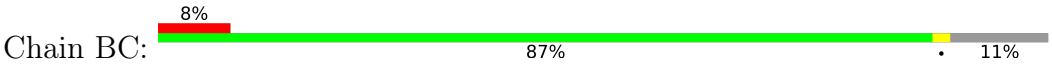
• Molecule 10: 60S ribosomal protein L8

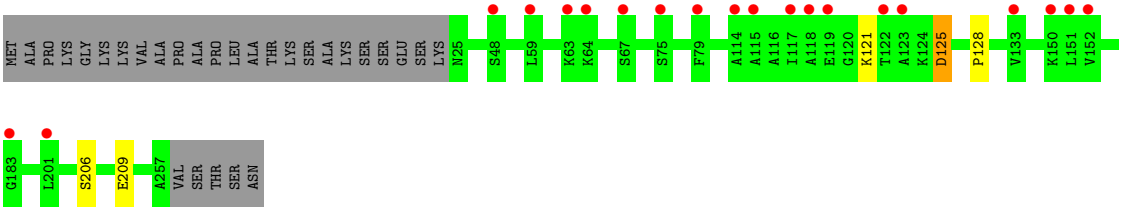
Chain p:



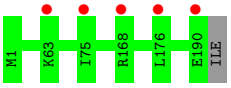


• Molecule 10: 60S ribosomal protein L8

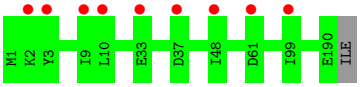




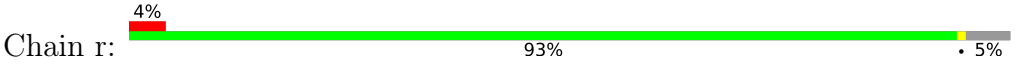
• Molecule 11: 60S ribosomal protein L9-B

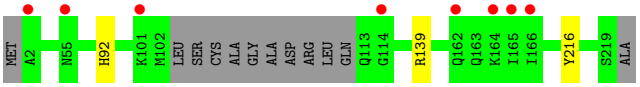


• Molecule 11: 60S ribosomal protein L9-B

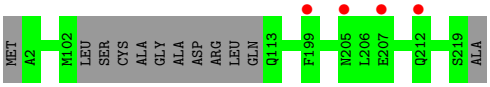


• Molecule 12: 60S ribosomal protein L10

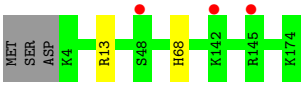




• Molecule 12: 60S ribosomal protein L10

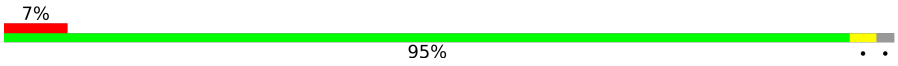


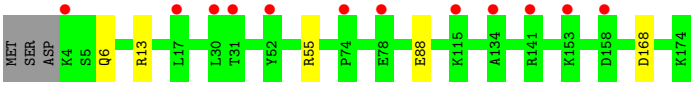
• Molecule 13: 60S ribosomal protein L11-B



• Molecule 13: 60S ribosomal protein L11-B

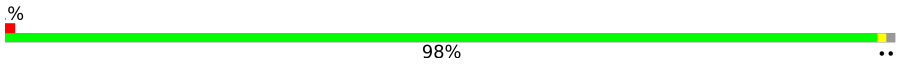
Chain BF:

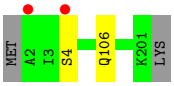




• Molecule 14: 60S ribosomal protein L13

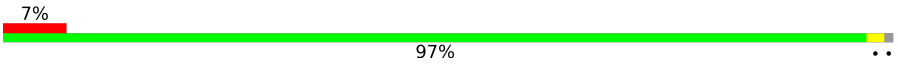
Chain t:

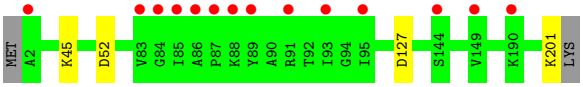




• Molecule 14: 60S ribosomal protein L13

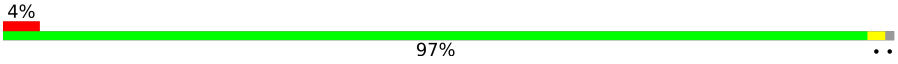
Chain BG:

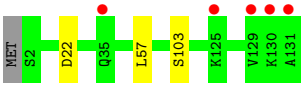




• Molecule 15: 60S ribosomal protein L14-B

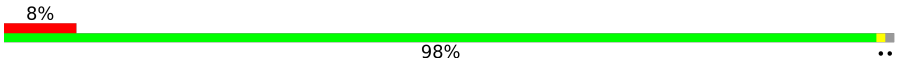
Chain u:

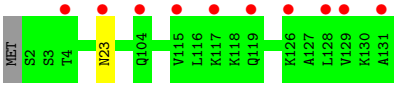




• Molecule 15: 60S ribosomal protein L14-B

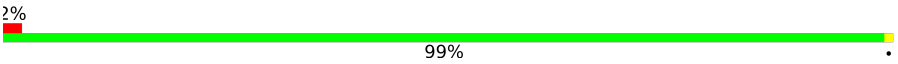
Chain BH:

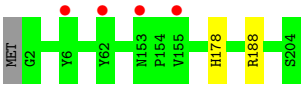




• Molecule 16: 60S ribosomal protein L15-A

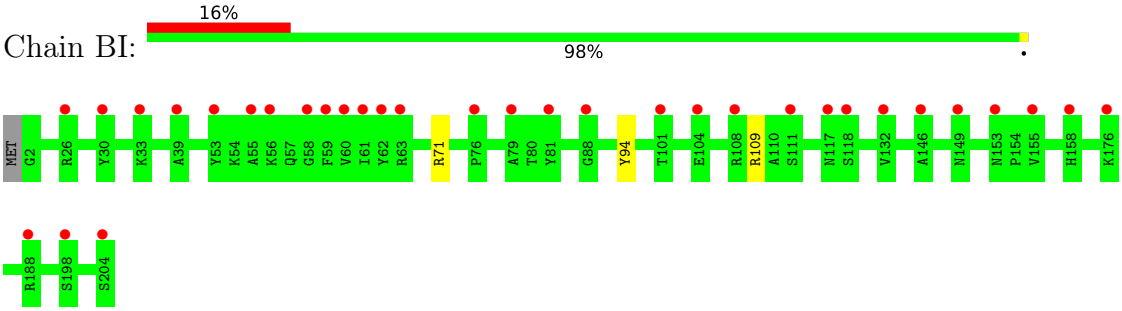
Chain v:





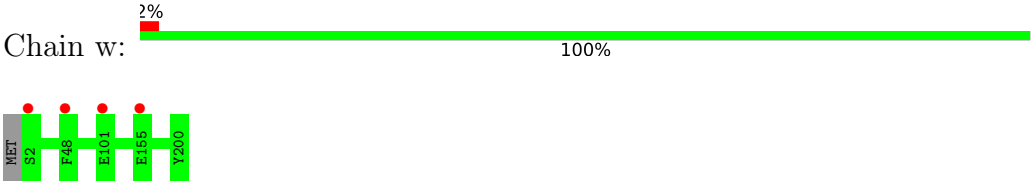
• Molecule 16: 60S ribosomal protein L15-A

Chain BI:



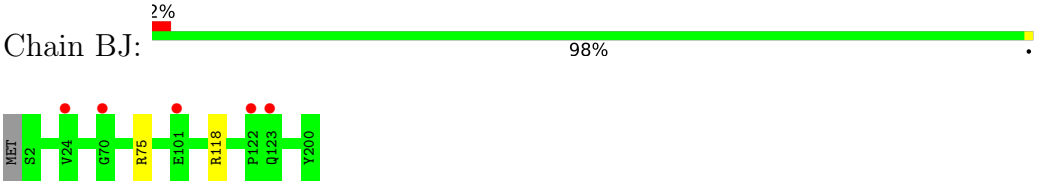
• Molecule 17: Ribosomal protein L13

Chain w:



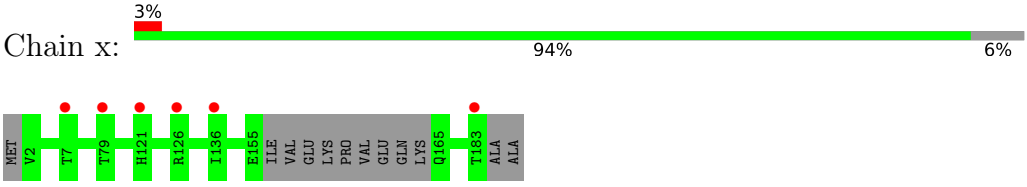
• Molecule 17: Ribosomal protein L13

Chain BJ:



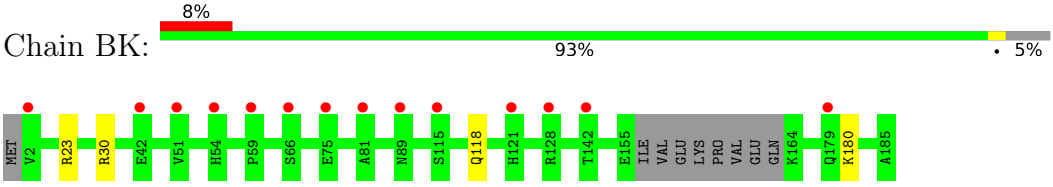
• Molecule 18: Ribosomal protein L22

Chain x:



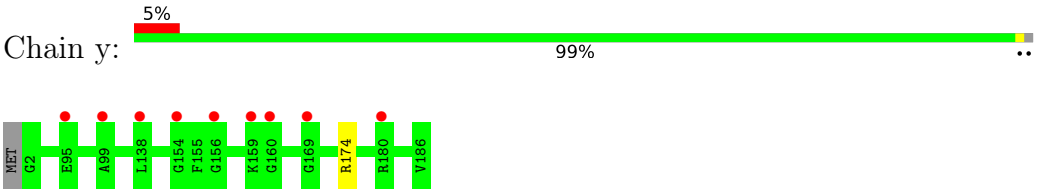
• Molecule 18: Ribosomal protein L22

Chain BK:



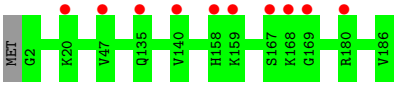
• Molecule 19: 60S ribosomal protein L18-A

Chain y:



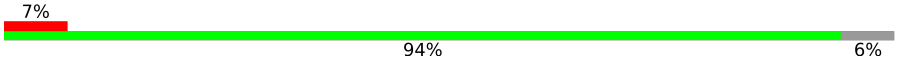
• Molecule 19: 60S ribosomal protein L18-A

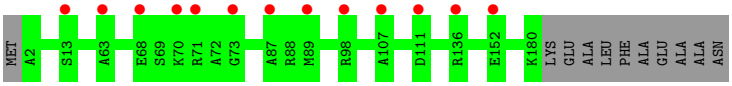
Chain BL:



• Molecule 20: 60S ribosomal protein L19-A

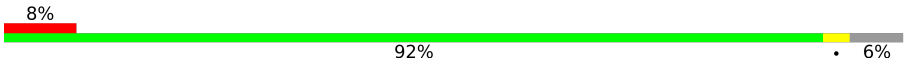
Chain z:

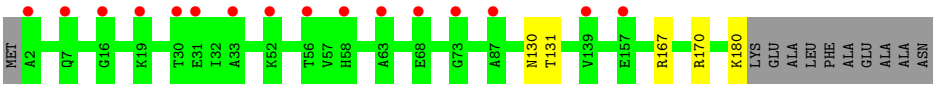




• Molecule 20: 60S ribosomal protein L19-A

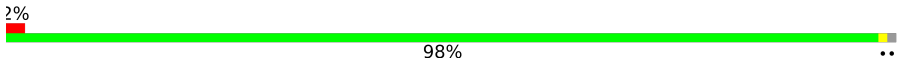
Chain BM:

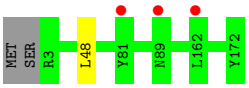




• Molecule 21: 60S ribosomal protein L20

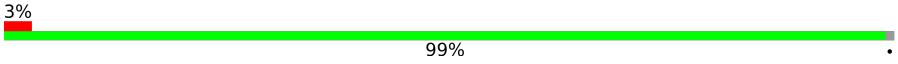
Chain 0:

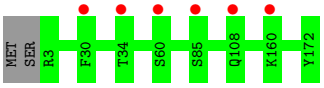




• Molecule 21: 60S ribosomal protein L20

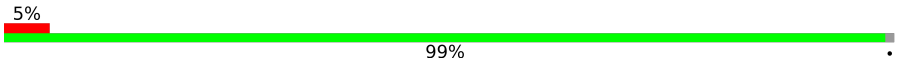
Chain BN:

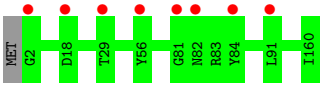




• Molecule 22: 60S ribosomal protein L21-A

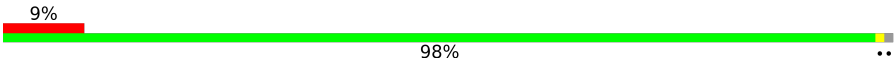
Chain 2:

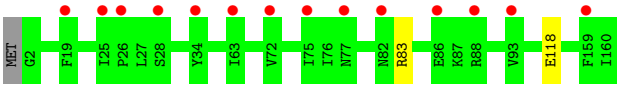




• Molecule 22: 60S ribosomal protein L21-A

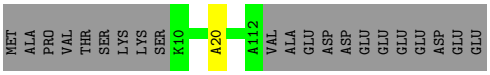
Chain BO:





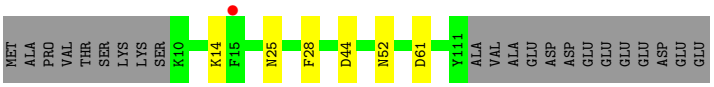
• Molecule 23: 60S ribosomal protein L22-B

Chain 5:



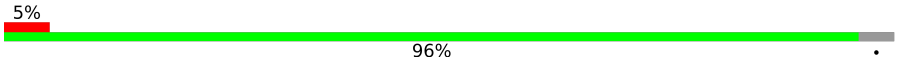
• Molecule 23: 60S ribosomal protein L22-B

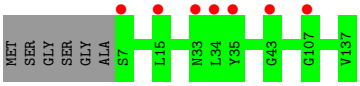
Chain BP:



• Molecule 24: 60S ribosomal protein L23-A

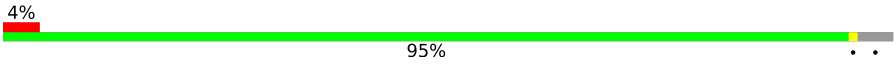
Chain 6:

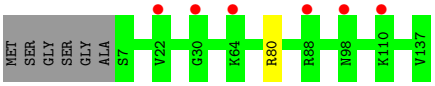




• Molecule 24: 60S ribosomal protein L23-A

Chain BQ:



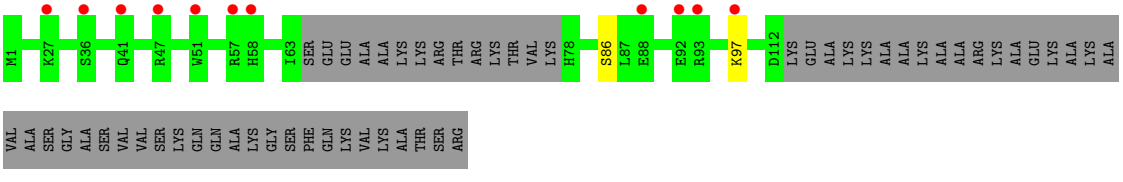


• Molecule 25: 60S ribosomal protein L24-A

Chain 7:

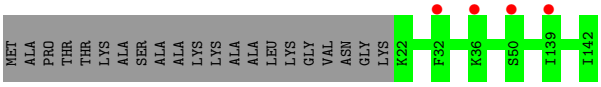
• Molecule 25: 60S ribosomal protein L24-A

Chain BR:

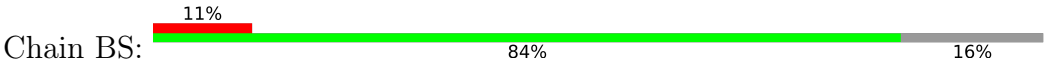


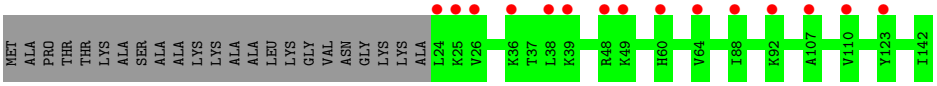
• Molecule 26: 60S ribosomal protein L25

Chain 8:

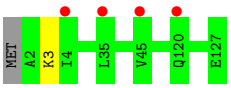


• Molecule 26: 60S ribosomal protein L25

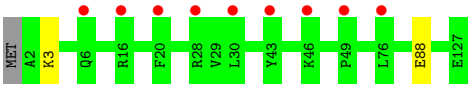




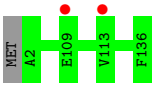
• Molecule 27: Ribosomal protein L24



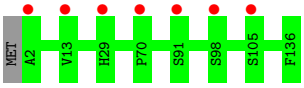
• Molecule 27: Ribosomal protein L24



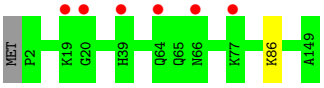
• Molecule 28: 60S ribosomal protein L27



• Molecule 28: 60S ribosomal protein L27

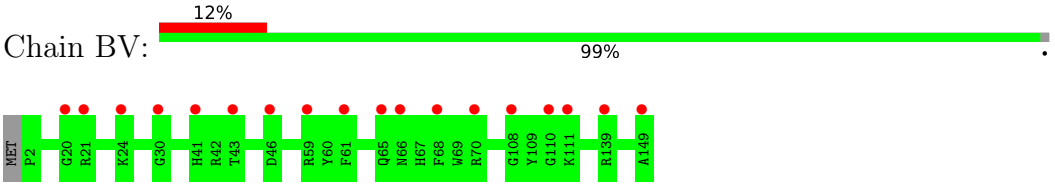


• Molecule 29: 60S ribosomal protein L28



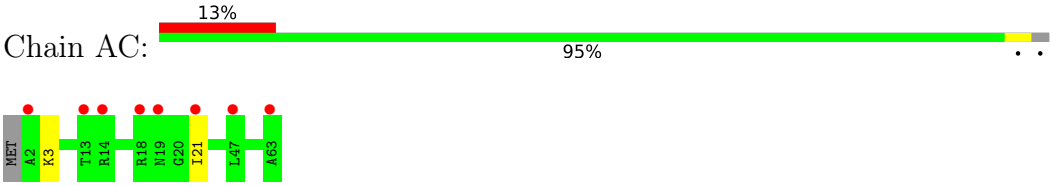
• Molecule 29: 60S ribosomal protein L28

Chain BV:



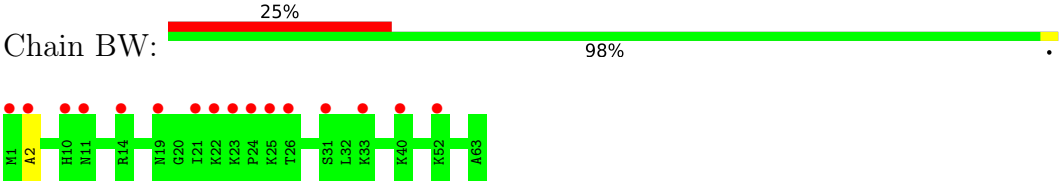
• Molecule 30: 60S ribosomal protein L29

Chain AC:



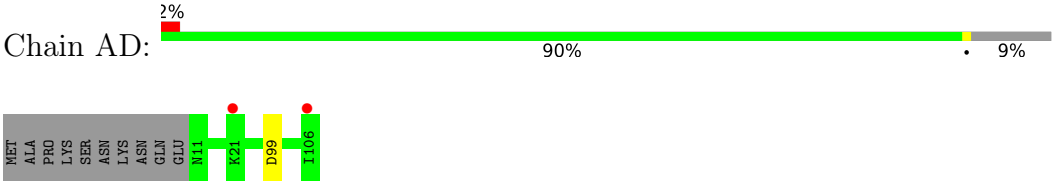
• Molecule 30: 60S ribosomal protein L29

Chain BW:



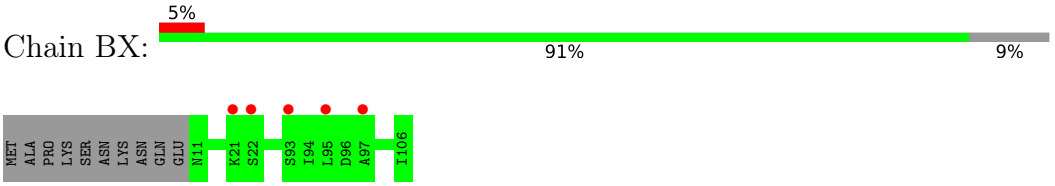
• Molecule 31: 60S ribosomal protein L30

Chain AD:



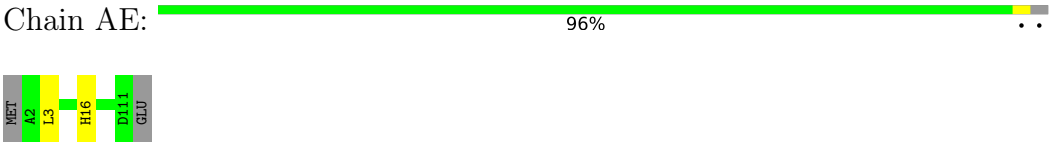
• Molecule 31: 60S ribosomal protein L30

Chain BX:



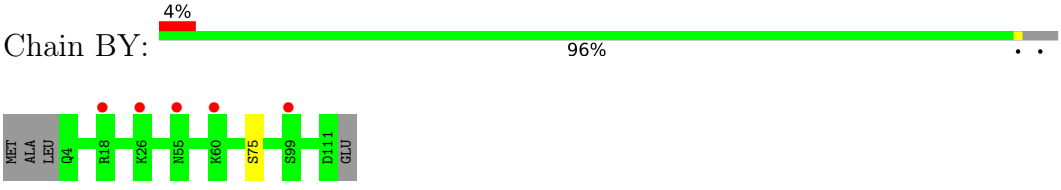
• Molecule 32: 60S ribosomal protein L31-B

Chain AE:



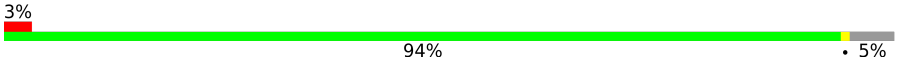
• Molecule 32: 60S ribosomal protein L31-B

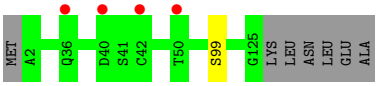
Chain BY:



• Molecule 33: 60S ribosomal protein L32

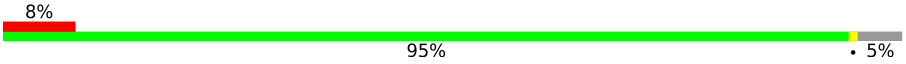
Chain AF:

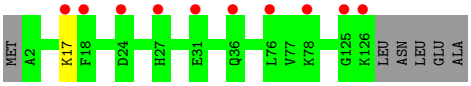




• Molecule 33: 60S ribosomal protein L32

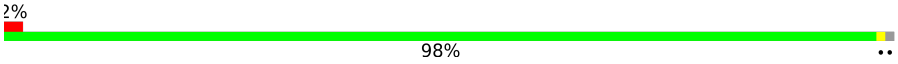
Chain BZ:

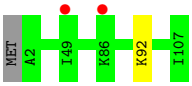




• Molecule 34: 60S ribosomal protein L33-A

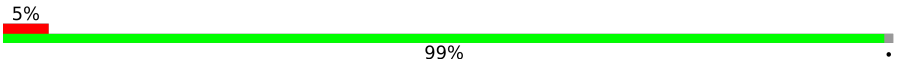
Chain AG:

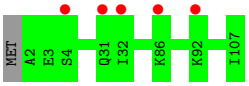




• Molecule 34: 60S ribosomal protein L33-A

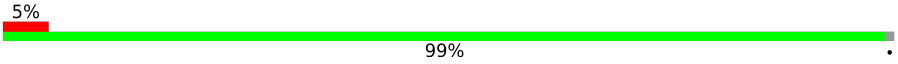
Chain CA:

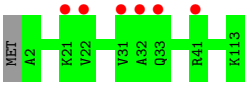




• Molecule 35: 60S ribosomal protein L34-B

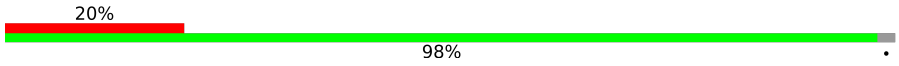
Chain AH:

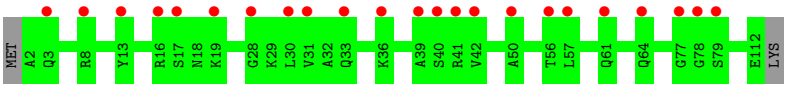




• Molecule 35: 60S ribosomal protein L34-B

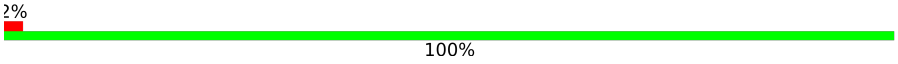
Chain CB:





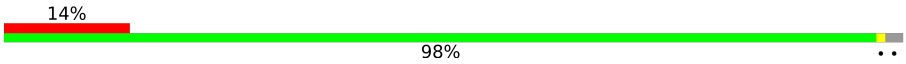
• Molecule 36: Ribosomal protein L29

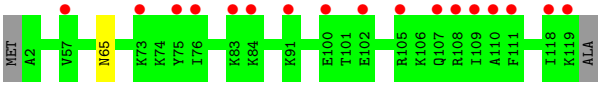
Chain AI:



• Molecule 36: Ribosomal protein L29

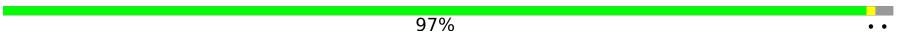
Chain CC:





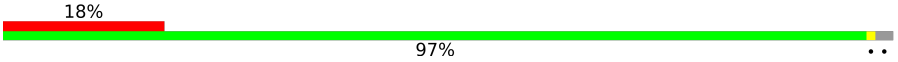
• Molecule 37: 60S ribosomal protein L36

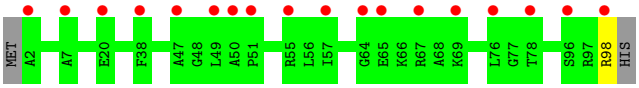
Chain AJ:



• Molecule 37: 60S ribosomal protein L36

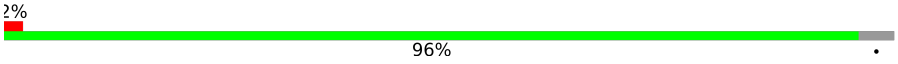
Chain CD:

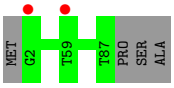




• Molecule 38: 60S ribosomal protein L37-B

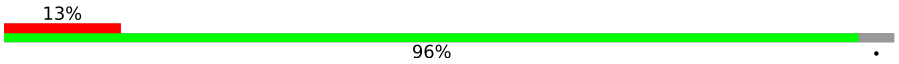
Chain AK:

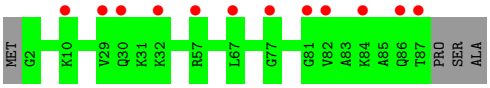




• Molecule 38: 60S ribosomal protein L37-B

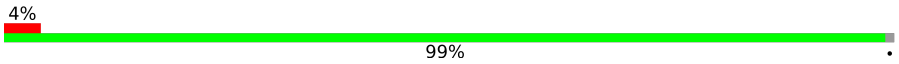
Chain CE:

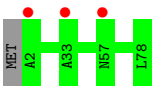




• Molecule 39: 60S ribosomal protein L38

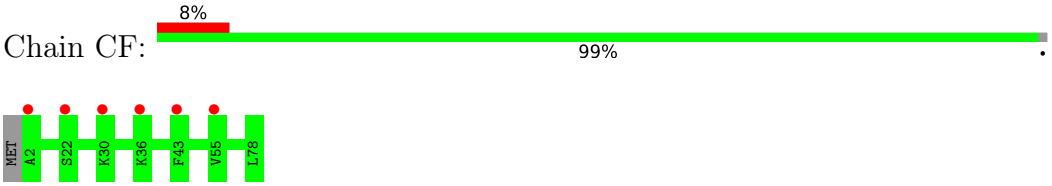
Chain AL:





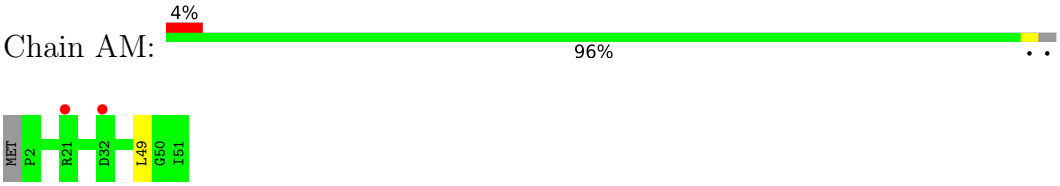
• Molecule 39: 60S ribosomal protein L38

Chain CF:



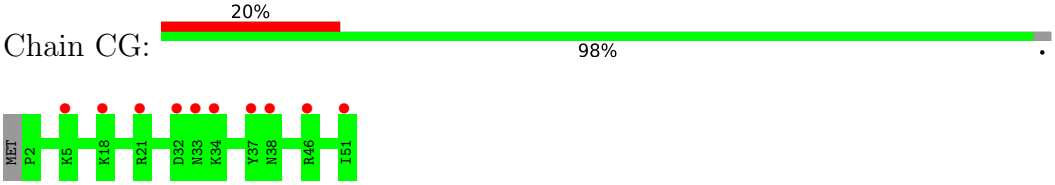
• Molecule 40: 60S ribosomal protein L39

Chain AM:



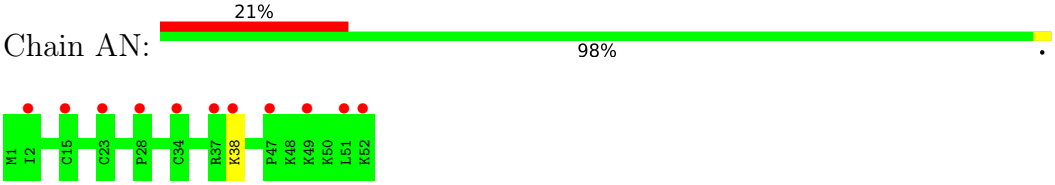
• Molecule 40: 60S ribosomal protein L39

Chain CG:



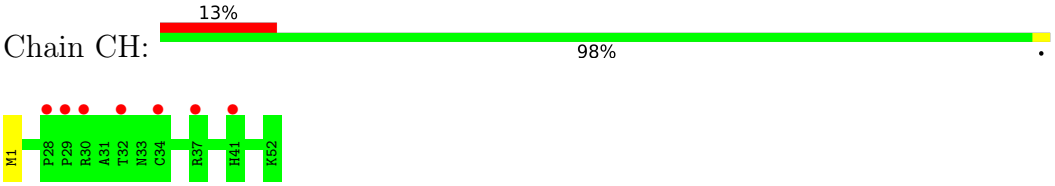
• Molecule 41: 60S ribosomal protein L40-B

Chain AN:



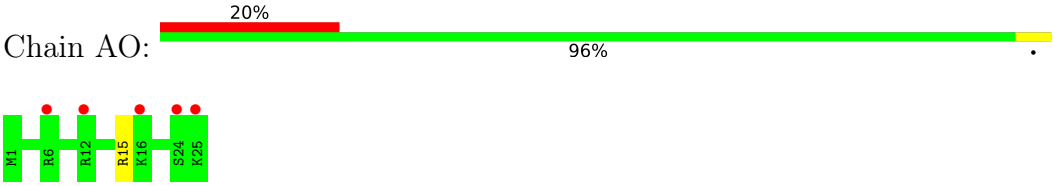
• Molecule 41: 60S ribosomal protein L40-B

Chain CH:



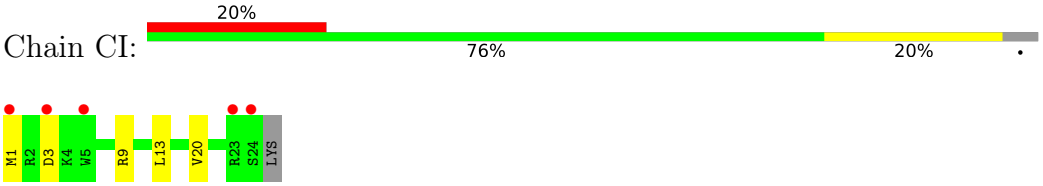
• Molecule 42: 60S ribosomal protein L41

Chain AO:



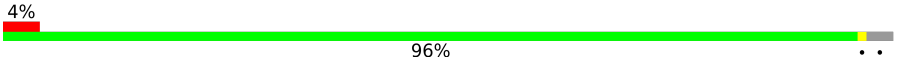
• Molecule 42: 60S ribosomal protein L41

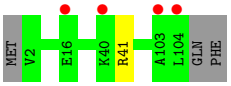
Chain CI:



• Molecule 43: 60S ribosomal protein L42-B

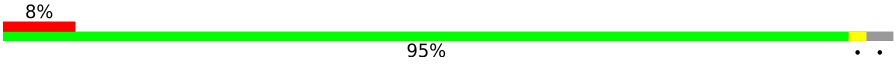
Chain AP:

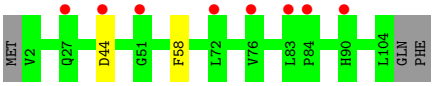




• Molecule 43: 60S ribosomal protein L42-B

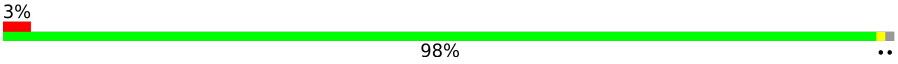
Chain CJ:

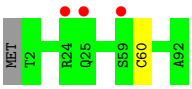




• Molecule 44: 60S ribosomal protein L43-A

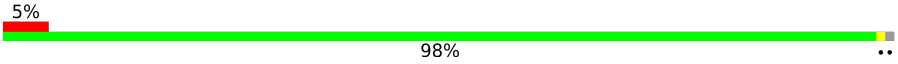
Chain AQ:

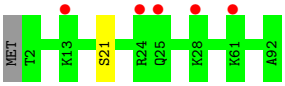




• Molecule 44: 60S ribosomal protein L43-A

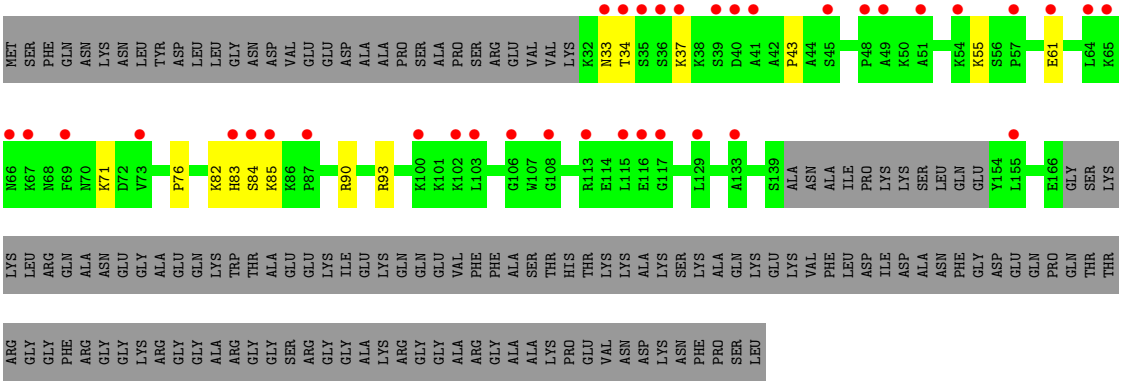
Chain CK:





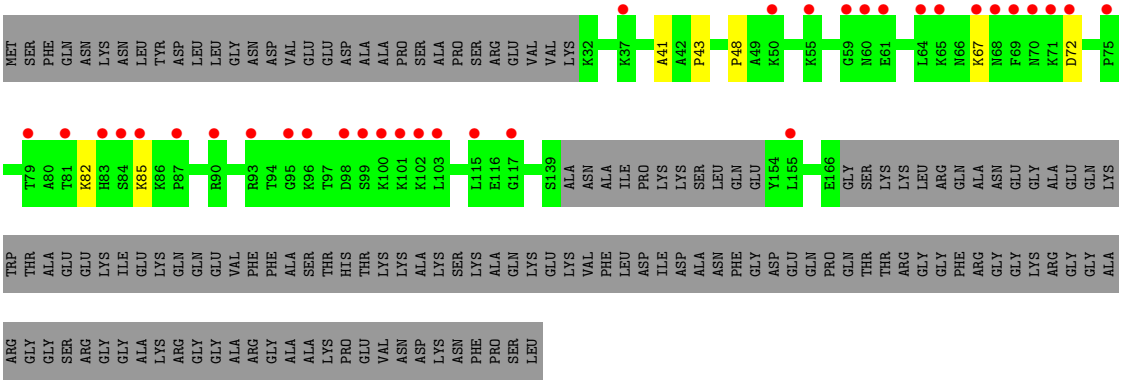
• Molecule 45: 60S ribosomal protein CAALFM_C304810CA

Chain i:



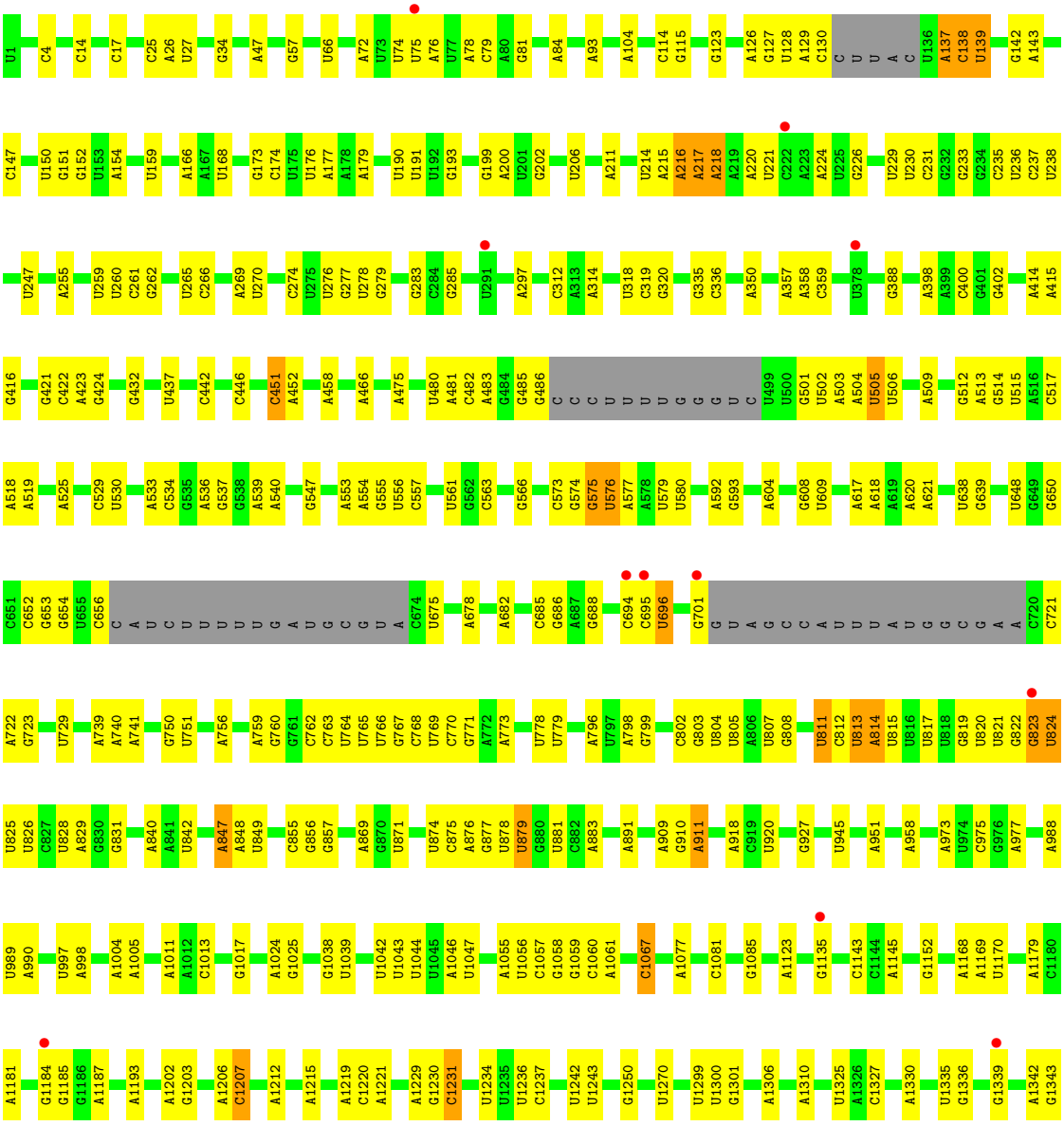
• Molecule 45: 60S ribosomal protein CAALFM_C304810CA

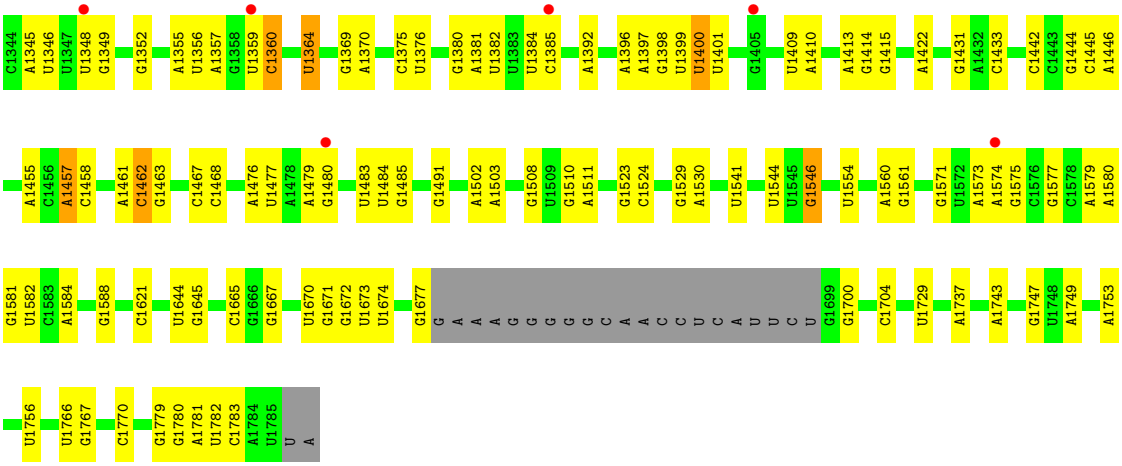
Chain CL:



• Molecule 46: 18S ribosomal RNA

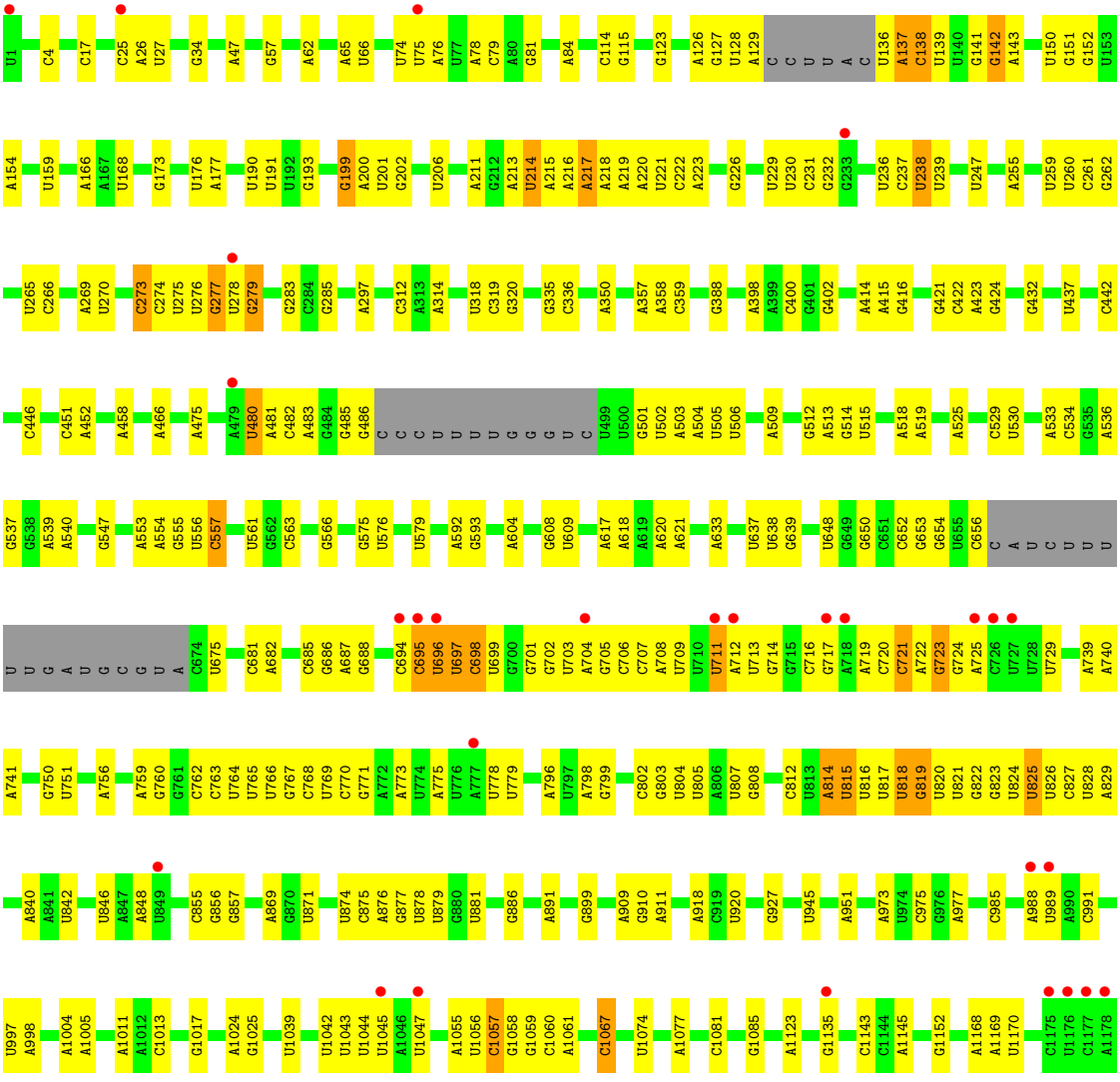
Chain B:

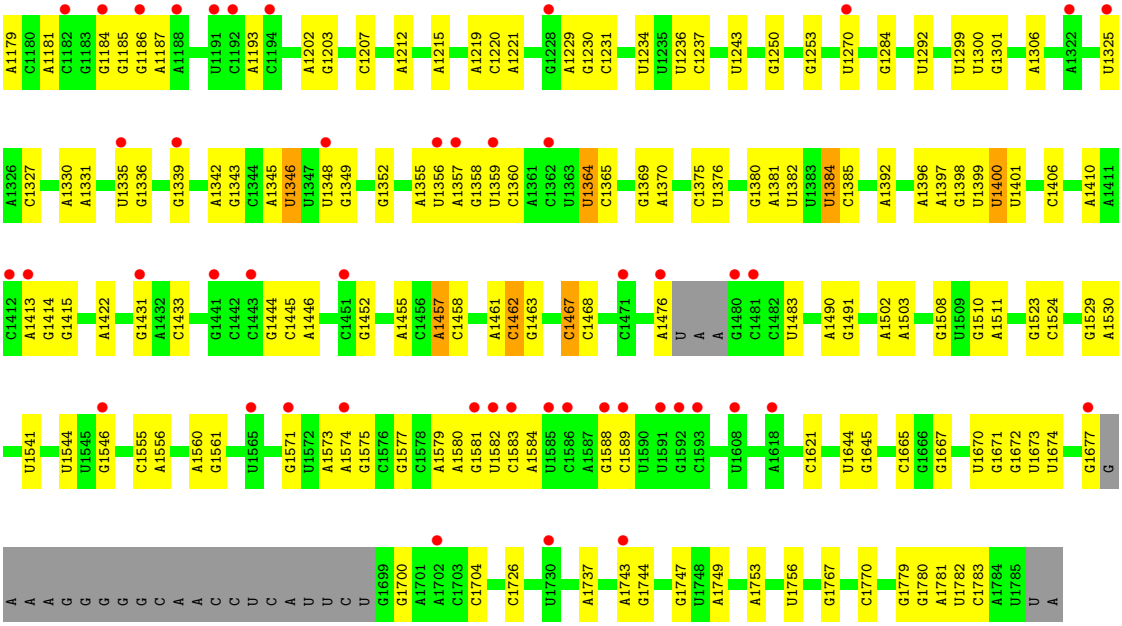




• Molecule 46: 18S ribosomal RNA

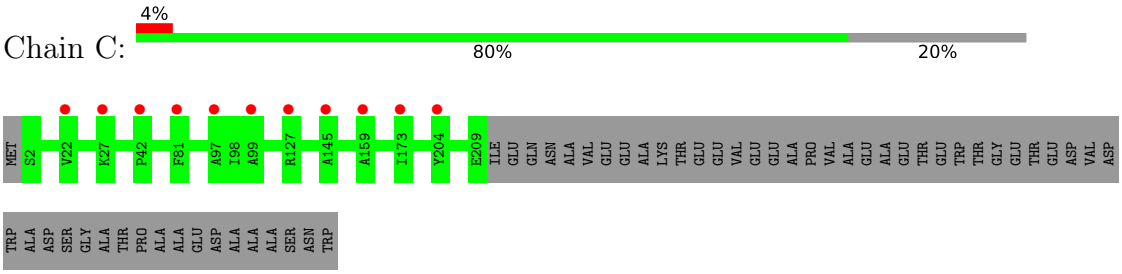
Chain CM:





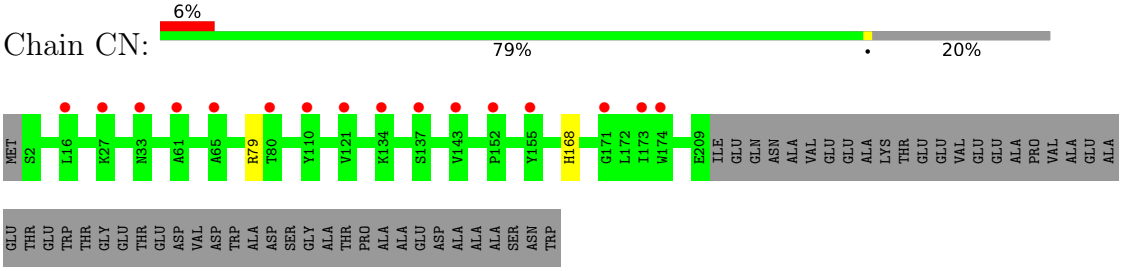
• Molecule 47: 40S ribosomal protein S0

Chain C:



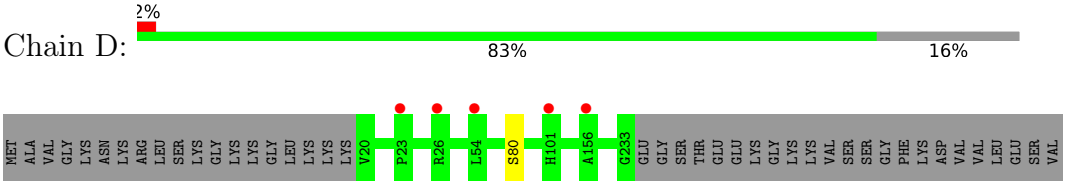
• Molecule 47: 40S ribosomal protein S0

Chain CN:



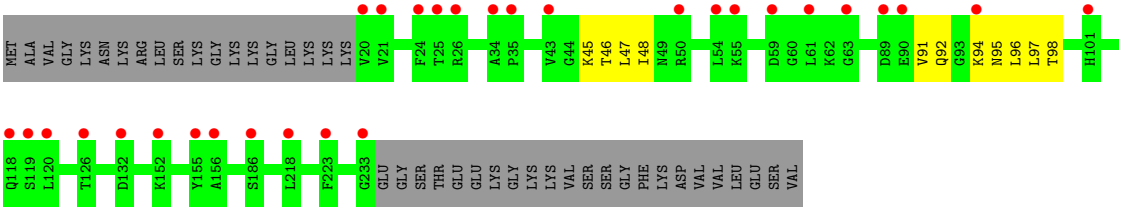
• Molecule 48: 40S ribosomal protein S1

Chain D:

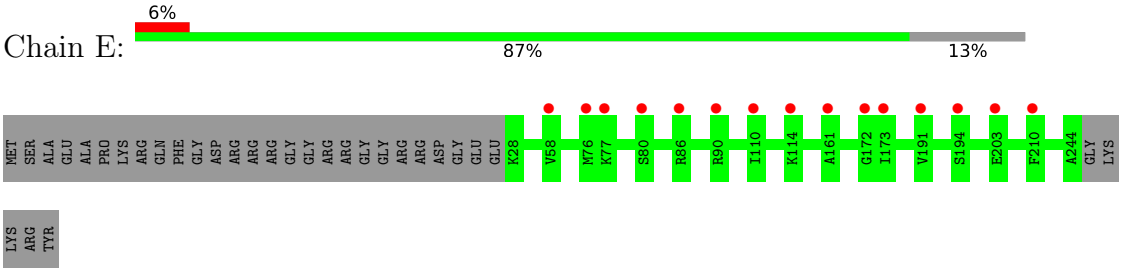


• Molecule 48: 40S ribosomal protein S1

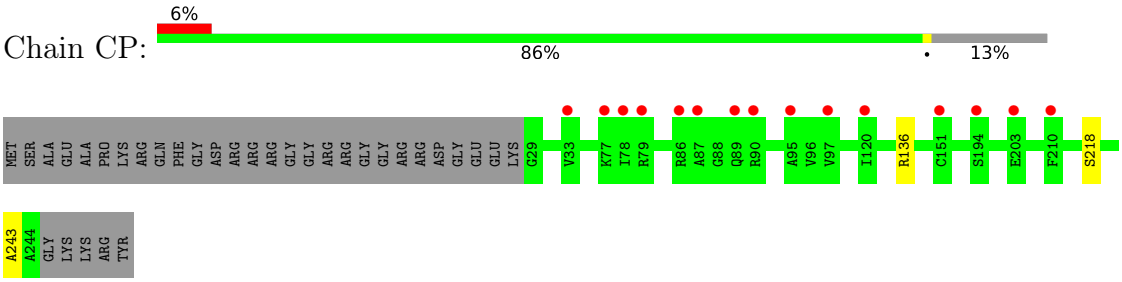
Chain CO:



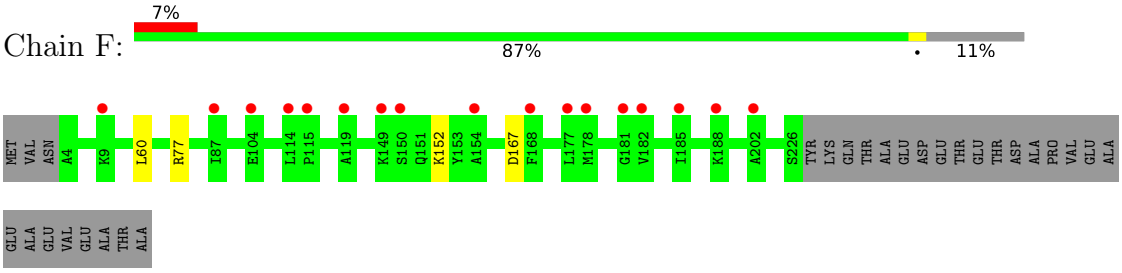
• Molecule 49: Ribosomal protein S5



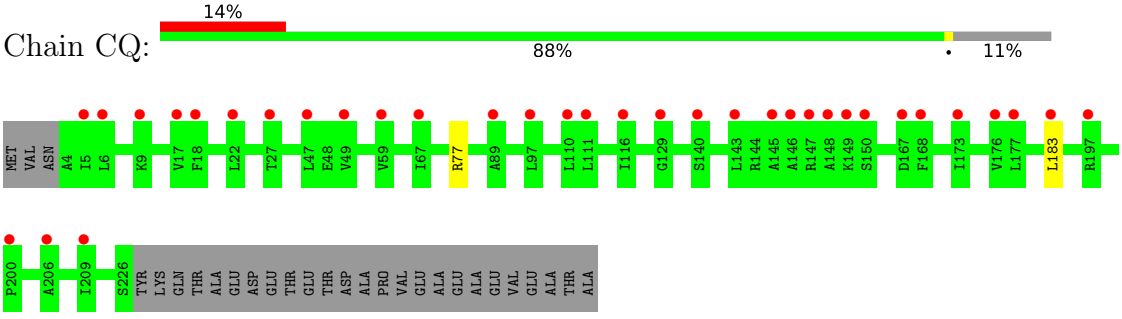
• Molecule 49: Ribosomal protein S5



• Molecule 50: Ribosomal protein S3

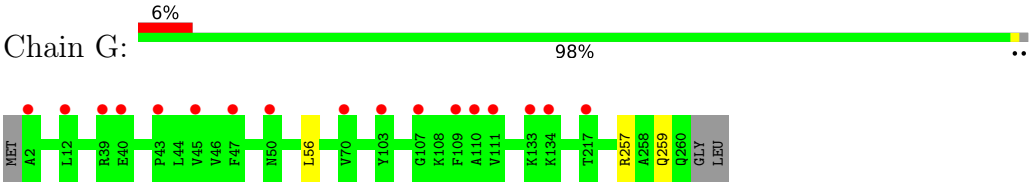


• Molecule 50: Ribosomal protein S3



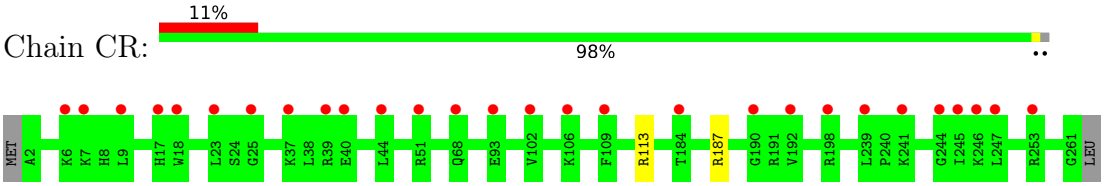
• Molecule 51: 40S ribosomal protein S4

Chain G:



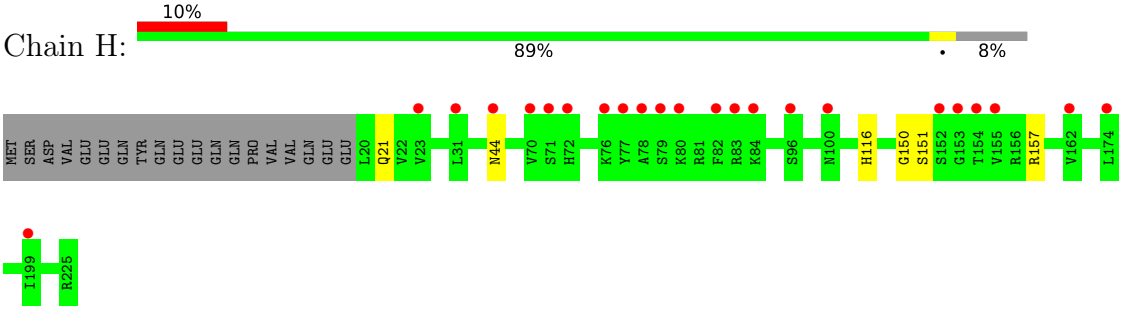
• Molecule 51: 40S ribosomal protein S4

Chain CR:



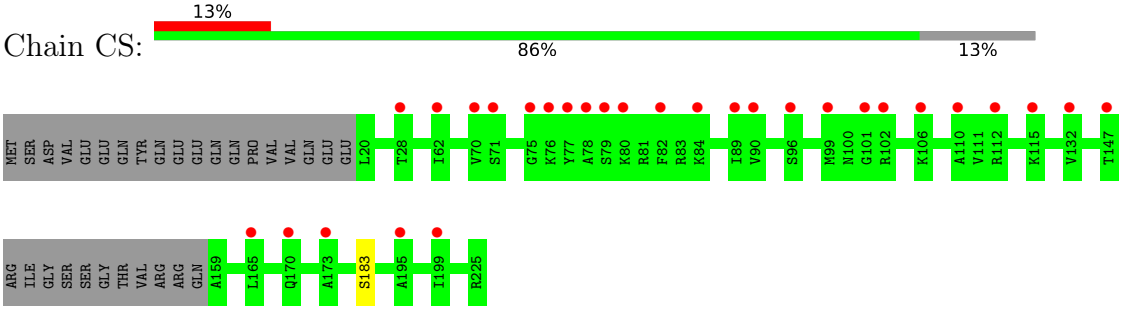
• Molecule 52: Ribosomal protein S7

Chain H:



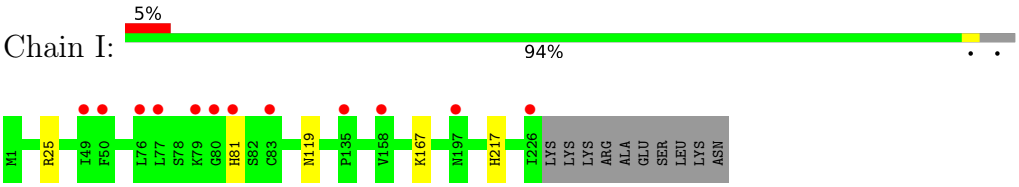
• Molecule 52: Ribosomal protein S7

Chain CS:



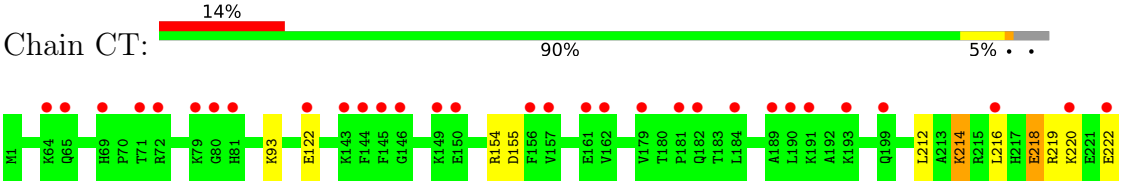
• Molecule 53: 40S ribosomal protein S6

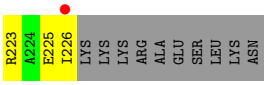
Chain I:



• Molecule 53: 40S ribosomal protein S6

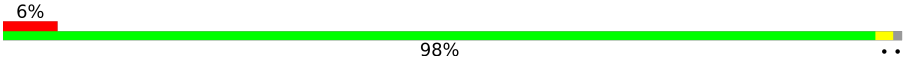
Chain CT:

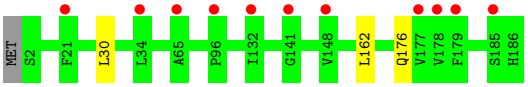




• Molecule 54: 40S ribosomal protein S7

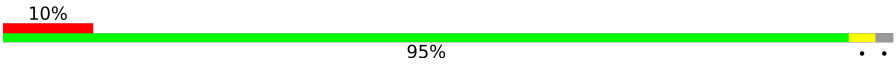
Chain J:





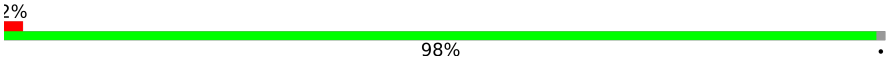
• Molecule 54: 40S ribosomal protein S7

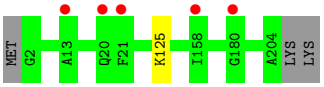
Chain CU:



• Molecule 55: 40S ribosomal protein S8

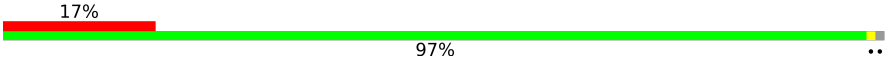
Chain K:

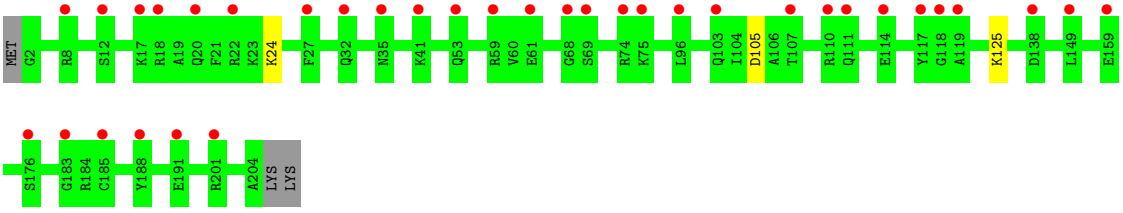




• Molecule 55: 40S ribosomal protein S8

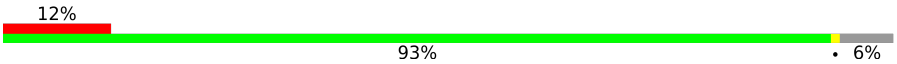
Chain CV:

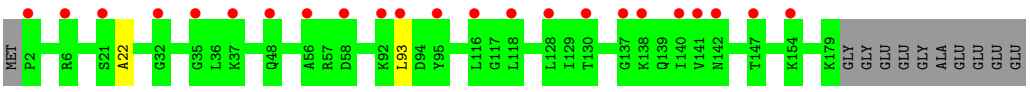




• Molecule 56: Ribosomal protein S4

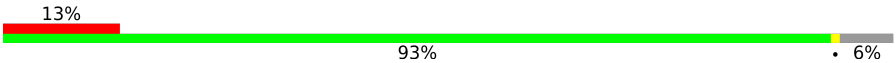
Chain L:

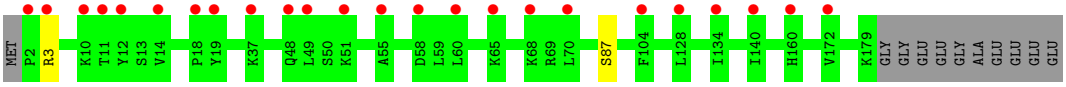




• Molecule 56: Ribosomal protein S4

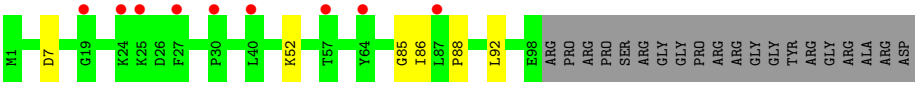
Chain CW:





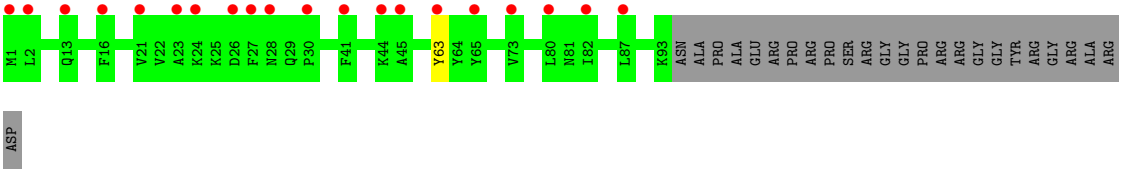
• Molecule 57: 40S ribosomal protein S10-A

Chain M:



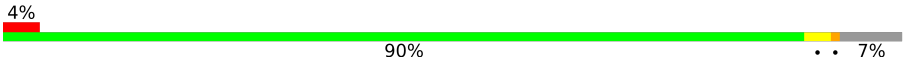
• Molecule 57: 40S ribosomal protein S10-A

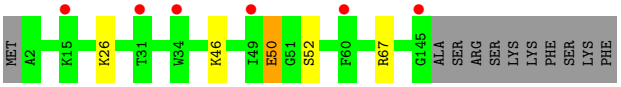
Chain CX:



• Molecule 58: 40S ribosomal protein S11A

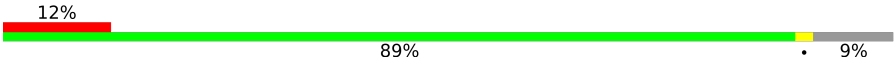
Chain N:

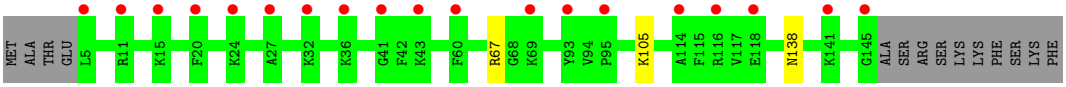




• Molecule 58: 40S ribosomal protein S11A

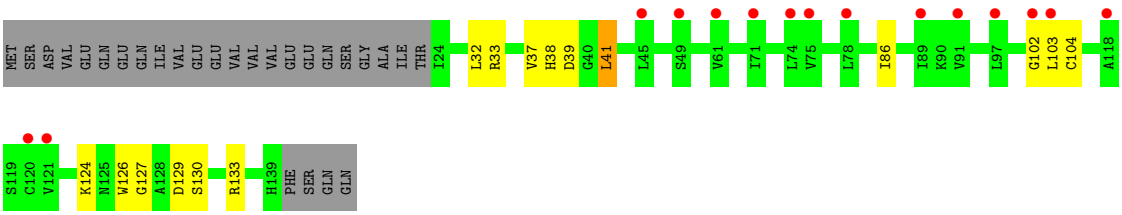
Chain CY:





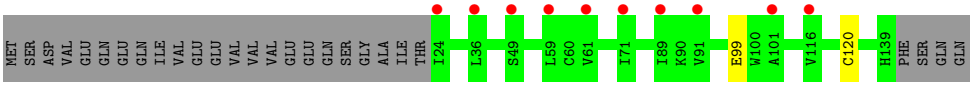
• Molecule 59: 40S ribosomal protein S12

Chain O:



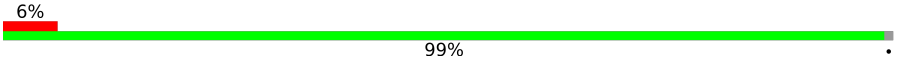
• Molecule 59: 40S ribosomal protein S12

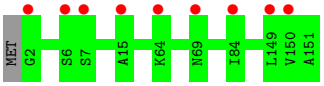
Chain CZ:



• Molecule 60: 40S ribosomal protein S13

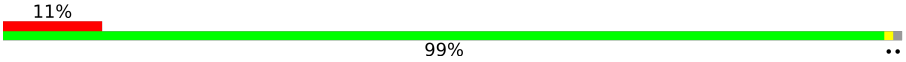
Chain P:

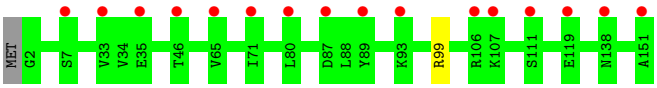




• Molecule 60: 40S ribosomal protein S13

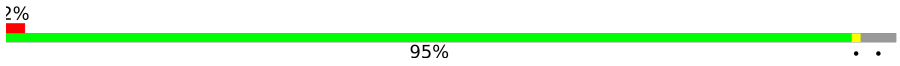
Chain DA:

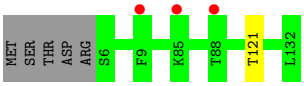




• Molecule 61: 40S ribosomal protein S14-A

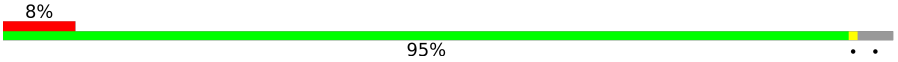
Chain Q:

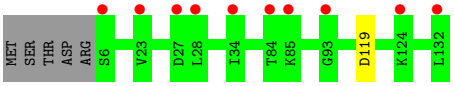




• Molecule 61: 40S ribosomal protein S14-A

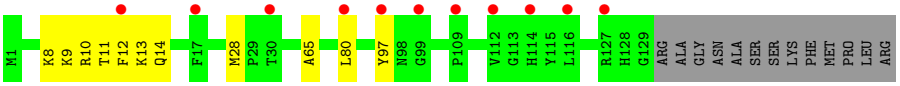
Chain DB:





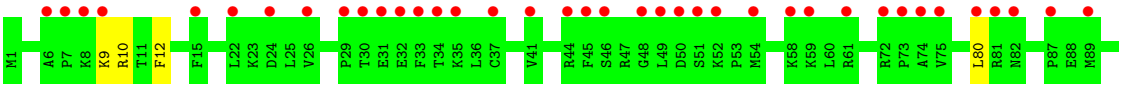
• Molecule 62: 40S ribosomal protein S15

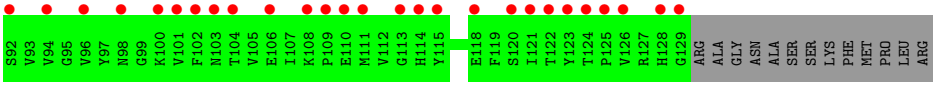
Chain R:



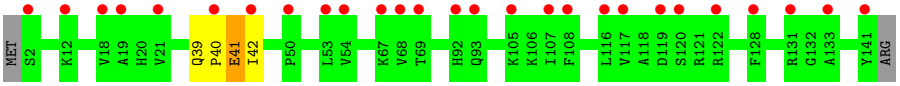
• Molecule 62: 40S ribosomal protein S15

Chain DC:

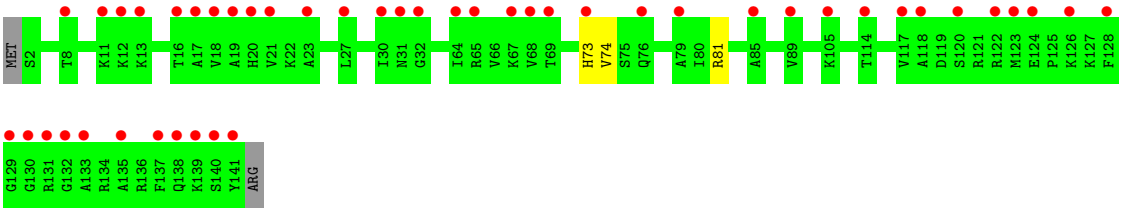




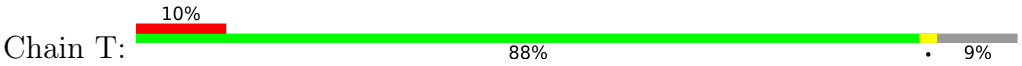
• Molecule 63: 40S ribosomal protein S16

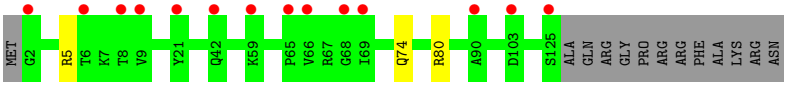


• Molecule 63: 40S ribosomal protein S16

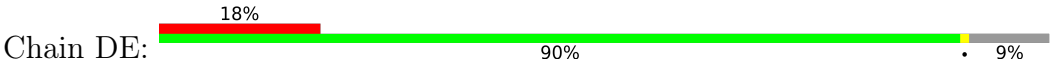


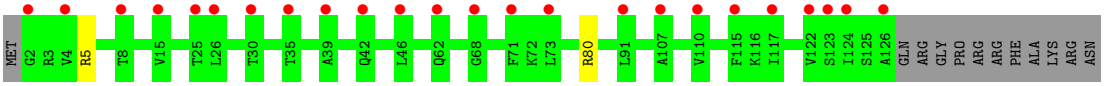
• Molecule 64: 40S ribosomal protein S17-B



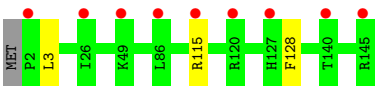


• Molecule 64: 40S ribosomal protein S17-B

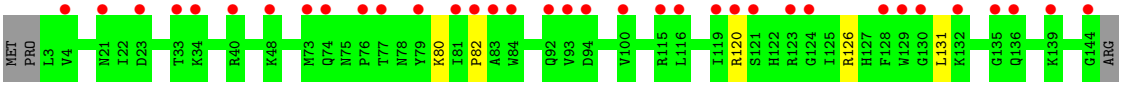




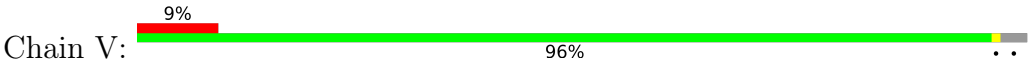
• Molecule 65: 40S ribosomal protein S18-B

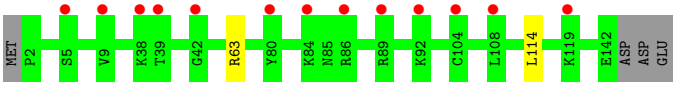


• Molecule 65: 40S ribosomal protein S18-B

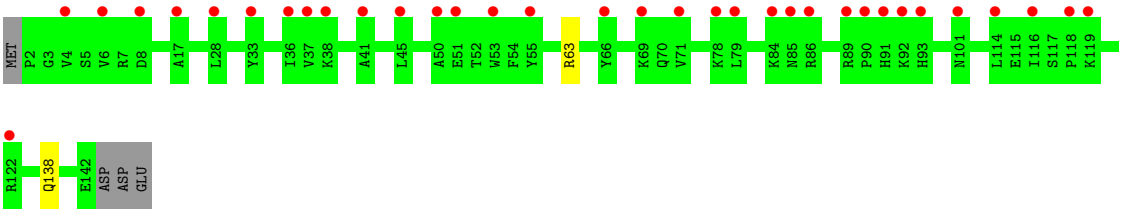


• Molecule 66: 40S ribosomal protein S19-A

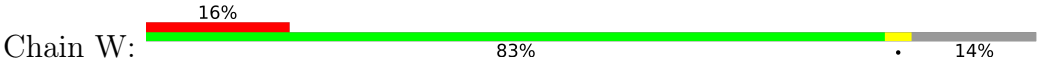


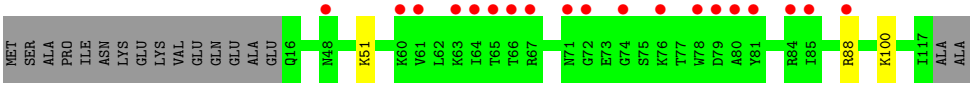


• Molecule 66: 40S ribosomal protein S19-A

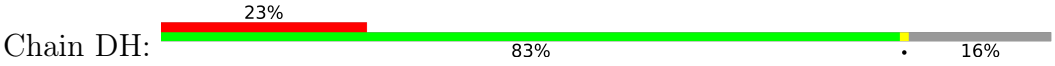


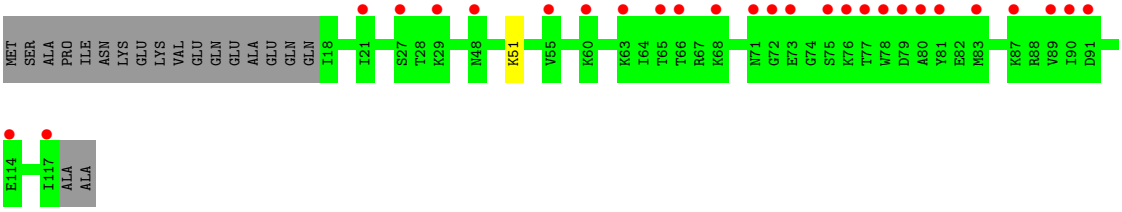
• Molecule 67: Ribosomal protein S10



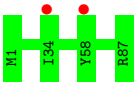


• Molecule 67: Ribosomal protein S10



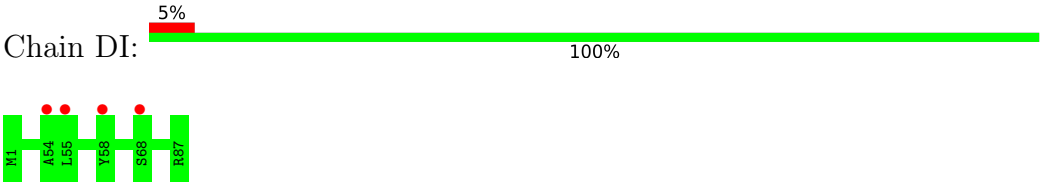


• Molecule 68: 40S ribosomal protein S21



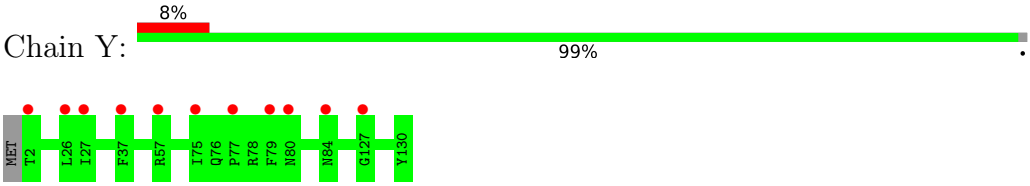
• Molecule 68: 40S ribosomal protein S21

Chain DI:



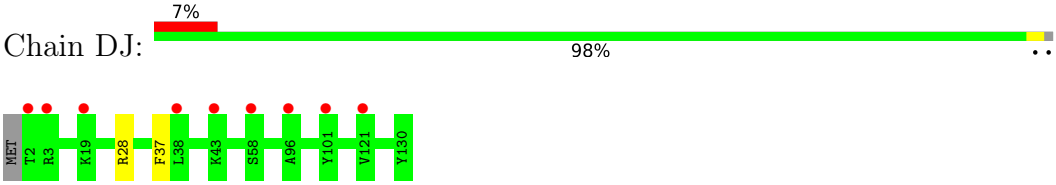
• Molecule 69: 40S ribosomal protein S22-A

Chain Y:



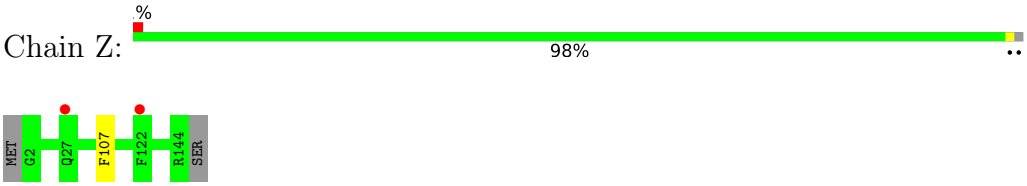
• Molecule 69: 40S ribosomal protein S22-A

Chain DJ:



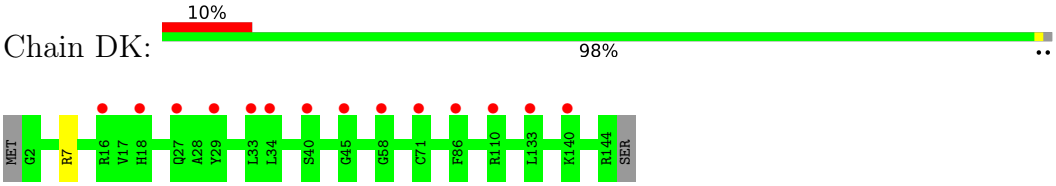
• Molecule 70: Ribosomal protein S23 (S12)

Chain Z:



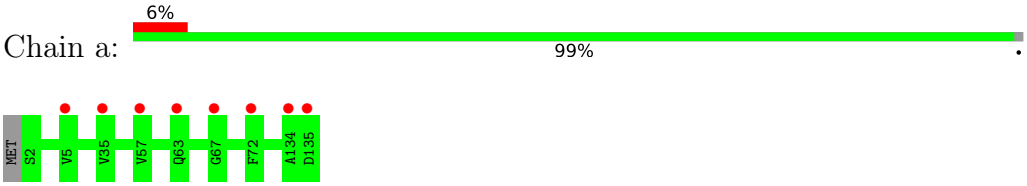
• Molecule 70: Ribosomal protein S23 (S12)

Chain DK:



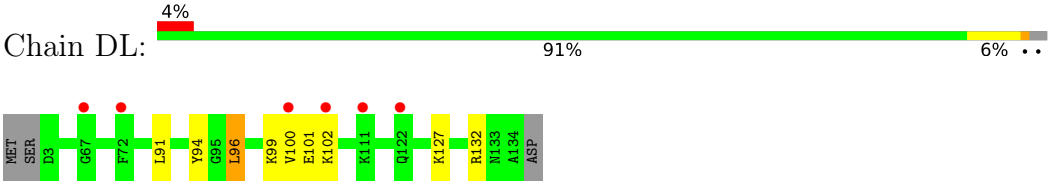
• Molecule 71: 40S ribosomal protein S24

Chain a:



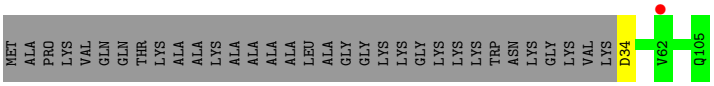
• Molecule 71: 40S ribosomal protein S24

Chain DL:



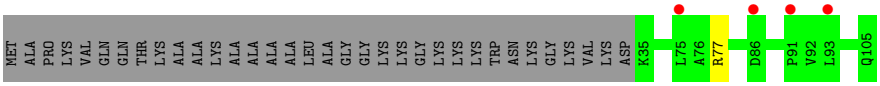
• Molecule 72: 40S ribosomal protein S25

Chain b:



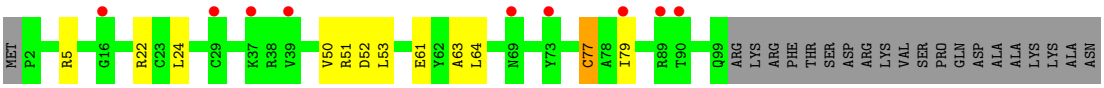
• Molecule 72: 40S ribosomal protein S25

Chain DM:



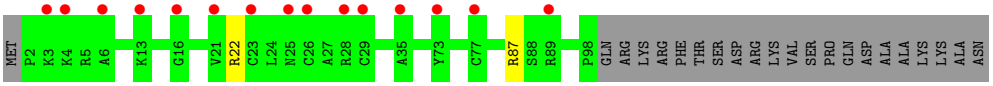
• Molecule 73: 40S ribosomal protein S26

Chain c:



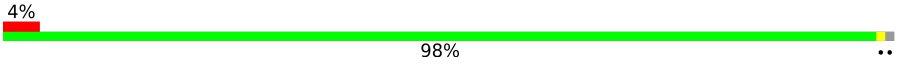
• Molecule 73: 40S ribosomal protein S26

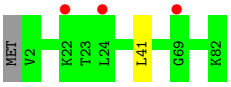
Chain DN:



• Molecule 74: 40S ribosomal protein S27

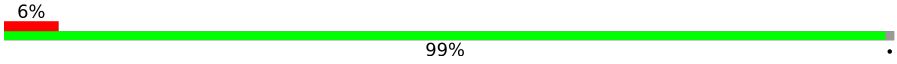
Chain d:

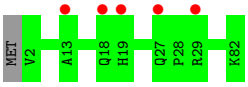




• Molecule 74: 40S ribosomal protein S27

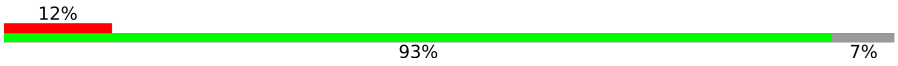
Chain DO:

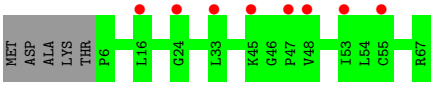




• Molecule 75: 40S ribosomal protein S28-B

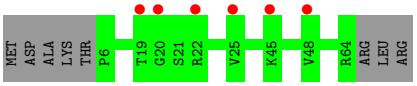
Chain e:





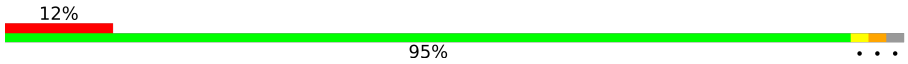
• Molecule 75: 40S ribosomal protein S28-B

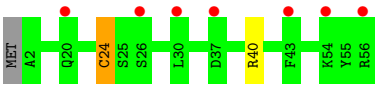
Chain DP:



• Molecule 76: 40S ribosomal protein S29A

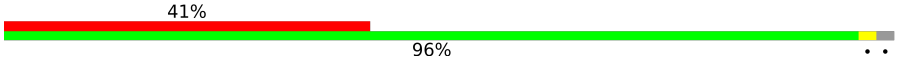
Chain f:

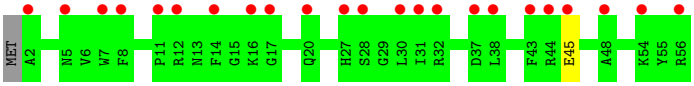




• Molecule 76: 40S ribosomal protein S29A

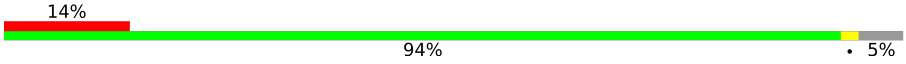
Chain DQ:

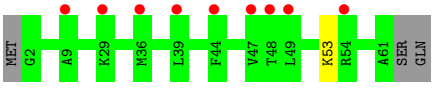




• Molecule 77: 40S ribosomal protein S30

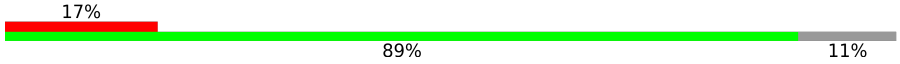
Chain g:

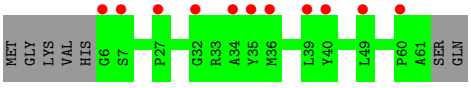




• Molecule 77: 40S ribosomal protein S30

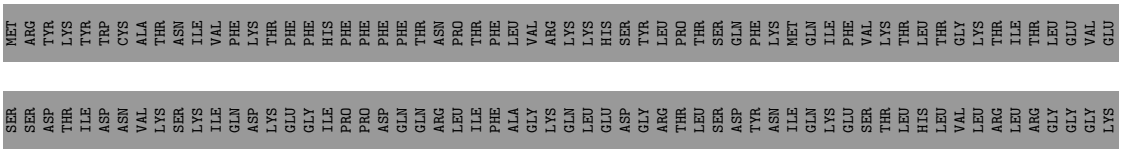
Chain DR:

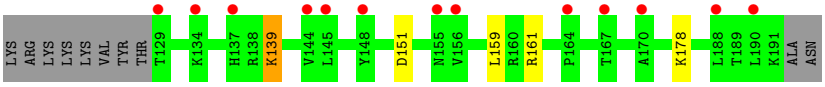




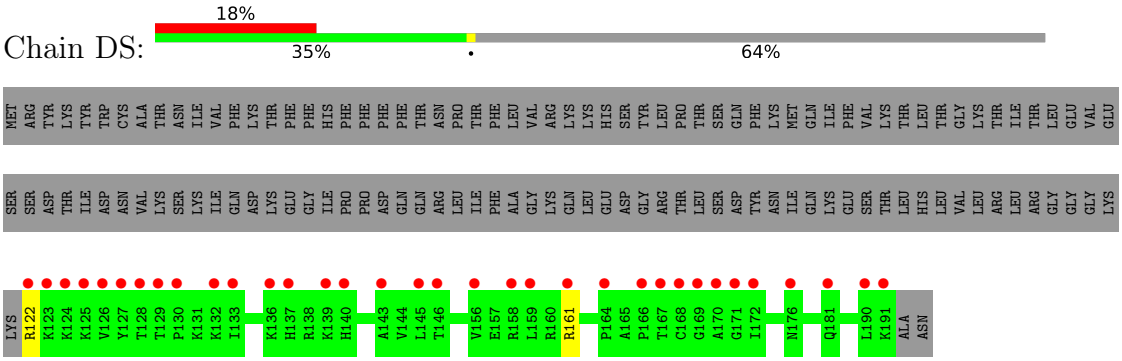
• Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein

Chain h:

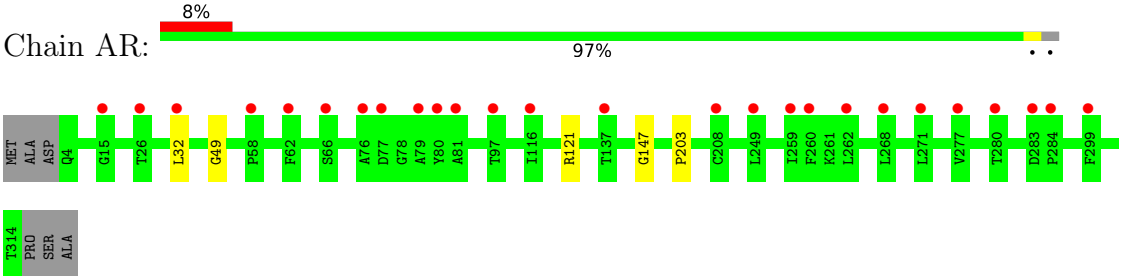




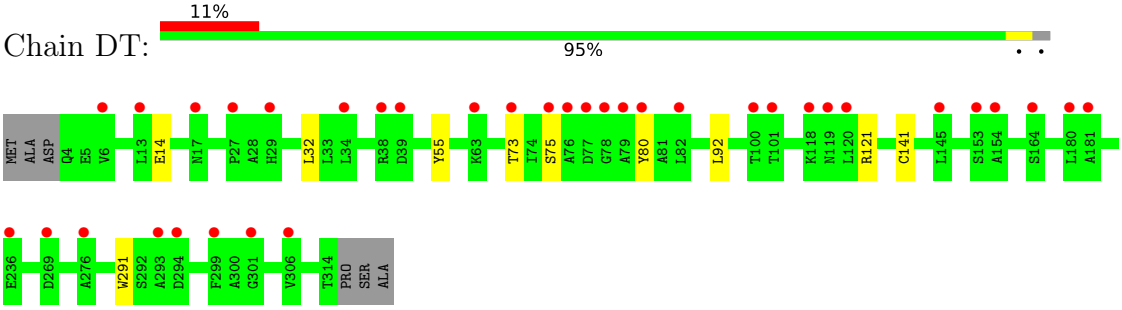
• Molecule 78: Ubiquitin-40S ribosomal protein S31 fusion protein



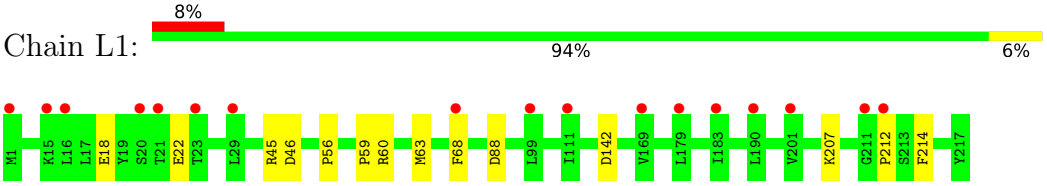
• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein



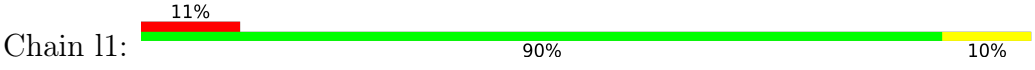
• Molecule 79: Guanine nucleotide-binding protein subunit beta-like protein

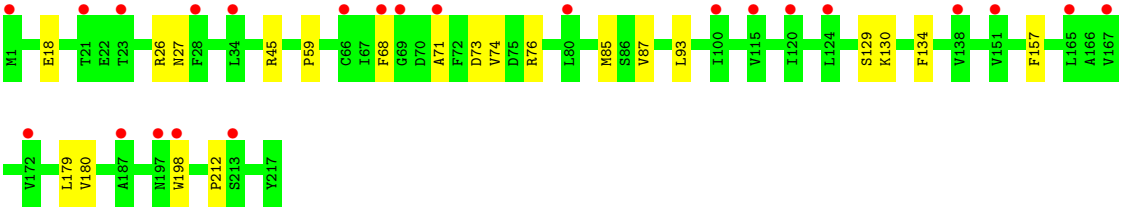


• Molecule 80: Ribosomal protein



• Molecule 80: Ribosomal protein

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E22
T23
R26
N27
F28
L34
R45
P59
C66
I67
F68
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A71
F72
D73
V74
D75
R76
L80
M85
S86
V87
L93
I100
V115
I120
L124
S129
K130
F134
V138
V151
F157
L165
A166
V167
V172
L179
V180
A187
N197
W198
P212
S213
Y217

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	0.74 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19rc4_4035	Depositor
R, R_{free}	0.254 , 0.297 0.256 , 0.296	Depositor DCC
R_{free} test set	1824 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)	0.24 , 57.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.41	0/76973	1.00	183/119996 (0.2%)
1	AS	0.40	0/76539	1.00	199/119319 (0.2%)
2	3	0.34	0/2884	0.85	1/4492 (0.0%)
2	AT	0.36	0/2884	0.85	0/4492
3	4	0.35	0/3724	0.90	5/5798 (0.1%)
3	AU	0.32	0/3746	0.89	6/5832 (0.1%)
4	AW	0.30	0/1922	0.62	0/2581
4	j	0.32	0/1922	0.65	0/2581
5	AX	0.32	0/3145	0.65	1/4231 (0.0%)
5	k	0.31	0/3145	0.65	1/4231 (0.0%)
6	AY	0.28	0/2799	0.62	0/3777
6	l	0.32	0/2799	0.66	0/3777
7	AZ	0.30	0/2447	0.64	0/3294
7	m	0.31	0/2479	0.61	0/3337
8	BA	0.30	0/1231	0.62	0/1662
8	n	0.31	0/1263	0.67	0/1703
9	BB	0.32	0/1918	0.59	0/2575
9	o	0.33	0/1918	0.60	0/2575
10	BC	0.30	0/1835	0.62	0/2472
10	p	0.33	0/1869	0.59	0/2519
11	BD	0.30	0/1537	0.62	0/2067
11	q	0.30	0/1537	0.65	0/2067
12	BE	0.31	0/1724	0.65	0/2314
12	r	0.31	0/1724	0.65	0/2314
13	BF	0.30	0/1390	0.68	0/1861
13	s	0.30	0/1390	0.67	0/1861
14	BG	0.29	0/1637	0.65	0/2195
14	t	0.31	0/1637	0.65	0/2195
15	BH	0.32	0/1044	0.64	0/1407
15	u	0.29	0/1044	0.63	1/1407 (0.1%)
16	BI	0.29	0/1753	0.68	0/2347
16	v	0.32	0/1753	0.68	0/2347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
17	BJ	0.31	0/1620	0.64	0/2167
17	w	0.32	0/1620	0.64	0/2167
18	BK	0.29	0/1429	0.65	0/1920
18	x	0.29	0/1410	0.66	0/1895
19	BL	0.30	0/1482	0.66	0/1985
19	y	0.31	0/1482	0.66	0/1985
20	BM	0.28	0/1475	0.70	0/1961
20	z	0.29	0/1475	0.68	0/1961
21	0	0.31	0/1457	0.65	0/1962
21	BN	0.30	0/1457	0.61	0/1962
22	2	0.30	0/1285	0.64	0/1723
22	BO	0.29	0/1285	0.62	0/1723
23	5	0.30	0/846	0.60	0/1140
23	BP	0.35	0/841	0.67	0/1133
24	6	0.30	0/993	0.64	0/1339
24	BQ	0.30	0/993	0.64	0/1339
25	7	0.31	0/958	0.58	0/1267
25	BR	0.30	0/814	0.60	0/1079
26	8	0.29	0/990	0.63	0/1337
26	BS	0.27	0/976	0.61	0/1319
27	9	0.29	0/999	0.61	0/1334
27	BT	0.29	0/999	0.63	0/1334
28	AA	0.31	0/1112	0.58	0/1488
28	BU	0.29	0/1112	0.58	0/1488
29	AB	0.30	0/1199	0.61	0/1607
29	BV	0.31	0/1199	0.63	0/1607
30	AC	0.28	0/503	0.71	0/668
30	BW	0.29	0/522	0.68	0/692
31	AD	0.30	0/738	0.59	0/994
31	BX	0.30	0/738	0.59	0/994
32	AE	0.30	0/907	0.67	2/1219 (0.2%)
32	BY	0.28	0/894	0.66	0/1201
33	AF	0.30	0/1021	0.62	0/1368
33	BZ	0.30	0/1039	0.65	0/1390
34	AG	0.31	0/866	0.60	0/1165
34	CA	0.32	0/895	0.63	0/1201
35	AH	0.31	0/896	0.66	0/1195
35	CB	0.29	0/925	0.66	0/1231
36	AI	0.28	0/1003	0.64	0/1336
36	CC	0.27	0/990	0.66	0/1319
37	AJ	0.29	0/763	0.67	0/1012
37	CD	0.30	0/772	0.67	0/1023
38	AK	0.34	0/690	0.71	0/916

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
38	CE	0.30	0/690	0.69	0/916
39	AL	0.29	0/623	0.61	0/831
39	CF	0.29	0/632	0.63	0/842
40	AM	0.29	0/447	0.67	0/594
40	CG	0.31	0/447	0.72	0/594
41	AN	0.31	0/425	0.69	0/563
41	CH	0.32	0/436	0.69	0/577
42	AO	0.30	0/237	0.80	0/304
42	CI	0.49	0/228	0.63	0/293
43	AP	0.32	0/840	0.65	0/1110
43	CJ	0.33	0/860	0.65	0/1136
44	AQ	0.34	0/705	0.69	0/940
44	CK	0.32	0/705	0.67	0/940
45	CL	0.34	0/942	0.66	0/1258
45	i	0.38	0/942	0.86	3/1258 (0.2%)
46	B	0.38	0/40832	1.02	84/63622 (0.1%)
46	CM	0.40	0/41169	1.01	92/64148 (0.1%)
47	C	0.27	0/1666	0.58	0/2273
47	CN	0.29	0/1666	0.62	0/2273
48	CO	0.32	0/1750	0.69	0/2354
48	D	0.29	0/1750	0.63	0/2354
49	CP	0.31	0/1648	0.60	0/2237
49	E	0.29	0/1657	0.62	0/2248
50	CQ	0.31	0/1731	0.68	1/2324 (0.0%)
50	F	0.33	0/1731	0.73	1/2324 (0.0%)
51	CR	0.30	0/2096	0.65	0/2822
51	G	0.29	0/2092	0.66	1/2817 (0.0%)
52	CS	0.31	0/1546	0.64	0/2085
52	H	0.30	0/1631	0.65	0/2199
53	CT	0.35	0/1845	0.63	0/2464
53	I	0.30	0/1845	0.68	0/2464
54	CU	0.30	0/1490	0.65	0/2004
54	J	0.31	0/1516	0.68	1/2039 (0.0%)
55	CV	0.30	0/1606	0.69	0/2150
55	K	0.30	0/1606	0.67	0/2150
56	CW	0.28	0/1478	0.65	0/1978
56	L	0.31	0/1478	0.69	1/1978 (0.1%)
57	CX	0.35	0/801	0.66	0/1081
57	M	0.35	0/836	0.71	2/1130 (0.2%)
58	CY	0.31	0/1154	0.66	0/1553
58	N	0.32	0/1175	0.70	1/1582 (0.1%)
59	CZ	0.31	0/892	0.75	0/1203
59	O	0.41	0/892	1.00	2/1203 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
60	DA	0.27	0/1210	0.61	0/1631
60	P	0.28	0/1210	0.60	0/1631
61	DB	0.30	0/953	0.73	0/1279
61	Q	0.31	0/953	0.71	0/1279
62	DC	0.36	0/1038	0.73	1/1395 (0.1%)
62	R	0.37	0/1038	0.73	1/1395 (0.1%)
63	DD	0.30	0/1109	0.63	0/1486
63	S	0.31	0/1109	0.63	0/1486
64	DE	0.28	0/1014	0.68	0/1361
64	T	0.31	0/1009	0.74	0/1354
65	DF	0.32	0/1186	0.80	1/1590 (0.1%)
65	U	0.31	0/1205	0.68	1/1615 (0.1%)
66	DG	0.30	0/1120	0.64	0/1508
66	V	0.31	0/1120	0.72	1/1508 (0.1%)
67	DH	0.29	0/800	0.64	0/1082
67	W	0.30	0/818	0.72	0/1106
68	DI	0.31	0/683	0.67	0/918
68	X	0.31	0/683	0.72	0/918
69	DJ	0.31	0/1049	0.65	0/1412
69	Y	0.29	0/1049	0.63	0/1412
70	DK	0.31	0/1128	0.70	0/1505
70	Z	0.29	0/1128	0.69	0/1505
71	DL	0.35	0/1086	0.67	0/1447
71	a	0.31	0/1100	0.70	0/1466
72	DM	0.29	0/577	0.70	0/778
72	b	0.29	0/585	0.62	0/789
73	DN	0.34	0/782	0.76	0/1048
73	c	0.49	0/791	1.08	5/1060 (0.5%)
74	DO	0.30	0/624	0.66	0/843
74	d	0.30	0/624	0.67	1/843 (0.1%)
75	DP	0.31	0/459	0.79	0/615
75	e	0.32	0/489	0.77	0/654
76	DQ	0.35	0/466	0.73	0/620
76	f	0.33	0/466	0.75	1/620 (0.2%)
77	DR	0.32	0/451	0.72	0/601
77	g	0.40	0/482	0.85	1/642 (0.2%)
78	DS	0.30	0/585	0.75	0/778
78	h	0.33	0/520	0.93	1/693 (0.1%)
79	AR	0.28	0/2451	0.65	1/3337 (0.0%)
79	DT	0.33	0/2451	0.71	3/3337 (0.1%)
80	L1	0.28	0/1737	0.53	0/2335
80	l1	0.29	0/1737	0.57	1/2335 (0.0%)
All	All	0.36	0/433095	0.88	607/635204 (0.1%)

There are no bond length outliers.

The worst 5 of 607 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AS	1224	C	O5'-P-OP2	-18.14	88.93	110.70
46	B	823	G	OP1-P-O3'	-15.09	72.01	105.20
46	B	824	U	O4'-C1'-N1	-13.61	97.31	108.20
73	c	53	LEU	CB-CG-CD2	-12.73	89.37	111.00
1	AS	1576	A	O4'-C1'-N9	11.75	117.60	108.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	AW	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
4	j	247/254 (97%)	239 (97%)	8 (3%)	0	100	100
5	AX	384/389 (99%)	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%)	13	42
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	BB	232/241 (96%)	225 (97%)	6 (3%)	1 (0%)	30	61
9	o	232/241 (96%)	223 (96%)	8 (3%)	1 (0%)	30	61
10	BC	231/262 (88%)	220 (95%)	9 (4%)	2 (1%)	14	44
10	p	236/262 (90%)	224 (95%)	9 (4%)	3 (1%)	10	36
11	BD	188/191 (98%)	182 (97%)	6 (3%)	0	100	100
11	q	188/191 (98%)	184 (98%)	4 (2%)	0	100	100
12	BE	204/220 (93%)	199 (98%)	5 (2%)	0	100	100
12	r	204/220 (93%)	201 (98%)	3 (2%)	0	100	100
13	BF	169/174 (97%)	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%)	25	56
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%)	13	42
23	BP	100/124 (81%)	85 (85%)	13 (13%)	2 (2%)	6	28
24	6	129/137 (94%)	126 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	BQ	129/137 (94%)	126 (98%)	3 (2%)	0	100	100
25	7	114/155 (74%)	100 (88%)	13 (11%)	1 (1%)	14	44
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
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%)	8	32
31	AD	94/106 (89%)	91 (97%)	2 (2%)	1 (1%)	12	40
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
40	AM	48/51 (94%)	46 (96%)	1 (2%)	1 (2%)	5 27
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
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 19
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%)	25 56
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 61
52	CS	191/225 (85%)	180 (94%)	11 (6%)	0	100 100
52	H	204/225 (91%)	187 (92%)	15 (7%)	2 (1%)	13 42
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%)	12 40
54	J	183/186 (98%)	171 (93%)	11 (6%)	1 (0%)	25 56
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
56	L	176/189 (93%)	173 (98%)	2 (1%)	1 (1%)	22 53
57	CX	91/118 (77%)	84 (92%)	7 (8%)	0	100 100
57	M	96/118 (81%)	83 (86%)	11 (12%)	2 (2%)	5 27
58	CY	139/155 (90%)	136 (98%)	3 (2%)	0	100 100
58	N	142/155 (92%)	132 (93%)	9 (6%)	1 (1%)	19 50
59	CZ	114/143 (80%)	98 (86%)	16 (14%)	0	100 100
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 46
61	Q	125/132 (95%)	122 (98%)	2 (2%)	1 (1%)	16 46
62	DC	127/142 (89%)	110 (87%)	16 (13%)	1 (1%)	16 46
62	R	127/142 (89%)	110 (87%)	16 (13%)	1 (1%)	16 46
63	DD	138/142 (97%)	131 (95%)	5 (4%)	2 (1%)	9 34
63	S	138/142 (97%)	131 (95%)	5 (4%)	2 (1%)	9 34
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 34
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 33
71	a	132/135 (98%)	129 (98%)	3 (2%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	13	42
74	DO	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
74	d	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
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%)	2	12
79	AR	309/317 (98%)	281 (91%)	25 (8%)	3 (1%)	13	42
79	DT	309/317 (98%)	285 (92%)	22 (7%)	2 (1%)	22	53
80	L1	215/217 (99%)	166 (77%)	45 (21%)	4 (2%)	6	29
80	l1	215/217 (99%)	124 (58%)	81 (38%)	10 (5%)	2	13
All	All	22518/24692 (91%)	21437 (95%)	995 (4%)	86 (0%)	30	61

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 (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	AW	190/194 (98%)	189 (100%)	1 (0%)	86 91
4	j	190/194 (98%)	190 (100%)	0	100 100
5	AX	325/328 (99%)	319 (98%)	6 (2%)	54 74
5	k	325/328 (99%)	322 (99%)	3 (1%)	75 85
6	AY	290/292 (99%)	287 (99%)	3 (1%)	73 84
6	l	290/292 (99%)	288 (99%)	2 (1%)	81 88
7	AZ	247/252 (98%)	243 (98%)	4 (2%)	58 76
7	m	250/252 (99%)	248 (99%)	2 (1%)	79 87
8	BA	132/154 (86%)	132 (100%)	0	100 100
8	n	136/154 (88%)	135 (99%)	1 (1%)	81 88
9	BB	198/204 (97%)	198 (100%)	0	100 100
9	o	198/204 (97%)	195 (98%)	3 (2%)	60 77
10	BC	193/216 (89%)	189 (98%)	4 (2%)	48 70
10	p	198/216 (92%)	197 (100%)	1 (0%)	86 91
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%)	175 (98%)	3 (2%)	56 74
13	BF	146/149 (98%)	141 (97%)	5 (3%)	32 59
13	s	146/149 (98%)	144 (99%)	2 (1%)	62 78
14	BG	166/168 (99%)	163 (98%)	3 (2%)	54 74
14	t	166/168 (99%)	164 (99%)	2 (1%)	67 80
15	BH	108/109 (99%)	107 (99%)	1 (1%)	75 85
15	u	108/109 (99%)	106 (98%)	2 (2%)	52 72
16	BI	177/178 (99%)	174 (98%)	3 (2%)	56 74
16	v	177/178 (99%)	175 (99%)	2 (1%)	70 82
17	BJ	166/167 (99%)	164 (99%)	2 (1%)	67 80
17	w	166/167 (99%)	166 (100%)	0	100 100
18	BK	145/154 (94%)	141 (97%)	4 (3%)	38 64
18	x	144/154 (94%)	144 (100%)	0	100 100
19	BL	153/154 (99%)	153 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	y	153/154 (99%)	152 (99%)	1 (1%)	81 88
20	BM	146/153 (95%)	141 (97%)	5 (3%)	32 59
20	z	146/153 (95%)	146 (100%)	0	100 100
21	0	155/157 (99%)	154 (99%)	1 (1%)	84 90
21	BN	155/157 (99%)	155 (100%)	0	100 100
22	2	133/134 (99%)	133 (100%)	0	100 100
22	BO	133/134 (99%)	131 (98%)	2 (2%)	60 77
23	5	93/112 (83%)	93 (100%)	0	100 100
23	BP	93/112 (83%)	89 (96%)	4 (4%)	25 53
24	6	101/104 (97%)	101 (100%)	0	100 100
24	BQ	101/104 (97%)	100 (99%)	1 (1%)	73 84
25	7	97/127 (76%)	95 (98%)	2 (2%)	48 70
25	BR	86/127 (68%)	84 (98%)	2 (2%)	45 68
26	8	108/121 (89%)	108 (100%)	0	100 100
26	BS	107/121 (88%)	107 (100%)	0	100 100
27	9	111/112 (99%)	110 (99%)	1 (1%)	75 85
27	BT	111/112 (99%)	109 (98%)	2 (2%)	54 74
28	AA	117/118 (99%)	117 (100%)	0	100 100
28	BU	117/118 (99%)	117 (100%)	0	100 100
29	AB	120/121 (99%)	119 (99%)	1 (1%)	79 87
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%)	97 (99%)	1 (1%)	73 84
32	BY	97/100 (97%)	96 (99%)	1 (1%)	73 84
33	AF	109/115 (95%)	108 (99%)	1 (1%)	75 85
33	BZ	111/115 (96%)	109 (98%)	2 (2%)	54 74
34	AG	91/92 (99%)	90 (99%)	1 (1%)	70 82
34	CA	94/92 (102%)	94 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
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%)	104 (99%)	1 (1%)	73 84
37	AJ	77/79 (98%)	76 (99%)	1 (1%)	65 79
37	CD	78/79 (99%)	77 (99%)	1 (1%)	65 79
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%)	46 (98%)	1 (2%)	48 70
41	CH	48/47 (102%)	47 (98%)	1 (2%)	48 70
42	AO	24/24 (100%)	23 (96%)	1 (4%)	25 53
42	CI	23/24 (96%)	20 (87%)	3 (13%)	3 14
43	AP	88/91 (97%)	87 (99%)	1 (1%)	70 82
43	CJ	90/91 (99%)	88 (98%)	2 (2%)	47 69
44	AQ	72/73 (99%)	71 (99%)	1 (1%)	62 78
44	CK	72/73 (99%)	71 (99%)	1 (1%)	62 78
45	CL	100/212 (47%)	97 (97%)	3 (3%)	36 62
45	i	100/212 (47%)	92 (92%)	8 (8%)	10 32
47	C	176/215 (82%)	176 (100%)	0	100 100
47	CN	176/215 (82%)	174 (99%)	2 (1%)	70 82
48	CO	194/229 (85%)	183 (94%)	11 (6%)	17 44
48	D	194/229 (85%)	193 (100%)	1 (0%)	86 91
49	CP	174/198 (88%)	172 (99%)	2 (1%)	70 82
49	E	175/198 (88%)	175 (100%)	0	100 100
50	CQ	174/196 (89%)	173 (99%)	1 (1%)	84 90
50	F	174/196 (89%)	171 (98%)	3 (2%)	56 74
51	CR	218/220 (99%)	216 (99%)	2 (1%)	75 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	G	218/220 (99%)	217 (100%)	1 (0%)	86 91
52	CS	169/197 (86%)	168 (99%)	1 (1%)	84 90
52	H	178/197 (90%)	174 (98%)	4 (2%)	47 69
53	CT	195/204 (96%)	184 (94%)	11 (6%)	17 45
53	I	195/204 (96%)	190 (97%)	5 (3%)	41 66
54	CU	163/167 (98%)	160 (98%)	3 (2%)	54 74
54	J	166/167 (99%)	165 (99%)	1 (1%)	84 90
55	CV	157/160 (98%)	154 (98%)	3 (2%)	52 72
55	K	157/160 (98%)	156 (99%)	1 (1%)	84 90
56	CW	153/160 (96%)	151 (99%)	2 (1%)	65 79
56	L	153/160 (96%)	153 (100%)	0	100 100
57	CX	87/104 (84%)	86 (99%)	1 (1%)	70 82
57	M	90/104 (86%)	88 (98%)	2 (2%)	47 69
58	CY	122/134 (91%)	119 (98%)	3 (2%)	42 67
58	N	124/134 (92%)	120 (97%)	4 (3%)	34 61
59	CZ	98/123 (80%)	96 (98%)	2 (2%)	50 71
59	O	98/123 (80%)	89 (91%)	9 (9%)	7 26
60	DA	129/130 (99%)	128 (99%)	1 (1%)	79 87
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%)	109 (98%)	2 (2%)	54 74
62	R	111/121 (92%)	102 (92%)	9 (8%)	9 31
63	DD	114/116 (98%)	113 (99%)	1 (1%)	75 85
63	S	114/116 (98%)	111 (97%)	3 (3%)	41 66
64	DE	112/122 (92%)	110 (98%)	2 (2%)	54 74
64	T	112/122 (92%)	109 (97%)	3 (3%)	40 65
65	DF	126/129 (98%)	124 (98%)	2 (2%)	58 76
65	U	128/129 (99%)	126 (98%)	2 (2%)	58 76
66	DG	113/117 (97%)	111 (98%)	2 (2%)	54 74
66	V	113/117 (97%)	112 (99%)	1 (1%)	75 85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
67	DH	90/105 (86%)	89 (99%)	1 (1%)	70 82
67	W	92/105 (88%)	89 (97%)	3 (3%)	33 60
68	DI	71/71 (100%)	71 (100%)	0	100 100
68	X	71/71 (100%)	71 (100%)	0	100 100
69	DJ	112/113 (99%)	110 (98%)	2 (2%)	54 74
69	Y	112/113 (99%)	112 (100%)	0	100 100
70	DK	116/118 (98%)	115 (99%)	1 (1%)	75 85
70	Z	116/118 (98%)	115 (99%)	1 (1%)	75 85
71	DL	109/112 (97%)	101 (93%)	8 (7%)	11 35
71	a	111/112 (99%)	111 (100%)	0	100 100
72	DM	63/85 (74%)	62 (98%)	1 (2%)	58 76
72	b	64/85 (75%)	63 (98%)	1 (2%)	58 76
73	DN	83/102 (81%)	81 (98%)	2 (2%)	44 68
73	c	84/102 (82%)	75 (89%)	9 (11%)	5 21
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%)	46 (98%)	1 (2%)	48 70
76	f	47/48 (98%)	45 (96%)	2 (4%)	25 53
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%)	60 (97%)	2 (3%)	34 61
78	h	55/175 (31%)	53 (96%)	2 (4%)	30 57
79	AR	259/263 (98%)	258 (100%)	1 (0%)	89 93
79	DT	259/263 (98%)	254 (98%)	5 (2%)	52 72
80	L1	196/196 (100%)	186 (95%)	10 (5%)	20 48
80	l1	196/196 (100%)	186 (95%)	10 (5%)	20 48
All	All	19326/20828 (93%)	19049 (99%)	277 (1%)	62 78

5 of 277 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
67	DH	51	LYS
71	DL	100	VAL
80	L1	88	ASP
70	Z	107	PHE
67	W	51	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
18	BK	120	ASN
47	CN	33	ASN
19	BL	158	HIS
28	BU	29	HIS
54	CU	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	3213/3359 (95%)	608 (18%)	43 (1%)
1	AS	3195/3359 (95%)	617 (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%)	2130 (20%)	197 (1%)

5 of 2130 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

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Mol	Chain	Res	Type
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	$\#\|Z\| > 2$
83	PAR	1	3967	-	45,45,45	0.50	0	64,67,67	1.18	5 (7%)
83	PAR	CM	1946	-	45,45,45	0.44	0	64,67,67	0.76	2 (3%)
82	3K5	CJ	202	-	62,63,63	0.32	0	82,95,95	0.62	1 (1%)
83	PAR	AS	3790	-	45,45,45	0.53	0	64,67,67	1.25	5 (7%)
83	PAR	AS	3789	-	45,45,45	0.51	0	64,67,67	0.72	1 (1%)
83	PAR	AS	3788	-	45,45,45	0.62	1 (2%)	64,67,67	1.05	3 (4%)
83	PAR	B	1970	-	45,45,45	0.59	0	64,67,67	1.83	13 (20%)
83	PAR	1	3969	-	45,45,45	0.69	1 (2%)	64,67,67	1.70	12 (18%)
83	PAR	1	3968	-	45,45,45	0.54	0	64,67,67	1.07	5 (7%)
82	3K5	1	3406	-	62,63,63	2.92	31 (50%)	82,95,95	1.96	20 (24%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
83	PAR	1	3967	-	-	9/18/94/94	0/4/4/4
83	PAR	CM	1946	-	-	4/18/94/94	0/4/4/4
82	3K5	CJ	202	-	-	12/29/121/121	0/7/7/7
83	PAR	AS	3790	-	-	9/18/94/94	1/4/4/4
83	PAR	AS	3789	-	-	10/18/94/94	0/4/4/4
83	PAR	AS	3788	-	-	6/18/94/94	0/4/4/4
83	PAR	B	1970	-	-	12/18/94/94	0/4/4/4
83	PAR	1	3969	-	-	10/18/94/94	0/4/4/4
83	PAR	1	3968	-	-	7/18/94/94	1/4/4/4
82	3K5	1	3406	-	-	6/29/121/121	0/7/7/7

The worst 5 of 33 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
82	1	3406	3K5	C17-C22	-9.42	1.35	1.53
82	1	3406	3K5	O4-C22	7.60	1.60	1.43
82	1	3406	3K5	C21-C22	5.77	1.62	1.52
82	1	3406	3K5	C37-C36	-4.91	1.39	1.51
82	1	3406	3K5	C29-C28	-4.66	1.40	1.51

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
83	B	1970	PAR	C13-C23-C33	-8.07	92.40	102.10
82	1	3406	3K5	O14-C38-C39	6.54	123.12	111.09
82	1	3406	3K5	C9-C8-C7	-6.34	112.41	126.91
83	1	3969	PAR	O54-C54-C64	5.61	116.45	106.01
83	1	3969	PAR	C52-C42-C32	-5.55	100.80	111.16

There are no chirality outliers.

5 of 85 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

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Mol	Chain	Res	Type	Atoms
82	CJ	202	3K5	O10-C30-O9-C26

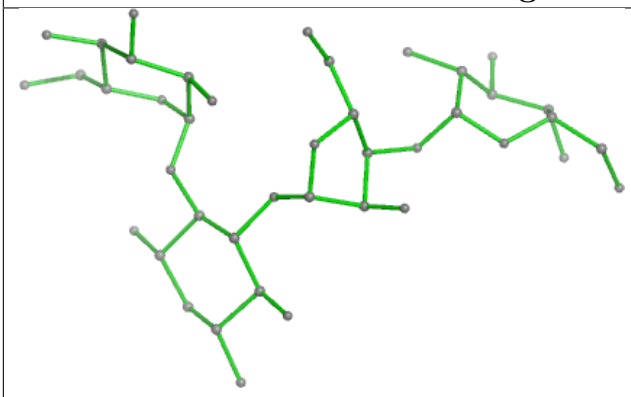
All (2) ring outliers are listed below:

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

No monomer is involved in short contacts.

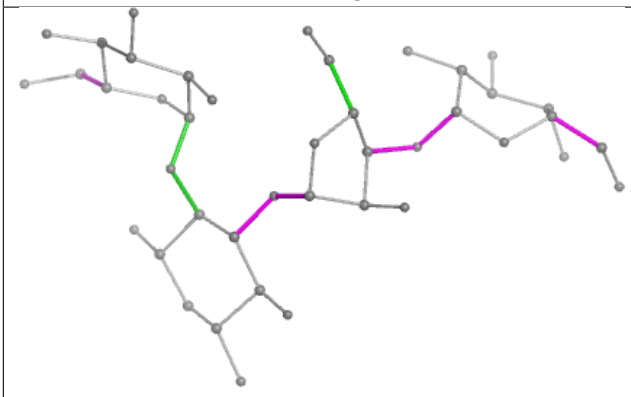
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand PAR 1 3967

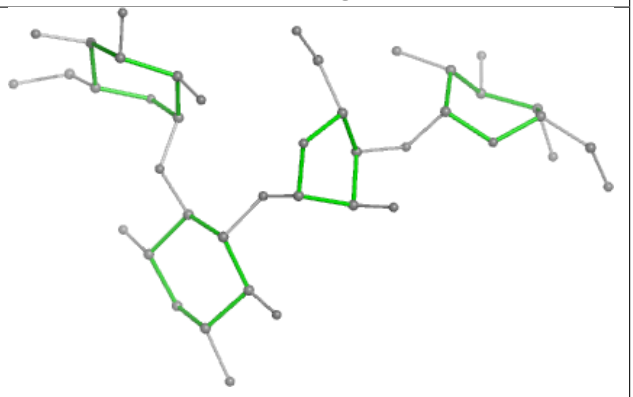


Bond lengths

Bond angles

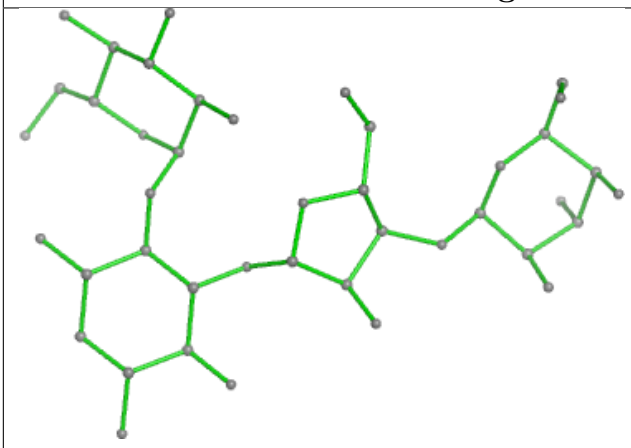


Torsions

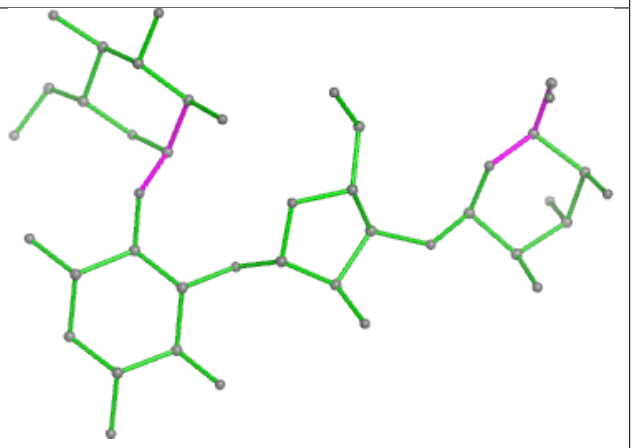


Rings

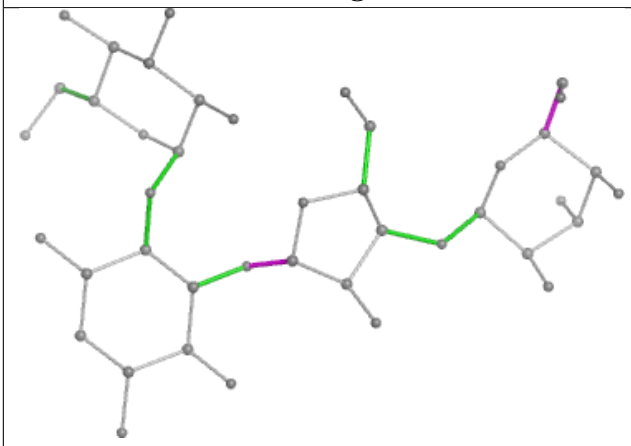
Ligand PAR CM 1946



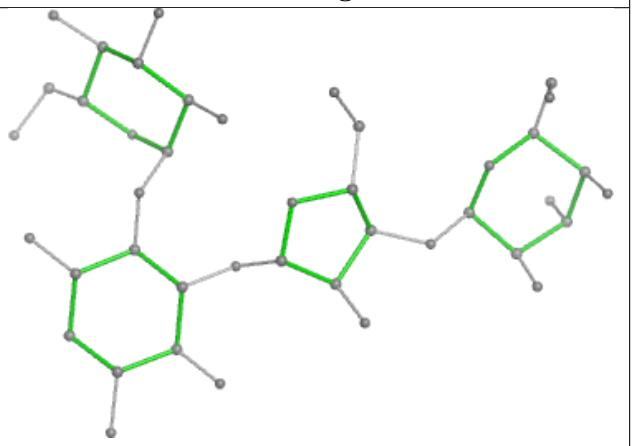
Bond lengths



Bond angles

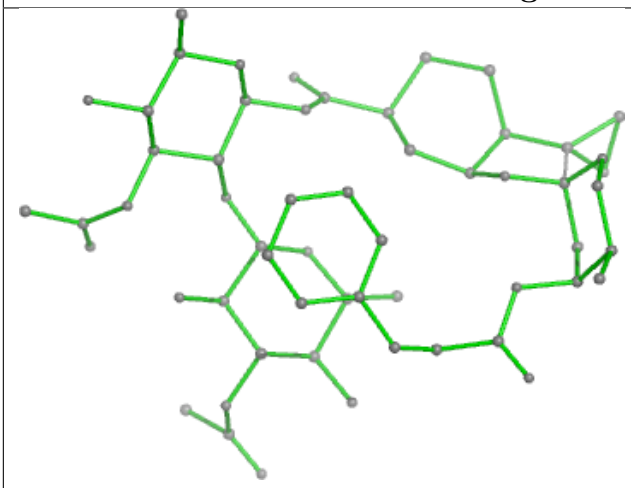


Torsions

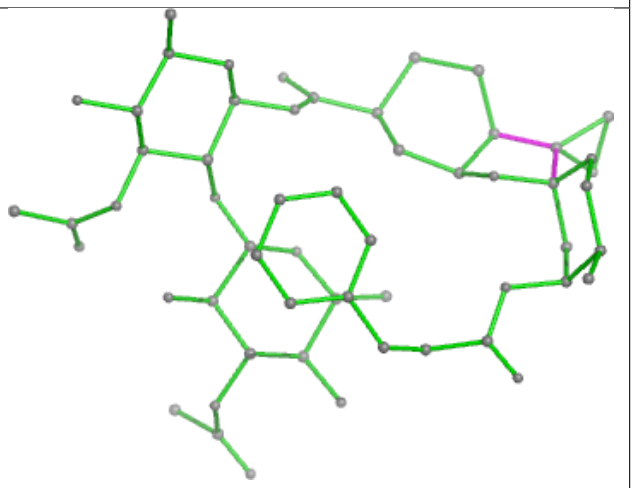


Rings

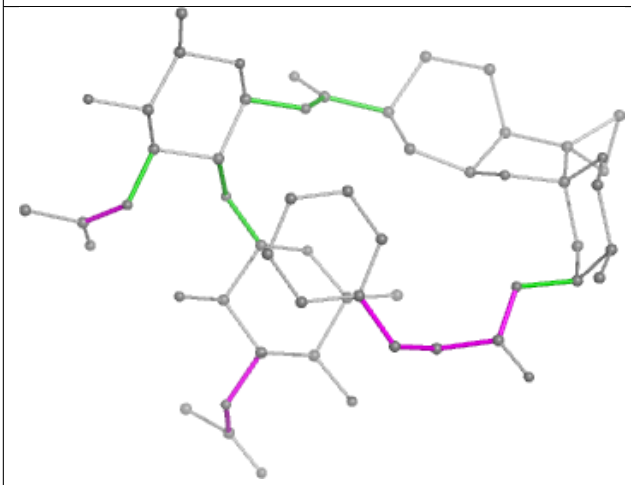
Ligand 3K5 CJ 202



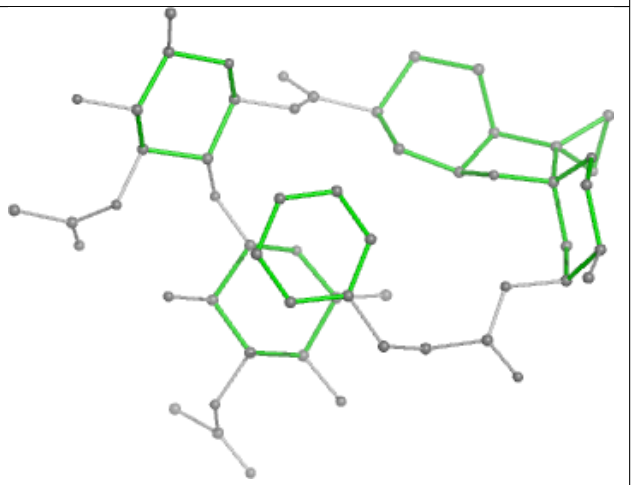
Bond lengths



Bond angles

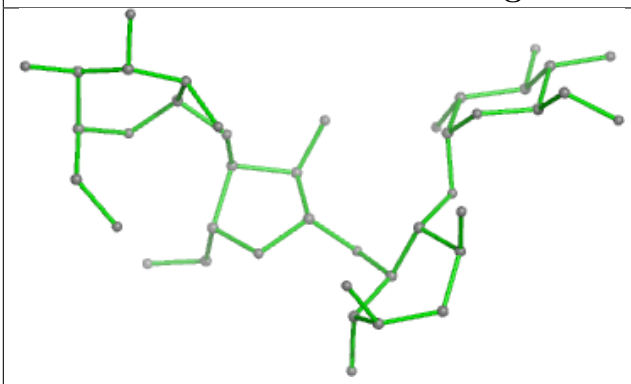


Torsions

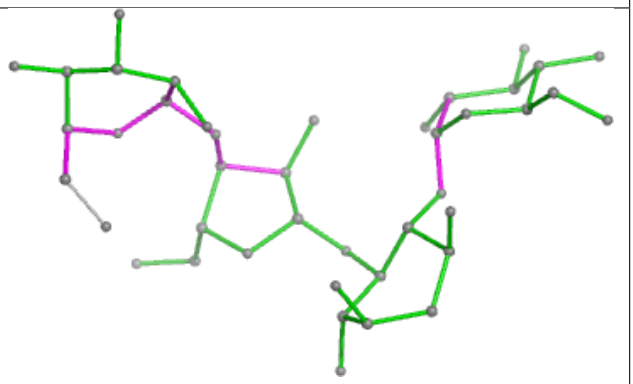


Rings

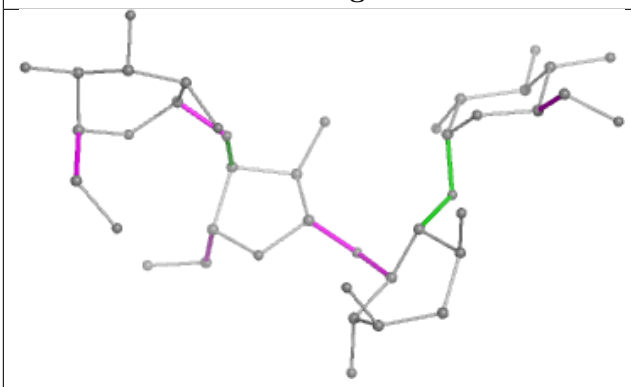
Ligand PAR AS 3790



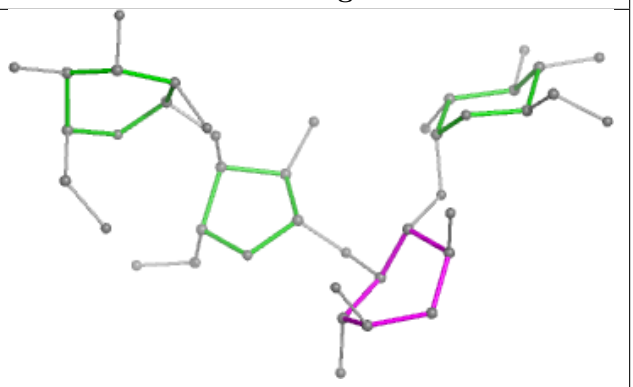
Bond lengths



Bond angles

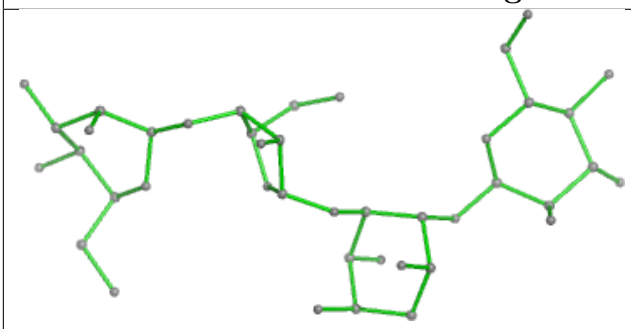


Torsions

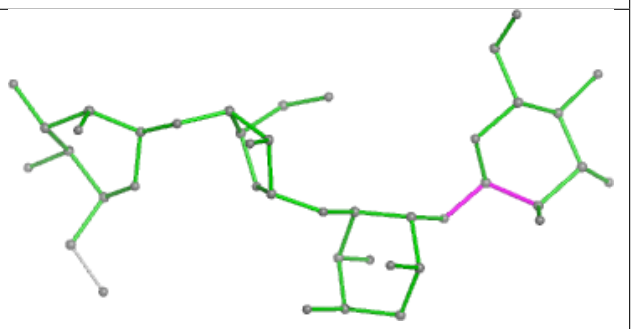


Rings

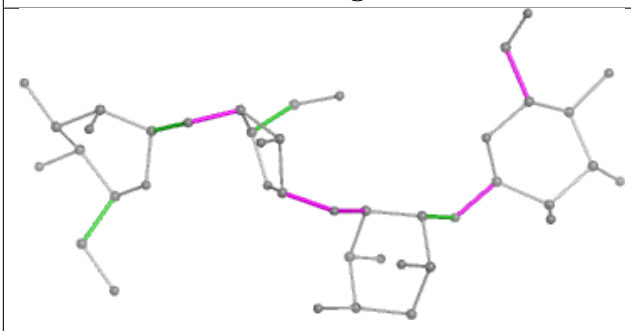
Ligand PAR AS 3789



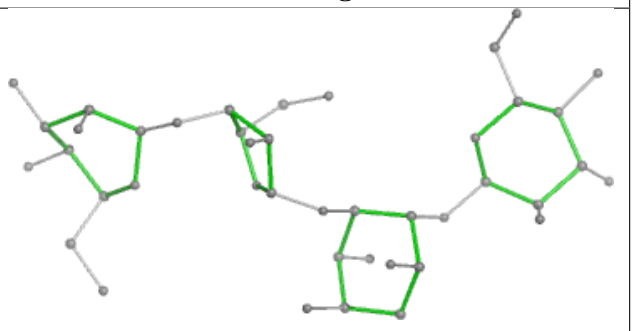
Bond lengths



Bond angles

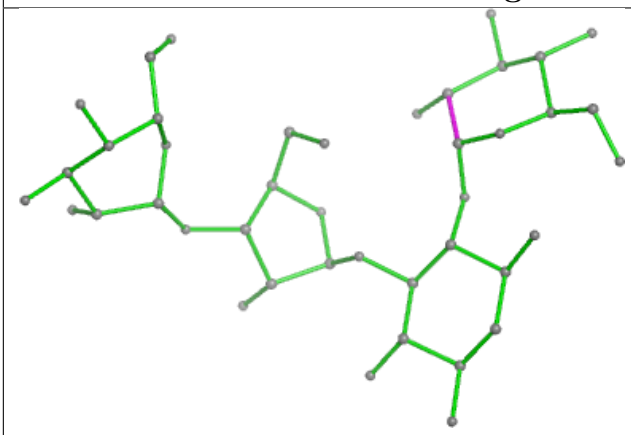


Torsions

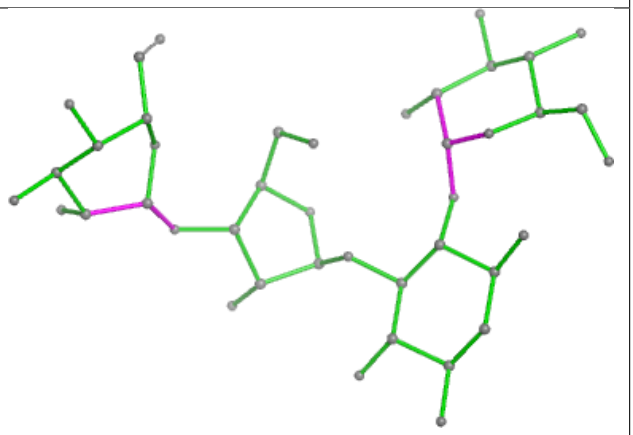


Rings

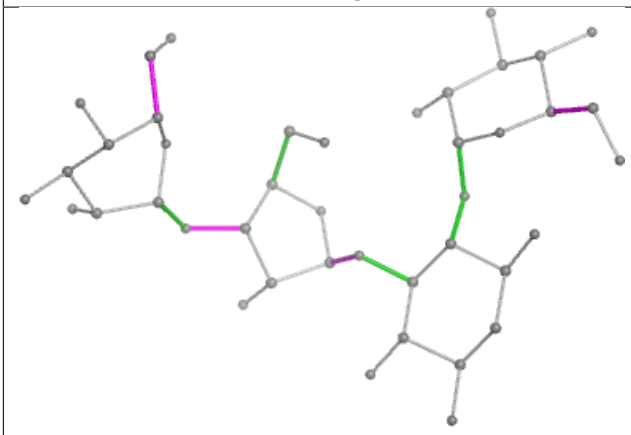
Ligand PAR AS 3788



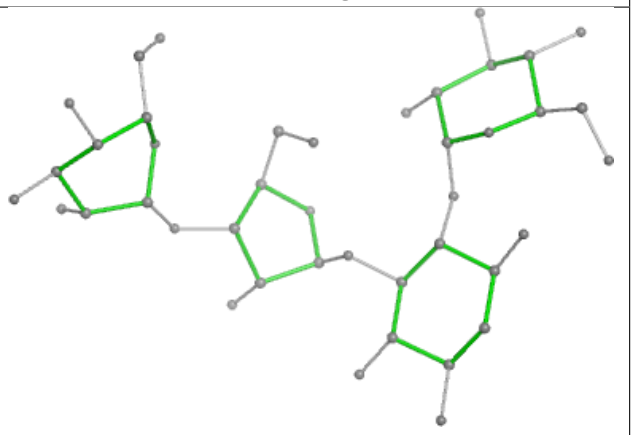
Bond lengths



Bond angles

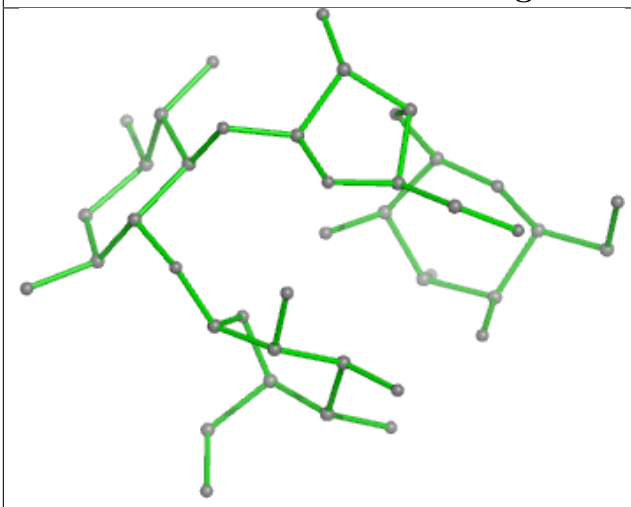


Torsions

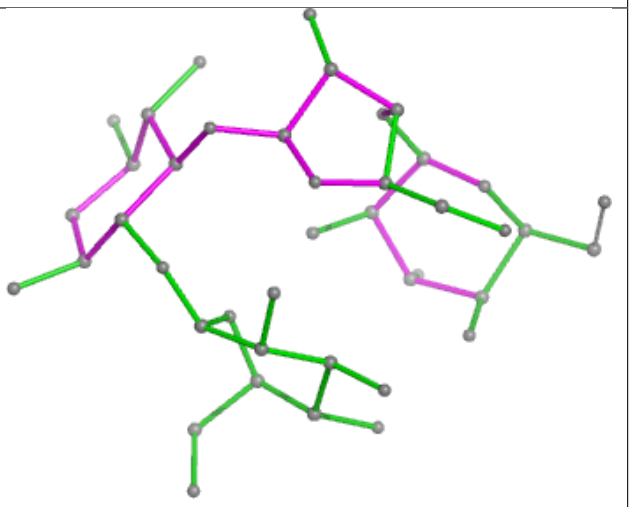


Rings

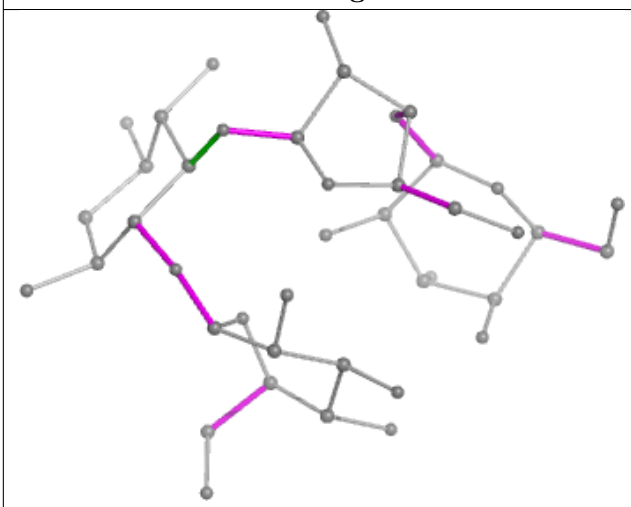
Ligand PAR B 1970



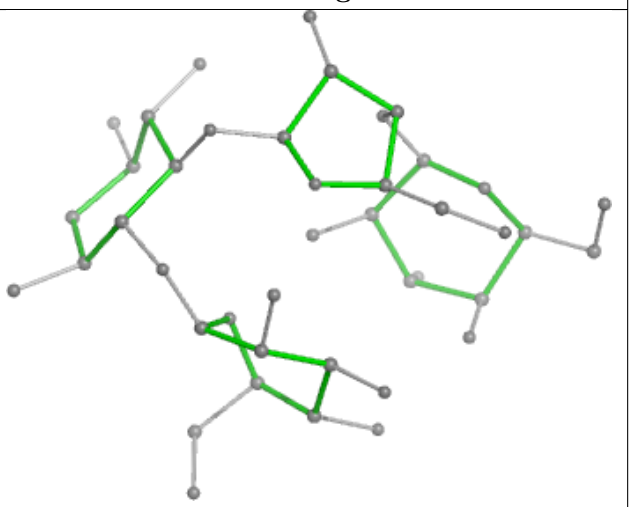
Bond lengths



Bond angles



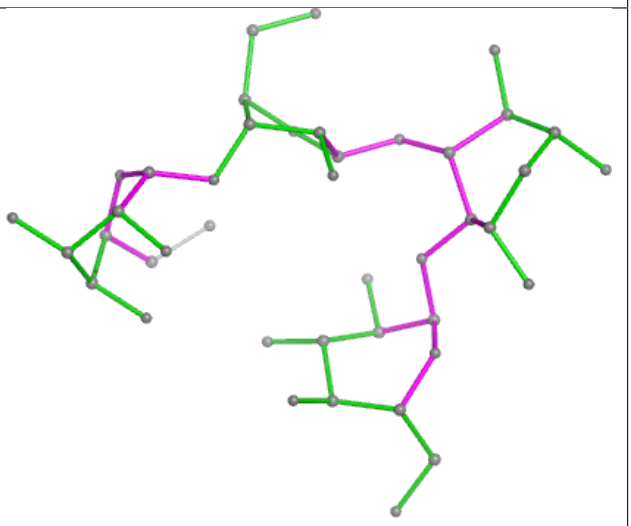
Torsions



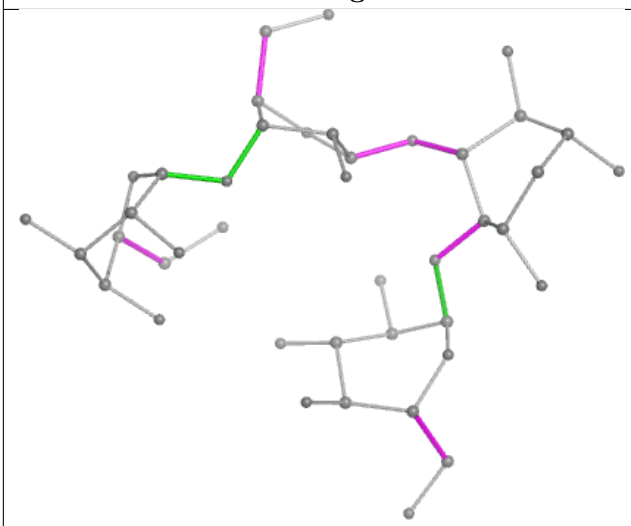
Rings

Ligand PAR 1 3969

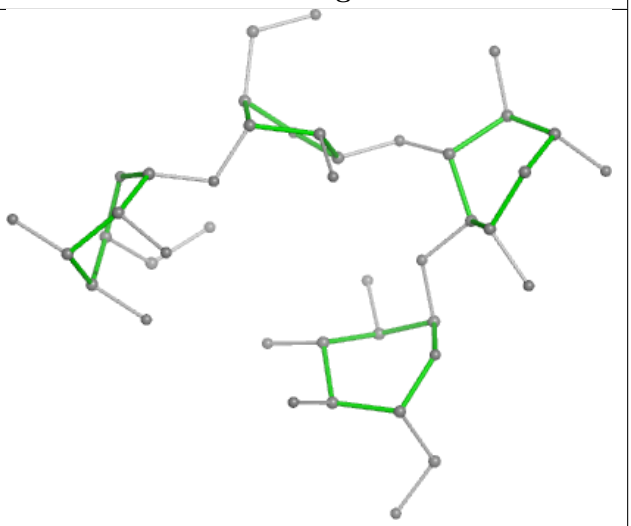
Bond lengths



Bond angles

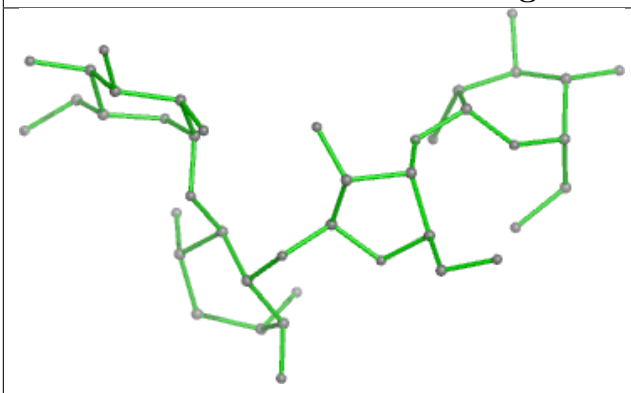


Torsions

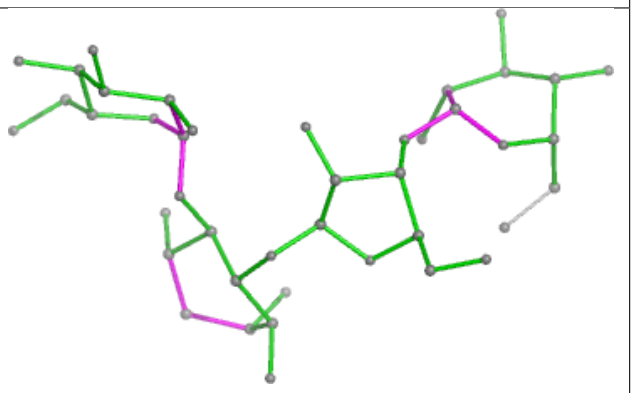


Rings

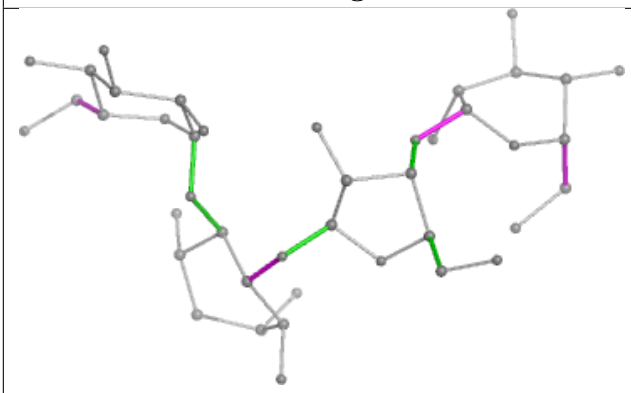
Ligand PAR 1 3968



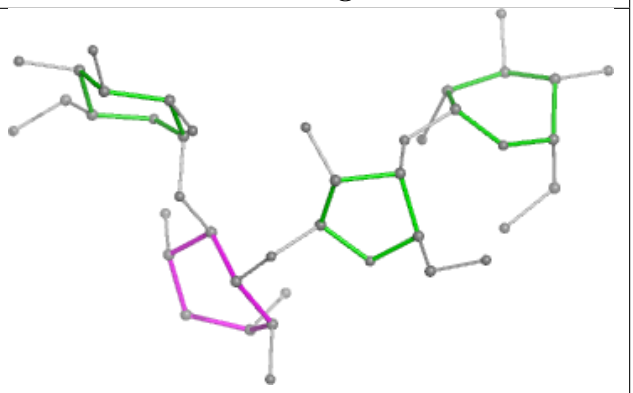
Bond lengths



Bond angles

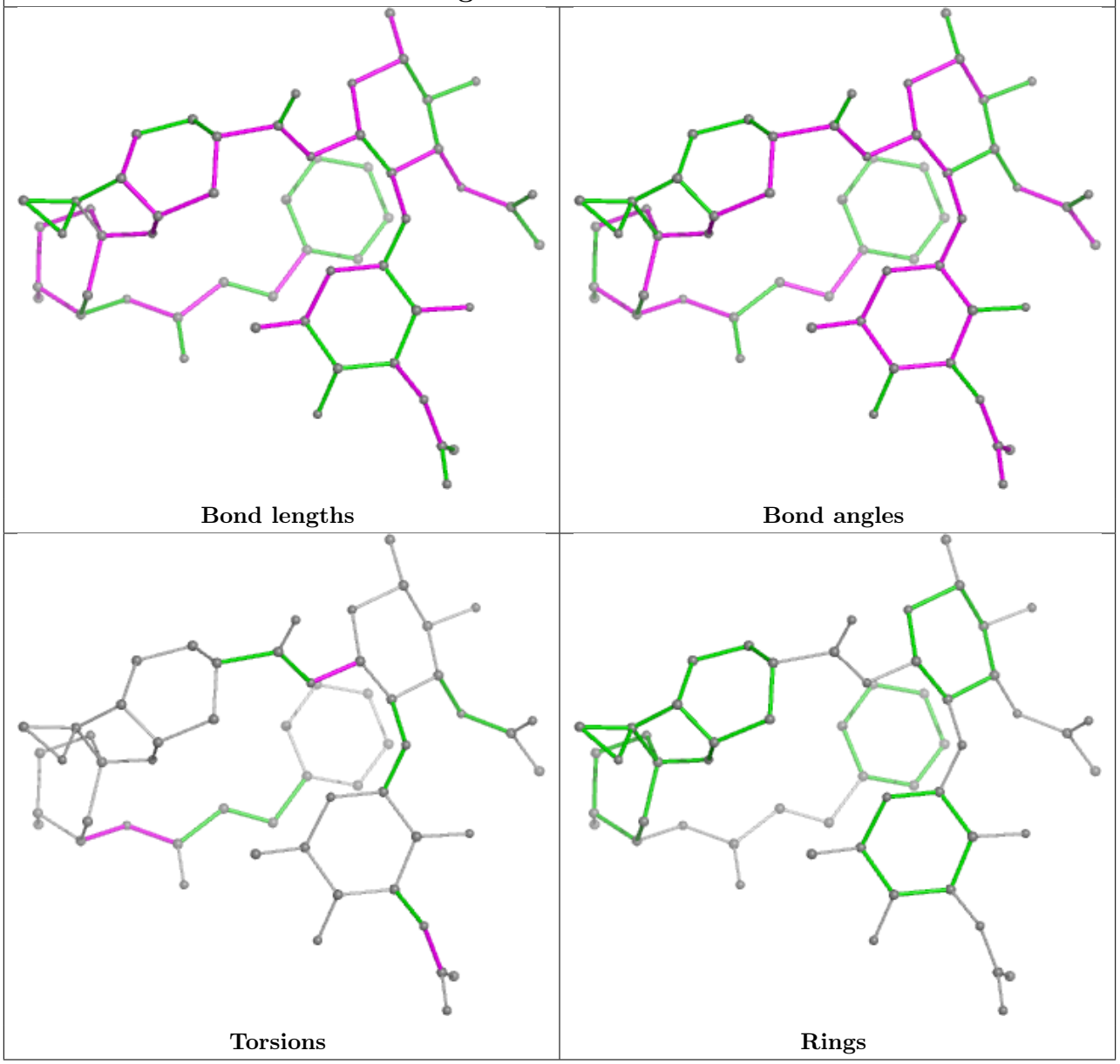


Torsions



Rings

Ligand 3K5 1 3406



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, 95^{th} 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%)	-0.26	26 (0%) 82 72	33, 71, 185, 393	0
1	AS	3199/3359 (95%)	-0.00	67 (2%) 63 48	49, 89, 219, 337	0
2	3	121/121 (100%)	-0.37	0 100 100	53, 92, 111, 143	0
2	AT	121/121 (100%)	-0.03	1 (0%) 82 72	53, 98, 122, 145	0
3	4	157/158 (99%)	-0.41	0 100 100	48, 71, 125, 166	0
3	AU	158/158 (100%)	0.01	1 (0%) 85 78	68, 108, 154, 217	0
4	AW	249/254 (98%)	0.64	22 (8%) 17 16	50, 91, 113, 132	0
4	j	249/254 (98%)	0.24	6 (2%) 59 44	26, 53, 80, 240	0
5	AX	386/389 (99%)	0.27	7 (1%) 67 53	47, 76, 110, 158	0
5	k	386/389 (99%)	0.31	13 (3%) 48 35	40, 67, 91, 136	0
6	AY	361/363 (99%)	1.06	51 (14%) 7 8	63, 95, 129, 159	0
6	l	361/363 (99%)	0.36	16 (4%) 39 30	38, 79, 114, 146	0
7	AZ	292/298 (97%)	1.24	57 (19%) 4 3	63, 120, 153, 172	0
7	m	296/298 (99%)	0.50	10 (3%) 48 35	64, 100, 125, 148	0
8	BA	153/176 (86%)	0.72	8 (5%) 34 27	66, 99, 128, 152	0
8	n	157/176 (89%)	0.36	2 (1%) 74 61	69, 92, 119, 145	0
9	BB	234/241 (97%)	0.46	9 (3%) 44 33	49, 79, 140, 187	0
9	o	234/241 (97%)	0.21	5 (2%) 63 48	48, 74, 120, 164	0
10	BC	233/262 (88%)	0.83	20 (8%) 18 16	100, 128, 169, 189	0
10	p	238/262 (90%)	0.21	6 (2%) 58 43	54, 81, 127, 159	0
11	BD	190/191 (99%)	0.61	9 (4%) 37 28	71, 101, 131, 160	0
11	q	190/191 (99%)	0.46	5 (2%) 57 42	69, 90, 115, 139	0
12	BE	208/220 (94%)	0.25	4 (1%) 66 51	50, 79, 129, 163	0
12	r	208/220 (94%)	0.43	8 (3%) 44 33	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%)	0.88	12 (7%) 24 20	85, 125, 151, 166	0
13	s	171/174 (98%)	0.52	3 (1%) 67 53	68, 103, 125, 135	0
14	BG	200/202 (99%)	0.77	14 (7%) 24 20	60, 112, 148, 175	0
14	t	200/202 (99%)	0.18	2 (1%) 79 68	48, 85, 119, 152	0
15	BH	130/131 (99%)	0.54	10 (7%) 21 18	62, 93, 126, 146	0
15	u	130/131 (99%)	0.21	5 (3%) 44 33	67, 86, 106, 121	0
16	BI	203/204 (99%)	1.25	33 (16%) 5 5	64, 101, 120, 130	0
16	v	203/204 (99%)	0.35	4 (1%) 64 50	41, 60, 77, 96	0
17	BJ	199/200 (99%)	0.36	5 (2%) 58 43	49, 72, 111, 148	0
17	w	199/200 (99%)	0.37	4 (2%) 64 50	44, 68, 101, 129	0
18	BK	176/185 (95%)	0.80	14 (7%) 20 18	51, 84, 115, 143	0
18	x	173/185 (93%)	0.46	6 (3%) 47 35	41, 68, 111, 132	0
19	BL	185/186 (99%)	0.67	10 (5%) 32 26	63, 90, 111, 128	0
19	y	185/186 (99%)	0.54	9 (4%) 36 28	50, 75, 97, 121	0
20	BM	179/190 (94%)	0.81	16 (8%) 17 16	68, 98, 166, 190	0
20	z	179/190 (94%)	0.46	13 (7%) 22 19	49, 75, 130, 160	0
21	0	170/172 (98%)	0.20	3 (1%) 67 53	56, 76, 97, 141	0
21	BN	170/172 (98%)	0.52	6 (3%) 47 35	54, 78, 109, 127	0
22	2	159/160 (99%)	0.47	8 (5%) 35 28	49, 74, 119, 141	0
22	BO	159/160 (99%)	0.89	14 (8%) 17 16	57, 84, 139, 157	0
23	5	103/124 (83%)	0.47	0 100 100	82, 112, 136, 152	0
23	BP	102/124 (82%)	0.47	1 (0%) 79 68	101, 139, 160, 183	0
24	6	131/137 (95%)	0.47	7 (5%) 33 26	40, 65, 90, 106	0
24	BQ	131/137 (95%)	0.61	6 (4%) 38 29	49, 70, 99, 123	0
25	7	118/155 (76%)	0.39	1 (0%) 82 72	44, 91, 134, 145	0
25	BR	98/155 (63%)	0.92	11 (11%) 11 11	62, 93, 145, 155	0
26	8	121/142 (85%)	0.41	4 (3%) 49 36	56, 76, 94, 135	0
26	BS	119/142 (83%)	0.94	15 (12%) 9 9	84, 109, 128, 137	0
27	9	126/127 (99%)	0.59	4 (3%) 50 37	60, 86, 110, 122	0
27	BT	126/127 (99%)	0.70	9 (7%) 23 20	71, 109, 138, 164	0
28	AA	135/136 (99%)	0.47	2 (1%) 71 58	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%)	0.75	7 (5%) 34 27	98, 127, 145, 166	0
29	AB	148/149 (99%)	0.38	6 (4%) 42 31	37, 70, 95, 125	0
29	BV	148/149 (99%)	0.98	18 (12%) 10 10	53, 95, 123, 144	0
30	AC	62/63 (98%)	1.02	8 (12%) 9 9	55, 87, 122, 137	0
30	BW	63/63 (100%)	1.57	16 (25%) 2 1	53, 105, 146, 167	1 (1%)
31	AD	96/106 (90%)	-0.03	2 (2%) 63 48	52, 79, 107, 130	0
31	BX	96/106 (90%)	0.65	5 (5%) 34 27	90, 116, 148, 155	0
32	AE	110/112 (98%)	0.22	0 100 100	53, 74, 122, 137	0
32	BY	108/112 (96%)	0.74	5 (4%) 38 29	63, 96, 138, 172	0
33	AF	124/131 (94%)	0.55	4 (3%) 50 37	51, 75, 95, 108	0
33	BZ	125/131 (95%)	0.81	10 (8%) 20 18	52, 84, 111, 128	1 (0%)
34	AG	106/107 (99%)	0.29	2 (1%) 66 51	51, 72, 97, 109	0
34	CA	106/107 (99%)	0.52	5 (4%) 37 28	44, 73, 98, 118	3 (2%)
35	AH	112/113 (99%)	0.62	6 (5%) 32 26	51, 72, 119, 139	0
35	CB	111/113 (98%)	1.25	23 (20%) 3 3	71, 109, 145, 171	4 (3%)
36	AI	120/120 (100%)	0.47	2 (1%) 69 55	62, 86, 116, 137	0
36	CC	118/120 (98%)	1.12	17 (14%) 7 7	87, 116, 139, 160	0
37	AJ	97/99 (97%)	0.23	0 100 100	52, 78, 109, 153	0
37	CD	97/99 (97%)	1.38	18 (18%) 4 4	90, 120, 159, 176	1 (1%)
38	AK	86/90 (95%)	0.42	2 (2%) 61 46	33, 56, 93, 130	0
38	CE	86/90 (95%)	0.88	12 (13%) 7 8	63, 88, 128, 161	0
39	AL	77/78 (98%)	0.50	3 (3%) 44 33	75, 97, 121, 146	0
39	CF	77/78 (98%)	0.79	6 (7%) 20 18	93, 129, 166, 184	1 (1%)
40	AM	50/51 (98%)	0.38	2 (4%) 43 32	44, 65, 96, 97	0
40	CG	50/51 (98%)	1.37	10 (20%) 3 3	78, 95, 117, 129	0
41	AN	52/52 (100%)	1.26	11 (21%) 3 2	90, 109, 125, 140	0
41	CH	52/52 (100%)	1.04	7 (13%) 8 8	81, 121, 140, 160	1 (1%)
42	AO	25/25 (100%)	1.38	5 (20%) 3 3	69, 80, 96, 100	0
42	CI	24/25 (96%)	1.11	5 (20%) 3 2	72, 81, 96, 109	0
43	AP	103/106 (97%)	0.21	4 (3%) 44 33	39, 71, 108, 129	0
43	CJ	103/106 (97%)	0.80	8 (7%) 20 18	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%)	0.25	3 (3%) 49 36	37, 59, 101, 127	0
44	CK	91/92 (98%)	0.57	5 (5%) 32 25	60, 93, 141, 151	0
45	CL	121/267 (45%)	1.45	34 (28%) 2 1	79, 119, 153, 163	0
45	i	121/267 (45%)	1.48	37 (30%) 1 1	88, 117, 147, 157	0
46	B	1712/1787 (95%)	-0.03	17 (0%) 79 68	52, 102, 183, 234	0
46	CM	1726/1787 (96%)	0.40	76 (4%) 39 30	60, 114, 210, 260	0
47	C	208/261 (79%)	0.59	11 (5%) 33 26	86, 116, 138, 150	0
47	CN	208/261 (79%)	0.81	16 (7%) 21 18	85, 128, 158, 190	0
48	CO	214/256 (83%)	1.03	30 (14%) 7 8	99, 136, 168, 188	0
48	D	214/256 (83%)	0.28	5 (2%) 61 46	69, 96, 117, 128	0
49	CP	216/249 (86%)	0.54	15 (6%) 24 20	52, 98, 135, 160	0
49	E	217/249 (87%)	0.61	15 (6%) 24 20	74, 100, 128, 146	0
50	CQ	223/251 (88%)	1.10	35 (15%) 6 6	99, 123, 165, 199	0
50	F	223/251 (88%)	0.74	17 (7%) 21 19	85, 116, 144, 157	0
51	CR	260/262 (99%)	0.89	28 (10%) 12 12	69, 108, 134, 170	0
51	G	259/262 (98%)	0.74	17 (6%) 26 21	76, 101, 118, 127	0
52	CS	195/225 (86%)	1.03	29 (14%) 7 6	108, 135, 155, 164	0
52	H	206/225 (91%)	0.73	23 (11%) 11 11	89, 111, 140, 166	0
53	CT	226/236 (95%)	0.92	32 (14%) 7 7	74, 121, 172, 204	0
53	I	226/236 (95%)	0.59	12 (5%) 33 26	65, 109, 141, 157	0
54	CU	182/186 (97%)	0.79	18 (9%) 14 14	81, 142, 173, 184	0
54	J	185/186 (99%)	0.70	11 (5%) 29 24	85, 119, 141, 156	0
55	CV	203/206 (98%)	1.18	35 (17%) 5 4	65, 100, 153, 194	0
55	K	203/206 (98%)	0.36	5 (2%) 58 43	46, 86, 131, 146	0
56	CW	178/189 (94%)	1.08	24 (13%) 8 8	81, 116, 146, 160	0
56	L	178/189 (94%)	1.15	23 (12%) 9 9	78, 110, 129, 140	0
57	CX	93/118 (78%)	1.22	20 (21%) 3 2	103, 137, 163, 177	0
57	M	98/118 (83%)	0.76	9 (9%) 16 15	94, 123, 141, 148	0
58	CY	141/155 (90%)	1.06	19 (13%) 8 8	68, 93, 131, 177	0
58	N	144/155 (92%)	0.59	6 (4%) 41 31	60, 85, 116, 178	0
59	CZ	116/143 (81%)	0.90	10 (8%) 18 16	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%)	1.03	15 (12%) 9 9	132, 157, 173, 175	0
60	DA	150/151 (99%)	1.03	16 (10%) 12 12	79, 113, 136, 154	0
60	P	150/151 (99%)	0.53	9 (6%) 29 23	58, 89, 115, 122	0
61	DB	127/132 (96%)	0.76	10 (7%) 20 18	84, 125, 146, 153	0
61	Q	127/132 (96%)	0.16	3 (2%) 59 44	59, 85, 104, 117	0
62	DC	129/142 (90%)	2.09	65 (50%) 0 0	113, 139, 164, 181	0
62	R	129/142 (90%)	0.85	11 (8%) 18 17	83, 113, 146, 157	0
63	DD	140/142 (98%)	1.79	46 (32%) 1 1	112, 140, 160, 173	0
63	S	140/142 (98%)	1.22	27 (19%) 4 3	90, 118, 138, 151	0
64	DE	125/137 (91%)	1.20	24 (19%) 4 3	102, 141, 182, 190	0
64	T	124/137 (90%)	0.93	14 (11%) 11 11	98, 122, 152, 158	0
65	DF	142/145 (97%)	1.53	35 (24%) 2 1	104, 136, 161, 196	0
65	U	144/145 (99%)	0.60	9 (6%) 27 22	85, 104, 126, 153	0
66	DG	141/145 (97%)	1.40	34 (24%) 2 2	105, 135, 160, 186	0
66	V	141/145 (97%)	0.79	13 (9%) 16 15	99, 118, 138, 163	0
67	DH	100/119 (84%)	1.38	27 (27%) 2 1	91, 136, 168, 175	0
67	W	102/119 (85%)	1.11	19 (18%) 4 4	86, 125, 141, 156	0
68	DI	87/87 (100%)	0.50	4 (4%) 38 29	83, 112, 147, 169	0
68	X	87/87 (100%)	0.49	2 (2%) 61 46	76, 104, 128, 144	0
69	DJ	129/130 (99%)	0.71	9 (6%) 24 20	70, 93, 113, 121	0
69	Y	129/130 (99%)	0.74	11 (8%) 18 17	71, 88, 108, 117	0
70	DK	143/145 (98%)	1.07	14 (9%) 14 14	64, 88, 115, 142	0
70	Z	143/145 (98%)	0.36	2 (1%) 73 60	65, 86, 108, 128	0
71	DL	132/135 (97%)	0.54	6 (4%) 39 29	98, 127, 151, 176	0
71	a	134/135 (99%)	0.72	8 (5%) 29 23	84, 114, 131, 142	0
72	DM	71/105 (67%)	0.56	4 (5%) 31 25	125, 148, 169, 177	0
72	b	72/105 (68%)	0.19	1 (1%) 73 60	94, 122, 140, 143	0
73	DN	97/119 (81%)	1.18	15 (15%) 6 6	85, 105, 154, 166	0
73	c	98/119 (82%)	0.84	9 (9%) 16 15	71, 91, 127, 138	0
74	DO	81/82 (98%)	0.88	5 (6%) 28 22	92, 128, 173, 190	0
74	d	81/82 (98%)	0.51	3 (3%) 45 33	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%)	0.75	6 (10%) 13 13	112, 139, 163, 178	0
75	e	62/67 (92%)	0.81	8 (12%) 9 9	100, 120, 139, 145	0
76	DQ	55/56 (98%)	1.91	23 (41%) 1 0	99, 119, 163, 182	0
76	f	55/56 (98%)	1.16	7 (12%) 9 9	88, 104, 133, 144	0
77	DR	56/63 (88%)	1.41	11 (19%) 4 3	91, 125, 176, 199	0
77	g	60/63 (95%)	0.87	9 (15%) 6 6	89, 116, 141, 158	0
78	DS	70/193 (36%)	1.93	34 (48%) 0 0	166, 184, 197, 204	0
78	h	63/193 (32%)	1.12	13 (20%) 3 3	132, 154, 164, 169	0
79	AR	311/317 (98%)	0.82	26 (8%) 18 17	112, 141, 163, 176	0
79	DT	311/317 (98%)	0.94	36 (11%) 11 11	131, 161, 184, 208	0
80	L1	217/217 (100%)	0.85	17 (7%) 20 18	116, 148, 185, 242	0
80	l1	217/217 (100%)	1.00	23 (10%) 13 12	132, 158, 182, 217	0
All	All	33241/35542 (93%)	0.48	2153 (6%) 26 21	26, 98, 166, 393	14 (0%)

The worst 5 of 2153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
51	G	110	ALA	9.1
63	DD	131	ARG	9.0
6	AY	363	ASN	8.5
48	CO	55	LYS	8.4
46	CM	1480	G	7.6

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

median, 95^{th} 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	0.21	106,106,106,106	0
81	MG	B	1834	1/1	0.24	0.24	241,241,241,241	0
81	MG	B	1848	1/1	0.43	0.18	57,57,57,57	0
81	MG	CM	1811	1/1	0.43	0.36	73,73,73,73	0
81	MG	1	3470	1/1	0.47	0.28	48,48,48,48	0
81	MG	B	1805	1/1	0.47	0.35	82,82,82,82	0
81	MG	8	201	1/1	0.51	0.15	55,55,55,55	0
81	MG	B	1960	1/1	0.53	0.20	41,41,41,41	0
81	MG	AS	3484	1/1	0.53	0.18	43,43,43,43	0
81	MG	1	3694	1/1	0.53	0.18	120,120,120,120	0
81	MG	B	1932	1/1	0.54	0.29	81,81,81,81	0
81	MG	1	3800	1/1	0.54	0.26	95,95,95,95	0
81	MG	1	3783	1/1	0.55	0.16	36,36,36,36	0
81	MG	CM	1871	1/1	0.56	0.18	99,99,99,99	0
81	MG	CM	1925	1/1	0.56	0.29	61,61,61,61	0
81	MG	B	1966	1/1	0.57	0.17	99,99,99,99	0
81	MG	CM	1833	1/1	0.57	0.36	69,69,69,69	0
81	MG	AS	3581	1/1	0.58	0.11	66,66,66,66	0
81	MG	AS	3595	1/1	0.58	0.25	47,47,47,47	0
81	MG	g	101	1/1	0.58	0.34	66,66,66,66	0
81	MG	B	1925	1/1	0.59	0.13	76,76,76,76	0
81	MG	1	3457	1/1	0.60	0.20	44,44,44,44	0
81	MG	B	1919	1/1	0.60	0.15	110,110,110,110	0
81	MG	AS	3588	1/1	0.61	0.36	79,79,79,79	0
81	MG	CM	1883	1/1	0.61	0.20	65,65,65,65	0
81	MG	AS	3497	1/1	0.61	0.25	75,75,75,75	0
81	MG	AS	3647	1/1	0.62	0.24	62,62,62,62	0
81	MG	k	403	1/1	0.62	0.34	78,78,78,78	0
81	MG	1	3869	1/1	0.63	0.28	61,61,61,61	0
81	MG	1	3755	1/1	0.63	0.16	51,51,51,51	0
81	MG	CM	1822	1/1	0.63	0.22	81,81,81,81	0
81	MG	1	3677	1/1	0.63	0.12	55,55,55,55	0
81	MG	B	1893	1/1	0.63	0.17	69,69,69,69	0
81	MG	1	3433	1/1	0.63	0.36	72,72,72,72	0
81	MG	AS	3632	1/1	0.63	0.16	91,91,91,91	0
81	MG	CM	1940	1/1	0.63	0.30	59,59,59,59	0
84	ZN	AP	201	1/1	0.63	0.28	234,234,234,234	0
81	MG	B	1836	1/1	0.64	0.35	78,78,78,78	0
81	MG	AS	3528	1/1	0.64	0.18	97,97,97,97	0
81	MG	B	1967	1/1	0.64	0.09	71,71,71,71	0
81	MG	AS	3704	1/1	0.65	0.24	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	AS	3762	1/1	0.65	0.11	57,57,57,57	0
81	MG	4	212	1/1	0.65	0.14	81,81,81,81	0
81	MG	1	3603	1/1	0.65	0.31	64,64,64,64	0
81	MG	1	3668	1/1	0.65	0.22	57,57,57,57	0
81	MG	AS	3550	1/1	0.66	0.26	48,48,48,48	0
81	MG	B	1871	1/1	0.66	0.24	64,64,64,64	0
81	MG	1	3844	1/1	0.66	0.22	75,75,75,75	0
81	MG	3	211	1/1	0.66	0.21	64,64,64,64	0
81	MG	B	1801	1/1	0.66	0.19	54,54,54,54	0
81	MG	CM	1897	1/1	0.66	0.25	105,105,105,105	0
81	MG	B	1931	1/1	0.66	0.25	72,72,72,72	0
81	MG	1	3857	1/1	0.66	0.16	49,49,49,49	0
81	MG	CL	302	1/1	0.66	0.32	43,43,43,43	0
81	MG	B	1956	1/1	0.66	0.12	67,67,67,67	0
81	MG	AS	3737	1/1	0.67	0.30	60,60,60,60	0
81	MG	1	3748	1/1	0.67	0.15	27,27,27,27	0
81	MG	B	1854	1/1	0.67	0.17	96,96,96,96	0
81	MG	1	3894	1/1	0.67	0.24	52,52,52,52	0
81	MG	1	3788	1/1	0.68	0.20	57,57,57,57	0
81	MG	DB	201	1/1	0.68	0.19	67,67,67,67	0
81	MG	AS	3464	1/1	0.68	0.24	81,81,81,81	0
81	MG	1	3879	1/1	0.68	0.23	63,63,63,63	0
81	MG	D	301	1/1	0.69	0.32	69,69,69,69	0
81	MG	DC	201	1/1	0.69	0.32	42,42,42,42	0
81	MG	AS	3729	1/1	0.69	0.47	79,79,79,79	0
81	MG	1	3839	1/1	0.69	0.15	50,50,50,50	0
81	MG	1	3715	1/1	0.70	0.25	51,51,51,51	0
81	MG	B	1923	1/1	0.70	0.16	92,92,92,92	0
81	MG	1	3502	1/1	0.70	0.19	55,55,55,55	0
81	MG	1	3852	1/1	0.70	0.33	62,62,62,62	0
81	MG	AS	3765	1/1	0.70	0.18	44,44,44,44	0
81	MG	AT	203	1/1	0.70	0.29	71,71,71,71	0
81	MG	1	3584	1/1	0.70	0.25	61,61,61,61	0
81	MG	B	1889	1/1	0.70	0.23	71,71,71,71	0
83	PAR	AS	3789	42/42	0.70	0.16	69,100,118,123	42
81	MG	1	3802	1/1	0.70	0.08	89,89,89,89	0
81	MG	B	1843	1/1	0.71	0.12	83,83,83,83	0
81	MG	1	3464	1/1	0.71	0.28	34,34,34,34	0
81	MG	B	1922	1/1	0.71	0.15	65,65,65,65	0
81	MG	3	207	1/1	0.71	0.24	87,87,87,87	0
81	MG	1	3766	1/1	0.71	0.12	63,63,63,63	0
81	MG	1	3789	1/1	0.71	0.31	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3796	1/1	0.71	0.13	62,62,62,62	0
81	MG	CM	1912	1/1	0.72	0.22	62,62,62,62	0
81	MG	1	3415	1/1	0.72	0.31	23,23,23,23	0
81	MG	AS	3535	1/1	0.72	0.18	88,88,88,88	0
81	MG	CM	1857	1/1	0.72	0.18	99,99,99,99	0
81	MG	1	3509	1/1	0.72	0.15	30,30,30,30	0
81	MG	1	3931	1/1	0.72	0.10	58,58,58,58	0
81	MG	CM	1890	1/1	0.72	0.17	57,57,57,57	0
81	MG	F	301	1/1	0.72	0.20	69,69,69,69	0
81	MG	B	1915	1/1	0.73	0.20	76,76,76,76	0
81	MG	BH	201	1/1	0.73	0.11	54,54,54,54	0
81	MG	DB	203	1/1	0.73	0.18	117,117,117,117	0
81	MG	AS	3507	1/1	0.73	0.28	72,72,72,72	0
81	MG	1	3890	1/1	0.73	0.09	45,45,45,45	0
81	MG	1	3798	1/1	0.73	0.21	50,50,50,50	0
83	PAR	AS	3790	42/42	0.73	0.19	81,107,127,140	0
81	MG	B	1815	1/1	0.73	0.32	59,59,59,59	0
84	ZN	CB	201	1/1	0.73	0.26	255,255,255,255	0
81	MG	1	3545	1/1	0.74	0.17	34,34,34,34	0
81	MG	AU	203	1/1	0.74	0.16	100,100,100,100	0
81	MG	1	3904	1/1	0.74	0.14	57,57,57,57	0
81	MG	1	3649	1/1	0.74	0.11	53,53,53,53	0
81	MG	CQ	304	1/1	0.74	0.11	71,71,71,71	0
81	MG	AS	3649	1/1	0.74	0.12	54,54,54,54	0
81	MG	1	3864	1/1	0.74	0.10	62,62,62,62	0
81	MG	1	3555	1/1	0.74	0.16	53,53,53,53	0
81	MG	CM	1862	1/1	0.74	0.26	64,64,64,64	0
83	PAR	B	1970	42/42	0.74	0.17	82,119,132,143	0
81	MG	1	3754	1/1	0.74	0.12	59,59,59,59	0
81	MG	CM	1873	1/1	0.74	0.33	40,40,40,40	0
81	MG	AS	3457	1/1	0.74	0.27	37,37,37,37	0
81	MG	1	3425	1/1	0.74	0.32	40,40,40,40	0
81	MG	B	1879	1/1	0.75	0.12	94,94,94,94	0
81	MG	AS	3671	1/1	0.75	0.25	46,46,46,46	0
81	MG	B	1946	1/1	0.75	0.10	72,72,72,72	0
81	MG	AS	3709	1/1	0.75	0.08	52,52,52,52	0
81	MG	B	1949	1/1	0.75	0.18	75,75,75,75	0
81	MG	4	215	1/1	0.75	0.15	56,56,56,56	0
81	MG	1	3843	1/1	0.75	0.25	63,63,63,63	0
81	MG	1	3909	1/1	0.75	0.14	44,44,44,44	0
81	MG	AS	3779	1/1	0.75	0.25	57,57,57,57	0
81	MG	AP	203	1/1	0.75	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	4	208	1/1	0.75	0.21	57,57,57,57	0
81	MG	1	3866	1/1	0.75	0.15	81,81,81,81	0
81	MG	DJ	202	1/1	0.75	0.11	53,53,53,53	0
81	MG	CM	1801	1/1	0.75	0.21	36,36,36,36	0
81	MG	4	213	1/1	0.75	0.13	49,49,49,49	0
81	MG	AS	3598	1/1	0.75	0.17	69,69,69,69	0
81	MG	AS	3615	1/1	0.75	0.19	50,50,50,50	0
81	MG	AS	3424	1/1	0.75	0.20	52,52,52,52	0
81	MG	B	1874	1/1	0.75	0.23	51,51,51,51	0
81	MG	B	1909	1/1	0.76	0.08	62,62,62,62	0
81	MG	B	1924	1/1	0.76	0.08	89,89,89,89	0
81	MG	j	304	1/1	0.76	0.20	42,42,42,42	0
83	PAR	1	3969	42/42	0.76	0.14	47,103,124,126	0
81	MG	AS	3781	1/1	0.76	0.13	49,49,49,49	0
81	MG	1	3585	1/1	0.76	0.12	53,53,53,53	0
81	MG	1	3645	1/1	0.76	0.17	56,56,56,56	0
84	ZN	AH	201	1/1	0.76	0.14	213,213,213,213	0
81	MG	AS	3618	1/1	0.76	0.15	58,58,58,58	0
81	MG	B	1945	1/1	0.76	0.15	61,61,61,61	0
81	MG	CM	1917	1/1	0.77	0.15	86,86,86,86	0
81	MG	AT	208	1/1	0.77	0.29	49,49,49,49	0
81	MG	1	3423	1/1	0.77	0.24	55,55,55,55	0
81	MG	1	3611	1/1	0.77	0.15	50,50,50,50	0
81	MG	DA	202	1/1	0.77	0.23	70,70,70,70	0
81	MG	AS	3522	1/1	0.77	0.24	36,36,36,36	0
81	MG	1	3771	1/1	0.77	0.16	109,109,109,109	0
81	MG	1	3838	1/1	0.77	0.25	35,35,35,35	0
81	MG	V	201	1/1	0.77	0.13	75,75,75,75	0
81	MG	1	3644	1/1	0.77	0.12	56,56,56,56	0
81	MG	AS	3585	1/1	0.77	0.33	58,58,58,58	0
81	MG	AR	401	1/1	0.77	0.16	83,83,83,83	0
83	PAR	AS	3788	42/42	0.77	0.15	84,114,125,131	0
81	MG	1	3535	1/1	0.77	0.22	84,84,84,84	0
81	MG	1	3597	1/1	0.77	0.49	78,78,78,78	0
81	MG	B	1959	1/1	0.77	0.29	44,44,44,44	0
81	MG	AS	3783	1/1	0.77	0.14	65,65,65,65	0
81	MG	1	3667	1/1	0.77	0.12	50,50,50,50	0
81	MG	CM	1915	1/1	0.78	0.24	66,66,66,66	0
81	MG	1	3856	1/1	0.78	0.14	54,54,54,54	0
81	MG	1	3466	1/1	0.78	0.36	47,47,47,47	0
81	MG	AS	3620	1/1	0.78	0.14	110,110,110,110	0
81	MG	CM	1945	1/1	0.78	0.18	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3420	1/1	0.78	0.12	38,38,38,38	0
81	MG	B	1911	1/1	0.78	0.17	58,58,58,58	0
81	MG	1	3471	1/1	0.78	0.16	41,41,41,41	0
81	MG	1	3811	1/1	0.78	0.16	38,38,38,38	0
81	MG	AS	3682	1/1	0.78	0.25	77,77,77,77	0
81	MG	CM	1830	1/1	0.78	0.23	81,81,81,81	0
81	MG	1	3484	1/1	0.78	0.19	60,60,60,60	0
83	PAR	1	3968	42/42	0.78	0.16	56,91,119,122	0
81	MG	1	3888	1/1	0.78	0.14	55,55,55,55	0
81	MG	1	3552	1/1	0.78	0.18	75,75,75,75	0
81	MG	I	301	1/1	0.78	0.17	85,85,85,85	0
81	MG	1	3490	1/1	0.78	0.15	45,45,45,45	0
81	MG	y	202	1/1	0.78	0.13	45,45,45,45	0
81	MG	1	3730	1/1	0.78	0.20	48,48,48,48	0
81	MG	1	3578	1/1	0.78	0.14	41,41,41,41	0
81	MG	AS	3782	1/1	0.78	0.12	37,37,37,37	0
81	MG	1	3764	1/1	0.79	0.32	63,63,63,63	0
81	MG	B	1863	1/1	0.79	0.09	103,103,103,103	0
81	MG	1	3842	1/1	0.79	0.12	27,27,27,27	0
81	MG	1	3635	1/1	0.79	0.20	61,61,61,61	0
81	MG	1	3558	1/1	0.79	0.13	65,65,65,65	0
81	MG	1	3926	1/1	0.79	0.10	37,37,37,37	0
81	MG	Z	201	1/1	0.79	0.21	61,61,61,61	0
81	MG	1	3830	1/1	0.79	0.14	28,28,28,28	0
81	MG	B	1901	1/1	0.79	0.12	74,74,74,74	0
81	MG	AS	3612	1/1	0.79	0.18	52,52,52,52	0
81	MG	B	1903	1/1	0.79	0.17	61,61,61,61	0
81	MG	CM	1891	1/1	0.79	0.13	48,48,48,48	0
81	MG	B	1906	1/1	0.79	0.24	43,43,43,43	0
81	MG	CM	1907	1/1	0.79	0.16	103,103,103,103	0
81	MG	1	3960	1/1	0.79	0.18	35,35,35,35	0
81	MG	B	1957	1/1	0.79	0.09	31,31,31,31	0
81	MG	1	3961	1/1	0.79	0.19	85,85,85,85	0
81	MG	1	3660	1/1	0.79	0.12	58,58,58,58	0
81	MG	AS	3775	1/1	0.80	0.15	47,47,47,47	0
81	MG	AS	3605	1/1	0.80	0.13	72,72,72,72	0
81	MG	AS	3609	1/1	0.80	0.23	55,55,55,55	0
81	MG	AS	3483	1/1	0.80	0.25	31,31,31,31	0
81	MG	1	3823	1/1	0.80	0.16	48,48,48,48	0
81	MG	AS	3495	1/1	0.80	0.26	51,51,51,51	0
81	MG	1	3556	1/1	0.80	0.17	66,66,66,66	0
81	MG	1	3898	1/1	0.80	0.25	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	AS	3516	1/1	0.80	0.36	48,48,48,48	0
81	MG	1	3477	1/1	0.80	0.16	18,18,18,18	0
81	MG	B	1862	1/1	0.80	0.10	80,80,80,80	0
81	MG	B	1809	1/1	0.80	0.12	37,37,37,37	0
81	MG	1	3561	1/1	0.80	0.25	53,53,53,53	0
81	MG	AS	3707	1/1	0.80	0.09	27,27,27,27	0
81	MG	B	1819	1/1	0.80	0.17	30,30,30,30	0
81	MG	CM	1858	1/1	0.80	0.17	113,113,113,113	0
81	MG	AS	3721	1/1	0.80	0.15	64,64,64,64	0
81	MG	1	3699	1/1	0.80	0.14	43,43,43,43	0
81	MG	AS	3735	1/1	0.80	0.18	56,56,56,56	0
81	MG	B	1880	1/1	0.80	0.12	49,49,49,49	0
81	MG	AS	3746	1/1	0.80	0.23	71,71,71,71	0
81	MG	5	201	1/1	0.80	0.15	65,65,65,65	0
81	MG	AS	3469	1/1	0.80	0.18	55,55,55,55	0
81	MG	B	1890	1/1	0.81	0.15	87,87,87,87	0
81	MG	1	3892	1/1	0.81	0.08	71,71,71,71	0
81	MG	BZ	201	1/1	0.81	0.29	67,67,67,67	0
81	MG	CM	1922	1/1	0.81	0.20	49,49,49,49	0
81	MG	1	3870	1/1	0.81	0.13	54,54,54,54	0
81	MG	CM	1936	1/1	0.81	0.10	62,62,62,62	0
81	MG	B	1841	1/1	0.81	0.17	55,55,55,55	0
81	MG	CM	1942	1/1	0.81	0.12	42,42,42,42	0
81	MG	CM	1816	1/1	0.81	0.22	45,45,45,45	0
81	MG	CM	1818	1/1	0.81	0.19	40,40,40,40	0
81	MG	AS	3583	1/1	0.81	0.16	61,61,61,61	0
81	MG	AS	3636	1/1	0.81	0.17	69,69,69,69	0
81	MG	AS	3641	1/1	0.81	0.14	80,80,80,80	0
81	MG	DB	204	1/1	0.81	0.14	26,26,26,26	0
81	MG	Y	201	1/1	0.81	0.20	69,69,69,69	0
81	MG	1	3760	1/1	0.81	0.16	43,43,43,43	0
81	MG	AS	3667	1/1	0.81	0.15	28,28,28,28	0
81	MG	CM	1864	1/1	0.81	0.22	54,54,54,54	0
81	MG	0	202	1/1	0.81	0.34	87,87,87,87	0
81	MG	AS	3677	1/1	0.81	0.09	65,65,65,65	0
81	MG	1	3782	1/1	0.81	0.18	66,66,66,66	0
81	MG	CM	1885	1/1	0.81	0.22	57,57,57,57	0
81	MG	AT	202	1/1	0.81	0.24	43,43,43,43	0
81	MG	1	3863	1/1	0.81	0.15	85,85,85,85	0
81	MG	AT	204	1/1	0.81	0.14	85,85,85,85	0
81	MG	AS	3436	1/1	0.81	0.21	65,65,65,65	0
81	MG	AS	3700	1/1	0.82	0.16	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3532	1/1	0.82	0.27	37,37,37,37	0
81	MG	BS	201	1/1	0.82	0.17	83,83,83,83	0
81	MG	B	1835	1/1	0.82	0.14	52,52,52,52	0
81	MG	o	304	1/1	0.82	0.20	47,47,47,47	0
81	MG	CM	1810	1/1	0.82	0.25	45,45,45,45	0
81	MG	1	3410	1/1	0.82	0.40	42,42,42,42	0
81	MG	3	206	1/1	0.82	0.19	55,55,55,55	0
81	MG	1	3572	1/1	0.82	0.11	44,44,44,44	0
81	MG	AS	3494	1/1	0.82	0.19	63,63,63,63	0
81	MG	AS	3742	1/1	0.82	0.10	72,72,72,72	0
81	MG	CM	1831	1/1	0.82	0.22	36,36,36,36	0
81	MG	1	3777	1/1	0.82	0.15	52,52,52,52	0
81	MG	CM	1855	1/1	0.82	0.08	131,131,131,131	0
81	MG	AI	201	1/1	0.82	0.13	66,66,66,66	0
81	MG	3	212	1/1	0.82	0.21	46,46,46,46	0
81	MG	1	3711	1/1	0.82	0.15	54,54,54,54	0
81	MG	B	1869	1/1	0.82	0.24	59,59,59,59	0
81	MG	1	3758	1/1	0.82	0.16	40,40,40,40	0
81	MG	1	3925	1/1	0.82	0.14	39,39,39,39	0
81	MG	1	3813	1/1	0.82	0.15	71,71,71,71	0
81	MG	AS	3670	1/1	0.82	0.14	63,63,63,63	0
81	MG	1	3483	1/1	0.82	0.17	30,30,30,30	0
81	MG	B	1882	1/1	0.82	0.10	56,56,56,56	0
81	MG	B	1883	1/1	0.82	0.30	82,82,82,82	0
81	MG	AT	212	1/1	0.82	0.12	41,41,41,41	0
81	MG	AS	3787	1/1	0.83	0.18	66,66,66,66	0
81	MG	AS	3651	1/1	0.83	0.10	22,22,22,22	0
81	MG	Z	202	1/1	0.83	0.35	69,69,69,69	0
81	MG	CM	1903	1/1	0.83	0.14	38,38,38,38	0
81	MG	AS	3554	1/1	0.83	0.15	44,44,44,44	0
81	MG	AS	3561	1/1	0.83	0.13	42,42,42,42	0
81	MG	o	303	1/1	0.83	0.19	52,52,52,52	0
81	MG	B	1938	1/1	0.83	0.07	51,51,51,51	0
81	MG	1	3707	1/1	0.83	0.09	82,82,82,82	0
81	MG	w	301	1/1	0.83	0.34	39,39,39,39	0
81	MG	w	303	1/1	0.83	0.51	64,64,64,64	0
81	MG	x	202	1/1	0.83	0.11	25,25,25,25	0
81	MG	CM	1808	1/1	0.83	0.26	63,63,63,63	0
81	MG	AS	3603	1/1	0.83	0.19	44,44,44,44	0
81	MG	AS	3727	1/1	0.83	0.27	73,73,73,73	0
81	MG	1	3805	1/1	0.83	0.11	28,28,28,28	0
81	MG	AS	3733	1/1	0.83	0.12	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	CM	1820	1/1	0.83	0.15	34,34,34,34	0
81	MG	1	3807	1/1	0.83	0.07	39,39,39,39	0
81	MG	1	3750	1/1	0.83	0.23	46,46,46,46	0
81	MG	1	3893	1/1	0.83	0.11	34,34,34,34	0
81	MG	AS	3617	1/1	0.83	0.14	62,62,62,62	0
81	MG	1	3544	1/1	0.83	0.37	47,47,47,47	0
81	MG	1	3769	1/1	0.83	0.22	37,37,37,37	0
81	MG	AS	3774	1/1	0.83	0.19	49,49,49,49	0
81	MG	1	3524	1/1	0.83	0.10	58,58,58,58	0
81	MG	AS	3776	1/1	0.83	0.12	52,52,52,52	0
81	MG	1	3831	1/1	0.83	0.17	38,38,38,38	0
81	MG	1	3772	1/1	0.83	0.22	49,49,49,49	0
81	MG	1	3560	1/1	0.83	0.24	73,73,73,73	0
81	MG	1	3840	1/1	0.83	0.22	52,52,52,52	0
81	MG	1	3918	1/1	0.84	0.09	43,43,43,43	0
81	MG	AS	3513	1/1	0.84	0.21	36,36,36,36	0
81	MG	CM	1832	1/1	0.84	0.15	63,63,63,63	0
81	MG	B	1867	1/1	0.84	0.19	65,65,65,65	0
81	MG	CM	1848	1/1	0.84	0.25	61,61,61,61	0
81	MG	CM	1849	1/1	0.84	0.25	53,53,53,53	0
81	MG	CM	1854	1/1	0.84	0.17	90,90,90,90	0
81	MG	1	3923	1/1	0.84	0.16	36,36,36,36	0
81	MG	AS	3717	1/1	0.84	0.23	64,64,64,64	0
81	MG	1	3860	1/1	0.84	0.15	70,70,70,70	0
81	MG	1	3812	1/1	0.84	0.27	58,58,58,58	0
81	MG	CM	1863	1/1	0.84	0.14	15,15,15,15	0
81	MG	AS	3540	1/1	0.84	0.28	55,55,55,55	0
81	MG	CM	1870	1/1	0.84	0.12	73,73,73,73	0
81	MG	AS	3548	1/1	0.84	0.17	49,49,49,49	0
81	MG	1	3574	1/1	0.84	0.25	53,53,53,53	0
81	MG	1	3434	1/1	0.84	0.24	25,25,25,25	0
81	MG	CM	1884	1/1	0.84	0.14	31,31,31,31	0
81	MG	AF	201	1/1	0.84	0.21	82,82,82,82	0
81	MG	1	3550	1/1	0.84	0.15	35,35,35,35	0
81	MG	AS	3747	1/1	0.84	0.22	48,48,48,48	0
81	MG	1	3787	1/1	0.84	0.17	43,43,43,43	0
81	MG	1	3873	1/1	0.84	0.07	57,57,57,57	0
81	MG	1	3693	1/1	0.84	0.13	36,36,36,36	0
81	MG	1	3882	1/1	0.84	0.12	31,31,31,31	0
81	MG	B	1813	1/1	0.84	0.18	42,42,42,42	0
81	MG	1	3636	1/1	0.84	0.11	34,34,34,34	0
81	MG	1	3563	1/1	0.84	0.32	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	AS	3608	1/1	0.84	0.22	65,65,65,65	0
81	MG	CM	1933	1/1	0.84	0.20	69,69,69,69	0
81	MG	f	102	1/1	0.84	0.09	53,53,53,53	0
81	MG	CM	1939	1/1	0.84	0.19	82,82,82,82	0
81	MG	AS	3784	1/1	0.84	0.15	54,54,54,54	0
81	MG	1	3590	1/1	0.84	0.09	36,36,36,36	0
81	MG	B	1914	1/1	0.84	0.18	62,62,62,62	0
81	MG	AS	3410	1/1	0.84	0.31	25,25,25,25	0
81	MG	1	3765	1/1	0.84	0.16	49,49,49,49	0
81	MG	4	216	1/1	0.84	0.12	42,42,42,42	0
81	MG	AS	3628	1/1	0.84	0.24	73,73,73,73	0
81	MG	AS	3437	1/1	0.84	0.23	36,36,36,36	0
81	MG	B	1837	1/1	0.84	0.12	78,78,78,78	0
81	MG	DG	201	1/1	0.84	0.20	49,49,49,49	0
81	MG	BJ	302	1/1	0.84	0.12	42,42,42,42	0
81	MG	1	3648	1/1	0.84	0.13	51,51,51,51	0
81	MG	AS	3643	1/1	0.84	0.25	37,37,37,37	0
81	MG	1	3427	1/1	0.84	0.25	36,36,36,36	0
81	MG	o	302	1/1	0.84	0.18	37,37,37,37	0
81	MG	B	1929	1/1	0.84	0.21	70,70,70,70	0
81	MG	AS	3492	1/1	0.84	0.09	24,24,24,24	0
81	MG	1	3598	1/1	0.84	0.09	44,44,44,44	0
81	MG	1	3737	1/1	0.84	0.21	43,43,43,43	0
81	MG	1	3910	1/1	0.84	0.10	50,50,50,50	0
81	MG	AS	3498	1/1	0.84	0.24	33,33,33,33	0
81	MG	3	214	1/1	0.85	0.17	48,48,48,48	0
81	MG	AS	3702	1/1	0.85	0.10	72,72,72,72	0
81	MG	B	1884	1/1	0.85	0.18	107,107,107,107	0
81	MG	AS	3523	1/1	0.85	0.33	49,49,49,49	0
81	MG	B	1887	1/1	0.85	0.09	51,51,51,51	0
81	MG	AS	3712	1/1	0.85	0.15	45,45,45,45	0
81	MG	4	204	1/1	0.85	0.07	37,37,37,37	0
81	MG	1	3646	1/1	0.85	0.10	73,73,73,73	0
81	MG	AS	3725	1/1	0.85	0.07	38,38,38,38	0
81	MG	1	3595	1/1	0.85	0.10	52,52,52,52	0
81	MG	AS	3728	1/1	0.85	0.12	21,21,21,21	0
81	MG	AS	3549	1/1	0.85	0.21	34,34,34,34	0
81	MG	B	1899	1/1	0.85	0.19	38,38,38,38	0
81	MG	1	3623	1/1	0.85	0.12	44,44,44,44	0
81	MG	1	3650	1/1	0.85	0.10	30,30,30,30	0
81	MG	1	3653	1/1	0.85	0.10	47,47,47,47	0
81	MG	AS	3743	1/1	0.85	0.16	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3503	1/1	0.85	0.07	62,62,62,62	0
81	MG	B	1910	1/1	0.85	0.16	76,76,76,76	0
81	MG	AS	3748	1/1	0.85	0.18	60,60,60,60	0
81	MG	AS	3760	1/1	0.85	0.11	146,146,146,146	0
81	MG	CM	1894	1/1	0.85	0.35	49,49,49,49	0
81	MG	Z	203	1/1	0.85	0.20	62,62,62,62	0
81	MG	CM	1901	1/1	0.85	0.10	53,53,53,53	0
81	MG	c	202	1/1	0.85	0.11	60,60,60,60	0
81	MG	AS	3596	1/1	0.85	0.21	43,43,43,43	0
81	MG	1	3768	1/1	0.85	0.12	38,38,38,38	0
81	MG	1	3722	1/1	0.85	0.10	45,45,45,45	0
81	MG	1	3728	1/1	0.85	0.14	53,53,53,53	0
81	MG	AS	3407	1/1	0.85	0.10	37,37,37,37	0
81	MG	1	3411	1/1	0.85	0.23	24,24,24,24	0
81	MG	s	201	1/1	0.85	0.17	49,49,49,49	0
81	MG	1	3403	1/1	0.85	0.34	31,31,31,31	0
81	MG	1	3867	1/1	0.85	0.14	45,45,45,45	0
81	MG	AS	3442	1/1	0.85	0.19	41,41,41,41	0
81	MG	1	3827	1/1	0.85	0.08	36,36,36,36	0
81	MG	AS	3621	1/1	0.85	0.16	60,60,60,60	0
81	MG	B	1926	1/1	0.85	0.17	70,70,70,70	0
81	MG	x	203	1/1	0.85	0.20	70,70,70,70	0
81	MG	AT	213	1/1	0.85	0.08	51,51,51,51	0
81	MG	AS	3476	1/1	0.85	0.20	37,37,37,37	0
81	MG	AX	401	1/1	0.85	0.10	43,43,43,43	0
81	MG	1	3959	1/1	0.85	0.12	48,48,48,48	0
81	MG	1	3747	1/1	0.85	0.19	34,34,34,34	0
81	MG	B	1936	1/1	0.85	0.12	59,59,59,59	0
81	MG	1	3606	1/1	0.85	0.20	35,35,35,35	0
81	MG	1	3877	1/1	0.85	0.31	36,36,36,36	0
81	MG	CM	1806	1/1	0.85	0.21	68,68,68,68	0
81	MG	1	3837	1/1	0.85	0.09	59,59,59,59	0
81	MG	1	3678	1/1	0.85	0.16	38,38,38,38	0
81	MG	AS	3506	1/1	0.85	0.19	40,40,40,40	0
81	MG	AS	3672	1/1	0.85	0.24	58,58,58,58	0
81	MG	B	1955	1/1	0.85	0.22	45,45,45,45	0
81	MG	1	3682	1/1	0.85	0.28	60,60,60,60	0
81	MG	AS	3687	1/1	0.85	0.16	44,44,44,44	0
81	MG	AS	3611	1/1	0.86	0.08	29,29,29,29	0
81	MG	1	3818	1/1	0.86	0.11	75,75,75,75	0
81	MG	AS	3517	1/1	0.86	0.23	34,34,34,34	0
81	MG	B	1846	1/1	0.86	0.19	56,56,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	AW	303	1/1	0.86	0.13	82,82,82,82	0
81	MG	1	3438	1/1	0.86	0.18	30,30,30,30	0
81	MG	AX	402	1/1	0.86	0.25	34,34,34,34	0
81	MG	AS	3526	1/1	0.86	0.15	50,50,50,50	0
81	MG	1	3402	1/1	0.86	0.25	16,16,16,16	0
81	MG	1	3460	1/1	0.86	0.16	23,23,23,23	0
81	MG	CM	1911	1/1	0.86	0.09	63,63,63,63	0
81	MG	AS	3731	1/1	0.86	0.14	49,49,49,49	0
81	MG	1	3577	1/1	0.86	0.29	53,53,53,53	0
81	MG	CM	1804	1/1	0.86	0.33	48,48,48,48	0
81	MG	AS	3734	1/1	0.86	0.15	37,37,37,37	0
81	MG	AF	204	1/1	0.86	0.12	55,55,55,55	0
81	MG	AS	3639	1/1	0.86	0.17	59,59,59,59	0
81	MG	1	3832	1/1	0.86	0.08	46,46,46,46	0
81	MG	1	3654	1/1	0.86	0.11	49,49,49,49	0
81	MG	AS	3645	1/1	0.86	0.14	45,45,45,45	0
81	MG	1	3553	1/1	0.86	0.11	43,43,43,43	0
81	MG	AS	3648	1/1	0.86	0.09	43,43,43,43	0
81	MG	CN	301	1/1	0.86	0.15	54,54,54,54	0
81	MG	B	1968	1/1	0.86	0.07	48,48,48,48	0
81	MG	AS	3576	1/1	0.86	0.43	84,84,84,84	0
81	MG	AS	3654	1/1	0.86	0.23	34,34,34,34	0
81	MG	B	1969	1/1	0.86	0.14	50,50,50,50	0
81	MG	CM	1841	1/1	0.86	0.09	118,118,118,118	0
81	MG	1	3661	1/1	0.86	0.20	63,63,63,63	0
81	MG	1	3408	1/1	0.86	0.21	39,39,39,39	0
81	MG	CM	1850	1/1	0.86	0.20	55,55,55,55	0
81	MG	AS	3778	1/1	0.86	0.08	38,38,38,38	0
81	MG	1	3950	1/1	0.86	0.49	50,50,50,50	0
81	MG	1	3953	1/1	0.86	0.21	57,57,57,57	0
81	MG	1	3409	1/1	0.86	0.31	29,29,29,29	0
81	MG	1	3485	1/1	0.86	0.19	54,54,54,54	0
81	MG	1	3543	1/1	0.86	0.14	39,39,39,39	0
81	MG	1	3467	1/1	0.86	0.25	37,37,37,37	0
81	MG	1	3853	1/1	0.86	0.12	63,63,63,63	0
81	MG	AS	3705	1/1	0.86	0.26	58,58,58,58	0
81	MG	1	3691	1/1	0.86	0.09	35,35,35,35	0
81	MG	1	3803	1/1	0.87	0.17	24,24,24,24	0
81	MG	1	3721	1/1	0.87	0.14	42,42,42,42	0
81	MG	1	3643	1/1	0.87	0.12	50,50,50,50	0
81	MG	AS	3777	1/1	0.87	0.14	82,82,82,82	0
81	MG	1	3419	1/1	0.87	0.16	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	CM	1869	1/1	0.87	0.12	55,55,55,55	0
81	MG	1	3911	1/1	0.87	0.10	39,39,39,39	0
81	MG	AS	3653	1/1	0.87	0.10	47,47,47,47	0
81	MG	1	3579	1/1	0.87	0.25	47,47,47,47	0
81	MG	1	3858	1/1	0.87	0.14	62,62,62,62	0
81	MG	AS	3668	1/1	0.87	0.18	78,78,78,78	0
81	MG	B	1847	1/1	0.87	0.09	28,28,28,28	0
81	MG	1	3604	1/1	0.87	0.13	46,46,46,46	0
81	MG	u	202	1/1	0.87	0.07	55,55,55,55	0
81	MG	AS	3566	1/1	0.87	0.27	37,37,37,37	0
81	MG	AT	207	1/1	0.87	0.12	80,80,80,80	0
81	MG	CM	1898	1/1	0.87	0.19	60,60,60,60	0
81	MG	AS	3574	1/1	0.87	0.12	48,48,48,48	0
81	MG	AT	209	1/1	0.87	0.07	24,24,24,24	0
81	MG	AS	3686	1/1	0.87	0.12	50,50,50,50	0
81	MG	1	3774	1/1	0.87	0.13	46,46,46,46	0
81	MG	AS	3698	1/1	0.87	0.21	48,48,48,48	0
81	MG	AS	3412	1/1	0.87	0.29	41,41,41,41	0
81	MG	B	1856	1/1	0.87	0.11	65,65,65,65	0
81	MG	AS	3430	1/1	0.87	0.21	39,39,39,39	0
81	MG	1	3738	1/1	0.87	0.10	22,22,22,22	0
81	MG	1	3936	1/1	0.87	0.29	43,43,43,43	0
81	MG	BO	201	1/1	0.87	0.18	65,65,65,65	0
81	MG	1	3495	1/1	0.87	0.11	50,50,50,50	0
81	MG	AS	3711	1/1	0.87	0.19	51,51,51,51	0
81	MG	BZ	203	1/1	0.87	0.21	83,83,83,83	0
81	MG	1	3829	1/1	0.87	0.21	61,61,61,61	0
81	MG	1	3565	1/1	0.87	0.22	31,31,31,31	0
81	MG	1	3525	1/1	0.87	0.19	46,46,46,46	0
81	MG	CW	201	1/1	0.87	0.19	83,83,83,83	0
81	MG	1	3629	1/1	0.87	0.33	60,60,60,60	0
81	MG	1	3965	1/1	0.87	0.09	42,42,42,42	0
81	MG	1	3833	1/1	0.87	0.14	47,47,47,47	0
81	MG	1	3698	1/1	0.87	0.16	26,26,26,26	0
81	MG	1	3880	1/1	0.87	0.12	30,30,30,30	0
81	MG	B	1886	1/1	0.87	0.13	52,52,52,52	0
81	MG	AQ	102	1/1	0.87	0.11	27,27,27,27	0
81	MG	1	3795	1/1	0.87	0.15	60,60,60,60	0
83	PAR	1	3967	42/42	0.87	0.17	62,83,103,110	0
81	MG	AS	3499	1/1	0.87	0.24	42,42,42,42	0
81	MG	1	3416	1/1	0.87	0.24	30,30,30,30	0
81	MG	AS	3630	1/1	0.87	0.13	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3478	1/1	0.87	0.16	25,25,25,25	0
81	MG	1	3841	1/1	0.87	0.16	55,55,55,55	0
81	MG	1	3638	1/1	0.87	0.27	48,48,48,48	0
83	PAR	CM	1946	42/42	0.87	0.30	80,100,118,130	42
81	MG	AS	3640	1/1	0.87	0.18	59,59,59,59	0
81	MG	B	1902	1/1	0.87	0.20	51,51,51,51	0
81	MG	1	3665	1/1	0.87	0.22	25,25,25,25	0
81	MG	CM	1845	1/1	0.88	0.22	60,60,60,60	0
81	MG	1	3447	1/1	0.88	0.18	96,96,96,96	0
81	MG	1	3570	1/1	0.88	0.17	61,61,61,61	0
81	MG	B	1907	1/1	0.88	0.19	54,54,54,54	0
81	MG	1	3546	1/1	0.88	0.26	54,54,54,54	0
81	MG	AS	3425	1/1	0.88	0.15	24,24,24,24	0
81	MG	1	3906	1/1	0.88	0.07	69,69,69,69	0
81	MG	B	1820	1/1	0.88	0.23	38,38,38,38	0
81	MG	B	1829	1/1	0.88	0.32	28,28,28,28	0
81	MG	AS	3751	1/1	0.88	0.14	70,70,70,70	0
81	MG	B	1832	1/1	0.88	0.13	63,63,63,63	0
81	MG	1	3907	1/1	0.88	0.20	77,77,77,77	0
81	MG	AS	3764	1/1	0.88	0.15	72,72,72,72	0
81	MG	1	3826	1/1	0.88	0.16	53,53,53,53	0
81	MG	1	3859	1/1	0.88	0.25	43,43,43,43	0
81	MG	CM	1881	1/1	0.88	0.19	34,34,34,34	0
81	MG	1	3612	1/1	0.88	0.14	21,21,21,21	0
81	MG	1	3914	1/1	0.88	0.15	31,31,31,31	0
81	MG	1	3757	1/1	0.88	0.17	38,38,38,38	0
81	MG	l	402	1/1	0.88	0.13	51,51,51,51	0
81	MG	1	3922	1/1	0.88	0.42	52,52,52,52	0
81	MG	1	3548	1/1	0.88	0.11	54,54,54,54	0
81	MG	CM	1895	1/1	0.88	0.07	30,30,30,30	0
81	MG	CM	1896	1/1	0.88	0.12	32,32,32,32	0
81	MG	B	1851	1/1	0.88	0.09	64,64,64,64	0
81	MG	1	3794	1/1	0.88	0.17	30,30,30,30	0
81	MG	1	3674	1/1	0.88	0.19	53,53,53,53	0
81	MG	CM	1902	1/1	0.88	0.10	63,63,63,63	0
81	MG	AS	3501	1/1	0.88	0.14	60,60,60,60	0
81	MG	1	3929	1/1	0.88	0.07	87,87,87,87	0
81	MG	B	1948	1/1	0.88	0.13	44,44,44,44	0
81	MG	1	3522	1/1	0.88	0.23	44,44,44,44	0
81	MG	AS	3515	1/1	0.88	0.30	55,55,55,55	0
81	MG	B	1952	1/1	0.88	0.21	64,64,64,64	0
81	MG	1	3933	1/1	0.88	0.08	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	B	1865	1/1	0.88	0.14	95,95,95,95	0
81	MG	1	3630	1/1	0.88	0.15	34,34,34,34	0
81	MG	1	3943	1/1	0.88	0.11	61,61,61,61	0
81	MG	1	3723	1/1	0.88	0.15	51,51,51,51	0
81	MG	1	3952	1/1	0.88	0.20	33,33,33,33	0
81	MG	AS	3683	1/1	0.88	0.22	49,49,49,49	0
81	MG	1	3681	1/1	0.88	0.11	20,20,20,20	0
81	MG	AS	3544	1/1	0.88	0.16	34,34,34,34	0
81	MG	1	3632	1/1	0.88	0.08	45,45,45,45	0
81	MG	B	1881	1/1	0.88	0.23	53,53,53,53	0
81	MG	AC	101	1/1	0.88	0.12	43,43,43,43	0
81	MG	1	3804	1/1	0.88	0.18	26,26,26,26	0
81	MG	AS	3557	1/1	0.88	0.11	28,28,28,28	0
81	MG	G	301	1/1	0.88	0.13	49,49,49,49	0
81	MG	AF	203	1/1	0.88	0.18	43,43,43,43	0
81	MG	1	3685	1/1	0.88	0.27	38,38,38,38	0
81	MG	1	3430	1/1	0.88	0.24	34,34,34,34	0
81	MG	AS	3714	1/1	0.88	0.08	81,81,81,81	0
81	MG	3	201	1/1	0.88	0.15	62,62,62,62	0
81	MG	AS	3719	1/1	0.88	0.08	48,48,48,48	0
81	MG	AS	3582	1/1	0.88	0.17	49,49,49,49	0
81	MG	1	3473	1/1	0.88	0.28	18,18,18,18	0
81	MG	CM	1824	1/1	0.88	0.20	35,35,35,35	0
81	MG	CM	1829	1/1	0.88	0.15	76,76,76,76	0
81	MG	i	301	1/1	0.88	0.22	59,59,59,59	0
81	MG	B	1898	1/1	0.88	0.08	50,50,50,50	0
81	MG	1	3849	1/1	0.88	0.39	50,50,50,50	0
81	MG	1	3776	1/1	0.88	0.14	63,63,63,63	0
81	MG	B	1806	1/1	0.88	0.17	42,42,42,42	0
81	MG	AS	3681	1/1	0.89	0.19	64,64,64,64	0
81	MG	CM	1809	1/1	0.89	0.24	34,34,34,34	0
81	MG	1	3655	1/1	0.89	0.09	40,40,40,40	0
81	MG	AS	3519	1/1	0.89	0.10	73,73,73,73	0
81	MG	z	201	1/1	0.89	0.08	51,51,51,51	0
81	MG	1	3955	1/1	0.89	0.27	61,61,61,61	0
81	MG	AS	3696	1/1	0.89	0.21	66,66,66,66	0
81	MG	0	203	1/1	0.89	0.13	57,57,57,57	0
81	MG	AS	3699	1/1	0.89	0.07	46,46,46,46	0
81	MG	B	1964	1/1	0.89	0.11	39,39,39,39	0
81	MG	AS	3701	1/1	0.89	0.14	43,43,43,43	0
81	MG	AS	3532	1/1	0.89	0.12	62,62,62,62	0
81	MG	1	3582	1/1	0.89	0.11	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3896	1/1	0.89	0.07	36,36,36,36	0
81	MG	CM	1840	1/1	0.89	0.19	35,35,35,35	0
81	MG	AS	3541	1/1	0.89	0.13	60,60,60,60	0
81	MG	1	3814	1/1	0.89	0.15	41,41,41,41	0
81	MG	1	3962	1/1	0.89	0.10	24,24,24,24	0
81	MG	1	3566	1/1	0.89	0.10	24,24,24,24	0
81	MG	1	3528	1/1	0.89	0.10	45,45,45,45	0
81	MG	1	3429	1/1	0.89	0.25	13,13,13,13	0
81	MG	1	3908	1/1	0.89	0.17	47,47,47,47	0
81	MG	1	3621	1/1	0.89	0.09	35,35,35,35	0
81	MG	1	3792	1/1	0.89	0.10	20,20,20,20	0
81	MG	AS	3570	1/1	0.89	0.24	37,37,37,37	0
81	MG	1	3591	1/1	0.89	0.09	35,35,35,35	0
81	MG	AS	3575	1/1	0.89	0.41	30,30,30,30	0
81	MG	B	1802	1/1	0.89	0.23	33,33,33,33	0
81	MG	1	3624	1/1	0.89	0.27	32,32,32,32	0
81	MG	4	205	1/1	0.89	0.12	76,76,76,76	0
81	MG	1	3917	1/1	0.89	0.18	27,27,27,27	0
81	MG	4	209	1/1	0.89	0.19	45,45,45,45	0
81	MG	1	3501	1/1	0.89	0.20	33,33,33,33	0
81	MG	1	3920	1/1	0.89	0.08	53,53,53,53	0
81	MG	4	214	1/1	0.89	0.09	25,25,25,25	0
81	MG	B	1823	1/1	0.89	0.16	32,32,32,32	0
81	MG	AS	3419	1/1	0.89	0.24	26,26,26,26	0
81	MG	AS	3604	1/1	0.89	0.13	61,61,61,61	0
81	MG	1	3523	1/1	0.89	0.10	28,28,28,28	0
81	MG	AS	3761	1/1	0.89	0.12	54,54,54,54	0
81	MG	1	3487	1/1	0.89	0.15	44,44,44,44	0
81	MG	j	302	1/1	0.89	0.09	35,35,35,35	0
81	MG	CM	1899	1/1	0.89	0.15	65,65,65,65	0
81	MG	B	1918	1/1	0.89	0.16	111,111,111,111	0
81	MG	AS	3766	1/1	0.89	0.05	29,29,29,29	0
81	MG	1	3684	1/1	0.89	0.12	35,35,35,35	0
81	MG	AS	3614	1/1	0.89	0.15	32,32,32,32	0
81	MG	B	1920	1/1	0.89	0.22	50,50,50,50	0
81	MG	AS	3451	1/1	0.89	0.18	35,35,35,35	0
81	MG	AS	3453	1/1	0.89	0.18	82,82,82,82	0
81	MG	B	1921	1/1	0.89	0.13	84,84,84,84	0
81	MG	AS	3780	1/1	0.89	0.12	22,22,22,22	0
81	MG	AS	3461	1/1	0.89	0.11	38,38,38,38	0
81	MG	CM	1932	1/1	0.89	0.15	78,78,78,78	0
81	MG	AS	3623	1/1	0.89	0.15	89,89,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3481	1/1	0.89	0.21	44,44,44,44	0
81	MG	1	3734	1/1	0.89	0.12	44,44,44,44	0
81	MG	1	3689	1/1	0.89	0.14	33,33,33,33	0
81	MG	AS	3634	1/1	0.89	0.20	19,19,19,19	0
81	MG	AS	3480	1/1	0.89	0.15	23,23,23,23	0
81	MG	AS	3481	1/1	0.89	0.38	38,38,38,38	0
81	MG	1	3690	1/1	0.89	0.24	45,45,45,45	0
81	MG	1	3934	1/1	0.89	0.12	20,20,20,20	0
81	MG	1	3883	1/1	0.89	0.21	35,35,35,35	0
81	MG	1	3940	1/1	0.89	0.14	44,44,44,44	0
81	MG	v	301	1/1	0.89	0.18	21,21,21,21	0
81	MG	v	302	1/1	0.89	0.18	54,54,54,54	0
81	MG	1	3808	1/1	0.89	0.29	42,42,42,42	0
81	MG	B	1939	1/1	0.89	0.16	87,87,87,87	0
81	MG	1	3946	1/1	0.89	0.05	40,40,40,40	0
81	MG	AS	3504	1/1	0.89	0.18	44,44,44,44	0
81	MG	AS	3658	1/1	0.89	0.08	49,49,49,49	0
81	MG	B	1857	1/1	0.89	0.12	51,51,51,51	0
81	MG	B	1860	1/1	0.89	0.20	42,42,42,42	0
81	MG	AS	3508	1/1	0.89	0.12	62,62,62,62	0
81	MG	x	201	1/1	0.89	0.20	11,11,11,11	0
81	MG	CJ	203	1/1	0.89	0.19	51,51,51,51	0
81	MG	CK	102	1/1	0.89	0.16	50,50,50,50	0
81	MG	1	3810	1/1	0.89	0.15	32,32,32,32	0
81	MG	CM	1802	1/1	0.89	0.30	18,18,18,18	0
81	MG	1	3745	1/1	0.89	0.14	42,42,42,42	0
81	MG	AS	3680	1/1	0.89	0.15	31,31,31,31	0
81	MG	1	3538	1/1	0.90	0.20	51,51,51,51	0
81	MG	AS	3403	1/1	0.90	0.28	18,18,18,18	0
81	MG	2	201	1/1	0.90	0.28	49,49,49,49	0
81	MG	1	3583	1/1	0.90	0.17	30,30,30,30	0
81	MG	AS	3547	1/1	0.90	0.13	36,36,36,36	0
81	MG	6	201	1/1	0.90	0.23	38,38,38,38	0
81	MG	1	3743	1/1	0.90	0.21	34,34,34,34	0
81	MG	4	211	1/1	0.90	0.10	59,59,59,59	0
81	MG	1	3539	1/1	0.90	0.19	28,28,28,28	0
81	MG	1	3941	1/1	0.90	0.21	50,50,50,50	0
81	MG	1	3942	1/1	0.90	0.14	44,44,44,44	0
81	MG	CM	1877	1/1	0.90	0.15	35,35,35,35	0
81	MG	AH	202	1/1	0.90	0.09	59,59,59,59	0
81	MG	CM	1882	1/1	0.90	0.09	36,36,36,36	0
81	MG	1	3454	1/1	0.90	0.18	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3836	1/1	0.90	0.09	49,49,49,49	0
81	MG	1	3948	1/1	0.90	0.09	35,35,35,35	0
81	MG	1	3587	1/1	0.90	0.19	37,37,37,37	0
81	MG	AS	3688	1/1	0.90	0.07	37,37,37,37	0
81	MG	1	3512	1/1	0.90	0.21	45,45,45,45	0
81	MG	AS	3697	1/1	0.90	0.17	49,49,49,49	0
81	MG	k	404	1/1	0.90	0.14	49,49,49,49	0
81	MG	AS	3466	1/1	0.90	0.20	46,46,46,46	0
81	MG	B	1803	1/1	0.90	0.22	50,50,50,50	0
81	MG	AU	206	1/1	0.90	0.14	30,30,30,30	0
81	MG	CM	1900	1/1	0.90	0.10	86,86,86,86	0
81	MG	AU	207	1/1	0.90	0.12	49,49,49,49	0
81	MG	1	3514	1/1	0.90	0.15	22,22,22,22	0
81	MG	AS	3594	1/1	0.90	0.15	46,46,46,46	0
81	MG	1	3594	1/1	0.90	0.15	46,46,46,46	0
81	MG	BG	302	1/1	0.90	0.07	28,28,28,28	0
81	MG	1	3956	1/1	0.90	0.16	55,55,55,55	0
81	MG	1	3421	1/1	0.90	0.23	17,17,17,17	0
81	MG	BN	201	1/1	0.90	0.07	33,33,33,33	0
81	MG	r	302	1/1	0.90	0.08	64,64,64,64	0
81	MG	AS	3485	1/1	0.90	0.15	47,47,47,47	0
81	MG	AS	3487	1/1	0.90	0.09	48,48,48,48	0
81	MG	B	1818	1/1	0.90	0.19	36,36,36,36	0
81	MG	r	303	1/1	0.90	0.12	42,42,42,42	0
81	MG	B	1961	1/1	0.90	0.07	48,48,48,48	0
81	MG	B	1962	1/1	0.90	0.12	29,29,29,29	0
81	MG	1	3874	1/1	0.90	0.14	48,48,48,48	0
81	MG	CM	1943	1/1	0.90	0.06	38,38,38,38	0
81	MG	CM	1944	1/1	0.90	0.13	60,60,60,60	0
81	MG	B	1822	1/1	0.90	0.17	34,34,34,34	0
81	MG	1	3875	1/1	0.90	0.08	32,32,32,32	0
81	MG	CP	301	1/1	0.90	0.18	19,19,19,19	0
81	MG	AS	3502	1/1	0.90	0.18	41,41,41,41	0
81	MG	AS	3730	1/1	0.90	0.28	44,44,44,44	0
81	MG	B	1900	1/1	0.90	0.22	42,42,42,42	0
81	MG	1	3534	1/1	0.90	0.11	30,30,30,30	0
81	MG	B	1830	1/1	0.90	0.20	39,39,39,39	0
81	MG	1	3497	1/1	0.90	0.24	15,15,15,15	0
81	MG	1	3816	1/1	0.90	0.14	51,51,51,51	0
81	MG	AS	3739	1/1	0.90	0.21	17,17,17,17	0
81	MG	3	202	1/1	0.90	0.22	50,50,50,50	0
81	MG	CM	1826	1/1	0.90	0.10	87,87,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
82	3K5	CJ	202	57/57	0.90	0.15	51,79,102,115	0
81	MG	B	1908	1/1	0.90	0.11	35,35,35,35	0
81	MG	1	3847	1/1	0.90	0.27	50,50,50,50	0
81	MG	1	3724	1/1	0.90	0.22	44,44,44,44	0
81	MG	1	3686	1/1	0.90	0.15	36,36,36,36	0
81	MG	1	3928	1/1	0.90	0.17	43,43,43,43	0
81	MG	1	3659	1/1	0.90	0.10	40,40,40,40	0
81	MG	AS	3527	1/1	0.90	0.20	64,64,64,64	0
81	MG	B	1917	1/1	0.90	0.11	28,28,28,28	0
81	MG	AS	3763	1/1	0.90	0.06	38,38,38,38	0
81	MG	AS	3531	1/1	0.90	0.17	51,51,51,51	0
84	ZN	c	201	1/1	0.90	0.08	91,91,91,91	0
81	MG	1	3580	1/1	0.90	0.15	44,44,44,44	0
81	MG	AF	202	1/1	0.91	0.17	26,26,26,26	0
81	MG	B	1943	1/1	0.91	0.10	65,65,65,65	0
81	MG	CM	1842	1/1	0.91	0.23	41,41,41,41	0
81	MG	4	210	1/1	0.91	0.10	49,49,49,49	0
81	MG	CM	1847	1/1	0.91	0.10	32,32,32,32	0
81	MG	1	3476	1/1	0.91	0.18	49,49,49,49	0
81	MG	1	3600	1/1	0.91	0.21	20,20,20,20	0
81	MG	1	3809	1/1	0.91	0.08	56,56,56,56	0
81	MG	CM	1851	1/1	0.91	0.22	45,45,45,45	0
81	MG	CM	1853	1/1	0.91	0.13	79,79,79,79	0
81	MG	1	3886	1/1	0.91	0.20	57,57,57,57	0
81	MG	AS	3750	1/1	0.91	0.06	21,21,21,21	0
81	MG	B	1953	1/1	0.91	0.09	37,37,37,37	0
81	MG	AS	3754	1/1	0.91	0.11	51,51,51,51	0
81	MG	CM	1861	1/1	0.91	0.09	57,57,57,57	0
81	MG	AS	3755	1/1	0.91	0.06	45,45,45,45	0
81	MG	AS	3757	1/1	0.91	0.09	29,29,29,29	0
81	MG	1	3938	1/1	0.91	0.14	30,30,30,30	0
81	MG	AS	3627	1/1	0.91	0.09	17,17,17,17	0
81	MG	1	3417	1/1	0.91	0.20	15,15,15,15	0
81	MG	1	3662	1/1	0.91	0.16	71,71,71,71	0
81	MG	1	3779	1/1	0.91	0.07	40,40,40,40	0
81	MG	1	3848	1/1	0.91	0.22	29,29,29,29	0
81	MG	B	1804	1/1	0.91	0.18	55,55,55,55	0
81	MG	1	3536	1/1	0.91	0.16	48,48,48,48	0
81	MG	1	3947	1/1	0.91	0.29	83,83,83,83	0
81	MG	1	3496	1/1	0.91	0.08	31,31,31,31	0
81	MG	1	3510	1/1	0.91	0.15	14,14,14,14	0
81	MG	1	3854	1/1	0.91	0.11	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	B	1816	1/1	0.91	0.18	49,49,49,49	0
81	MG	CM	1893	1/1	0.91	0.26	32,32,32,32	0
81	MG	B	1891	1/1	0.91	0.27	26,26,26,26	0
81	MG	1	3905	1/1	0.91	0.06	39,39,39,39	0
81	MG	1	3540	1/1	0.91	0.10	33,33,33,33	0
81	MG	1	3819	1/1	0.91	0.08	34,34,34,34	0
81	MG	1	3821	1/1	0.91	0.07	56,56,56,56	0
81	MG	1	3822	1/1	0.91	0.14	42,42,42,42	0
81	MG	AS	3659	1/1	0.91	0.09	25,25,25,25	0
81	MG	AS	3660	1/1	0.91	0.15	34,34,34,34	0
81	MG	AS	3665	1/1	0.91	0.12	24,24,24,24	0
81	MG	B	1827	1/1	0.91	0.24	32,32,32,32	0
81	MG	1	3675	1/1	0.91	0.11	69,69,69,69	0
81	MG	1	3616	1/1	0.91	0.14	44,44,44,44	0
81	MG	AS	3533	1/1	0.91	0.23	19,19,19,19	0
81	MG	B	1831	1/1	0.91	0.17	37,37,37,37	0
81	MG	AS	3673	1/1	0.91	0.08	10,10,10,10	0
81	MG	CM	1918	1/1	0.91	0.10	86,86,86,86	0
81	MG	1	3913	1/1	0.91	0.18	43,43,43,43	0
81	MG	CM	1923	1/1	0.91	0.14	71,71,71,71	0
81	MG	B	1833	1/1	0.91	0.24	25,25,25,25	0
81	MG	1	3573	1/1	0.91	0.21	40,40,40,40	0
81	MG	AS	3546	1/1	0.91	0.11	45,45,45,45	0
81	MG	1	3413	1/1	0.91	0.18	9,9,9,9	0
81	MG	CM	1937	1/1	0.91	0.07	33,33,33,33	0
81	MG	BB	301	1/1	0.91	0.15	25,25,25,25	0
81	MG	AS	3404	1/1	0.91	0.32	33,33,33,33	0
81	MG	AS	3405	1/1	0.91	0.34	18,18,18,18	0
81	MG	1	3529	1/1	0.91	0.13	10,10,10,10	0
81	MG	AS	3553	1/1	0.91	0.08	23,23,23,23	0
81	MG	1	3797	1/1	0.91	0.27	23,23,23,23	0
81	MG	AS	3411	1/1	0.91	0.07	12,12,12,12	0
81	MG	B	1916	1/1	0.91	0.13	44,44,44,44	0
81	MG	B	1838	1/1	0.91	0.19	68,68,68,68	0
81	MG	1	3625	1/1	0.91	0.19	20,20,20,20	0
81	MG	B	1842	1/1	0.91	0.12	25,25,25,25	0
81	MG	AS	3427	1/1	0.91	0.18	22,22,22,22	0
81	MG	1	3726	1/1	0.91	0.22	59,59,59,59	0
81	MG	AS	3579	1/1	0.91	0.17	77,77,77,77	0
81	MG	AS	3431	1/1	0.91	0.21	16,16,16,16	0
81	MG	3	213	1/1	0.91	0.08	26,26,26,26	0
81	MG	1	3559	1/1	0.91	0.18	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	4	203	1/1	0.91	0.14	29,29,29,29	0
81	MG	1	3729	1/1	0.91	0.21	30,30,30,30	0
81	MG	B	1853	1/1	0.91	0.20	37,37,37,37	0
81	MG	1	3461	1/1	0.91	0.24	14,14,14,14	0
81	MG	9	202	1/1	0.91	0.25	93,93,93,93	0
81	MG	1	3731	1/1	0.91	0.52	30,30,30,30	0
81	MG	AS	3600	1/1	0.91	0.06	43,43,43,43	0
81	MG	AS	3602	1/1	0.91	0.27	49,49,49,49	0
81	MG	CM	1827	1/1	0.91	0.19	20,20,20,20	0
81	MG	1	3930	1/1	0.91	0.15	79,79,79,79	0
81	MG	AS	3468	1/1	0.91	0.22	44,44,44,44	0
81	MG	B	1934	1/1	0.91	0.09	69,69,69,69	0
81	MG	B	1858	1/1	0.91	0.08	77,77,77,77	0
81	MG	B	1859	1/1	0.91	0.22	45,45,45,45	0
81	MG	B	1944	1/1	0.92	0.28	51,51,51,51	0
81	MG	1	3944	1/1	0.92	0.10	52,52,52,52	0
81	MG	AS	3655	1/1	0.92	0.08	33,33,33,33	0
81	MG	1	3945	1/1	0.92	0.14	30,30,30,30	0
81	MG	1	3426	1/1	0.92	0.37	31,31,31,31	0
81	MG	1	3878	1/1	0.92	0.06	40,40,40,40	0
81	MG	AS	3663	1/1	0.92	0.18	31,31,31,31	0
81	MG	AS	3664	1/1	0.92	0.14	31,31,31,31	0
81	MG	B	1951	1/1	0.92	0.13	67,67,67,67	0
81	MG	AS	3514	1/1	0.92	0.16	18,18,18,18	0
81	MG	y	201	1/1	0.92	0.11	32,32,32,32	0
81	MG	AS	3669	1/1	0.92	0.17	12,12,12,12	0
81	MG	1	3442	1/1	0.92	0.25	33,33,33,33	0
81	MG	B	1954	1/1	0.92	0.11	63,63,63,63	0
81	MG	1	3703	1/1	0.92	0.08	49,49,49,49	0
81	MG	1	3825	1/1	0.92	0.06	31,31,31,31	0
81	MG	CM	1813	1/1	0.92	0.17	22,22,22,22	0
81	MG	1	3704	1/1	0.92	0.13	79,79,79,79	0
81	MG	1	3705	1/1	0.92	0.11	37,37,37,37	0
81	MG	1	3576	1/1	0.92	0.20	29,29,29,29	0
81	MG	1	3708	1/1	0.92	0.13	10,10,10,10	0
81	MG	6	202	1/1	0.92	0.07	8,8,8,8	0
81	MG	AS	3685	1/1	0.92	0.12	25,25,25,25	0
81	MG	B	1870	1/1	0.92	0.09	106,106,106,106	0
81	MG	CM	1828	1/1	0.92	0.19	41,41,41,41	0
81	MG	1	3891	1/1	0.92	0.20	48,48,48,48	0
81	MG	AS	3534	1/1	0.92	0.17	30,30,30,30	0
81	MG	AS	3690	1/1	0.92	0.11	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	AS	3693	1/1	0.92	0.10	77,77,77,77	0
81	MG	AS	3695	1/1	0.92	0.17	36,36,36,36	0
81	MG	CM	1835	1/1	0.92	0.13	15,15,15,15	0
81	MG	CM	1838	1/1	0.92	0.15	32,32,32,32	0
81	MG	CM	1839	1/1	0.92	0.18	46,46,46,46	0
81	MG	B	1873	1/1	0.92	0.17	50,50,50,50	0
81	MG	AS	3538	1/1	0.92	0.18	27,27,27,27	0
81	MG	1	3709	1/1	0.92	0.29	12,12,12,12	0
81	MG	B	1878	1/1	0.92	0.08	86,86,86,86	0
81	MG	1	3445	1/1	0.92	0.21	35,35,35,35	0
81	MG	1	3714	1/1	0.92	0.17	21,21,21,21	0
81	MG	1	3966	1/1	0.92	0.08	63,63,63,63	0
81	MG	1	3895	1/1	0.92	0.15	54,54,54,54	0
81	MG	K	301	1/1	0.92	0.06	35,35,35,35	0
81	MG	AS	3706	1/1	0.92	0.07	29,29,29,29	0
81	MG	1	3526	1/1	0.92	0.17	34,34,34,34	0
81	MG	3	204	1/1	0.92	0.13	39,39,39,39	0
81	MG	1	3720	1/1	0.92	0.11	47,47,47,47	0
81	MG	AP	202	1/1	0.92	0.20	37,37,37,37	0
81	MG	1	3899	1/1	0.92	0.12	48,48,48,48	0
81	MG	AS	3562	1/1	0.92	0.08	33,33,33,33	0
81	MG	3	208	1/1	0.92	0.14	35,35,35,35	0
81	MG	AS	3720	1/1	0.92	0.07	41,41,41,41	0
81	MG	CM	1865	1/1	0.92	0.09	32,32,32,32	0
81	MG	AS	3568	1/1	0.92	0.08	61,61,61,61	0
81	MG	AS	3724	1/1	0.92	0.08	43,43,43,43	0
81	MG	3	210	1/1	0.92	0.16	38,38,38,38	0
81	MG	AS	3572	1/1	0.92	0.14	58,58,58,58	0
81	MG	B	1892	1/1	0.92	0.18	55,55,55,55	0
81	MG	1	3901	1/1	0.92	0.06	39,39,39,39	0
81	MG	1	3784	1/1	0.92	0.10	45,45,45,45	0
81	MG	1	3617	1/1	0.92	0.17	29,29,29,29	0
81	MG	1	3500	1/1	0.92	0.18	37,37,37,37	0
81	MG	1	3463	1/1	0.92	0.20	12,12,12,12	0
81	MG	CM	1886	1/1	0.92	0.07	25,25,25,25	0
81	MG	1	3663	1/1	0.92	0.04	83,83,83,83	0
81	MG	AS	3736	1/1	0.92	0.07	35,35,35,35	0
81	MG	1	3479	1/1	0.92	0.18	21,21,21,21	0
81	MG	AS	3587	1/1	0.92	0.14	37,37,37,37	0
81	MG	AS	3740	1/1	0.92	0.09	33,33,33,33	0
81	MG	1	3412	1/1	0.92	0.28	26,26,26,26	0
81	MG	AS	3416	1/1	0.92	0.30	16,16,16,16	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3627	1/1	0.92	0.20	25,25,25,25	0
81	MG	1	3448	1/1	0.92	0.27	20,20,20,20	0
81	MG	B	1817	1/1	0.92	0.22	19,19,19,19	0
81	MG	1	3450	1/1	0.92	0.16	82,82,82,82	0
81	MG	1	3537	1/1	0.92	0.28	52,52,52,52	0
81	MG	B	1912	1/1	0.92	0.09	59,59,59,59	0
81	MG	1	3468	1/1	0.92	0.18	28,28,28,28	0
81	MG	AS	3756	1/1	0.92	0.05	47,47,47,47	0
81	MG	1	3452	1/1	0.92	0.23	22,22,22,22	0
81	MG	CM	1913	1/1	0.92	0.17	60,60,60,60	0
81	MG	AS	3606	1/1	0.92	0.24	38,38,38,38	0
81	MG	AS	3607	1/1	0.92	0.12	63,63,63,63	0
81	MG	AS	3439	1/1	0.92	0.17	22,22,22,22	0
81	MG	1	3516	1/1	0.92	0.21	34,34,34,34	0
81	MG	AS	3610	1/1	0.92	0.14	64,64,64,64	0
81	MG	CM	1924	1/1	0.92	0.19	40,40,40,40	0
81	MG	AS	3444	1/1	0.92	0.06	5,5,5,5	0
81	MG	1	3639	1/1	0.92	0.26	28,28,28,28	0
81	MG	AS	3769	1/1	0.92	0.10	45,45,45,45	0
81	MG	AS	3772	1/1	0.92	0.11	65,65,65,65	0
81	MG	AS	3773	1/1	0.92	0.08	29,29,29,29	0
81	MG	AS	3613	1/1	0.92	0.07	46,46,46,46	0
81	MG	1	3542	1/1	0.92	0.16	42,42,42,42	0
81	MG	1	3596	1/1	0.92	0.09	31,31,31,31	0
81	MG	AS	3616	1/1	0.92	0.09	52,52,52,52	0
81	MG	k	401	1/1	0.92	0.12	41,41,41,41	0
81	MG	1	3568	1/1	0.92	0.21	29,29,29,29	0
81	MG	1	3862	1/1	0.92	0.16	23,23,23,23	0
81	MG	l	401	1/1	0.92	0.07	31,31,31,31	0
81	MG	1	3753	1/1	0.92	0.16	44,44,44,44	0
81	MG	AS	3624	1/1	0.92	0.14	67,67,67,67	0
81	MG	1	3569	1/1	0.92	0.12	46,46,46,46	0
81	MG	1	3647	1/1	0.92	0.16	50,50,50,50	0
81	MG	B	1927	1/1	0.92	0.19	39,39,39,39	0
81	MG	AS	3631	1/1	0.92	0.39	65,65,65,65	0
81	MG	1	3692	1/1	0.92	0.07	35,35,35,35	0
81	MG	B	1930	1/1	0.92	0.15	60,60,60,60	0
81	MG	1	3935	1/1	0.92	0.04	31,31,31,31	0
81	MG	CL	301	1/1	0.92	0.06	22,22,22,22	0
81	MG	AS	3637	1/1	0.92	0.08	61,61,61,61	0
82	3K5	1	3406	57/57	0.92	0.15	46,67,95,99	0
81	MG	AT	211	1/1	0.92	0.20	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3518	1/1	0.92	0.15	26,26,26,26	0
81	MG	AS	3488	1/1	0.92	0.20	35,35,35,35	0
81	MG	B	1933	1/1	0.92	0.18	50,50,50,50	0
81	MG	1	3815	1/1	0.92	0.10	38,38,38,38	0
81	MG	AS	3644	1/1	0.92	0.08	22,22,22,22	0
81	MG	AW	302	1/1	0.92	0.12	23,23,23,23	0
81	MG	B	1935	1/1	0.92	0.21	56,56,56,56	0
81	MG	1	3871	1/1	0.92	0.08	93,93,93,93	0
81	MG	1	3405	1/1	0.92	0.20	16,16,16,16	0
81	MG	1	3763	1/1	0.92	0.21	40,40,40,40	0
81	MG	AS	3650	1/1	0.92	0.07	40,40,40,40	0
81	MG	1	3697	1/1	0.92	0.10	35,35,35,35	0
81	MG	1	3456	1/1	0.93	0.10	6,6,6,6	0
81	MG	AS	3703	1/1	0.93	0.15	32,32,32,32	0
81	MG	1	3887	1/1	0.93	0.06	18,18,18,18	0
81	MG	CM	1823	1/1	0.93	0.21	33,33,33,33	0
81	MG	B	1840	1/1	0.93	0.12	34,34,34,34	0
81	MG	AS	3434	1/1	0.93	0.08	19,19,19,19	0
81	MG	1	3401	1/1	0.93	0.33	24,24,24,24	0
81	MG	1	3609	1/1	0.93	0.16	63,63,63,63	0
81	MG	AS	3593	1/1	0.93	0.21	61,61,61,61	0
81	MG	1	3610	1/1	0.93	0.21	34,34,34,34	0
81	MG	1	3562	1/1	0.93	0.19	12,12,12,12	0
81	MG	AS	3716	1/1	0.93	0.09	85,85,85,85	0
81	MG	1	3435	1/1	0.93	0.16	10,10,10,10	0
81	MG	AS	3597	1/1	0.93	0.16	37,37,37,37	0
81	MG	CM	1836	1/1	0.93	0.15	41,41,41,41	0
81	MG	1	3954	1/1	0.93	0.11	17,17,17,17	0
81	MG	AS	3599	1/1	0.93	0.07	40,40,40,40	0
81	MG	AS	3722	1/1	0.93	0.10	43,43,43,43	0
81	MG	1	3652	1/1	0.93	0.06	38,38,38,38	0
81	MG	AS	3601	1/1	0.93	0.10	82,82,82,82	0
81	MG	AS	3456	1/1	0.93	0.17	13,13,13,13	0
81	MG	x	204	1/1	0.93	0.10	32,32,32,32	0
81	MG	1	3739	1/1	0.93	0.16	22,22,22,22	0
81	MG	1	3740	1/1	0.93	0.09	28,28,28,28	0
81	MG	1	3505	1/1	0.93	0.16	24,24,24,24	0
81	MG	0	201	1/1	0.93	0.32	59,59,59,59	0
81	MG	1	3696	1/1	0.93	0.12	50,50,50,50	0
81	MG	AS	3473	1/1	0.93	0.17	33,33,33,33	0
81	MG	1	3746	1/1	0.93	0.25	34,34,34,34	0
81	MG	1	3963	1/1	0.93	0.11	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3903	1/1	0.93	0.44	67,67,67,67	0
81	MG	CM	1860	1/1	0.93	0.16	45,45,45,45	0
81	MG	1	3506	1/1	0.93	0.17	13,13,13,13	0
81	MG	1	3586	1/1	0.93	0.09	54,54,54,54	0
81	MG	1	3851	1/1	0.93	0.16	25,25,25,25	0
81	MG	B	1868	1/1	0.93	0.12	39,39,39,39	0
81	MG	1	3436	1/1	0.93	0.12	20,20,20,20	0
81	MG	3	205	1/1	0.93	0.11	42,42,42,42	0
81	MG	1	3702	1/1	0.93	0.13	34,34,34,34	0
81	MG	1	3806	1/1	0.93	0.09	28,28,28,28	0
81	MG	1	3855	1/1	0.93	0.05	96,96,96,96	0
81	MG	CM	1874	1/1	0.93	0.10	48,48,48,48	0
81	MG	1	3588	1/1	0.93	0.12	31,31,31,31	0
81	MG	CM	1880	1/1	0.93	0.16	13,13,13,13	0
81	MG	AS	3625	1/1	0.93	0.09	51,51,51,51	0
81	MG	AS	3626	1/1	0.93	0.18	51,51,51,51	0
81	MG	1	3475	1/1	0.93	0.23	16,16,16,16	0
81	MG	1	3551	1/1	0.93	0.08	57,57,57,57	0
81	MG	AS	3629	1/1	0.93	0.09	41,41,41,41	0
81	MG	B	1958	1/1	0.93	0.12	29,29,29,29	0
81	MG	CM	1888	1/1	0.93	0.14	35,35,35,35	0
81	MG	AS	3503	1/1	0.93	0.17	10,10,10,10	0
81	MG	1	3916	1/1	0.93	0.15	29,29,29,29	0
81	MG	AS	3505	1/1	0.93	0.16	23,23,23,23	0
81	MG	AS	3768	1/1	0.93	0.11	38,38,38,38	0
81	MG	1	3706	1/1	0.93	0.47	77,77,77,77	0
81	MG	1	3488	1/1	0.93	0.23	10,10,10,10	0
81	MG	1	3437	1/1	0.93	0.16	13,13,13,13	0
81	MG	AS	3509	1/1	0.93	0.11	33,33,33,33	0
81	MG	AS	3510	1/1	0.93	0.22	26,26,26,26	0
81	MG	B	1963	1/1	0.93	0.08	33,33,33,33	0
81	MG	1	3418	1/1	0.93	0.20	18,18,18,18	0
81	MG	1	3633	1/1	0.93	0.17	33,33,33,33	0
81	MG	AS	3646	1/1	0.93	0.15	36,36,36,36	0
81	MG	CM	1904	1/1	0.93	0.07	28,28,28,28	0
81	MG	B	1888	1/1	0.93	0.12	52,52,52,52	0
81	MG	1	3924	1/1	0.93	0.07	24,24,24,24	0
81	MG	1	3713	1/1	0.93	0.22	29,29,29,29	0
81	MG	1	3767	1/1	0.93	0.24	51,51,51,51	0
81	MG	CM	1914	1/1	0.93	0.18	49,49,49,49	0
81	MG	E	302	1/1	0.93	0.16	22,22,22,22	0
81	MG	CM	1916	1/1	0.93	0.23	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3927	1/1	0.93	0.14	45,45,45,45	0
81	MG	1	3673	1/1	0.93	0.13	55,55,55,55	0
81	MG	B	1895	1/1	0.93	0.05	5,5,5,5	0
81	MG	B	1897	1/1	0.93	0.15	35,35,35,35	0
81	MG	Q	201	1/1	0.93	0.03	10,10,10,10	0
81	MG	1	3575	1/1	0.93	0.09	25,25,25,25	0
81	MG	CM	1928	1/1	0.93	0.13	78,78,78,78	0
81	MG	CM	1929	1/1	0.93	0.09	61,61,61,61	0
81	MG	AS	3662	1/1	0.93	0.14	39,39,39,39	0
81	MG	1	3716	1/1	0.93	0.18	25,25,25,25	0
81	MG	1	3414	1/1	0.93	0.24	12,12,12,12	0
81	MG	AS	3536	1/1	0.93	0.10	27,27,27,27	0
81	MG	CM	1938	1/1	0.93	0.10	20,20,20,20	0
81	MG	AU	201	1/1	0.93	0.17	34,34,34,34	0
81	MG	AS	3537	1/1	0.93	0.11	38,38,38,38	0
81	MG	1	3932	1/1	0.93	0.07	27,27,27,27	0
81	MG	1	3637	1/1	0.93	0.17	45,45,45,45	0
81	MG	1	3455	1/1	0.93	0.21	22,22,22,22	0
81	MG	B	1904	1/1	0.93	0.09	72,72,72,72	0
81	MG	1	3876	1/1	0.93	0.15	40,40,40,40	0
81	MG	B	1821	1/1	0.93	0.19	30,30,30,30	0
81	MG	CQ	302	1/1	0.93	0.09	99,99,99,99	0
81	MG	CQ	303	1/1	0.93	0.07	12,12,12,12	0
81	MG	AY	401	1/1	0.93	0.09	45,45,45,45	0
81	MG	1	3601	1/1	0.93	0.32	39,39,39,39	0
81	MG	BE	302	1/1	0.93	0.15	45,45,45,45	0
81	MG	AS	3679	1/1	0.93	0.07	62,62,62,62	0
81	MG	1	3778	1/1	0.93	0.10	49,49,49,49	0
81	MG	1	3939	1/1	0.93	0.15	22,22,22,22	0
81	MG	BJ	304	1/1	0.93	0.10	21,21,21,21	0
81	MG	AS	3406	1/1	0.93	0.24	16,16,16,16	0
81	MG	m	301	1/1	0.93	0.10	60,60,60,60	0
81	MG	AS	3684	1/1	0.93	0.07	57,57,57,57	0
81	MG	o	301	1/1	0.93	0.12	29,29,29,29	0
81	MG	AS	3560	1/1	0.93	0.13	34,34,34,34	0
81	MG	BZ	204	1/1	0.93	0.11	57,57,57,57	0
81	MG	1	3828	1/1	0.93	0.06	19,19,19,19	0
81	MG	1	3602	1/1	0.93	0.20	20,20,20,20	0
81	MG	AS	3689	1/1	0.93	0.12	52,52,52,52	0
81	MG	AS	3413	1/1	0.93	0.20	18,18,18,18	0
81	MG	1	3881	1/1	0.93	0.12	39,39,39,39	0
81	MG	AS	3418	1/1	0.93	0.20	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	r	301	1/1	0.93	0.16	41,41,41,41	0
81	MG	AS	3420	1/1	0.93	0.14	18,18,18,18	0
81	MG	1	3781	1/1	0.93	0.06	22,22,22,22	0
84	ZN	AK	101	1/1	0.93	0.19	42,42,42,42	0
81	MG	1	3480	1/1	0.93	0.20	15,15,15,15	0
81	MG	AS	3578	1/1	0.93	0.17	74,74,74,74	0
81	MG	AS	3426	1/1	0.93	0.16	16,16,16,16	0
81	MG	CM	1843	1/1	0.94	0.10	41,41,41,41	0
81	MG	3	203	1/1	0.94	0.19	31,31,31,31	0
81	MG	CM	1846	1/1	0.94	0.18	29,29,29,29	0
81	MG	AS	3429	1/1	0.94	0.26	30,30,30,30	0
81	MG	1	3507	1/1	0.94	0.14	17,17,17,17	0
81	MG	1	3680	1/1	0.94	0.14	26,26,26,26	0
81	MG	B	1947	1/1	0.94	0.13	62,62,62,62	0
81	MG	AS	3543	1/1	0.94	0.16	17,17,17,17	0
81	MG	1	3845	1/1	0.94	0.14	34,34,34,34	0
81	MG	AS	3545	1/1	0.94	0.20	22,22,22,22	0
81	MG	B	1826	1/1	0.94	0.10	54,54,54,54	0
81	MG	1	3443	1/1	0.94	0.15	53,53,53,53	0
81	MG	B	1828	1/1	0.94	0.17	41,41,41,41	0
81	MG	CM	1859	1/1	0.94	0.12	34,34,34,34	0
81	MG	1	3884	1/1	0.94	0.10	43,43,43,43	0
81	MG	AS	3446	1/1	0.94	0.18	36,36,36,36	0
81	MG	AS	3450	1/1	0.94	0.17	9,9,9,9	0
81	MG	1	3541	1/1	0.94	0.22	15,15,15,15	0
81	MG	AS	3767	1/1	0.94	0.07	56,56,56,56	0
81	MG	AS	3452	1/1	0.94	0.14	8,8,8,8	0
81	MG	CM	1866	1/1	0.94	0.07	24,24,24,24	0
81	MG	CM	1867	1/1	0.94	0.17	35,35,35,35	0
81	MG	1	3742	1/1	0.94	0.07	29,29,29,29	0
81	MG	AS	3771	1/1	0.94	0.10	37,37,37,37	0
81	MG	AS	3661	1/1	0.94	0.17	27,27,27,27	0
81	MG	CM	1872	1/1	0.94	0.04	26,26,26,26	0
81	MG	AS	3454	1/1	0.94	0.07	48,48,48,48	0
81	MG	1	3850	1/1	0.94	0.07	28,28,28,28	0
81	MG	B	1896	1/1	0.94	0.14	23,23,23,23	0
81	MG	AS	3460	1/1	0.94	0.12	26,26,26,26	0
81	MG	AS	3569	1/1	0.94	0.18	29,29,29,29	0
81	MG	1	3683	1/1	0.94	0.15	28,28,28,28	0
81	MG	AS	3463	1/1	0.94	0.20	25,25,25,25	0
81	MG	1	3474	1/1	0.94	0.23	16,16,16,16	0
81	MG	4	201	1/1	0.94	0.07	29,29,29,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	4	202	1/1	0.94	0.10	29,29,29,29	0
81	MG	CM	1887	1/1	0.94	0.20	8,8,8,8	0
81	MG	1	3656	1/1	0.94	0.12	64,64,64,64	0
81	MG	AS	3675	1/1	0.94	0.13	54,54,54,54	0
81	MG	AS	3676	1/1	0.94	0.06	43,43,43,43	0
81	MG	AS	3472	1/1	0.94	0.14	16,16,16,16	0
81	MG	1	3511	1/1	0.94	0.18	16,16,16,16	0
81	MG	1	3687	1/1	0.94	0.15	32,32,32,32	0
81	MG	AS	3478	1/1	0.94	0.16	28,28,28,28	0
81	MG	AS	3584	1/1	0.94	0.06	37,37,37,37	0
81	MG	AS	3479	1/1	0.94	0.16	25,25,25,25	0
81	MG	AS	3586	1/1	0.94	0.11	11,11,11,11	0
81	MG	1	3786	1/1	0.94	0.26	33,33,33,33	0
81	MG	1	3489	1/1	0.94	0.12	41,41,41,41	0
81	MG	AS	3592	1/1	0.94	0.06	29,29,29,29	0
81	MG	8	202	1/1	0.94	0.11	34,34,34,34	0
81	MG	AU	205	1/1	0.94	0.18	50,50,50,50	0
81	MG	B	1845	1/1	0.94	0.18	30,30,30,30	0
81	MG	9	201	1/1	0.94	0.30	36,36,36,36	0
81	MG	1	3897	1/1	0.94	0.17	29,29,29,29	0
81	MG	AS	3694	1/1	0.94	0.17	62,62,62,62	0
81	MG	1	3751	1/1	0.94	0.12	28,28,28,28	0
81	MG	AS	3490	1/1	0.94	0.15	27,27,27,27	0
81	MG	1	3615	1/1	0.94	0.07	10,10,10,10	0
81	MG	B	1913	1/1	0.94	0.10	37,37,37,37	0
81	MG	BB	302	1/1	0.94	0.05	36,36,36,36	0
81	MG	CM	1920	1/1	0.94	0.10	58,58,58,58	0
81	MG	CM	1921	1/1	0.94	0.13	38,38,38,38	0
81	MG	1	3900	1/1	0.94	0.09	45,45,45,45	0
81	MG	BF	201	1/1	0.94	0.11	49,49,49,49	0
81	MG	AS	3496	1/1	0.94	0.21	21,21,21,21	0
81	MG	1	3530	1/1	0.94	0.15	19,19,19,19	0
81	MG	CM	1927	1/1	0.94	0.08	41,41,41,41	0
81	MG	1	3861	1/1	0.94	0.06	54,54,54,54	0
81	MG	1	3441	1/1	0.94	0.15	20,20,20,20	0
81	MG	CM	1931	1/1	0.94	0.10	58,58,58,58	0
81	MG	BK	202	1/1	0.94	0.07	45,45,45,45	0
81	MG	1	3491	1/1	0.94	0.24	37,37,37,37	0
81	MG	1	3581	1/1	0.94	0.13	12,12,12,12	0
81	MG	1	3517	1/1	0.94	0.08	66,66,66,66	0
81	MG	BV	201	1/1	0.94	0.14	51,51,51,51	0
81	MG	1	3951	1/1	0.94	0.18	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3761	1/1	0.94	0.11	33,33,33,33	0
81	MG	AS	3710	1/1	0.94	0.10	27,27,27,27	0
81	MG	1	3671	1/1	0.94	0.14	9,9,9,9	0
81	MG	1	3801	1/1	0.94	0.06	19,19,19,19	0
81	MG	AS	3713	1/1	0.94	0.11	36,36,36,36	0
81	MG	AS	3401	1/1	0.94	0.24	10,10,10,10	0
81	MG	B	1866	1/1	0.94	0.09	63,63,63,63	0
81	MG	1	3834	1/1	0.94	0.11	18,18,18,18	0
81	MG	AS	3511	1/1	0.94	0.15	28,28,28,28	0
81	MG	1	3872	1/1	0.94	0.05	42,42,42,42	0
81	MG	1	3493	1/1	0.94	0.07	22,22,22,22	0
81	MG	1	3915	1/1	0.94	0.12	43,43,43,43	0
81	MG	AS	3723	1/1	0.94	0.20	50,50,50,50	0
81	MG	1	3626	1/1	0.94	0.19	27,27,27,27	0
81	MG	CM	1817	1/1	0.94	0.20	48,48,48,48	0
81	MG	B	1811	1/1	0.94	0.18	42,42,42,42	0
81	MG	AS	3726	1/1	0.94	0.17	39,39,39,39	0
81	MG	1	3701	1/1	0.94	0.09	25,25,25,25	0
81	MG	AS	3520	1/1	0.94	0.18	29,29,29,29	0
81	MG	B	1876	1/1	0.94	0.14	33,33,33,33	0
81	MG	1	3494	1/1	0.94	0.21	20,20,20,20	0
81	MG	AS	3417	1/1	0.94	0.21	24,24,24,24	0
81	MG	1	3919	1/1	0.94	0.17	34,34,34,34	0
81	MG	1	3732	1/1	0.94	0.13	24,24,24,24	0
81	MG	AS	3529	1/1	0.94	0.06	91,91,91,91	0
81	MG	1	3458	1/1	0.94	0.14	10,10,10,10	0
81	MG	AS	3633	1/1	0.94	0.06	15,15,15,15	0
81	MG	AS	3738	1/1	0.94	0.10	17,17,17,17	0
81	MG	AS	3422	1/1	0.94	0.18	13,13,13,13	0
81	MG	B	1940	1/1	0.94	0.07	61,61,61,61	0
81	MG	AS	3741	1/1	0.94	0.18	43,43,43,43	0
81	MG	B	1942	1/1	0.94	0.13	49,49,49,49	0
81	MG	AS	3638	1/1	0.94	0.20	14,14,14,14	0
81	MG	AS	3745	1/1	0.94	0.08	41,41,41,41	0
81	MG	1	3735	1/1	0.94	0.09	28,28,28,28	0
84	ZN	CE	101	1/1	0.94	0.07	119,119,119,119	0
81	MG	CM	1875	1/1	0.95	0.18	48,48,48,48	0
81	MG	AS	3571	1/1	0.95	0.15	35,35,35,35	0
81	MG	BB	303	1/1	0.95	0.22	28,28,28,28	0
81	MG	1	3719	1/1	0.95	0.15	15,15,15,15	0
81	MG	1	3513	1/1	0.95	0.12	36,36,36,36	0
81	MG	1	3571	1/1	0.95	0.13	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	B	1877	1/1	0.95	0.19	30,30,30,30	0
81	MG	BI	301	1/1	0.95	0.11	53,53,53,53	0
81	MG	BJ	301	1/1	0.95	0.10	47,47,47,47	0
81	MG	1	3835	1/1	0.95	0.09	44,44,44,44	0
81	MG	AS	3657	1/1	0.95	0.14	19,19,19,19	0
81	MG	1	3641	1/1	0.95	0.14	31,31,31,31	0
81	MG	w	302	1/1	0.95	0.13	60,60,60,60	0
81	MG	CM	1892	1/1	0.95	0.10	50,50,50,50	0
81	MG	BN	202	1/1	0.95	0.08	31,31,31,31	0
81	MG	1	3439	1/1	0.95	0.27	25,25,25,25	0
81	MG	1	3759	1/1	0.95	0.43	28,28,28,28	0
81	MG	1	3666	1/1	0.95	0.17	41,41,41,41	0
81	MG	AS	3500	1/1	0.95	0.04	42,42,42,42	0
81	MG	AS	3415	1/1	0.95	0.21	17,17,17,17	0
81	MG	1	3424	1/1	0.95	0.23	7,7,7,7	0
81	MG	B	1885	1/1	0.95	0.09	34,34,34,34	0
81	MG	1	3727	1/1	0.95	0.14	39,39,39,39	0
81	MG	1	3482	1/1	0.95	0.19	26,26,26,26	0
81	MG	1	3669	1/1	0.95	0.15	48,48,48,48	0
81	MG	CM	1803	1/1	0.95	0.13	19,19,19,19	0
81	MG	CM	1906	1/1	0.95	0.16	48,48,48,48	0
81	MG	1	3670	1/1	0.95	0.21	25,25,25,25	0
81	MG	CM	1805	1/1	0.95	0.12	16,16,16,16	0
81	MG	1	3472	1/1	0.95	0.12	29,29,29,29	0
81	MG	1	3846	1/1	0.95	0.07	27,27,27,27	0
81	MG	1	3889	1/1	0.95	0.13	35,35,35,35	0
81	MG	1	3564	1/1	0.95	0.11	15,15,15,15	0
81	MG	AS	3428	1/1	0.95	0.18	23,23,23,23	0
81	MG	CM	1812	1/1	0.95	0.13	47,47,47,47	0
81	MG	AS	3758	1/1	0.95	0.08	22,22,22,22	0
81	MG	CM	1919	1/1	0.95	0.06	16,16,16,16	0
81	MG	CM	1814	1/1	0.95	0.19	22,22,22,22	0
81	MG	B	1894	1/1	0.95	0.06	21,21,21,21	0
81	MG	1	3521	1/1	0.95	0.16	32,32,32,32	0
81	MG	1	3608	1/1	0.95	0.11	24,24,24,24	0
81	MG	CM	1819	1/1	0.95	0.09	20,20,20,20	0
81	MG	4	206	1/1	0.95	0.09	32,32,32,32	0
81	MG	AS	3518	1/1	0.95	0.06	27,27,27,27	0
81	MG	1	3736	1/1	0.95	0.15	42,42,42,42	0
81	MG	B	1839	1/1	0.95	0.15	24,24,24,24	0
81	MG	1	3773	1/1	0.95	0.07	40,40,40,40	0
81	MG	1	3451	1/1	0.95	0.10	12,12,12,12	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3651	1/1	0.95	0.22	29,29,29,29	0
81	MG	AS	3770	1/1	0.95	0.07	40,40,40,40	0
81	MG	AB	201	1/1	0.95	0.18	64,64,64,64	0
81	MG	AS	3449	1/1	0.95	0.15	28,28,28,28	0
81	MG	AS	3691	1/1	0.95	0.08	51,51,51,51	0
81	MG	1	3631	1/1	0.95	0.09	37,37,37,37	0
81	MG	AD	201	1/1	0.95	0.13	88,88,88,88	0
81	MG	1	3592	1/1	0.95	0.09	68,68,68,68	0
81	MG	1	3817	1/1	0.95	0.09	87,87,87,87	0
81	MG	1	3567	1/1	0.95	0.15	42,42,42,42	0
81	MG	AS	3455	1/1	0.95	0.17	26,26,26,26	0
81	MG	B	1852	1/1	0.95	0.10	27,27,27,27	0
81	MG	1	3634	1/1	0.95	0.16	27,27,27,27	0
81	MG	AS	3459	1/1	0.95	0.20	6,6,6,6	0
81	MG	AG	201	1/1	0.95	0.09	59,59,59,59	0
81	MG	1	3820	1/1	0.95	0.09	48,48,48,48	0
81	MG	DA	201	1/1	0.95	0.16	38,38,38,38	0
81	MG	AS	3542	1/1	0.95	0.18	15,15,15,15	0
81	MG	AT	201	1/1	0.95	0.18	13,13,13,13	0
81	MG	DB	202	1/1	0.95	0.09	35,35,35,35	0
81	MG	1	3744	1/1	0.95	0.10	45,45,45,45	0
81	MG	1	3407	1/1	0.95	0.17	14,14,14,14	0
81	MG	AS	3465	1/1	0.95	0.08	41,41,41,41	0
81	MG	1	3658	1/1	0.95	0.15	20,20,20,20	0
81	MG	1	3824	1/1	0.95	0.06	29,29,29,29	0
81	MG	1	3785	1/1	0.95	0.13	15,15,15,15	0
81	MG	AT	210	1/1	0.95	0.13	27,27,27,27	0
81	MG	Q	202	1/1	0.95	0.08	62,62,62,62	0
81	MG	1	3865	1/1	0.95	0.10	53,53,53,53	0
81	MG	AS	3551	1/1	0.95	0.20	42,42,42,42	0
81	MG	AS	3474	1/1	0.95	0.14	29,29,29,29	0
81	MG	AU	202	1/1	0.95	0.13	47,47,47,47	0
81	MG	1	3614	1/1	0.95	0.15	49,49,49,49	0
81	MG	AU	204	1/1	0.95	0.06	39,39,39,39	0
81	MG	AS	3477	1/1	0.95	0.12	16,16,16,16	0
81	MG	1	3958	1/1	0.95	0.14	24,24,24,24	0
81	MG	1	3486	1/1	0.95	0.15	29,29,29,29	0
81	MG	1	3868	1/1	0.95	0.09	67,67,67,67	0
81	MG	1	3688	1/1	0.95	0.13	14,14,14,14	0
81	MG	AS	3567	1/1	0.95	0.15	9,9,9,9	0
81	MG	1	3717	1/1	0.95	0.13	37,37,37,37	0
81	MG	1	3790	1/1	0.95	0.08	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3752	1/1	0.95	0.22	47,47,47,47	0
81	MG	B	1807	1/1	0.96	0.07	101,101,101,101	0
81	MG	CM	1879	1/1	0.96	0.15	18,18,18,18	0
81	MG	AS	3432	1/1	0.96	0.11	24,24,24,24	0
81	MG	B	1808	1/1	0.96	0.20	54,54,54,54	0
81	MG	AS	3435	1/1	0.96	0.06	73,73,73,73	0
81	MG	BJ	303	1/1	0.96	0.13	20,20,20,20	0
81	MG	1	3492	1/1	0.96	0.10	43,43,43,43	0
81	MG	BK	201	1/1	0.96	0.15	27,27,27,27	0
81	MG	B	1810	1/1	0.96	0.10	11,11,11,11	0
81	MG	1	3593	1/1	0.96	0.14	14,14,14,14	0
81	MG	AS	3589	1/1	0.96	0.18	37,37,37,37	0
81	MG	AS	3591	1/1	0.96	0.06	28,28,28,28	0
81	MG	AS	3744	1/1	0.96	0.11	49,49,49,49	0
81	MG	AS	3666	1/1	0.96	0.19	17,17,17,17	0
81	MG	AS	3440	1/1	0.96	0.06	21,21,21,21	0
81	MG	B	1861	1/1	0.96	0.10	62,62,62,62	0
81	MG	AS	3443	1/1	0.96	0.07	36,36,36,36	0
81	MG	B	1812	1/1	0.96	0.13	24,24,24,24	0
81	MG	AS	3445	1/1	0.96	0.24	54,54,54,54	0
81	MG	AS	3753	1/1	0.96	0.10	27,27,27,27	0
81	MG	1	3672	1/1	0.96	0.05	8,8,8,8	0
81	MG	B	1864	1/1	0.96	0.13	49,49,49,49	0
81	MG	AS	3674	1/1	0.96	0.08	22,22,22,22	0
81	MG	x	205	1/1	0.96	0.21	30,30,30,30	0
81	MG	1	3628	1/1	0.96	0.08	17,17,17,17	0
81	MG	CM	1807	1/1	0.96	0.13	28,28,28,28	0
81	MG	AS	3759	1/1	0.96	0.04	39,39,39,39	0
81	MG	1	3921	1/1	0.96	0.13	33,33,33,33	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	1	3453	1/1	0.96	0.11	6,6,6,6	0
81	MG	1	3422	1/1	0.96	0.19	1,1,1,1	0
81	MG	1	3957	1/1	0.96	0.22	46,46,46,46	0
81	MG	1	3733	1/1	0.96	0.06	33,33,33,33	0
81	MG	B	1872	1/1	0.96	0.06	12,12,12,12	0
81	MG	CM	1815	1/1	0.96	0.14	19,19,19,19	0
81	MG	AS	3530	1/1	0.96	0.11	52,52,52,52	0
81	MG	1	3676	1/1	0.96	0.09	12,12,12,12	0
81	MG	1	3431	1/1	0.96	0.21	20,20,20,20	0
81	MG	B	1824	1/1	0.96	0.04	32,32,32,32	0
81	MG	AS	3462	1/1	0.96	0.20	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	CM	1821	1/1	0.96	0.10	16,16,16,16	0
81	MG	1	3504	1/1	0.96	0.14	27,27,27,27	0
81	MG	1	3679	1/1	0.96	0.27	21,21,21,21	0
81	MG	1	3770	1/1	0.96	0.18	25,25,25,25	0
81	MG	CM	1825	1/1	0.96	0.21	37,37,37,37	0
81	MG	AS	3692	1/1	0.96	0.09	47,47,47,47	0
81	MG	k	402	1/1	0.96	0.08	55,55,55,55	0
81	MG	AS	3539	1/1	0.96	0.10	57,57,57,57	0
81	MG	AS	3467	1/1	0.96	0.11	19,19,19,19	0
81	MG	1	3613	1/1	0.96	0.10	22,22,22,22	0
81	MG	1	3446	1/1	0.96	0.09	5,5,5,5	0
81	MG	AS	3471	1/1	0.96	0.13	9,9,9,9	0
81	MG	k	405	1/1	0.96	0.17	61,61,61,61	0
81	MG	1	3657	1/1	0.96	0.07	20,20,20,20	0
81	MG	1	3741	1/1	0.96	0.06	42,42,42,42	0
81	MG	B	1937	1/1	0.96	0.08	70,70,70,70	0
81	MG	AD	202	1/1	0.96	0.13	17,17,17,17	0
81	MG	1	3599	1/1	0.96	0.10	19,19,19,19	0
81	MG	AS	3408	1/1	0.96	0.19	1,1,1,1	0
81	MG	1	3712	1/1	0.96	0.18	20,20,20,20	0
81	MG	1	3432	1/1	0.96	0.27	21,21,21,21	0
81	MG	CP	302	1/1	0.96	0.10	54,54,54,54	0
81	MG	AT	205	1/1	0.96	0.10	13,13,13,13	0
81	MG	1	3498	1/1	0.96	0.13	73,73,73,73	0
81	MG	1	3618	1/1	0.96	0.10	11,11,11,11	0
81	MG	1	3619	1/1	0.96	0.11	39,39,39,39	0
81	MG	AS	3486	1/1	0.96	0.14	32,32,32,32	0
81	MG	3	209	1/1	0.96	0.13	25,25,25,25	0
81	MG	AS	3563	1/1	0.96	0.17	53,53,53,53	0
81	MG	CM	1852	1/1	0.96	0.12	47,47,47,47	0
81	MG	AS	3715	1/1	0.96	0.07	73,73,73,73	0
81	MG	AS	3564	1/1	0.96	0.14	47,47,47,47	0
81	MG	1	3620	1/1	0.96	0.05	27,27,27,27	0
81	MG	CM	1856	1/1	0.96	0.10	36,36,36,36	0
81	MG	B	1844	1/1	0.96	0.10	15,15,15,15	0
81	MG	DQ	101	1/1	0.96	0.09	61,61,61,61	0
81	MG	1	3664	1/1	0.96	0.13	54,54,54,54	0
81	MG	u	201	1/1	0.96	0.06	42,42,42,42	0
81	MG	CL	303	1/1	0.96	0.09	66,66,66,66	0
81	MG	1	3508	1/1	0.96	0.12	27,27,27,27	0
81	MG	AS	3423	1/1	0.96	0.17	10,10,10,10	0
81	MG	AW	301	1/1	0.96	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3622	1/1	0.96	0.16	8,8,8,8	0
81	MG	AS	3573	1/1	0.96	0.23	16,16,16,16	0
81	MG	B	1849	1/1	0.96	0.18	28,28,28,28	0
81	MG	1	3519	1/1	0.96	0.28	45,45,45,45	0
81	MG	1	3557	1/1	0.96	0.13	33,33,33,33	0
81	MG	AS	3652	1/1	0.96	0.13	57,57,57,57	0
81	MG	1	3605	1/1	0.96	0.14	17,17,17,17	0
81	MG	1	3695	1/1	0.96	0.12	29,29,29,29	0
81	MG	BE	301	1/1	0.96	0.16	34,34,34,34	0
81	MG	AS	3732	1/1	0.96	0.10	74,74,74,74	0
81	MG	1	3949	1/1	0.96	0.07	42,42,42,42	0
84	ZN	f	101	1/1	0.96	0.10	123,123,123,123	0
81	MG	AS	3656	1/1	0.96	0.32	19,19,19,19	0
81	MG	CM	1876	1/1	0.96	0.19	19,19,19,19	0
81	MG	1	3444	1/1	0.97	0.13	18,18,18,18	0
81	MG	1	3520	1/1	0.97	0.05	14,14,14,14	0
81	MG	AS	3475	1/1	0.97	0.11	10,10,10,10	0
81	MG	1	3902	1/1	0.97	0.04	32,32,32,32	0
81	MG	BG	301	1/1	0.97	0.09	56,56,56,56	0
81	MG	CM	1844	1/1	0.97	0.10	34,34,34,34	0
81	MG	1	3749	1/1	0.97	0.12	24,24,24,24	0
81	MG	1	3791	1/1	0.97	0.12	22,22,22,22	0
81	MG	AS	3433	1/1	0.97	0.16	12,12,12,12	0
81	MG	AS	3590	1/1	0.97	0.06	55,55,55,55	0
81	MG	1	3700	1/1	0.97	0.09	41,41,41,41	0
81	MG	B	1814	1/1	0.97	0.07	79,79,79,79	0
81	MG	AS	3482	1/1	0.97	0.07	54,54,54,54	0
81	MG	1	3527	1/1	0.97	0.20	33,33,33,33	0
81	MG	1	3499	1/1	0.97	0.14	11,11,11,11	0
81	MG	AS	3708	1/1	0.97	0.19	43,43,43,43	0
81	MG	AS	3438	1/1	0.97	0.16	15,15,15,15	0
81	MG	1	3718	1/1	0.97	0.12	42,42,42,42	0
81	MG	B	1950	1/1	0.97	0.06	54,54,54,54	0
81	MG	AS	3441	1/1	0.97	0.17	22,22,22,22	0
81	MG	CM	1930	1/1	0.97	0.04	29,29,29,29	0
81	MG	B	1850	1/1	0.97	0.06	44,44,44,44	0
81	MG	BZ	202	1/1	0.97	0.16	102,102,102,102	0
81	MG	AS	3491	1/1	0.97	0.07	28,28,28,28	0
81	MG	CM	1934	1/1	0.97	0.06	49,49,49,49	0
81	MG	CM	1935	1/1	0.97	0.07	109,109,109,109	0
81	MG	4	207	1/1	0.97	0.07	35,35,35,35	0
81	MG	CA	201	1/1	0.97	0.07	46,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3885	1/1	0.97	0.06	33,33,33,33	0
81	MG	AS	3402	1/1	0.97	0.26	16,16,16,16	0
81	MG	AS	3718	1/1	0.97	0.05	7,7,7,7	0
81	MG	CM	1941	1/1	0.97	0.06	29,29,29,29	0
81	MG	1	3462	1/1	0.97	0.12	13,13,13,13	0
81	MG	AS	3447	1/1	0.97	0.13	16,16,16,16	0
81	MG	1	3465	1/1	0.97	0.13	17,17,17,17	0
81	MG	1	3937	1/1	0.97	0.07	64,64,64,64	0
81	MG	1	3912	1/1	0.97	0.07	24,24,24,24	0
81	MG	AS	3552	1/1	0.97	0.09	39,39,39,39	0
81	MG	1	3799	1/1	0.97	0.09	15,15,15,15	0
81	MG	CQ	301	1/1	0.97	0.10	16,16,16,16	0
81	MG	1	3756	1/1	0.97	0.11	20,20,20,20	0
81	MG	AS	3409	1/1	0.97	0.06	91,91,91,91	0
81	MG	AS	3558	1/1	0.97	0.15	25,25,25,25	0
81	MG	CM	1878	1/1	0.97	0.09	13,13,13,13	0
81	MG	AS	3559	1/1	0.97	0.12	17,17,17,17	0
81	MG	AH	203	1/1	0.97	0.07	79,79,79,79	0
81	MG	1	3549	1/1	0.97	0.14	43,43,43,43	0
81	MG	1	3640	1/1	0.97	0.17	37,37,37,37	0
81	MG	AS	3458	1/1	0.97	0.12	11,11,11,11	0
81	MG	j	301	1/1	0.97	0.06	11,11,11,11	0
81	MG	AS	3678	1/1	0.97	0.22	16,16,16,16	0
81	MG	1	3780	1/1	0.97	0.11	33,33,33,33	0
81	MG	DJ	201	1/1	0.97	0.13	17,17,17,17	0
81	MG	B	1965	1/1	0.97	0.12	35,35,35,35	0
81	MG	j	303	1/1	0.97	0.08	13,13,13,13	0
81	MG	CM	1889	1/1	0.97	0.07	62,62,62,62	0
81	MG	AS	3512	1/1	0.97	0.14	17,17,17,17	0
81	MG	1	3607	1/1	0.97	0.04	13,13,13,13	0
81	MG	1	3642	1/1	0.97	0.14	18,18,18,18	0
81	MG	1	3725	1/1	0.97	0.09	6,6,6,6	0
81	MG	1	3531	1/1	0.97	0.04	25,25,25,25	0
81	MG	E	301	1/1	0.97	0.07	63,63,63,63	0
81	MG	1	3710	1/1	0.97	0.15	26,26,26,26	0
81	MG	1	3469	1/1	0.97	0.24	33,33,33,33	0
81	MG	AS	3470	1/1	0.97	0.16	18,18,18,18	0
81	MG	AS	3635	1/1	0.97	0.17	13,13,13,13	0
81	MG	AS	3749	1/1	0.97	0.07	51,51,51,51	0
81	MG	1	3589	1/1	0.97	0.10	44,44,44,44	0
81	MG	CM	1834	1/1	0.97	0.05	38,38,38,38	0
81	MG	H	1001	1/1	0.97	0.04	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	AS	3752	1/1	0.97	0.08	33,33,33,33	0
84	ZN	AQ	101	1/1	0.97	0.05	95,95,95,95	0
81	MG	CM	1905	1/1	0.97	0.14	29,29,29,29	0
81	MG	CM	1837	1/1	0.97	0.07	12,12,12,12	0
81	MG	AS	3524	1/1	0.97	0.09	38,38,38,38	0
81	MG	CM	1908	1/1	0.97	0.07	23,23,23,23	0
81	MG	AS	3414	1/1	0.98	0.06	71,71,71,71	0
81	MG	AG	202	1/1	0.98	0.04	43,43,43,43	0
81	MG	CM	1926	1/1	0.98	0.05	36,36,36,36	0
81	MG	AS	3577	1/1	0.98	0.12	20,20,20,20	0
81	MG	AS	3555	1/1	0.98	0.08	39,39,39,39	0
81	MG	CM	1868	1/1	0.98	0.12	37,37,37,37	0
81	MG	AT	206	1/1	0.98	0.12	50,50,50,50	0
81	MG	AS	3556	1/1	0.98	0.06	38,38,38,38	0
81	MG	AS	3580	1/1	0.98	0.06	42,42,42,42	0
81	MG	B	1928	1/1	0.98	0.03	17,17,17,17	0
81	MG	B	1875	1/1	0.98	0.05	103,103,103,103	0
81	MG	1	3428	1/1	0.98	0.30	16,16,16,16	0
81	MG	1	3533	1/1	0.98	0.12	15,15,15,15	0
81	MG	AS	3521	1/1	0.98	0.08	59,59,59,59	0
81	MG	1	3964	1/1	0.98	0.08	76,76,76,76	0
81	MG	1	3404	1/1	0.98	0.14	13,13,13,13	0
81	MG	1	3554	1/1	0.98	0.10	36,36,36,36	0
81	MG	AS	3565	1/1	0.98	0.10	19,19,19,19	0
81	MG	AS	3525	1/1	0.98	0.14	25,25,25,25	0
81	MG	AS	3489	1/1	0.98	0.08	23,23,23,23	0
81	MG	AS	3642	1/1	0.98	0.04	99,99,99,99	0
81	MG	AP	204	1/1	0.98	0.04	49,49,49,49	0
81	MG	1	3547	1/1	0.98	0.14	24,24,24,24	0
81	MG	1	3449	1/1	0.98	0.21	14,14,14,14	0
81	MG	AS	3619	1/1	0.98	0.08	47,47,47,47	0
84	ZN	AN	101	1/1	0.98	0.08	149,149,149,149	0
81	MG	1	3515	1/1	0.98	0.14	11,11,11,11	0
81	MG	1	3459	1/1	0.98	0.17	16,16,16,16	0
81	MG	AS	3622	1/1	0.98	0.05	22,22,22,22	0
81	MG	AS	3786	1/1	0.98	0.03	31,31,31,31	0
81	MG	B	1825	1/1	0.98	0.13	22,22,22,22	0
81	MG	B	1941	1/1	0.98	0.05	48,48,48,48	0
84	ZN	CK	101	1/1	0.98	0.06	137,137,137,137	0
84	ZN	DQ	102	1/1	0.98	0.04	47,47,47,47	0
81	MG	AS	3448	1/1	0.99	0.05	6,6,6,6	0
81	MG	1	3793	1/1	0.99	0.03	26,26,26,26	0

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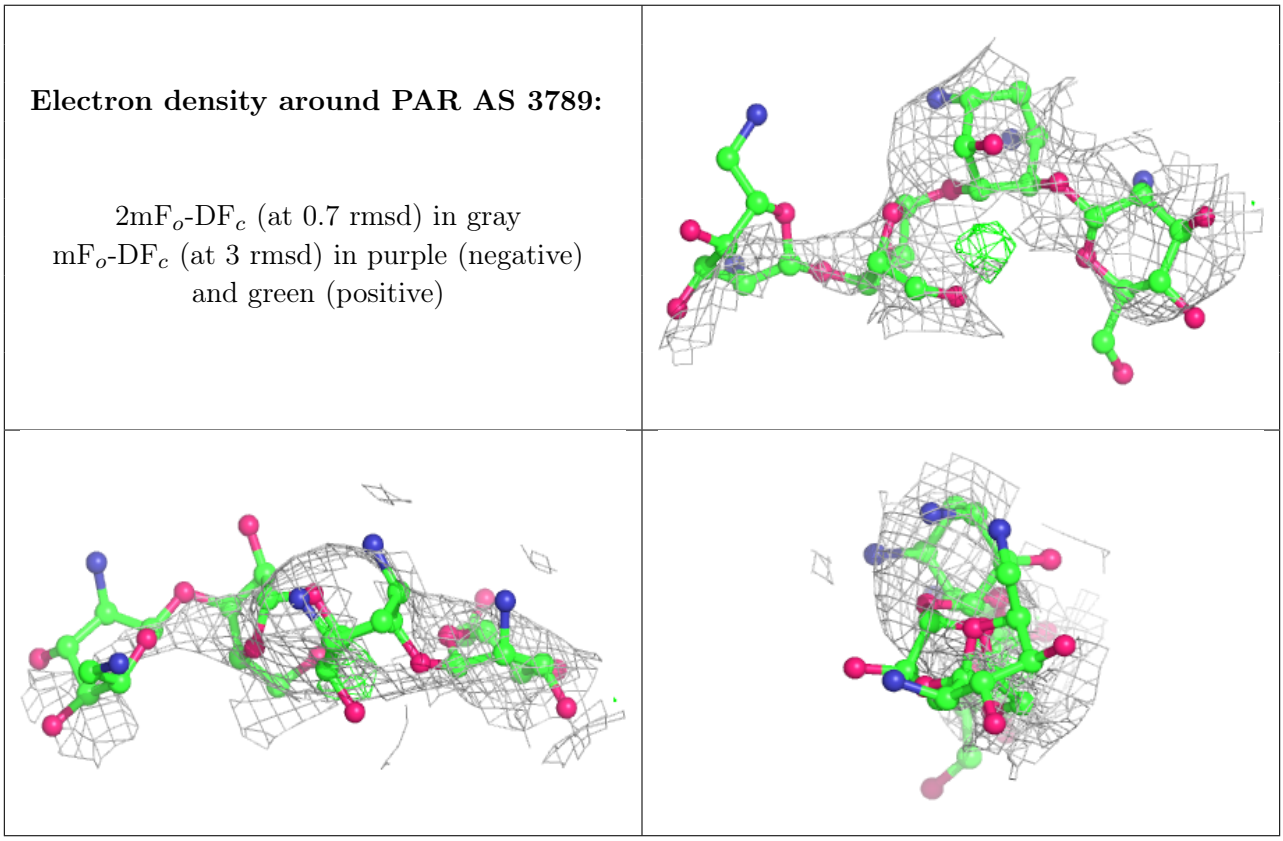
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
81	MG	1	3775	1/1	0.99	0.05	31,31,31,31	0
81	MG	AS	3493	1/1	0.99	0.07	7,7,7,7	0
81	MG	1	3440	1/1	0.99	0.09	50,50,50,50	0
81	MG	AS	3421	1/1	0.99	0.04	63,63,63,63	0
81	MG	1	3762	1/1	0.99	0.04	50,50,50,50	0
81	MG	AS	3785	1/1	0.99	0.07	13,13,13,13	0
81	MG	B	1905	1/1	0.99	0.06	93,93,93,93	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.

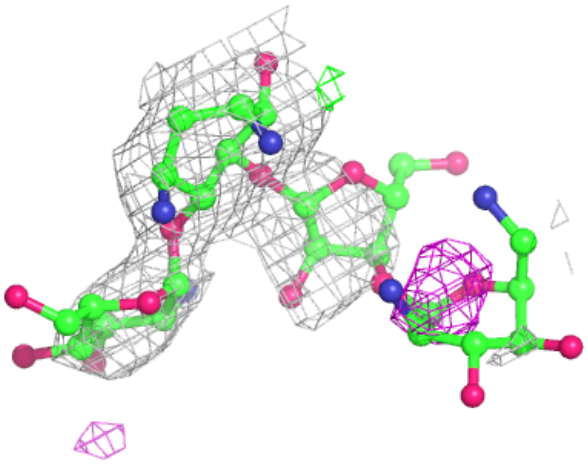
Electron density around PAR AS 3789:

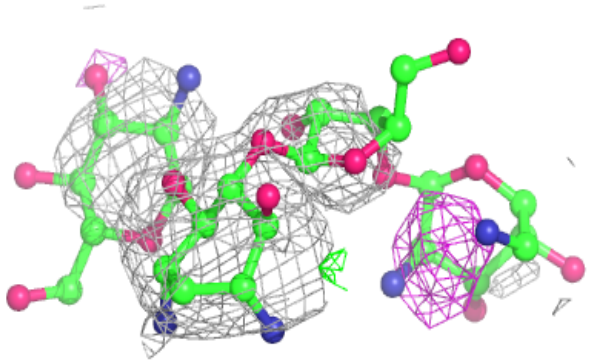
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

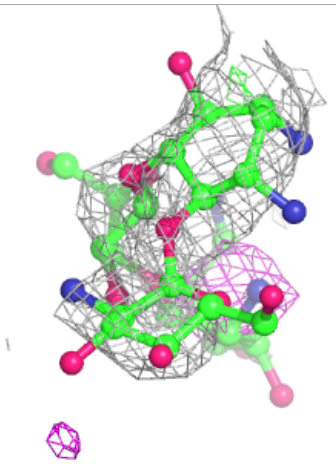


Electron density around PAR AS 3790:

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

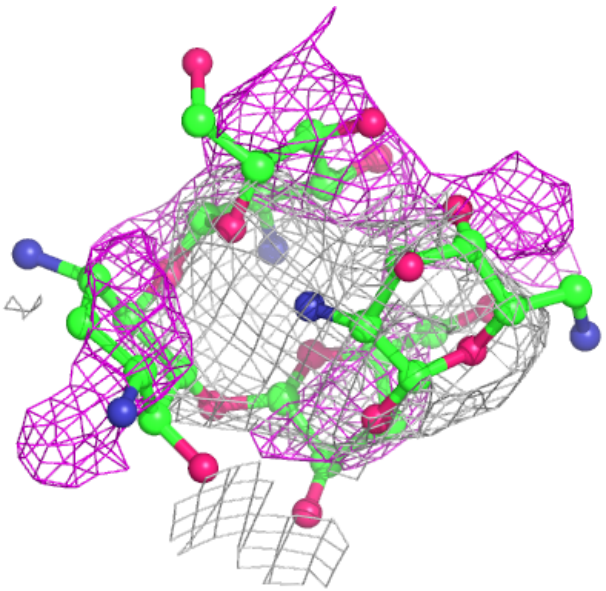


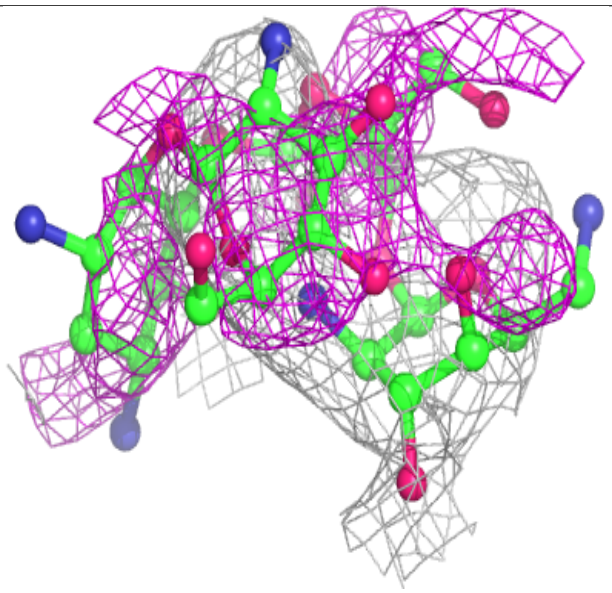


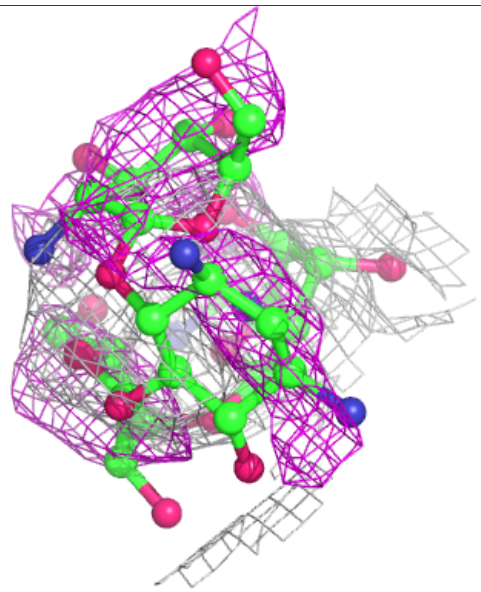


Electron density around PAR B 1970:

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

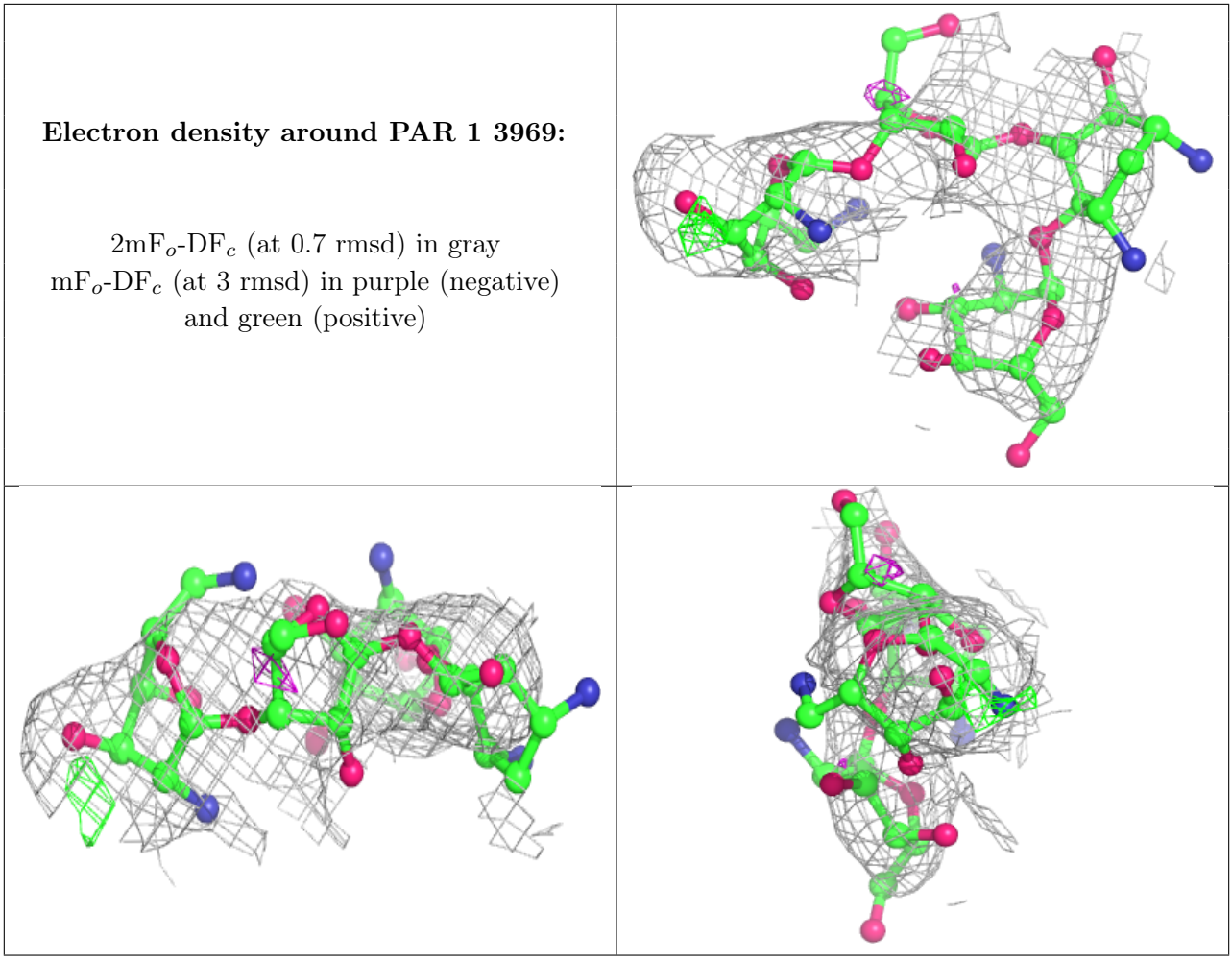






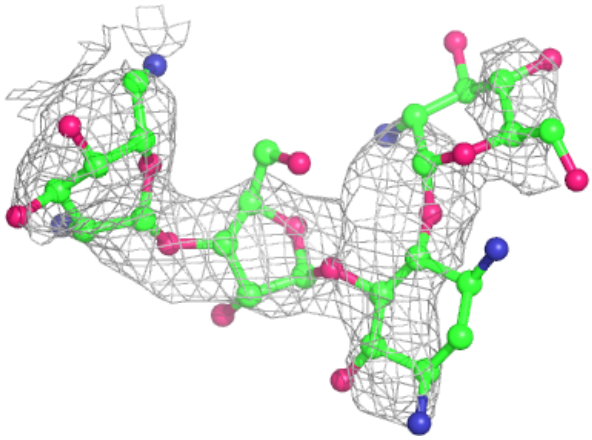
Electron density around PAR 1 3969:

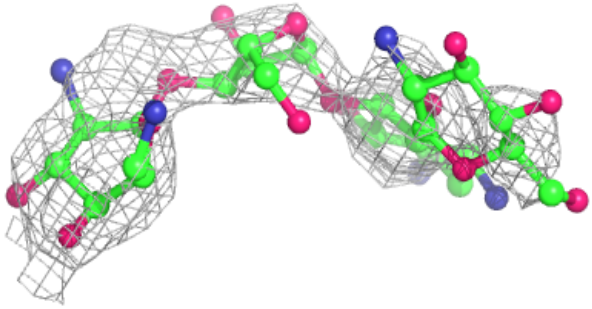
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

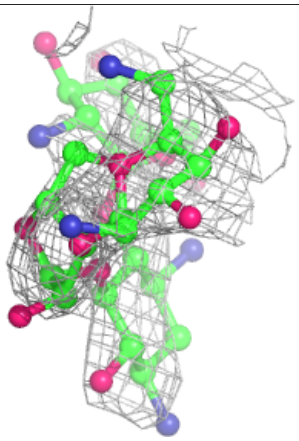


Electron density around PAR AS 3788:

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

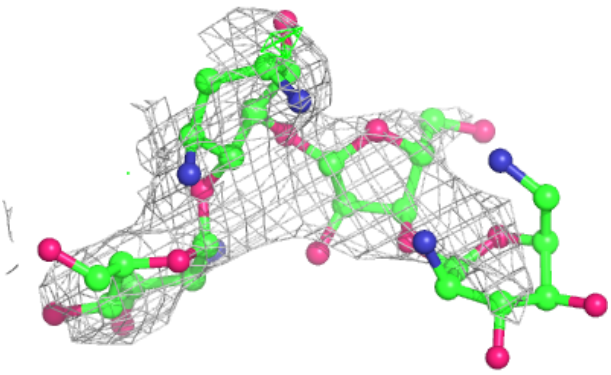


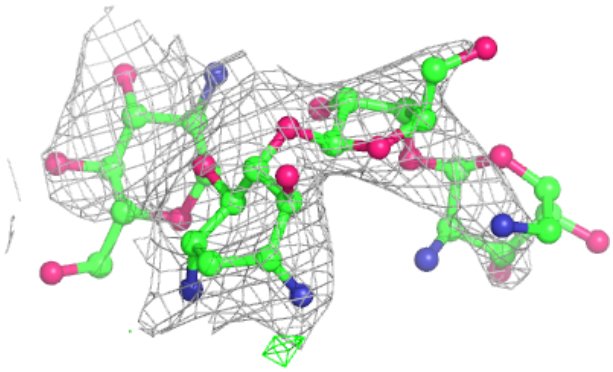


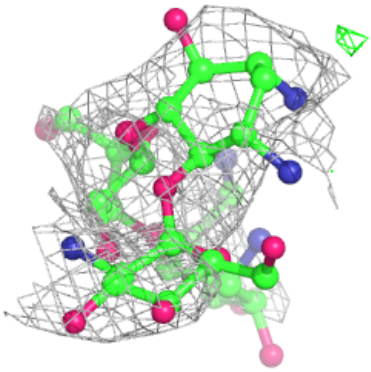


Electron density around PAR 1 3968:

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

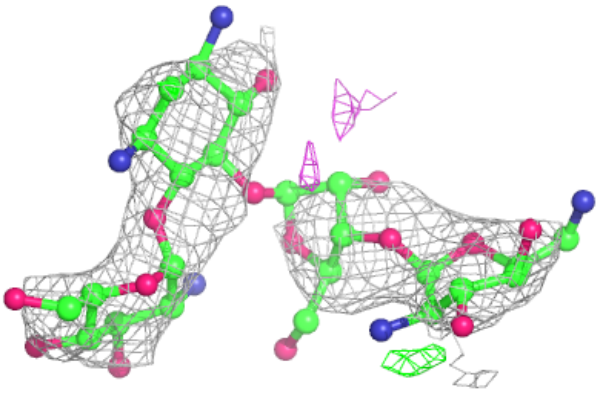


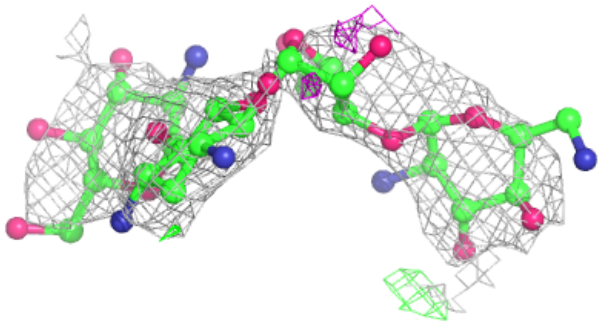


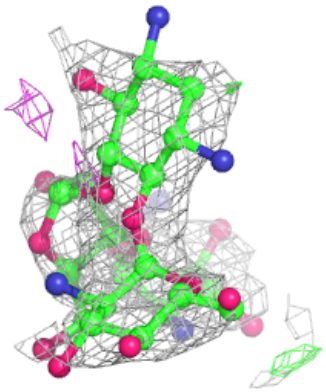


Electron density around PAR 1 3967:

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

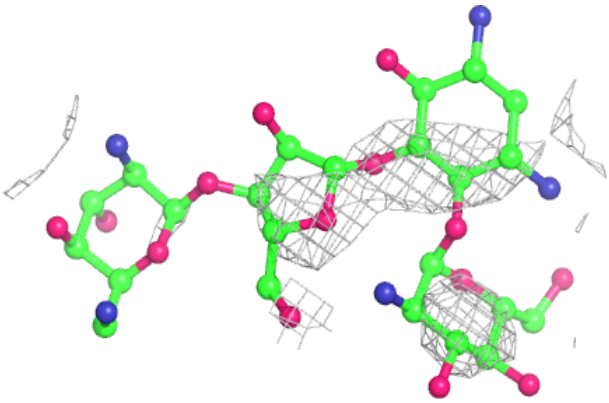


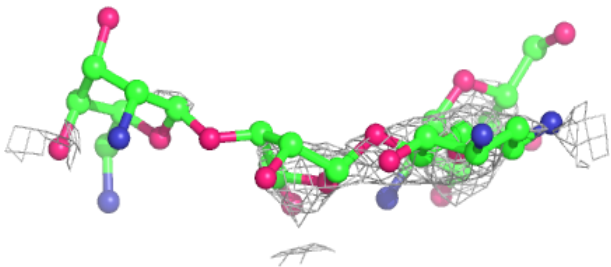


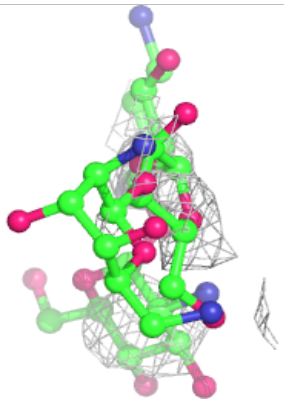


Electron density around PAR CM 1946:

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

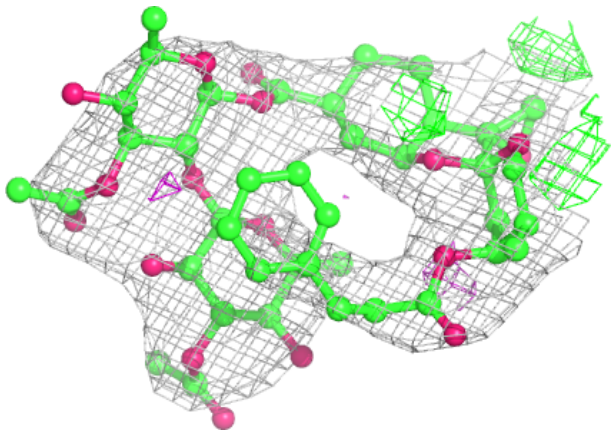


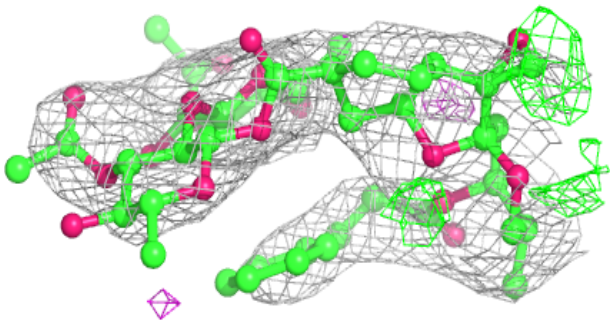


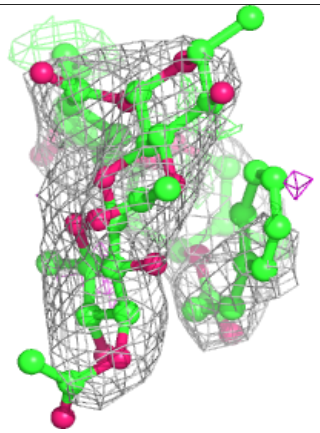


Electron density around 3K5 CJ 202:

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

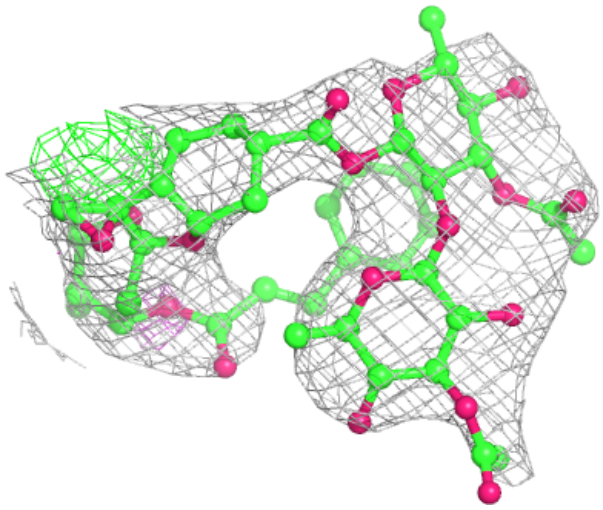


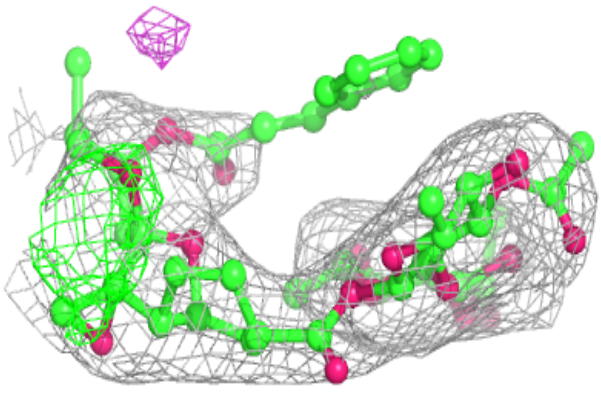


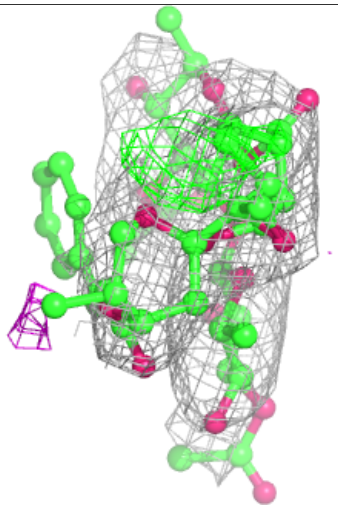


Electron density around 3K5 1 3406:

$2mF_o$-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

There are no such residues in this entry.