



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 07:33 AM UTC

PDB ID : 4V7L / pdb_00004v7l
Title : The structures of viomycin bound to the 70S ribosome.
Authors : Stanley, R.E.; Blaha, G.
Deposited on : 2009-11-12
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

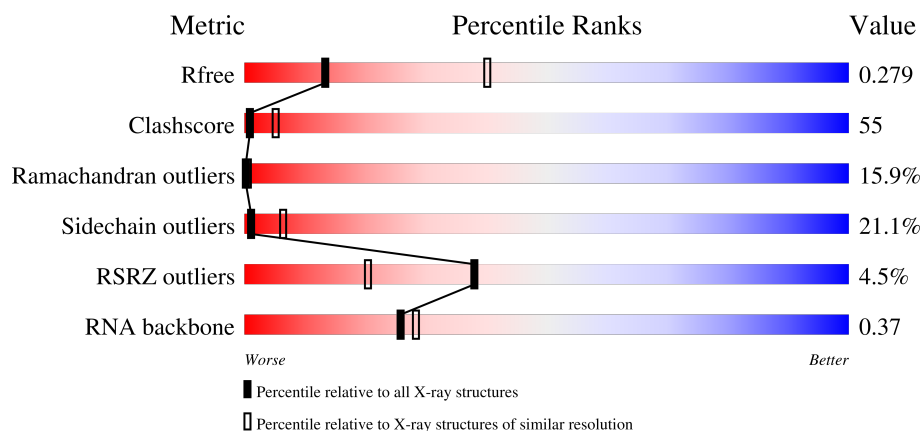
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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

Mol	Chain	Length	Quality of chain
1	AA	1509	
1	CA	1509	
2	AB	256	
2	CB	256	

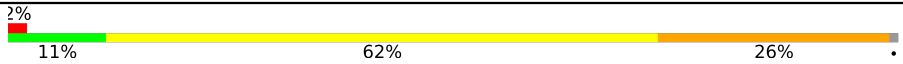
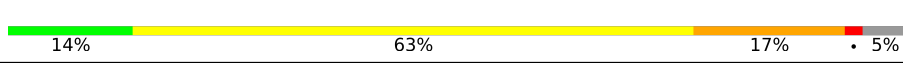
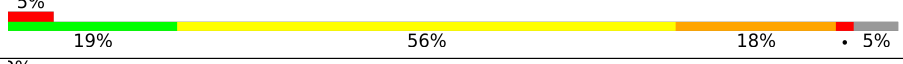
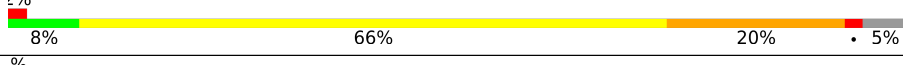
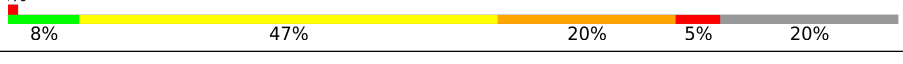
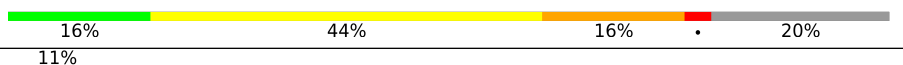
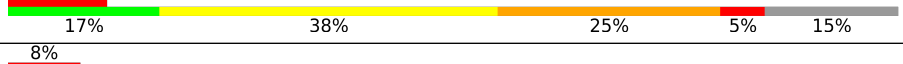
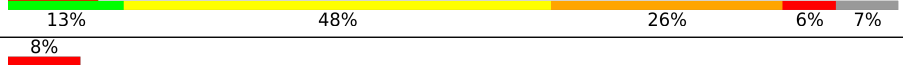
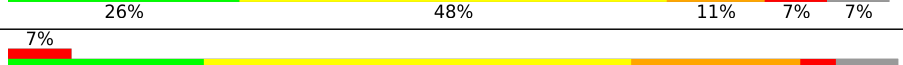
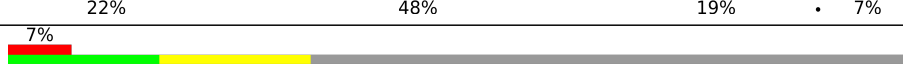
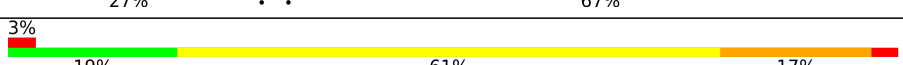
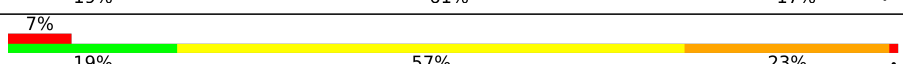
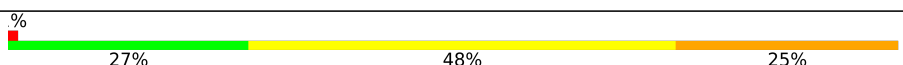
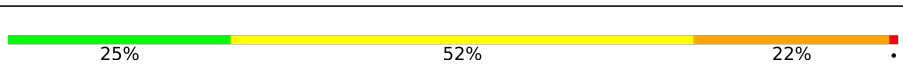
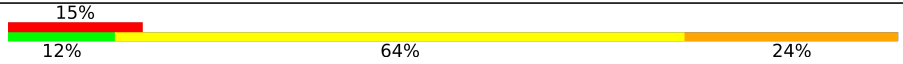
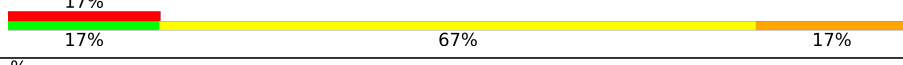
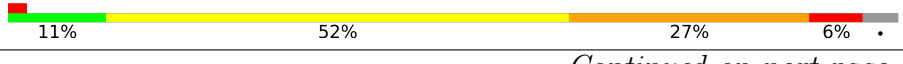
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126	
13	CM	126	
14	AN	61	
14	CN	61	
15	AO	89	

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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	30	
22	CV	30	
23	AW	75	
23	CW	75	
24	AX	77	
24	CX	77	
25	AY	75	
25	CY	75	
26	AZ	6	
26	CZ	6	
27	BA	2915	
27	DA	2915	

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Mol	Chain	Length	Quality of chain
28	BB	122	
28	DB	122	
29	BC	229	
29	DC	229	
30	BD	276	
30	DD	276	
31	BE	206	
31	DE	206	
32	BF	210	
32	DF	210	
33	BG	182	
33	DG	182	
34	BH	180	
34	DH	180	
35	BI	148	
35	DI	148	
36	BN	140	
36	DN	140	
37	BO	122	
37	DO	122	
38	BP	150	
38	DP	150	
39	BQ	141	
39	DQ	141	
40	BR	118	

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Mol	Chain	Length	Quality of chain
40	DR	118	
41	BS	112	
41	DS	112	
42	BT	146	
42	DT	146	
43	BU	118	
43	DU	118	
44	BV	101	
44	DV	101	
45	BW	113	
45	DW	113	
46	BX	96	
46	DX	96	
47	BY	110	
47	DY	110	
48	BZ	206	
48	DZ	206	
49	B0	85	
49	D0	85	
50	B1	98	
50	D1	98	
51	B2	72	
51	D2	72	
52	B3	60	
52	D3	60	

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Mol	Chain	Length	Quality of chain
53	B4	71	
53	D4	71	
54	B5	60	
54	D5	60	
55	B6	54	
55	D6	54	
56	B7	49	
56	D7	49	
57	B8	65	
57	D8	65	
58	B9	37	
58	D9	37	

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
26	UAL	AZ	5	-	-	X	-
26	UAL	CZ	5	-	-	X	-
26	5OH	CZ	6	-	-	X	-
59	MG	BA	3298	-	-	-	X
59	MG	BA	3322	-	-	-	X
59	MG	DA	3203	-	-	-	X
59	MG	DA	3236	-	-	-	X
59	MG	DA	3238	-	-	-	X
59	MG	DA	3273	-	-	-	X

2 Entry composition

There are 60 unique types of molecules in this entry. The entry contains 294559 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 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1495	Total	C	N	O	P	0	0	0
			32141	14306	5964	10377	1494			
1	CA	1495	Total	C	N	O	P	0	0	0
			32141	14306	5964	10377	1494			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	AB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			
2	CB	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	AC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			
3	CC	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	AD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			
4	CD	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	AE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			
5	CE	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	AF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			
6	CF	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	AG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			
7	CG	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	AH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			
8	CH	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	AI	127	Total	C	N	O		0	0	0
			1005	636	195	174				
9	CI	127	Total	C	N	O		0	0	0
			1006	637	195	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	AJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	CJ	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	AK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			
11	CK	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			
12	CL	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	120	Total	C	N	O	S	0	0	0
			947	585	195	165	2			
13	CM	119	Total	C	N	O	S	0	0	0
			910	564	180	164	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	AN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			
14	CN	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	AO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			
15	CO	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	AP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			
16	CP	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	AQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			
17	CQ	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	AR	70	Total	C	N	O	0	0	0
			574	367	112	95			
18	CR	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	AS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			
19	CS	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	AT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			
20	CT	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	AU	25	Total	C	N	O	0	0	1
			209	128	51	30			
21	CU	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			
22	CV	10	Total	C	N	O	P	0	0	0
			213	97	42	65	9			

- Molecule 23 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AW	75	Total	C	N	O	P	0	0	0
			1593	711	281	526	75			
23	CW	75	Total	C	N	O	P	0	0	0
			1593	711	281	526	75			

- Molecule 24 is a RNA chain called tRNA-Met.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			
24	CX	77	Total	C	N	O	P	0	0	0
			1640	732	297	535	76			

- Molecule 25 is a RNA chain called tRNA-Gln.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	AY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			
25	CY	75	Total	C	N	O	P	0	0	0
			1591	711	280	526	74			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	33	G	C	conflict	GB CP001637.1
AY	44	U	A	conflict	GB CP001637.1

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Chain	Residue	Modelled	Actual	Comment	Reference
CY	33	G	C	conflict	GB CP001637.1
CY	44	U	A	conflict	GB CP001637.1

- Molecule 26 is a protein called Viomycin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	AZ	6	Total	C	N	O	0	0	0
			48	25	13	10			
26	CZ	6	Total	C	N	O	0	0	0
			48	25	13	10			

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	BA	2800	Total	C	N	O	P	0	0	0
			60311	26841	11284	19387	2799			
27	DA	2800	Total	C	N	O	P	0	0	0
			60313	26842	11286	19386	2799			

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	BB	118	Total	C	N	O	P	0	0	0
			2528	1126	466	819	117			
28	DB	118	Total	C	N	O	P	0	0	0
			2528	1126	466	819	117			

- Molecule 29 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
29	BC	191	Total	C	N	O	0	0	1
			1142	691	221	230			
29	DC	191	Total	C	N	O	0	0	1
			1142	691	221	230			

- Molecule 30 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	BD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			
30	DD	272	Total	C	N	O	S	0	0	1
			2105	1329	417	356	3			

- Molecule 31 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			
31	DE	205	Total	C	N	O	S	0	0	1
			1564	988	300	270	6			

- Molecule 32 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			
32	DF	208	Total	C	N	O	S	0	0	1
			1624	1035	304	282	3			

- Molecule 33 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	BG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			
33	DG	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 34 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
34	BH	164	Total	C	N	O	S	0	0	1
			1252	794	233	224	1			
34	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 35 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BI	146	Total	C	N	O	S	0	0	1
			1042	668	175	198	1			
35	DI	146	Total	C	N	O	S	0	0	1
			1046	670	175	200	1			

- Molecule 36 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	BN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			
36	DN	139	Total	C	N	O	S	0	0	1
			1105	712	207	182	4			

- Molecule 37 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			
37	DO	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 38 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			
38	DP	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 39 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
39	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
39	DQ	139	Total	C	N	O	S	0	0	0
			1107	707	209	184	7			

- Molecule 40 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
40	BR	117	Total	C	N	O		0	0	0
			960	599	202	159				
40	DR	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 41 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
41	BS	99	Total	C	N	O		0	0	1
			771	486	155	130				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
41	DS	101	Total	C	N	O	0	0	1
			777	489	156	132			

- Molecule 42 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
42	BT	138	Total	C	N	O	0	0	1
			1142	710	235	196			
42	DT	138	Total	C	N	O	0	0	1
			1142	710	235	196			

- Molecule 43 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
43	BU	117	Total	C	N	O	0	0	0
			958	604	202	151			
43	DU	117	Total	C	N	O	0	0	0
			958	604	202	151			

- Molecule 44 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BV	101	Total	C	N	O	0	0	0
			779	501	142	135			
44	DV	101	Total	C	N	O	0	0	0
			779	501	142	135			

- Molecule 45 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
45	BW	113	Total	C	N	O	0	0	0
			896	563	176	155			
45	DW	113	Total	C	N	O	0	0	0
			896	563	176	155			

- Molecule 46 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
46	BX	93	Total	C	N	O	0	0	1
			726	471	132	123			
46	DX	93	Total	C	N	O	0	0	1
			726	471	132	123			

- Molecule 47 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			
47	DY	101	Total	C	N	O	S	0	0	1
			776	500	149	123	4			

- Molecule 48 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			
48	DZ	177	Total	C	N	O	S	0	0	1
			1404	897	253	252	2			

- Molecule 49 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	B0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			
49	D0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

- Molecule 50 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
50	B1	94	Total	C	N	O	S	0	0	1
			715	448	141	125	1			
50	D1	94	Total	C	N	O	S	0	0	1
			732	460	146	125	1			

- Molecule 51 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
51	B2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			
51	D2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 52 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
52	B3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			
52	D3	60	Total	C	N	O	S	0	0	1
			468	298	91	78	1			

- Molecule 53 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
53	B4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			
53	D4	31	Total	C	N	O	S	0	0	1
			226	142	37	43	4			

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
54	B5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			
54	D5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 55 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
55	B6	51	Total	C	N	O	S	0	0	1
			411	253	84	70	4			
55	D6	46	Total	C	N	O	S	0	0	1
			390	241	80	65	4			

- Molecule 56 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
56	B7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			
56	D7	49	Total	C	N	O	S	0	0	1
			419	257	105	55	2			

- Molecule 57 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
57	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 58 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
58	B9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			
58	D9	36	Total	C	N	O	S	0	0	0
			299	183	67	46	3			

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	AA	133	Total	Mg	0	0
			133	133		
59	AC	1	Total	Mg	0	0
			1	1		
59	AD	1	Total	Mg	0	0
			1	1		
59	AE	1	Total	Mg	0	0
			1	1		
59	AF	1	Total	Mg	0	0
			1	1		
59	AH	1	Total	Mg	0	0
			1	1		
59	AK	2	Total	Mg	0	0
			2	2		
59	AL	1	Total	Mg	0	0
			1	1		
59	AO	1	Total	Mg	0	0
			1	1		
59	AT	2	Total	Mg	0	0
			2	2		
59	AW	7	Total	Mg	0	0
			7	7		
59	AX	7	Total	Mg	0	0
			7	7		
59	AY	2	Total	Mg	0	0
			2	2		
59	BA	400	Total	Mg	0	0
			400	400		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	BB	1	Total 1	Mg 1	0	0
59	BD	1	Total 1	Mg 1	0	0
59	BE	1	Total 1	Mg 1	0	0
59	BF	2	Total 2	Mg 2	0	0
59	BH	1	Total 1	Mg 1	0	0
59	BN	1	Total 1	Mg 1	0	0
59	BP	1	Total 1	Mg 1	0	0
59	BQ	1	Total 1	Mg 1	0	0
59	BR	1	Total 1	Mg 1	0	0
59	BU	1	Total 1	Mg 1	0	0
59	BX	1	Total 1	Mg 1	0	0
59	BY	1	Total 1	Mg 1	0	0
59	BZ	1	Total 1	Mg 1	0	0
59	B0	2	Total 2	Mg 2	0	0
59	B5	1	Total 1	Mg 1	0	0
59	CA	92	Total 92	Mg 92	0	0
59	CE	2	Total 2	Mg 2	0	0
59	CQ	1	Total 1	Mg 1	0	0
59	CV	2	Total 2	Mg 2	0	0
59	CX	3	Total 3	Mg 3	0	0
59	DA	275	Total 275	Mg 275	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
59	DB	1	Total 1	Mg 1	0	0
59	DD	3	Total 3	Mg 3	0	0
59	DE	3	Total 3	Mg 3	0	0
59	DF	1	Total 1	Mg 1	0	0
59	DR	1	Total 1	Mg 1	0	0
59	DZ	1	Total 1	Mg 1	0	0
59	D5	2	Total 2	Mg 2	0	0
59	D6	1	Total 1	Mg 1	0	0

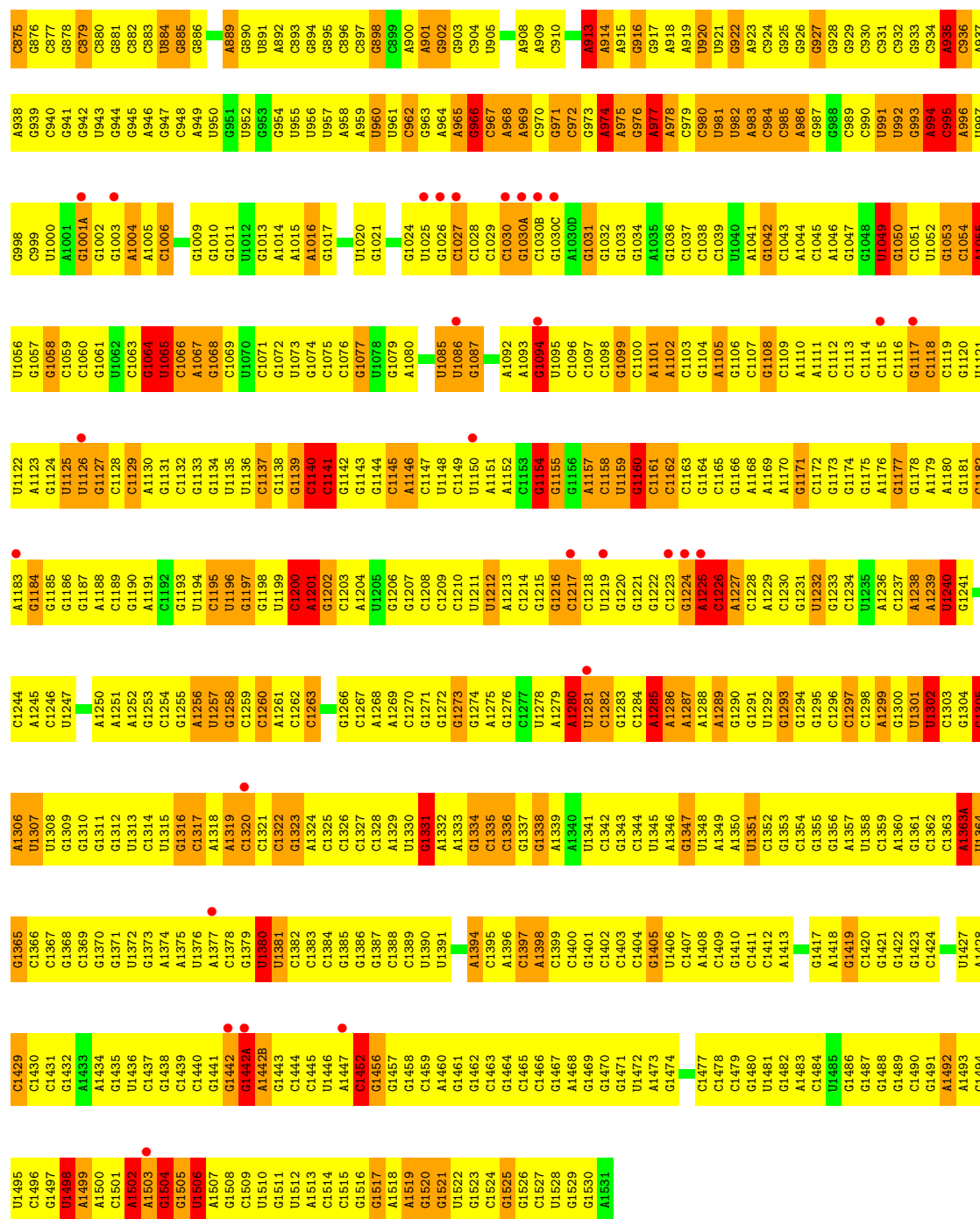
- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AD	1	Total 1	Zn 1	0	0
60	B4	1	Total 1	Zn 1	0	0
60	B5	1	Total 1	Zn 1	0	0
60	B9	1	Total 1	Zn 1	0	0
60	CD	1	Total 1	Zn 1	0	0
60	D4	1	Total 1	Zn 1	0	0
60	D5	1	Total 1	Zn 1	0	0
60	D9	1	Total 1	Zn 1	0	0

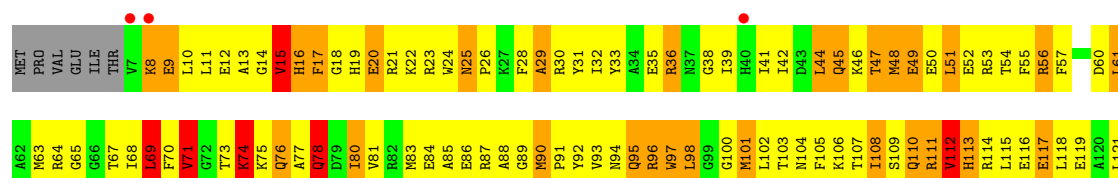
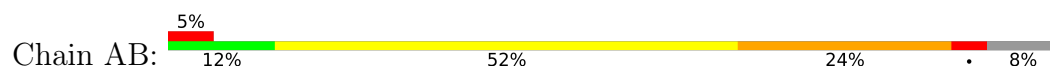


Chain CA:

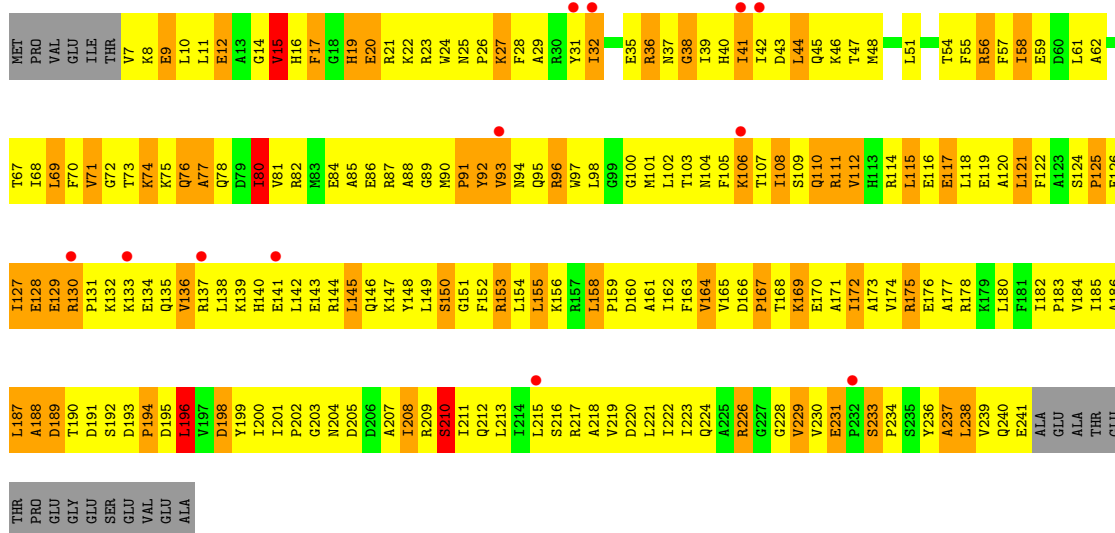
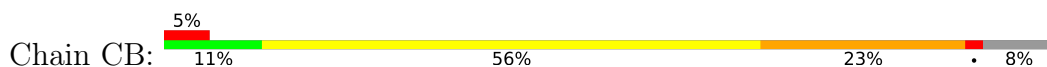




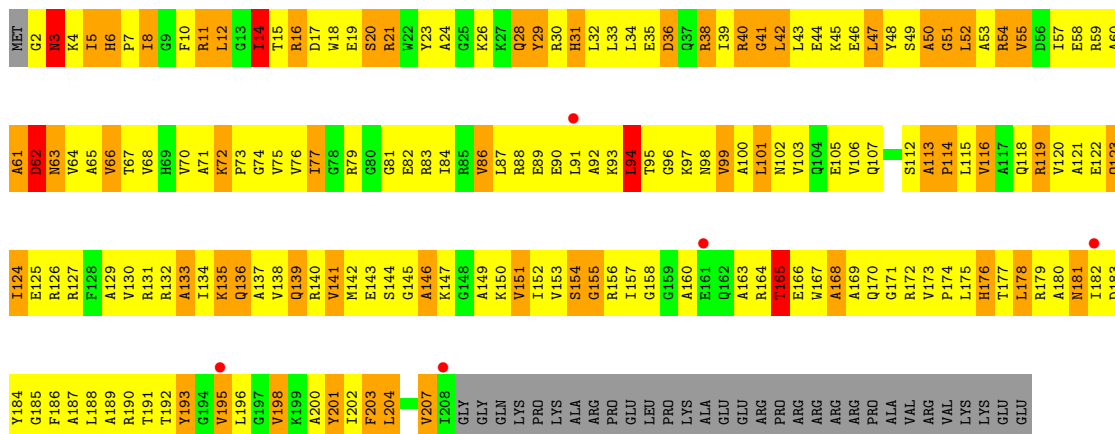
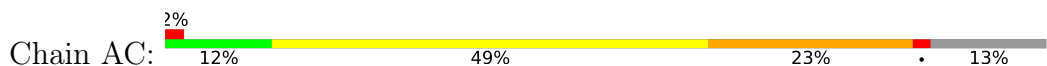
● Molecule 2: 30S ribosomal protein S2



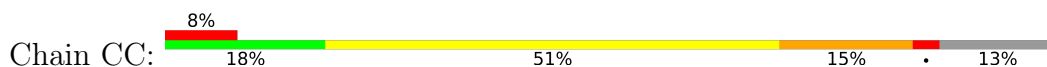
- Molecule 2: 30S ribosomal protein S2

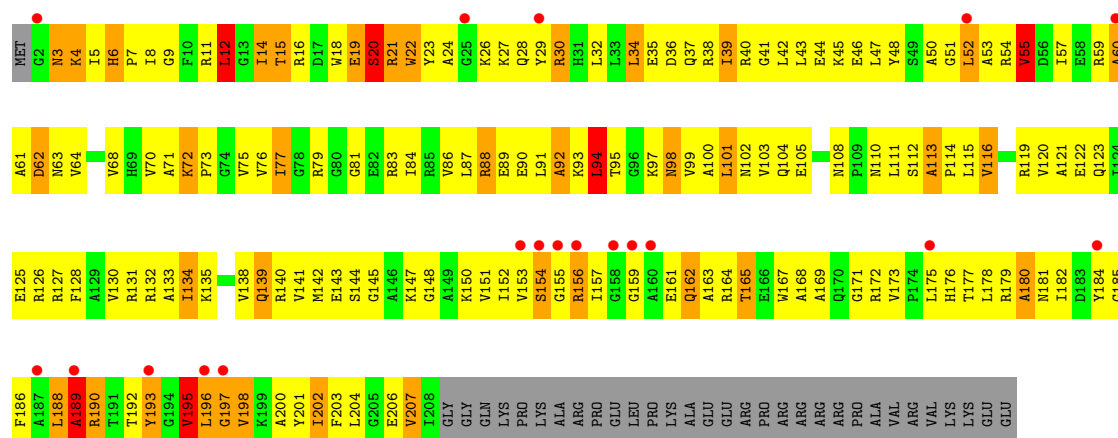


- Molecule 3: 30S ribosomal protein S3

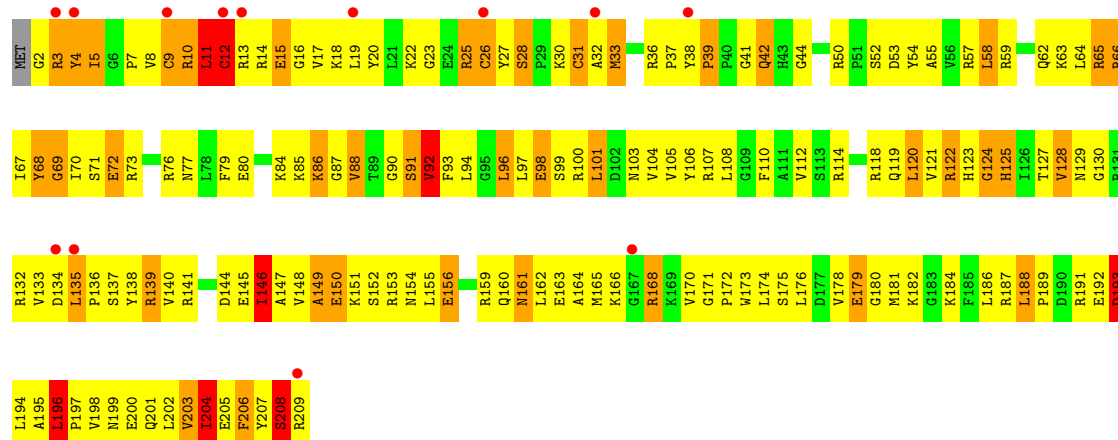


- Molecule 3: 30S ribosomal protein S3

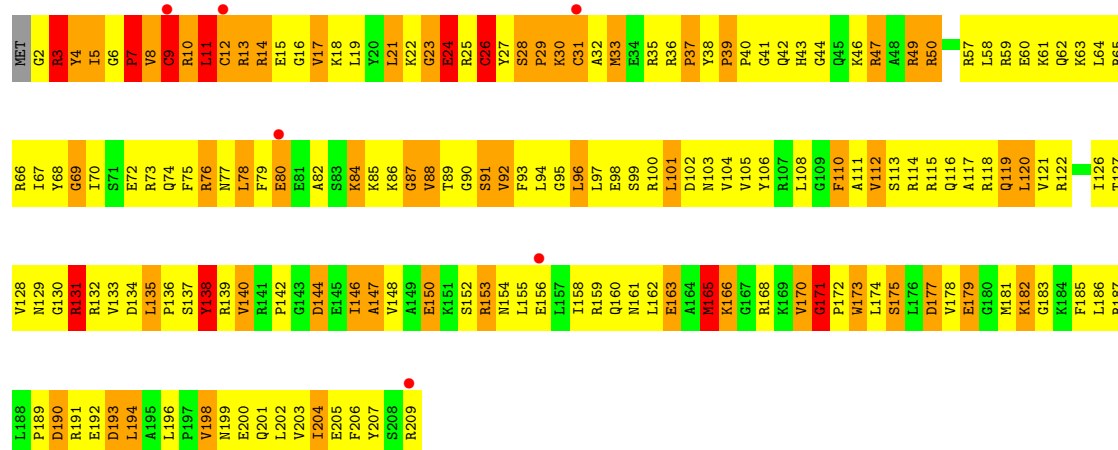
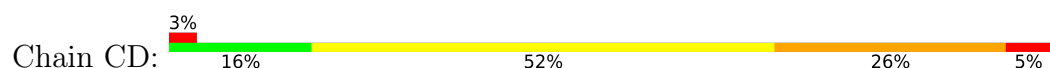




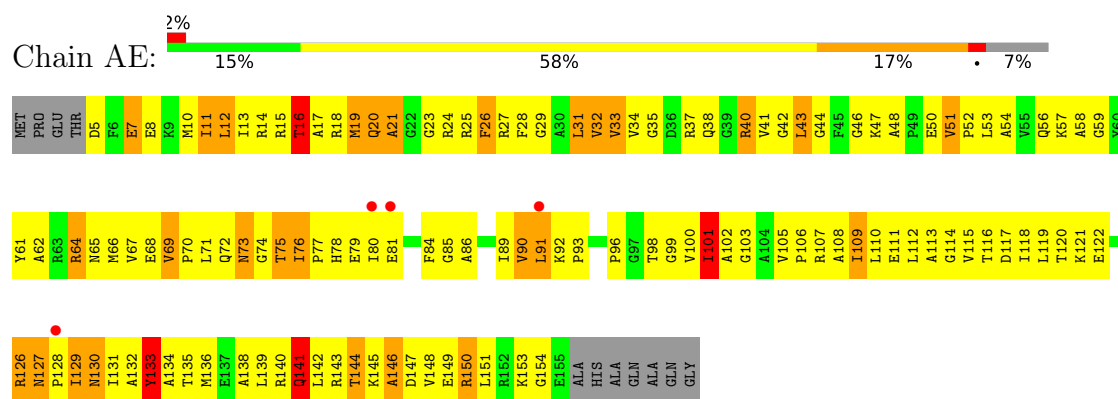
• Molecule 4: 30S ribosomal protein S4



• Molecule 4: 30S ribosomal protein S4



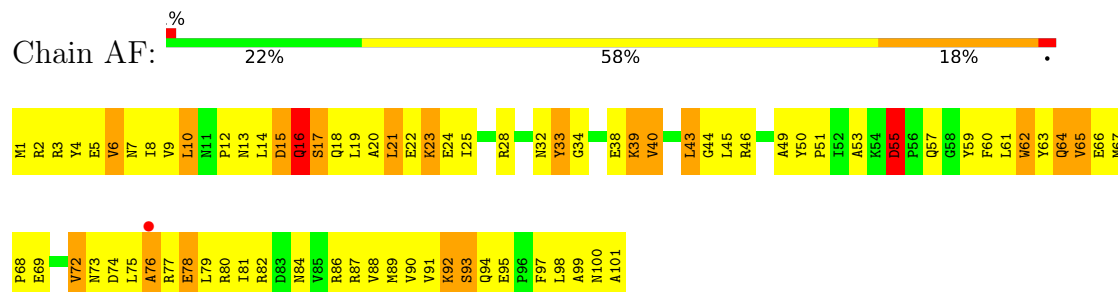
• Molecule 5: 30S ribosomal protein S5



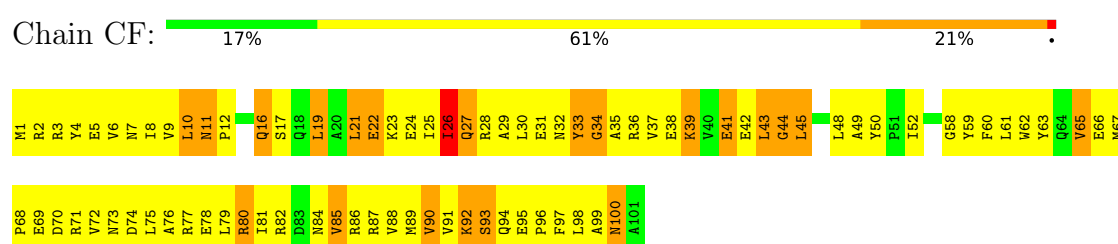
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

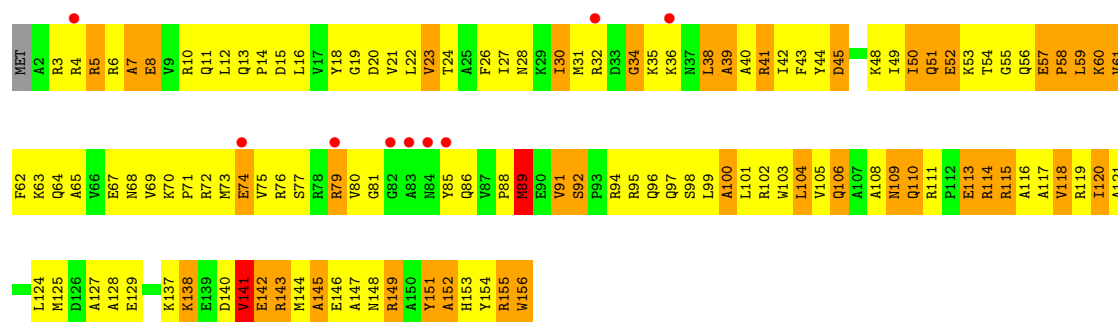


• Molecule 6: 30S ribosomal protein S6



• Molecule 7: 30S ribosomal protein S7

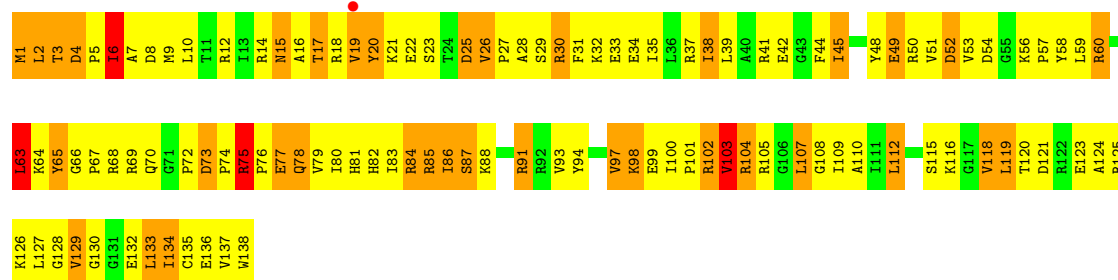
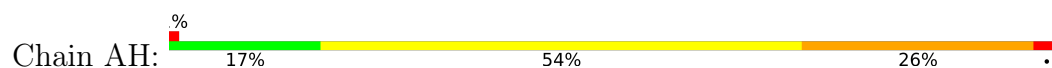




• Molecule 7: 30S ribosomal protein S7



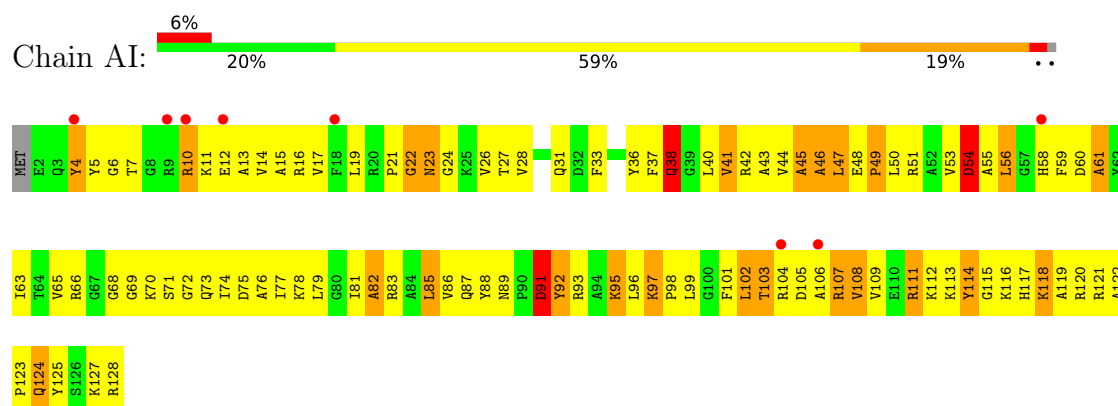
• Molecule 8: 30S ribosomal protein S8



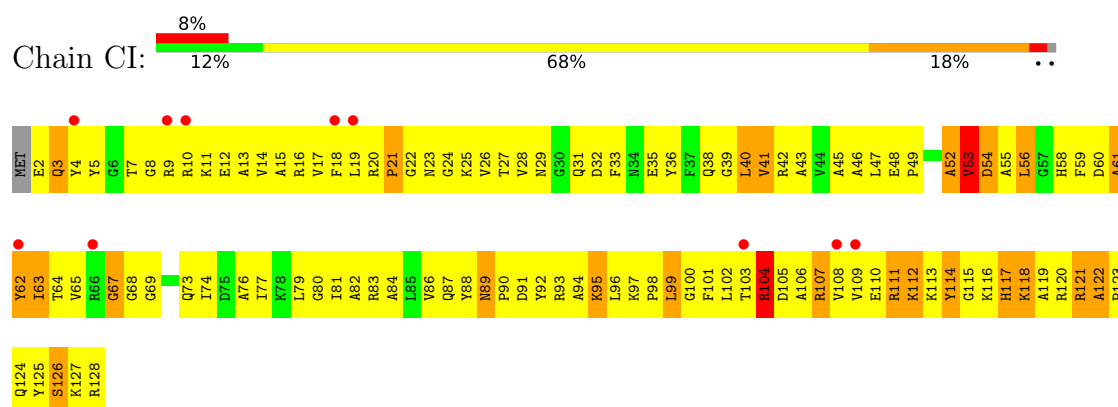
• Molecule 8: 30S ribosomal protein S8



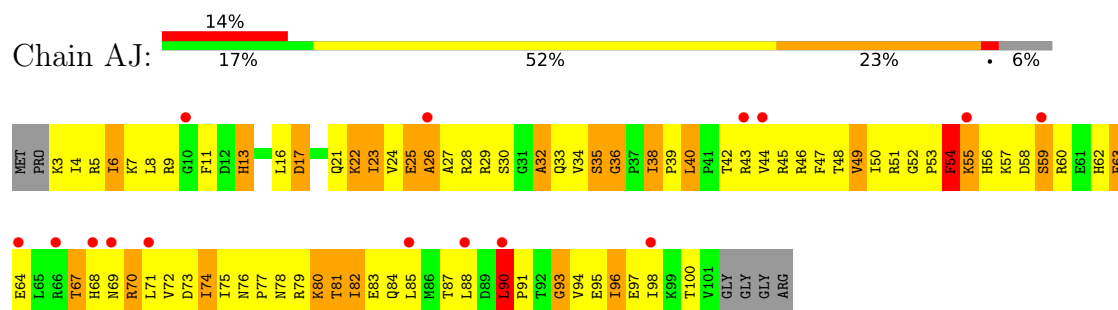
- Molecule 9: 30S ribosomal protein S9



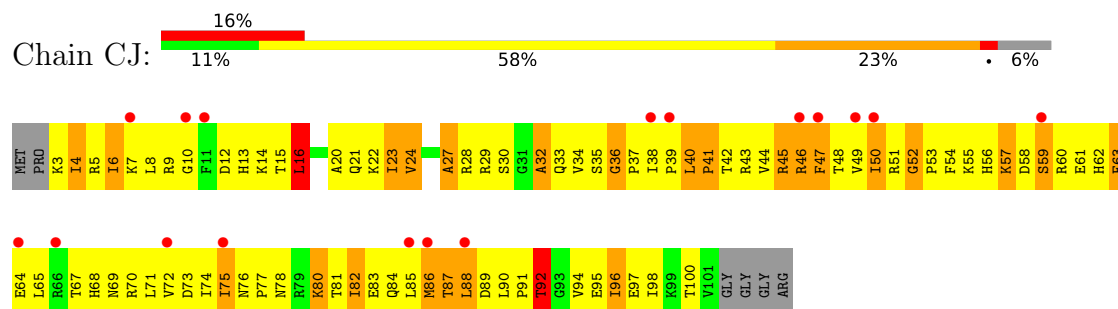
- Molecule 9: 30S ribosomal protein S9



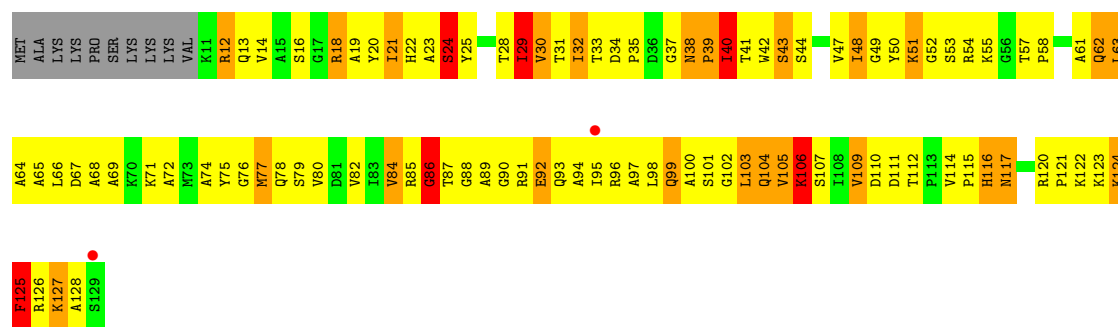
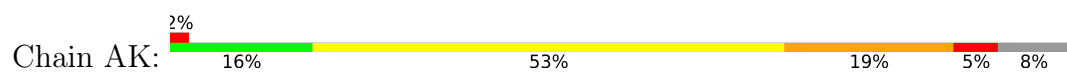
- Molecule 10: 30S ribosomal protein S10



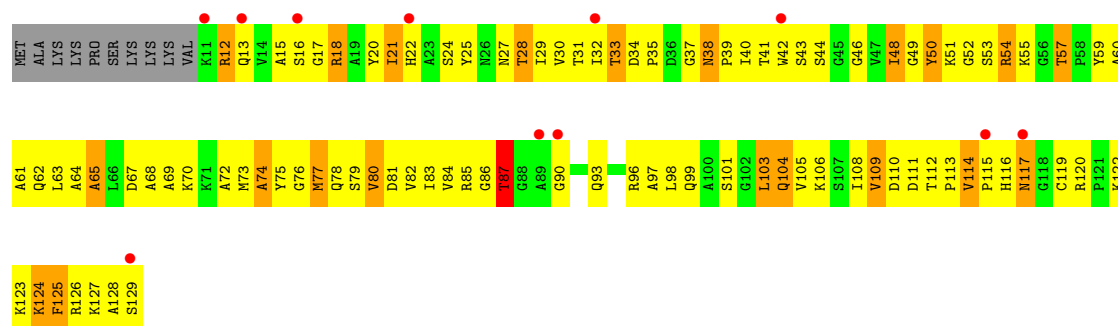
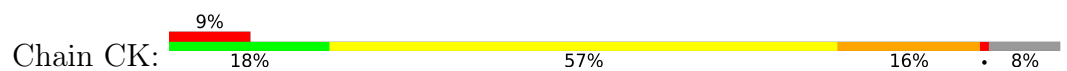
- Molecule 10: 30S ribosomal protein S10



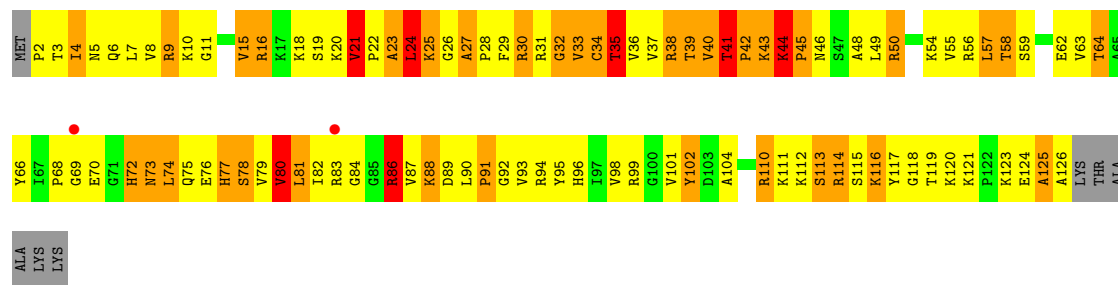
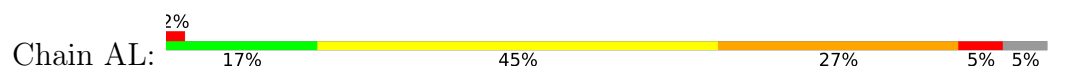
- Molecule 11: 30S ribosomal protein S11



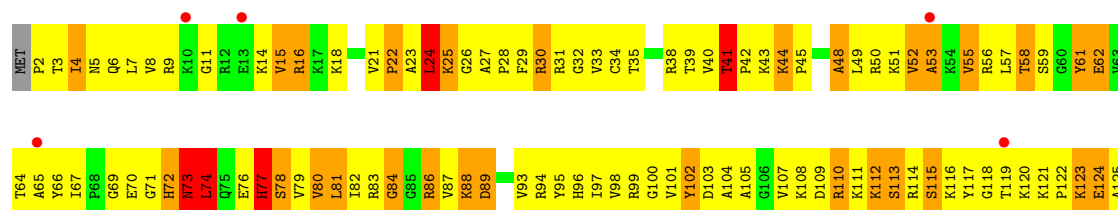
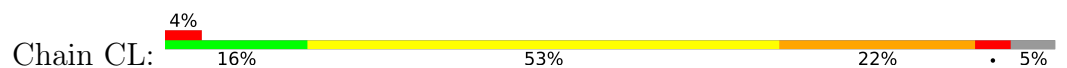
• Molecule 11: 30S ribosomal protein S11



• Molecule 12: 30S ribosomal protein S12



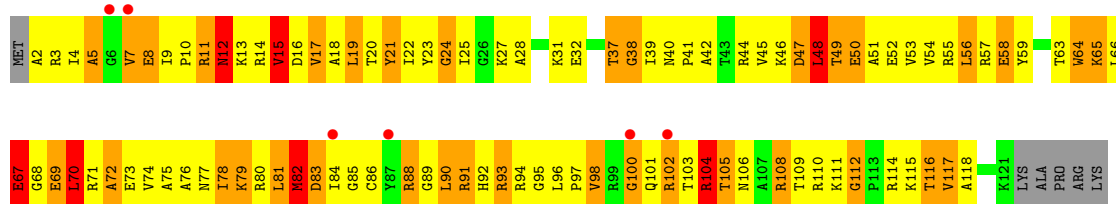
• Molecule 12: 30S ribosomal protein S12



A126
LYS
THR
ALA
ALA
LYS
LYS

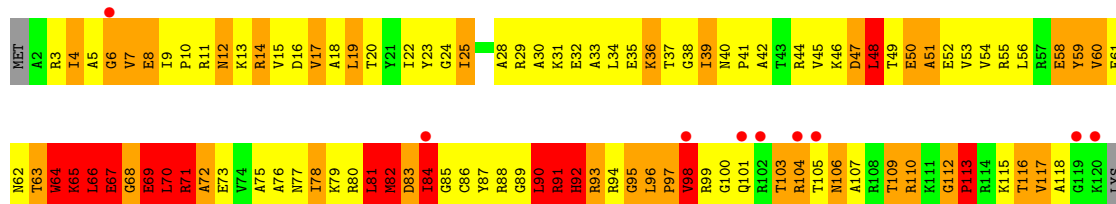
- Molecule 13: 30S ribosomal protein S13

Chain AM: 5% 15% 47% 28% 6% 5%



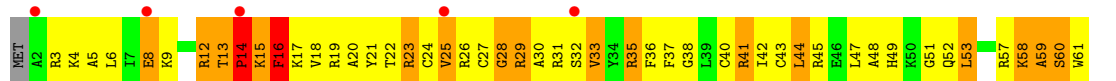
- Molecule 13: 30S ribosomal protein S13

Chain CM: 7% 10% 44% 27% 13% 6%



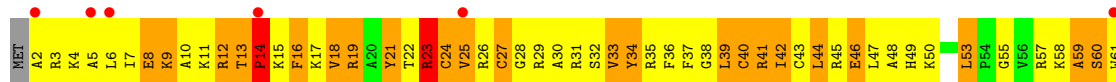
- Molecule 14: 30S ribosomal protein S14

Chain AN: 8% 18% 51% 26% . .



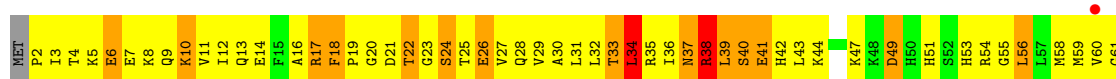
- Molecule 14: 30S ribosomal protein S14

Chain CN: 10% 8% 51% 36% . .



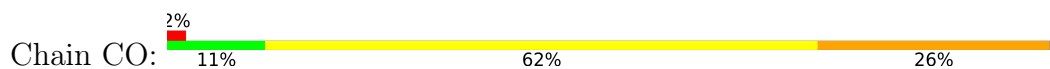
- Molecule 15: 30S ribosomal protein S15

Chain AO: 6% 12% 60% 25% . .

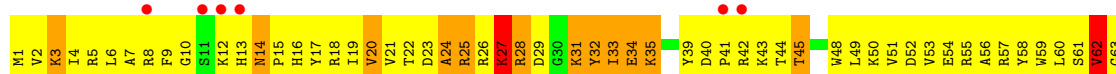
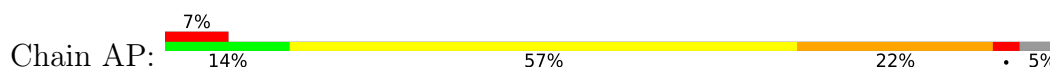




• Molecule 15: 30S ribosomal protein S15



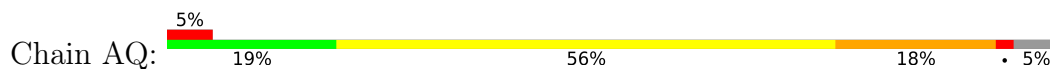
• Molecule 16: 30S ribosomal protein S16



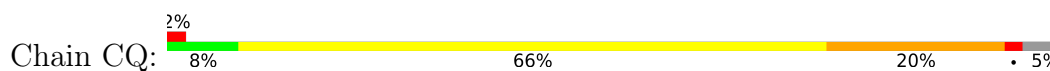
• Molecule 16: 30S ribosomal protein S16

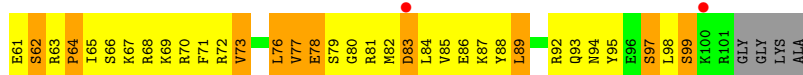


• Molecule 17: 30S ribosomal protein S17

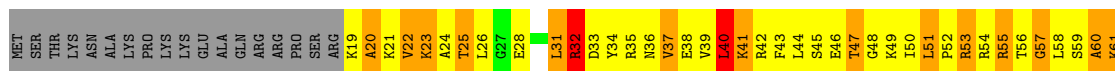


• Molecule 17: 30S ribosomal protein S17

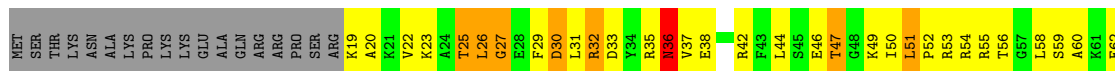
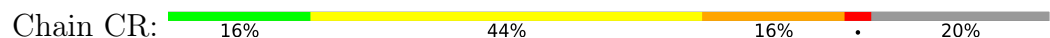




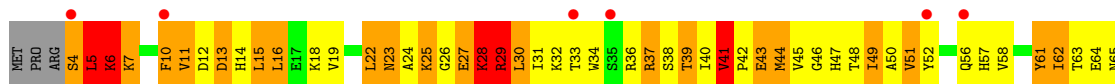
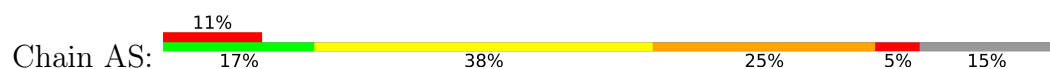
- Molecule 18: 30S ribosomal protein S18



- Molecule 18: 30S ribosomal protein S18



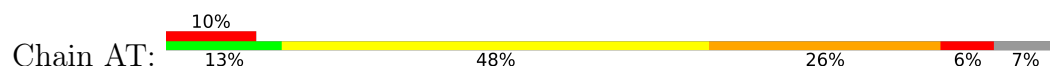
- Molecule 19: 30S ribosomal protein S19

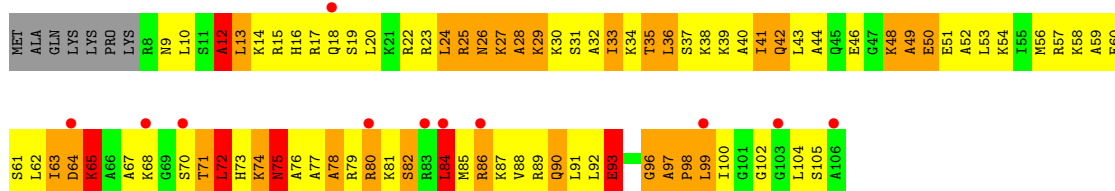


- Molecule 19: 30S ribosomal protein S19

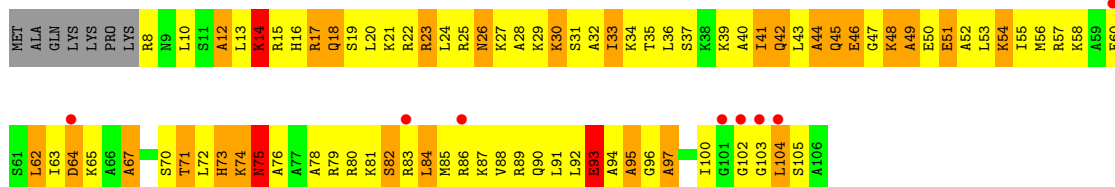
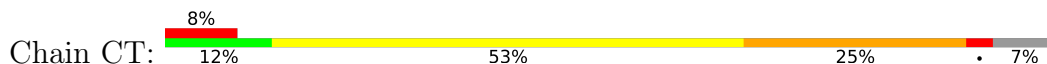


- Molecule 20: 30S ribosomal protein S20





• Molecule 20: 30S ribosomal protein S20



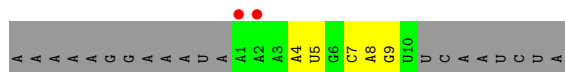
• Molecule 21: 30S ribosomal protein Thx



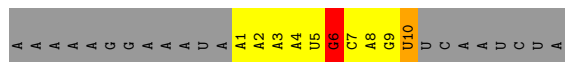
• Molecule 21: 30S ribosomal protein Thx



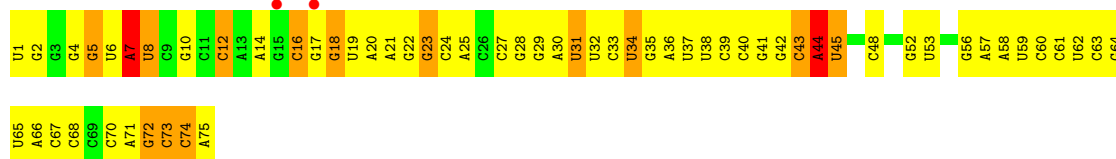
• Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')



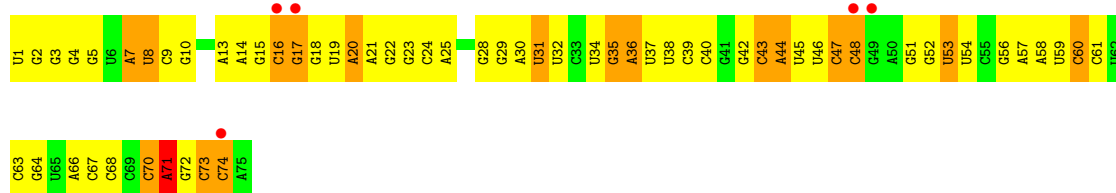
• Molecule 22: RNA (5'-R(*AP*AP*AP*AP*AP*GP*GP*AP*AP*AP*UP*A*AP*AP*AP*AP*UP*GP*CP*AP*GP*UP*UP*CP*AP*AP*UP*CP*UP*A)-3')



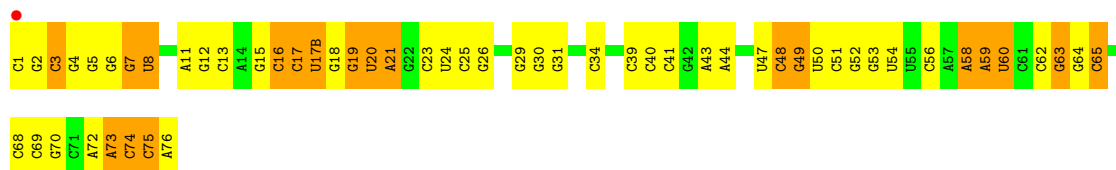
• Molecule 23: tRNA-Gln



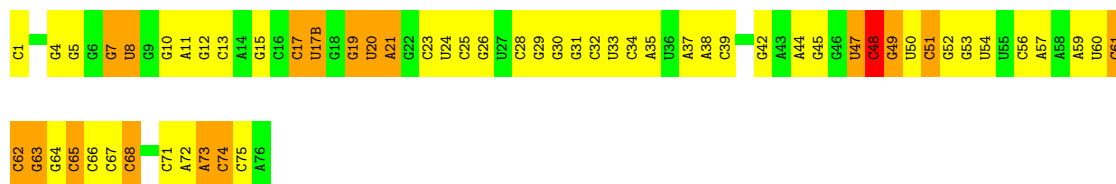
• Molecule 23: tRNA-Gln



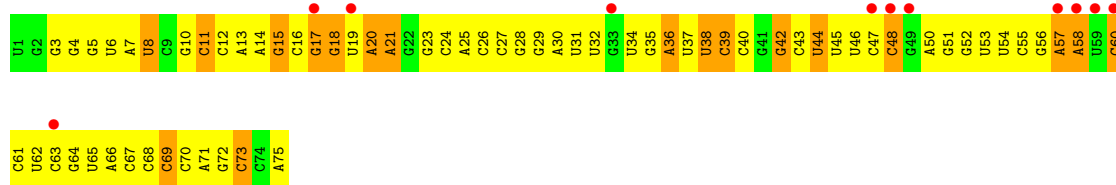
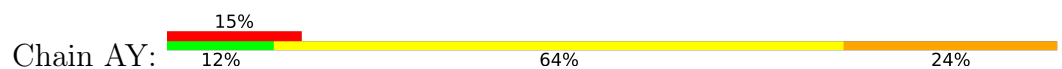
• Molecule 24: tRNA-Met



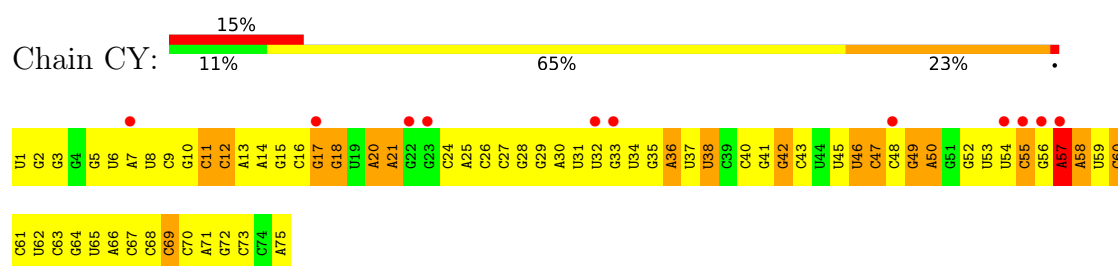
• Molecule 24: tRNA-Met



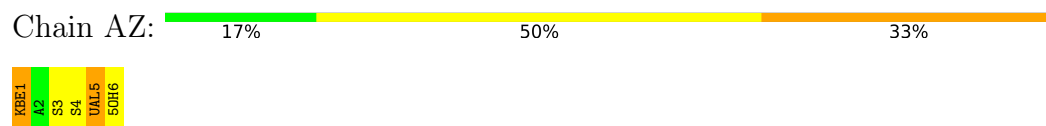
• Molecule 25: tRNA-Gln



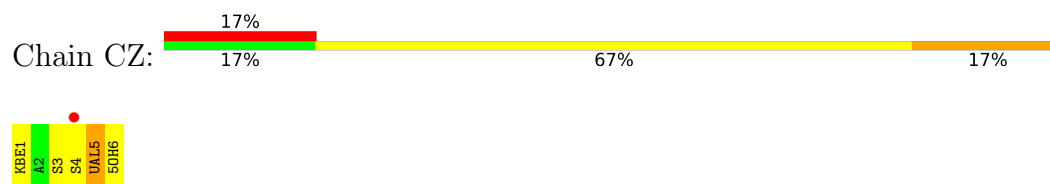
• Molecule 25: tRNA-Gln



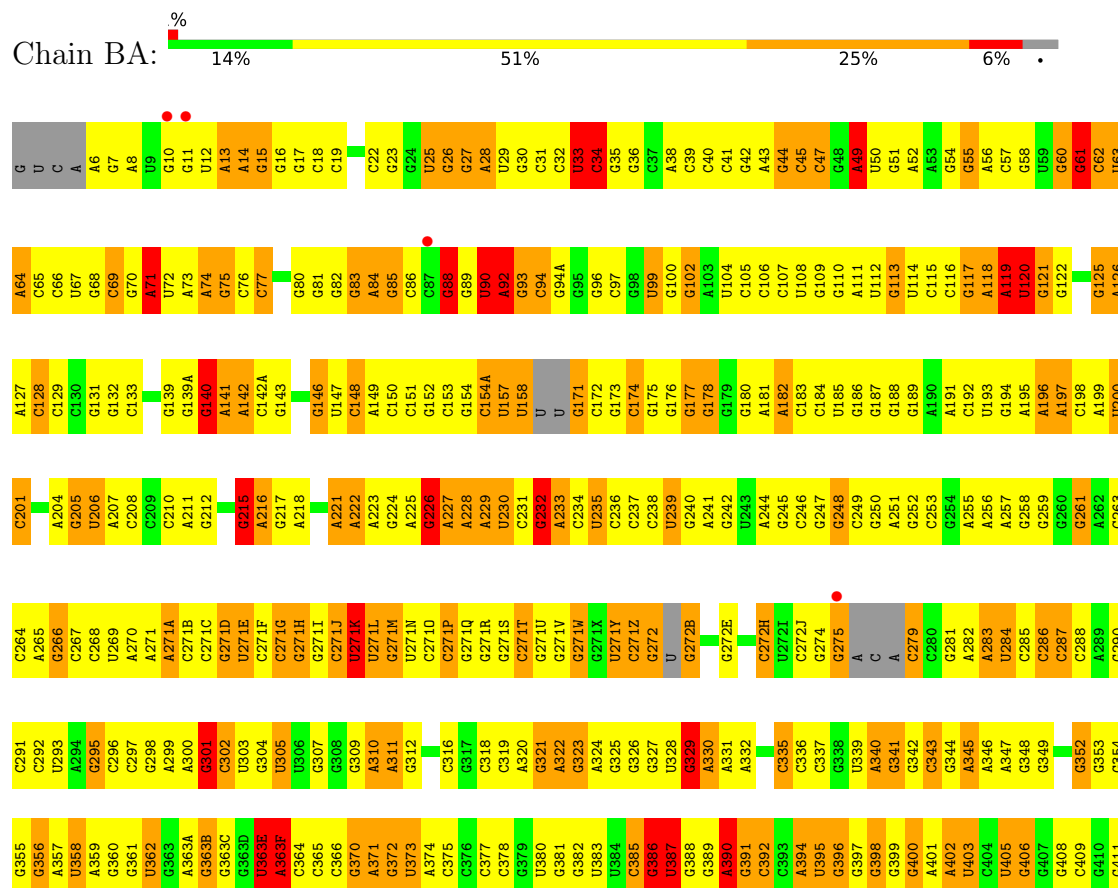
• Molecule 26: Viomycin



• Molecule 26: Viomycin

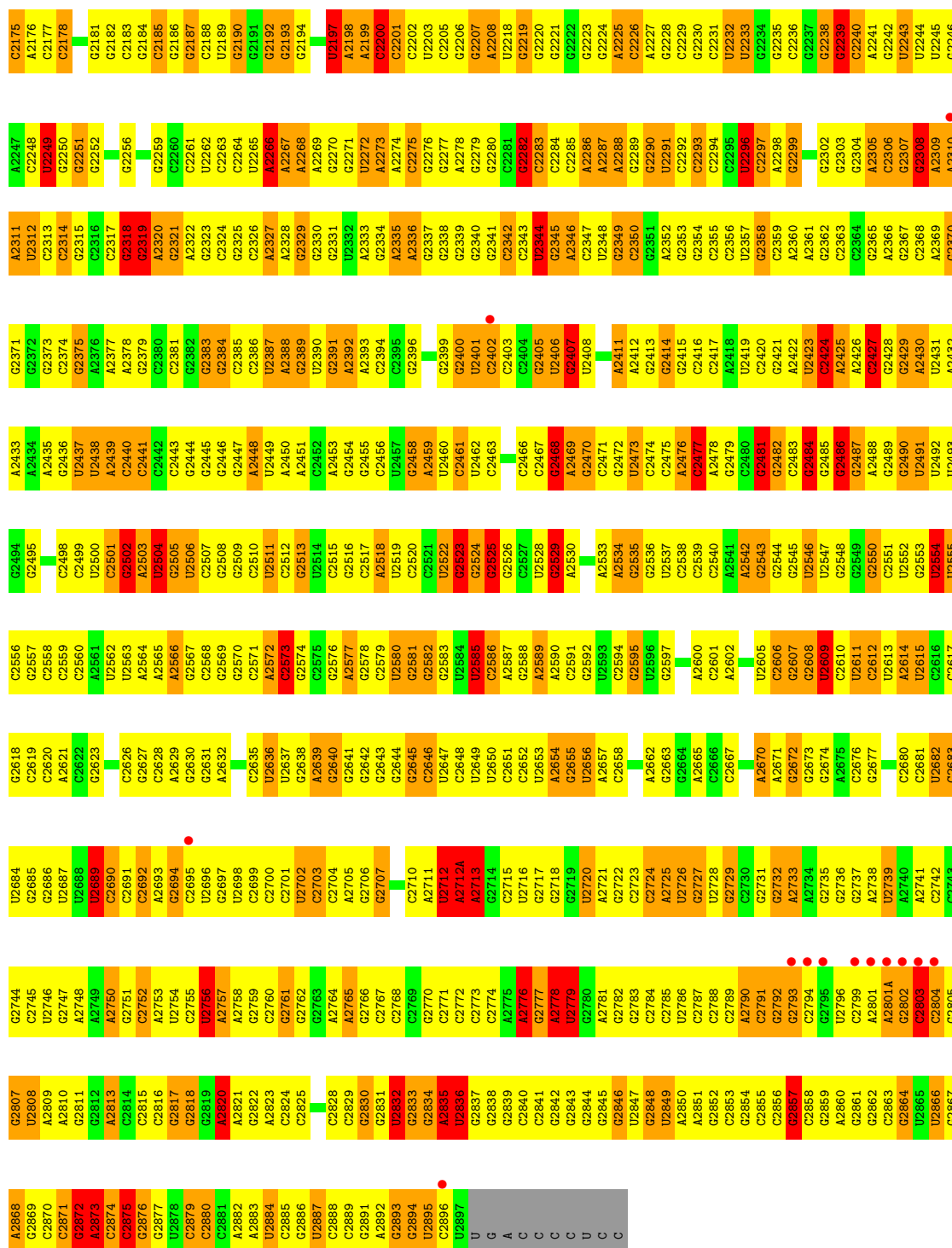


• Molecule 27: 23S ribosomal RNA

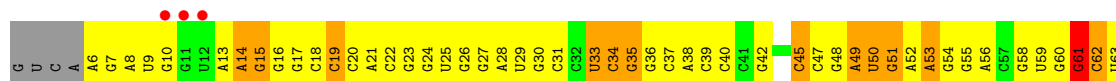
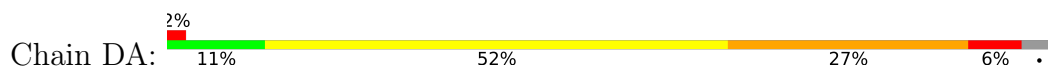


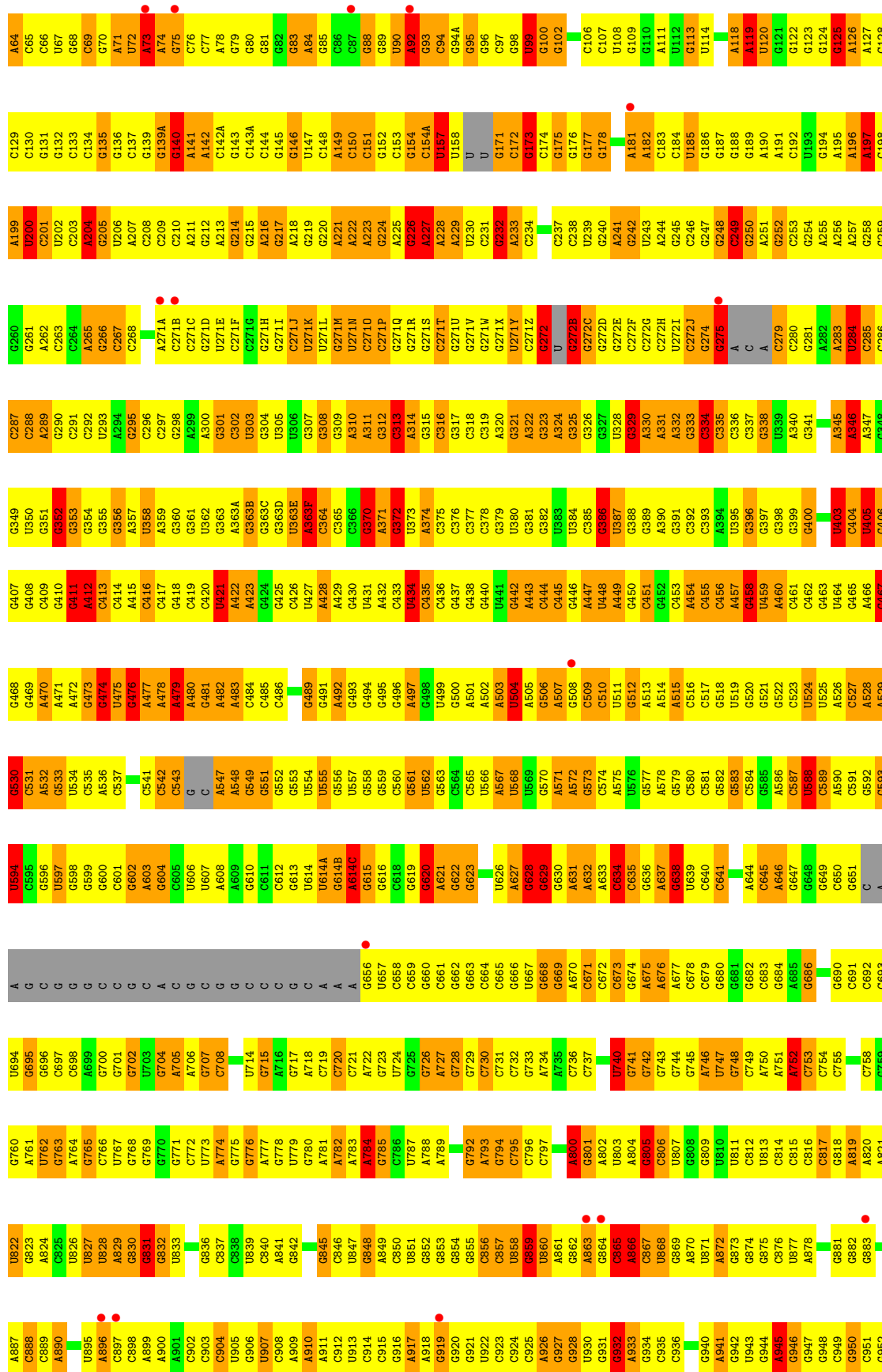
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G1215	G1151	G1024	G962	A900	C834	U767	G704	C605	C541	A480	
G1216	C1152	G1025	U963		A835	G768	A705	U606	C542	G481	C420
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	C1180	A1054	C988	A926	G859	G792	C731	G629	U567	G506	C445
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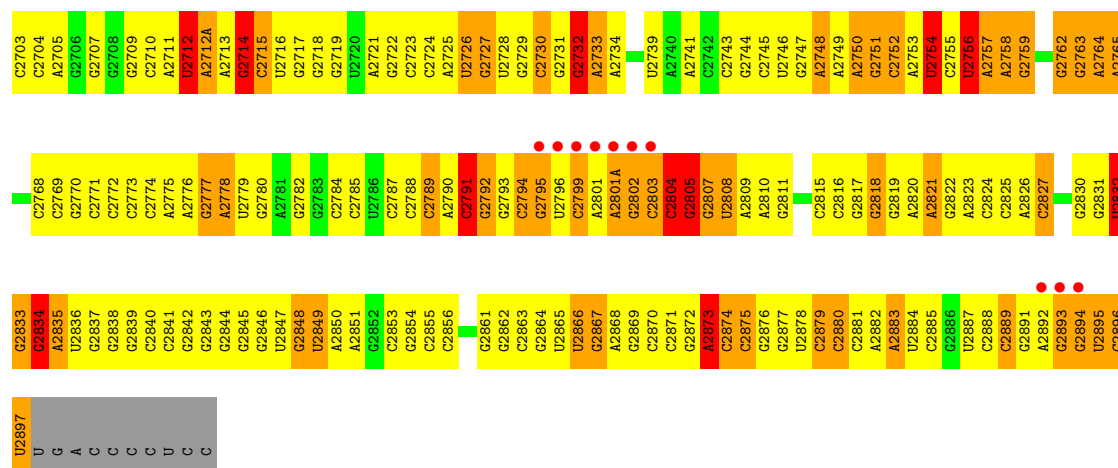
• Molecule 27: 23S ribosomal RNA



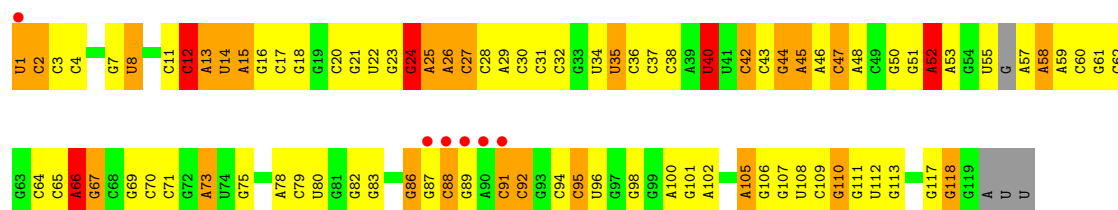


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G1776	G1699	A1632	A1569	A1508	G1444	G1382	C1320	G1259	C1200	C1140	A	G1017	U958
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A1780	G1703	C1638	U1576	C1513	G1448	C1387	G1325	G1264	U1205	A1143	C	A1021	G962
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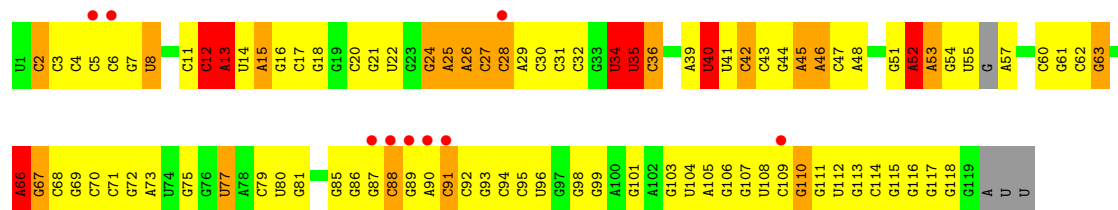
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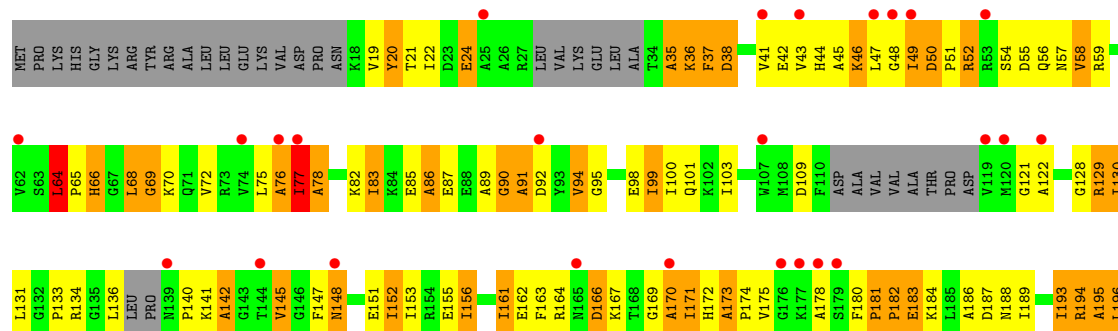
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• Molecule 28: 5S ribosomal RNA

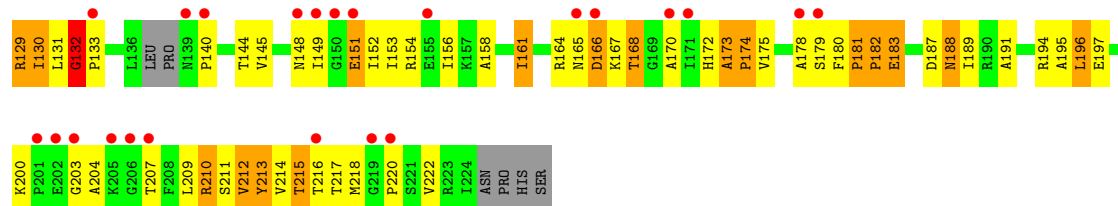
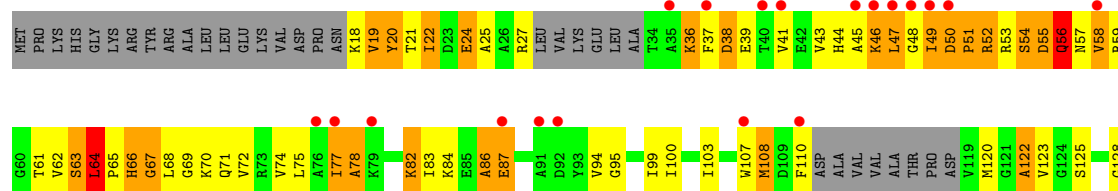


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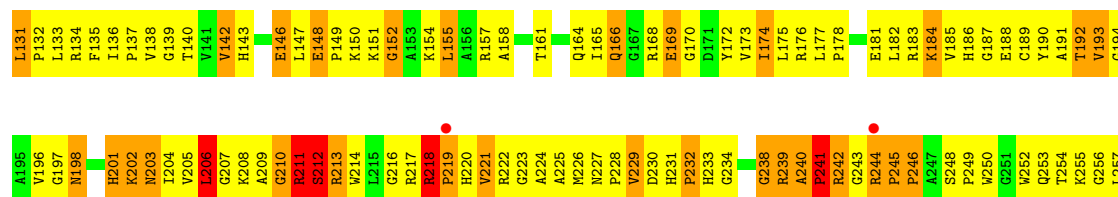
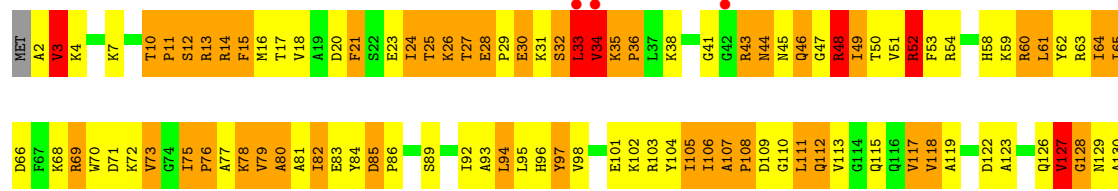
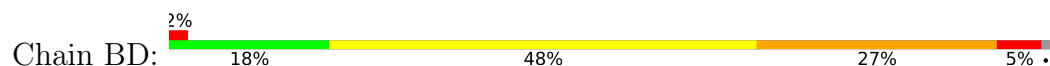




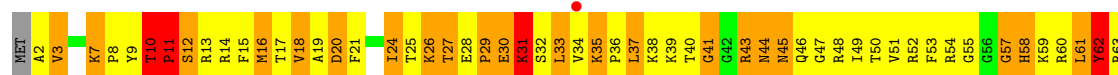
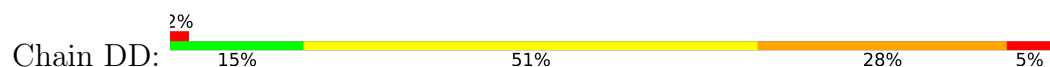
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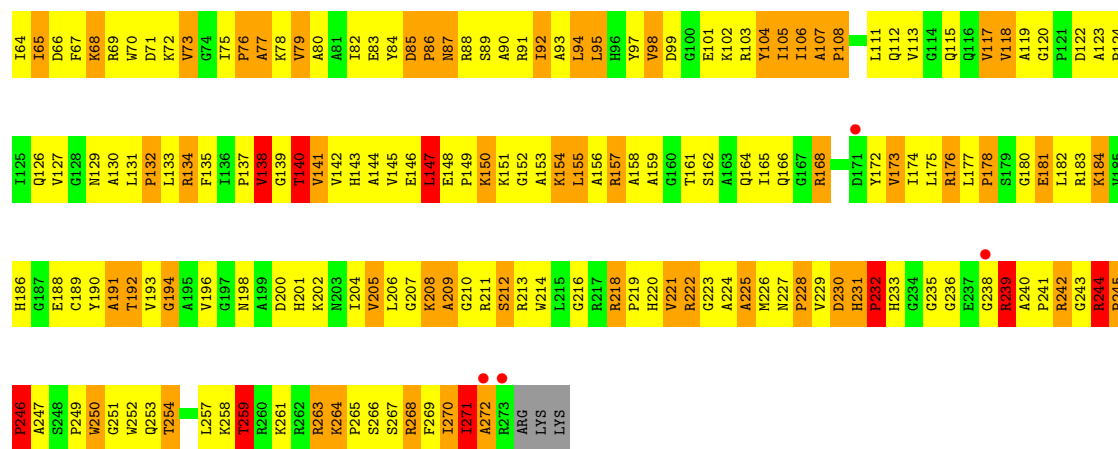


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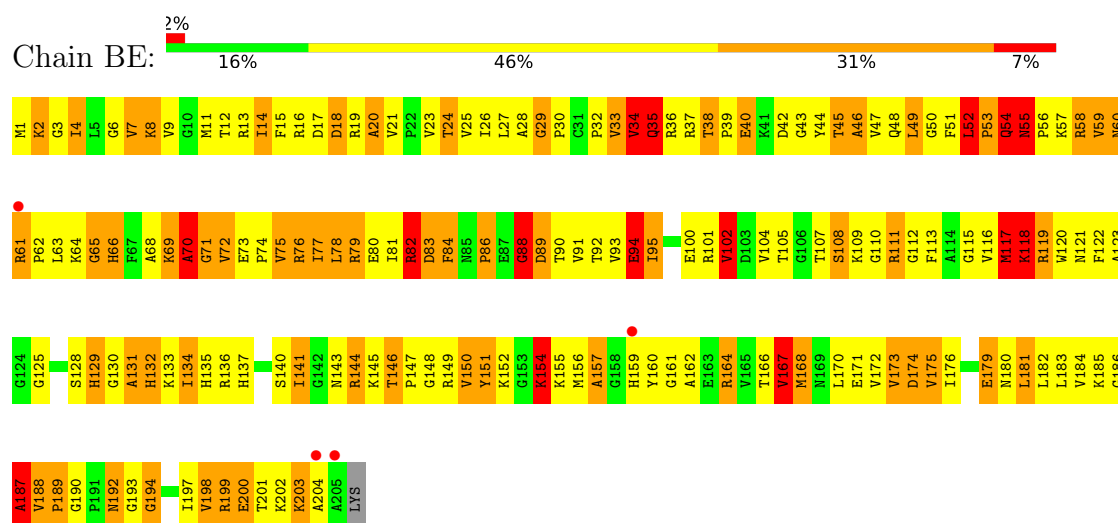


• Molecule 30: 50S ribosomal protein L2

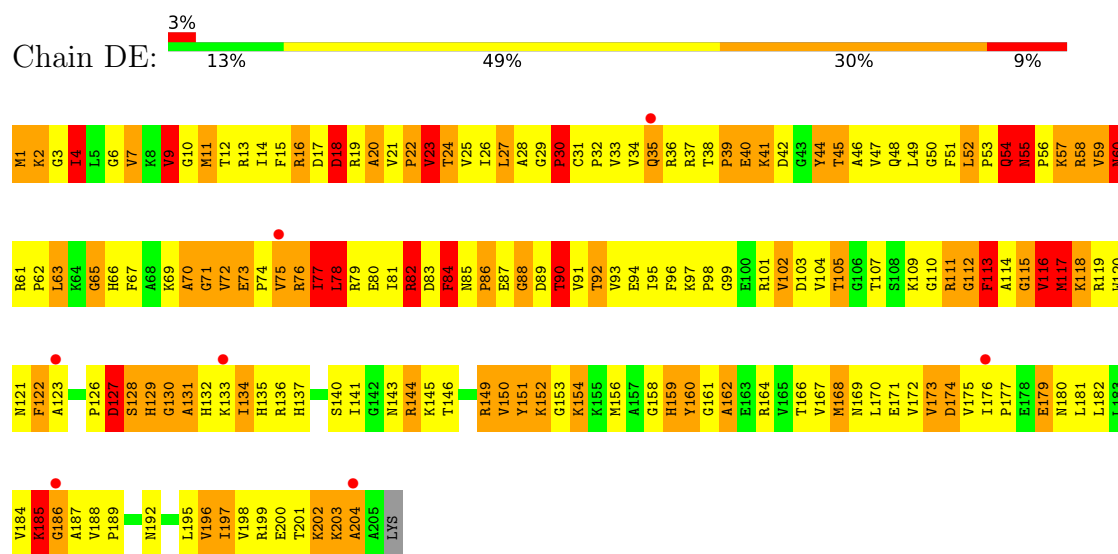




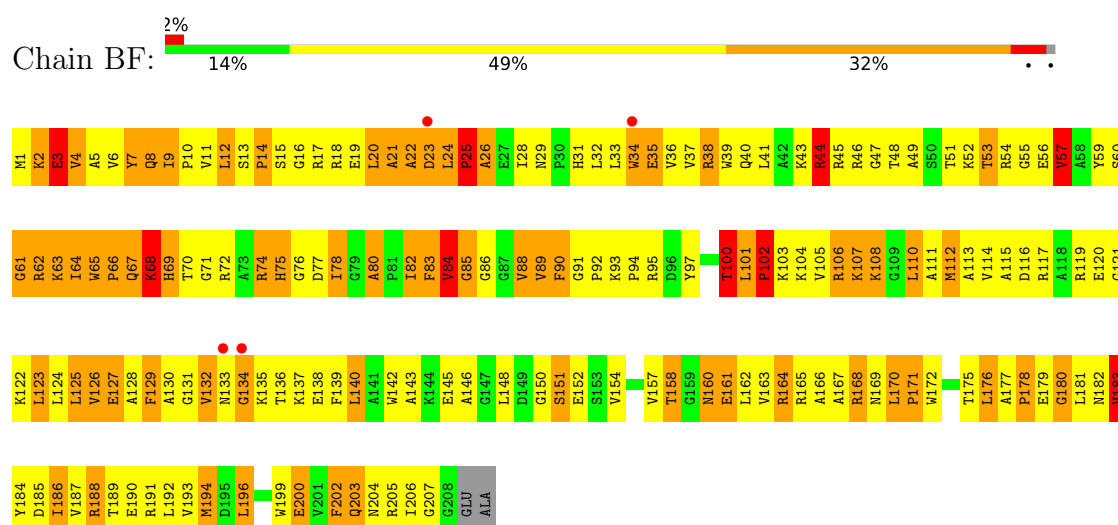
• Molecule 31: 50S ribosomal protein L3



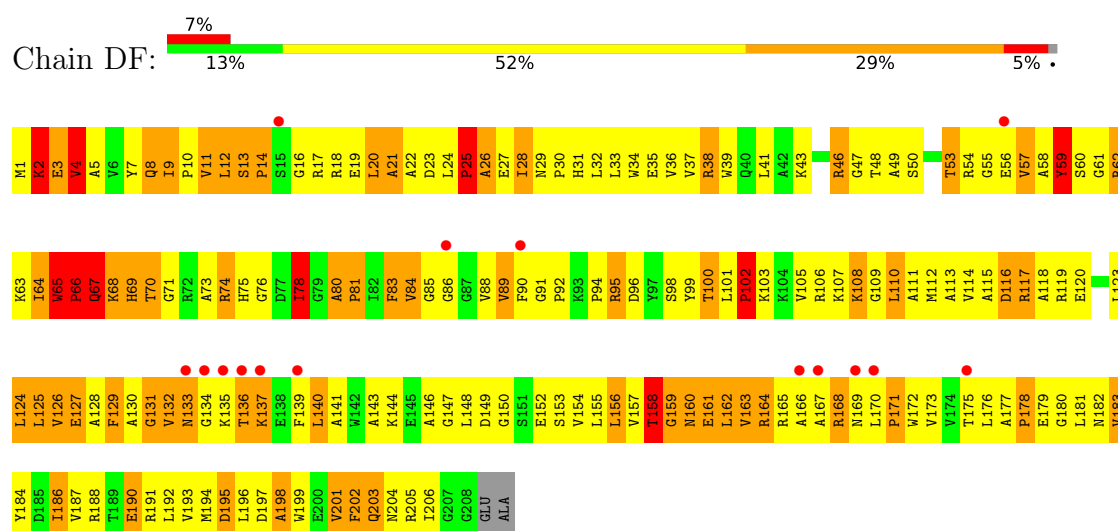
• Molecule 31: 50S ribosomal protein L3



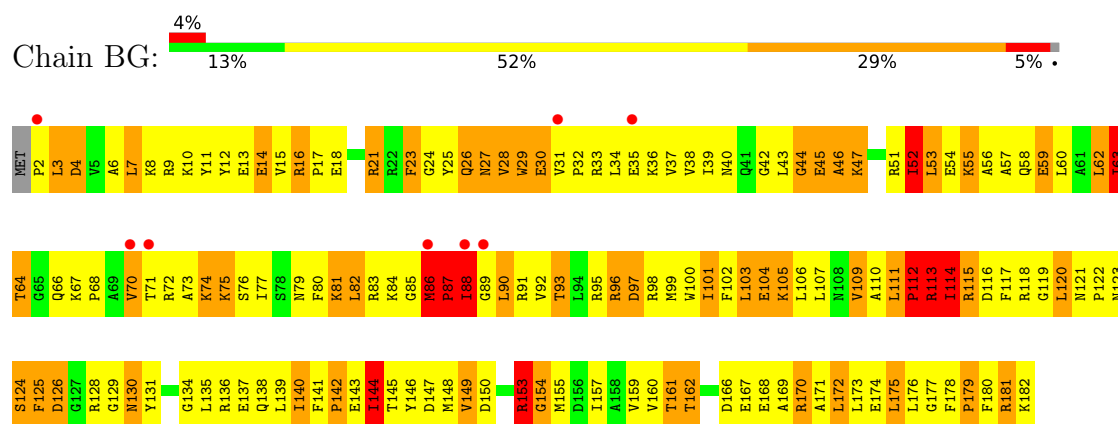
• Molecule 32: 50S ribosomal protein L4



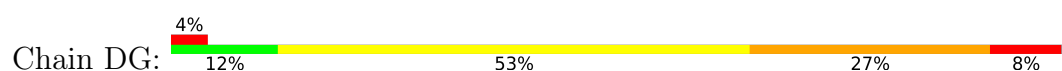
• Molecule 32: 50S ribosomal protein L4

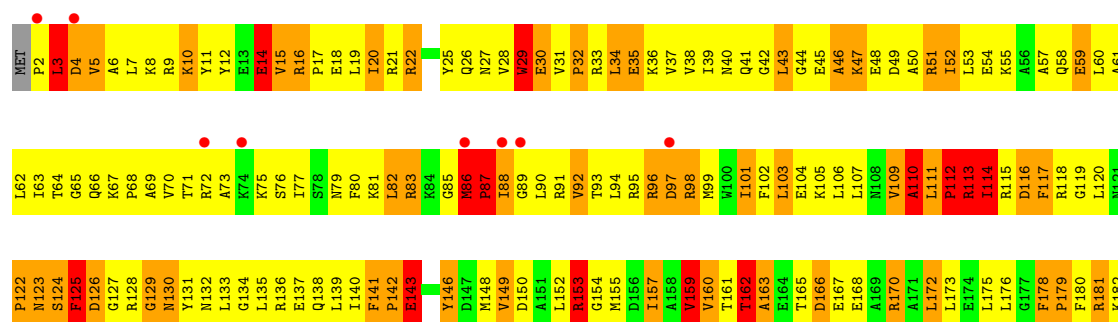


• Molecule 33: 50S ribosomal protein L5

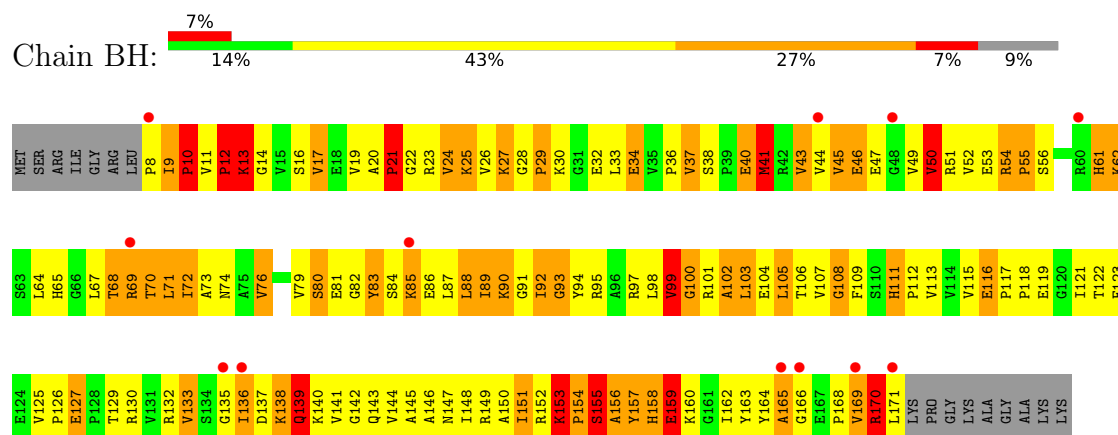


• Molecule 33: 50S ribosomal protein L5

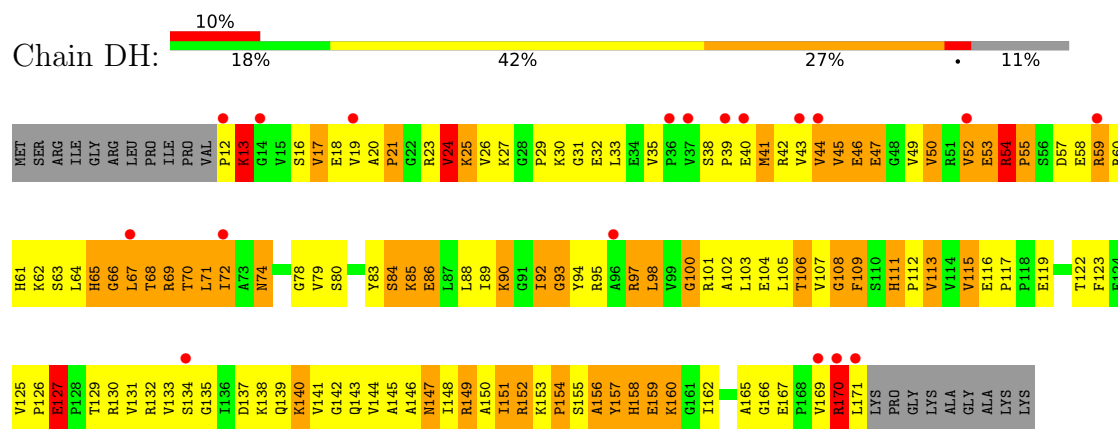




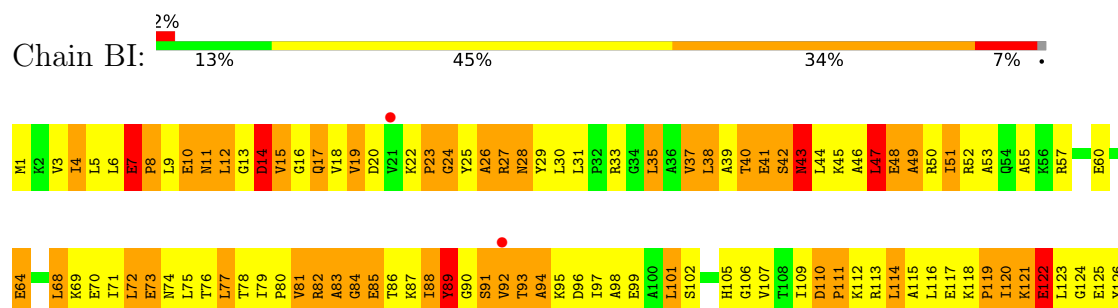
• Molecule 34: 50S ribosomal protein L6

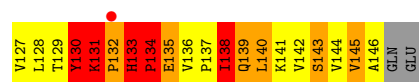


• Molecule 34: 50S ribosomal protein L6

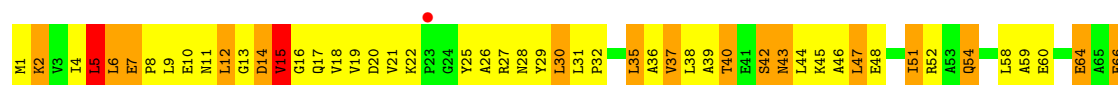
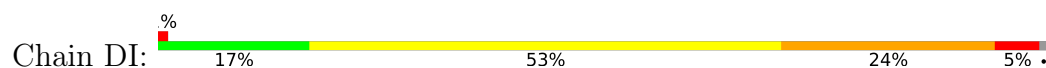


• Molecule 35: 50S ribosomal protein L9

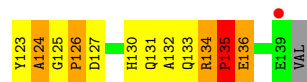
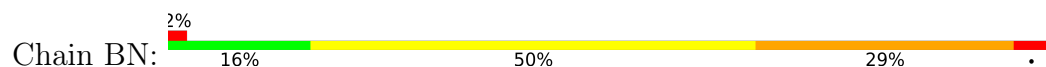




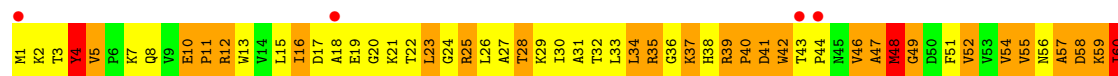
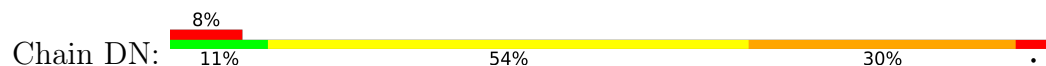
• Molecule 35: 50S ribosomal protein L9



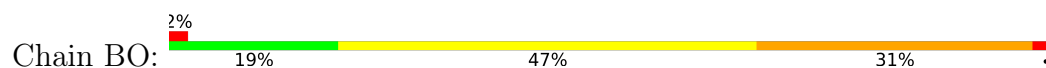
• Molecule 36: 50S ribosomal protein L13

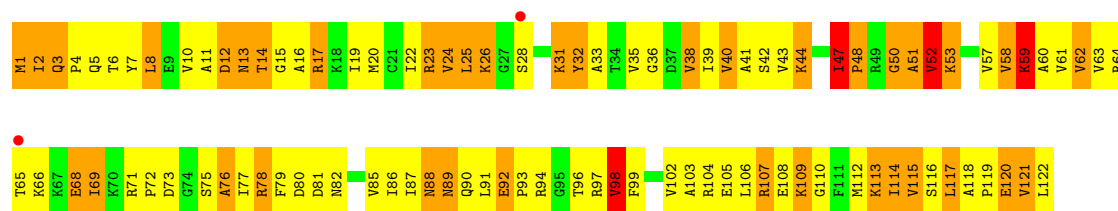


• Molecule 36: 50S ribosomal protein L13



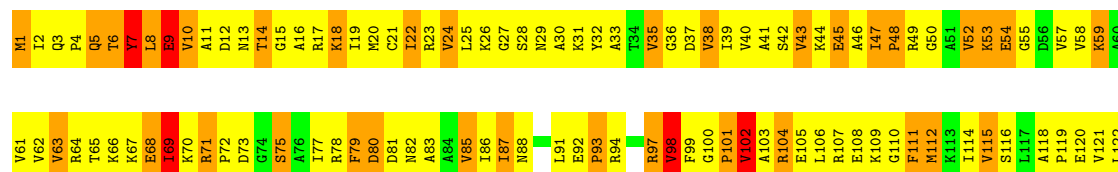
• Molecule 37: 50S ribosomal protein L14





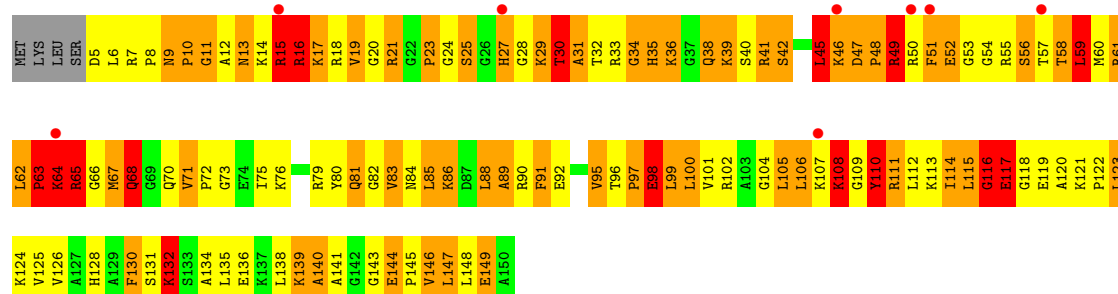
• Molecule 37: 50S ribosomal protein L14

Chain DO: 11% 57% 28%



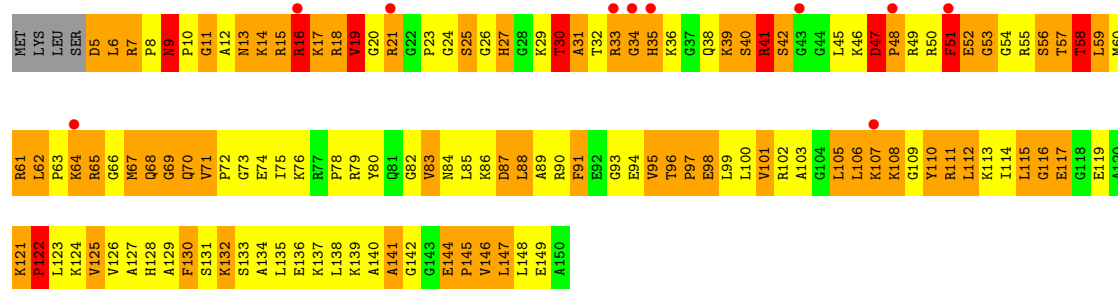
• Molecule 38: 50S ribosomal protein L15

Chain BP: 5% 13% 38% 36% 11%



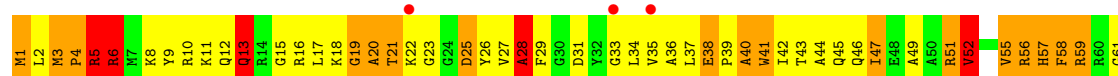
• Molecule 38: 50S ribosomal protein L15

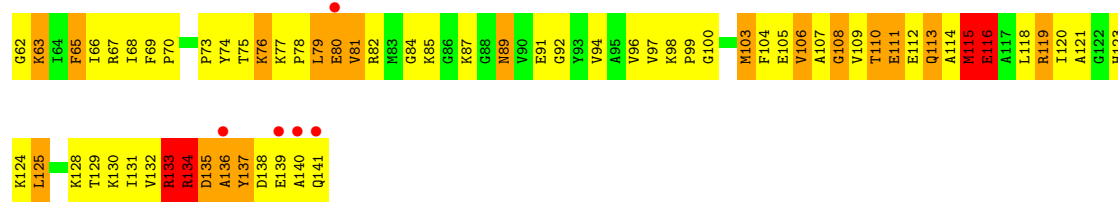
Chain DP: 7% 9% 41% 41% 6%



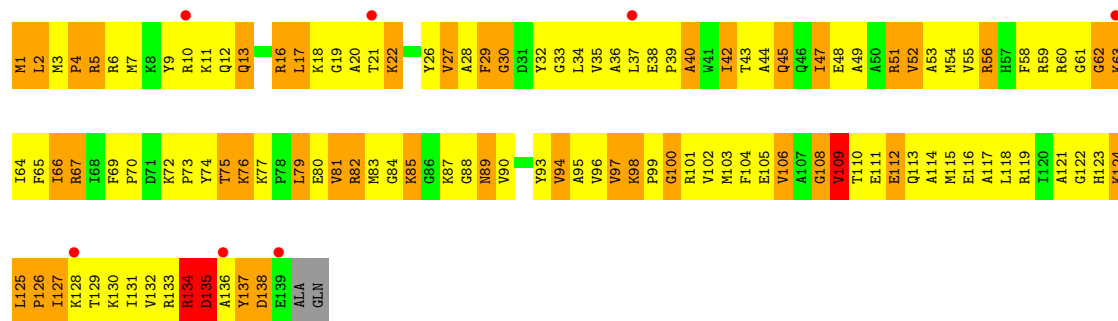
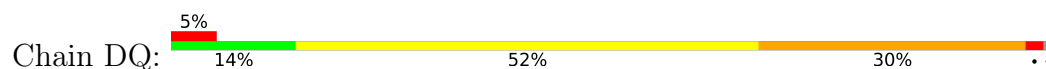
• Molecule 39: 50S ribosomal protein L16

Chain BQ: 6% 18% 51% 25% 6%

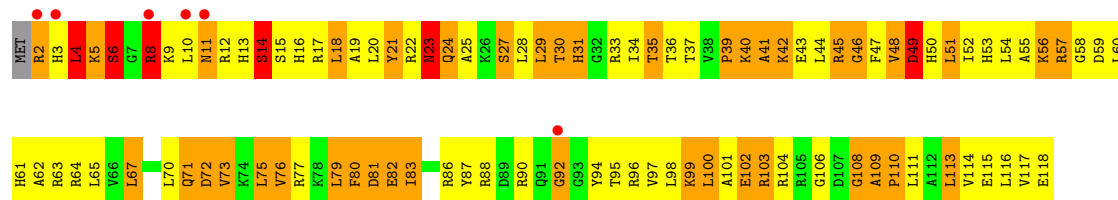
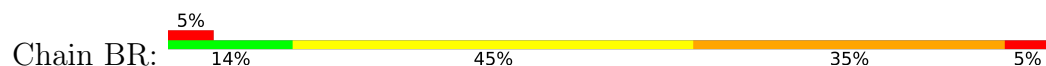




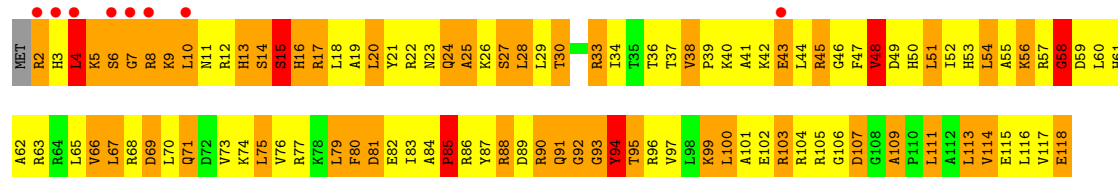
• Molecule 39: 50S ribosomal protein L16



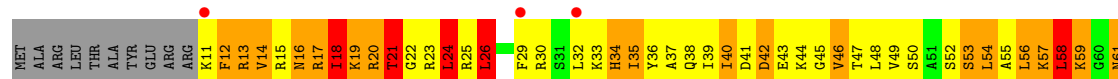
• Molecule 40: 50S ribosomal protein L17

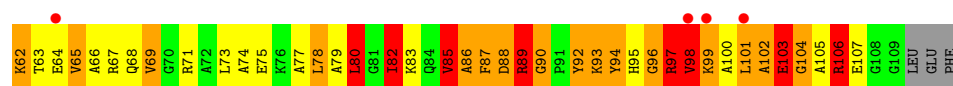


• Molecule 40: 50S ribosomal protein L17

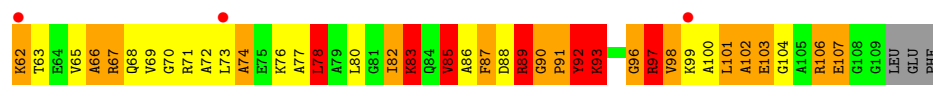
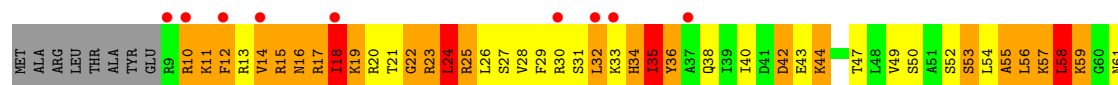


• Molecule 41: 50S ribosomal protein L18

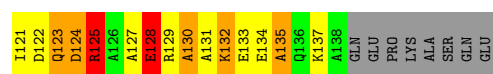
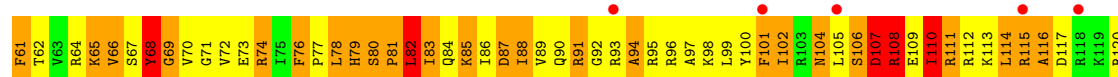




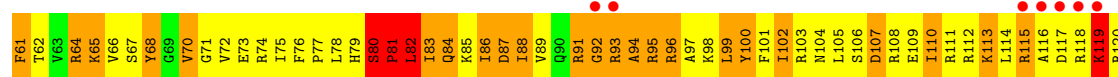
• Molecule 41: 50S ribosomal protein L18



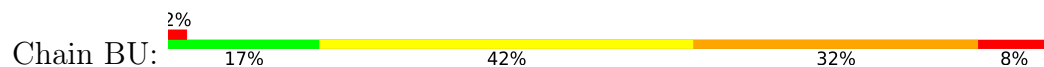
• Molecule 42: 50S ribosomal protein L19



• Molecule 42: 50S ribosomal protein L19

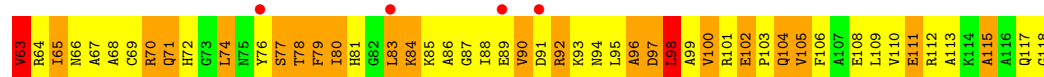
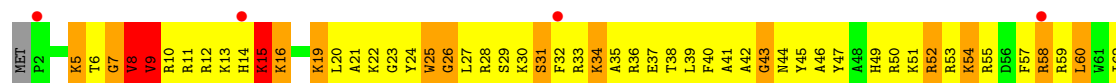
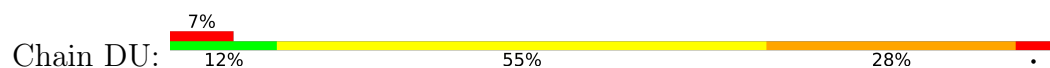


• Molecule 43: 50S ribosomal protein L20

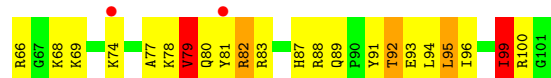
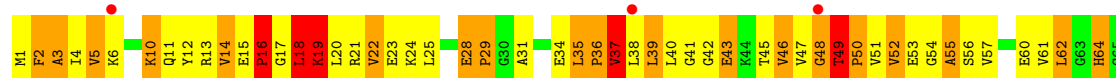




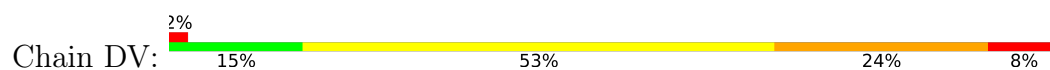
- Molecule 43: 50S ribosomal protein L20



- Molecule 44: 50S ribosomal protein L21



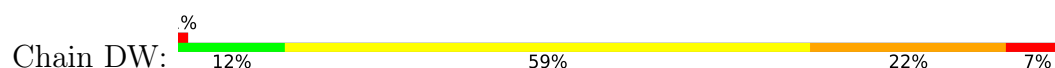
- Molecule 44: 50S ribosomal protein L21

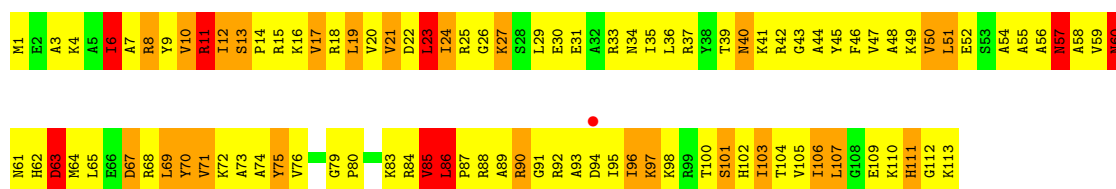


- Molecule 45: 50S ribosomal protein L22

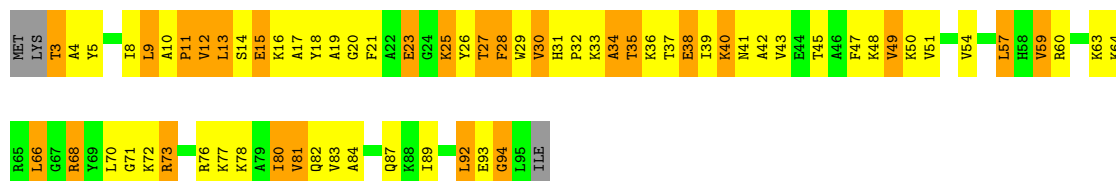


- Molecule 45: 50S ribosomal protein L22

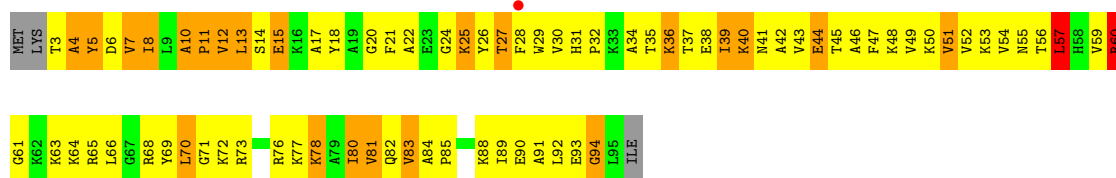
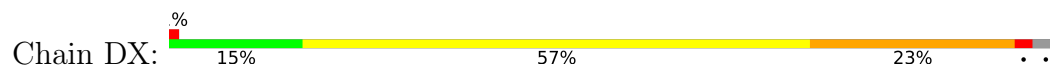




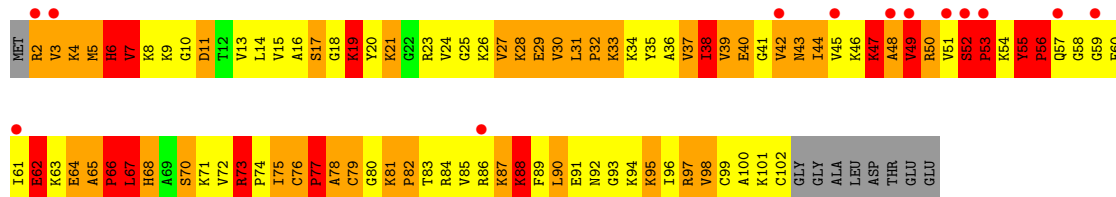
• Molecule 46: 50S ribosomal protein L23



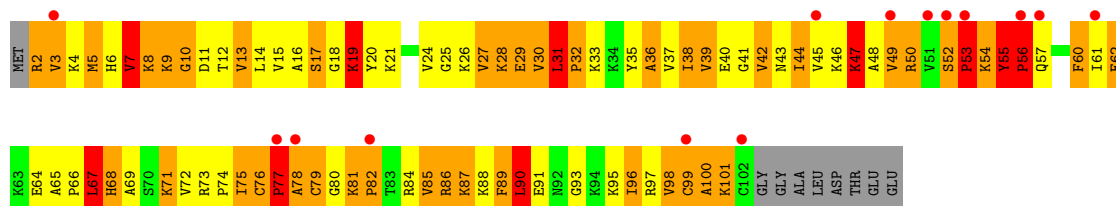
• Molecule 46: 50S ribosomal protein L23



• Molecule 47: 50S ribosomal protein L24

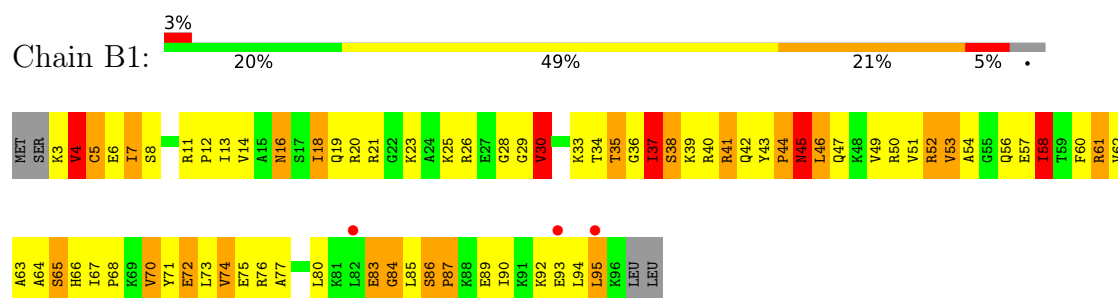


• Molecule 47: 50S ribosomal protein L24

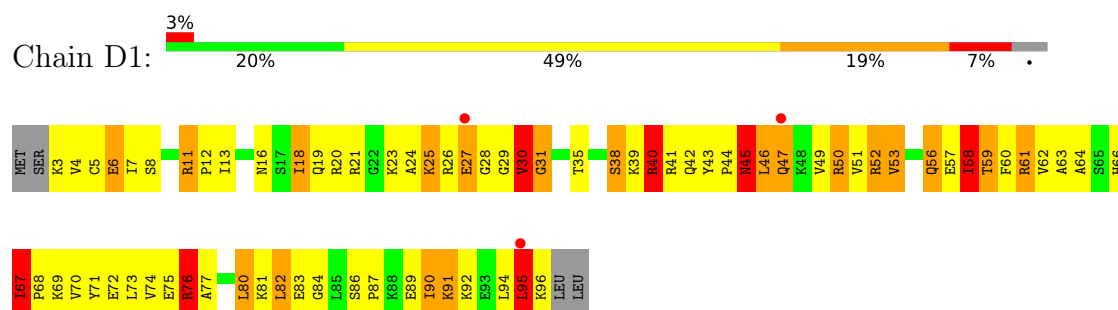


• Molecule 48: 50S ribosomal protein L25

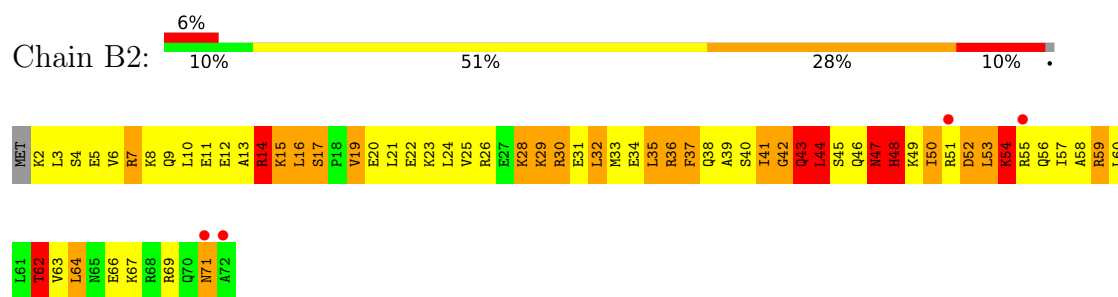
- Molecule 50: 50S ribosomal protein L28



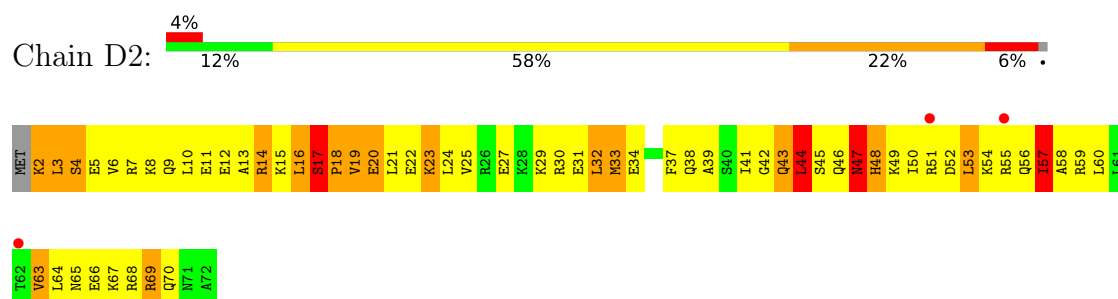
- Molecule 50: 50S ribosomal protein L28



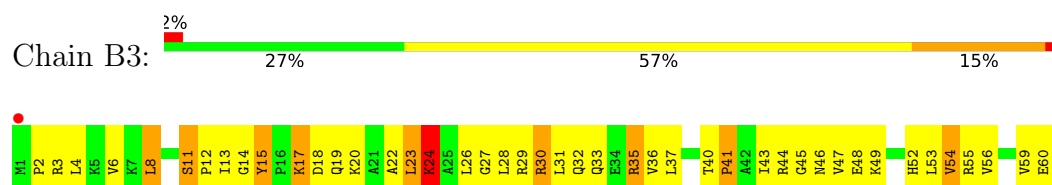
- Molecule 51: 50S ribosomal protein L29



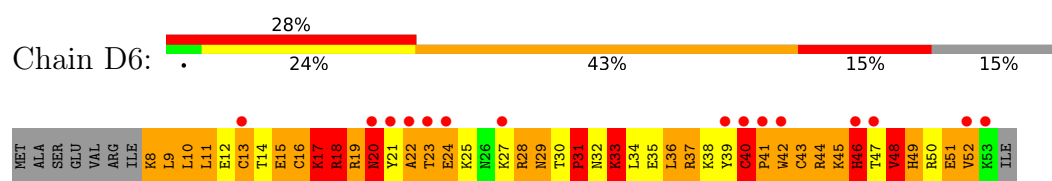
- Molecule 51: 50S ribosomal protein L29



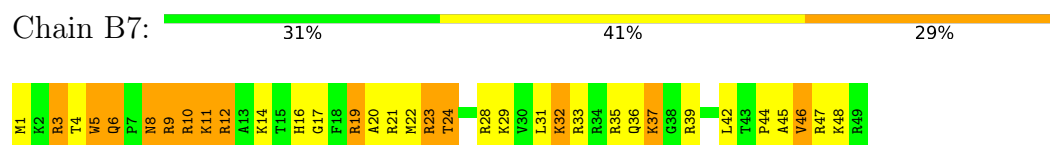
- Molecule 52: 50S ribosomal protein L30



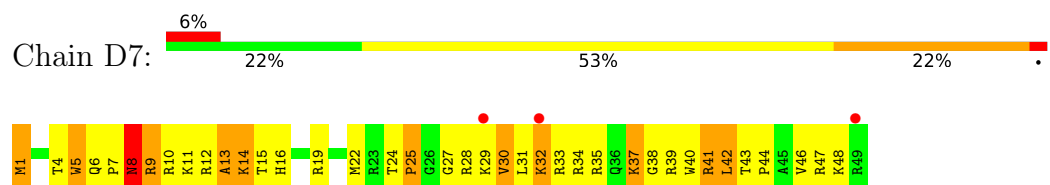
- Molecule 55: 50S ribosomal protein L33



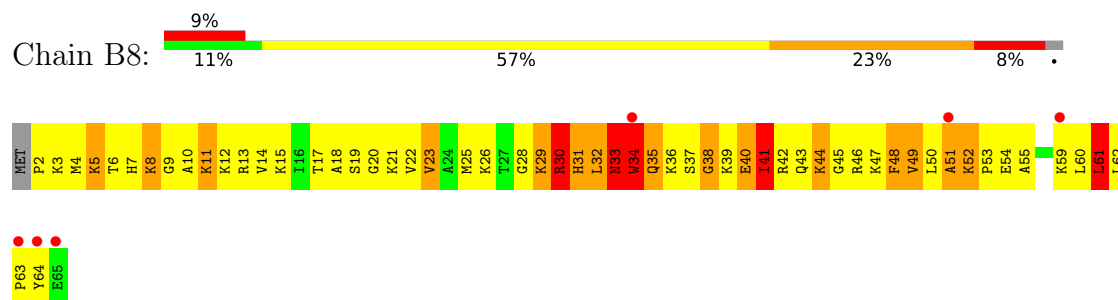
- Molecule 56: 50S ribosomal protein L34



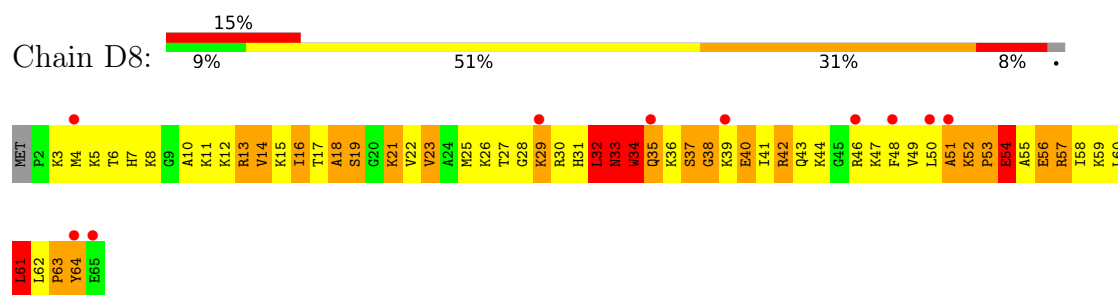
- Molecule 56: 50S ribosomal protein L34



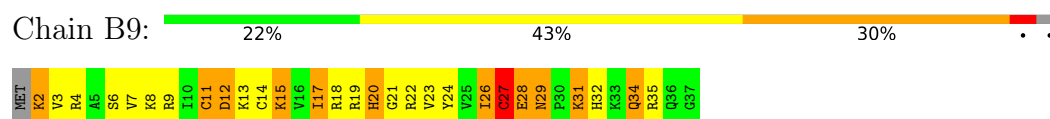
- Molecule 57: 50S ribosomal protein L35



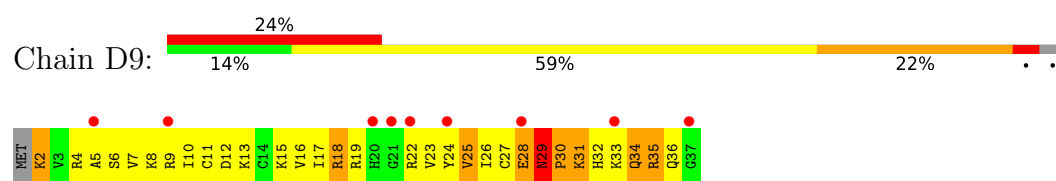
- Molecule 57: 50S ribosomal protein L35



- Molecule 58: 50S ribosomal protein L36



- Molecule 58: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.23Å 448.51Å 633.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 94.1 (50.00-3.00)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.272 0.249 , 0.279	Depositor DCC
R_{free} test set	55515 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 102.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	294559	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KBE, 5OH, MG, DPP, ZN, UAL

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	AA	0.40	0/35980	0.81	73/56157 (0.1%)
1	CA	0.39	0/35980	0.81	65/56157 (0.1%)
2	AB	0.44	0/1936	1.16	28/2611 (1.1%)
2	CB	0.44	0/1936	1.15	23/2611 (0.9%)
3	AC	0.47	0/1637	1.19	22/2207 (1.0%)
3	CC	0.46	0/1637	1.14	19/2207 (0.9%)
4	AD	0.55	0/1733	1.19	12/2318 (0.5%)
4	CD	0.52	0/1733	1.18	15/2318 (0.6%)
5	AE	0.59	1/1163 (0.1%)	1.21	14/1566 (0.9%)
5	CE	0.52	0/1163	1.24	22/1566 (1.4%)
6	AF	0.51	0/856	1.11	7/1154 (0.6%)
6	CF	0.50	0/856	1.07	7/1154 (0.6%)
7	AG	0.49	0/1276	1.24	24/1709 (1.4%)
7	CG	0.49	0/1276	1.14	15/1709 (0.9%)
8	AH	0.51	0/1136	1.18	10/1527 (0.7%)
8	CH	0.48	0/1136	1.14	10/1527 (0.7%)
9	AI	0.42	0/1023	1.15	11/1371 (0.8%)
9	CI	0.44	0/1024	1.04	11/1372 (0.8%)
10	AJ	0.47	0/808	1.14	6/1087 (0.6%)
10	CJ	0.52	0/808	1.12	4/1087 (0.4%)
11	AK	0.50	0/900	1.17	11/1213 (0.9%)
11	CK	0.50	0/900	1.22	12/1213 (1.0%)
12	AL	0.59	0/987	1.40	20/1322 (1.5%)
12	CL	0.54	0/987	1.19	11/1322 (0.8%)
13	AM	0.54	0/957	1.26	13/1284 (1.0%)
13	CM	1.31	16/920 (1.7%)	1.72	27/1241 (2.2%)
14	AN	0.53	0/501	0.99	1/664 (0.2%)
14	CN	0.49	0/501	1.17	8/664 (1.2%)
15	AO	0.54	0/745	1.14	7/992 (0.7%)
15	CO	0.49	0/745	0.99	2/992 (0.2%)
16	AP	0.53	0/717	1.30	11/965 (1.1%)
16	CP	0.48	0/717	1.03	6/965 (0.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.55	0/837	1.12	3/1119 (0.3%)
17	CQ	0.48	0/837	1.09	5/1119 (0.4%)
18	AR	0.57	0/579	1.30	11/768 (1.4%)
18	CR	0.55	0/579	1.30	9/768 (1.2%)
19	AS	0.48	0/643	1.12	6/867 (0.7%)
19	CS	0.50	0/643	1.05	5/867 (0.6%)
20	AT	0.46	0/765	1.24	10/1007 (1.0%)
20	CT	0.51	0/765	1.25	15/1007 (1.5%)
21	AU	0.58	0/213	1.19	1/279 (0.4%)
21	CU	0.44	0/213	0.99	2/279 (0.7%)
22	AV	0.43	0/239	0.62	0/371
22	CV	0.37	0/239	0.86	2/371 (0.5%)
23	AW	0.40	0/1778	0.73	2/2768 (0.1%)
23	CW	0.36	0/1778	0.70	1/2768 (0.0%)
24	AX	0.39	0/1832	0.72	3/2855 (0.1%)
24	CX	0.38	0/1832	0.69	3/2855 (0.1%)
25	AY	0.31	0/1776	0.62	0/2766
25	CY	0.33	0/1776	0.65	1/2766 (0.0%)
26	AZ	0.84	0/11	0.67	0/13
26	CZ	1.00	0/11	0.91	0/13
27	BA	0.46	0/67544	0.87	180/105433 (0.2%)
27	DA	0.42	0/67547	0.86	150/105438 (0.1%)
28	BB	0.44	0/2826	0.86	8/4406 (0.2%)
28	DB	0.40	0/2826	0.85	4/4406 (0.1%)
29	BC	0.43	0/1145	1.17	10/1556 (0.6%)
29	DC	0.45	0/1145	1.26	17/1556 (1.1%)
30	BD	0.76	4/2155 (0.2%)	1.44	37/2907 (1.3%)
30	DD	0.64	0/2155	1.38	45/2907 (1.5%)
31	BE	0.69	0/1597	1.38	31/2155 (1.4%)
31	DE	0.60	0/1597	1.35	35/2155 (1.6%)
32	BF	0.63	0/1659	1.33	33/2246 (1.5%)
32	DF	0.55	0/1659	1.30	28/2246 (1.2%)
33	BG	0.65	0/1499	1.37	30/2016 (1.5%)
33	DG	0.65	2/1499 (0.1%)	1.39	34/2016 (1.7%)
34	BH	0.73	2/1277 (0.2%)	1.32	20/1729 (1.2%)
34	DH	0.45	0/1246	1.23	14/1684 (0.8%)
35	BI	0.53	0/1057	1.32	18/1453 (1.2%)
35	DI	0.53	0/1061	1.31	22/1458 (1.5%)
36	BN	0.67	0/1132	1.33	22/1527 (1.4%)
36	DN	0.51	0/1132	1.28	13/1527 (0.9%)
37	BO	0.62	0/943	1.34	13/1269 (1.0%)
37	DO	0.58	0/943	1.26	8/1269 (0.6%)
38	BP	0.72	1/1131 (0.1%)	1.60	25/1504 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DP	0.59	0/1131	1.39	18/1504 (1.2%)
39	BQ	0.68	0/1143	1.27	17/1527 (1.1%)
39	DQ	0.53	1/1128 (0.1%)	1.13	9/1508 (0.6%)
40	BR	0.70	0/974	1.39	15/1302 (1.2%)
40	DR	0.57	0/974	1.29	20/1302 (1.5%)
41	BS	0.60	0/779	1.59	20/1038 (1.9%)
41	DS	0.53	0/785	1.29	10/1048 (1.0%)
42	BT	0.69	1/1156 (0.1%)	1.41	23/1544 (1.5%)
42	DT	0.57	0/1156	1.36	18/1544 (1.2%)
43	BU	0.68	0/975	1.40	19/1297 (1.5%)
43	DU	0.52	0/975	1.39	20/1297 (1.5%)
44	BV	0.69	0/790	1.39	13/1057 (1.2%)
44	DV	0.52	0/790	1.25	11/1057 (1.0%)
45	BW	0.67	0/907	1.22	11/1216 (0.9%)
45	DW	0.64	0/907	1.33	20/1216 (1.6%)
46	BX	0.65	0/740	1.30	7/995 (0.7%)
46	DX	0.60	0/740	1.27	9/995 (0.9%)
47	BY	0.74	0/789	1.66	20/1053 (1.9%)
47	DY	0.61	0/789	1.49	13/1053 (1.2%)
48	BZ	0.53	0/1436	1.13	15/1951 (0.8%)
48	DZ	0.46	0/1436	1.12	19/1951 (1.0%)
49	B0	0.60	0/671	1.13	4/892 (0.4%)
49	D0	0.50	0/671	1.11	5/892 (0.6%)
50	B1	0.62	0/722	1.20	5/964 (0.5%)
50	D1	0.58	0/739	1.18	8/983 (0.8%)
51	B2	0.66	0/600	1.34	9/793 (1.1%)
51	D2	0.50	0/600	1.12	4/793 (0.5%)
52	B3	0.65	0/473	1.27	8/636 (1.3%)
52	D3	0.55	0/473	1.40	12/636 (1.9%)
53	B4	0.51	0/229	1.36	2/311 (0.6%)
53	D4	0.65	0/229	1.61	7/311 (2.3%)
54	B5	0.70	0/473	1.49	9/639 (1.4%)
54	D5	0.56	0/473	1.27	5/639 (0.8%)
55	B6	0.91	0/418	1.59	11/562 (2.0%)
55	D6	1.09	2/397 (0.5%)	1.78	11/531 (2.1%)
56	B7	0.72	0/427	1.33	9/563 (1.6%)
56	D7	0.63	0/427	1.26	8/563 (1.4%)
57	B8	0.72	0/516	1.44	10/681 (1.5%)
57	D8	0.61	0/516	1.34	9/681 (1.3%)
58	B9	0.75	0/302	1.38	3/397 (0.8%)
58	D9	0.44	0/302	1.15	4/397 (1.0%)
All	All	0.48	30/318953 (0.0%)	0.97	1873/477060 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	90
1	CA	1	81
13	CM	0	1
22	CV	0	2
23	AW	0	1
23	CW	0	2
27	BA	0	223
27	DA	0	164
28	BB	0	6
28	DB	0	6
30	DD	0	1
36	DN	0	1
47	BY	0	1
54	D5	0	1
55	B6	0	1
55	D6	0	1
All	All	1	582

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	CM	65	LYS	CA-C	11.98	1.67	1.52
55	D6	46	HIS	C-N	-10.66	1.18	1.33
13	CM	65	LYS	C-N	10.36	1.48	1.33
34	BH	11	VAL	N-CA	10.04	1.54	1.46
13	CM	69	GLU	CA-C	-9.10	1.40	1.52

The worst 5 of 1873 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	CM	70	LEU	N-CA-C	-22.04	78.50	111.34
47	DY	7	VAL	N-CA-C	18.17	129.13	110.23
55	D6	48	VAL	N-CA-C	17.09	129.70	111.58
41	DS	16	ASN	N-CA-C	-16.16	91.86	112.23
43	BU	27	LEU	N-CA-C	-14.85	95.20	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	CA	517	G	C3'

5 of 582 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	12	U	Sidechain
1	AA	17	U	Sidechain
1	AA	34	C	Sidechain
1	AA	49	U	Sidechain
1	AA	52	G	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32141	0	16225	1911	0
1	CA	32141	0	16225	2193	0
2	AB	1901	0	1951	293	0
2	CB	1901	0	1951	284	0
3	AC	1613	0	1677	249	0
3	CC	1613	0	1677	226	0
4	AD	1703	0	1764	232	0
4	CD	1703	0	1764	272	0
5	AE	1147	0	1207	186	0
5	CE	1147	0	1207	198	0
6	AF	843	0	857	120	0
6	CF	843	0	857	130	0
7	AG	1257	0	1296	192	0
7	CG	1257	0	1296	154	0
8	AH	1116	0	1177	221	0
8	CH	1116	0	1177	182	0
9	AI	1005	0	1032	161	0
9	CI	1006	0	1034	155	0
10	AJ	795	0	840	168	0
10	CJ	795	0	840	165	0
11	AK	885	0	904	131	0
11	CK	885	0	904	123	0
12	AL	971	0	1057	170	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	CL	971	0	1057	187	0
13	AM	947	0	999	211	0
13	CM	910	0	931	197	0
14	AN	492	0	533	102	0
14	CN	492	0	533	112	0
15	AO	734	0	771	125	0
15	CO	734	0	771	112	0
16	AP	701	0	720	119	0
16	CP	701	0	720	99	0
17	AQ	824	0	891	115	0
17	CQ	824	0	891	125	0
18	AR	574	0	644	95	0
18	CR	574	0	644	79	0
19	AS	630	0	652	116	0
19	CS	630	0	652	116	0
20	AT	763	0	861	134	0
20	CT	763	0	861	140	0
21	AU	209	0	221	25	0
21	CU	209	0	221	33	0
22	AV	213	0	110	6	0
22	CV	213	0	110	12	0
23	AW	1593	0	810	79	0
23	CW	1593	0	810	76	0
24	AX	1640	0	837	69	0
24	CX	1640	0	837	74	0
25	AY	1591	0	810	84	0
25	CY	1591	0	810	88	0
26	AZ	48	0	40	13	0
26	CZ	48	0	40	20	0
27	BA	60311	0	30410	3527	0
27	DA	60313	0	30409	3994	0
28	BB	2528	0	1285	121	0
28	DB	2528	0	1285	141	0
29	BC	1142	0	865	107	0
29	DC	1142	0	865	145	0
30	BD	2105	0	2182	432	0
30	DD	2105	0	2182	399	0
31	BE	1564	0	1629	309	0
31	DE	1564	0	1629	334	0
32	BF	1624	0	1677	336	0
32	DF	1624	0	1677	270	0
33	BG	1474	0	1535	238	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	DG	1474	0	1535	270	0
34	BH	1252	0	1316	243	0
34	DH	1223	0	1282	199	0
35	BI	1042	0	1031	203	0
35	DI	1046	0	1035	157	0
36	BN	1105	0	1180	181	0
36	DN	1105	0	1180	224	0
37	BO	933	0	996	172	0
37	DO	933	0	996	171	0
38	BP	1114	0	1187	304	0
38	DP	1114	0	1187	341	0
39	BQ	1122	0	1179	190	0
39	DQ	1107	0	1166	206	0
40	BR	960	0	1021	173	0
40	DR	960	0	1021	188	0
41	BS	771	0	832	166	0
41	DS	777	0	825	150	0
42	BT	1142	0	1202	287	0
42	DT	1142	0	1202	284	0
43	BU	958	0	1015	199	0
43	DU	958	0	1015	211	0
44	BV	779	0	852	170	0
44	DV	779	0	852	172	0
45	BW	896	0	953	109	0
45	DW	896	0	953	164	0
46	BX	726	0	778	106	0
46	DX	726	0	778	136	0
47	BY	776	0	870	218	0
47	DY	776	0	870	197	0
48	BZ	1404	0	1432	197	0
48	DZ	1404	0	1432	230	0
49	B0	662	0	688	93	0
49	D0	662	0	688	106	0
50	B1	715	0	766	120	0
50	D1	732	0	808	104	0
51	B2	598	0	653	119	0
51	D2	598	0	653	95	0
52	B3	468	0	523	57	0
52	D3	468	0	523	89	0
53	B4	226	0	226	42	0
53	D4	226	0	227	34	0
54	B5	459	0	476	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
54	D5	459	0	476	73	0
55	B6	411	0	403	125	0
55	D6	390	0	404	105	0
56	B7	419	0	467	51	0
56	D7	419	0	467	82	0
57	B8	508	0	576	133	0
57	D8	508	0	576	136	0
58	B9	299	0	323	51	0
58	D9	299	0	323	53	0
59	AA	133	0	0	0	0
59	AC	1	0	0	0	0
59	AD	1	0	0	0	0
59	AE	1	0	0	0	0
59	AF	1	0	0	0	0
59	AH	1	0	0	0	0
59	AK	2	0	0	0	0
59	AL	1	0	0	0	0
59	AO	1	0	0	0	0
59	AT	2	0	0	0	0
59	AW	7	0	0	0	0
59	AX	7	0	0	0	0
59	AY	2	0	0	0	0
59	B0	2	0	0	0	0
59	B5	1	0	0	0	0
59	BA	400	0	0	0	0
59	BB	1	0	0	0	0
59	BD	1	0	0	0	0
59	BE	1	0	0	0	0
59	BF	2	0	0	0	0
59	BH	1	0	0	0	0
59	BN	1	0	0	0	0
59	BP	1	0	0	0	0
59	BQ	1	0	0	0	0
59	BR	1	0	0	0	0
59	BU	1	0	0	0	0
59	BX	1	0	0	0	0
59	BY	1	0	0	1	0
59	BZ	1	0	0	0	0
59	CA	92	0	0	0	0
59	CE	2	0	0	0	0
59	CQ	1	0	0	0	0
59	CV	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	CX	3	0	0	0	0
59	D5	2	0	0	0	0
59	D6	1	0	0	0	0
59	DA	275	0	0	0	0
59	DB	1	0	0	0	0
59	DD	3	0	0	0	0
59	DE	3	0	0	0	0
59	DF	1	0	0	0	0
59	DR	1	0	0	0	0
59	DZ	1	0	0	0	0
60	AD	1	0	0	1	0
60	B4	1	0	0	0	0
60	B5	1	0	0	0	0
60	B9	1	0	0	0	0
60	CD	1	0	0	1	0
60	D4	1	0	0	0	0
60	D5	1	0	0	0	0
60	D9	1	0	0	0	0
All	All	294559	0	198755	26706	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

The worst 5 of 26706 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:BP:59:LEU:HA	38:BP:61:ARG:CZ	1.58	1.32
30:DD:231:HIS:ND1	30:DD:232:PRO:HD2	1.55	1.20
1:CA:1363(A):A:H1'	1:CA:1365:G:N7	1.57	1.19
40:BR:100:LEU:HD21	40:BR:113:LEU:HD13	1.24	1.19
27:BA:2787:C:H1'	31:BE:61:ARG:HG3	1.25	1.18

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	
2	AB	233/256 (91%)	126 (54%)	73 (31%)	34 (15%)	0	0
2	CB	233/256 (91%)	151 (65%)	50 (22%)	32 (14%)	0	1
3	AC	205/239 (86%)	123 (60%)	54 (26%)	28 (14%)	0	1
3	CC	205/239 (86%)	121 (59%)	59 (29%)	25 (12%)	0	1
4	AD	206/209 (99%)	129 (63%)	52 (25%)	25 (12%)	0	1
4	CD	206/209 (99%)	126 (61%)	51 (25%)	29 (14%)	0	1
5	AE	149/162 (92%)	94 (63%)	38 (26%)	17 (11%)	0	1
5	CE	149/162 (92%)	103 (69%)	27 (18%)	19 (13%)	0	1
6	AF	99/101 (98%)	71 (72%)	18 (18%)	10 (10%)	0	2
6	CF	99/101 (98%)	76 (77%)	16 (16%)	7 (7%)	1	4
7	AG	153/156 (98%)	101 (66%)	39 (26%)	13 (8%)	0	3
7	CG	153/156 (98%)	102 (67%)	38 (25%)	13 (8%)	0	3
8	AH	136/138 (99%)	98 (72%)	27 (20%)	11 (8%)	1	3
8	CH	136/138 (99%)	81 (60%)	38 (28%)	17 (12%)	0	1
9	AI	125/128 (98%)	83 (66%)	29 (23%)	13 (10%)	0	2
9	CI	125/128 (98%)	82 (66%)	26 (21%)	17 (14%)	0	1
10	AJ	97/105 (92%)	64 (66%)	26 (27%)	7 (7%)	1	4
10	CJ	97/105 (92%)	55 (57%)	28 (29%)	14 (14%)	0	0
11	AK	117/129 (91%)	70 (60%)	34 (29%)	13 (11%)	0	1
11	CK	117/129 (91%)	87 (74%)	22 (19%)	8 (7%)	1	5
12	AL	123/132 (93%)	75 (61%)	25 (20%)	23 (19%)	0	0
12	CL	123/132 (93%)	76 (62%)	24 (20%)	23 (19%)	0	0
13	AM	118/126 (94%)	64 (54%)	33 (28%)	21 (18%)	0	0
13	CM	117/126 (93%)	64 (55%)	29 (25%)	24 (20%)	0	0
14	AN	58/61 (95%)	29 (50%)	19 (33%)	10 (17%)	0	0
14	CN	58/61 (95%)	35 (60%)	12 (21%)	11 (19%)	0	0
15	AO	86/89 (97%)	56 (65%)	19 (22%)	11 (13%)	0	1
15	CO	86/89 (97%)	49 (57%)	28 (33%)	9 (10%)	0	2
16	AP	82/88 (93%)	49 (60%)	21 (26%)	12 (15%)	0	0
16	CP	82/88 (93%)	45 (55%)	28 (34%)	9 (11%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	AQ	98/105 (93%)	73 (74%)	15 (15%)	10 (10%)	0	2
17	CQ	98/105 (93%)	70 (71%)	22 (22%)	6 (6%)	1	7
18	AR	68/88 (77%)	35 (52%)	21 (31%)	12 (18%)	0	0
18	CR	68/88 (77%)	41 (60%)	16 (24%)	11 (16%)	0	0
19	AS	77/93 (83%)	51 (66%)	15 (20%)	11 (14%)	0	1
19	CS	77/93 (83%)	46 (60%)	18 (23%)	13 (17%)	0	0
20	AT	97/106 (92%)	59 (61%)	20 (21%)	18 (19%)	0	0
20	CT	97/106 (92%)	52 (54%)	36 (37%)	9 (9%)	0	2
21	AU	23/27 (85%)	16 (70%)	4 (17%)	3 (13%)	0	1
21	CU	23/27 (85%)	14 (61%)	5 (22%)	4 (17%)	0	0
26	AZ	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
26	CZ	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
29	BC	183/229 (80%)	69 (38%)	49 (27%)	65 (36%)	0	0
29	DC	183/229 (80%)	69 (38%)	59 (32%)	55 (30%)	0	0
30	BD	270/276 (98%)	172 (64%)	66 (24%)	32 (12%)	0	1
30	DD	270/276 (98%)	180 (67%)	57 (21%)	33 (12%)	0	1
31	BE	203/206 (98%)	130 (64%)	38 (19%)	35 (17%)	0	0
31	DE	203/206 (98%)	125 (62%)	34 (17%)	44 (22%)	0	0
32	BF	206/210 (98%)	137 (66%)	31 (15%)	38 (18%)	0	0
32	DF	206/210 (98%)	125 (61%)	40 (19%)	41 (20%)	0	0
33	BG	179/182 (98%)	107 (60%)	47 (26%)	25 (14%)	0	1
33	DG	179/182 (98%)	109 (61%)	42 (24%)	28 (16%)	0	0
34	BH	162/180 (90%)	87 (54%)	43 (26%)	32 (20%)	0	0
34	DH	158/180 (88%)	88 (56%)	35 (22%)	35 (22%)	0	0
35	BI	144/148 (97%)	73 (51%)	33 (23%)	38 (26%)	0	0
35	DI	144/148 (97%)	80 (56%)	41 (28%)	23 (16%)	0	0
36	BN	137/140 (98%)	91 (66%)	27 (20%)	19 (14%)	0	1
36	DN	137/140 (98%)	82 (60%)	28 (20%)	27 (20%)	0	0
37	BO	120/122 (98%)	84 (70%)	25 (21%)	11 (9%)	0	2
37	DO	120/122 (98%)	80 (67%)	23 (19%)	17 (14%)	0	1
38	BP	144/150 (96%)	71 (49%)	42 (29%)	31 (22%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	DP	144/150 (96%)	72 (50%)	36 (25%)	36 (25%)	0	0
39	BQ	139/141 (99%)	98 (70%)	21 (15%)	20 (14%)	0	0
39	DQ	137/141 (97%)	88 (64%)	29 (21%)	20 (15%)	0	0
40	BR	115/118 (98%)	75 (65%)	25 (22%)	15 (13%)	0	1
40	DR	115/118 (98%)	66 (57%)	31 (27%)	18 (16%)	0	0
41	BS	97/112 (87%)	45 (46%)	24 (25%)	28 (29%)	0	0
41	DS	99/112 (88%)	51 (52%)	14 (14%)	34 (34%)	0	0
42	BT	136/146 (93%)	78 (57%)	26 (19%)	32 (24%)	0	0
42	DT	136/146 (93%)	68 (50%)	32 (24%)	36 (26%)	0	0
43	BU	115/118 (98%)	70 (61%)	27 (24%)	18 (16%)	0	0
43	DU	115/118 (98%)	69 (60%)	30 (26%)	16 (14%)	0	1
44	BV	99/101 (98%)	61 (62%)	24 (24%)	14 (14%)	0	1
44	DV	99/101 (98%)	61 (62%)	19 (19%)	19 (19%)	0	0
45	BW	111/113 (98%)	77 (69%)	23 (21%)	11 (10%)	0	2
45	DW	111/113 (98%)	71 (64%)	29 (26%)	11 (10%)	0	2
46	BX	91/96 (95%)	67 (74%)	16 (18%)	8 (9%)	0	3
46	DX	91/96 (95%)	60 (66%)	17 (19%)	14 (15%)	0	0
47	BY	99/110 (90%)	42 (42%)	22 (22%)	35 (35%)	0	0
47	DY	99/110 (90%)	37 (37%)	29 (29%)	33 (33%)	0	0
48	BZ	175/206 (85%)	99 (57%)	49 (28%)	27 (15%)	0	0
48	DZ	175/206 (85%)	97 (55%)	51 (29%)	27 (15%)	0	0
49	B0	82/85 (96%)	62 (76%)	12 (15%)	8 (10%)	0	2
49	D0	82/85 (96%)	61 (74%)	14 (17%)	7 (8%)	0	3
50	B1	92/98 (94%)	60 (65%)	20 (22%)	12 (13%)	0	1
50	D1	92/98 (94%)	65 (71%)	16 (17%)	11 (12%)	0	1
51	B2	69/72 (96%)	46 (67%)	14 (20%)	9 (13%)	0	1
51	D2	69/72 (96%)	37 (54%)	20 (29%)	12 (17%)	0	0
52	B3	58/60 (97%)	49 (84%)	7 (12%)	2 (3%)	3	17
52	D3	58/60 (97%)	46 (79%)	10 (17%)	2 (3%)	3	17
53	B4	29/71 (41%)	18 (62%)	6 (21%)	5 (17%)	0	0
53	D4	29/71 (41%)	17 (59%)	9 (31%)	3 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	B5	57/60 (95%)	34 (60%)	13 (23%)	10 (18%)	0	0
54	D5	57/60 (95%)	33 (58%)	14 (25%)	10 (18%)	0	0
55	B6	49/54 (91%)	17 (35%)	14 (29%)	18 (37%)	0	0
55	D6	44/54 (82%)	16 (36%)	11 (25%)	17 (39%)	0	0
56	B7	47/49 (96%)	35 (74%)	8 (17%)	4 (8%)	0	3
56	D7	47/49 (96%)	30 (64%)	13 (28%)	4 (8%)	0	3
57	B8	62/65 (95%)	34 (55%)	19 (31%)	9 (14%)	0	1
57	D8	62/65 (95%)	32 (52%)	15 (24%)	15 (24%)	0	0
58	B9	34/37 (92%)	25 (74%)	8 (24%)	1 (3%)	3	20
58	D9	34/37 (92%)	18 (53%)	13 (38%)	3 (9%)	0	3
All	All	11702/12598 (93%)	7090 (61%)	2747 (24%)	1865 (16%)	0	0

5 of 1865 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	9	GLU
2	AB	15	VAL
2	AB	20	GLU
2	AB	96	ARG
2	AB	101	MET

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	AB	202/220 (92%)	168 (83%)	34 (17%)	2	11
2	CB	202/220 (92%)	173 (86%)	29 (14%)	3	15
3	AC	160/188 (85%)	127 (79%)	33 (21%)	1	7
3	CC	160/188 (85%)	139 (87%)	21 (13%)	4	19
4	AD	180/181 (99%)	147 (82%)	33 (18%)	2	9
4	CD	180/181 (99%)	142 (79%)	38 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	AE	115/123 (94%)	98 (85%)	17 (15%)	3	15
5	CE	115/123 (94%)	94 (82%)	21 (18%)	2	9
6	AF	90/90 (100%)	76 (84%)	14 (16%)	2	13
6	CF	90/90 (100%)	77 (86%)	13 (14%)	3	15
7	AG	126/127 (99%)	101 (80%)	25 (20%)	1	8
7	CG	126/127 (99%)	105 (83%)	21 (17%)	2	12
8	AH	119/119 (100%)	91 (76%)	28 (24%)	1	4
8	CH	119/119 (100%)	100 (84%)	19 (16%)	2	12
9	AI	97/99 (98%)	83 (86%)	14 (14%)	3	15
9	CI	97/99 (98%)	85 (88%)	12 (12%)	4	20
10	AJ	88/92 (96%)	71 (81%)	17 (19%)	1	8
10	CJ	88/92 (96%)	75 (85%)	13 (15%)	3	15
11	AK	90/99 (91%)	71 (79%)	19 (21%)	1	6
11	CK	90/99 (91%)	76 (84%)	14 (16%)	2	13
12	AL	104/109 (95%)	86 (83%)	18 (17%)	2	10
12	CL	104/109 (95%)	90 (86%)	14 (14%)	4	18
13	AM	94/101 (93%)	75 (80%)	19 (20%)	1	7
13	CM	88/101 (87%)	63 (72%)	25 (28%)	0	2
14	AN	49/50 (98%)	39 (80%)	10 (20%)	1	7
14	CN	49/50 (98%)	38 (78%)	11 (22%)	1	5
15	AO	79/80 (99%)	63 (80%)	16 (20%)	1	7
15	CO	79/80 (99%)	63 (80%)	16 (20%)	1	7
16	AP	72/74 (97%)	64 (89%)	8 (11%)	6	25
16	CP	72/74 (97%)	59 (82%)	13 (18%)	2	9
17	AQ	94/97 (97%)	78 (83%)	16 (17%)	2	11
17	CQ	94/97 (97%)	77 (82%)	17 (18%)	2	9
18	AR	61/77 (79%)	53 (87%)	8 (13%)	4	19
18	CR	61/77 (79%)	54 (88%)	7 (12%)	5	24
19	AS	69/80 (86%)	51 (74%)	18 (26%)	0	3
19	CS	69/80 (86%)	48 (70%)	21 (30%)	0	1
20	AT	76/82 (93%)	60 (79%)	16 (21%)	1	6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	CT	76/82 (93%)	63 (83%)	13 (17%)	2	11
21	AU	19/22 (86%)	16 (84%)	3 (16%)	2	13
21	CU	19/22 (86%)	17 (90%)	2 (10%)	6	27
26	AZ	2/2 (100%)	2 (100%)	0	100	100
26	CZ	2/2 (100%)	2 (100%)	0	100	100
29	BC	61/181 (34%)	55 (90%)	6 (10%)	7	30
29	DC	61/181 (34%)	52 (85%)	9 (15%)	3	15
30	BD	213/218 (98%)	158 (74%)	55 (26%)	0	3
30	DD	213/218 (98%)	165 (78%)	48 (22%)	1	5
31	BE	165/166 (99%)	121 (73%)	44 (27%)	0	3
31	DE	165/166 (99%)	123 (74%)	42 (26%)	0	3
32	BF	165/166 (99%)	135 (82%)	30 (18%)	2	9
32	DF	165/166 (99%)	135 (82%)	30 (18%)	2	9
33	BG	155/156 (99%)	116 (75%)	39 (25%)	0	3
33	DG	155/156 (99%)	126 (81%)	29 (19%)	1	9
34	BH	136/148 (92%)	105 (77%)	31 (23%)	1	5
34	DH	132/148 (89%)	112 (85%)	20 (15%)	3	14
35	BI	102/124 (82%)	75 (74%)	27 (26%)	0	3
35	DI	103/124 (83%)	83 (81%)	20 (19%)	1	8
36	BN	117/119 (98%)	88 (75%)	29 (25%)	1	3
36	DN	117/119 (98%)	94 (80%)	23 (20%)	1	8
37	BO	100/100 (100%)	72 (72%)	28 (28%)	0	2
37	DO	100/100 (100%)	71 (71%)	29 (29%)	0	2
38	BP	112/116 (97%)	74 (66%)	38 (34%)	0	1
38	DP	112/116 (97%)	80 (71%)	32 (29%)	0	2
39	BQ	111/111 (100%)	81 (73%)	30 (27%)	0	2
39	DQ	110/111 (99%)	85 (77%)	25 (23%)	1	5
40	BR	100/101 (99%)	71 (71%)	29 (29%)	0	2
40	DR	100/101 (99%)	68 (68%)	32 (32%)	0	1
41	BS	77/88 (88%)	58 (75%)	19 (25%)	1	4
41	DS	76/88 (86%)	58 (76%)	18 (24%)	1	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	BT	120/127 (94%)	84 (70%)	36 (30%)	0	1
42	DT	120/127 (94%)	90 (75%)	30 (25%)	0	3
43	BU	92/94 (98%)	69 (75%)	23 (25%)	0	3
43	DU	92/94 (98%)	77 (84%)	15 (16%)	2	12
44	BV	82/82 (100%)	57 (70%)	25 (30%)	0	1
44	DV	82/82 (100%)	62 (76%)	20 (24%)	1	4
45	BW	91/92 (99%)	68 (75%)	23 (25%)	0	3
45	DW	91/92 (99%)	68 (75%)	23 (25%)	0	3
46	BX	74/78 (95%)	57 (77%)	17 (23%)	1	5
46	DX	74/78 (95%)	58 (78%)	16 (22%)	1	6
47	BY	84/91 (92%)	56 (67%)	28 (33%)	0	1
47	DY	84/91 (92%)	59 (70%)	25 (30%)	0	2
48	BZ	155/179 (87%)	125 (81%)	30 (19%)	1	8
48	DZ	155/179 (87%)	133 (86%)	22 (14%)	3	16
49	B0	66/67 (98%)	53 (80%)	13 (20%)	1	8
49	D0	66/67 (98%)	57 (86%)	9 (14%)	3	17
50	B1	74/83 (89%)	51 (69%)	23 (31%)	0	1
50	D1	78/83 (94%)	59 (76%)	19 (24%)	1	4
51	B2	66/67 (98%)	47 (71%)	19 (29%)	0	2
51	D2	66/67 (98%)	53 (80%)	13 (20%)	1	8
52	B3	51/52 (98%)	42 (82%)	9 (18%)	2	10
52	D3	51/52 (98%)	42 (82%)	9 (18%)	2	10
53	B4	27/63 (43%)	24 (89%)	3 (11%)	6	25
53	D4	27/63 (43%)	25 (93%)	2 (7%)	13	42
54	B5	51/52 (98%)	38 (74%)	13 (26%)	0	3
54	D5	51/52 (98%)	40 (78%)	11 (22%)	1	6
55	B6	43/52 (83%)	30 (70%)	13 (30%)	0	1
55	D6	44/52 (85%)	29 (66%)	15 (34%)	0	1
56	B7	41/42 (98%)	32 (78%)	9 (22%)	1	5
56	D7	41/42 (98%)	36 (88%)	5 (12%)	5	21
57	B8	53/55 (96%)	44 (83%)	9 (17%)	2	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	D8	53/55 (96%)	41 (77%)	12 (23%)	1	5
58	B9	33/34 (97%)	22 (67%)	11 (33%)	0	1
58	D9	33/34 (97%)	28 (85%)	5 (15%)	3	14
All	All	9600/10432 (92%)	7577 (79%)	2023 (21%)	1	6

5 of 2023 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
48	BZ	38	VAL
42	DT	11	GLU
4	CD	138	TYR
41	DS	12	PHE
47	DY	71	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 323 such sidechains are listed below:

Mol	Chain	Res	Type
30	DD	164	GLN
44	DV	11	GLN
31	DE	66	HIS
38	DP	13	ASN
48	DZ	131	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1493/1509 (98%)	360 (24%)	136 (9%)
1	CA	1493/1509 (98%)	371 (24%)	120 (8%)
22	AV	9/30 (30%)	0	0
22	CV	9/30 (30%)	0	0
23	AW	74/75 (98%)	17 (22%)	2 (2%)
23	CW	74/75 (98%)	16 (21%)	4 (5%)
24	AX	76/77 (98%)	19 (25%)	1 (1%)
24	CX	76/77 (98%)	19 (25%)	0
25	AY	74/75 (98%)	23 (31%)	1 (1%)
25	CY	74/75 (98%)	22 (29%)	1 (1%)
27	BA	2796/2915 (95%)	815 (29%)	220 (7%)
27	DA	2797/2915 (95%)	924 (33%)	280 (10%)
28	BB	116/122 (95%)	26 (22%)	5 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	DB	116/122 (95%)	28 (24%)	8 (6%)
All	All	9277/9606 (96%)	2640 (28%)	778 (8%)

5 of 2640 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	8	A
1	AA	9	G
1	AA	13	U
1	AA	31	G
1	AA	32	A

5 of 778 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	1211	U
27	DA	740	U
1	CA	1397	C
1	CA	1201	A
27	DA	284	U

5.4 Non-standard residues in protein, DNA, RNA chains

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
26	KBE	AZ	1	26	8,8,9	0.57	0	6,8,10	1.30	1 (16%)
26	UAL	AZ	5	26	6,8,9	2.55	2 (33%)	4,9,11	1.30	1 (25%)
26	UAL	CZ	5	26	6,8,9	3.20	2 (33%)	4,9,11	3.50	3 (75%)
26	5OH	AZ	6	26	7,12,13	0.54	0	4,16,18	0.73	0
26	5OH	CZ	6	26	7,12,13	0.76	0	4,16,18	0.94	0
26	KBE	CZ	1	26	8,8,9	0.62	0	6,8,10	0.78	0
26	DPP	CZ	2	26	4,5,6	0.71	0	1,5,7	0.01	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	DPP	AZ	2	26	4,5,6	0.38	0	1,5,7	0.18	0

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
26	KBE	AZ	1	26	-	1/7/7/8	-
26	UAL	AZ	5	26	-	0/3/7/9	-
26	UAL	CZ	5	26	-	0/3/7/9	-
26	5OH	AZ	6	26	-	0/2/18/20	0/1/1/1
26	5OH	CZ	6	26	-	0/2/18/20	0/1/1/1
26	KBE	CZ	1	26	-	0/7/7/8	-
26	DPP	CZ	2	26	-	0/2/4/6	-
26	DPP	AZ	2	26	-	0/2/4/6	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	CZ	5	UAL	C1-N1	-6.82	1.29	1.40
26	AZ	5	UAL	C-CA	4.93	1.53	1.45
26	CZ	5	UAL	C-CA	3.55	1.51	1.45
26	AZ	5	UAL	C1-N1	-3.16	1.35	1.40

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	CZ	5	UAL	O2-C1-N2	-5.59	111.92	123.18
26	CZ	5	UAL	N2-C1-N1	2.82	121.55	115.39
26	CZ	5	UAL	O2-C1-N1	2.63	126.51	120.37
26	AZ	1	KBE	CB-CA-C	2.59	116.35	112.17
26	AZ	5	UAL	O-C-CA	-2.35	122.45	125.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	AZ	1	KBE	C-CA-CB-N

There are no ring outliers.

6 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	AZ	1	KBE	3	0
26	AZ	5	UAL	4	0
26	CZ	5	UAL	5	0
26	AZ	6	5OH	3	0
26	CZ	6	5OH	11	0
26	CZ	1	KBE	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 973 ligands modelled in this entry, 973 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	D6	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D6	46:HIS	C	47:THR	N	1.18

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1495/1509 (99%)	0.04	29 (1%) 66 43	48, 83, 149, 196	0
1	CA	1495/1509 (99%)	0.13	34 (2%) 61 38	59, 91, 155, 196	0
2	AB	235/256 (91%)	0.49	12 (5%) 33 17	80, 114, 144, 161	0
2	CB	235/256 (91%)	0.56	12 (5%) 33 17	81, 118, 152, 171	0
3	AC	207/239 (86%)	0.29	5 (2%) 59 36	76, 101, 140, 153	0
3	CC	207/239 (86%)	0.62	19 (9%) 14 8	89, 109, 136, 147	0
4	AD	208/209 (99%)	0.39	13 (6%) 26 13	65, 84, 101, 114	0
4	CD	208/209 (99%)	0.15	6 (2%) 53 31	55, 77, 98, 107	0
5	AE	151/162 (93%)	0.11	4 (2%) 57 34	59, 81, 107, 122	0
5	CE	151/162 (93%)	0.17	0 100 100	72, 88, 109, 145	0
6	AF	101/101 (100%)	-0.07	1 (0%) 79 59	63, 84, 93, 110	0
6	CF	101/101 (100%)	-0.09	0 100 100	76, 88, 101, 134	0
7	AG	155/156 (99%)	0.37	9 (5%) 29 15	74, 94, 129, 151	0
7	CG	155/156 (99%)	0.54	12 (7%) 19 10	84, 103, 128, 140	0
8	AH	138/138 (100%)	0.08	1 (0%) 84 66	69, 84, 96, 107	0
8	CH	138/138 (100%)	0.21	4 (2%) 53 31	74, 91, 102, 117	0
9	AI	127/128 (99%)	0.65	8 (6%) 26 13	76, 115, 136, 144	0
9	CI	127/128 (99%)	0.83	10 (7%) 18 10	89, 121, 139, 143	0
10	AJ	99/105 (94%)	1.04	15 (15%) 5 3	80, 127, 152, 164	0
10	CJ	99/105 (94%)	1.12	17 (17%) 4 3	88, 125, 148, 154	0
11	AK	119/129 (92%)	0.14	2 (1%) 69 45	55, 79, 107, 127	0
11	CK	119/129 (92%)	0.39	11 (9%) 14 8	69, 88, 108, 124	0
12	AL	125/132 (94%)	0.08	2 (1%) 70 47	55, 69, 91, 126	0
12	CL	125/132 (94%)	0.33	5 (4%) 42 23	66, 82, 98, 129	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	120/126 (95%)	0.33	6 (5%) 34 18	58, 86, 98, 107	0
13	CM	119/126 (94%)	0.67	9 (7%) 20 10	80, 108, 125, 136	0
14	AN	60/61 (98%)	0.75	5 (8%) 17 9	76, 92, 110, 122	0
14	CN	60/61 (98%)	0.92	6 (10%) 12 7	90, 105, 120, 123	0
15	AO	88/89 (98%)	0.25	5 (5%) 29 15	64, 76, 99, 114	0
15	CO	88/89 (98%)	0.32	2 (2%) 61 38	71, 84, 106, 117	0
16	AP	84/88 (95%)	0.57	6 (7%) 22 11	68, 86, 108, 124	0
16	CP	84/88 (95%)	0.17	0 100 100	71, 81, 105, 136	0
17	AQ	100/105 (95%)	0.19	5 (5%) 34 18	62, 79, 95, 99	0
17	CQ	100/105 (95%)	0.29	2 (2%) 65 41	64, 85, 100, 103	0
18	AR	70/88 (79%)	0.04	1 (1%) 73 51	67, 83, 106, 134	0
18	CR	70/88 (79%)	0.02	0 100 100	72, 86, 107, 134	0
19	AS	79/93 (84%)	0.81	10 (12%) 8 5	87, 105, 127, 134	0
19	CS	79/93 (84%)	0.92	7 (8%) 15 8	101, 122, 143, 154	0
20	AT	99/106 (93%)	0.74	11 (11%) 10 6	71, 89, 118, 130	0
20	CT	99/106 (93%)	0.65	8 (8%) 18 9	74, 90, 114, 125	0
21	AU	25/27 (92%)	1.35	4 (16%) 5 3	86, 92, 100, 118	0
21	CU	25/27 (92%)	1.05	2 (8%) 18 9	89, 104, 116, 119	0
22	AV	10/30 (33%)	0.50	2 (20%) 3 2	63, 73, 124, 133	0
22	CV	10/30 (33%)	0.68	0 100 100	68, 85, 125, 130	0
23	AW	75/75 (100%)	0.45	2 (2%) 56 33	46, 119, 161, 185	0
23	CW	75/75 (100%)	0.64	5 (6%) 24 12	79, 141, 174, 184	0
24	AX	77/77 (100%)	0.12	1 (1%) 75 53	48, 89, 121, 130	0
24	CX	77/77 (100%)	0.18	0 100 100	69, 98, 125, 132	0
25	AY	75/75 (100%)	0.84	11 (14%) 6 3	51, 157, 193, 194	0
25	CY	75/75 (100%)	1.04	11 (14%) 6 3	67, 167, 194, 194	0
26	AZ	2/6 (33%)	0.69	0 100 100	85, 85, 85, 88	0
26	CZ	2/6 (33%)	1.75	1 (50%) 0 0	99, 99, 99, 100	0
27	BA	2800/2915 (96%)	-0.29	43 (1%) 72 49	30, 56, 157, 198	0
27	DA	2800/2915 (96%)	0.06	66 (2%) 59 36	49, 77, 168, 197	0
28	BB	118/122 (96%)	-0.05	6 (5%) 33 17	47, 76, 119, 164	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
28	DB	118/122 (96%)	0.52	9 (7%)	20 10	80, 104, 136, 162	0
29	BC	191/229 (83%)	1.24	31 (16%)	4 3	130, 167, 187, 195	0
29	DC	191/229 (83%)	1.38	42 (21%)	2 1	122, 173, 188, 191	0
30	BD	272/276 (98%)	-0.15	6 (2%)	62 39	32, 52, 68, 79	0
30	DD	272/276 (98%)	0.09	5 (1%)	67 44	46, 61, 78, 92	0
31	BE	205/206 (99%)	-0.00	4 (1%)	65 41	33, 58, 93, 104	0
31	DE	205/206 (99%)	0.41	7 (3%)	48 27	57, 84, 112, 121	0
32	BF	208/210 (99%)	-0.03	4 (1%)	66 43	29, 60, 125, 149	0
32	DF	208/210 (99%)	0.40	15 (7%)	21 11	54, 86, 132, 152	0
33	BG	181/182 (99%)	0.30	8 (4%)	39 21	64, 83, 116, 146	0
33	DG	181/182 (99%)	0.51	8 (4%)	39 21	79, 106, 132, 153	0
34	BH	164/180 (91%)	0.62	12 (7%)	21 11	68, 97, 124, 142	0
34	DH	160/180 (88%)	0.78	18 (11%)	10 6	110, 139, 159, 163	0
35	BI	146/148 (98%)	0.51	3 (2%)	63 40	62, 119, 140, 144	0
35	DI	146/148 (98%)	0.29	2 (1%)	73 51	67, 105, 128, 136	0
36	BN	139/140 (99%)	-0.06	3 (2%)	62 39	42, 57, 86, 104	0
36	DN	139/140 (99%)	0.55	11 (7%)	18 10	65, 91, 115, 124	0
37	BO	122/122 (100%)	-0.07	2 (1%)	70 47	38, 57, 75, 88	0
37	DO	122/122 (100%)	0.03	0	100 100	60, 77, 93, 100	0
38	BP	146/150 (97%)	0.54	8 (5%)	30 15	37, 69, 102, 156	0
38	DP	146/150 (97%)	0.75	10 (6%)	23 12	61, 93, 122, 148	0
39	BQ	141/141 (100%)	0.30	8 (5%)	29 15	42, 60, 92, 118	0
39	DQ	139/141 (98%)	0.52	7 (5%)	34 18	68, 90, 120, 134	0
40	BR	117/118 (99%)	-0.06	6 (5%)	33 17	35, 52, 69, 82	0
40	DR	117/118 (99%)	0.34	8 (6%)	23 12	58, 71, 83, 96	0
41	BS	99/112 (88%)	0.39	7 (7%)	22 11	48, 76, 94, 105	0
41	DS	101/112 (90%)	0.77	12 (11%)	9 5	68, 100, 117, 122	0
42	BT	138/146 (94%)	0.30	10 (7%)	21 11	51, 70, 126, 152	0
42	DT	138/146 (94%)	0.65	13 (9%)	14 7	61, 90, 149, 175	0
43	BU	117/118 (99%)	-0.03	2 (1%)	69 45	37, 49, 73, 95	0
43	DU	117/118 (99%)	0.65	8 (6%)	23 12	60, 91, 111, 124	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
44	BV	101/101 (100%)	0.16	5 (4%) 34 18	35, 65, 90, 116	0
44	DV	101/101 (100%)	0.39	2 (1%) 65 41	59, 106, 121, 129	0
45	BW	113/113 (100%)	-0.38	2 (1%) 67 44	32, 46, 76, 136	0
45	DW	113/113 (100%)	-0.10	1 (0%) 81 61	43, 64, 95, 130	0
46	BX	93/96 (96%)	-0.14	0 100 100	43, 53, 70, 91	0
46	DX	93/96 (96%)	0.13	1 (1%) 78 57	56, 71, 89, 95	0
47	BY	101/110 (91%)	0.90	13 (12%) 7 5	58, 78, 145, 163	0
47	DY	101/110 (91%)	0.85	14 (13%) 6 4	73, 94, 149, 156	0
48	BZ	177/206 (85%)	0.89	30 (16%) 4 3	65, 107, 169, 177	0
48	DZ	177/206 (85%)	1.13	37 (20%) 2 2	104, 130, 177, 191	0
49	B0	84/85 (98%)	0.07	6 (7%) 22 11	43, 56, 83, 103	0
49	D0	84/85 (98%)	0.45	5 (5%) 27 14	71, 83, 100, 118	0
50	B1	94/98 (95%)	0.17	3 (3%) 50 29	44, 61, 92, 109	0
50	D1	94/98 (95%)	0.36	3 (3%) 50 29	54, 70, 94, 110	0
51	B2	71/72 (98%)	0.04	4 (5%) 30 15	46, 66, 86, 117	0
51	D2	71/72 (98%)	0.19	3 (4%) 40 22	65, 86, 103, 107	0
52	B3	60/60 (100%)	0.06	1 (1%) 69 45	43, 58, 85, 110	0
52	D3	60/60 (100%)	0.60	2 (3%) 49 28	75, 90, 112, 116	0
53	B4	31/71 (43%)	0.34	1 (3%) 50 29	92, 107, 120, 126	0
53	D4	31/71 (43%)	0.35	3 (9%) 13 7	108, 119, 128, 135	0
54	B5	59/60 (98%)	0.27	8 (13%) 7 4	33, 51, 115, 135	0
54	D5	59/60 (98%)	0.42	1 (1%) 69 45	60, 71, 143, 177	0
55	B6	51/54 (94%)	1.29	8 (15%) 5 3	59, 83, 106, 112	0
55	D6	46/54 (85%)	1.70	15 (32%) 1 1	56, 103, 116, 117	0
56	B7	49/49 (100%)	0.06	0 100 100	28, 44, 84, 115	0
56	D7	49/49 (100%)	0.34	3 (6%) 27 14	46, 59, 90, 101	0
57	B8	64/65 (98%)	0.44	6 (9%) 14 7	40, 56, 73, 97	0
57	D8	64/65 (98%)	1.06	10 (15%) 5 3	60, 74, 87, 118	0
58	B9	36/37 (97%)	0.17	0 100 100	46, 63, 80, 93	0
58	D9	36/37 (97%)	1.33	9 (25%) 2 1	88, 122, 133, 137	0
All	All	21214/22204 (95%)	0.23	953 (4%) 38 20	28, 83, 154, 198	0

The worst 5 of 953 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
48	DZ	175	PRO	11.5
39	BQ	140	ALA	9.9
27	BA	2802	G	9.2
28	DB	88	C	8.8
27	DA	2802	G	8.8

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
26	UAL	AZ	5	9/10	0.69	0.16	81,82,83,84	0
26	UAL	CZ	5	9/10	0.74	0.18	97,99,99,99	0
26	KBE	CZ	1	9/10	0.75	0.29	89,91,93,94	0
26	5OH	AZ	6	12/13	0.78	0.13	84,89,92,94	0
26	5OH	CZ	6	12/13	0.81	0.14	99,101,102,102	0
26	KBE	AZ	1	9/10	0.84	0.23	78,79,82,82	0
26	DPP	CZ	2	6/7	0.88	0.12	94,96,97,97	0
26	DPP	AZ	2	6/7	0.94	0.10	79,82,82,84	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
59	MG	CA	1675	1/1	0.06	0.30	150,150,150,150	0
59	MG	DA	3203	1/1	0.33	0.47	97,97,97,97	0
59	MG	CA	1605	1/1	0.40	0.14	99,99,99,99	0
59	MG	DA	3236	1/1	0.44	0.50	91,91,91,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DD	301	1/1	0.53	0.21	110,110,110,110	0
59	MG	DA	3183	1/1	0.54	0.13	100,100,100,100	0
59	MG	BA	3290	1/1	0.54	0.20	69,69,69,69	0
59	MG	CA	1619	1/1	0.58	0.29	80,80,80,80	0
59	MG	AW	106	1/1	0.59	0.29	94,94,94,94	0
59	MG	BA	3297	1/1	0.60	0.34	95,95,95,95	0
59	MG	AX	105	1/1	0.61	0.26	82,82,82,82	0
59	MG	BA	3298	1/1	0.63	0.72	178,178,178,178	0
59	MG	AW	101	1/1	0.64	0.32	135,135,135,135	0
59	MG	BA	3322	1/1	0.65	0.46	147,147,147,147	0
59	MG	CA	1603	1/1	0.67	0.35	113,113,113,113	0
59	MG	CA	1639	1/1	0.67	0.18	74,74,74,74	0
59	MG	AA	1671	1/1	0.67	0.23	83,83,83,83	0
59	MG	DA	3171	1/1	0.67	0.36	75,75,75,75	0
59	MG	AX	107	1/1	0.69	0.28	80,80,80,80	0
59	MG	AA	1710	1/1	0.70	0.28	113,113,113,113	0
59	MG	AT	201	1/1	0.72	0.18	92,92,92,92	0
59	MG	AA	1667	1/1	0.73	0.19	59,59,59,59	0
59	MG	AA	1707	1/1	0.73	0.23	59,59,59,59	0
59	MG	DA	3271	1/1	0.74	0.13	80,80,80,80	0
59	MG	DA	3197	1/1	0.74	0.34	84,84,84,84	0
59	MG	DA	3218	1/1	0.75	0.27	75,75,75,75	0
59	MG	CA	1638	1/1	0.75	0.21	46,46,46,46	0
59	MG	BA	3332	1/1	0.75	0.36	105,105,105,105	0
59	MG	DA	3273	1/1	0.75	0.45	106,106,106,106	0
59	MG	DA	3181	1/1	0.75	0.17	52,52,52,52	0
59	MG	BA	3357	1/1	0.76	0.21	54,54,54,54	0
59	MG	DA	3095	1/1	0.76	0.21	64,64,64,64	0
59	MG	AA	1634	1/1	0.77	0.15	72,72,72,72	0
59	MG	BA	3004	1/1	0.77	0.30	81,81,81,81	0
59	MG	CA	1674	1/1	0.77	0.26	63,63,63,63	0
59	MG	BA	3275	1/1	0.77	0.13	93,93,93,93	0
59	MG	AA	1676	1/1	0.77	0.14	77,77,77,77	0
59	MG	BA	3227	1/1	0.78	0.16	69,69,69,69	0
59	MG	AK	202	1/1	0.78	0.17	90,90,90,90	0
59	MG	DA	3112	1/1	0.78	0.12	70,70,70,70	0
59	MG	DA	3229	1/1	0.78	0.20	76,76,76,76	0
59	MG	DD	303	1/1	0.78	0.24	95,95,95,95	0
59	MG	DA	3238	1/1	0.79	0.43	101,101,101,101	0
59	MG	AY	102	1/1	0.79	0.29	96,96,96,96	0
59	MG	BA	3333	1/1	0.79	0.27	55,55,55,55	0
59	MG	AA	1620	1/1	0.79	0.12	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3165	1/1	0.79	0.27	60,60,60,60	0
59	MG	CA	1686	1/1	0.81	0.21	64,64,64,64	0
59	MG	DA	3077	1/1	0.81	0.40	73,73,73,73	0
59	MG	BA	3347	1/1	0.81	0.26	78,78,78,78	0
59	MG	AC	301	1/1	0.81	0.13	64,64,64,64	0
59	MG	BA	3243	1/1	0.81	0.20	35,35,35,35	0
59	MG	CA	1652	1/1	0.81	0.25	86,86,86,86	0
59	MG	BA	3320	1/1	0.81	0.74	89,89,89,89	0
59	MG	DA	3184	1/1	0.81	0.07	50,50,50,50	0
59	MG	CA	1618	1/1	0.81	0.28	69,69,69,69	0
59	MG	CA	1630	1/1	0.82	0.21	55,55,55,55	0
59	MG	BA	3341	1/1	0.82	0.36	86,86,86,86	0
59	MG	BA	3360	1/1	0.82	0.33	68,68,68,68	0
59	MG	DA	3045	1/1	0.82	0.09	41,41,41,41	0
59	MG	BA	3174	1/1	0.82	0.11	43,43,43,43	0
59	MG	DA	3234	1/1	0.82	0.47	84,84,84,84	0
59	MG	DA	3172	1/1	0.83	0.24	55,55,55,55	0
59	MG	DA	3175	1/1	0.83	0.23	53,53,53,53	0
59	MG	BA	3307	1/1	0.83	0.23	64,64,64,64	0
59	MG	AA	1700	1/1	0.83	0.20	58,58,58,58	0
59	MG	BA	3366	1/1	0.83	0.17	64,64,64,64	0
59	MG	CA	1672	1/1	0.83	0.10	45,45,45,45	0
59	MG	BX	101	1/1	0.83	0.28	53,53,53,53	0
59	MG	DA	3211	1/1	0.83	0.34	78,78,78,78	0
59	MG	BA	3260	1/1	0.83	0.23	58,58,58,58	0
59	MG	AK	201	1/1	0.83	0.21	66,66,66,66	0
59	MG	CA	1691	1/1	0.83	0.11	55,55,55,55	0
59	MG	CA	1612	1/1	0.83	0.28	80,80,80,80	0
59	MG	AA	1624	1/1	0.83	0.08	54,54,54,54	0
59	MG	DA	3253	1/1	0.83	0.12	46,46,46,46	0
59	MG	AA	1632	1/1	0.83	0.21	53,53,53,53	0
59	MG	CA	1623	1/1	0.83	0.23	91,91,91,91	0
59	MG	DA	3163	1/1	0.83	0.20	62,62,62,62	0
59	MG	AY	101	1/1	0.83	0.18	71,71,71,71	0
59	MG	BA	3276	1/1	0.84	0.19	45,45,45,45	0
59	MG	AA	1645	1/1	0.84	0.23	64,64,64,64	0
59	MG	DA	3053	1/1	0.84	0.13	47,47,47,47	0
59	MG	BA	3270	1/1	0.84	0.19	64,64,64,64	0
59	MG	DA	3078	1/1	0.84	0.20	58,58,58,58	0
59	MG	BA	3325	1/1	0.84	0.09	61,61,61,61	0
59	MG	CA	1631	1/1	0.84	0.21	45,45,45,45	0
59	MG	DA	3157	1/1	0.84	0.20	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3210	1/1	0.84	0.25	57,57,57,57	0
59	MG	AW	103	1/1	0.84	0.28	73,73,73,73	0
59	MG	CA	1692	1/1	0.85	0.22	73,73,73,73	0
59	MG	DA	3227	1/1	0.85	0.09	72,72,72,72	0
59	MG	AE	201	1/1	0.85	0.18	87,87,87,87	0
59	MG	BA	3170	1/1	0.85	0.18	57,57,57,57	0
59	MG	DA	3074	1/1	0.85	0.19	59,59,59,59	0
59	MG	BA	3269	1/1	0.85	0.44	83,83,83,83	0
59	MG	AA	1725	1/1	0.85	0.20	84,84,84,84	0
59	MG	DA	3265	1/1	0.85	0.20	51,51,51,51	0
59	MG	BA	3177	1/1	0.85	0.27	65,65,65,65	0
59	MG	BA	3224	1/1	0.85	0.09	63,63,63,63	0
59	MG	BA	3389	1/1	0.85	0.17	44,44,44,44	0
59	MG	AA	1603	1/1	0.85	0.34	58,58,58,58	0
60	ZN	D4	101	1/1	0.85	0.15	147,147,147,147	0
59	MG	DA	3189	1/1	0.86	0.44	92,92,92,92	0
59	MG	BA	3265	1/1	0.86	0.07	28,28,28,28	0
59	MG	DA	3200	1/1	0.86	0.09	46,46,46,46	0
59	MG	AA	1604	1/1	0.86	0.23	56,56,56,56	0
59	MG	CA	1643	1/1	0.86	0.13	51,51,51,51	0
59	MG	CA	1650	1/1	0.86	0.28	69,69,69,69	0
59	MG	BA	3205	1/1	0.86	0.49	86,86,86,86	0
59	MG	DA	3097	1/1	0.86	0.34	65,65,65,65	0
59	MG	BA	3112	1/1	0.86	0.09	52,52,52,52	0
59	MG	DA	3232	1/1	0.86	0.17	80,80,80,80	0
59	MG	DA	3144	1/1	0.86	0.32	57,57,57,57	0
59	MG	DA	3152	1/1	0.86	0.19	54,54,54,54	0
59	MG	AA	1626	1/1	0.86	0.13	48,48,48,48	0
59	MG	BA	3230	1/1	0.86	0.15	48,48,48,48	0
59	MG	AW	105	1/1	0.86	0.06	41,41,41,41	0
59	MG	BA	3246	1/1	0.86	0.10	46,46,46,46	0
59	MG	BA	3299	1/1	0.86	0.51	85,85,85,85	0
59	MG	CQ	201	1/1	0.86	0.18	94,94,94,94	0
59	MG	DA	3009	1/1	0.86	0.11	20,20,20,20	0
59	MG	AA	1689	1/1	0.86	0.23	73,73,73,73	0
59	MG	DA	3111	1/1	0.87	0.20	71,71,71,71	0
59	MG	CA	1683	1/1	0.87	0.27	55,55,55,55	0
59	MG	DA	3120	1/1	0.87	0.08	55,55,55,55	0
59	MG	DA	3136	1/1	0.87	0.12	47,47,47,47	0
59	MG	AA	1728	1/1	0.87	0.07	59,59,59,59	0
59	MG	AT	202	1/1	0.87	0.30	70,70,70,70	0
59	MG	BA	3390	1/1	0.87	0.11	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BQ	201	1/1	0.87	0.15	48,48,48,48	0
59	MG	DA	3235	1/1	0.87	0.21	68,68,68,68	0
59	MG	BA	3296	1/1	0.87	0.15	61,61,61,61	0
59	MG	AA	1685	1/1	0.87	0.17	50,50,50,50	0
59	MG	DA	3245	1/1	0.87	0.26	86,86,86,86	0
59	MG	DA	3050	1/1	0.87	0.21	70,70,70,70	0
59	MG	DA	3254	1/1	0.87	0.09	54,54,54,54	0
59	MG	DA	3260	1/1	0.87	0.13	35,35,35,35	0
59	MG	AA	1646	1/1	0.87	0.10	61,61,61,61	0
59	MG	AW	104	1/1	0.87	0.13	57,57,57,57	0
59	MG	CA	1670	1/1	0.87	0.23	67,67,67,67	0
59	MG	CA	1614	1/1	0.87	0.11	49,49,49,49	0
59	MG	AA	1716	1/1	0.87	0.15	44,44,44,44	0
59	MG	AA	1677	1/1	0.87	0.19	75,75,75,75	0
59	MG	CA	1626	1/1	0.88	0.26	46,46,46,46	0
59	MG	CA	1689	1/1	0.88	0.21	63,63,63,63	0
59	MG	DA	3213	1/1	0.88	0.24	62,62,62,62	0
59	MG	DA	3217	1/1	0.88	0.30	85,85,85,85	0
59	MG	BA	3134	1/1	0.88	0.32	39,39,39,39	0
59	MG	DA	3220	1/1	0.88	0.22	64,64,64,64	0
59	MG	BA	3262	1/1	0.88	0.12	27,27,27,27	0
59	MG	BA	3338	1/1	0.88	0.13	60,60,60,60	0
59	MG	AA	1640	1/1	0.88	0.16	37,37,37,37	0
59	MG	DA	3016	1/1	0.88	0.13	54,54,54,54	0
59	MG	DA	3164	1/1	0.88	0.20	51,51,51,51	0
59	MG	DA	3020	1/1	0.88	0.12	45,45,45,45	0
59	MG	AA	1727	1/1	0.88	0.20	71,71,71,71	0
59	MG	CA	1607	1/1	0.88	0.26	36,36,36,36	0
59	MG	DA	3247	1/1	0.88	0.13	82,82,82,82	0
59	MG	DA	3250	1/1	0.88	0.26	61,61,61,61	0
59	MG	DA	3176	1/1	0.88	0.18	51,51,51,51	0
59	MG	CA	1608	1/1	0.88	0.21	57,57,57,57	0
59	MG	AA	1691	1/1	0.88	0.27	56,56,56,56	0
59	MG	BA	3240	1/1	0.88	0.17	60,60,60,60	0
59	MG	DA	3266	1/1	0.88	0.19	72,72,72,72	0
59	MG	BA	3175	1/1	0.88	0.15	43,43,43,43	0
59	MG	BA	3373	1/1	0.88	0.20	55,55,55,55	0
59	MG	CA	1682	1/1	0.88	0.28	61,61,61,61	0
59	MG	AA	1721	1/1	0.88	0.13	54,54,54,54	0
59	MG	DA	3209	1/1	0.88	0.26	69,69,69,69	0
59	MG	DA	3178	1/1	0.89	0.22	36,36,36,36	0
59	MG	AA	1665	1/1	0.89	0.07	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	AA	1719	1/1	0.89	0.24	58,58,58,58	0
59	MG	DA	3014	1/1	0.89	0.13	79,79,79,79	0
59	MG	AX	106	1/1	0.89	0.11	43,43,43,43	0
59	MG	AA	1666	1/1	0.89	0.28	75,75,75,75	0
59	MG	BA	3274	1/1	0.89	0.06	36,36,36,36	0
59	MG	AA	1641	1/1	0.89	0.07	62,62,62,62	0
59	MG	BA	3353	1/1	0.89	0.24	50,50,50,50	0
59	MG	DA	3069	1/1	0.89	0.36	78,78,78,78	0
59	MG	BA	3182	1/1	0.89	0.18	81,81,81,81	0
59	MG	AA	1699	1/1	0.89	0.21	61,61,61,61	0
59	MG	BA	3291	1/1	0.89	0.14	42,42,42,42	0
59	MG	DA	3091	1/1	0.89	0.12	67,67,67,67	0
59	MG	AA	1629	1/1	0.89	0.07	78,78,78,78	0
59	MG	BA	3016	1/1	0.89	0.21	27,27,27,27	0
59	MG	DA	3098	1/1	0.89	0.06	37,37,37,37	0
59	MG	DA	3102	1/1	0.89	0.19	84,84,84,84	0
59	MG	DA	3109	1/1	0.89	0.13	65,65,65,65	0
59	MG	CA	1651	1/1	0.89	0.06	50,50,50,50	0
59	MG	BA	3034	1/1	0.89	0.20	37,37,37,37	0
59	MG	BA	3392	1/1	0.89	0.24	63,63,63,63	0
59	MG	DA	3132	1/1	0.89	0.20	60,60,60,60	0
59	MG	BA	3084	1/1	0.89	0.13	19,19,19,19	0
59	MG	BA	3302	1/1	0.89	0.10	42,42,42,42	0
59	MG	DA	3145	1/1	0.89	0.17	45,45,45,45	0
59	MG	DA	3146	1/1	0.89	0.21	70,70,70,70	0
59	MG	BZ	301	1/1	0.89	0.09	42,42,42,42	0
59	MG	B0	101	1/1	0.89	0.20	58,58,58,58	0
59	MG	B0	102	1/1	0.89	0.30	49,49,49,49	0
59	MG	AA	1627	1/1	0.89	0.29	55,55,55,55	0
59	MG	CA	1688	1/1	0.89	0.19	59,59,59,59	0
59	MG	BA	3315	1/1	0.89	0.11	46,46,46,46	0
59	MG	BA	3132	1/1	0.89	0.18	87,87,87,87	0
59	MG	DE	302	1/1	0.89	0.42	65,65,65,65	0
59	MG	AA	1657	1/1	0.89	0.15	53,53,53,53	0
59	MG	CE	201	1/1	0.90	0.13	71,71,71,71	0
59	MG	AA	1712	1/1	0.90	0.20	53,53,53,53	0
59	MG	DA	3173	1/1	0.90	0.05	57,57,57,57	0
59	MG	CX	101	1/1	0.90	0.10	42,42,42,42	0
59	MG	BA	3331	1/1	0.90	0.14	52,52,52,52	0
59	MG	CA	1609	1/1	0.90	0.25	52,52,52,52	0
59	MG	AA	1714	1/1	0.90	0.26	66,66,66,66	0
59	MG	AA	1693	1/1	0.90	0.07	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3039	1/1	0.90	0.21	58,58,58,58	0
59	MG	BA	3181	1/1	0.90	0.07	46,46,46,46	0
59	MG	DA	3193	1/1	0.90	0.13	40,40,40,40	0
59	MG	BA	3340	1/1	0.90	0.05	42,42,42,42	0
59	MG	BA	3054	1/1	0.90	0.07	22,22,22,22	0
59	MG	DA	3068	1/1	0.90	0.17	60,60,60,60	0
59	MG	AA	1698	1/1	0.90	0.10	49,49,49,49	0
59	MG	BA	3277	1/1	0.90	0.15	60,60,60,60	0
59	MG	DA	3076	1/1	0.90	0.19	48,48,48,48	0
59	MG	BA	3284	1/1	0.90	0.16	33,33,33,33	0
59	MG	BA	3288	1/1	0.90	0.11	33,33,33,33	0
59	MG	DA	3082	1/1	0.90	0.19	37,37,37,37	0
59	MG	DA	3088	1/1	0.90	0.07	36,36,36,36	0
59	MG	BA	3219	1/1	0.90	0.07	43,43,43,43	0
59	MG	BA	3367	1/1	0.90	0.20	35,35,35,35	0
59	MG	CA	1647	1/1	0.90	0.27	51,51,51,51	0
59	MG	BA	3102	1/1	0.90	0.10	49,49,49,49	0
59	MG	AA	1680	1/1	0.90	0.22	63,63,63,63	0
59	MG	BA	3113	1/1	0.90	0.19	34,34,34,34	0
59	MG	CA	1657	1/1	0.90	0.25	62,62,62,62	0
59	MG	AA	1638	1/1	0.90	0.14	50,50,50,50	0
59	MG	DA	3119	1/1	0.90	0.16	62,62,62,62	0
59	MG	BA	3397	1/1	0.90	0.25	66,66,66,66	0
59	MG	DA	3127	1/1	0.90	0.20	48,48,48,48	0
59	MG	BH	201	1/1	0.90	0.09	71,71,71,71	0
59	MG	DA	3257	1/1	0.90	0.20	40,40,40,40	0
59	MG	DA	3135	1/1	0.90	0.19	58,58,58,58	0
59	MG	AA	1649	1/1	0.90	0.35	71,71,71,71	0
59	MG	BA	3159	1/1	0.90	0.15	46,46,46,46	0
59	MG	BA	3255	1/1	0.90	0.06	22,22,22,22	0
59	MG	BA	3308	1/1	0.90	0.24	49,49,49,49	0
59	MG	AA	1602	1/1	0.90	0.17	44,44,44,44	0
59	MG	CA	1602	1/1	0.90	0.20	46,46,46,46	0
59	MG	BA	3261	1/1	0.90	0.20	53,53,53,53	0
59	MG	DR	201	1/1	0.90	0.22	65,65,65,65	0
59	MG	BA	3002	1/1	0.90	0.14	59,59,59,59	0
59	MG	DA	3028	1/1	0.91	0.16	35,35,35,35	0
59	MG	BA	3213	1/1	0.91	0.19	54,54,54,54	0
59	MG	BA	3287	1/1	0.91	0.14	56,56,56,56	0
59	MG	BA	3216	1/1	0.91	0.22	42,42,42,42	0
59	MG	AA	1659	1/1	0.91	0.18	73,73,73,73	0
59	MG	AA	1661	1/1	0.91	0.07	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3293	1/1	0.91	0.26	44,44,44,44	0
59	MG	CA	1642	1/1	0.91	0.13	29,29,29,29	0
59	MG	DA	3190	1/1	0.91	0.06	33,33,33,33	0
59	MG	BA	3376	1/1	0.91	0.43	66,66,66,66	0
59	MG	BA	3110	1/1	0.91	0.15	39,39,39,39	0
59	MG	AA	1711	1/1	0.91	0.15	68,68,68,68	0
59	MG	BA	3233	1/1	0.91	0.12	32,32,32,32	0
59	MG	DA	3208	1/1	0.91	0.33	62,62,62,62	0
59	MG	DA	3083	1/1	0.91	0.17	35,35,35,35	0
59	MG	AA	1605	1/1	0.91	0.18	54,54,54,54	0
59	MG	AA	1713	1/1	0.91	0.14	57,57,57,57	0
59	MG	CA	1666	1/1	0.91	0.19	68,68,68,68	0
59	MG	CA	1669	1/1	0.91	0.09	36,36,36,36	0
59	MG	AA	1647	1/1	0.91	0.28	80,80,80,80	0
59	MG	BA	3001	1/1	0.91	0.28	72,72,72,72	0
59	MG	DA	3226	1/1	0.91	0.28	70,70,70,70	0
59	MG	DA	3103	1/1	0.91	0.05	38,38,38,38	0
59	MG	DA	3104	1/1	0.91	0.07	36,36,36,36	0
59	MG	DA	3108	1/1	0.91	0.11	51,51,51,51	0
59	MG	DA	3233	1/1	0.91	0.22	58,58,58,58	0
59	MG	BA	3257	1/1	0.91	0.10	21,21,21,21	0
59	MG	BA	3317	1/1	0.91	0.26	50,50,50,50	0
59	MG	BA	3164	1/1	0.91	0.27	37,37,37,37	0
59	MG	AA	1637	1/1	0.91	0.06	40,40,40,40	0
59	MG	DA	3239	1/1	0.91	0.37	78,78,78,78	0
59	MG	DA	3241	1/1	0.91	0.14	42,42,42,42	0
59	MG	BA	3323	1/1	0.91	0.12	61,61,61,61	0
59	MG	DA	3123	1/1	0.91	0.16	32,32,32,32	0
59	MG	DA	3126	1/1	0.91	0.10	48,48,48,48	0
59	MG	DA	3251	1/1	0.91	0.15	44,44,44,44	0
59	MG	BA	3166	1/1	0.91	0.10	35,35,35,35	0
59	MG	CA	1606	1/1	0.91	0.27	52,52,52,52	0
59	MG	CA	1690	1/1	0.91	0.12	46,46,46,46	0
59	MG	AA	1695	1/1	0.91	0.07	55,55,55,55	0
59	MG	DA	3262	1/1	0.91	0.10	58,58,58,58	0
59	MG	BA	3009	1/1	0.91	0.12	30,30,30,30	0
59	MG	AA	1651	1/1	0.91	0.17	37,37,37,37	0
59	MG	DA	3270	1/1	0.91	0.12	61,61,61,61	0
59	MG	BA	3027	1/1	0.91	0.12	35,35,35,35	0
59	MG	AA	1654	1/1	0.91	0.06	100,100,100,100	0
59	MG	CA	1616	1/1	0.91	0.20	46,46,46,46	0
59	MG	DA	3011	1/1	0.91	0.20	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3035	1/1	0.91	0.11	22,22,22,22	0
59	MG	AA	1614	1/1	0.91	0.10	45,45,45,45	0
59	MG	CA	1622	1/1	0.91	0.18	49,49,49,49	0
59	MG	BA	3381	1/1	0.92	0.08	43,43,43,43	0
59	MG	CA	1645	1/1	0.92	0.05	27,27,27,27	0
59	MG	BA	3386	1/1	0.92	0.08	20,20,20,20	0
59	MG	DA	3186	1/1	0.92	0.04	41,41,41,41	0
59	MG	BA	3184	1/1	0.92	0.23	56,56,56,56	0
59	MG	BA	3303	1/1	0.92	0.31	91,91,91,91	0
59	MG	DA	3191	1/1	0.92	0.12	77,77,77,77	0
59	MG	BA	3192	1/1	0.92	0.10	29,29,29,29	0
59	MG	DA	3081	1/1	0.92	0.17	48,48,48,48	0
59	MG	CA	1653	1/1	0.92	0.10	46,46,46,46	0
59	MG	BA	3199	1/1	0.92	0.24	54,54,54,54	0
59	MG	DA	3207	1/1	0.92	0.48	69,69,69,69	0
59	MG	CA	1658	1/1	0.92	0.11	40,40,40,40	0
59	MG	CA	1665	1/1	0.92	0.13	34,34,34,34	0
59	MG	BA	3311	1/1	0.92	0.21	54,54,54,54	0
59	MG	AA	1658	1/1	0.92	0.26	42,42,42,42	0
59	MG	BA	3144	1/1	0.92	0.12	37,37,37,37	0
59	MG	DA	3214	1/1	0.92	0.05	34,34,34,34	0
59	MG	DA	3215	1/1	0.92	0.26	63,63,63,63	0
59	MG	CA	1671	1/1	0.92	0.19	54,54,54,54	0
59	MG	AA	1703	1/1	0.92	0.09	41,41,41,41	0
59	MG	BA	3321	1/1	0.92	0.08	51,51,51,51	0
59	MG	DA	3224	1/1	0.92	0.06	53,53,53,53	0
59	MG	BA	3099	1/1	0.92	0.38	51,51,51,51	0
59	MG	BA	3272	1/1	0.92	0.15	30,30,30,30	0
59	MG	AA	1729	1/1	0.92	0.17	57,57,57,57	0
59	MG	DA	3230	1/1	0.92	0.12	46,46,46,46	0
59	MG	BA	3103	1/1	0.92	0.23	65,65,65,65	0
59	MG	DA	3116	1/1	0.92	0.08	43,43,43,43	0
59	MG	BA	3106	1/1	0.92	0.16	29,29,29,29	0
59	MG	BA	3231	1/1	0.92	0.17	54,54,54,54	0
59	MG	BA	3337	1/1	0.92	0.14	61,61,61,61	0
59	MG	BA	3280	1/1	0.92	0.21	54,54,54,54	0
59	MG	AA	1672	1/1	0.92	0.14	51,51,51,51	0
59	MG	BA	3234	1/1	0.92	0.18	35,35,35,35	0
59	MG	BA	3235	1/1	0.92	0.18	51,51,51,51	0
59	MG	CV	102	1/1	0.92	0.13	44,44,44,44	0
59	MG	BA	3352	1/1	0.92	0.25	51,51,51,51	0
59	MG	AX	102	1/1	0.92	0.17	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3241	1/1	0.92	0.15	38,38,38,38	0
59	MG	DA	3149	1/1	0.92	0.19	42,42,42,42	0
59	MG	AA	1670	1/1	0.92	0.16	36,36,36,36	0
59	MG	BA	3127	1/1	0.92	0.06	48,48,48,48	0
59	MG	DA	3162	1/1	0.92	0.08	40,40,40,40	0
59	MG	BA	3247	1/1	0.92	0.16	29,29,29,29	0
59	MG	BA	3371	1/1	0.92	0.17	57,57,57,57	0
59	MG	DA	3267	1/1	0.92	0.24	53,53,53,53	0
59	MG	DA	3166	1/1	0.92	0.10	41,41,41,41	0
59	MG	DA	3169	1/1	0.92	0.07	37,37,37,37	0
59	MG	DA	3036	1/1	0.92	0.21	31,31,31,31	0
59	MG	DA	3274	1/1	0.92	0.12	62,62,62,62	0
59	MG	DB	201	1/1	0.92	0.07	44,44,44,44	0
59	MG	CA	1633	1/1	0.92	0.15	38,38,38,38	0
59	MG	DA	3043	1/1	0.92	0.17	48,48,48,48	0
59	MG	BA	3248	1/1	0.92	0.15	37,37,37,37	0
59	MG	BA	3037	1/1	0.92	0.21	27,27,27,27	0
59	MG	D6	101	1/1	0.92	0.12	37,37,37,37	0
59	MG	BA	3379	1/1	0.92	0.18	52,52,52,52	0
59	MG	DA	3168	1/1	0.93	0.12	43,43,43,43	0
59	MG	BA	3056	1/1	0.93	0.27	59,59,59,59	0
59	MG	BA	3318	1/1	0.93	0.13	41,41,41,41	0
59	MG	BA	3319	1/1	0.93	0.15	25,25,25,25	0
59	MG	BA	3067	1/1	0.93	0.22	36,36,36,36	0
59	MG	BA	3249	1/1	0.93	0.28	50,50,50,50	0
59	MG	AA	1639	1/1	0.93	0.08	54,54,54,54	0
59	MG	DA	3035	1/1	0.93	0.43	63,63,63,63	0
59	MG	BA	3088	1/1	0.93	0.18	22,22,22,22	0
59	MG	BA	3095	1/1	0.93	0.12	30,30,30,30	0
59	MG	BA	3326	1/1	0.93	0.06	35,35,35,35	0
59	MG	DA	3185	1/1	0.93	0.06	42,42,42,42	0
59	MG	DA	3044	1/1	0.93	0.11	22,22,22,22	0
59	MG	BA	3329	1/1	0.93	0.06	48,48,48,48	0
59	MG	DA	3049	1/1	0.93	0.11	41,41,41,41	0
59	MG	AA	1635	1/1	0.93	0.10	46,46,46,46	0
59	MG	DA	3192	1/1	0.93	0.15	39,39,39,39	0
59	MG	AA	1687	1/1	0.93	0.05	27,27,27,27	0
59	MG	DA	3055	1/1	0.93	0.17	42,42,42,42	0
59	MG	BA	3187	1/1	0.93	0.20	35,35,35,35	0
59	MG	CA	1629	1/1	0.93	0.16	52,52,52,52	0
59	MG	AA	1628	1/1	0.93	0.21	46,46,46,46	0
59	MG	BA	3193	1/1	0.93	0.10	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3271	1/1	0.93	0.17	64,64,64,64	0
59	MG	BA	3196	1/1	0.93	0.18	49,49,49,49	0
59	MG	BA	3197	1/1	0.93	0.29	45,45,45,45	0
59	MG	BA	3348	1/1	0.93	0.20	62,62,62,62	0
59	MG	BA	3349	1/1	0.93	0.18	53,53,53,53	0
59	MG	AA	1726	1/1	0.93	0.10	32,32,32,32	0
59	MG	DA	3089	1/1	0.93	0.24	26,26,26,26	0
59	MG	BA	3200	1/1	0.93	0.10	51,51,51,51	0
59	MG	DA	3092	1/1	0.93	0.24	51,51,51,51	0
59	MG	DA	3223	1/1	0.93	0.22	61,61,61,61	0
59	MG	BA	3202	1/1	0.93	0.11	28,28,28,28	0
59	MG	BA	3359	1/1	0.93	0.12	51,51,51,51	0
59	MG	BA	3278	1/1	0.93	0.25	50,50,50,50	0
59	MG	AW	102	1/1	0.93	0.04	53,53,53,53	0
59	MG	BA	3283	1/1	0.93	0.19	46,46,46,46	0
59	MG	BA	3008	1/1	0.93	0.15	13,13,13,13	0
59	MG	CA	1659	1/1	0.93	0.13	64,64,64,64	0
59	MG	AA	1690	1/1	0.93	0.10	40,40,40,40	0
59	MG	BA	3117	1/1	0.93	0.17	38,38,38,38	0
59	MG	BA	3223	1/1	0.93	0.10	46,46,46,46	0
59	MG	BA	3120	1/1	0.93	0.08	49,49,49,49	0
59	MG	DA	3118	1/1	0.93	0.19	41,41,41,41	0
59	MG	AA	1660	1/1	0.93	0.26	40,40,40,40	0
59	MG	DA	3243	1/1	0.93	0.17	35,35,35,35	0
59	MG	BA	3294	1/1	0.93	0.37	72,72,72,72	0
59	MG	DA	3121	1/1	0.93	0.07	37,37,37,37	0
59	MG	BA	3019	1/1	0.93	0.22	21,21,21,21	0
59	MG	BA	3026	1/1	0.93	0.16	29,29,29,29	0
59	MG	BA	3394	1/1	0.93	0.11	49,49,49,49	0
59	MG	AA	1644	1/1	0.93	0.20	48,48,48,48	0
59	MG	DA	3134	1/1	0.93	0.14	42,42,42,42	0
59	MG	BF	302	1/1	0.93	0.05	26,26,26,26	0
59	MG	BA	3156	1/1	0.93	0.13	25,25,25,25	0
59	MG	DA	3263	1/1	0.93	0.29	62,62,62,62	0
59	MG	DA	3141	1/1	0.93	0.12	46,46,46,46	0
59	MG	AA	1730	1/1	0.93	0.11	60,60,60,60	0
59	MG	BA	3238	1/1	0.93	0.10	26,26,26,26	0
59	MG	DA	3268	1/1	0.93	0.19	47,47,47,47	0
59	MG	BA	3161	1/1	0.93	0.20	16,16,16,16	0
59	MG	AA	1733	1/1	0.93	0.05	30,30,30,30	0
59	MG	DA	3272	1/1	0.93	0.26	60,60,60,60	0
59	MG	AA	1663	1/1	0.93	0.26	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3153	1/1	0.93	0.17	28,28,28,28	0
59	MG	DA	3275	1/1	0.93	0.19	54,54,54,54	0
59	MG	CA	1601	1/1	0.93	0.14	29,29,29,29	0
59	MG	DA	3160	1/1	0.93	0.13	28,28,28,28	0
59	MG	CV	101	1/1	0.93	0.19	36,36,36,36	0
59	MG	BA	3313	1/1	0.93	0.24	55,55,55,55	0
59	MG	AA	1622	1/1	0.93	0.22	44,44,44,44	0
59	MG	D5	101	1/1	0.93	0.09	28,28,28,28	0
59	MG	DA	3004	1/1	0.93	0.16	54,54,54,54	0
59	MG	DA	3167	1/1	0.93	0.11	42,42,42,42	0
59	MG	BA	3053	1/1	0.94	0.14	11,11,11,11	0
59	MG	BA	3204	1/1	0.94	0.03	2,2,2,2	0
59	MG	BA	3128	1/1	0.94	0.17	34,34,34,34	0
59	MG	BA	3334	1/1	0.94	0.07	32,32,32,32	0
59	MG	BA	3208	1/1	0.94	0.22	54,54,54,54	0
59	MG	BA	3210	1/1	0.94	0.14	57,57,57,57	0
59	MG	AA	1648	1/1	0.94	0.20	48,48,48,48	0
59	MG	BA	3214	1/1	0.94	0.22	87,87,87,87	0
59	MG	DA	3182	1/1	0.94	0.10	33,33,33,33	0
59	MG	BA	3133	1/1	0.94	0.05	20,20,20,20	0
59	MG	AA	1678	1/1	0.94	0.07	52,52,52,52	0
59	MG	DA	3054	1/1	0.94	0.11	42,42,42,42	0
59	MG	CA	1632	1/1	0.94	0.22	47,47,47,47	0
59	MG	DA	3187	1/1	0.94	0.23	51,51,51,51	0
59	MG	DA	3064	1/1	0.94	0.12	48,48,48,48	0
59	MG	DA	3066	1/1	0.94	0.14	31,31,31,31	0
59	MG	BA	3281	1/1	0.94	0.18	41,41,41,41	0
59	MG	BA	3351	1/1	0.94	0.22	60,60,60,60	0
59	MG	BA	3282	1/1	0.94	0.05	48,48,48,48	0
59	MG	DA	3196	1/1	0.94	0.25	48,48,48,48	0
59	MG	CA	1640	1/1	0.94	0.08	47,47,47,47	0
59	MG	DA	3198	1/1	0.94	0.27	56,56,56,56	0
59	MG	CA	1641	1/1	0.94	0.12	28,28,28,28	0
59	MG	BA	3061	1/1	0.94	0.18	21,21,21,21	0
59	MG	DA	3204	1/1	0.94	0.08	41,41,41,41	0
59	MG	AA	1606	1/1	0.94	0.17	63,63,63,63	0
59	MG	BA	3078	1/1	0.94	0.06	20,20,20,20	0
59	MG	BA	3229	1/1	0.94	0.09	37,37,37,37	0
59	MG	BA	3079	1/1	0.94	0.12	23,23,23,23	0
59	MG	BA	3003	1/1	0.94	0.14	42,42,42,42	0
59	MG	BA	3087	1/1	0.94	0.08	39,39,39,39	0
59	MG	AA	1617	1/1	0.94	0.07	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3093	1/1	0.94	0.20	40,40,40,40	0
59	MG	DA	3216	1/1	0.94	0.09	35,35,35,35	0
59	MG	BA	3375	1/1	0.94	0.16	38,38,38,38	0
59	MG	DA	3096	1/1	0.94	0.15	38,38,38,38	0
59	MG	BA	3091	1/1	0.94	0.13	34,34,34,34	0
59	MG	DA	3221	1/1	0.94	0.14	59,59,59,59	0
59	MG	DA	3222	1/1	0.94	0.12	50,50,50,50	0
59	MG	BA	3172	1/1	0.94	0.19	40,40,40,40	0
59	MG	BA	3380	1/1	0.94	0.11	47,47,47,47	0
59	MG	AA	1732	1/1	0.94	0.06	32,32,32,32	0
59	MG	BA	3383	1/1	0.94	0.08	36,36,36,36	0
59	MG	AA	1653	1/1	0.94	0.15	47,47,47,47	0
59	MG	BA	3300	1/1	0.94	0.14	40,40,40,40	0
59	MG	BA	3242	1/1	0.94	0.24	44,44,44,44	0
59	MG	AA	1702	1/1	0.94	0.32	59,59,59,59	0
59	MG	BA	3306	1/1	0.94	0.10	29,29,29,29	0
59	MG	CA	1677	1/1	0.94	0.10	53,53,53,53	0
59	MG	CA	1681	1/1	0.94	0.07	58,58,58,58	0
59	MG	AW	107	1/1	0.94	0.05	41,41,41,41	0
59	MG	BE	301	1/1	0.94	0.11	12,12,12,12	0
59	MG	DA	3240	1/1	0.94	0.06	49,49,49,49	0
59	MG	CA	1684	1/1	0.94	0.23	49,49,49,49	0
59	MG	DA	3242	1/1	0.94	0.13	34,34,34,34	0
59	MG	BA	3104	1/1	0.94	0.22	52,52,52,52	0
59	MG	DA	3244	1/1	0.94	0.10	33,33,33,33	0
59	MG	CA	1687	1/1	0.94	0.19	56,56,56,56	0
59	MG	DA	3128	1/1	0.94	0.12	26,26,26,26	0
59	MG	DA	3129	1/1	0.94	0.15	35,35,35,35	0
59	MG	AA	1619	1/1	0.94	0.27	47,47,47,47	0
59	MG	DA	3133	1/1	0.94	0.05	69,69,69,69	0
59	MG	BA	3185	1/1	0.94	0.13	62,62,62,62	0
59	MG	BA	3251	1/1	0.94	0.19	34,34,34,34	0
59	MG	BA	3316	1/1	0.94	0.40	68,68,68,68	0
59	MG	DA	3261	1/1	0.94	0.17	50,50,50,50	0
59	MG	DA	3137	1/1	0.94	0.05	28,28,28,28	0
59	MG	BA	3253	1/1	0.94	0.13	56,56,56,56	0
59	MG	BA	3109	1/1	0.94	0.10	34,34,34,34	0
59	MG	B5	101	1/1	0.94	0.19	37,37,37,37	0
59	MG	AA	1724	1/1	0.94	0.15	56,56,56,56	0
59	MG	DA	3147	1/1	0.94	0.20	44,44,44,44	0
59	MG	AA	1674	1/1	0.94	0.05	42,42,42,42	0
59	MG	AO	101	1/1	0.94	0.10	62,62,62,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CX	102	1/1	0.94	0.39	78,78,78,78	0
59	MG	DA	3154	1/1	0.94	0.13	64,64,64,64	0
59	MG	DA	3155	1/1	0.94	0.12	56,56,56,56	0
59	MG	DA	3156	1/1	0.94	0.19	28,28,28,28	0
59	MG	DA	3002	1/1	0.94	0.10	31,31,31,31	0
59	MG	AA	1642	1/1	0.94	0.08	55,55,55,55	0
59	MG	BA	3264	1/1	0.94	0.18	34,34,34,34	0
59	MG	BA	3119	1/1	0.94	0.10	20,20,20,20	0
59	MG	DA	3013	1/1	0.94	0.17	32,32,32,32	0
59	MG	BA	3268	1/1	0.94	0.30	44,44,44,44	0
59	MG	BA	3328	1/1	0.94	0.11	35,35,35,35	0
59	MG	BA	3052	1/1	0.94	0.23	37,37,37,37	0
59	MG	AA	1656	1/1	0.95	0.07	42,42,42,42	0
59	MG	BA	3080	1/1	0.95	0.08	26,26,26,26	0
59	MG	CX	103	1/1	0.95	0.06	50,50,50,50	0
59	MG	BA	3171	1/1	0.95	0.20	51,51,51,51	0
59	MG	DA	3003	1/1	0.95	0.16	36,36,36,36	0
59	MG	AA	1688	1/1	0.95	0.23	47,47,47,47	0
59	MG	DA	3005	1/1	0.95	0.22	50,50,50,50	0
59	MG	DA	3006	1/1	0.95	0.13	20,20,20,20	0
59	MG	BA	3005	1/1	0.95	0.03	17,17,17,17	0
59	MG	DA	3170	1/1	0.95	0.06	52,52,52,52	0
59	MG	AA	1601	1/1	0.95	0.06	38,38,38,38	0
59	MG	BA	3259	1/1	0.95	0.07	35,35,35,35	0
59	MG	BA	3090	1/1	0.95	0.10	32,32,32,32	0
59	MG	AA	1675	1/1	0.95	0.25	38,38,38,38	0
59	MG	BA	3010	1/1	0.95	0.16	29,29,29,29	0
59	MG	DA	3027	1/1	0.95	0.17	28,28,28,28	0
59	MG	BA	3327	1/1	0.95	0.22	44,44,44,44	0
59	MG	DA	3029	1/1	0.95	0.09	34,34,34,34	0
59	MG	BA	3097	1/1	0.95	0.04	21,21,21,21	0
59	MG	BA	3012	1/1	0.95	0.16	31,31,31,31	0
59	MG	BA	3266	1/1	0.95	0.14	27,27,27,27	0
59	MG	BA	3100	1/1	0.95	0.17	22,22,22,22	0
59	MG	CA	1617	1/1	0.95	0.10	39,39,39,39	0
59	MG	DA	3188	1/1	0.95	0.13	40,40,40,40	0
59	MG	AA	1607	1/1	0.95	0.29	43,43,43,43	0
59	MG	DA	3048	1/1	0.95	0.12	48,48,48,48	0
59	MG	AA	1652	1/1	0.95	0.27	55,55,55,55	0
59	MG	BA	3335	1/1	0.95	0.32	52,52,52,52	0
59	MG	DA	3051	1/1	0.95	0.32	51,51,51,51	0
59	MG	BA	3336	1/1	0.95	0.16	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3020	1/1	0.95	0.13	22,22,22,22	0
59	MG	CA	1628	1/1	0.95	0.04	27,27,27,27	0
59	MG	BA	3024	1/1	0.95	0.07	22,22,22,22	0
59	MG	DA	3201	1/1	0.95	0.07	33,33,33,33	0
59	MG	AA	1694	1/1	0.95	0.12	24,24,24,24	0
59	MG	DA	3067	1/1	0.95	0.19	50,50,50,50	0
59	MG	AA	1669	1/1	0.95	0.10	36,36,36,36	0
59	MG	BA	3028	1/1	0.95	0.18	41,41,41,41	0
59	MG	BA	3029	1/1	0.95	0.23	23,23,23,23	0
59	MG	BA	3115	1/1	0.95	0.16	22,22,22,22	0
59	MG	BA	3116	1/1	0.95	0.11	54,54,54,54	0
59	MG	DA	3212	1/1	0.95	0.27	61,61,61,61	0
59	MG	BA	3031	1/1	0.95	0.12	12,12,12,12	0
59	MG	DA	3079	1/1	0.95	0.09	16,16,16,16	0
59	MG	AX	101	1/1	0.95	0.17	57,57,57,57	0
59	MG	AA	1715	1/1	0.95	0.08	34,34,34,34	0
59	MG	BA	3122	1/1	0.95	0.11	38,38,38,38	0
59	MG	DA	3084	1/1	0.95	0.09	48,48,48,48	0
59	MG	DA	3219	1/1	0.95	0.16	40,40,40,40	0
59	MG	CA	1644	1/1	0.95	0.43	68,68,68,68	0
59	MG	BA	3286	1/1	0.95	0.14	26,26,26,26	0
59	MG	BA	3361	1/1	0.95	0.06	25,25,25,25	0
59	MG	CA	1648	1/1	0.95	0.10	56,56,56,56	0
59	MG	CA	1649	1/1	0.95	0.04	48,48,48,48	0
59	MG	DA	3225	1/1	0.95	0.28	55,55,55,55	0
59	MG	DA	3094	1/1	0.95	0.16	27,27,27,27	0
59	MG	BA	3362	1/1	0.95	0.20	51,51,51,51	0
59	MG	BA	3363	1/1	0.95	0.07	56,56,56,56	0
59	MG	AX	104	1/1	0.95	0.23	45,45,45,45	0
59	MG	BA	3220	1/1	0.95	0.26	52,52,52,52	0
59	MG	DA	3099	1/1	0.95	0.12	45,45,45,45	0
59	MG	DA	3100	1/1	0.95	0.05	57,57,57,57	0
59	MG	CA	1655	1/1	0.95	0.15	41,41,41,41	0
59	MG	CA	1656	1/1	0.95	0.19	51,51,51,51	0
59	MG	BA	3370	1/1	0.95	0.10	28,28,28,28	0
59	MG	DA	3106	1/1	0.95	0.20	51,51,51,51	0
59	MG	BA	3042	1/1	0.95	0.10	22,22,22,22	0
59	MG	BA	3372	1/1	0.95	0.10	26,26,26,26	0
59	MG	CA	1663	1/1	0.95	0.08	50,50,50,50	0
59	MG	AA	1633	1/1	0.95	0.04	37,37,37,37	0
59	MG	AF	201	1/1	0.95	0.07	39,39,39,39	0
59	MG	CA	1668	1/1	0.95	0.04	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3228	1/1	0.95	0.16	21,21,21,21	0
59	MG	DA	3248	1/1	0.95	0.28	60,60,60,60	0
59	MG	AA	1717	1/1	0.95	0.17	50,50,50,50	0
59	MG	BA	3135	1/1	0.95	0.13	38,38,38,38	0
59	MG	BA	3139	1/1	0.95	0.05	15,15,15,15	0
59	MG	DA	3125	1/1	0.95	0.25	59,59,59,59	0
59	MG	CA	1673	1/1	0.95	0.04	71,71,71,71	0
59	MG	DA	3258	1/1	0.95	0.06	29,29,29,29	0
59	MG	AA	1611	1/1	0.95	0.13	52,52,52,52	0
59	MG	BA	3384	1/1	0.95	0.11	39,39,39,39	0
59	MG	BA	3147	1/1	0.95	0.19	33,33,33,33	0
59	MG	DA	3130	1/1	0.95	0.17	27,27,27,27	0
59	MG	DA	3264	1/1	0.95	0.11	41,41,41,41	0
59	MG	CA	1679	1/1	0.95	0.15	46,46,46,46	0
59	MG	CA	1680	1/1	0.95	0.13	59,59,59,59	0
59	MG	BA	3149	1/1	0.95	0.15	31,31,31,31	0
59	MG	BA	3151	1/1	0.95	0.16	22,22,22,22	0
59	MG	DA	3269	1/1	0.95	0.04	43,43,43,43	0
59	MG	BA	3391	1/1	0.95	0.11	31,31,31,31	0
59	MG	BA	3305	1/1	0.95	0.16	32,32,32,32	0
59	MG	AL	201	1/1	0.95	0.13	44,44,44,44	0
59	MG	DA	3142	1/1	0.95	0.09	44,44,44,44	0
59	MG	BA	3396	1/1	0.95	0.04	37,37,37,37	0
59	MG	AA	1686	1/1	0.95	0.09	58,58,58,58	0
59	MG	BA	3072	1/1	0.95	0.14	16,16,16,16	0
59	MG	BF	301	1/1	0.95	0.10	37,37,37,37	0
59	MG	BA	3162	1/1	0.95	0.27	66,66,66,66	0
59	MG	BA	3075	1/1	0.95	0.17	32,32,32,32	0
59	MG	DE	303	1/1	0.95	0.07	32,32,32,32	0
59	MG	BN	201	1/1	0.95	0.14	67,67,67,67	0
59	MG	BA	3314	1/1	0.95	0.22	68,68,68,68	0
59	MG	D5	102	1/1	0.95	0.08	91,91,91,91	0
59	MG	BR	201	1/1	0.95	0.25	41,41,41,41	0
60	ZN	B4	101	1/1	0.95	0.09	117,117,117,117	0
59	MG	AA	1701	1/1	0.95	0.09	36,36,36,36	0
59	MG	BA	3121	1/1	0.96	0.09	38,38,38,38	0
59	MG	BA	3188	1/1	0.96	0.19	22,22,22,22	0
59	MG	DA	3021	1/1	0.96	0.11	28,28,28,28	0
59	MG	DA	3024	1/1	0.96	0.06	29,29,29,29	0
59	MG	BA	3189	1/1	0.96	0.17	18,18,18,18	0
59	MG	BA	3191	1/1	0.96	0.07	31,31,31,31	0
59	MG	BA	3076	1/1	0.96	0.22	34,34,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3031	1/1	0.96	0.12	31,31,31,31	0
59	MG	DA	3034	1/1	0.96	0.04	30,30,30,30	0
59	MG	DA	3174	1/1	0.96	0.04	47,47,47,47	0
59	MG	BA	3123	1/1	0.96	0.11	45,45,45,45	0
59	MG	BA	3195	1/1	0.96	0.11	79,79,79,79	0
59	MG	DA	3037	1/1	0.96	0.10	26,26,26,26	0
59	MG	DA	3180	1/1	0.96	0.17	27,27,27,27	0
59	MG	BA	3339	1/1	0.96	0.28	66,66,66,66	0
59	MG	BA	3126	1/1	0.96	0.14	52,52,52,52	0
59	MG	CA	1625	1/1	0.96	0.39	54,54,54,54	0
59	MG	AA	1697	1/1	0.96	0.10	73,73,73,73	0
59	MG	CA	1627	1/1	0.96	0.10	62,62,62,62	0
59	MG	BA	3345	1/1	0.96	0.07	31,31,31,31	0
59	MG	BA	3346	1/1	0.96	0.16	35,35,35,35	0
59	MG	AA	1673	1/1	0.96	0.09	35,35,35,35	0
59	MG	BA	3273	1/1	0.96	0.06	26,26,26,26	0
59	MG	BA	3131	1/1	0.96	0.35	68,68,68,68	0
59	MG	BA	3350	1/1	0.96	0.05	20,20,20,20	0
59	MG	DA	3056	1/1	0.96	0.09	31,31,31,31	0
59	MG	DA	3058	1/1	0.96	0.05	33,33,33,33	0
59	MG	DA	3194	1/1	0.96	0.09	52,52,52,52	0
59	MG	DA	3061	1/1	0.96	0.15	28,28,28,28	0
59	MG	DA	3063	1/1	0.96	0.07	53,53,53,53	0
59	MG	CA	1636	1/1	0.96	0.17	55,55,55,55	0
59	MG	AA	1623	1/1	0.96	0.09	27,27,27,27	0
59	MG	BA	3082	1/1	0.96	0.06	15,15,15,15	0
59	MG	AA	1643	1/1	0.96	0.12	51,51,51,51	0
59	MG	BA	3354	1/1	0.96	0.13	41,41,41,41	0
59	MG	DA	3205	1/1	0.96	0.10	27,27,27,27	0
59	MG	BA	3206	1/1	0.96	0.18	36,36,36,36	0
59	MG	AA	1613	1/1	0.96	0.05	51,51,51,51	0
59	MG	AA	1609	1/1	0.96	0.07	23,23,23,23	0
59	MG	BA	3211	1/1	0.96	0.03	16,16,16,16	0
59	MG	CA	1646	1/1	0.96	0.19	40,40,40,40	0
59	MG	BA	3140	1/1	0.96	0.09	30,30,30,30	0
59	MG	BA	3142	1/1	0.96	0.07	18,18,18,18	0
59	MG	BA	3365	1/1	0.96	0.13	36,36,36,36	0
59	MG	BA	3033	1/1	0.96	0.09	26,26,26,26	0
59	MG	DA	3085	1/1	0.96	0.10	22,22,22,22	0
59	MG	DA	3087	1/1	0.96	0.40	59,59,59,59	0
59	MG	BA	3145	1/1	0.96	0.13	13,13,13,13	0
59	MG	BA	3369	1/1	0.96	0.22	38,38,38,38	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3090	1/1	0.96	0.12	24,24,24,24	0
59	MG	AA	1718	1/1	0.96	0.12	36,36,36,36	0
59	MG	CA	1654	1/1	0.96	0.12	63,63,63,63	0
59	MG	BA	3148	1/1	0.96	0.14	27,27,27,27	0
59	MG	AA	1621	1/1	0.96	0.20	54,54,54,54	0
59	MG	BA	3292	1/1	0.96	0.17	40,40,40,40	0
59	MG	BA	3374	1/1	0.96	0.09	31,31,31,31	0
59	MG	BA	3225	1/1	0.96	0.10	43,43,43,43	0
59	MG	CA	1660	1/1	0.96	0.10	45,45,45,45	0
59	MG	BA	3226	1/1	0.96	0.05	33,33,33,33	0
59	MG	DA	3231	1/1	0.96	0.15	43,43,43,43	0
59	MG	CA	1664	1/1	0.96	0.14	44,44,44,44	0
59	MG	DA	3101	1/1	0.96	0.04	28,28,28,28	0
59	MG	BA	3377	1/1	0.96	0.28	43,43,43,43	0
59	MG	BA	3036	1/1	0.96	0.18	20,20,20,20	0
59	MG	BA	3007	1/1	0.96	0.18	39,39,39,39	0
59	MG	DA	3237	1/1	0.96	0.04	39,39,39,39	0
59	MG	BA	3157	1/1	0.96	0.04	42,42,42,42	0
59	MG	BA	3039	1/1	0.96	0.18	18,18,18,18	0
59	MG	AA	1706	1/1	0.96	0.13	43,43,43,43	0
59	MG	BA	3232	1/1	0.96	0.20	25,25,25,25	0
59	MG	BA	3387	1/1	0.96	0.10	46,46,46,46	0
59	MG	AH	201	1/1	0.96	0.14	31,31,31,31	0
59	MG	BA	3304	1/1	0.96	0.16	22,22,22,22	0
59	MG	AA	1723	1/1	0.96	0.05	36,36,36,36	0
59	MG	AX	103	1/1	0.96	0.10	32,32,32,32	0
59	MG	BA	3393	1/1	0.96	0.05	40,40,40,40	0
59	MG	DA	3249	1/1	0.96	0.15	54,54,54,54	0
59	MG	DA	3122	1/1	0.96	0.09	31,31,31,31	0
59	MG	BA	3237	1/1	0.96	0.27	32,32,32,32	0
59	MG	DA	3252	1/1	0.96	0.19	47,47,47,47	0
59	MG	BA	3395	1/1	0.96	0.05	46,46,46,46	0
59	MG	BA	3108	1/1	0.96	0.07	44,44,44,44	0
59	MG	DA	3255	1/1	0.96	0.04	13,13,13,13	0
59	MG	BA	3310	1/1	0.96	0.25	55,55,55,55	0
59	MG	BA	3398	1/1	0.96	0.22	66,66,66,66	0
59	MG	BA	3400	1/1	0.96	0.13	39,39,39,39	0
59	MG	BA	3168	1/1	0.96	0.04	37,37,37,37	0
59	MG	DA	3131	1/1	0.96	0.17	38,38,38,38	0
59	MG	BA	3312	1/1	0.96	0.09	42,42,42,42	0
59	MG	BA	3013	1/1	0.96	0.08	6,6,6,6	0
59	MG	BA	3057	1/1	0.96	0.06	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3058	1/1	0.96	0.12	20,20,20,20	0
59	MG	BA	3244	1/1	0.96	0.07	31,31,31,31	0
59	MG	CE	202	1/1	0.96	0.13	40,40,40,40	0
59	MG	BA	3245	1/1	0.96	0.33	48,48,48,48	0
59	MG	BU	201	1/1	0.96	0.16	22,22,22,22	0
59	MG	BA	3015	1/1	0.96	0.19	25,25,25,25	0
59	MG	BA	3064	1/1	0.96	0.15	32,32,32,32	0
59	MG	AA	1612	1/1	0.96	0.04	32,32,32,32	0
59	MG	BA	3180	1/1	0.96	0.18	22,22,22,22	0
59	MG	BA	3071	1/1	0.96	0.05	42,42,42,42	0
59	MG	DA	3150	1/1	0.96	0.04	43,43,43,43	0
59	MG	BA	3252	1/1	0.96	0.04	18,18,18,18	0
59	MG	BA	3118	1/1	0.96	0.11	18,18,18,18	0
59	MG	BA	3183	1/1	0.96	0.07	37,37,37,37	0
59	MG	CA	1604	1/1	0.96	0.07	21,21,21,21	0
59	MG	BA	3256	1/1	0.96	0.21	56,56,56,56	0
59	MG	AA	1684	1/1	0.96	0.03	42,42,42,42	0
59	MG	DA	3158	1/1	0.96	0.21	38,38,38,38	0
59	MG	DA	3012	1/1	0.96	0.07	33,33,33,33	0
59	MG	AA	1655	1/1	0.96	0.20	28,28,28,28	0
59	MG	BA	3186	1/1	0.96	0.15	30,30,30,30	0
59	MG	CA	1667	1/1	0.97	0.19	37,37,37,37	0
59	MG	DA	3177	1/1	0.97	0.14	29,29,29,29	0
59	MG	DA	3071	1/1	0.97	0.09	27,27,27,27	0
59	MG	DA	3072	1/1	0.97	0.09	28,28,28,28	0
59	MG	DA	3073	1/1	0.97	0.07	18,18,18,18	0
59	MG	BA	3221	1/1	0.97	0.04	25,25,25,25	0
59	MG	DA	3075	1/1	0.97	0.08	32,32,32,32	0
59	MG	BA	3060	1/1	0.97	0.04	13,13,13,13	0
59	MG	AA	1668	1/1	0.97	0.09	194,194,194,194	0
59	MG	BA	3163	1/1	0.97	0.03	22,22,22,22	0
59	MG	AA	1692	1/1	0.97	0.04	55,55,55,55	0
59	MG	DA	3080	1/1	0.97	0.15	41,41,41,41	0
59	MG	AA	1662	1/1	0.97	0.14	23,23,23,23	0
59	MG	BA	3285	1/1	0.97	0.04	28,28,28,28	0
59	MG	BA	3114	1/1	0.97	0.40	53,53,53,53	0
59	MG	CA	1676	1/1	0.97	0.06	55,55,55,55	0
59	MG	BA	3068	1/1	0.97	0.11	15,15,15,15	0
59	MG	DA	3086	1/1	0.97	0.14	26,26,26,26	0
59	MG	DA	3195	1/1	0.97	0.10	38,38,38,38	0
59	MG	BA	3069	1/1	0.97	0.12	20,20,20,20	0
59	MG	BA	3289	1/1	0.97	0.16	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3014	1/1	0.97	0.09	63,63,63,63	0
59	MG	DA	3199	1/1	0.97	0.20	38,38,38,38	0
59	MG	AA	1616	1/1	0.97	0.04	16,16,16,16	0
59	MG	AA	1610	1/1	0.97	0.04	29,29,29,29	0
59	MG	BA	3017	1/1	0.97	0.08	14,14,14,14	0
59	MG	BA	3355	1/1	0.97	0.07	33,33,33,33	0
59	MG	BA	3038	1/1	0.97	0.14	20,20,20,20	0
59	MG	CA	1610	1/1	0.97	0.12	27,27,27,27	0
59	MG	BA	3358	1/1	0.97	0.08	49,49,49,49	0
59	MG	CA	1613	1/1	0.97	0.05	66,66,66,66	0
59	MG	BA	3295	1/1	0.97	0.06	47,47,47,47	0
59	MG	CA	1615	1/1	0.97	0.25	51,51,51,51	0
59	MG	BA	3178	1/1	0.97	0.07	11,11,11,11	0
59	MG	BA	3018	1/1	0.97	0.08	23,23,23,23	0
59	MG	BA	3239	1/1	0.97	0.10	25,25,25,25	0
59	MG	BA	3041	1/1	0.97	0.05	20,20,20,20	0
59	MG	CA	1620	1/1	0.97	0.14	40,40,40,40	0
59	MG	DA	3105	1/1	0.97	0.10	28,28,28,28	0
59	MG	CA	1621	1/1	0.97	0.23	42,42,42,42	0
59	MG	DA	3107	1/1	0.97	0.04	32,32,32,32	0
59	MG	AA	1696	1/1	0.97	0.15	34,34,34,34	0
59	MG	BA	3083	1/1	0.97	0.12	6,6,6,6	0
59	MG	DA	3110	1/1	0.97	0.03	38,38,38,38	0
59	MG	CA	1624	1/1	0.97	0.13	24,24,24,24	0
59	MG	BA	3043	1/1	0.97	0.13	22,22,22,22	0
59	MG	DA	3113	1/1	0.97	0.05	49,49,49,49	0
59	MG	DA	3115	1/1	0.97	0.06	59,59,59,59	0
59	MG	BA	3085	1/1	0.97	0.18	18,18,18,18	0
59	MG	BA	3086	1/1	0.97	0.17	46,46,46,46	0
59	MG	BA	3044	1/1	0.97	0.16	28,28,28,28	0
59	MG	DA	3007	1/1	0.97	0.28	42,42,42,42	0
59	MG	DA	3008	1/1	0.97	0.06	39,39,39,39	0
59	MG	BA	3047	1/1	0.97	0.20	30,30,30,30	0
59	MG	BA	3089	1/1	0.97	0.06	55,55,55,55	0
59	MG	DA	3124	1/1	0.97	0.03	43,43,43,43	0
59	MG	BA	3309	1/1	0.97	0.07	41,41,41,41	0
59	MG	BA	3138	1/1	0.97	0.09	17,17,17,17	0
59	MG	BA	3049	1/1	0.97	0.04	12,12,12,12	0
59	MG	CA	1635	1/1	0.97	0.10	32,32,32,32	0
59	MG	BA	3050	1/1	0.97	0.12	4,4,4,4	0
59	MG	BA	3378	1/1	0.97	0.06	25,25,25,25	0
59	MG	BA	3141	1/1	0.97	0.12	1,1,1,1	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3026	1/1	0.97	0.07	36,36,36,36	0
59	MG	BA	3094	1/1	0.97	0.04	12,12,12,12	0
59	MG	BA	3143	1/1	0.97	0.25	37,37,37,37	0
59	MG	BA	3382	1/1	0.97	0.14	37,37,37,37	0
59	MG	BA	3051	1/1	0.97	0.09	1,1,1,1	0
59	MG	AA	1618	1/1	0.97	0.15	22,22,22,22	0
59	MG	DA	3139	1/1	0.97	0.03	18,18,18,18	0
59	MG	DA	3140	1/1	0.97	0.14	38,38,38,38	0
59	MG	BA	3201	1/1	0.97	0.09	111,111,111,111	0
59	MG	BA	3023	1/1	0.97	0.11	23,23,23,23	0
59	MG	DA	3143	1/1	0.97	0.09	30,30,30,30	0
59	MG	BA	3388	1/1	0.97	0.07	13,13,13,13	0
59	MG	DA	3038	1/1	0.97	0.05	25,25,25,25	0
59	MG	AA	1625	1/1	0.97	0.17	32,32,32,32	0
59	MG	DA	3259	1/1	0.97	0.21	43,43,43,43	0
59	MG	DA	3041	1/1	0.97	0.07	7,7,7,7	0
59	MG	DA	3148	1/1	0.97	0.31	40,40,40,40	0
59	MG	DA	3042	1/1	0.97	0.18	41,41,41,41	0
59	MG	BA	3263	1/1	0.97	0.06	37,37,37,37	0
59	MG	DA	3151	1/1	0.97	0.03	14,14,14,14	0
59	MG	BA	3055	1/1	0.97	0.04	21,21,21,21	0
59	MG	AA	1722	1/1	0.97	0.04	35,35,35,35	0
59	MG	BA	3324	1/1	0.97	0.20	35,35,35,35	0
59	MG	BA	3207	1/1	0.97	0.07	24,24,24,24	0
59	MG	BA	3152	1/1	0.97	0.13	18,18,18,18	0
59	MG	BA	3209	1/1	0.97	0.06	27,27,27,27	0
59	MG	DA	3052	1/1	0.97	0.08	30,30,30,30	0
59	MG	BA	3153	1/1	0.97	0.05	37,37,37,37	0
59	MG	BA	3154	1/1	0.97	0.15	44,44,44,44	0
59	MG	AA	1681	1/1	0.97	0.05	30,30,30,30	0
59	MG	AD	301	1/1	0.97	0.10	49,49,49,49	0
59	MG	DA	3165	1/1	0.97	0.04	49,49,49,49	0
59	MG	DA	3057	1/1	0.97	0.04	21,21,21,21	0
59	MG	BA	3158	1/1	0.97	0.08	40,40,40,40	0
59	MG	DE	301	1/1	0.97	0.08	43,43,43,43	0
59	MG	DA	3060	1/1	0.97	0.03	16,16,16,16	0
59	MG	CA	1661	1/1	0.97	0.26	42,42,42,42	0
59	MG	CA	1662	1/1	0.97	0.04	23,23,23,23	0
59	MG	DZ	301	1/1	0.97	0.15	55,55,55,55	0
59	MG	BA	3218	1/1	0.97	0.05	21,21,21,21	0
59	MG	DA	3065	1/1	0.97	0.20	51,51,51,51	0
59	MG	BA	3059	1/1	0.97	0.04	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	BA	3160	1/1	0.97	0.12	13,13,13,13	0
60	ZN	B5	102	1/1	0.97	0.15	75,75,75,75	0
59	MG	BP	201	1/1	0.97	0.04	21,21,21,21	0
60	ZN	D5	103	1/1	0.97	0.09	92,92,92,92	0
59	MG	BD	301	1/1	0.98	0.06	13,13,13,13	0
59	MG	BA	3173	1/1	0.98	0.04	17,17,17,17	0
59	MG	BA	3081	1/1	0.98	0.15	6,6,6,6	0
59	MG	BA	3254	1/1	0.98	0.05	43,43,43,43	0
59	MG	BA	3212	1/1	0.98	0.04	25,25,25,25	0
59	MG	BA	3022	1/1	0.98	0.08	12,12,12,12	0
59	MG	BA	3176	1/1	0.98	0.16	27,27,27,27	0
59	MG	BA	3215	1/1	0.98	0.04	12,12,12,12	0
59	MG	DA	3010	1/1	0.98	0.15	39,39,39,39	0
59	MG	AA	1664	1/1	0.98	0.05	20,20,20,20	0
59	MG	BA	3356	1/1	0.98	0.07	41,41,41,41	0
59	MG	DA	3228	1/1	0.98	0.03	16,16,16,16	0
59	MG	BA	3217	1/1	0.98	0.12	11,11,11,11	0
59	MG	BY	201	1/1	0.98	0.12	32,32,32,32	0
59	MG	DA	3015	1/1	0.98	0.22	37,37,37,37	0
59	MG	BA	3011	1/1	0.98	0.13	31,31,31,31	0
59	MG	DA	3159	1/1	0.98	0.03	16,16,16,16	0
59	MG	DA	3017	1/1	0.98	0.12	16,16,16,16	0
59	MG	DA	3161	1/1	0.98	0.08	32,32,32,32	0
59	MG	DA	3018	1/1	0.98	0.08	14,14,14,14	0
59	MG	DA	3019	1/1	0.98	0.06	13,13,13,13	0
59	MG	BA	3179	1/1	0.98	0.17	31,31,31,31	0
59	MG	AA	1682	1/1	0.98	0.07	53,53,53,53	0
59	MG	DA	3022	1/1	0.98	0.07	14,14,14,14	0
59	MG	AA	1683	1/1	0.98	0.05	31,31,31,31	0
59	MG	BA	3222	1/1	0.98	0.08	18,18,18,18	0
59	MG	BA	3267	1/1	0.98	0.10	31,31,31,31	0
59	MG	AA	1636	1/1	0.98	0.13	21,21,21,21	0
59	MG	BA	3045	1/1	0.98	0.04	23,23,23,23	0
59	MG	DA	3246	1/1	0.98	0.09	23,23,23,23	0
59	MG	DA	3030	1/1	0.98	0.03	17,17,17,17	0
59	MG	BA	3150	1/1	0.98	0.04	33,33,33,33	0
59	MG	DA	3033	1/1	0.98	0.03	10,10,10,10	0
59	MG	BA	3368	1/1	0.98	0.04	24,24,24,24	0
59	MG	BA	3066	1/1	0.98	0.13	20,20,20,20	0
59	MG	BA	3046	1/1	0.98	0.05	30,30,30,30	0
59	MG	AA	1720	1/1	0.98	0.04	52,52,52,52	0
59	MG	BA	3092	1/1	0.98	0.04	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1611	1/1	0.98	0.09	38,38,38,38	0
59	MG	BA	3155	1/1	0.98	0.07	9,9,9,9	0
59	MG	BA	3190	1/1	0.98	0.09	29,29,29,29	0
59	MG	BA	3048	1/1	0.98	0.05	6,6,6,6	0
59	MG	BA	3030	1/1	0.98	0.09	18,18,18,18	0
59	MG	BA	3279	1/1	0.98	0.10	62,62,62,62	0
59	MG	DA	3047	1/1	0.98	0.04	25,25,25,25	0
59	MG	DA	3117	1/1	0.98	0.10	32,32,32,32	0
59	MG	BA	3125	1/1	0.98	0.17	43,43,43,43	0
59	MG	BA	3194	1/1	0.98	0.07	33,33,33,33	0
59	MG	BA	3236	1/1	0.98	0.13	23,23,23,23	0
59	MG	AA	1615	1/1	0.98	0.12	42,42,42,42	0
59	MG	BA	3073	1/1	0.98	0.09	10,10,10,10	0
59	MG	BA	3006	1/1	0.98	0.18	16,16,16,16	0
59	MG	BA	3101	1/1	0.98	0.05	25,25,25,25	0
59	MG	BA	3385	1/1	0.98	0.03	32,32,32,32	0
59	MG	AA	1705	1/1	0.98	0.04	47,47,47,47	0
59	MG	BA	3077	1/1	0.98	0.04	23,23,23,23	0
59	MG	AA	1731	1/1	0.98	0.03	22,22,22,22	0
59	MG	DA	3059	1/1	0.98	0.03	28,28,28,28	0
59	MG	BA	3203	1/1	0.98	0.10	38,38,38,38	0
59	MG	DA	3202	1/1	0.98	0.04	34,34,34,34	0
59	MG	DD	302	1/1	0.98	0.24	34,34,34,34	0
59	MG	BA	3105	1/1	0.98	0.09	14,14,14,14	0
59	MG	BA	3167	1/1	0.98	0.16	31,31,31,31	0
59	MG	BA	3137	1/1	0.98	0.10	34,34,34,34	0
59	MG	AA	1630	1/1	0.98	0.07	26,26,26,26	0
59	MG	DF	301	1/1	0.98	0.05	31,31,31,31	0
59	MG	BA	3342	1/1	0.98	0.06	21,21,21,21	0
59	MG	BA	3343	1/1	0.98	0.04	34,34,34,34	0
59	MG	BA	3344	1/1	0.98	0.04	37,37,37,37	0
59	MG	DA	3138	1/1	0.98	0.04	19,19,19,19	0
59	MG	BA	3107	1/1	0.98	0.07	13,13,13,13	0
59	MG	BA	3250	1/1	0.98	0.06	21,21,21,21	0
59	MG	BA	3399	1/1	0.98	0.07	41,41,41,41	0
59	MG	BA	3021	1/1	0.98	0.09	3,3,3,3	0
59	MG	BB	201	1/1	0.98	0.03	18,18,18,18	0
59	MG	BA	3070	1/1	0.99	0.02	14,14,14,14	0
59	MG	BA	3364	1/1	0.99	0.05	8,8,8,8	0
59	MG	BA	3111	1/1	0.99	0.11	28,28,28,28	0
59	MG	BA	3129	1/1	0.99	0.06	27,27,27,27	0
59	MG	BA	3130	1/1	0.99	0.06	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	DA	3256	1/1	0.99	0.03	27,27,27,27	0
59	MG	BA	3096	1/1	0.99	0.03	17,17,17,17	0
59	MG	DA	3023	1/1	0.99	0.02	33,33,33,33	0
59	MG	AA	1650	1/1	0.99	0.06	26,26,26,26	0
59	MG	DA	3025	1/1	0.99	0.05	5,5,5,5	0
59	MG	DA	3062	1/1	0.99	0.03	24,24,24,24	0
59	MG	DA	3179	1/1	0.99	0.10	33,33,33,33	0
59	MG	BA	3198	1/1	0.99	0.03	16,16,16,16	0
59	MG	BA	3098	1/1	0.99	0.15	18,18,18,18	0
59	MG	CA	1637	1/1	0.99	0.04	29,29,29,29	0
59	MG	AA	1679	1/1	0.99	0.02	27,27,27,27	0
59	MG	AA	1708	1/1	0.99	0.03	64,64,64,64	0
59	MG	BA	3136	1/1	0.99	0.04	30,30,30,30	0
59	MG	DA	3032	1/1	0.99	0.04	9,9,9,9	0
59	MG	DA	3070	1/1	0.99	0.09	10,10,10,10	0
59	MG	BA	3074	1/1	0.99	0.04	12,12,12,12	0
59	MG	BA	3063	1/1	0.99	0.09	19,19,19,19	0
59	MG	DA	3001	1/1	0.99	0.03	25,25,25,25	0
59	MG	BA	3025	1/1	0.99	0.03	20,20,20,20	0
59	MG	BA	3065	1/1	0.99	0.06	13,13,13,13	0
59	MG	DA	3114	1/1	0.99	0.03	42,42,42,42	0
59	MG	BA	3301	1/1	0.99	0.04	21,21,21,21	0
59	MG	BA	3032	1/1	0.99	0.08	21,21,21,21	0
59	MG	DA	3040	1/1	0.99	0.03	34,34,34,34	0
59	MG	BA	3040	1/1	0.99	0.03	9,9,9,9	0
59	MG	AA	1704	1/1	0.99	0.03	40,40,40,40	0
59	MG	BA	3330	1/1	0.99	0.07	21,21,21,21	0
59	MG	CA	1678	1/1	0.99	0.03	45,45,45,45	0
59	MG	BA	3124	1/1	0.99	0.14	27,27,27,27	0
59	MG	DA	3046	1/1	0.99	0.08	15,15,15,15	0
59	MG	BA	3093	1/1	0.99	0.08	10,10,10,10	0
59	MG	BA	3258	1/1	0.99	0.05	26,26,26,26	0
59	MG	BA	3146	1/1	0.99	0.15	12,12,12,12	0
60	ZN	AD	302	1/1	0.99	0.12	67,67,67,67	0
59	MG	DA	3206	1/1	0.99	0.10	27,27,27,27	0
59	MG	AA	1608	1/1	0.99	0.04	26,26,26,26	0
60	ZN	B9	101	1/1	0.99	0.04	64,64,64,64	0
60	ZN	CD	301	1/1	0.99	0.14	61,61,61,61	0
59	MG	BA	3169	1/1	0.99	0.05	51,51,51,51	0
59	MG	CA	1685	1/1	0.99	0.02	36,36,36,36	0
60	ZN	D9	101	1/1	0.99	0.04	109,109,109,109	0
59	MG	AA	1631	1/1	1.00	0.02	25,25,25,25	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
59	MG	CA	1634	1/1	1.00	0.02	17,17,17,17	0
59	MG	AA	1709	1/1	1.00	0.02	44,44,44,44	0
59	MG	BA	3062	1/1	1.00	0.04	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.