



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 07:25 AM UTC

PDB ID : 4V7Y / pdb_00004v7y
Title : Structure of the *Thermus thermophilus* 70S ribosome complexed with azithromycin.
Authors : Bulkley, D.P.; Innis, C.A.; Blaha, G.; Steitz, T.A.
Deposited on : 2010-08-18
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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

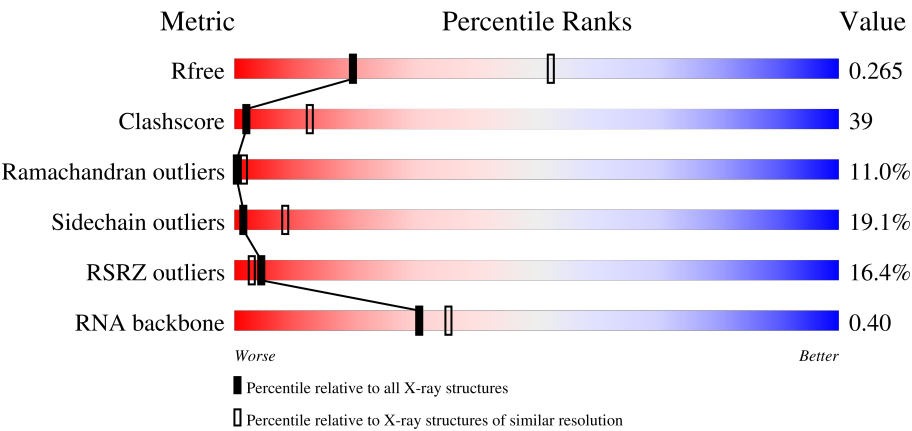
1 Overall quality at a glance i

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	1522	11% 27% 57% 15%
1	CA	1522	9% 27% 57% 15%
2	AB	256	19% 34% 43% 14% 8%
2	CB	256	19% 33% 44% 13% 8%

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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	135	
12	CL	135	
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	B0	85	
22	D0	85	
23	B1	98	
23	D1	98	
24	B2	72	
24	D2	72	
25	B3	60	
25	D3	60	
26	B4	71	
26	D4	71	
27	B5	60	
27	D5	60	

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Mol	Chain	Length	Quality of chain
28	B6	54	
28	D6	54	
29	B7	49	
29	D7	49	
30	B8	65	
30	D8	65	
31	BA	2787	
31	DA	2787	
32	BB	122	
32	DB	122	
33	BD	276	
33	DD	276	
34	BE	206	
34	DE	206	
35	BF	210	
35	DF	210	
36	BG	182	
36	DG	182	
37	BH	180	
37	DH	180	
38	BI	148	
38	DI	148	
39	BN	140	
39	DN	140	
40	BO	122	

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Mol	Chain	Length	Quality of chain
40	DO	122	
41	BP	150	
41	DP	150	
42	BQ	141	
42	DQ	141	
43	BR	118	
43	DR	118	
44	BS	112	
44	DS	112	
45	BT	146	
45	DT	146	
46	BU	118	
46	DU	118	
47	BV	101	
47	DV	101	
48	BW	113	
48	DW	113	
49	BX	96	
49	DX	96	
50	BY	110	
50	DY	110	
51	BZ	206	
51	DZ	206	

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
52	MG	AA	1622	-	-	-	X
52	MG	AA	1646	-	-	-	X
52	MG	CA	1633	-	-	-	X
52	MG	CA	1641	-	-	-	X
52	MG	DA	3125	-	-	-	X
52	MG	DA	3179	-	-	-	X
52	MG	DA	3216	-	-	-	X
52	MG	DA	3280	-	-	-	X
52	MG	DA	3289	-	-	-	X
52	MG	DA	3302	-	-	-	X
54	K	DA	3310	-	-	-	X

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 278000 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 rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			
1	CA	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- 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
			1011	639	198	174			
9	CI	127	Total	C	N	O	0	0	0
			1011	639	198	174			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AI	58	ARG	HIS	conflict	UNP P80374
CI	58	ARG	HIS	conflict	UNP P80374

- 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			
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			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AL	2	VAL	-	insertion	UNP Q5SHN3
AL	3	ALA	-	insertion	UNP Q5SHN3
AL	4	LEU	-	insertion	UNP Q5SHN3
CL	2	VAL	-	insertion	UNP Q5SHN3
CL	3	ALA	-	insertion	UNP Q5SHN3
CL	4	LEU	-	insertion	UNP Q5SHN3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	2			
13	CM	115	Total	C	N	O	S	0	0	0
			921	569	190	160	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			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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 protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	B0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			
22	D0	85	Total	C	N	O	S	0	0	0
			650	401	137	111	1			

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	B1	89	Total	C	N	O	0	0	1
			693	435	140	118			
23	D1	89	Total	C	N	O	0	0	1
			693	435	140	118			

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	B2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			
24	D2	51	Total	C	N	O	S	0	0	1
			421	263	85	72	1			

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
26	B4	32	Total	C	N	O	0	0	0
			157	93	32	32			
26	D4	32	Total	C	N	O	0	0	0
			157	93	32	32			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	B5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			
27	D5	59	Total	C	N	O	S	9	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	B6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			
28	D6	45	Total	C	N	O	S	0	0	1
			381	235	78	64	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	B8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			
30	D8	64	Total	C	N	O	S	0	0	1
			508	326	102	78	2			

- Molecule 31 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	BA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			
31	DA	2725	Total	C	N	O	P	0	0	0
			58698	26124	10986	18864	2724			

- Molecule 32 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	BB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			
32	DB	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

- Molecule 33 is a protein called 50S ribosomal protein L2.

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

- Molecule 34 is a protein called 50S ribosomal protein L3.

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

- Molecule 35 is a protein called 50S ribosomal protein L4.

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

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

- Molecule 36 is a protein called 50S ribosomal protein L5.

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

- Molecule 37 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
37	BH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			
37	DH	160	Total	C	N	O	S	0	0	1
			1223	773	229	220	1			

- Molecule 38 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
38	BI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			
38	DI	146	Total	C	N	O	S	0	0	1
			1132	723	201	207	1			

- Molecule 39 is a protein called 50S ribosomal protein L13.

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

- Molecule 40 is a protein called 50S ribosomal protein L14.

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

- Molecule 41 is a protein called 50S ribosomal protein L15.

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

- Molecule 42 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
42	BQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			
42	DQ	136	Total	C	N	O	S	0	0	0
			1080	688	204	183	5			

- Molecule 43 is a protein called 50S ribosomal protein L17.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

- Molecule 45 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			
45	DT	132	Total	C	N	O	S	0	0	0
			1100	686	227	186	1			

- Molecule 46 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
46	BU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			
46	DU	117	Total	C	N	O	S	0	0	0
			958	604	202	151	1			

- Molecule 47 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
47	BV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			
47	DV	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 48 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
48	BW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			
48	DW	113	Total	C	N	O	S	0	0	0
			896	563	176	155	2			

- Molecule 49 is a protein called 50S ribosomal protein L23.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L25.

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

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

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	AA	51	Total	Mg	0	0
			51	51		
52	B0	1	Total	Mg	0	0
			1	1		
52	B1	1	Total	Mg	0	0
			1	1		
52	B5	2	Total	Mg	0	0
			2	2		
52	B7	1	Total	Mg	0	0
			1	1		
52	BA	349	Total	Mg	0	0
			349	349		
52	BB	5	Total	Mg	0	0
			5	5		
52	BD	1	Total	Mg	0	0
			1	1		
52	BE	1	Total	Mg	0	0
			1	1		
52	BF	1	Total	Mg	0	0
			1	1		
52	BP	3	Total	Mg	0	0
			3	3		
52	BQ	2	Total	Mg	0	0
			2	2		
52	BR	1	Total	Mg	0	0
			1	1		
52	BU	1	Total	Mg	0	0
			1	1		
52	BX	1	Total	Mg	0	0
			1	1		
52	CA	48	Total	Mg	0	0
			48	48		
52	D0	1	Total	Mg	0	0
			1	1		
52	D1	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
52	D5	2	Total 2	Mg 2	0	0
52	D7	1	Total 1	Mg 1	0	0
52	DA	309	Total 309	Mg 309	0	0
52	DB	3	Total 3	Mg 3	0	0
52	DD	1	Total 1	Mg 1	0	0
52	DE	1	Total 1	Mg 1	0	0
52	DF	1	Total 1	Mg 1	0	0
52	DP	1	Total 1	Mg 1	0	0
52	DQ	1	Total 1	Mg 1	0	0
52	DR	1	Total 1	Mg 1	0	0
52	DU	1	Total 1	Mg 1	0	0
52	DX	1	Total 1	Mg 1	0	0

- Molecule 53 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
53	AD	1	Total 1	Zn 1	0	0
53	AN	1	Total 1	Zn 1	0	0
53	CD	1	Total 1	Zn 1	0	0
53	CN	1	Total 1	Zn 1	0	0

- Molecule 54 is POTASSIUM ION (CCD ID: K) (formula: K).

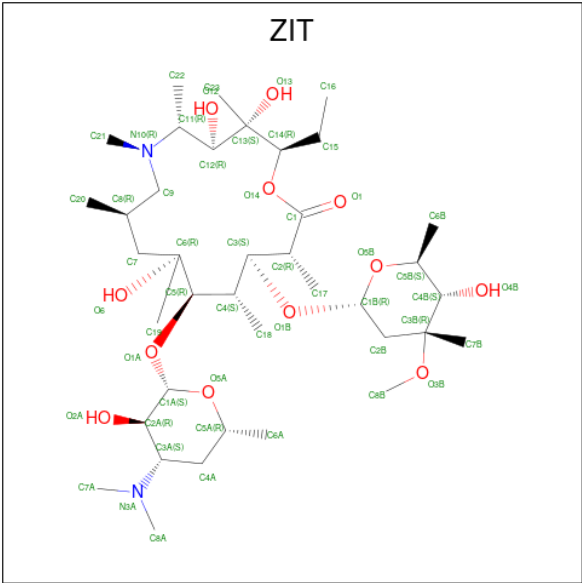
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
54	BA	1	Total 1	K 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
54	DA	1	Total	K		0	0
			1	1			

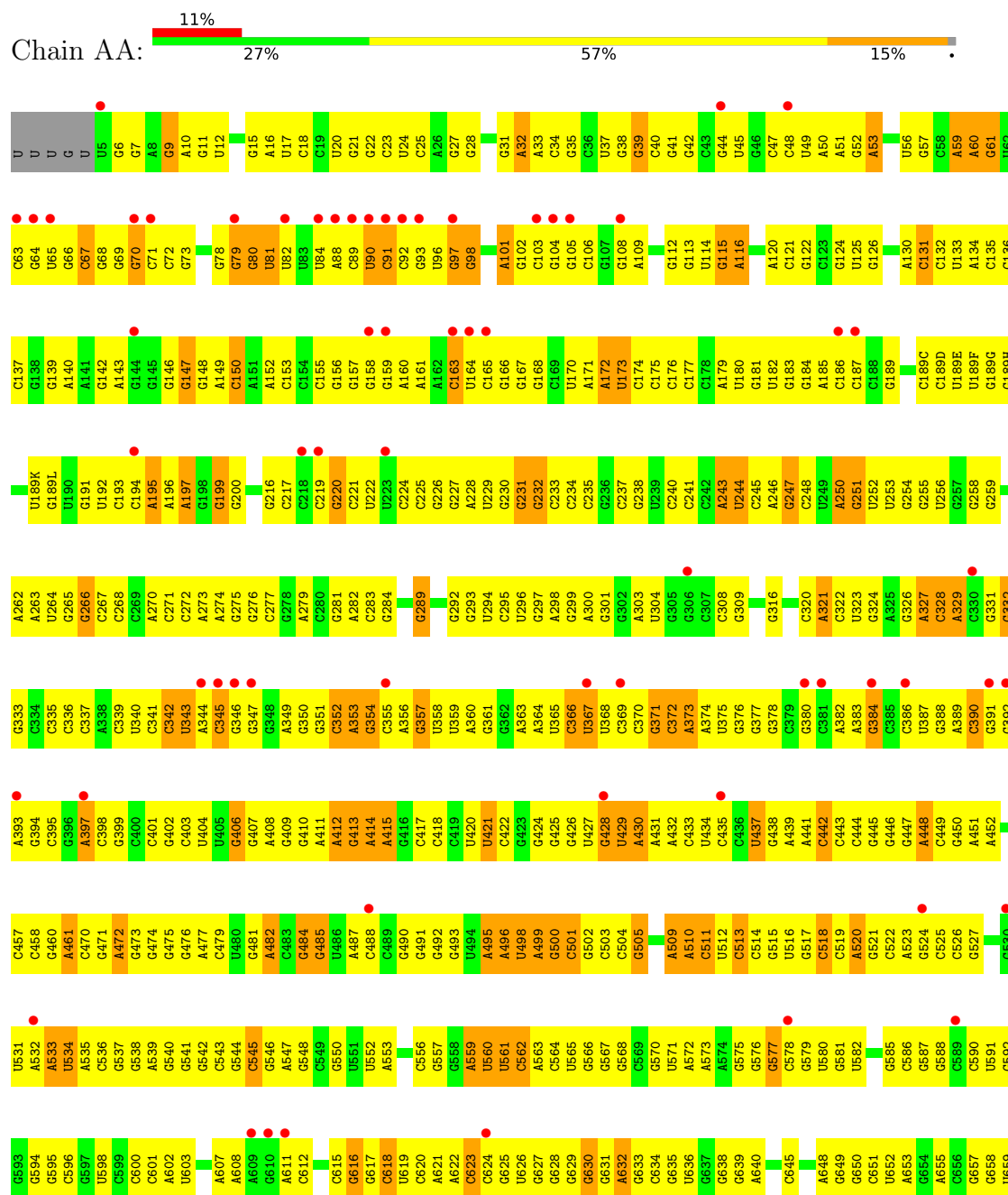
- Molecule 55 is AZITHROMYCIN (CCD ID: ZIT) (formula: C₃₈H₇₂N₂O₁₂).

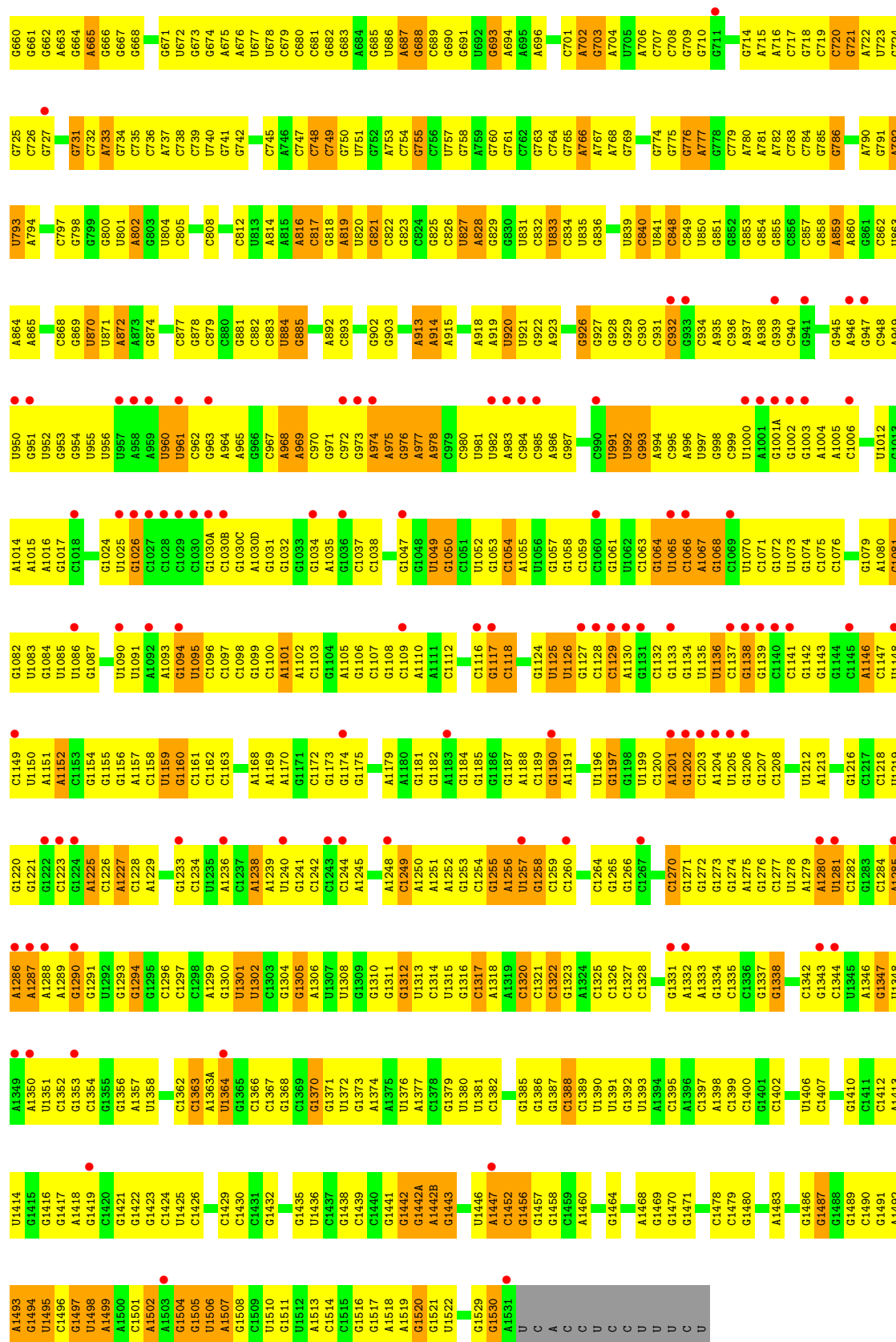


3 Residue-property plots

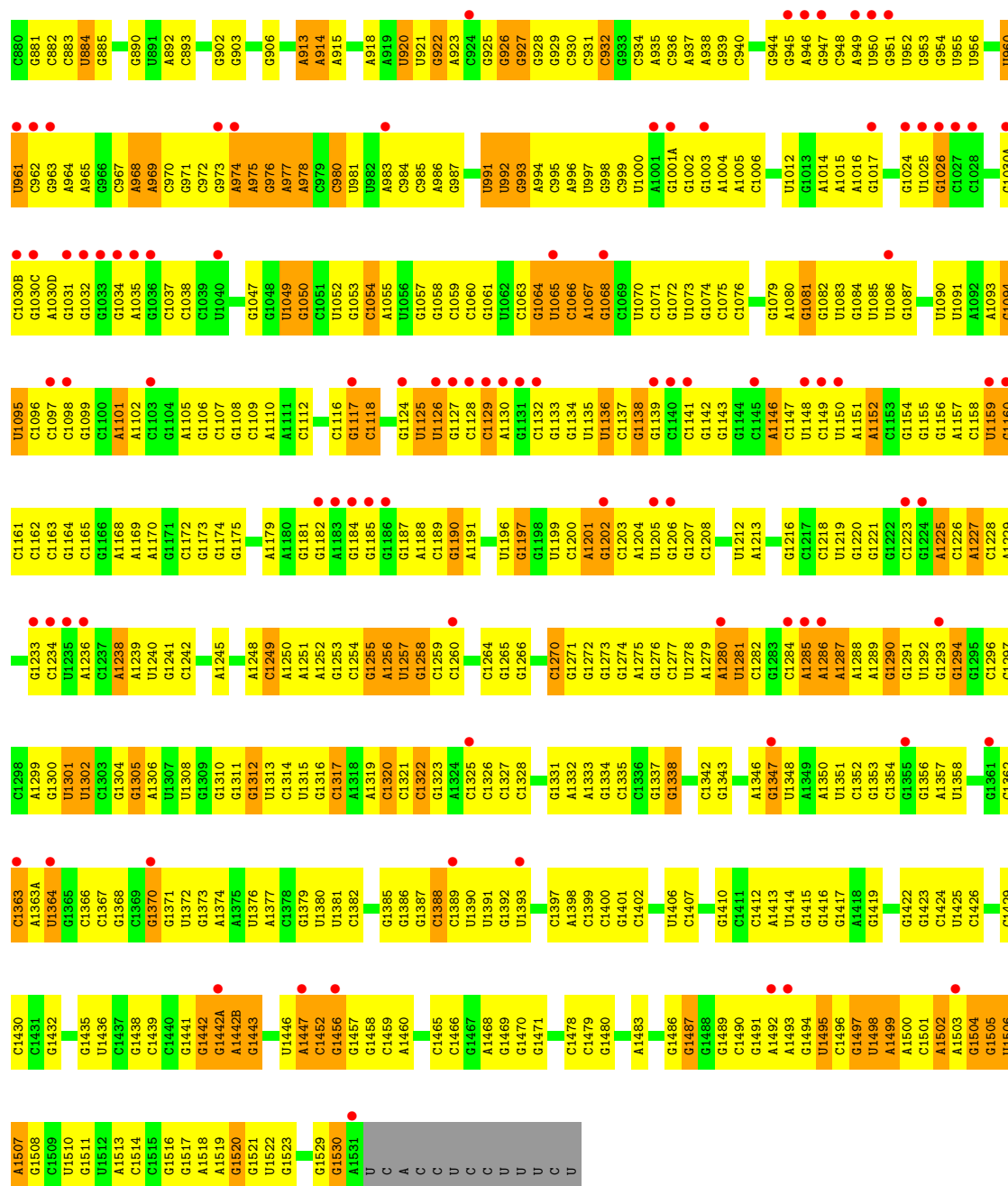
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: 16S rRNA



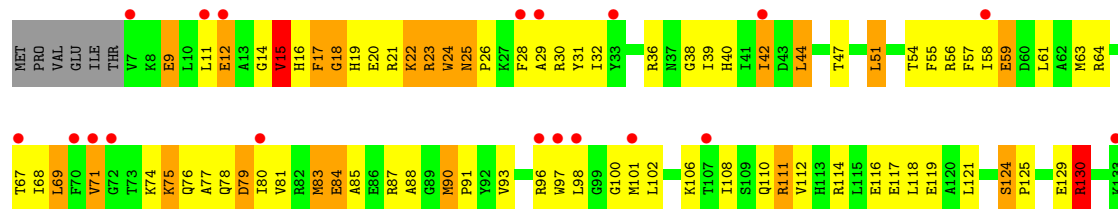


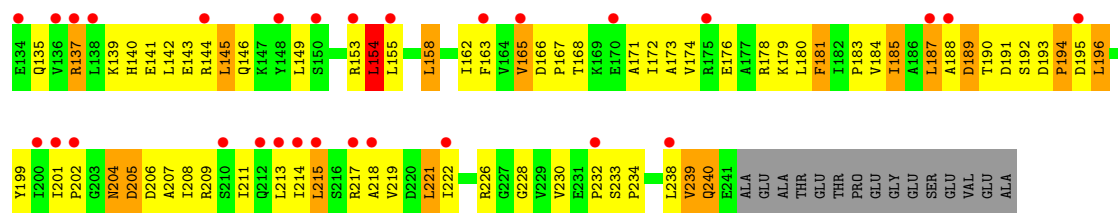




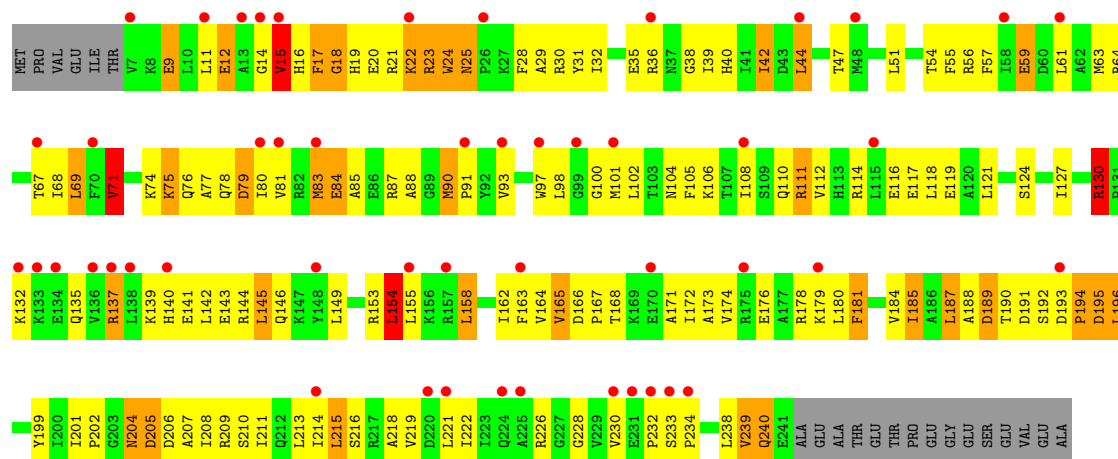
• Molecule 2: 30S ribosomal protein S2

Chain AB: 19% 34% 43% 14% 8%

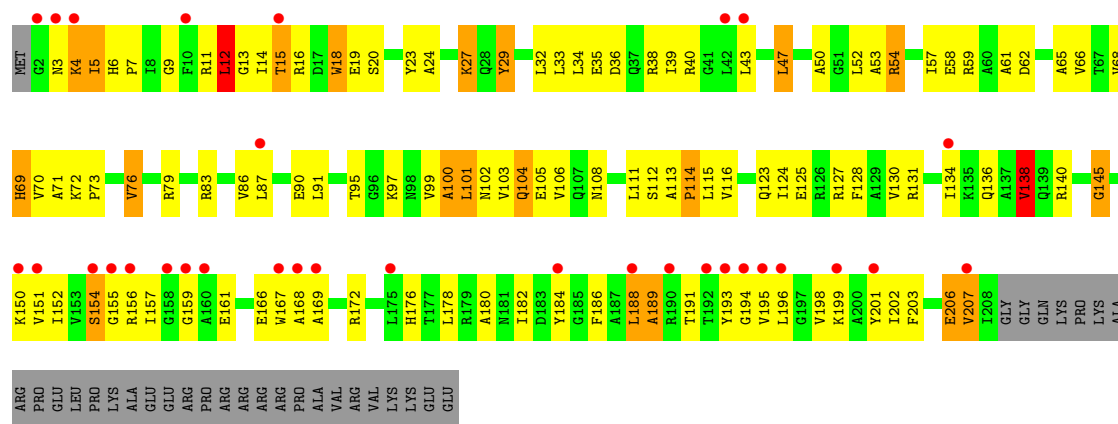




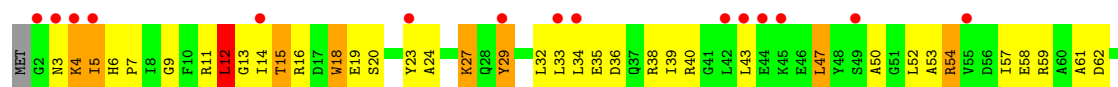
• Molecule 2: 30S ribosomal protein S2

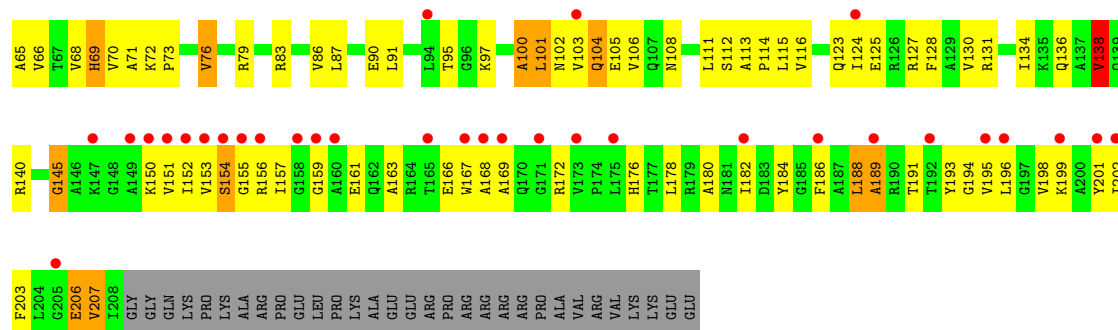


• Molecule 3: 30S ribosomal protein S3

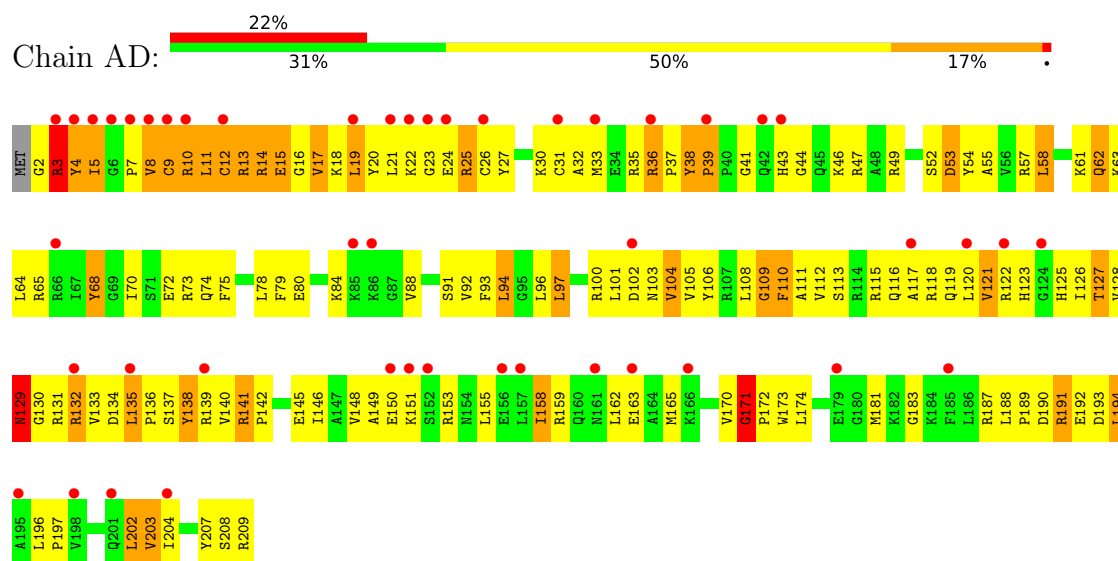


• Molecule 3: 30S ribosomal protein S3

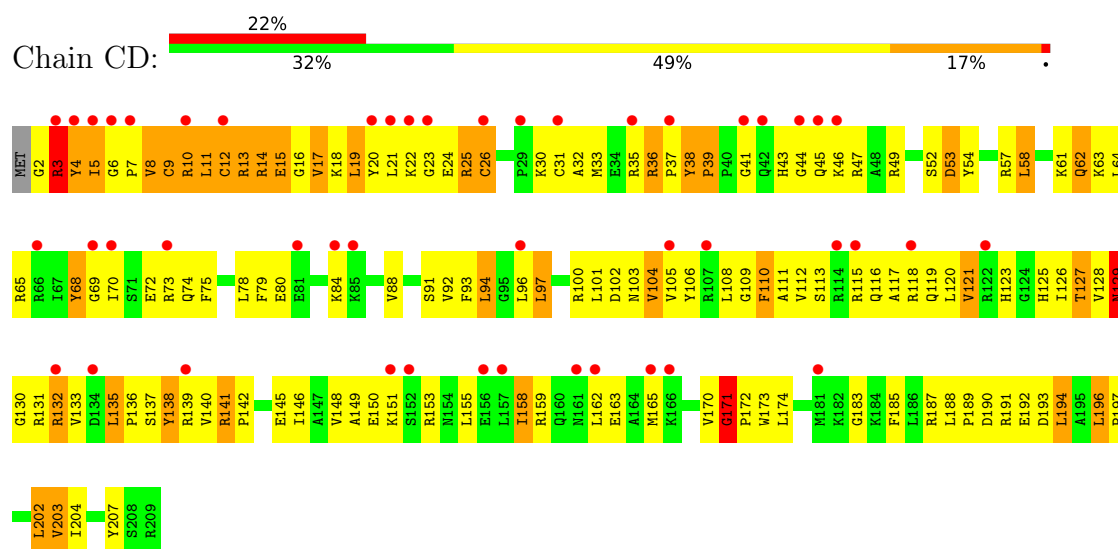




• Molecule 4: 30S ribosomal protein S4

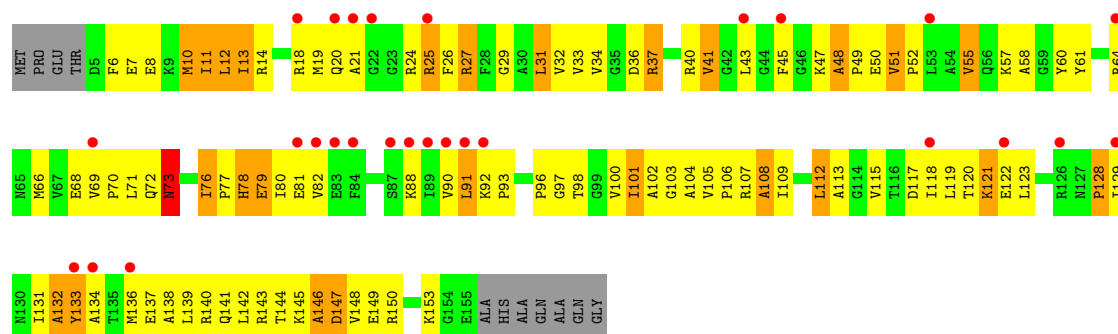


• Molecule 4: 30S ribosomal protein S4

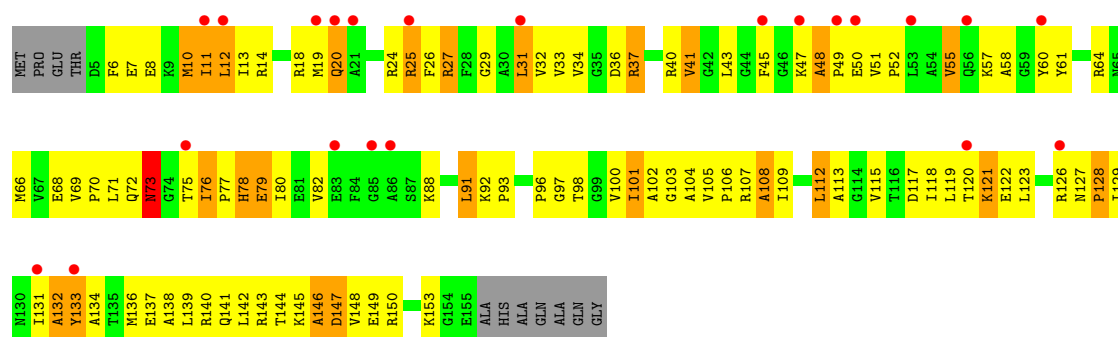


• Molecule 5: 30S ribosomal protein S5

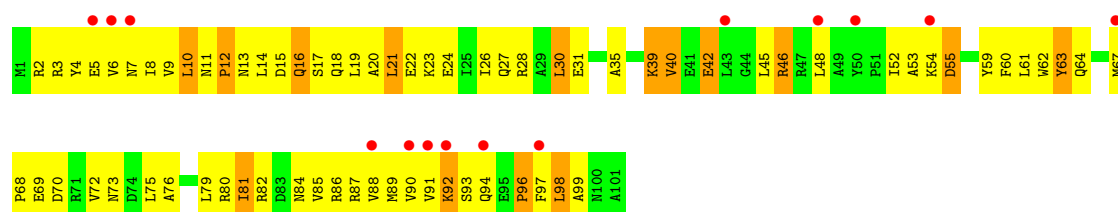




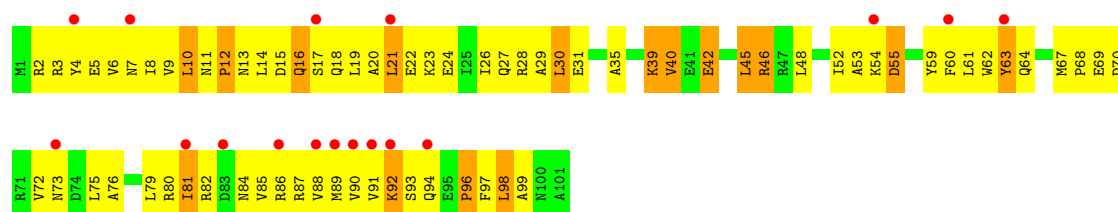
• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

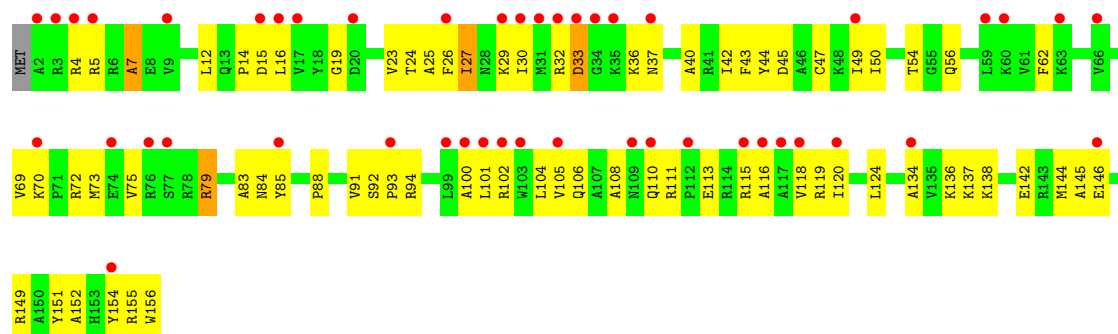


• Molecule 6: 30S ribosomal protein S6

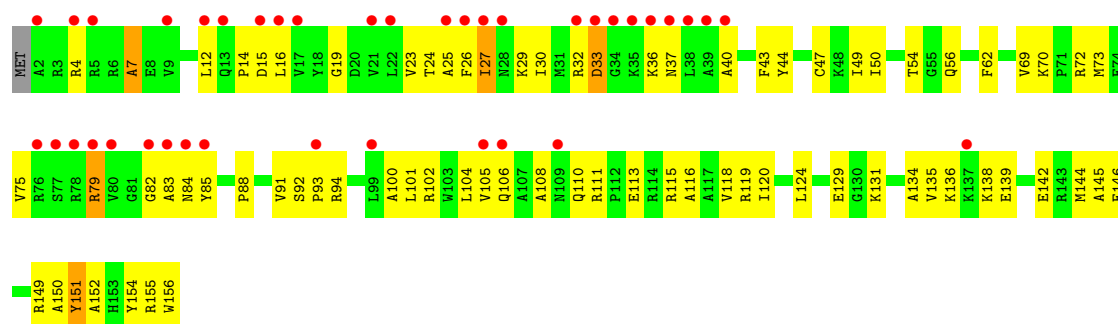


• Molecule 7: 30S ribosomal protein S7

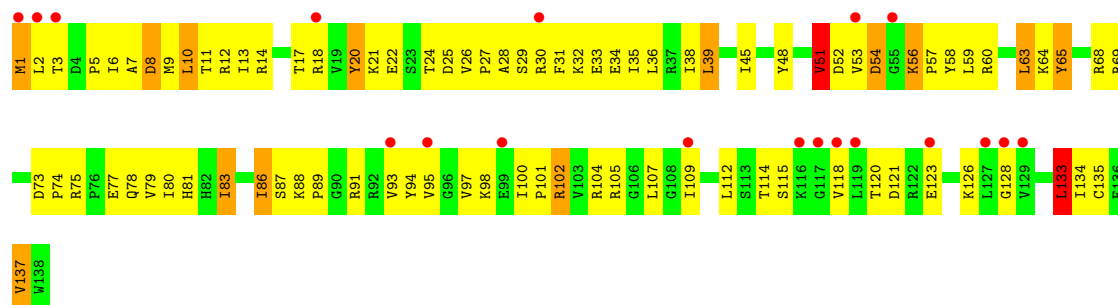




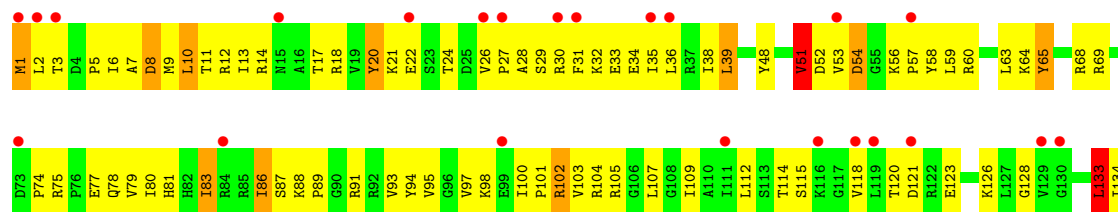
• Molecule 7: 30S ribosomal protein S7



• Molecule 8: 30S ribosomal protein S8

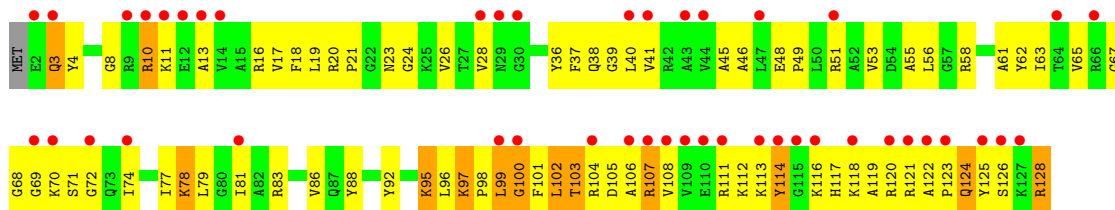


• Molecule 8: 30S ribosomal protein S8

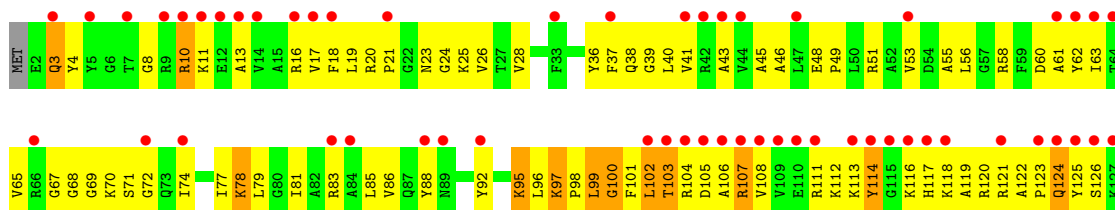




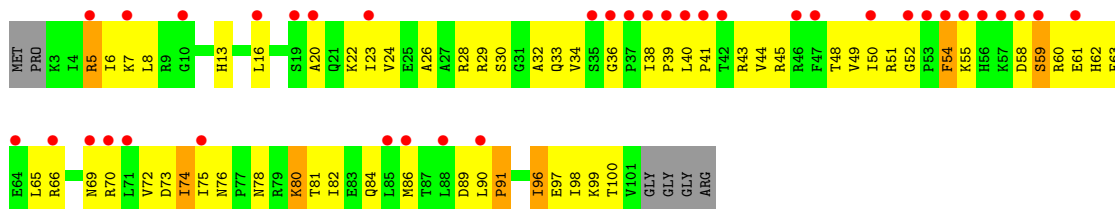
• Molecule 9: 30S ribosomal protein S9



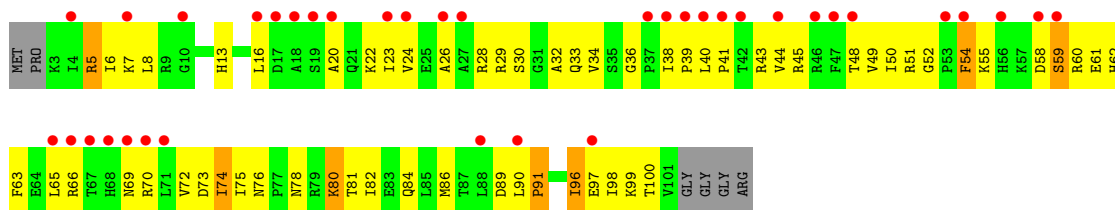
• Molecule 9: 30S ribosomal protein S9



• Molecule 10: 30S ribosomal protein S10

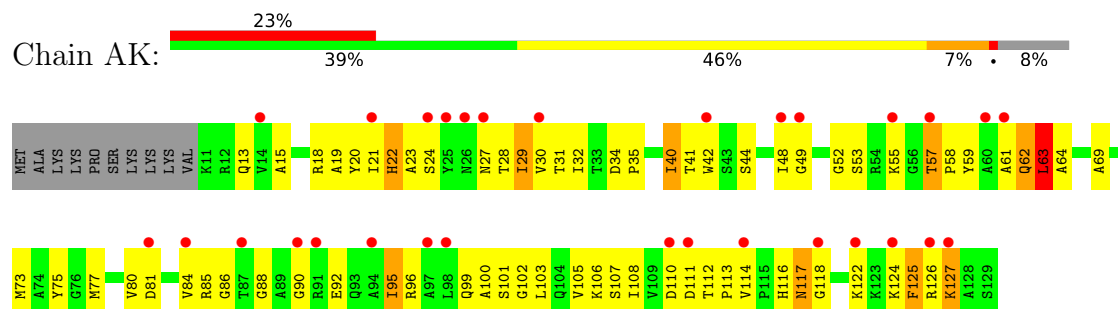


• Molecule 10: 30S ribosomal protein S10



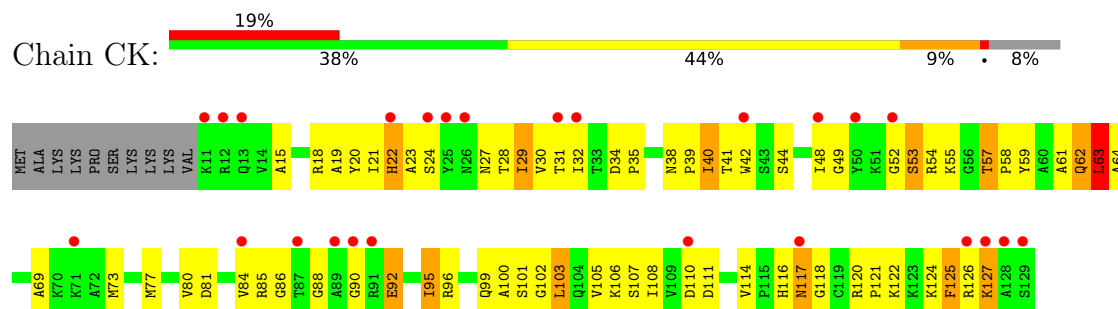
- Molecule 11: 30S ribosomal protein S11

Chain AK:



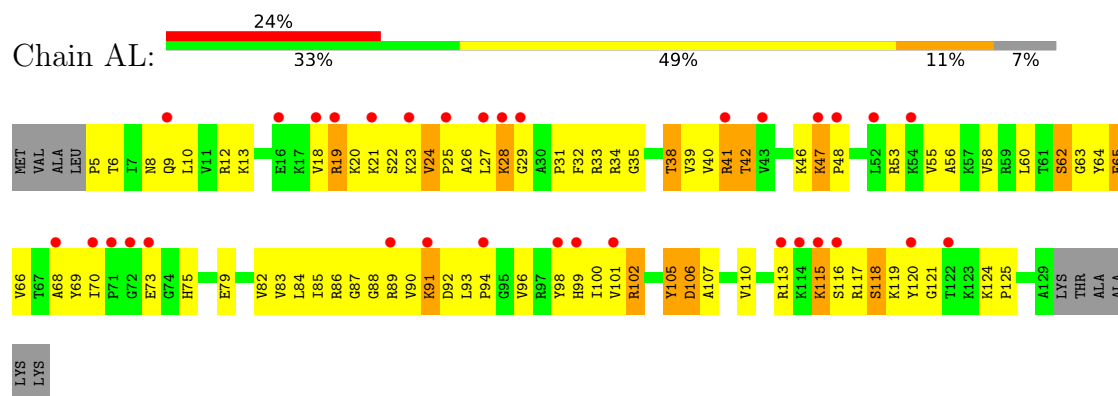
- Molecule 11: 30S ribosomal protein S11

Chain CK:



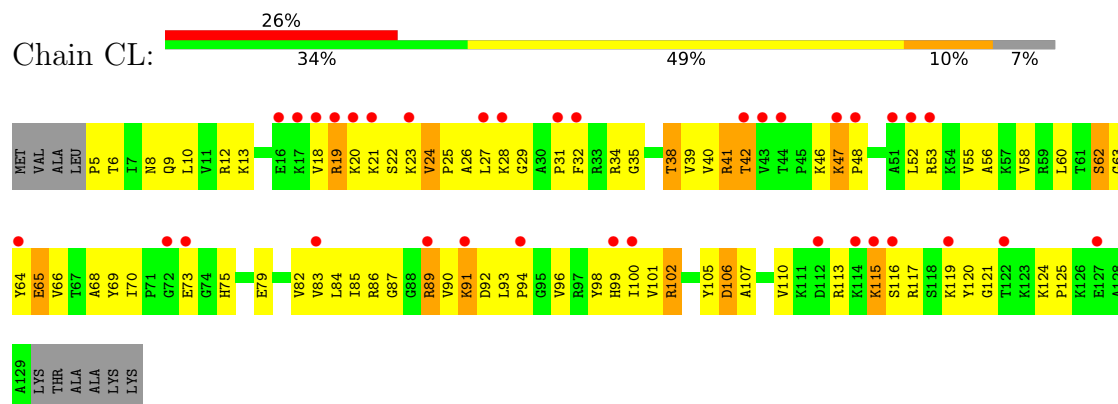
- Molecule 12: 30S ribosomal protein S12

Chain AL:

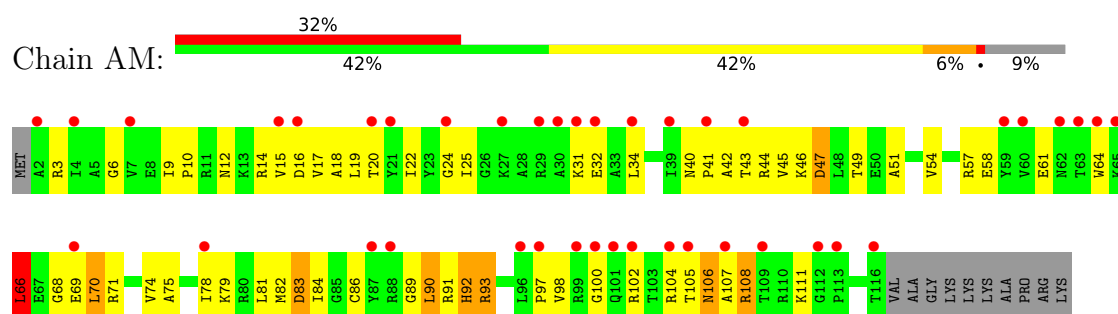


- Molecule 12: 30S ribosomal protein S12

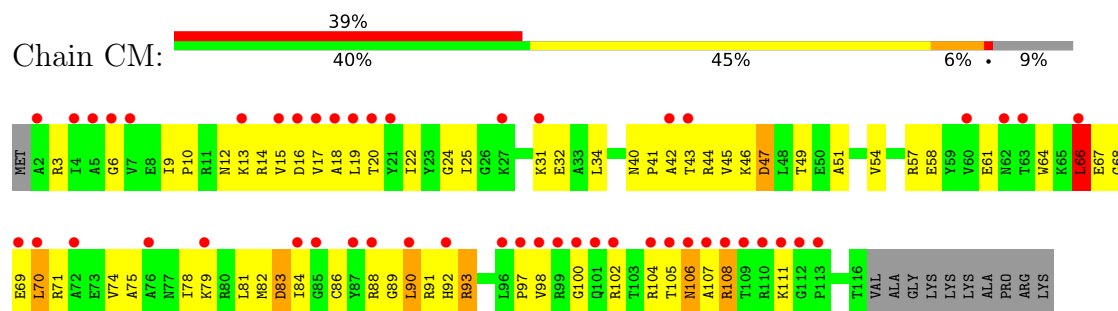
Chain CL:



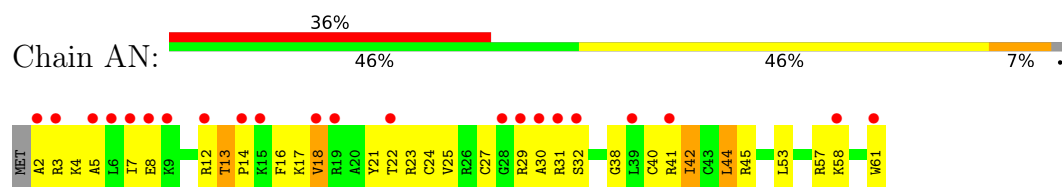
- Molecule 13: 30S ribosomal protein S13



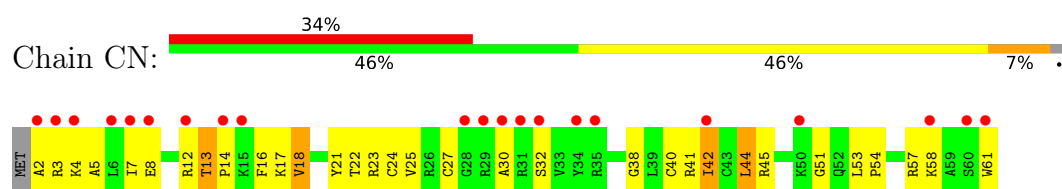
- Molecule 13: 30S ribosomal protein S13



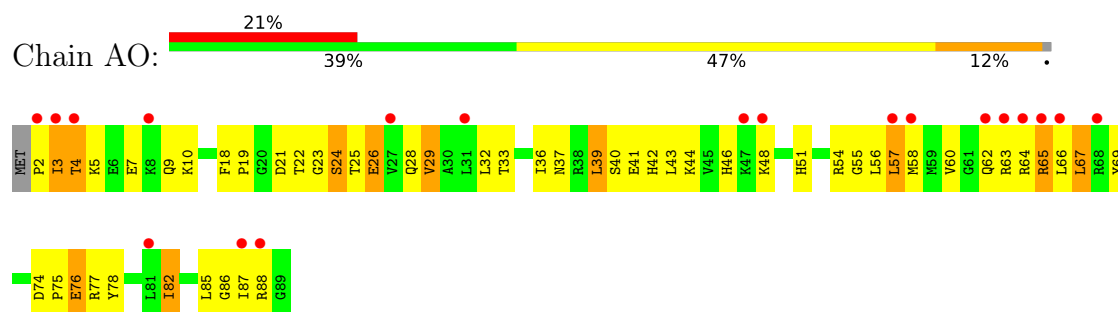
- Molecule 14: 30S ribosomal protein S14



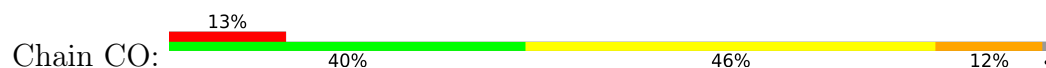
- Molecule 14: 30S ribosomal protein S14

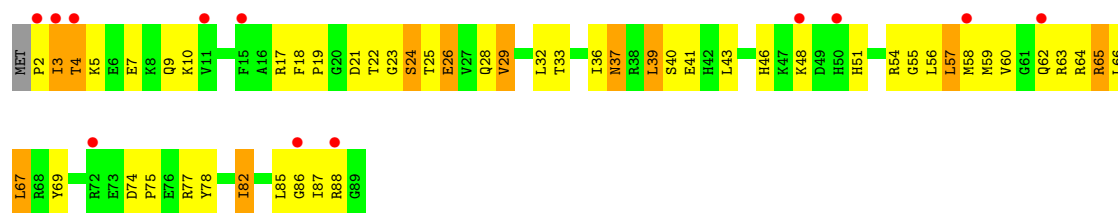


- Molecule 15: 30S ribosomal protein S15

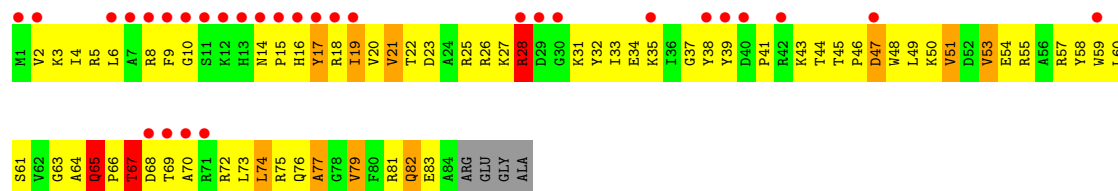


- Molecule 15: 30S ribosomal protein S15

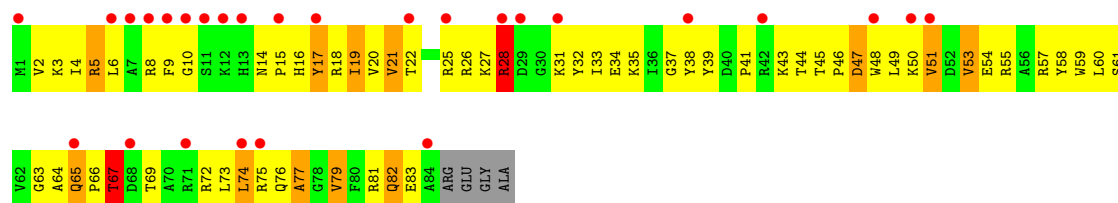




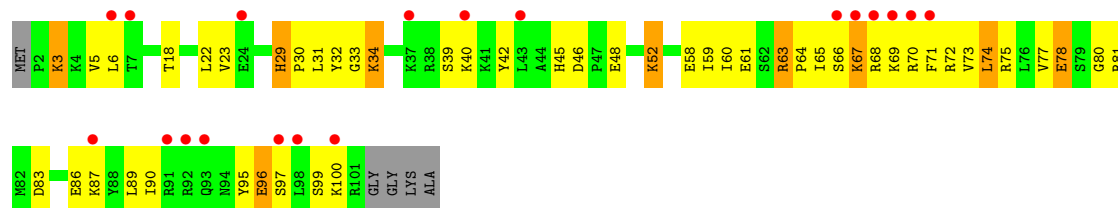
• Molecule 16: 30S ribosomal protein S16



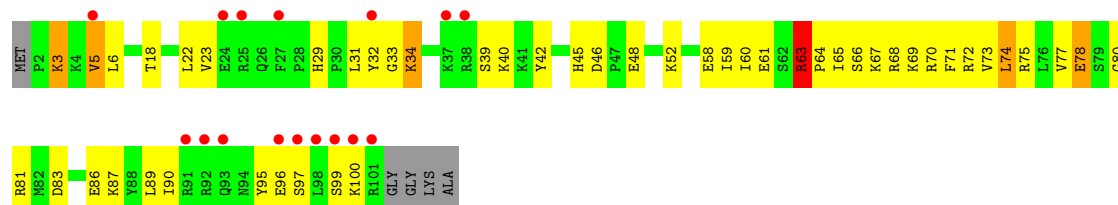
• Molecule 16: 30S ribosomal protein S16



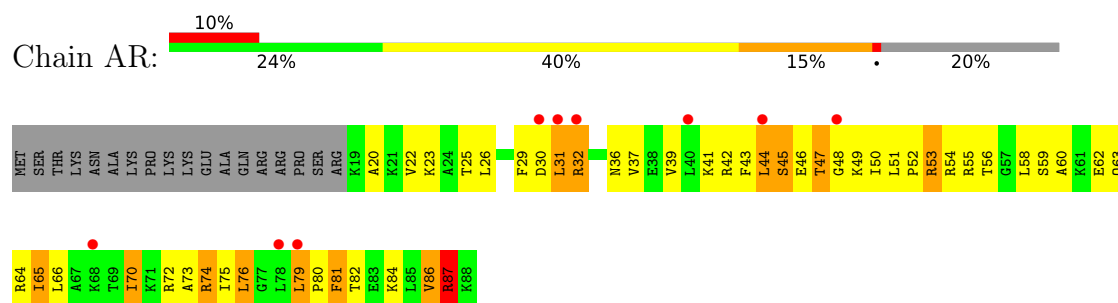
• Molecule 17: 30S ribosomal protein S17



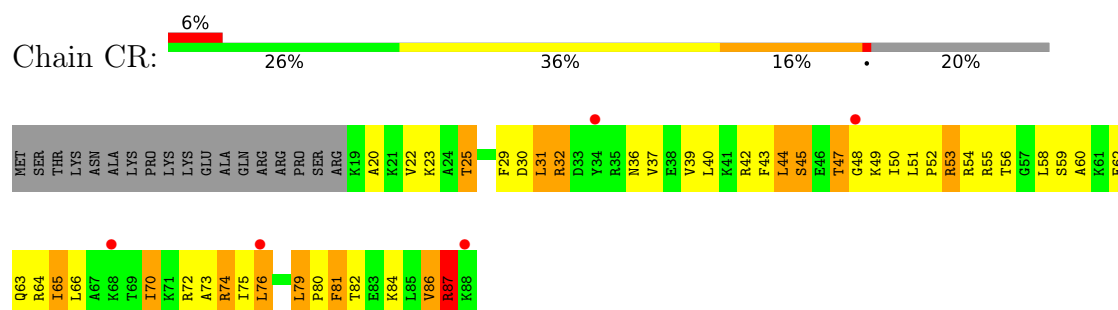
• Molecule 17: 30S ribosomal protein S17



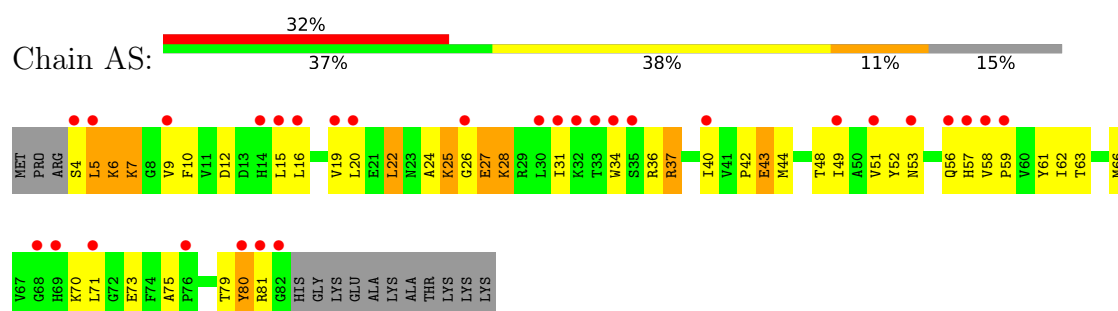
- Molecule 18: 30S ribosomal protein S18



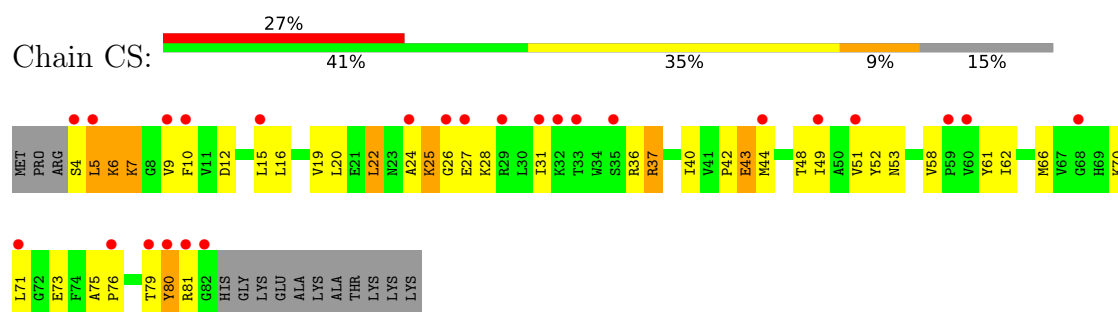
- Molecule 18: 30S ribosomal protein S18



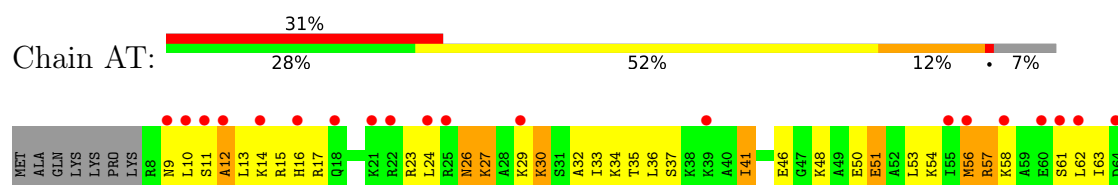
- Molecule 19: 30S ribosomal protein S19

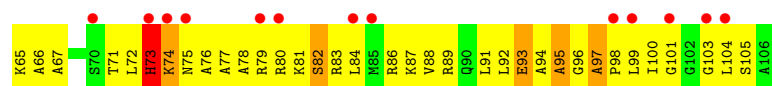


- Molecule 19: 30S ribosomal protein S19

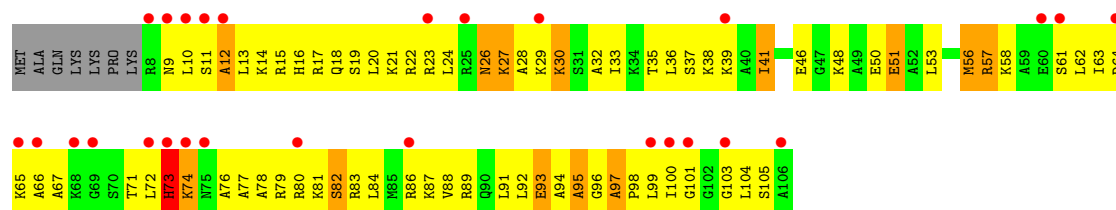


- Molecule 20: 30S ribosomal protein S20

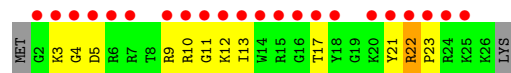
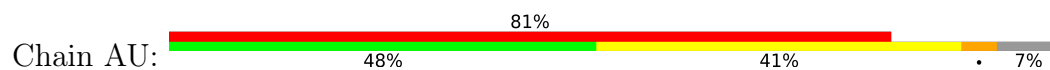




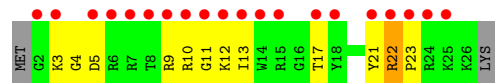
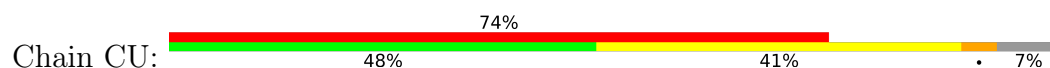
- Molecule 20: 30S ribosomal protein S20



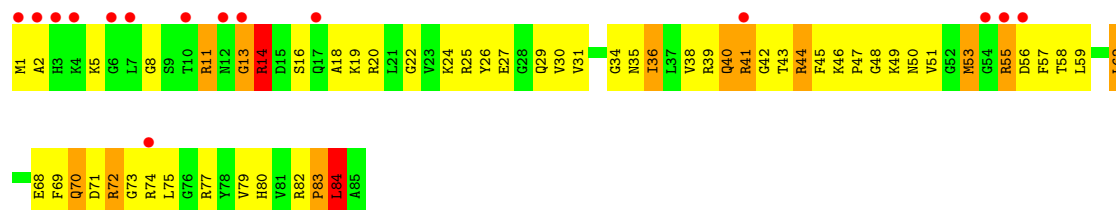
- Molecule 21: 30S ribosomal protein Thx



- Molecule 21: 30S ribosomal protein Thx



- Molecule 22: 50S ribosomal protein L27

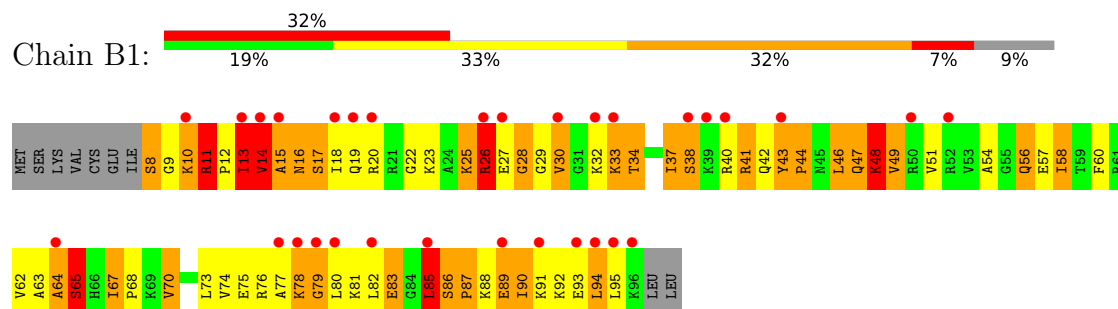


- Molecule 22: 50S ribosomal protein L27



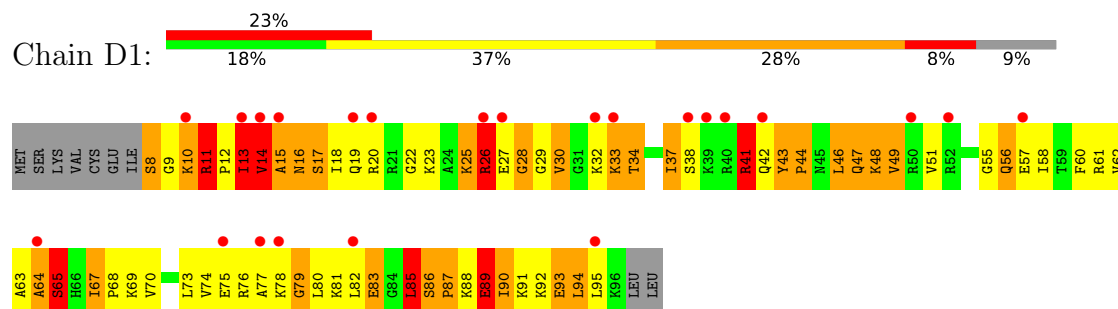
- Molecule 23: 50S ribosomal protein L28

Chain B1:



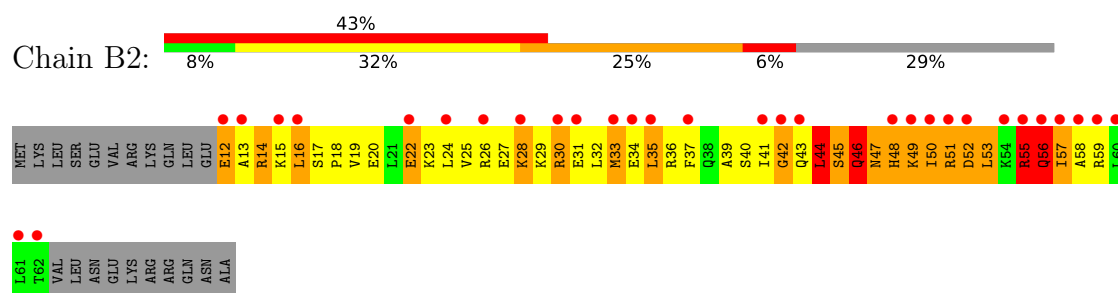
- Molecule 23: 50S ribosomal protein L28

Chain D1:



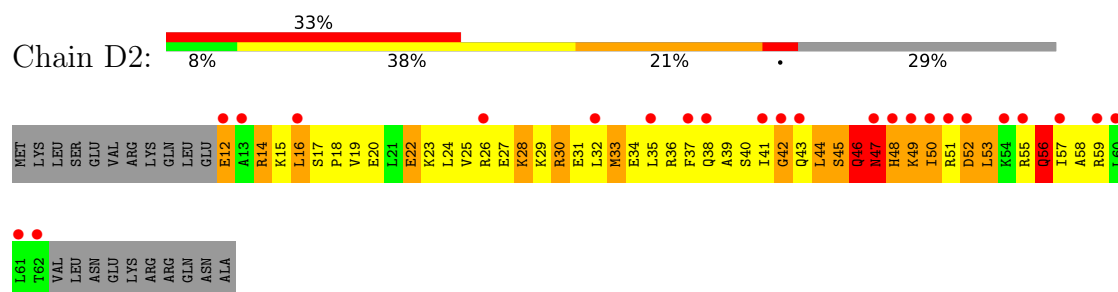
- Molecule 24: 50S ribosomal protein L29

Chain B2:



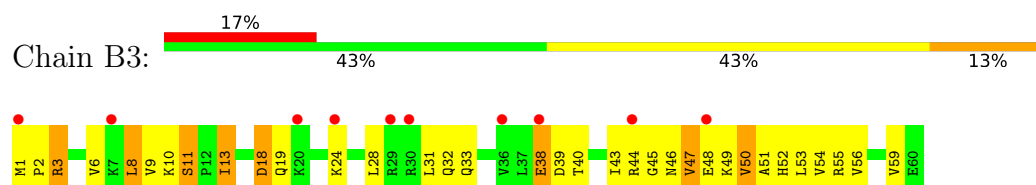
- Molecule 24: 50S ribosomal protein L29

Chain D2:

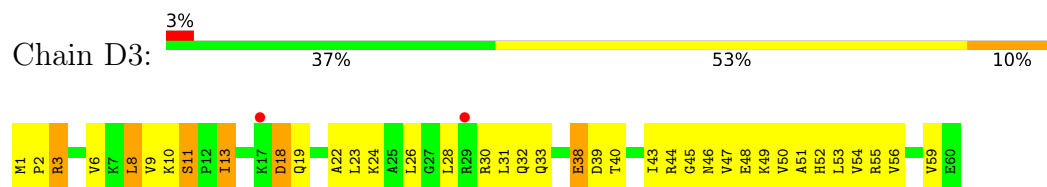


- Molecule 25: 50S ribosomal protein L30

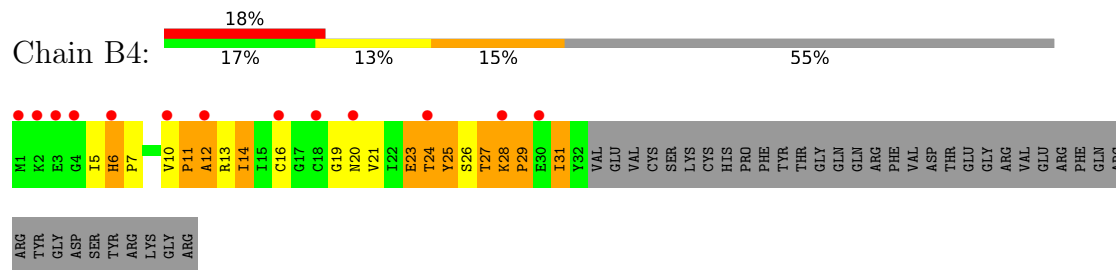
Chain B3:



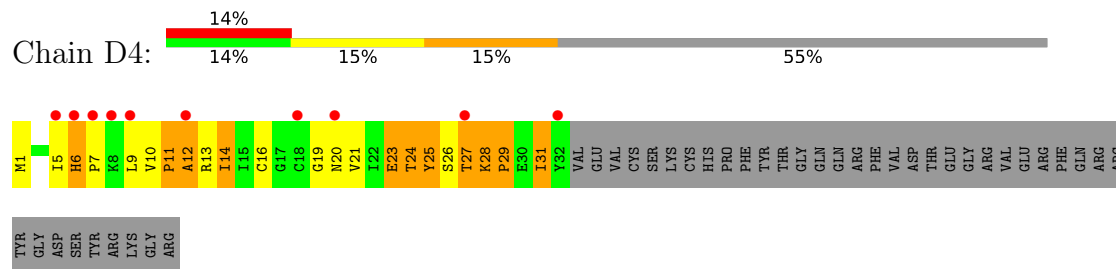
- Molecule 25: 50S ribosomal protein L30



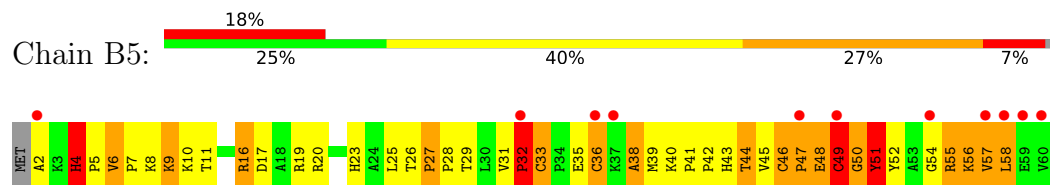
- Molecule 26: 50S ribosomal protein L31



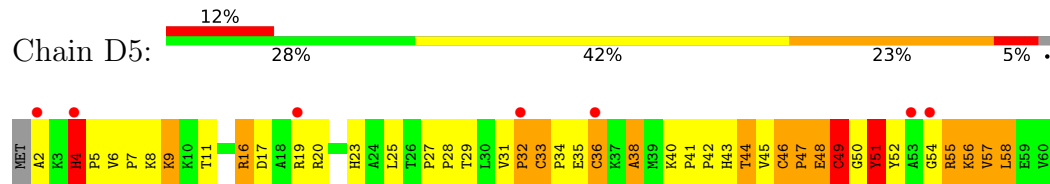
- Molecule 26: 50S ribosomal protein L31



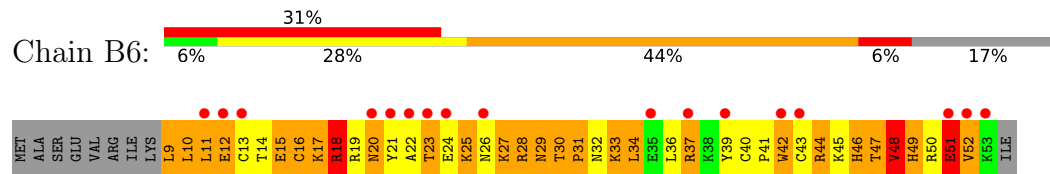
- Molecule 27: 50S ribosomal protein L32



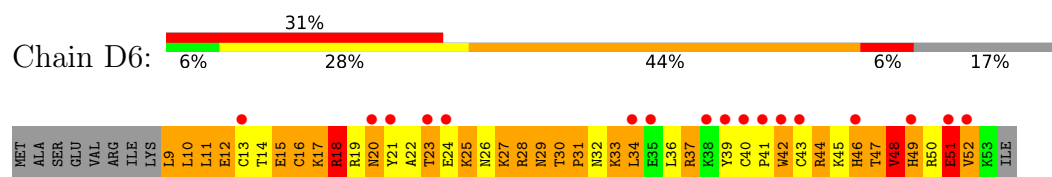
- Molecule 27: 50S ribosomal protein L32



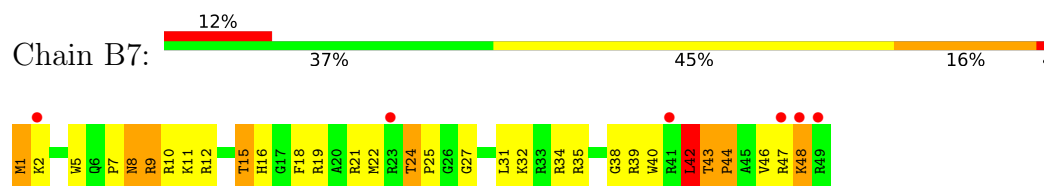
- Molecule 28: 50S ribosomal protein L33



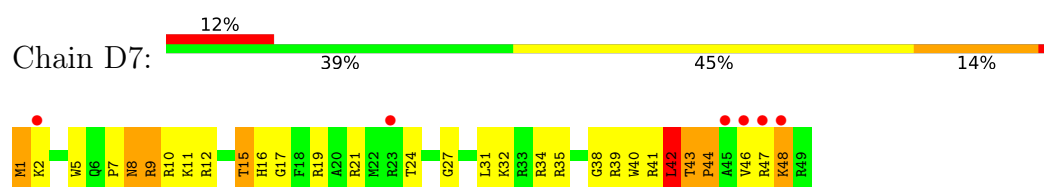
- Molecule 28: 50S ribosomal protein L33



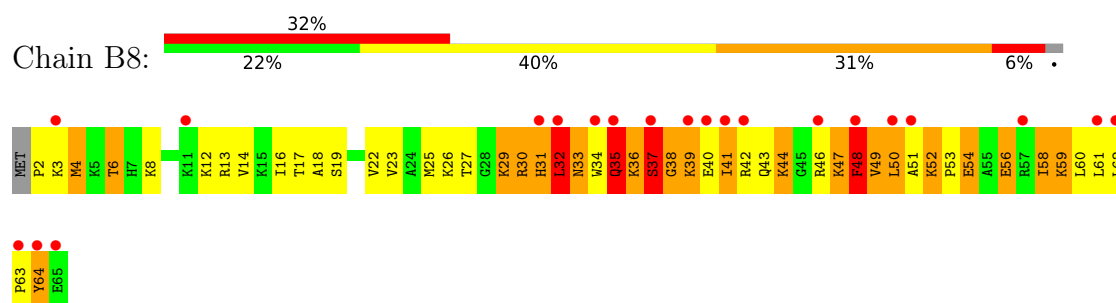
- Molecule 29: 50S ribosomal protein L34



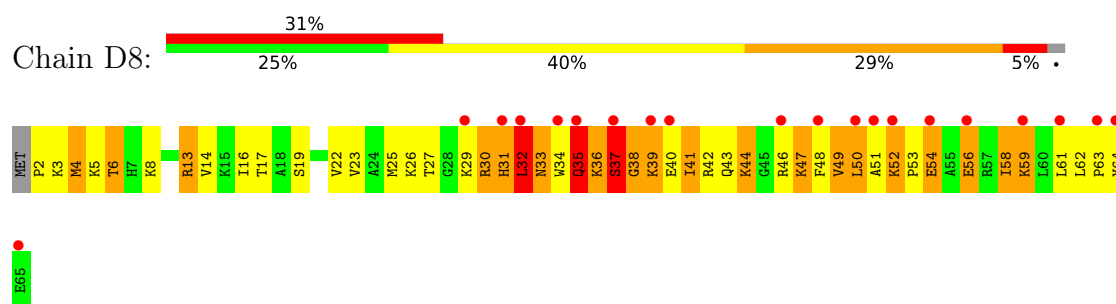
- Molecule 29: 50S ribosomal protein L34



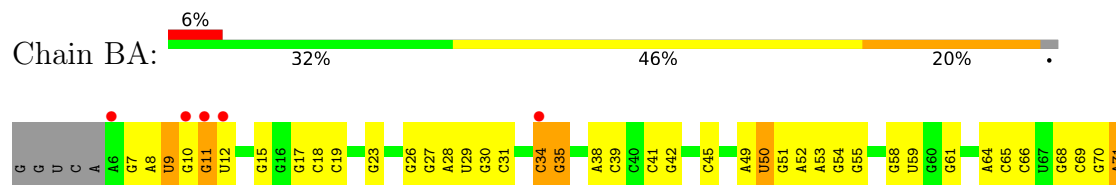
- Molecule 30: 50S ribosomal protein L35



- Molecule 30: 50S ribosomal protein L35



- Molecule 31: 23S ribosomal RNA



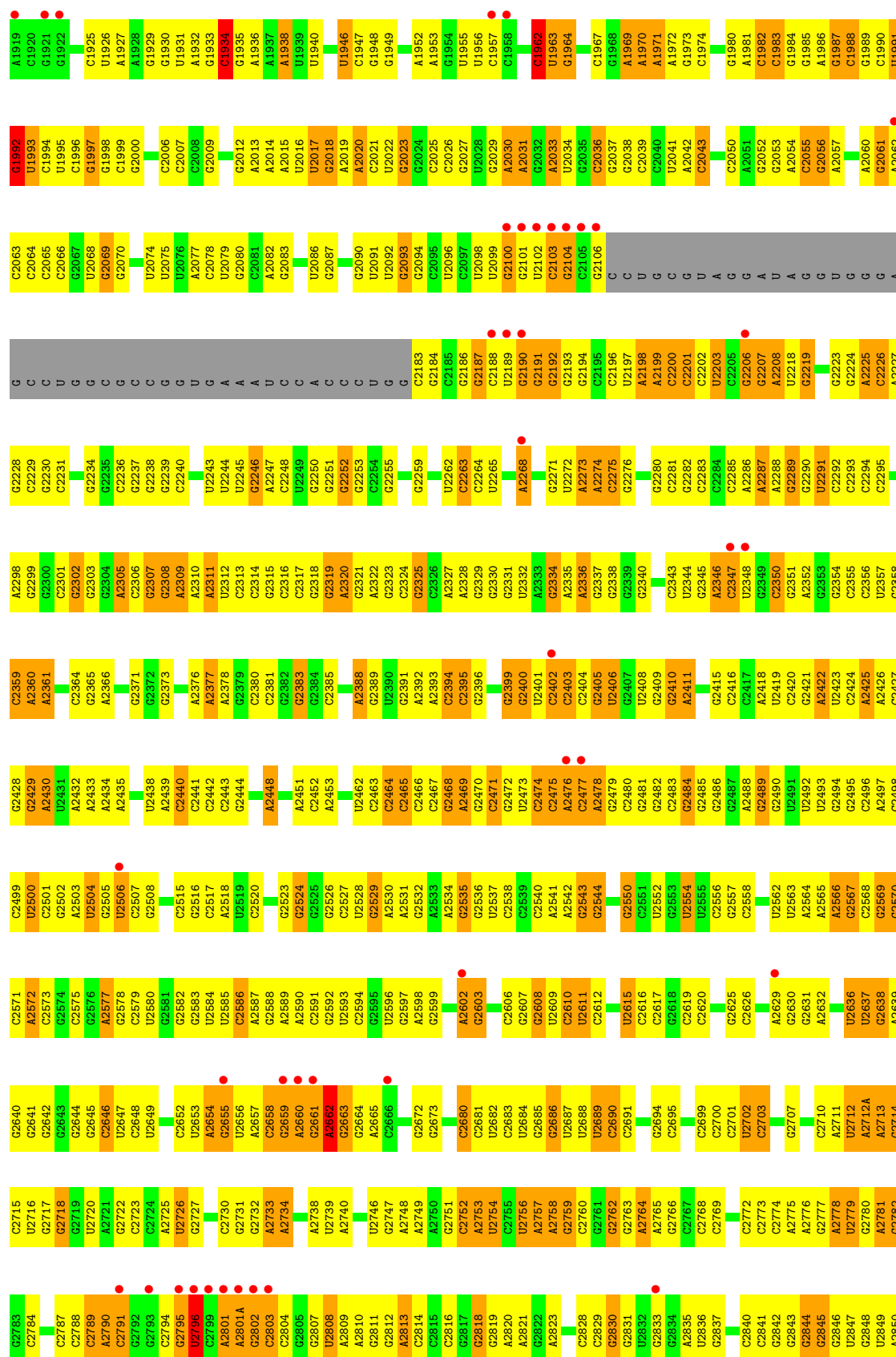
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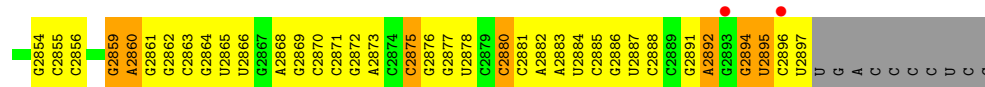
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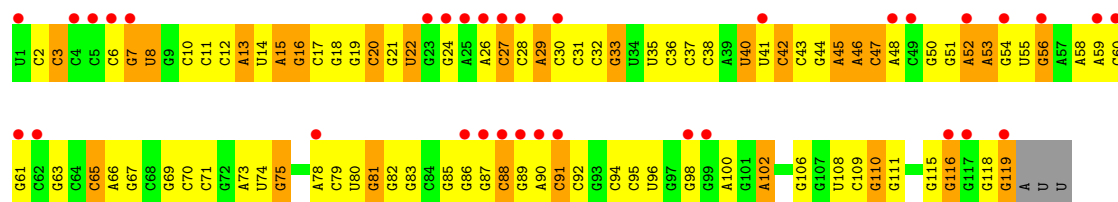


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C1831	U1766	C1675	A1610	C1532	G1473	G1473	U1407	U1340	G1277	A1210	G1144	G1025
G1833	C1767	G1678	C1613	C1533	A1474	G1474	C1408	U1341	A1278	U1211	C1145	U1026
U1834	U1768	U1679	G1613	G1534	A1475	G1475	C1409	G1344	G1279	G1212	C1146	A1027
G1835	C1771	U1680	G1614	A1544	G1476	G1476	G1410	A1214	G1280	A1148	A1148	A1029
A1912	G1772	G1681	C1615	C1545	G1477	G1477	C1411	C1345	G1281	G1149	G1149	G1030
A1913	C1773	C1682	C1616	C1546	G1478	G1478						
C1914	A1773	C1683	A1617	C1547	G1479	G1479						
U1915	C1774	C1684	A1618	C1548	G1480	G1480						
U1916	U1777	C1685	G1619	C1549	G1480	G1480						
U1917		C1686										
A1918		C1686										

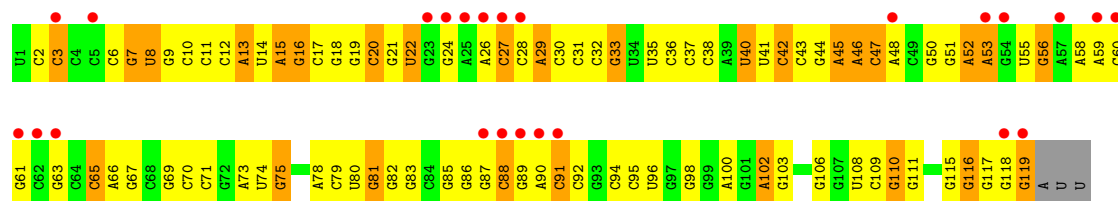




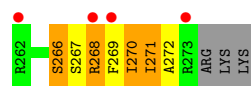
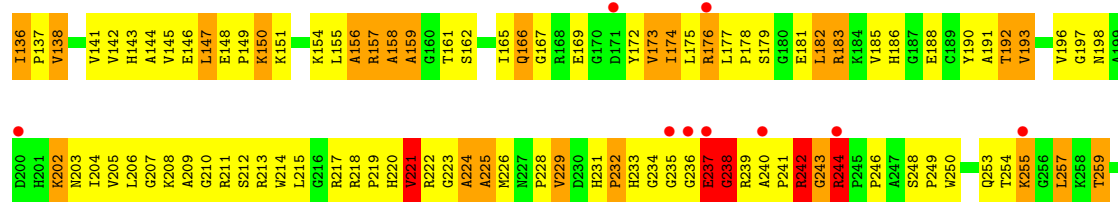
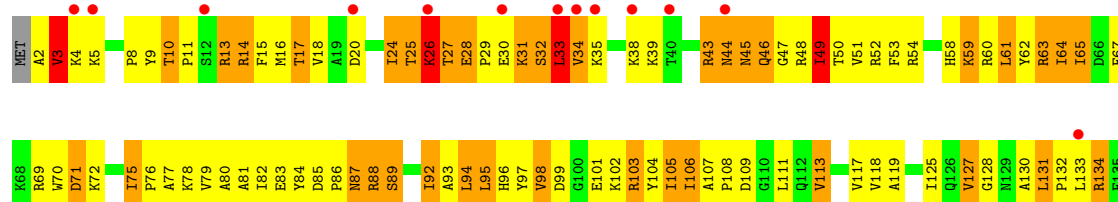
• Molecule 32: 5S ribosomal RNA



• Molecule 32: 5S ribosomal RNA

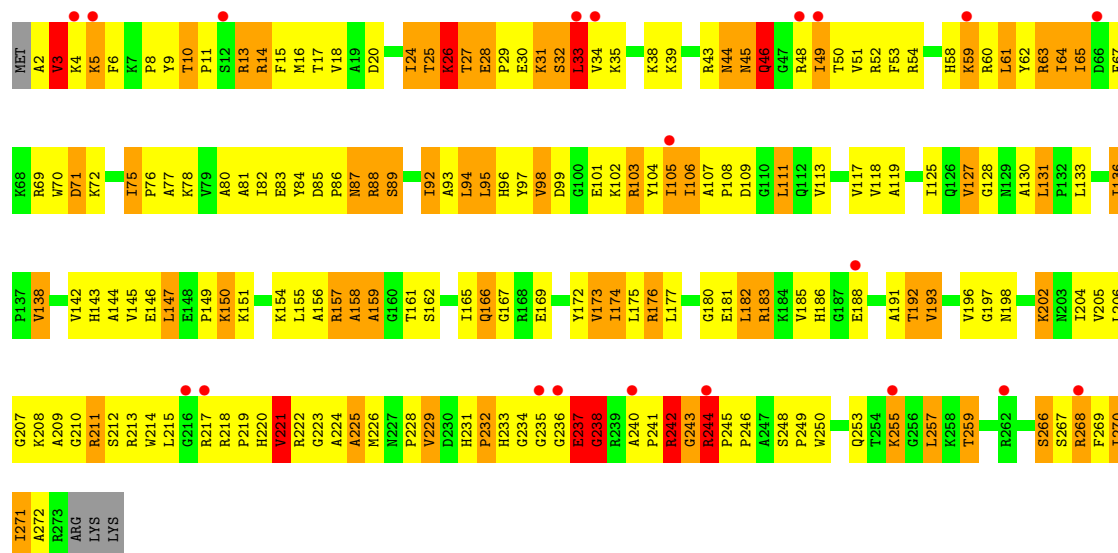


• Molecule 33: 50S ribosomal protein L2

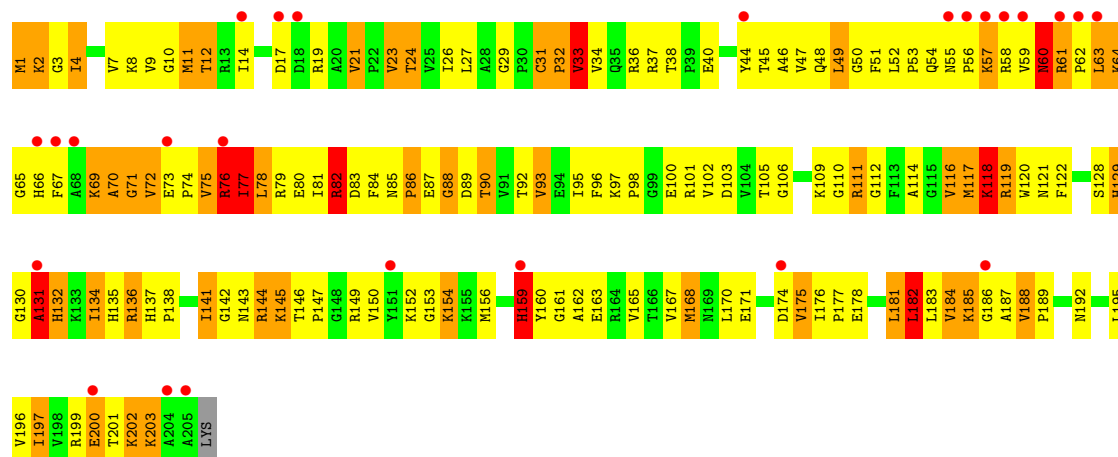


• Molecule 33: 50S ribosomal protein L2

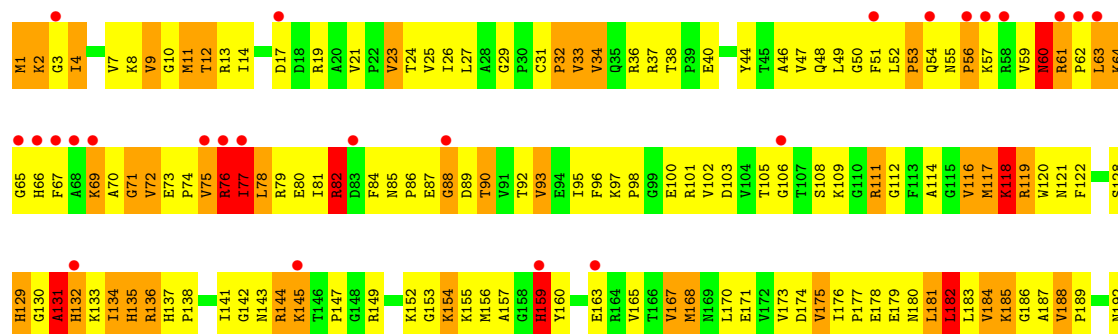




• Molecule 34: 50S ribosomal protein L3

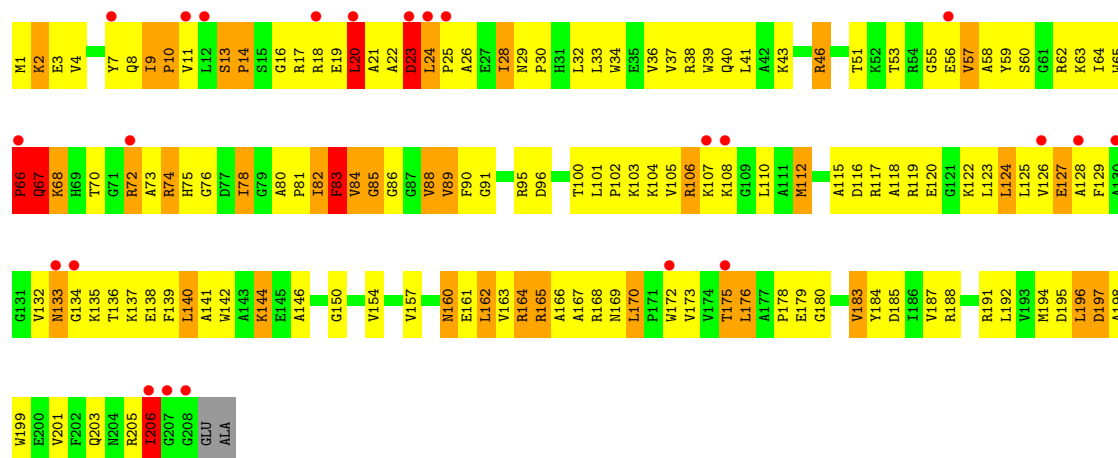


• Molecule 34: 50S ribosomal protein L3

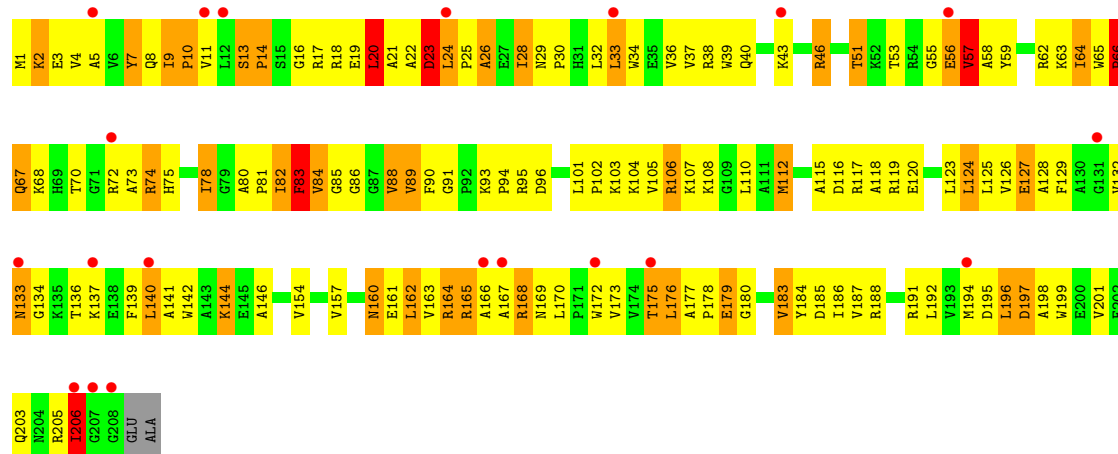




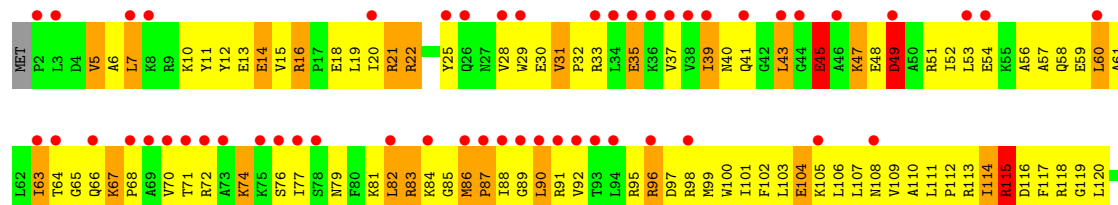
• Molecule 35: 50S ribosomal protein L4



• Molecule 35: 50S ribosomal protein L4

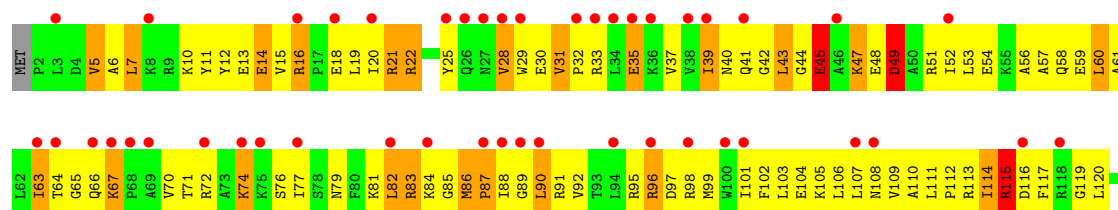


• Molecule 36: 50S ribosomal protein L5

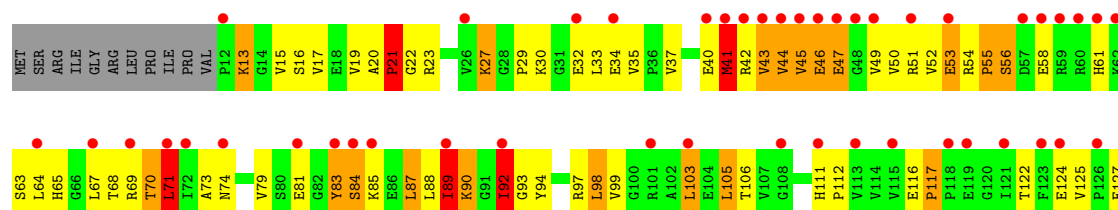




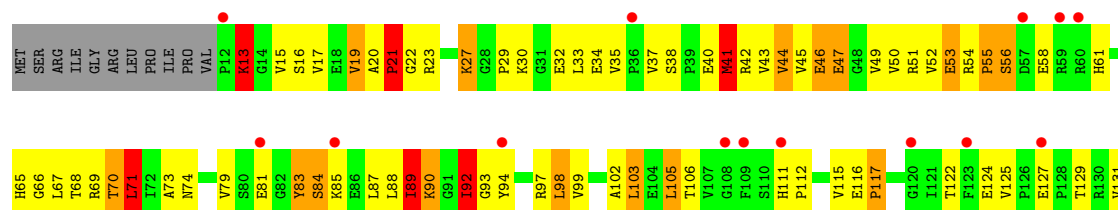
• Molecule 36: 50S ribosomal protein L5



• Molecule 37: 50S ribosomal protein L6

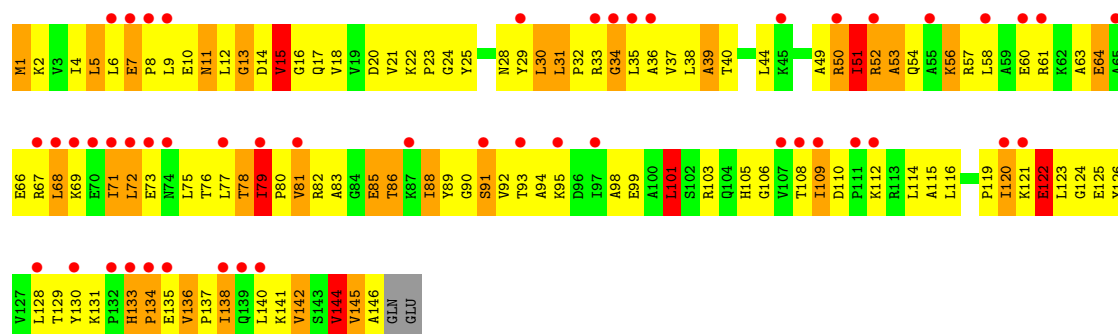


• Molecule 37: 50S ribosomal protein L6

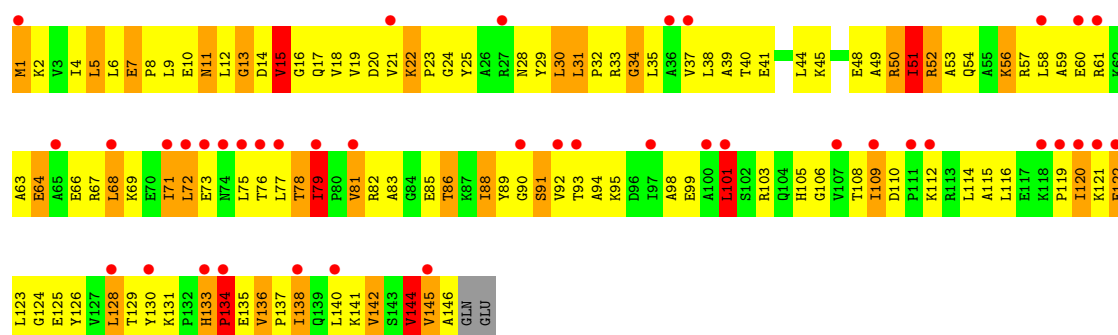


• Molecule 38: 50S ribosomal protein L9

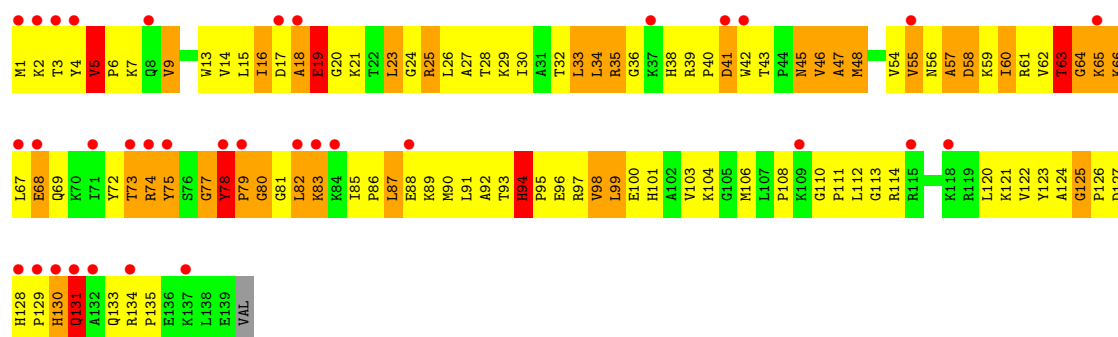




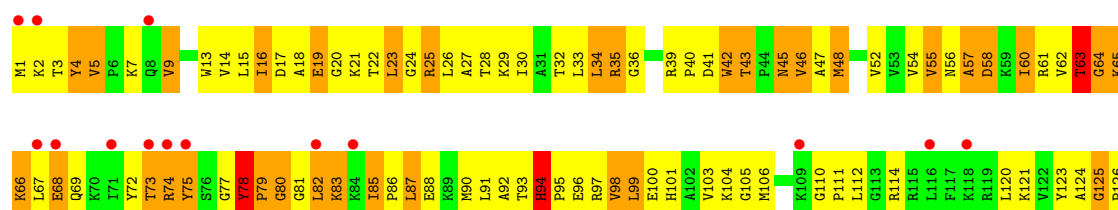
• Molecule 38: 50S ribosomal protein L9



• Molecule 39: 50S ribosomal protein L13

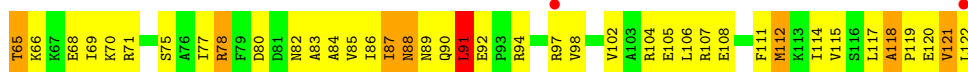
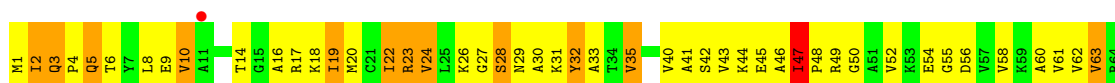


• Molecule 39: 50S ribosomal protein L13





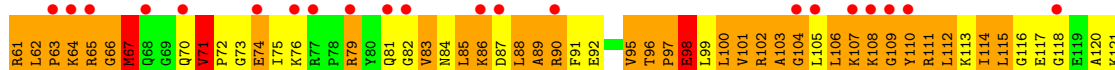
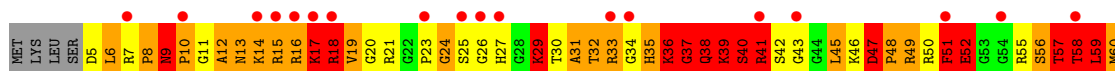
- Molecule 40: 50S ribosomal protein L14



- Molecule 40: 50S ribosomal protein L14



- Molecule 41: 50S ribosomal protein L15

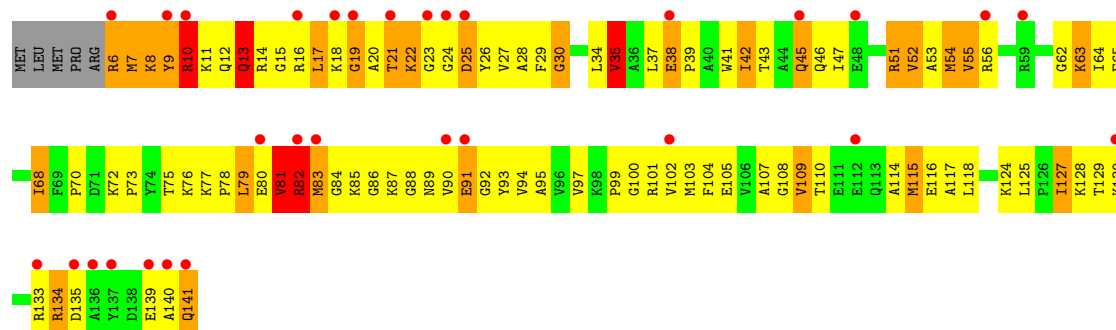


- Molecule 41: 50S ribosomal protein L15

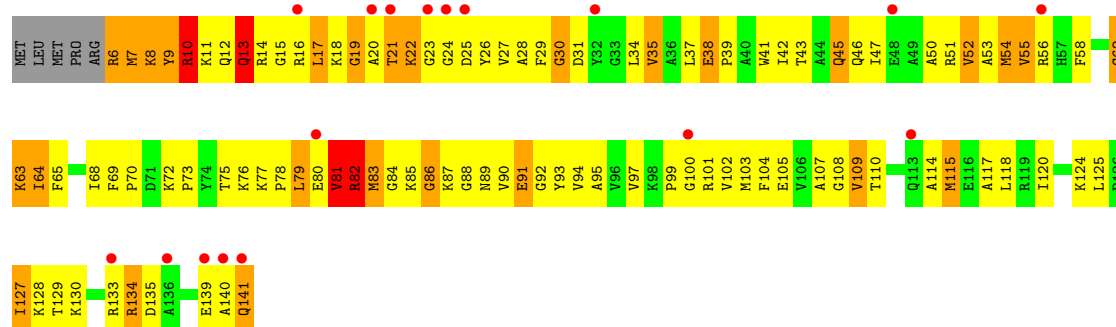




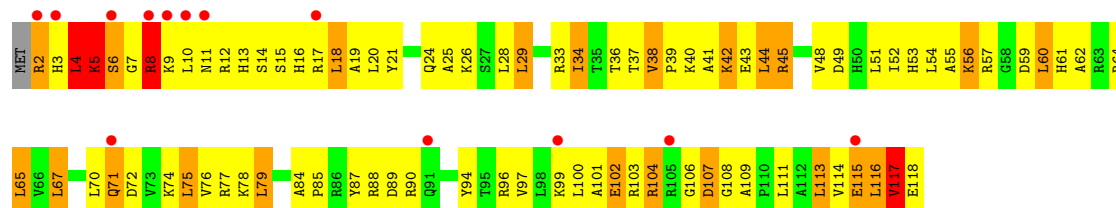
• Molecule 42: 50S ribosomal protein L16



• Molecule 42: 50S ribosomal protein L16

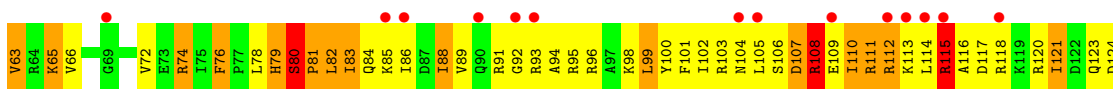


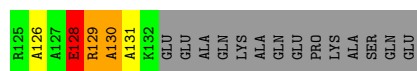
• Molecule 43: 50S ribosomal protein L17



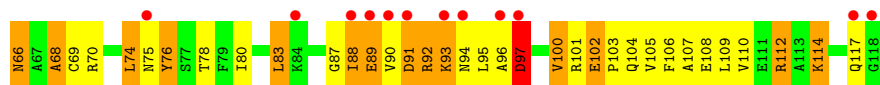
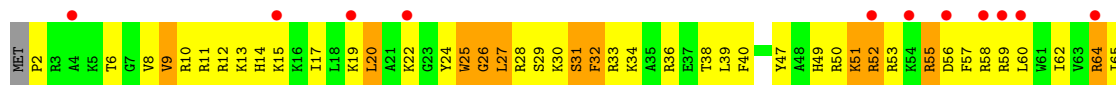
• Molecule 43: 50S ribosomal protein L17



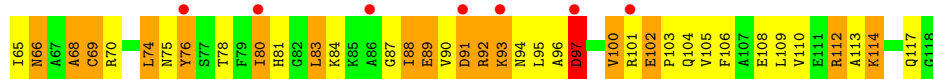
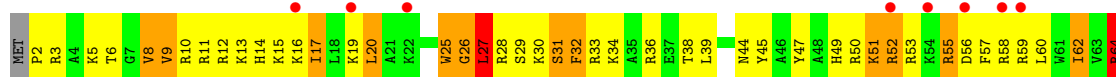




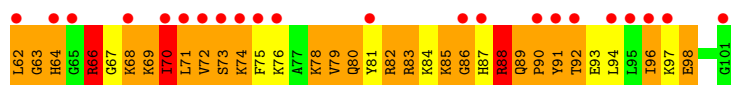
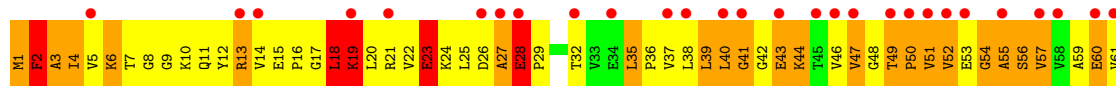
• Molecule 46: 50S ribosomal protein L20



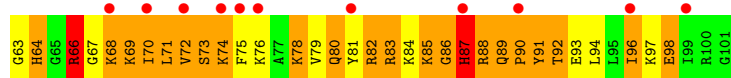
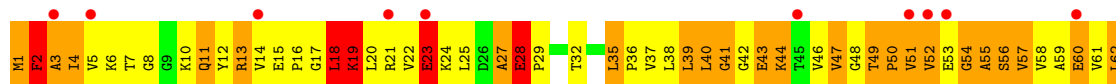
• Molecule 46: 50S ribosomal protein L20



• Molecule 47: 50S ribosomal protein L21

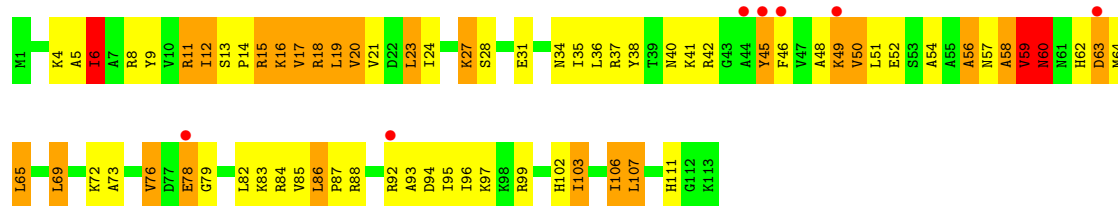


• Molecule 47: 50S ribosomal protein L21

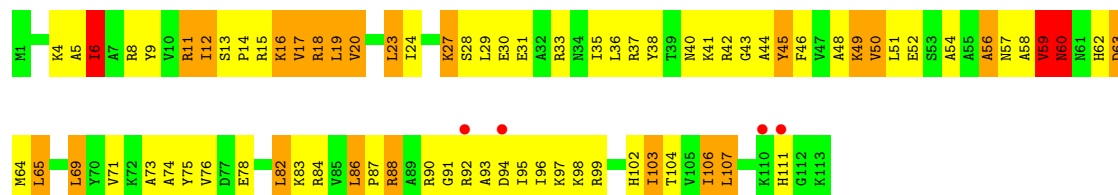


• Molecule 48: 50S ribosomal protein L22

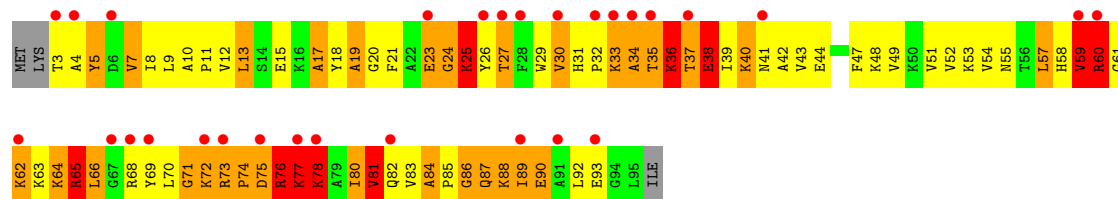
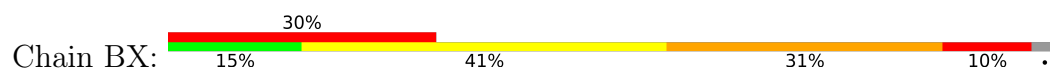




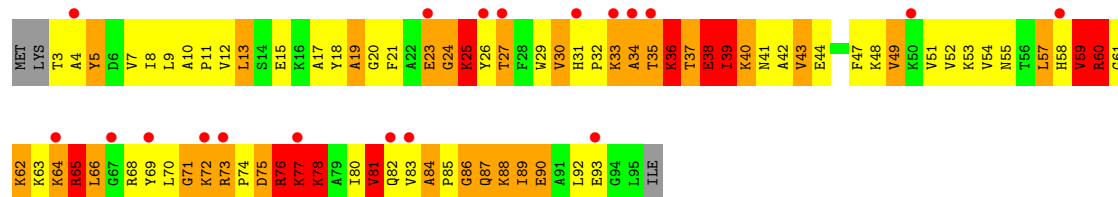
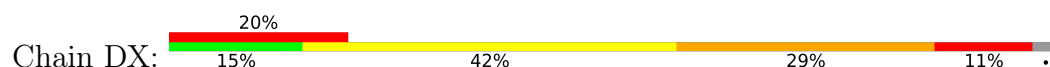
• Molecule 48: 50S ribosomal protein L22



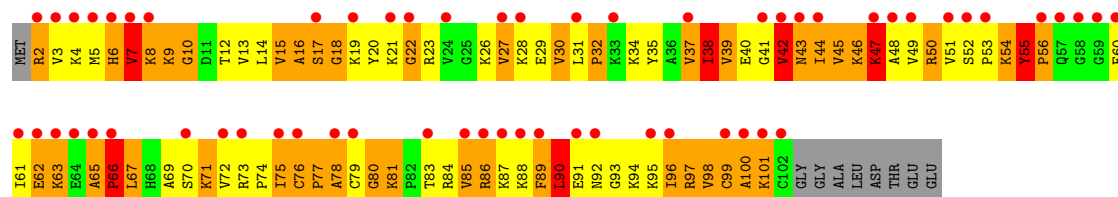
• Molecule 49: 50S ribosomal protein L23



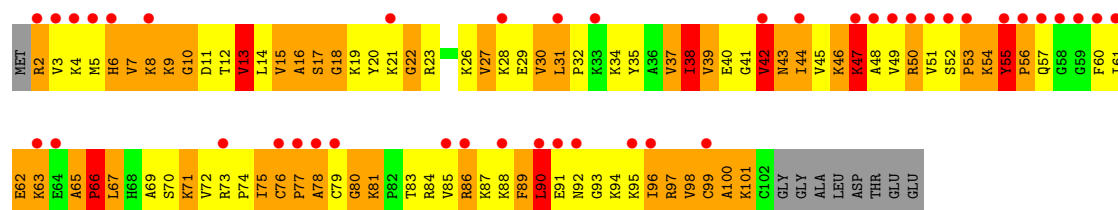
• Molecule 49: 50S ribosomal protein L23



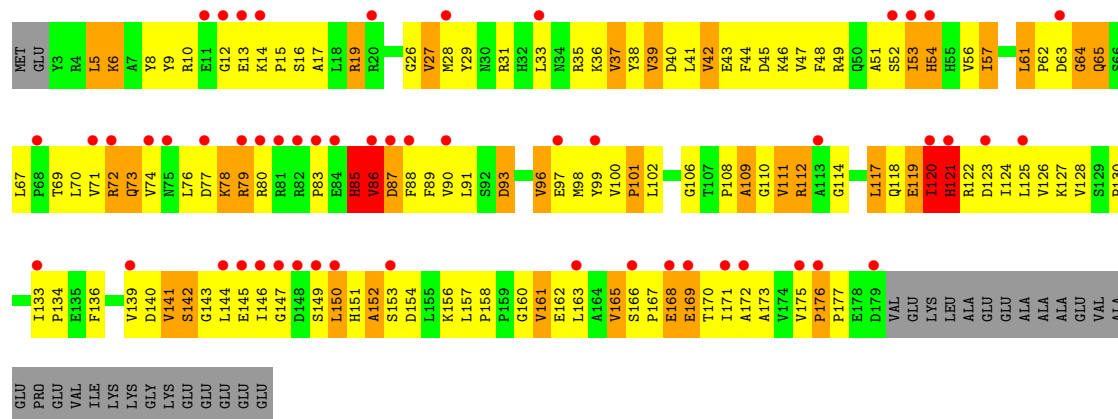
• Molecule 50: 50S ribosomal protein L24



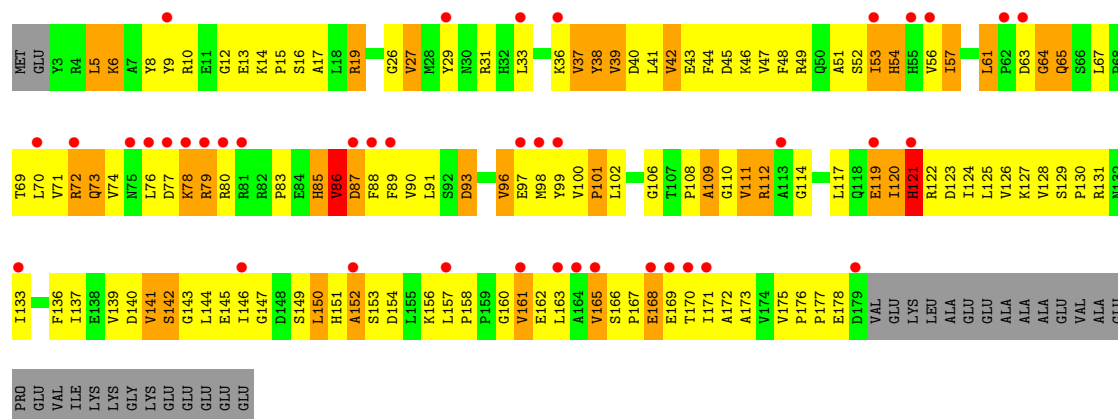
Chain DY:



Chain BZ:



Chain DZ:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.22Å 450.25Å 623.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.80 – 3.00 49.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.80-3.00) 88.7 (49.80-3.00)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.235 , 0.269 0.232 , 0.265	Depositor DCC
R_{free} test set	51892 reflections (4.45%)	wwPDB-VP
Wilson B-factor (Å ²)	73.9	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 101.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	278000	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: K, MG, ZN, ZIT

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	0.29	0/36190	0.39	0/56486
1	CA	0.29	0/36190	0.39	0/56486
2	AB	0.37	0/1936	0.86	4/2611 (0.2%)
2	CB	0.37	0/1936	0.85	5/2611 (0.2%)
3	AC	0.37	0/1637	0.84	5/2207 (0.2%)
3	CC	0.36	0/1637	0.83	5/2207 (0.2%)
4	AD	0.42	0/1733	0.87	6/2318 (0.3%)
4	CD	0.42	0/1733	0.88	7/2318 (0.3%)
5	AE	0.46	0/1163	0.90	1/1566 (0.1%)
5	CE	0.43	0/1163	0.90	2/1566 (0.1%)
6	AF	0.45	0/856	0.82	0/1154
6	CF	0.44	0/856	0.81	0/1154
7	AG	0.35	0/1276	0.78	0/1709
7	CG	0.36	0/1276	0.79	0/1709
8	AH	0.44	0/1136	0.88	2/1527 (0.1%)
8	CH	0.43	0/1136	0.86	2/1527 (0.1%)
9	AI	0.35	0/1028	0.76	0/1375
9	CI	0.35	0/1028	0.74	0/1375
10	AJ	0.41	0/808	0.83	0/1087
10	CJ	0.40	0/808	0.84	0/1087
11	AK	0.40	0/900	0.85	3/1213 (0.2%)
11	CK	0.41	0/900	0.86	4/1213 (0.3%)
12	AL	0.50	0/987	0.90	3/1322 (0.2%)
12	CL	0.51	0/987	0.90	0/1322
13	AM	0.36	0/928	0.83	4/1238 (0.3%)
13	CM	0.37	0/928	0.85	3/1238 (0.2%)
14	AN	0.35	0/501	0.75	0/664
14	CN	0.34	0/501	0.75	0/664
15	AO	0.46	0/745	0.84	0/992
15	CO	0.42	0/745	0.85	0/992
16	AP	0.41	0/717	0.85	2/965 (0.2%)
16	CP	0.44	0/717	0.85	3/965 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.41	0/837	0.92	3/1119 (0.3%)
17	CQ	0.42	0/837	0.94	4/1119 (0.4%)
18	AR	0.43	0/579	0.98	4/768 (0.5%)
18	CR	0.43	0/579	0.96	5/768 (0.7%)
19	AS	0.40	0/643	0.78	0/867
19	CS	0.39	0/643	0.78	0/867
20	AT	0.44	0/765	0.91	1/1007 (0.1%)
20	CT	0.44	0/765	0.90	1/1007 (0.1%)
21	AU	0.37	0/213	0.78	0/279
21	CU	0.37	0/213	0.77	0/279
22	B0	0.74	0/658	1.18	3/878 (0.3%)
22	D0	0.61	0/658	1.17	4/878 (0.5%)
23	B1	0.98	0/700	1.42	11/931 (1.2%)
23	D1	0.87	1/700 (0.1%)	1.38	11/931 (1.2%)
24	B2	0.94	0/423	1.20	5/560 (0.9%)
24	D2	0.74	0/423	1.19	2/560 (0.4%)
25	B3	0.78	0/473	1.13	3/636 (0.5%)
25	D3	0.59	0/473	1.12	2/636 (0.3%)
26	B4	0.49	0/156	1.30	3/215 (1.4%)
26	D4	0.50	0/156	1.31	3/215 (1.4%)
27	B5	1.03	0/473	1.87	12/639 (1.9%)
27	D5	0.89	0/473	1.72	9/639 (1.4%)
28	B6	0.95	0/387	1.29	2/517 (0.4%)
28	D6	0.81	0/387	1.26	2/517 (0.4%)
29	B7	0.84	0/427	1.04	0/563
29	D7	0.68	0/427	1.05	0/563
30	B8	0.97	0/516	1.51	11/681 (1.6%)
30	D8	0.81	0/516	1.44	8/681 (1.2%)
31	BA	0.61	5/65745 (0.0%)	0.55	13/102639 (0.0%)
31	DA	0.48	4/65745 (0.0%)	0.53	12/102639 (0.0%)
32	BB	0.50	0/2853	0.50	0/4451
32	DB	0.40	0/2853	0.48	0/4451
33	BD	0.80	0/2155	1.20	16/2907 (0.6%)
33	DD	0.72	1/2155 (0.0%)	1.19	13/2907 (0.4%)
34	BE	0.83	1/1597 (0.1%)	1.18	9/2155 (0.4%)
34	DE	0.73	0/1597	1.16	7/2155 (0.3%)
35	BF	0.83	0/1659	1.14	7/2246 (0.3%)
35	DF	0.64	1/1659 (0.1%)	1.12	10/2246 (0.4%)
36	BG	0.43	0/1498	0.87	4/2013 (0.2%)
36	DG	0.40	0/1498	0.86	4/2013 (0.2%)
37	BH	0.79	0/1246	1.08	7/1684 (0.4%)
37	DH	0.54	0/1246	1.01	6/1684 (0.4%)
38	BI	0.56	0/1147	0.96	7/1553 (0.5%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
38	DI	0.51	0/1147	0.94	6/1553 (0.4%)
39	BN	0.87	0/1132	1.26	14/1527 (0.9%)
39	DN	0.66	0/1132	1.17	9/1527 (0.6%)
40	BO	0.71	0/943	1.09	4/1269 (0.3%)
40	DO	0.60	0/943	1.06	4/1269 (0.3%)
41	BP	0.92	1/1131 (0.1%)	1.42	14/1504 (0.9%)
41	DP	0.77	1/1131 (0.1%)	1.33	15/1504 (1.0%)
42	BQ	0.86	0/1100	1.28	7/1470 (0.5%)
42	DQ	0.73	0/1100	1.19	7/1470 (0.5%)
43	BR	0.91	2/974 (0.2%)	1.18	3/1302 (0.2%)
43	DR	0.74	0/974	1.18	8/1302 (0.6%)
44	BS	0.71	0/779	1.12	3/1038 (0.3%)
44	DS	0.56	0/779	1.07	4/1038 (0.4%)
45	BT	0.79	0/1114	1.29	16/1488 (1.1%)
45	DT	0.66	1/1114 (0.1%)	1.27	18/1488 (1.2%)
46	BU	0.96	0/975	1.08	3/1297 (0.2%)
46	DU	0.70	0/975	1.04	5/1297 (0.4%)
47	BV	0.97	1/789 (0.1%)	1.36	11/1054 (1.0%)
47	DV	0.74	0/789	1.26	5/1054 (0.5%)
48	BW	0.88	0/907	1.17	6/1216 (0.5%)
48	DW	0.74	0/907	1.13	4/1216 (0.3%)
49	BX	0.99	0/740	1.36	13/995 (1.3%)
49	DX	0.85	1/740 (0.1%)	1.30	11/995 (1.1%)
50	BY	0.90	1/789 (0.1%)	1.31	12/1053 (1.1%)
50	DY	0.76	1/789 (0.1%)	1.28	13/1053 (1.2%)
51	BZ	0.63	0/1436	1.01	10/1951 (0.5%)
51	DZ	0.49	0/1436	1.00	8/1951 (0.4%)
All	All	0.52	22/301000 (0.0%)	0.69	518/449812 (0.1%)

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
23	B1	0	1
23	D1	0	1
24	B2	0	3
24	D2	0	1
27	B5	0	1
27	D5	0	1
31	BA	21	0

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Mol	Chain	#Chirality outliers	#Planarity outliers
31	DA	21	0
33	BD	0	2
33	DD	0	2
34	BE	0	2
34	DE	0	2
35	BF	0	1
37	BH	0	2
37	DH	0	2
41	BP	0	5
41	DP	0	4
42	BQ	0	1
42	DQ	0	1
43	BR	0	1
43	DR	0	1
44	BS	0	1
44	DS	0	1
45	BT	0	1
45	DT	0	1
47	BV	0	1
47	DV	0	2
49	BX	0	3
49	DX	0	3
All	All	42	47

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	BA	669	G	C4'-C3'	-8.47	1.40	1.53
31	DA	669	G	C4'-C3'	-6.99	1.42	1.53
31	BA	1300	U	C4'-C3'	-6.73	1.43	1.53
43	BR	38	VAL	CA-CB	-6.71	1.50	1.54
31	DA	1300	U	C4'-C3'	-6.64	1.43	1.53

The worst 5 of 518 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	B5	46	CYS	CA-C-N	16.33	140.25	119.84
27	B5	46	CYS	C-N-CA	16.33	140.25	119.84
27	D5	46	CYS	CA-C-N	14.91	138.48	119.84
27	D5	46	CYS	C-N-CA	14.91	138.48	119.84
41	BP	59	LEU	N-CA-C	-13.90	95.64	112.59

5 of 42 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	BA	100	G	C1'
31	BA	472	A	C3'
31	BA	669	G	C1',C3',C4'
31	BA	945	A	C1'
31	BA	1300	U	C1',C3',C4'

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	B1	30	VAL	Peptide
24	B2	55	ARG	Peptide
24	B2	56	GLN	Peptide
24	B2	57	ILE	Peptide
27	B5	51	TYR	Peptide

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	32329	0	16318	1411	0
1	CA	32329	0	16318	1383	0
2	AB	1901	0	1951	177	0
2	CB	1901	0	1951	175	0
3	AC	1613	0	1677	119	0
3	CC	1613	0	1677	120	0
4	AD	1703	0	1763	175	0
4	CD	1703	0	1763	175	0
5	AE	1147	0	1207	113	0
5	CE	1147	0	1207	119	0
6	AF	843	0	857	83	0
6	CF	843	0	857	90	0
7	AG	1257	0	1296	60	0
7	CG	1257	0	1296	63	0
8	AH	1116	0	1177	89	0
8	CH	1116	0	1177	89	0
9	AI	1011	0	1042	87	0
9	CI	1011	0	1042	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	AJ	795	0	840	85	0
10	CJ	795	0	840	87	0
11	AK	885	0	904	67	0
11	CK	885	0	904	73	0
12	AL	971	0	1057	111	0
12	CL	971	0	1057	110	0
13	AM	921	0	976	64	0
13	CM	921	0	976	68	0
14	AN	492	0	530	35	0
14	CN	492	0	529	35	0
15	AO	734	0	771	61	0
15	CO	734	0	771	60	0
16	AP	701	0	720	95	0
16	CP	701	0	720	97	0
17	AQ	824	0	891	48	0
17	CQ	824	0	891	50	0
18	AR	574	0	644	63	0
18	CR	574	0	644	64	0
19	AS	630	0	652	42	0
19	CS	630	0	652	36	0
20	AT	763	0	861	81	0
20	CT	763	0	861	84	0
21	AU	209	0	221	12	0
21	CU	209	0	221	12	0
22	B0	650	0	654	71	0
22	D0	650	0	654	67	0
23	B1	693	0	764	150	0
23	D1	693	0	764	147	0
24	B2	421	0	461	124	1
24	D2	421	0	461	128	0
25	B3	468	0	523	38	0
25	D3	468	0	523	54	0
26	B4	157	0	69	15	0
26	D4	157	0	69	15	0
27	B5	459	0	478	88	0
27	D5	459	0	480	88	0
28	B6	381	0	390	97	0
28	D6	381	0	390	93	0
29	B7	419	0	467	40	0
29	D7	419	0	467	41	0
30	B8	508	0	576	158	0
30	D8	508	0	576	147	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	BA	58698	0	29590	2399	0
31	DA	58698	0	29591	2594	1
32	BB	2551	0	1295	154	0
32	DB	2551	0	1295	171	0
33	BD	2105	0	2182	348	0
33	DD	2105	0	2182	343	0
34	BE	1564	0	1629	219	0
34	DE	1564	0	1629	221	0
35	BF	1624	0	1677	183	0
35	DF	1624	0	1677	186	0
36	BG	1474	0	1534	158	0
36	DG	1474	0	1534	158	0
37	BH	1223	0	1282	144	0
37	DH	1223	0	1282	133	0
38	BI	1132	0	1218	145	0
38	DI	1132	0	1218	163	0
39	BN	1105	0	1180	187	0
39	DN	1105	0	1180	189	0
40	BO	933	0	996	89	0
40	DO	933	0	996	81	0
41	BP	1114	0	1187	277	0
41	DP	1114	0	1187	266	0
42	BQ	1080	0	1127	167	0
42	DQ	1080	0	1127	167	0
43	BR	960	0	1021	123	0
43	DR	960	0	1021	123	0
44	BS	771	0	832	152	0
44	DS	771	0	832	153	0
45	BT	1100	0	1164	184	0
45	DT	1100	0	1164	174	0
46	BU	958	0	1015	150	0
46	DU	958	0	1015	161	0
47	BV	779	0	851	221	0
47	DV	779	0	851	226	0
48	BW	896	0	953	78	0
48	DW	896	0	953	86	0
49	BX	726	0	778	172	0
49	DX	726	0	778	174	0
50	BY	776	0	870	184	0
50	DY	776	0	870	191	0
51	BZ	1404	0	1432	148	0
51	DZ	1404	0	1432	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	AA	51	0	0	0	0
52	B0	1	0	0	0	0
52	B1	1	0	0	0	0
52	B5	2	0	0	0	0
52	B7	1	0	0	0	0
52	BA	349	0	0	0	0
52	BB	5	0	0	0	0
52	BD	1	0	0	0	0
52	BE	1	0	0	0	0
52	BF	1	0	0	0	0
52	BP	3	0	0	0	0
52	BQ	2	0	0	0	0
52	BR	1	0	0	0	0
52	BU	1	0	0	0	0
52	BX	1	0	0	0	0
52	CA	48	0	0	0	0
52	D0	1	0	0	0	0
52	D1	1	0	0	0	0
52	D5	2	0	0	0	0
52	D7	1	0	0	0	0
52	DA	309	0	0	0	0
52	DB	3	0	0	0	0
52	DD	1	0	0	0	0
52	DE	1	0	0	0	0
52	DF	1	0	0	0	0
52	DP	1	0	0	0	0
52	DQ	1	0	0	0	0
52	DR	1	0	0	0	0
52	DU	1	0	0	0	0
52	DX	1	0	0	0	0
53	AD	1	0	0	0	0
53	AN	1	0	0	0	0
53	CD	1	0	0	0	0
53	CN	1	0	0	0	0
54	BA	1	0	0	0	0
54	DA	1	0	0	0	0
55	BA	52	0	72	3	0
55	DA	52	0	72	3	0
All	All	278000	0	189246	17928	1

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 39.

The worst 5 of 17928 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)
42:BQ:81:VAL:O	42:BQ:82:ARG:HG2	1.13	1.31
42:DQ:81:VAL:O	42:DQ:82:ARG:HG2	1.25	1.27
41:BP:59:LEU:HA	41:BP:61:ARG:NH1	1.49	1.25
41:DP:59:LEU:HA	41:DP:61:ARG:NH1	1.55	1.20
31:DA:2206:G:N2	31:DA:2207:G:H5'	1.58	1.19

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:B2:12:GLU:CB	31:DA:306:U:OP1[1_455]	2.15	0.05

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%)	178 (76%)	38 (16%)	17 (7%)	1	4
2	CB	233/256 (91%)	177 (76%)	39 (17%)	17 (7%)	1	4
3	AC	205/239 (86%)	155 (76%)	36 (18%)	14 (7%)	1	5
3	CC	205/239 (86%)	155 (76%)	37 (18%)	13 (6%)	1	6
4	AD	206/209 (99%)	138 (67%)	52 (25%)	16 (8%)	1	4
4	CD	206/209 (99%)	137 (66%)	55 (27%)	14 (7%)	1	5
5	AE	149/162 (92%)	105 (70%)	31 (21%)	13 (9%)	0	3
5	CE	149/162 (92%)	103 (69%)	33 (22%)	13 (9%)	0	3
6	AF	99/101 (98%)	76 (77%)	15 (15%)	8 (8%)	1	3
6	CF	99/101 (98%)	76 (77%)	14 (14%)	9 (9%)	0	2
7	AG	153/156 (98%)	130 (85%)	19 (12%)	4 (3%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	CG	153/156 (98%)	131 (86%)	18 (12%)	4 (3%)	4	23
8	AH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	1	10
8	CH	136/138 (99%)	98 (72%)	31 (23%)	7 (5%)	1	10
9	AI	123/128 (96%)	92 (75%)	24 (20%)	7 (6%)	1	8
9	CI	123/128 (96%)	94 (76%)	22 (18%)	7 (6%)	1	8
10	AJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	1	9
10	CJ	97/105 (92%)	81 (84%)	11 (11%)	5 (5%)	1	9
11	AK	117/129 (91%)	87 (74%)	26 (22%)	4 (3%)	3	17
11	CK	117/129 (91%)	86 (74%)	27 (23%)	4 (3%)	3	17
12	AL	123/135 (91%)	82 (67%)	31 (25%)	10 (8%)	1	3
12	CL	123/135 (91%)	83 (68%)	29 (24%)	11 (9%)	0	3
13	AM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	1	8
13	CM	107/126 (85%)	84 (78%)	17 (16%)	6 (6%)	1	8
14	AN	58/61 (95%)	45 (78%)	11 (19%)	2 (3%)	3	17
14	CN	58/61 (95%)	44 (76%)	12 (21%)	2 (3%)	3	17
15	AO	86/89 (97%)	62 (72%)	19 (22%)	5 (6%)	1	8
15	CO	86/89 (97%)	61 (71%)	21 (24%)	4 (5%)	2	11
16	AP	82/88 (93%)	48 (58%)	27 (33%)	7 (8%)	0	3
16	CP	82/88 (93%)	47 (57%)	29 (35%)	6 (7%)	1	4
17	AQ	98/105 (93%)	74 (76%)	18 (18%)	6 (6%)	1	7
17	CQ	98/105 (93%)	73 (74%)	19 (19%)	6 (6%)	1	7
18	AR	68/88 (77%)	52 (76%)	11 (16%)	5 (7%)	1	4
18	CR	68/88 (77%)	51 (75%)	13 (19%)	4 (6%)	1	7
19	AS	77/93 (83%)	58 (75%)	13 (17%)	6 (8%)	1	4
19	CS	77/93 (83%)	59 (77%)	12 (16%)	6 (8%)	1	4
20	AT	97/106 (92%)	69 (71%)	19 (20%)	9 (9%)	0	2
20	CT	97/106 (92%)	65 (67%)	23 (24%)	9 (9%)	0	2
21	AU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	12
21	CU	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	2	12
22	B0	83/85 (98%)	65 (78%)	14 (17%)	4 (5%)	2	11
22	D0	83/85 (98%)	64 (77%)	15 (18%)	4 (5%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	B1	87/98 (89%)	48 (55%)	17 (20%)	22 (25%)	0	0
23	D1	87/98 (89%)	45 (52%)	19 (22%)	23 (26%)	0	0
24	B2	49/72 (68%)	23 (47%)	19 (39%)	7 (14%)	0	1
24	D2	49/72 (68%)	23 (47%)	18 (37%)	8 (16%)	0	0
25	B3	58/60 (97%)	52 (90%)	4 (7%)	2 (3%)	3	17
25	D3	58/60 (97%)	51 (88%)	5 (9%)	2 (3%)	3	17
26	B4	30/71 (42%)	5 (17%)	11 (37%)	14 (47%)	0	0
26	D4	30/71 (42%)	5 (17%)	10 (33%)	15 (50%)	0	0
27	B5	57/60 (95%)	38 (67%)	11 (19%)	8 (14%)	0	1
27	D5	57/60 (95%)	36 (63%)	14 (25%)	7 (12%)	0	1
28	B6	41/54 (76%)	21 (51%)	6 (15%)	14 (34%)	0	0
28	D6	41/54 (76%)	19 (46%)	8 (20%)	14 (34%)	0	0
29	B7	47/49 (96%)	41 (87%)	4 (8%)	2 (4%)	2	12
29	D7	47/49 (96%)	40 (85%)	4 (8%)	3 (6%)	1	6
30	B8	62/65 (95%)	42 (68%)	11 (18%)	9 (14%)	0	1
30	D8	62/65 (95%)	41 (66%)	12 (19%)	9 (14%)	0	1
33	BD	270/276 (98%)	208 (77%)	45 (17%)	17 (6%)	1	6
33	DD	270/276 (98%)	207 (77%)	47 (17%)	16 (6%)	1	7
34	BE	203/206 (98%)	138 (68%)	37 (18%)	28 (14%)	0	1
34	DE	203/206 (98%)	138 (68%)	38 (19%)	27 (13%)	0	1
35	BF	206/210 (98%)	160 (78%)	30 (15%)	16 (8%)	1	4
35	DF	206/210 (98%)	156 (76%)	33 (16%)	17 (8%)	0	3
36	BG	177/182 (97%)	128 (72%)	35 (20%)	14 (8%)	1	3
36	DG	177/182 (97%)	127 (72%)	36 (20%)	14 (8%)	1	3
37	BH	158/180 (88%)	92 (58%)	41 (26%)	25 (16%)	0	0
37	DH	158/180 (88%)	93 (59%)	39 (25%)	26 (16%)	0	0
38	BI	144/148 (97%)	88 (61%)	32 (22%)	24 (17%)	0	0
38	DI	144/148 (97%)	87 (60%)	35 (24%)	22 (15%)	0	0
39	BN	137/140 (98%)	87 (64%)	32 (23%)	18 (13%)	0	1
39	DN	137/140 (98%)	88 (64%)	32 (23%)	17 (12%)	0	1
40	BO	120/122 (98%)	101 (84%)	16 (13%)	3 (2%)	4	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	DO	120/122 (98%)	99 (82%)	17 (14%)	4 (3%)	3	17
41	BP	144/150 (96%)	77 (54%)	17 (12%)	50 (35%)	0	0
41	DP	144/150 (96%)	76 (53%)	18 (12%)	50 (35%)	0	0
42	BQ	134/141 (95%)	92 (69%)	28 (21%)	14 (10%)	0	2
42	DQ	134/141 (95%)	96 (72%)	23 (17%)	15 (11%)	0	1
43	BR	115/118 (98%)	78 (68%)	29 (25%)	8 (7%)	1	4
43	DR	115/118 (98%)	82 (71%)	24 (21%)	9 (8%)	1	4
44	BS	97/112 (87%)	49 (50%)	24 (25%)	24 (25%)	0	0
44	DS	97/112 (87%)	49 (50%)	23 (24%)	25 (26%)	0	0
45	BT	130/146 (89%)	89 (68%)	21 (16%)	20 (15%)	0	0
45	DT	130/146 (89%)	90 (69%)	21 (16%)	19 (15%)	0	0
46	BU	115/118 (98%)	77 (67%)	27 (24%)	11 (10%)	0	2
46	DU	115/118 (98%)	74 (64%)	29 (25%)	12 (10%)	0	2
47	BV	97/101 (96%)	54 (56%)	15 (16%)	28 (29%)	0	0
47	DV	97/101 (96%)	52 (54%)	18 (19%)	27 (28%)	0	0
48	BW	111/113 (98%)	88 (79%)	15 (14%)	8 (7%)	1	4
48	DW	111/113 (98%)	89 (80%)	15 (14%)	7 (6%)	1	6
49	BX	91/96 (95%)	47 (52%)	22 (24%)	22 (24%)	0	0
49	DX	91/96 (95%)	48 (53%)	22 (24%)	21 (23%)	0	0
50	BY	99/110 (90%)	45 (46%)	22 (22%)	32 (32%)	0	0
50	DY	99/110 (90%)	46 (46%)	21 (21%)	32 (32%)	0	0
51	BZ	175/206 (85%)	113 (65%)	43 (25%)	19 (11%)	0	1
51	DZ	175/206 (85%)	113 (65%)	44 (25%)	18 (10%)	0	2
All	All	11148/12060 (92%)	7735 (69%)	2187 (20%)	1226 (11%)	0	1

5 of 1226 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	24	TRP
2	AB	154	LEU
2	AB	165	VAL
2	AB	194	PRO

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%)	171 (85%)	31 (15%)	3	14
2	CB	202/220 (92%)	171 (85%)	31 (15%)	3	14
3	AC	160/188 (85%)	151 (94%)	9 (6%)	19	52
3	CC	160/188 (85%)	151 (94%)	9 (6%)	19	52
4	AD	180/181 (99%)	153 (85%)	27 (15%)	3	14
4	CD	180/181 (99%)	153 (85%)	27 (15%)	3	14
5	AE	115/123 (94%)	96 (84%)	19 (16%)	2	12
5	CE	115/123 (94%)	97 (84%)	18 (16%)	2	13
6	AF	90/90 (100%)	79 (88%)	11 (12%)	5	21
6	CF	90/90 (100%)	79 (88%)	11 (12%)	5	21
7	AG	126/127 (99%)	121 (96%)	5 (4%)	28	62
7	CG	126/127 (99%)	121 (96%)	5 (4%)	28	62
8	AH	119/119 (100%)	104 (87%)	15 (13%)	4	20
8	CH	119/119 (100%)	104 (87%)	15 (13%)	4	20
9	AI	98/99 (99%)	89 (91%)	9 (9%)	8	33
9	CI	98/99 (99%)	89 (91%)	9 (9%)	8	33
10	AJ	88/92 (96%)	83 (94%)	5 (6%)	18	52
10	CJ	88/92 (96%)	83 (94%)	5 (6%)	18	52
11	AK	90/99 (91%)	79 (88%)	11 (12%)	5	21
11	CK	90/99 (91%)	78 (87%)	12 (13%)	4	18
12	AL	104/111 (94%)	94 (90%)	10 (10%)	8	31
12	CL	104/111 (94%)	94 (90%)	10 (10%)	8	31
13	AM	93/101 (92%)	88 (95%)	5 (5%)	20	53
13	CM	93/101 (92%)	88 (95%)	5 (5%)	20	53
14	AN	49/50 (98%)	46 (94%)	3 (6%)	17	49
14	CN	49/50 (98%)	46 (94%)	3 (6%)	17	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	AO	79/80 (99%)	71 (90%)	8 (10%)	7	29
15	CO	79/80 (99%)	70 (89%)	9 (11%)	5	24
16	AP	72/74 (97%)	61 (85%)	11 (15%)	3	14
16	CP	72/74 (97%)	61 (85%)	11 (15%)	3	14
17	AQ	94/97 (97%)	89 (95%)	5 (5%)	20	54
17	CQ	94/97 (97%)	89 (95%)	5 (5%)	20	54
18	AR	61/77 (79%)	51 (84%)	10 (16%)	2	12
18	CR	61/77 (79%)	51 (84%)	10 (16%)	2	12
19	AS	69/80 (86%)	63 (91%)	6 (9%)	9	35
19	CS	69/80 (86%)	63 (91%)	6 (9%)	9	35
20	AT	76/82 (93%)	65 (86%)	11 (14%)	3	15
20	CT	76/82 (93%)	64 (84%)	12 (16%)	2	13
21	AU	19/22 (86%)	19 (100%)	0	100	100
21	CU	19/22 (86%)	19 (100%)	0	100	100
22	B0	61/67 (91%)	47 (77%)	14 (23%)	1	5
22	D0	61/67 (91%)	47 (77%)	14 (23%)	1	5
23	B1	73/83 (88%)	54 (74%)	19 (26%)	0	3
23	D1	73/83 (88%)	56 (77%)	17 (23%)	1	4
24	B2	46/67 (69%)	34 (74%)	12 (26%)	0	3
24	D2	46/67 (69%)	34 (74%)	12 (26%)	0	3
25	B3	51/52 (98%)	42 (82%)	9 (18%)	2	10
25	D3	51/52 (98%)	43 (84%)	8 (16%)	2	13
27	B5	51/52 (98%)	37 (72%)	14 (28%)	0	2
27	D5	51/52 (98%)	38 (74%)	13 (26%)	0	3
28	B6	43/52 (83%)	29 (67%)	14 (33%)	0	1
28	D6	43/52 (83%)	29 (67%)	14 (33%)	0	1
29	B7	41/42 (98%)	33 (80%)	8 (20%)	1	8
29	D7	41/42 (98%)	33 (80%)	8 (20%)	1	8
30	B8	53/55 (96%)	37 (70%)	16 (30%)	0	1
30	D8	53/55 (96%)	38 (72%)	15 (28%)	0	2
33	BD	213/218 (98%)	150 (70%)	63 (30%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	DD	213/218 (98%)	151 (71%)	62 (29%)	0	2
34	BE	165/166 (99%)	124 (75%)	41 (25%)	1	3
34	DE	165/166 (99%)	127 (77%)	38 (23%)	1	5
35	BF	165/166 (99%)	128 (78%)	37 (22%)	1	5
35	DF	165/166 (99%)	126 (76%)	39 (24%)	1	4
36	BG	155/156 (99%)	126 (81%)	29 (19%)	1	9
36	DG	155/156 (99%)	126 (81%)	29 (19%)	1	9
37	BH	132/148 (89%)	106 (80%)	26 (20%)	1	8
37	DH	132/148 (89%)	107 (81%)	25 (19%)	1	9
38	BI	122/124 (98%)	98 (80%)	24 (20%)	1	8
38	DI	122/124 (98%)	98 (80%)	24 (20%)	1	8
39	BN	117/119 (98%)	88 (75%)	29 (25%)	1	3
39	DN	117/119 (98%)	86 (74%)	31 (26%)	0	3
40	BO	100/100 (100%)	71 (71%)	29 (29%)	0	2
40	DO	100/100 (100%)	71 (71%)	29 (29%)	0	2
41	BP	112/116 (97%)	65 (58%)	47 (42%)	0	0
41	DP	112/116 (97%)	66 (59%)	46 (41%)	0	0
42	BQ	106/111 (96%)	82 (77%)	24 (23%)	1	5
42	DQ	106/111 (96%)	83 (78%)	23 (22%)	1	6
43	BR	100/101 (99%)	75 (75%)	25 (25%)	0	3
43	DR	100/101 (99%)	75 (75%)	25 (25%)	0	3
44	BS	77/88 (88%)	53 (69%)	24 (31%)	0	1
44	DS	77/88 (88%)	55 (71%)	22 (29%)	0	2
45	BT	116/127 (91%)	83 (72%)	33 (28%)	0	2
45	DT	116/127 (91%)	83 (72%)	33 (28%)	0	2
46	BU	92/94 (98%)	72 (78%)	20 (22%)	1	6
46	DU	92/94 (98%)	71 (77%)	21 (23%)	1	5
47	BV	82/82 (100%)	51 (62%)	31 (38%)	0	1
47	DV	82/82 (100%)	50 (61%)	32 (39%)	0	1
48	BW	91/92 (99%)	67 (74%)	24 (26%)	0	3
48	DW	91/92 (99%)	67 (74%)	24 (26%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	BX	74/78 (95%)	53 (72%)	21 (28%)	0	2
49	DX	74/78 (95%)	53 (72%)	21 (28%)	0	2
50	BY	84/91 (92%)	62 (74%)	22 (26%)	0	3
50	DY	84/91 (92%)	63 (75%)	21 (25%)	0	3
51	BZ	155/179 (87%)	128 (83%)	27 (17%)	2	10
51	DZ	155/179 (87%)	128 (83%)	27 (17%)	2	10
All	All	9322/9876 (94%)	7543 (81%)	1779 (19%)	1	8

5 of 1779 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CC	27	LYS
51	DZ	120	ILE
24	D2	47	ASN
51	DZ	19	ARG
44	DS	101	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 290 such sidechains are listed below:

Mol	Chain	Res	Type
34	DE	192	ASN
51	DZ	55	HIS
37	DH	65	HIS
43	DR	71	GLN
39	BN	45	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	287 (19%)	31 (2%)
1	CA	1503/1522 (98%)	288 (19%)	31 (2%)
31	BA	2723/2787 (97%)	741 (27%)	71 (2%)
31	DA	2723/2787 (97%)	735 (26%)	70 (2%)
32	BB	118/122 (96%)	35 (29%)	1 (0%)
32	DB	118/122 (96%)	35 (29%)	0
All	All	8688/8862 (98%)	2121 (24%)	204 (2%)

5 of 2121 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	AA	9	G
1	AA	31	G
1	AA	32	A
1	AA	39	G
1	AA	47	C

5 of 204 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	499	A
31	DA	387	U
31	DA	2662	A
1	CA	687	A
1	CA	1285	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 802 ligands modelled in this entry, 800 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
55	ZIT	BA	3351	-	54,54,54	1.42	7 (12%)	82,83,83	1.10	5 (6%)
55	ZIT	DA	3311	-	54,54,54	1.42	6 (11%)	82,83,83	1.10	5 (6%)

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
55	ZIT	BA	3351	-	-	3/72/107/107	0/3/3/3
55	ZIT	DA	3311	-	-	3/72/107/107	0/3/3/3

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	DA	3311	ZIT	C13-C14	3.34	1.60	1.55
55	BA	3351	ZIT	C22-C11	3.34	1.58	1.52
55	DA	3311	ZIT	C22-C11	3.32	1.58	1.52
55	BA	3351	ZIT	C13-C14	3.29	1.60	1.55
55	DA	3311	ZIT	O13-C13	2.73	1.48	1.44

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	BA	3351	ZIT	C9-N10-C11	-3.08	106.95	112.06
55	DA	3311	ZIT	C9-N10-C11	-3.05	106.99	112.06
55	DA	3311	ZIT	C7-C8-C9	2.83	116.09	112.10
55	BA	3351	ZIT	C7-C8-C9	2.82	116.09	112.10
55	DA	3311	ZIT	O6-C6-C7	2.20	113.84	108.34

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

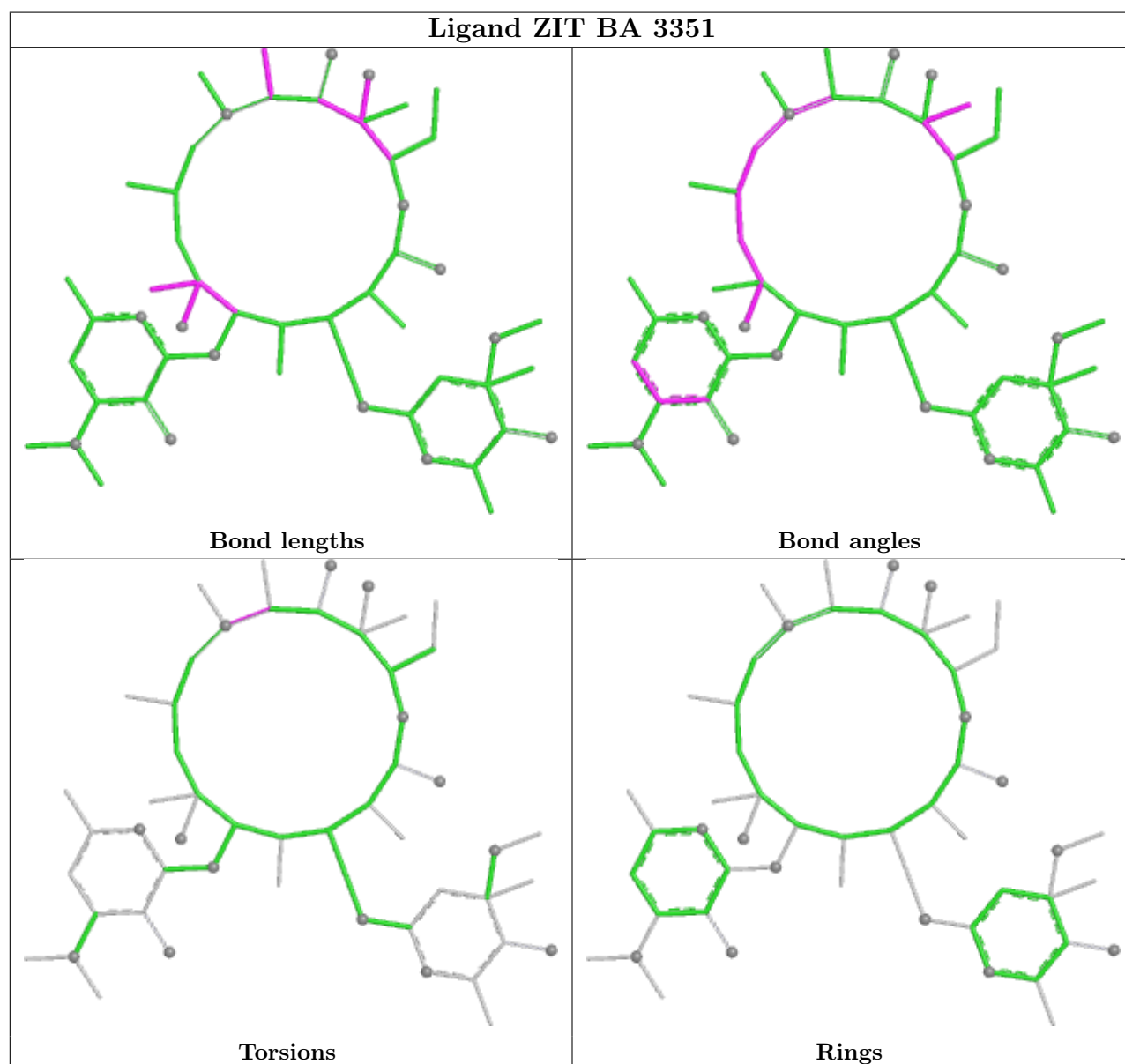
Mol	Chain	Res	Type	Atoms
55	BA	3351	ZIT	C12-C11-N10-C21
55	BA	3351	ZIT	C22-C11-N10-C21
55	DA	3311	ZIT	C12-C11-N10-C21
55	DA	3311	ZIT	C22-C11-N10-C21
55	BA	3351	ZIT	C12-C11-N10-C9

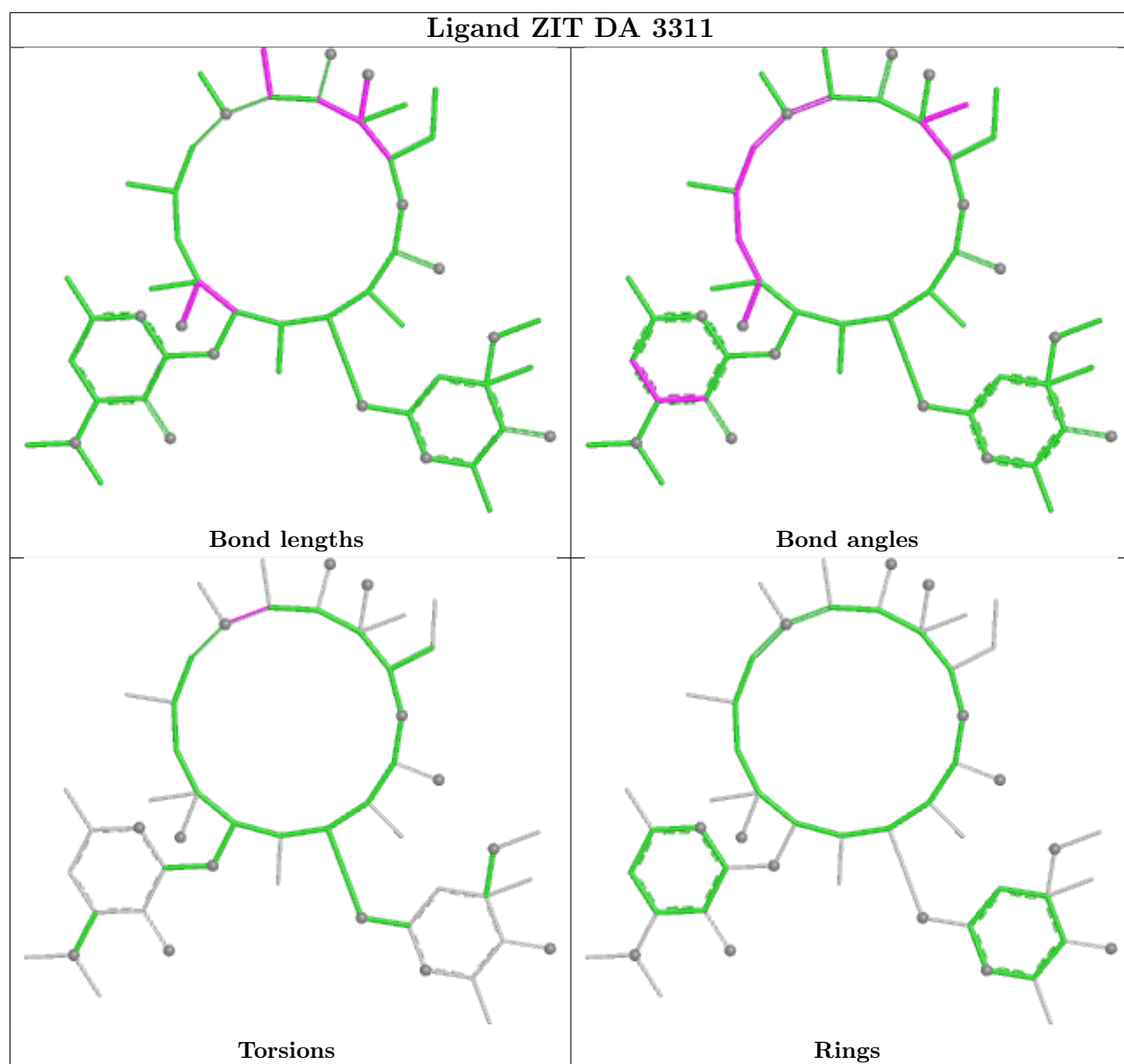
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	BA	3351	ZIT	3	0
55	DA	3311	ZIT	3	0

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





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
13	CM	3
13	AM	3
36	DG	1

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Mol	Chain	Number of breaks
36	BG	1
28	B6	1
28	D6	1
9	AI	1
9	CI	1
47	BV	1
47	DV	1

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	CM	69:GLU	C	70:LEU	N	5.29
1	AM	69:GLU	C	70:LEU	N	5.28
1	DG	112:PRO	C	113:ARG	N	4.77
1	BG	112:PRO	C	113:ARG	N	4.76
1	AM	112:GLY	C	113:PRO	N	4.20

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	1504/1522 (98%)	0.82	169 (11%) 10 6	60, 125, 191, 194	0
1	CA	1504/1522 (98%)	0.74	134 (8%) 15 8	61, 125, 191, 194	0
2	AB	235/256 (91%)	1.19	48 (20%) 3 2	107, 156, 184, 191	0
2	CB	235/256 (91%)	1.26	49 (20%) 2 2	107, 158, 185, 191	0
3	AC	207/239 (86%)	1.04	32 (15%) 5 3	115, 163, 184, 189	0
3	CC	207/239 (86%)	1.32	47 (22%) 2 1	119, 166, 184, 191	0
4	AD	208/209 (99%)	1.36	46 (22%) 2 1	83, 131, 170, 181	0
4	CD	208/209 (99%)	1.42	47 (22%) 2 1	82, 131, 168, 182	0
5	AE	151/162 (93%)	1.02	27 (17%) 3 2	83, 116, 160, 188	0
5	CE	151/162 (93%)	1.02	22 (14%) 6 3	84, 117, 162, 189	0
6	AF	101/101 (100%)	1.03	14 (13%) 6 4	85, 132, 164, 180	0
6	CF	101/101 (100%)	1.19	17 (16%) 4 3	86, 132, 165, 182	0
7	AG	155/156 (99%)	1.49	46 (29%) 1 1	140, 171, 188, 191	0
7	CG	155/156 (99%)	1.39	39 (25%) 1 1	140, 171, 188, 190	0
8	AH	138/138 (100%)	1.01	19 (13%) 6 4	85, 121, 155, 164	0
8	CH	138/138 (100%)	1.09	23 (16%) 4 3	85, 123, 156, 162	0
9	AI	127/128 (99%)	1.79	45 (35%) 1 1	142, 182, 190, 192	0
9	CI	127/128 (99%)	1.90	56 (44%) 0 1	143, 183, 190, 191	0
10	AJ	99/105 (94%)	1.90	37 (37%) 1 1	130, 176, 189, 191	0
10	CJ	99/105 (94%)	1.72	37 (37%) 1 1	130, 177, 190, 193	0
11	AK	119/129 (92%)	1.31	30 (25%) 1 1	82, 123, 164, 187	0
11	CK	119/129 (92%)	1.27	25 (21%) 2 1	84, 123, 165, 186	0
12	AL	125/135 (92%)	1.41	33 (26%) 1 1	80, 108, 163, 189	0
12	CL	125/135 (92%)	1.49	35 (28%) 1 1	82, 109, 164, 188	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
13	AM	115/126 (91%)	1.93	40 (34%)	1	1	150, 185, 190, 193	0
13	CM	115/126 (91%)	1.92	49 (42%)	0	1	149, 185, 190, 192	0
14	AN	60/61 (98%)	1.83	22 (36%)	1	1	131, 168, 185, 189	0
14	CN	60/61 (98%)	1.82	21 (35%)	1	1	132, 170, 186, 189	0
15	AO	88/89 (98%)	1.22	19 (21%)	2	2	74, 111, 157, 162	0
15	CO	88/89 (98%)	0.82	12 (13%)	7	4	74, 112, 159, 165	0
16	AP	84/88 (95%)	1.85	30 (35%)	1	1	91, 118, 161, 179	0
16	CP	84/88 (95%)	1.63	27 (32%)	1	1	89, 116, 160, 180	0
17	AQ	100/105 (95%)	1.14	19 (19%)	3	2	80, 109, 153, 163	0
17	CQ	100/105 (95%)	1.28	16 (16%)	5	3	85, 110, 153, 159	0
18	AR	70/88 (79%)	1.12	9 (12%)	7	5	93, 121, 170, 183	0
18	CR	70/88 (79%)	0.78	5 (7%)	22	11	93, 122, 171, 183	0
19	AS	79/93 (84%)	1.73	30 (37%)	1	1	142, 186, 190, 191	0
19	CS	79/93 (84%)	1.63	25 (31%)	1	1	142, 186, 191, 192	0
20	AT	99/106 (93%)	1.68	33 (33%)	1	1	84, 119, 157, 177	0
20	CT	99/106 (93%)	1.40	27 (27%)	1	1	84, 119, 157, 179	0
21	AU	25/27 (92%)	3.73	22 (88%)	0	0	143, 174, 188, 190	0
21	CU	25/27 (92%)	3.81	20 (80%)	0	0	141, 172, 188, 189	0
22	B0	85/85 (100%)	1.14	15 (17%)	4	3	49, 70, 175, 187	0
22	D0	85/85 (100%)	0.83	14 (16%)	4	3	54, 74, 173, 188	0
23	B1	89/98 (90%)	1.92	31 (34%)	1	1	50, 79, 150, 187	0
23	D1	89/98 (90%)	1.55	23 (25%)	1	1	51, 81, 151, 190	0
24	B2	51/72 (70%)	2.81	31 (60%)	0	0	59, 99, 175, 186	0
24	D2	51/72 (70%)	2.32	24 (47%)	0	0	62, 100, 175, 188	0
25	B3	60/60 (100%)	0.92	10 (16%)	4	3	46, 69, 132, 168	0
25	D3	60/60 (100%)	0.43	2 (3%)	49	28	51, 72, 136, 161	0
26	B4	32/71 (45%)	1.96	13 (40%)	0	1	133, 161, 182, 184	0
26	D4	32/71 (45%)	1.70	10 (31%)	1	1	133, 164, 182, 186	0
27	B5	58/60 (96%)	1.00	11 (18%)	3	2	34, 61, 165, 188	0
27	D5	58/60 (96%)	0.80	7 (12%)	8	5	39, 63, 163, 190	0
28	B6	45/54 (83%)	2.30	17 (37%)	1	1	49, 85, 141, 173	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
28	D6	45/54 (83%)	1.79	17 (37%) 1 1	52, 87, 142, 172	0
29	B7	49/49 (100%)	0.48	6 (12%) 8 5	36, 45, 119, 172	0
29	D7	49/49 (100%)	0.50	6 (12%) 8 5	38, 49, 120, 173	0
30	B8	64/65 (98%)	1.79	21 (32%) 1 1	46, 68, 140, 165	0
30	D8	64/65 (98%)	1.48	20 (31%) 1 1	49, 73, 141, 169	0
31	BA	2725/2787 (97%)	0.09	164 (6%) 27 14	33, 59, 153, 194	0
31	DA	2725/2787 (97%)	-0.01	105 (3%) 43 24	38, 64, 157, 194	0
32	BB	119/122 (97%)	1.43	34 (28%) 1 1	50, 101, 149, 184	0
32	DB	119/122 (97%)	1.12	24 (20%) 3 2	59, 105, 157, 184	0
33	BD	272/276 (98%)	0.46	26 (9%) 13 7	37, 62, 120, 168	0
33	DD	272/276 (98%)	0.45	20 (7%) 20 10	40, 65, 122, 165	0
34	BE	205/206 (99%)	0.83	25 (12%) 8 5	36, 65, 153, 181	0
34	DE	205/206 (99%)	0.71	26 (12%) 8 5	40, 69, 154, 182	0
35	BF	208/210 (99%)	0.79	23 (11%) 10 6	35, 77, 175, 189	0
35	DF	208/210 (99%)	0.62	20 (9%) 13 7	39, 79, 176, 188	0
36	BG	181/182 (99%)	1.96	73 (40%) 0 1	100, 152, 186, 192	0
36	DG	181/182 (99%)	1.79	65 (35%) 1 1	106, 159, 189, 191	0
37	BH	160/180 (88%)	2.15	70 (43%) 0 1	69, 111, 151, 182	0
37	DH	160/180 (88%)	1.15	22 (13%) 6 4	74, 114, 157, 185	0
38	BI	146/148 (98%)	1.73	49 (33%) 1 1	67, 152, 187, 190	0
38	DI	146/148 (98%)	1.63	41 (28%) 1 1	69, 156, 189, 191	0
39	BN	139/140 (99%)	1.34	34 (24%) 2 1	45, 75, 143, 182	0
39	DN	139/140 (99%)	0.75	17 (12%) 8 5	49, 78, 143, 183	0
40	BO	122/122 (100%)	0.38	3 (2%) 58 35	45, 67, 123, 147	0
40	DO	122/122 (100%)	0.35	8 (6%) 24 12	48, 69, 125, 149	0
41	BP	146/150 (97%)	1.72	47 (32%) 1 1	29, 93, 149, 190	0
41	DP	146/150 (97%)	1.24	38 (26%) 1 1	38, 95, 152, 188	0
42	BQ	136/141 (96%)	1.66	30 (22%) 2 1	50, 77, 147, 183	0
42	DQ	136/141 (96%)	1.19	17 (12%) 8 5	52, 79, 147, 183	0
43	BR	117/118 (99%)	0.69	13 (11%) 10 6	40, 60, 130, 139	0
43	DR	117/118 (99%)	0.55	17 (14%) 6 3	42, 62, 131, 140	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
44	BS	99/112 (88%)	2.13	48 (48%)	0	0	54, 111, 148, 165	0
44	DS	99/112 (88%)	1.69	31 (31%)	1	1	62, 113, 154, 170	0
45	BT	132/146 (90%)	1.29	31 (23%)	2	1	55, 87, 154, 181	0
45	DT	132/146 (90%)	1.04	29 (21%)	2	1	58, 90, 156, 179	0
46	BU	117/118 (99%)	1.02	23 (19%)	3	2	40, 62, 124, 176	0
46	DU	117/118 (99%)	0.92	15 (12%)	7	5	44, 67, 130, 175	0
47	BV	101/101 (100%)	2.21	50 (49%)	0	0	38, 103, 176, 188	0
47	DV	101/101 (100%)	1.22	21 (20%)	2	2	44, 109, 177, 188	0
48	BW	113/113 (100%)	0.30	7 (6%)	26	14	38, 51, 112, 179	0
48	DW	113/113 (100%)	0.16	4 (3%)	47	27	41, 54, 119, 181	0
49	BX	93/96 (96%)	1.60	29 (31%)	1	1	47, 74, 145, 179	0
49	DX	93/96 (96%)	1.38	19 (20%)	3	2	52, 76, 146, 179	0
50	BY	101/110 (91%)	2.54	59 (58%)	0	0	57, 107, 184, 192	0
50	DY	101/110 (91%)	2.02	42 (41%)	0	1	60, 108, 183, 193	0
51	BZ	177/206 (85%)	1.61	53 (29%)	1	1	68, 113, 158, 169	0
51	DZ	177/206 (85%)	1.22	40 (22%)	2	1	74, 117, 161, 168	0
All	All	20062/20922 (95%)	0.87	3293 (16%)	4	3	29, 99, 187, 194	0

The worst 5 of 3293 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
42	BQ	140	ALA	31.8
42	BQ	141	GLN	22.8
39	BN	68	GLU	15.8
42	DQ	24	GLY	15.8
42	BQ	24	GLY	15.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
52	MG	DA	3291	1/1	0.53	0.32	86,86,86,86	0
52	MG	BA	3246	1/1	0.57	0.34	75,75,75,75	0
52	MG	DA	3126	1/1	0.64	0.35	73,73,73,73	0
52	MG	DA	3306	1/1	0.65	0.39	87,87,87,87	0
52	MG	AA	1604	1/1	0.66	0.33	95,95,95,95	0
52	MG	CA	1623	1/1	0.67	0.24	67,67,67,67	0
52	MG	AA	1646	1/1	0.68	0.50	82,82,82,82	0
52	MG	DA	3245	1/1	0.70	0.25	78,78,78,78	0
52	MG	BA	3312	1/1	0.70	0.32	87,87,87,87	0
52	MG	DA	3191	1/1	0.70	0.32	91,91,91,91	0
52	MG	AA	1640	1/1	0.71	0.34	83,83,83,83	0
52	MG	DA	3302	1/1	0.71	0.50	86,86,86,86	0
52	MG	DA	3255	1/1	0.71	0.22	75,75,75,75	0
52	MG	DA	3298	1/1	0.72	0.29	71,71,71,71	0
52	MG	DA	3261	1/1	0.72	0.31	95,95,95,95	0
52	MG	DA	3219	1/1	0.72	0.29	75,75,75,75	0
52	MG	BA	3303	1/1	0.73	0.27	68,68,68,68	0
52	MG	DA	3264	1/1	0.73	0.39	80,80,80,80	0
52	MG	DA	3223	1/1	0.73	0.22	65,65,65,65	0
52	MG	AA	1641	1/1	0.74	0.16	69,69,69,69	0
52	MG	DA	3216	1/1	0.74	0.52	85,85,85,85	0
54	K	DA	3310	1/1	0.74	0.42	106,106,106,106	0
52	MG	CA	1647	1/1	0.75	0.22	84,84,84,84	0
52	MG	CA	1611	1/1	0.75	0.40	81,81,81,81	0
52	MG	DA	3179	1/1	0.75	0.47	77,77,77,77	0
52	MG	AA	1622	1/1	0.75	0.44	75,75,75,75	0
52	MG	DA	3102	1/1	0.76	0.27	80,80,80,80	0
52	MG	AA	1645	1/1	0.77	0.28	81,81,81,81	0
52	MG	CA	1641	1/1	0.78	0.59	87,87,87,87	0
52	MG	AA	1627	1/1	0.78	0.25	66,66,66,66	0
52	MG	CA	1633	1/1	0.78	0.56	87,87,87,87	0
52	MG	DA	3105	1/1	0.78	0.35	47,47,47,47	0
52	MG	DF	301	1/1	0.78	0.27	92,92,92,92	0
52	MG	DA	3125	1/1	0.78	0.41	58,58,58,58	0
52	MG	DA	3020	1/1	0.79	0.29	64,64,64,64	0
52	MG	BA	3097	1/1	0.79	0.15	70,70,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3190	1/1	0.79	0.20	53,53,53,53	0
52	MG	DA	3280	1/1	0.79	0.43	77,77,77,77	0
52	MG	DA	3289	1/1	0.79	0.41	92,92,92,92	0
52	MG	CA	1609	1/1	0.79	0.14	94,94,94,94	0
52	MG	AA	1633	1/1	0.79	0.16	81,81,81,81	0
52	MG	DA	3240	1/1	0.79	0.26	89,89,89,89	0
52	MG	DA	3146	1/1	0.79	0.24	69,69,69,69	0
52	MG	DA	3247	1/1	0.79	0.40	87,87,87,87	0
52	MG	DA	3250	1/1	0.79	0.17	75,75,75,75	0
52	MG	CA	1646	1/1	0.80	0.22	80,80,80,80	0
52	MG	DA	3294	1/1	0.80	0.15	67,67,67,67	0
52	MG	BA	3031	1/1	0.80	0.30	77,77,77,77	0
52	MG	CA	1632	1/1	0.80	0.34	79,79,79,79	0
52	MG	BA	3302	1/1	0.80	0.22	72,72,72,72	0
52	MG	DA	3190	1/1	0.80	0.30	63,63,63,63	0
52	MG	CA	1620	1/1	0.80	0.28	66,66,66,66	0
52	MG	DA	3111	1/1	0.81	0.37	71,71,71,71	0
52	MG	BA	3307	1/1	0.81	0.39	76,76,76,76	0
52	MG	DA	3308	1/1	0.81	0.31	81,81,81,81	0
52	MG	DA	3266	1/1	0.81	0.28	75,75,75,75	0
52	MG	BA	3195	1/1	0.81	0.46	58,58,58,58	0
52	MG	BA	3087	1/1	0.82	0.22	58,58,58,58	0
52	MG	CA	1625	1/1	0.82	0.40	74,74,74,74	0
52	MG	BA	3092	1/1	0.82	0.49	52,52,52,52	0
52	MG	DA	3265	1/1	0.82	0.34	79,79,79,79	0
52	MG	DA	3175	1/1	0.82	0.43	67,67,67,67	0
52	MG	AA	1651	1/1	0.82	0.25	75,75,75,75	0
52	MG	CA	1637	1/1	0.82	0.35	80,80,80,80	0
52	MG	CA	1638	1/1	0.82	0.27	71,71,71,71	0
52	MG	BA	3148	1/1	0.82	0.21	58,58,58,58	0
52	MG	BA	3341	1/1	0.82	0.22	63,63,63,63	0
52	MG	CA	1605	1/1	0.82	0.36	61,61,61,61	0
52	MG	CA	1607	1/1	0.82	0.35	82,82,82,82	0
52	MG	AA	1619	1/1	0.82	0.31	56,56,56,56	0
52	MG	BA	3039	1/1	0.82	0.36	60,60,60,60	0
54	K	BA	3350	1/1	0.82	0.34	95,95,95,95	0
52	MG	BA	3076	1/1	0.82	0.26	43,43,43,43	0
52	MG	DA	3208	1/1	0.83	0.38	62,62,62,62	0
52	MG	DA	3209	1/1	0.83	0.22	59,59,59,59	0
52	MG	DA	3013	1/1	0.83	0.44	77,77,77,77	0
52	MG	AA	1643	1/1	0.83	0.13	78,78,78,78	0
52	MG	DA	3100	1/1	0.83	0.22	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3235	1/1	0.83	0.31	79,79,79,79	0
52	MG	DA	3166	1/1	0.83	0.28	46,46,46,46	0
52	MG	BA	3332	1/1	0.83	0.25	61,61,61,61	0
52	MG	BA	3336	1/1	0.83	0.31	65,65,65,65	0
52	MG	DA	3001	1/1	0.83	0.31	76,76,76,76	0
52	MG	DA	3124	1/1	0.83	0.40	83,83,83,83	0
52	MG	DA	3198	1/1	0.83	0.49	70,70,70,70	0
52	MG	DA	3207	1/1	0.83	0.38	78,78,78,78	0
52	MG	DA	3189	1/1	0.84	0.33	63,63,63,63	0
52	MG	AA	1644	1/1	0.84	0.31	99,99,99,99	0
52	MG	DA	3062	1/1	0.84	0.33	65,65,65,65	0
52	MG	BA	3321	1/1	0.84	0.35	75,75,75,75	0
52	MG	CA	1630	1/1	0.84	0.28	77,77,77,77	0
52	MG	BA	3330	1/1	0.84	0.41	71,71,71,71	0
52	MG	DA	3284	1/1	0.84	0.30	65,65,65,65	0
52	MG	AA	1636	1/1	0.84	0.24	63,63,63,63	0
52	MG	BA	3235	1/1	0.84	0.33	72,72,72,72	0
52	MG	AA	1603	1/1	0.84	0.32	62,62,62,62	0
52	MG	BA	3249	1/1	0.84	0.14	40,40,40,40	0
52	MG	DA	3233	1/1	0.84	0.31	68,68,68,68	0
52	MG	BA	3259	1/1	0.84	0.30	46,46,46,46	0
52	MG	AA	1650	1/1	0.84	0.20	68,68,68,68	0
52	MG	BA	3157	1/1	0.84	0.40	74,74,74,74	0
52	MG	DA	3178	1/1	0.84	0.22	65,65,65,65	0
52	MG	BA	3180	1/1	0.84	0.30	64,64,64,64	0
52	MG	DA	3067	1/1	0.85	0.28	81,81,81,81	0
52	MG	DA	3081	1/1	0.85	0.26	43,43,43,43	0
52	MG	DA	3094	1/1	0.85	0.31	56,56,56,56	0
52	MG	BA	3280	1/1	0.85	0.35	75,75,75,75	0
52	MG	BA	3289	1/1	0.85	0.22	55,55,55,55	0
52	MG	CA	1644	1/1	0.85	0.34	74,74,74,74	0
52	MG	DA	3279	1/1	0.85	0.21	64,64,64,64	0
52	MG	BA	3121	1/1	0.85	0.31	57,57,57,57	0
52	MG	DA	3115	1/1	0.85	0.42	72,72,72,72	0
52	MG	DA	3288	1/1	0.85	0.26	72,72,72,72	0
52	MG	BA	3240	1/1	0.85	0.34	60,60,60,60	0
52	MG	DA	3211	1/1	0.85	0.28	79,79,79,79	0
52	MG	BA	3082	1/1	0.85	0.33	49,49,49,49	0
52	MG	CA	1606	1/1	0.85	0.39	72,72,72,72	0
52	MG	BA	3192	1/1	0.85	0.32	58,58,58,58	0
52	MG	DA	3149	1/1	0.85	0.19	55,55,55,55	0
52	MG	DA	3153	1/1	0.85	0.29	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3037	1/1	0.85	0.24	74,74,74,74	0
52	MG	DA	3167	1/1	0.85	0.25	48,48,48,48	0
52	MG	BA	3110	1/1	0.85	0.42	45,45,45,45	0
52	MG	DA	3246	1/1	0.86	0.29	87,87,87,87	0
52	MG	DA	3070	1/1	0.86	0.46	74,74,74,74	0
52	MG	DA	3248	1/1	0.86	0.39	74,74,74,74	0
52	MG	DA	3249	1/1	0.86	0.40	79,79,79,79	0
52	MG	BA	3263	1/1	0.86	0.40	62,62,62,62	0
52	MG	BA	3178	1/1	0.86	0.28	78,78,78,78	0
52	MG	DA	3182	1/1	0.86	0.13	55,55,55,55	0
52	MG	CA	1645	1/1	0.86	0.19	97,97,97,97	0
52	MG	BA	3074	1/1	0.86	0.31	36,36,36,36	0
52	MG	AA	1637	1/1	0.86	0.32	69,69,69,69	0
52	MG	D5	102	1/1	0.86	0.27	79,79,79,79	0
52	MG	BA	3238	1/1	0.86	0.19	49,49,49,49	0
52	MG	DA	3120	1/1	0.86	0.30	71,71,71,71	0
52	MG	BA	3306	1/1	0.86	0.11	56,56,56,56	0
52	MG	CA	1634	1/1	0.86	0.51	87,87,87,87	0
52	MG	DA	3027	1/1	0.86	0.31	61,61,61,61	0
52	MG	DA	3145	1/1	0.86	0.40	88,88,88,88	0
52	MG	CA	1636	1/1	0.86	0.38	79,79,79,79	0
52	MG	DA	3300	1/1	0.86	0.13	75,75,75,75	0
52	MG	DA	3040	1/1	0.86	0.18	43,43,43,43	0
52	MG	DA	3303	1/1	0.86	0.33	49,49,49,49	0
52	MG	DA	3305	1/1	0.86	0.35	76,76,76,76	0
52	MG	DA	3043	1/1	0.86	0.26	35,35,35,35	0
52	MG	DA	3236	1/1	0.86	0.31	67,67,67,67	0
52	MG	DA	3309	1/1	0.86	0.29	84,84,84,84	0
52	MG	CA	1616	1/1	0.86	0.30	73,73,73,73	0
52	MG	DA	3243	1/1	0.86	0.30	70,70,70,70	0
52	MG	CA	1618	1/1	0.86	0.27	62,62,62,62	0
52	MG	AA	1613	1/1	0.87	0.19	70,70,70,70	0
52	MG	BA	3274	1/1	0.87	0.25	81,81,81,81	0
52	MG	DA	3152	1/1	0.87	0.26	43,43,43,43	0
52	MG	BA	3320	1/1	0.87	0.14	54,54,54,54	0
52	MG	CA	1640	1/1	0.87	0.23	68,68,68,68	0
52	MG	BA	3095	1/1	0.87	0.32	38,38,38,38	0
52	MG	DA	3169	1/1	0.87	0.36	51,51,51,51	0
52	MG	DA	3079	1/1	0.87	0.23	59,59,59,59	0
52	MG	BA	3066	1/1	0.87	0.25	43,43,43,43	0
52	MG	DA	3087	1/1	0.87	0.27	55,55,55,55	0
52	MG	DA	3089	1/1	0.87	0.37	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3184	1/1	0.87	0.32	63,63,63,63	0
52	MG	DA	3090	1/1	0.87	0.32	76,76,76,76	0
52	MG	DA	3282	1/1	0.87	0.27	62,62,62,62	0
52	MG	CA	1619	1/1	0.87	0.34	75,75,75,75	0
52	MG	BA	3298	1/1	0.87	0.26	61,61,61,61	0
52	MG	BA	3334	1/1	0.87	0.27	53,53,53,53	0
52	MG	BA	3300	1/1	0.87	0.24	59,59,59,59	0
52	MG	DA	3110	1/1	0.87	0.33	73,73,73,73	0
52	MG	CA	1628	1/1	0.87	0.33	75,75,75,75	0
52	MG	DA	3299	1/1	0.87	0.21	66,66,66,66	0
52	MG	DA	3113	1/1	0.87	0.30	62,62,62,62	0
52	MG	DA	3114	1/1	0.87	0.31	65,65,65,65	0
52	MG	AA	1632	1/1	0.87	0.45	72,72,72,72	0
52	MG	DA	3222	1/1	0.87	0.29	67,67,67,67	0
52	MG	BQ	202	1/1	0.87	0.28	59,59,59,59	0
52	MG	DA	3025	1/1	0.87	0.40	50,50,50,50	0
52	MG	BA	3214	1/1	0.87	0.42	66,66,66,66	0
52	MG	DA	3029	1/1	0.87	0.23	87,87,87,87	0
52	MG	DA	3135	1/1	0.87	0.24	71,71,71,71	0
52	MG	BA	3229	1/1	0.87	0.19	50,50,50,50	0
52	MG	BA	3292	1/1	0.88	0.29	60,60,60,60	0
52	MG	BA	3080	1/1	0.88	0.31	34,34,34,34	0
52	MG	DA	3154	1/1	0.88	0.36	62,62,62,62	0
52	MG	DA	3160	1/1	0.88	0.14	59,59,59,59	0
52	MG	DA	3164	1/1	0.88	0.19	71,71,71,71	0
52	MG	DA	3083	1/1	0.88	0.22	47,47,47,47	0
52	MG	BA	3151	1/1	0.88	0.26	74,74,74,74	0
52	MG	BA	3232	1/1	0.88	0.31	70,70,70,70	0
52	MG	DA	3172	1/1	0.88	0.39	64,64,64,64	0
52	MG	CA	1615	1/1	0.88	0.38	67,67,67,67	0
52	MG	DA	3176	1/1	0.88	0.19	78,78,78,78	0
52	MG	BA	3027	1/1	0.88	0.34	42,42,42,42	0
52	MG	DA	3273	1/1	0.88	0.33	75,75,75,75	0
52	MG	BA	3237	1/1	0.88	0.18	61,61,61,61	0
52	MG	BA	3162	1/1	0.88	0.14	47,47,47,47	0
52	MG	DA	3281	1/1	0.88	0.11	30,30,30,30	0
52	MG	BA	3170	1/1	0.88	0.17	69,69,69,69	0
52	MG	BA	3171	1/1	0.88	0.32	62,62,62,62	0
52	MG	BA	3176	1/1	0.88	0.27	48,48,48,48	0
52	MG	BA	3104	1/1	0.88	0.27	37,37,37,37	0
52	MG	AA	1638	1/1	0.88	0.16	82,82,82,82	0
52	MG	BA	3270	1/1	0.88	0.12	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3039	1/1	0.88	0.23	43,43,43,43	0
52	MG	BA	3272	1/1	0.88	0.23	51,51,51,51	0
52	MG	BA	3120	1/1	0.88	0.30	52,52,52,52	0
52	MG	AA	1639	1/1	0.88	0.26	95,95,95,95	0
52	MG	DA	3127	1/1	0.88	0.28	35,35,35,35	0
52	MG	DA	3129	1/1	0.88	0.18	87,87,87,87	0
52	MG	CA	1601	1/1	0.88	0.28	83,83,83,83	0
52	MG	DA	3226	1/1	0.88	0.28	64,64,64,64	0
52	MG	BA	3138	1/1	0.88	0.18	74,74,74,74	0
52	MG	DA	3075	1/1	0.88	0.32	55,55,55,55	0
52	MG	DA	3078	1/1	0.88	0.28	46,46,46,46	0
52	MG	DA	3150	1/1	0.88	0.51	77,77,77,77	0
52	MG	DA	3197	1/1	0.89	0.23	75,75,75,75	0
52	MG	BA	3183	1/1	0.89	0.23	72,72,72,72	0
52	MG	DA	3203	1/1	0.89	0.37	67,67,67,67	0
52	MG	DA	3267	1/1	0.89	0.42	72,72,72,72	0
52	MG	BA	3166	1/1	0.89	0.27	39,39,39,39	0
52	MG	DA	3278	1/1	0.89	0.31	68,68,68,68	0
52	MG	CA	1602	1/1	0.89	0.36	70,70,70,70	0
52	MG	BA	3310	1/1	0.89	0.14	47,47,47,47	0
52	MG	DA	3031	1/1	0.89	0.22	47,47,47,47	0
52	MG	BA	3060	1/1	0.89	0.24	40,40,40,40	0
52	MG	DA	3155	1/1	0.89	0.25	62,62,62,62	0
52	MG	DA	3159	1/1	0.89	0.24	61,61,61,61	0
52	MG	BA	3315	1/1	0.89	0.31	69,69,69,69	0
52	MG	BA	3288	1/1	0.89	0.24	72,72,72,72	0
52	MG	BA	3009	1/1	0.89	0.33	38,38,38,38	0
52	MG	DA	3297	1/1	0.89	0.32	74,74,74,74	0
52	MG	DA	3057	1/1	0.89	0.29	40,40,40,40	0
52	MG	BA	3071	1/1	0.89	0.30	47,47,47,47	0
52	MG	DA	3066	1/1	0.89	0.24	60,60,60,60	0
52	MG	BA	3252	1/1	0.89	0.22	50,50,50,50	0
52	MG	BA	3034	1/1	0.89	0.29	62,62,62,62	0
52	MG	AA	1649	1/1	0.89	0.20	86,86,86,86	0
52	MG	BA	3338	1/1	0.89	0.21	73,73,73,73	0
52	MG	BA	3181	1/1	0.89	0.20	51,51,51,51	0
52	MG	BA	3346	1/1	0.89	0.34	80,80,80,80	0
52	MG	BA	3349	1/1	0.89	0.21	61,61,61,61	0
52	MG	DA	3143	1/1	0.89	0.27	57,57,57,57	0
52	MG	DA	3084	1/1	0.89	0.17	54,54,54,54	0
52	MG	BA	3186	1/1	0.90	0.16	66,66,66,66	0
52	MG	BA	3279	1/1	0.90	0.18	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3244	1/1	0.90	0.22	86,86,86,86	0
52	MG	BA	3116	1/1	0.90	0.23	51,51,51,51	0
52	MG	BA	3179	1/1	0.90	0.24	59,59,59,59	0
52	MG	BA	3090	1/1	0.90	0.18	38,38,38,38	0
52	MG	BA	3245	1/1	0.90	0.29	45,45,45,45	0
52	MG	BA	3200	1/1	0.90	0.42	59,59,59,59	0
52	MG	DA	3091	1/1	0.90	0.31	41,41,41,41	0
52	MG	DA	3093	1/1	0.90	0.29	64,64,64,64	0
52	MG	DA	3257	1/1	0.90	0.33	63,63,63,63	0
52	MG	DA	3260	1/1	0.90	0.42	73,73,73,73	0
52	MG	DA	3024	1/1	0.90	0.27	61,61,61,61	0
52	MG	DA	3262	1/1	0.90	0.25	77,77,77,77	0
52	MG	DA	3095	1/1	0.90	0.34	53,53,53,53	0
52	MG	DA	3173	1/1	0.90	0.24	65,65,65,65	0
52	MG	DA	3098	1/1	0.90	0.14	49,49,49,49	0
52	MG	BA	3073	1/1	0.90	0.27	53,53,53,53	0
52	MG	DA	3270	1/1	0.90	0.42	65,65,65,65	0
52	MG	BA	3343	1/1	0.90	0.24	58,58,58,58	0
52	MG	DA	3275	1/1	0.90	0.26	62,62,62,62	0
52	MG	CA	1626	1/1	0.90	0.29	78,78,78,78	0
52	MG	DA	3109	1/1	0.90	0.43	71,71,71,71	0
52	MG	BA	3344	1/1	0.90	0.32	48,48,48,48	0
52	MG	DA	3036	1/1	0.90	0.31	39,39,39,39	0
52	MG	CA	1629	1/1	0.90	0.15	82,82,82,82	0
52	MG	BA	3345	1/1	0.90	0.28	60,60,60,60	0
52	MG	BA	3219	1/1	0.90	0.05	38,38,38,38	0
52	MG	DA	3041	1/1	0.90	0.14	37,37,37,37	0
52	MG	DA	3290	1/1	0.90	0.27	52,52,52,52	0
52	MG	BA	3253	1/1	0.90	0.18	51,51,51,51	0
52	MG	DA	3205	1/1	0.90	0.38	54,54,54,54	0
52	MG	DA	3295	1/1	0.90	0.19	88,88,88,88	0
52	MG	BA	3254	1/1	0.90	0.18	53,53,53,53	0
52	MG	BA	3223	1/1	0.90	0.28	36,36,36,36	0
52	MG	BA	3182	1/1	0.90	0.22	68,68,68,68	0
52	MG	CA	1603	1/1	0.90	0.35	63,63,63,63	0
52	MG	DA	3132	1/1	0.90	0.29	43,43,43,43	0
52	MG	DA	3133	1/1	0.90	0.36	53,53,53,53	0
52	MG	BA	3230	1/1	0.90	0.30	38,38,38,38	0
52	MG	DA	3072	1/1	0.90	0.24	46,46,46,46	0
52	MG	DA	3074	1/1	0.90	0.24	53,53,53,53	0
52	MG	DA	3230	1/1	0.90	0.17	56,56,56,56	0
52	MG	BA	3081	1/1	0.90	0.16	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3076	1/1	0.90	0.29	55,55,55,55	0
52	MG	BA	3319	1/1	0.90	0.17	40,40,40,40	0
52	MG	BA	3149	1/1	0.91	0.17	51,51,51,51	0
52	MG	BA	3293	1/1	0.91	0.25	55,55,55,55	0
52	MG	BA	3295	1/1	0.91	0.22	70,70,70,70	0
52	MG	CA	1604	1/1	0.91	0.21	86,86,86,86	0
52	MG	DA	3085	1/1	0.91	0.25	54,54,54,54	0
52	MG	DA	3158	1/1	0.91	0.20	61,61,61,61	0
52	MG	D5	101	1/1	0.91	0.31	47,47,47,47	0
52	MG	BA	3085	1/1	0.91	0.21	40,40,40,40	0
52	MG	DA	3161	1/1	0.91	0.33	72,72,72,72	0
52	MG	BA	3049	1/1	0.91	0.37	41,41,41,41	0
52	MG	DA	3005	1/1	0.91	0.20	73,73,73,73	0
52	MG	BA	3158	1/1	0.91	0.20	49,49,49,49	0
52	MG	DA	3168	1/1	0.91	0.08	53,53,53,53	0
52	MG	BA	3058	1/1	0.91	0.29	39,39,39,39	0
52	MG	AA	1625	1/1	0.91	0.17	73,73,73,73	0
52	MG	CA	1614	1/1	0.91	0.33	76,76,76,76	0
52	MG	BA	3093	1/1	0.91	0.36	43,43,43,43	0
52	MG	BA	3008	1/1	0.91	0.29	34,34,34,34	0
52	MG	BA	3067	1/1	0.91	0.29	37,37,37,37	0
52	MG	DA	3032	1/1	0.91	0.35	69,69,69,69	0
52	MG	BA	3101	1/1	0.91	0.23	39,39,39,39	0
52	MG	DA	3274	1/1	0.91	0.17	63,63,63,63	0
52	MG	BA	3103	1/1	0.91	0.15	42,42,42,42	0
52	MG	DA	3188	1/1	0.91	0.17	48,48,48,48	0
52	MG	AA	1618	1/1	0.91	0.42	72,72,72,72	0
52	MG	BA	3010	1/1	0.91	0.26	38,38,38,38	0
52	MG	BA	3112	1/1	0.91	0.16	43,43,43,43	0
52	MG	DA	3195	1/1	0.91	0.28	56,56,56,56	0
52	MG	DA	3283	1/1	0.91	0.48	72,72,72,72	0
52	MG	DA	3117	1/1	0.91	0.07	59,59,59,59	0
52	MG	AA	1629	1/1	0.91	0.29	67,67,67,67	0
52	MG	DA	3047	1/1	0.91	0.29	45,45,45,45	0
52	MG	BA	3184	1/1	0.91	0.24	50,50,50,50	0
52	MG	DA	3059	1/1	0.91	0.23	53,53,53,53	0
52	MG	DA	3292	1/1	0.91	0.36	75,75,75,75	0
52	MG	BA	3119	1/1	0.91	0.23	52,52,52,52	0
52	MG	BA	3189	1/1	0.91	0.26	45,45,45,45	0
52	MG	DA	3296	1/1	0.91	0.13	60,60,60,60	0
52	MG	AA	1611	1/1	0.91	0.21	75,75,75,75	0
52	MG	AA	1614	1/1	0.91	0.12	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3134	1/1	0.91	0.25	47,47,47,47	0
52	MG	DA	3221	1/1	0.91	0.23	53,53,53,53	0
52	MG	AA	1634	1/1	0.91	0.29	58,58,58,58	0
52	MG	DA	3141	1/1	0.91	0.35	61,61,61,61	0
52	MG	BA	3196	1/1	0.91	0.25	65,65,65,65	0
52	MG	DA	3228	1/1	0.91	0.10	60,60,60,60	0
52	MG	DA	3307	1/1	0.91	0.32	80,80,80,80	0
52	MG	DA	3229	1/1	0.91	0.07	45,45,45,45	0
52	MG	BA	3197	1/1	0.91	0.24	52,52,52,52	0
52	MG	DB	202	1/1	0.91	0.28	63,63,63,63	0
52	MG	DB	203	1/1	0.91	0.31	56,56,56,56	0
52	MG	DA	3231	1/1	0.91	0.24	79,79,79,79	0
52	MG	DR	201	1/1	0.91	0.09	43,43,43,43	0
52	MG	BA	3198	1/1	0.91	0.24	44,44,44,44	0
52	MG	BA	3047	1/1	0.91	0.21	21,21,21,21	0
52	MG	BA	3133	1/1	0.92	0.27	35,35,35,35	0
52	MG	DA	3162	1/1	0.92	0.25	69,69,69,69	0
52	MG	BA	3134	1/1	0.92	0.23	46,46,46,46	0
52	MG	DA	3096	1/1	0.92	0.17	45,45,45,45	0
52	MG	BA	3137	1/1	0.92	0.26	61,61,61,61	0
52	MG	BA	3007	1/1	0.92	0.26	48,48,48,48	0
52	MG	BA	3301	1/1	0.92	0.23	57,57,57,57	0
52	MG	DA	3104	1/1	0.92	0.44	48,48,48,48	0
52	MG	DA	3259	1/1	0.92	0.38	74,74,74,74	0
52	MG	BA	3140	1/1	0.92	0.22	40,40,40,40	0
52	MG	DA	3108	1/1	0.92	0.18	48,48,48,48	0
52	MG	DA	3042	1/1	0.92	0.23	47,47,47,47	0
52	MG	BA	3204	1/1	0.92	0.23	46,46,46,46	0
52	MG	DA	3045	1/1	0.92	0.30	39,39,39,39	0
52	MG	DA	3112	1/1	0.92	0.27	68,68,68,68	0
52	MG	BA	3305	1/1	0.92	0.25	54,54,54,54	0
52	MG	DA	3268	1/1	0.92	0.52	81,81,81,81	0
52	MG	DA	3185	1/1	0.92	0.26	61,61,61,61	0
52	MG	DA	3272	1/1	0.92	0.20	74,74,74,74	0
52	MG	DA	3056	1/1	0.92	0.27	60,60,60,60	0
52	MG	BA	3209	1/1	0.92	0.31	56,56,56,56	0
52	MG	DA	3116	1/1	0.92	0.24	41,41,41,41	0
52	MG	DA	3277	1/1	0.92	0.26	68,68,68,68	0
52	MG	DA	3058	1/1	0.92	0.18	58,58,58,58	0
52	MG	BA	3142	1/1	0.92	0.36	39,39,39,39	0
52	MG	DA	3196	1/1	0.92	0.19	51,51,51,51	0
52	MG	BA	3013	1/1	0.92	0.19	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3041	1/1	0.92	0.23	29,29,29,29	0
52	MG	DA	3201	1/1	0.92	0.21	59,59,59,59	0
52	MG	BA	3114	1/1	0.92	0.25	56,56,56,56	0
52	MG	DA	3285	1/1	0.92	0.34	66,66,66,66	0
52	MG	DA	3287	1/1	0.92	0.08	51,51,51,51	0
52	MG	DA	3204	1/1	0.92	0.29	45,45,45,45	0
52	MG	DA	3069	1/1	0.92	0.36	51,51,51,51	0
52	MG	BA	3316	1/1	0.92	0.15	56,56,56,56	0
52	MG	BA	3152	1/1	0.92	0.32	61,61,61,61	0
52	MG	CA	1613	1/1	0.92	0.26	80,80,80,80	0
52	MG	BA	3275	1/1	0.92	0.27	47,47,47,47	0
52	MG	DA	3212	1/1	0.92	0.22	68,68,68,68	0
52	MG	BA	3277	1/1	0.92	0.34	62,62,62,62	0
52	MG	DA	3077	1/1	0.92	0.39	49,49,49,49	0
52	MG	DA	3142	1/1	0.92	0.34	41,41,41,41	0
52	MG	AA	1608	1/1	0.92	0.25	54,54,54,54	0
52	MG	DA	3144	1/1	0.92	0.18	47,47,47,47	0
52	MG	BA	3233	1/1	0.92	0.12	63,63,63,63	0
52	MG	DA	3227	1/1	0.92	0.24	74,74,74,74	0
52	MG	DA	3009	1/1	0.92	0.25	54,54,54,54	0
52	MG	BA	3284	1/1	0.92	0.25	71,71,71,71	0
52	MG	DA	3017	1/1	0.92	0.15	47,47,47,47	0
52	MG	BA	3068	1/1	0.92	0.25	54,54,54,54	0
52	MG	CA	1621	1/1	0.92	0.20	68,68,68,68	0
52	MG	DA	3088	1/1	0.92	0.29	34,34,34,34	0
52	MG	CA	1622	1/1	0.92	0.15	78,78,78,78	0
52	MG	AA	1626	1/1	0.92	0.33	76,76,76,76	0
52	MG	DA	3242	1/1	0.92	0.14	69,69,69,69	0
52	MG	DX	101	1/1	0.92	0.12	77,77,77,77	0
52	MG	CA	1624	1/1	0.92	0.30	65,65,65,65	0
52	MG	BA	3057	1/1	0.92	0.22	44,44,44,44	0
52	MG	DA	3048	1/1	0.93	0.17	40,40,40,40	0
52	MG	DA	3052	1/1	0.93	0.26	63,63,63,63	0
52	MG	DA	3054	1/1	0.93	0.18	36,36,36,36	0
52	MG	DA	3055	1/1	0.93	0.23	42,42,42,42	0
52	MG	BA	3187	1/1	0.93	0.28	42,42,42,42	0
52	MG	DA	3234	1/1	0.93	0.22	60,60,60,60	0
52	MG	DA	3140	1/1	0.93	0.19	49,49,49,49	0
52	MG	BA	3313	1/1	0.93	0.30	54,54,54,54	0
52	MG	BA	3005	1/1	0.93	0.22	47,47,47,47	0
52	MG	BA	3150	1/1	0.93	0.36	50,50,50,50	0
52	MG	DA	3061	1/1	0.93	0.28	57,57,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	AA	1606	1/1	0.93	0.35	73,73,73,73	0
52	MG	DA	3064	1/1	0.93	0.23	68,68,68,68	0
52	MG	DA	3147	1/1	0.93	0.11	63,63,63,63	0
52	MG	BA	3258	1/1	0.93	0.22	61,61,61,61	0
52	MG	BA	3194	1/1	0.93	0.32	44,44,44,44	0
52	MG	DA	3151	1/1	0.93	0.31	72,72,72,72	0
52	MG	BA	3326	1/1	0.93	0.09	54,54,54,54	0
52	MG	DA	3251	1/1	0.93	0.36	63,63,63,63	0
52	MG	DA	3254	1/1	0.93	0.11	65,65,65,65	0
52	MG	BA	3328	1/1	0.93	0.20	65,65,65,65	0
52	MG	BA	3329	1/1	0.93	0.25	68,68,68,68	0
52	MG	BA	3262	1/1	0.93	0.26	75,75,75,75	0
52	MG	AA	1631	1/1	0.93	0.11	60,60,60,60	0
52	MG	BA	3155	1/1	0.93	0.19	41,41,41,41	0
52	MG	BA	3271	1/1	0.93	0.25	46,46,46,46	0
52	MG	BA	3156	1/1	0.93	0.28	53,53,53,53	0
52	MG	BA	3054	1/1	0.93	0.16	68,68,68,68	0
52	MG	DA	3163	1/1	0.93	0.27	68,68,68,68	0
52	MG	CA	1642	1/1	0.93	0.17	62,62,62,62	0
52	MG	AA	1607	1/1	0.93	0.28	74,74,74,74	0
52	MG	BA	3159	1/1	0.93	0.24	45,45,45,45	0
52	MG	BA	3160	1/1	0.93	0.26	39,39,39,39	0
52	MG	DA	3086	1/1	0.93	0.23	38,38,38,38	0
52	MG	DA	3171	1/1	0.93	0.26	43,43,43,43	0
52	MG	BA	3211	1/1	0.93	0.13	39,39,39,39	0
52	MG	BA	3282	1/1	0.93	0.18	67,67,67,67	0
52	MG	BP	201	1/1	0.93	0.14	13,13,13,13	0
52	MG	D7	101	1/1	0.93	0.18	62,62,62,62	0
52	MG	DA	3177	1/1	0.93	0.35	61,61,61,61	0
52	MG	AA	1647	1/1	0.93	0.19	66,66,66,66	0
52	MG	DA	3004	1/1	0.93	0.27	49,49,49,49	0
52	MG	BA	3285	1/1	0.93	0.31	57,57,57,57	0
52	MG	BA	3088	1/1	0.93	0.10	10,10,10,10	0
52	MG	BA	3089	1/1	0.93	0.20	26,26,26,26	0
52	MG	DA	3014	1/1	0.93	0.25	68,68,68,68	0
52	MG	DA	3099	1/1	0.93	0.34	46,46,46,46	0
52	MG	BA	3122	1/1	0.93	0.29	40,40,40,40	0
52	MG	DA	3019	1/1	0.93	0.34	42,42,42,42	0
52	MG	BA	3126	1/1	0.93	0.30	50,50,50,50	0
52	MG	DA	3023	1/1	0.93	0.13	47,47,47,47	0
52	MG	DA	3106	1/1	0.93	0.30	76,76,76,76	0
52	MG	BA	3129	1/1	0.93	0.07	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3011	1/1	0.93	0.13	7,7,7,7	0
52	MG	DA	3202	1/1	0.93	0.17	40,40,40,40	0
52	MG	BA	3234	1/1	0.93	0.25	45,45,45,45	0
52	MG	CA	1610	1/1	0.93	0.12	61,61,61,61	0
52	MG	AA	1648	1/1	0.93	0.38	62,62,62,62	0
52	MG	DA	3301	1/1	0.93	0.21	57,57,57,57	0
52	MG	CA	1612	1/1	0.93	0.14	77,77,77,77	0
52	MG	BA	3236	1/1	0.93	0.46	70,70,70,70	0
52	MG	BA	3023	1/1	0.93	0.19	34,34,34,34	0
52	MG	BA	3304	1/1	0.93	0.47	86,86,86,86	0
52	MG	AA	1605	1/1	0.93	0.23	75,75,75,75	0
52	MG	DA	3118	1/1	0.93	0.15	66,66,66,66	0
52	MG	DA	3218	1/1	0.93	0.35	78,78,78,78	0
52	MG	CA	1617	1/1	0.93	0.26	61,61,61,61	0
52	MG	DA	3121	1/1	0.93	0.11	37,37,37,37	0
52	MG	DD	301	1/1	0.93	0.06	35,35,35,35	0
52	MG	AA	1616	1/1	0.93	0.19	77,77,77,77	0
52	MG	AA	1609	1/1	0.93	0.27	51,51,51,51	0
52	MG	DA	3225	1/1	0.93	0.12	54,54,54,54	0
52	MG	BA	3309	1/1	0.93	0.28	61,61,61,61	0
52	MG	B5	102	1/1	0.93	0.20	56,56,56,56	0
55	ZIT	DA	3311	52/52	0.93	0.20	100,100,100,100	0
52	MG	DA	3238	1/1	0.94	0.34	73,73,73,73	0
52	MG	BB	202	1/1	0.94	0.16	30,30,30,30	0
52	MG	DA	3241	1/1	0.94	0.18	60,60,60,60	0
52	MG	BB	203	1/1	0.94	0.20	41,41,41,41	0
52	MG	BB	205	1/1	0.94	0.18	78,78,78,78	0
52	MG	BF	301	1/1	0.94	0.07	62,62,62,62	0
52	MG	DA	3082	1/1	0.94	0.11	17,17,17,17	0
52	MG	AA	1635	1/1	0.94	0.41	63,63,63,63	0
52	MG	AA	1623	1/1	0.94	0.27	54,54,54,54	0
52	MG	BA	3296	1/1	0.94	0.40	67,67,67,67	0
52	MG	BA	3118	1/1	0.94	0.29	59,59,59,59	0
52	MG	DA	3012	1/1	0.94	0.12	23,23,23,23	0
52	MG	AA	1617	1/1	0.94	0.36	64,64,64,64	0
52	MG	BA	3188	1/1	0.94	0.29	62,62,62,62	0
52	MG	AA	1621	1/1	0.94	0.27	46,46,46,46	0
52	MG	BA	3241	1/1	0.94	0.24	79,79,79,79	0
52	MG	DA	3092	1/1	0.94	0.15	61,61,61,61	0
52	MG	AA	1615	1/1	0.94	0.34	76,76,76,76	0
52	MG	BA	3191	1/1	0.94	0.31	64,64,64,64	0
52	MG	B7	101	1/1	0.94	0.07	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3250	1/1	0.94	0.26	54,54,54,54	0
52	MG	DA	3097	1/1	0.94	0.18	44,44,44,44	0
52	MG	DA	3026	1/1	0.94	0.41	43,43,43,43	0
52	MG	BA	3096	1/1	0.94	0.21	55,55,55,55	0
52	MG	BA	3128	1/1	0.94	0.28	54,54,54,54	0
52	MG	DA	3269	1/1	0.94	0.09	61,61,61,61	0
52	MG	BA	3161	1/1	0.94	0.20	42,42,42,42	0
52	MG	DA	3181	1/1	0.94	0.20	50,50,50,50	0
52	MG	BA	3257	1/1	0.94	0.19	48,48,48,48	0
52	MG	DA	3033	1/1	0.94	0.21	44,44,44,44	0
52	MG	DA	3034	1/1	0.94	0.29	39,39,39,39	0
52	MG	DA	3276	1/1	0.94	0.16	70,70,70,70	0
52	MG	DA	3035	1/1	0.94	0.36	54,54,54,54	0
52	MG	BA	3014	1/1	0.94	0.27	32,32,32,32	0
52	MG	BA	3165	1/1	0.94	0.28	50,50,50,50	0
52	MG	DA	3038	1/1	0.94	0.24	48,48,48,48	0
52	MG	BA	3098	1/1	0.94	0.23	46,46,46,46	0
52	MG	BA	3167	1/1	0.94	0.39	52,52,52,52	0
52	MG	BA	3208	1/1	0.94	0.05	23,23,23,23	0
52	MG	BA	3324	1/1	0.94	0.24	59,59,59,59	0
52	MG	BA	3001	1/1	0.94	0.26	49,49,49,49	0
52	MG	DA	3286	1/1	0.94	0.23	58,58,58,58	0
52	MG	BA	3327	1/1	0.94	0.20	47,47,47,47	0
52	MG	BA	3210	1/1	0.94	0.20	37,37,37,37	0
52	MG	DA	3119	1/1	0.94	0.10	64,64,64,64	0
52	MG	BA	3003	1/1	0.94	0.11	43,43,43,43	0
52	MG	DA	3206	1/1	0.94	0.08	48,48,48,48	0
52	MG	BA	3174	1/1	0.94	0.40	57,57,57,57	0
52	MG	CA	1627	1/1	0.94	0.08	66,66,66,66	0
52	MG	BA	3331	1/1	0.94	0.21	46,46,46,46	0
52	MG	BA	3084	1/1	0.94	0.03	14,14,14,14	0
52	MG	BA	3107	1/1	0.94	0.11	34,34,34,34	0
52	MG	DA	3214	1/1	0.94	0.12	65,65,65,65	0
52	MG	DA	3215	1/1	0.94	0.27	59,59,59,59	0
52	MG	BA	3224	1/1	0.94	0.07	40,40,40,40	0
52	MG	BA	3337	1/1	0.94	0.34	58,58,58,58	0
52	MG	BA	3227	1/1	0.94	0.07	39,39,39,39	0
52	MG	CA	1635	1/1	0.94	0.07	86,86,86,86	0
52	MG	BA	3283	1/1	0.94	0.13	53,53,53,53	0
52	MG	DA	3137	1/1	0.94	0.26	38,38,38,38	0
52	MG	DA	3224	1/1	0.94	0.17	68,68,68,68	0
52	MG	DA	3138	1/1	0.94	0.21	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DA	3065	1/1	0.94	0.10	49,49,49,49	0
52	MG	BA	3342	1/1	0.94	0.19	49,49,49,49	0
52	MG	BA	3228	1/1	0.94	0.33	69,69,69,69	0
52	MG	DA	3068	1/1	0.94	0.30	49,49,49,49	0
52	MG	BA	3141	1/1	0.94	0.23	27,27,27,27	0
52	MG	BA	3063	1/1	0.94	0.23	48,48,48,48	0
52	MG	BA	3111	1/1	0.94	0.08	19,19,19,19	0
52	MG	BA	3347	1/1	0.94	0.20	66,66,66,66	0
52	MG	BA	3348	1/1	0.94	0.19	61,61,61,61	0
55	ZIT	BA	3351	52/52	0.94	0.20	100,100,100,100	0
52	MG	AA	1628	1/1	0.94	0.31	66,66,66,66	0
52	MG	BA	3339	1/1	0.95	0.20	41,41,41,41	0
52	MG	CA	1639	1/1	0.95	0.24	64,64,64,64	0
52	MG	BA	3105	1/1	0.95	0.32	46,46,46,46	0
52	MG	BA	3278	1/1	0.95	0.13	41,41,41,41	0
52	MG	DA	3237	1/1	0.95	0.12	53,53,53,53	0
52	MG	BA	3135	1/1	0.95	0.15	8,8,8,8	0
52	MG	DA	3239	1/1	0.95	0.17	59,59,59,59	0
52	MG	CA	1643	1/1	0.95	0.32	62,62,62,62	0
52	MG	DA	3071	1/1	0.95	0.21	40,40,40,40	0
52	MG	BA	3019	1/1	0.95	0.24	24,24,24,24	0
52	MG	DA	3073	1/1	0.95	0.21	42,42,42,42	0
52	MG	BA	3217	1/1	0.95	0.24	50,50,50,50	0
52	MG	BA	3109	1/1	0.95	0.30	34,34,34,34	0
52	MG	BA	3139	1/1	0.95	0.22	24,24,24,24	0
52	MG	CA	1648	1/1	0.95	0.21	79,79,79,79	0
52	MG	DA	3157	1/1	0.95	0.40	65,65,65,65	0
52	MG	D0	101	1/1	0.95	0.18	62,62,62,62	0
52	MG	D1	101	1/1	0.95	0.18	50,50,50,50	0
52	MG	DA	3080	1/1	0.95	0.30	40,40,40,40	0
52	MG	DA	3252	1/1	0.95	0.38	66,66,66,66	0
52	MG	BA	3175	1/1	0.95	0.18	49,49,49,49	0
52	MG	BA	3287	1/1	0.95	0.33	58,58,58,58	0
52	MG	BA	3226	1/1	0.95	0.14	32,32,32,32	0
52	MG	DA	3258	1/1	0.95	0.08	61,61,61,61	0
52	MG	BA	3043	1/1	0.95	0.10	36,36,36,36	0
52	MG	BA	3177	1/1	0.95	0.22	52,52,52,52	0
52	MG	BA	3045	1/1	0.95	0.20	26,26,26,26	0
52	MG	BA	3006	1/1	0.95	0.23	29,29,29,29	0
52	MG	DA	3263	1/1	0.95	0.19	67,67,67,67	0
52	MG	DA	3011	1/1	0.95	0.26	50,50,50,50	0
52	MG	BA	3144	1/1	0.95	0.19	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BX	101	1/1	0.95	0.11	61,61,61,61	0
52	MG	BA	3297	1/1	0.95	0.31	61,61,61,61	0
52	MG	DA	3174	1/1	0.95	0.39	63,63,63,63	0
52	MG	BA	3145	1/1	0.95	0.23	40,40,40,40	0
52	MG	DA	3018	1/1	0.95	0.30	32,32,32,32	0
52	MG	BA	3146	1/1	0.95	0.23	42,42,42,42	0
52	MG	BA	3113	1/1	0.95	0.25	26,26,26,26	0
52	MG	DA	3022	1/1	0.95	0.33	47,47,47,47	0
52	MG	BA	3025	1/1	0.95	0.20	54,54,54,54	0
52	MG	BA	3185	1/1	0.95	0.18	14,14,14,14	0
52	MG	BA	3050	1/1	0.95	0.23	38,38,38,38	0
52	MG	BA	3094	1/1	0.95	0.28	52,52,52,52	0
52	MG	DA	3186	1/1	0.95	0.19	63,63,63,63	0
52	MG	BA	3051	1/1	0.95	0.18	14,14,14,14	0
52	MG	BA	3242	1/1	0.95	0.16	48,48,48,48	0
52	MG	BA	3244	1/1	0.95	0.20	40,40,40,40	0
52	MG	BA	3153	1/1	0.95	0.26	25,25,25,25	0
52	MG	DA	3194	1/1	0.95	0.28	60,60,60,60	0
52	MG	BA	3311	1/1	0.95	0.15	46,46,46,46	0
52	MG	BA	3154	1/1	0.95	0.13	32,32,32,32	0
52	MG	BA	3077	1/1	0.95	0.26	28,28,28,28	0
52	MG	AA	1610	1/1	0.95	0.31	65,65,65,65	0
52	MG	DA	3199	1/1	0.95	0.13	47,47,47,47	0
52	MG	AA	1630	1/1	0.95	0.32	59,59,59,59	0
52	MG	BA	3317	1/1	0.95	0.10	41,41,41,41	0
52	MG	BA	3125	1/1	0.95	0.17	46,46,46,46	0
52	MG	AA	1612	1/1	0.95	0.24	66,66,66,66	0
52	MG	BA	3255	1/1	0.95	0.16	45,45,45,45	0
52	MG	BA	3323	1/1	0.95	0.11	64,64,64,64	0
52	MG	BA	3256	1/1	0.95	0.32	63,63,63,63	0
52	MG	DA	3044	1/1	0.95	0.24	46,46,46,46	0
52	MG	BA	3102	1/1	0.95	0.16	24,24,24,24	0
52	MG	BA	3038	1/1	0.95	0.31	25,25,25,25	0
52	MG	DA	3122	1/1	0.95	0.20	61,61,61,61	0
52	MG	BA	3132	1/1	0.95	0.26	55,55,55,55	0
52	MG	DA	3049	1/1	0.95	0.22	35,35,35,35	0
52	MG	DA	3304	1/1	0.95	0.22	52,52,52,52	0
52	MG	DA	3050	1/1	0.95	0.20	42,42,42,42	0
52	MG	BA	3201	1/1	0.95	0.20	29,29,29,29	0
52	MG	DA	3128	1/1	0.95	0.41	51,51,51,51	0
52	MG	BA	3202	1/1	0.95	0.18	41,41,41,41	0
52	MG	BA	3269	1/1	0.95	0.11	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	DB	201	1/1	0.95	0.26	52,52,52,52	0
52	MG	CA	1631	1/1	0.95	0.43	70,70,70,70	0
52	MG	BA	3203	1/1	0.95	0.25	35,35,35,35	0
52	MG	BA	3333	1/1	0.95	0.27	80,80,80,80	0
52	MG	DA	3136	1/1	0.95	0.29	59,59,59,59	0
52	MG	DP	201	1/1	0.95	0.08	50,50,50,50	0
52	MG	DQ	201	1/1	0.95	0.27	78,78,78,78	0
52	MG	BA	3163	1/1	0.95	0.29	47,47,47,47	0
52	MG	BA	3205	1/1	0.95	0.21	55,55,55,55	0
52	MG	DA	3139	1/1	0.95	0.21	68,68,68,68	0
52	MG	BA	3164	1/1	0.95	0.20	47,47,47,47	0
52	MG	BA	3015	1/1	0.95	0.20	48,48,48,48	0
52	MG	DA	3232	1/1	0.95	0.16	72,72,72,72	0
52	MG	BA	3221	1/1	0.96	0.33	40,40,40,40	0
52	MG	BA	3059	1/1	0.96	0.23	39,39,39,39	0
52	MG	AA	1624	1/1	0.96	0.35	56,56,56,56	0
52	MG	BA	3026	1/1	0.96	0.11	49,49,49,49	0
52	MG	BA	3136	1/1	0.96	0.28	32,32,32,32	0
52	MG	BA	3308	1/1	0.96	0.34	64,64,64,64	0
52	MG	BD	301	1/1	0.96	0.12	43,43,43,43	0
52	MG	BA	3267	1/1	0.96	0.22	38,38,38,38	0
52	MG	BA	3268	1/1	0.96	0.09	40,40,40,40	0
52	MG	DA	3210	1/1	0.96	0.16	63,63,63,63	0
52	MG	DA	3148	1/1	0.96	0.21	48,48,48,48	0
52	MG	BA	3064	1/1	0.96	0.15	28,28,28,28	0
52	MG	DA	3213	1/1	0.96	0.24	36,36,36,36	0
52	MG	BU	201	1/1	0.96	0.17	26,26,26,26	0
52	MG	BA	3044	1/1	0.96	0.20	26,26,26,26	0
52	MG	AA	1601	1/1	0.96	0.21	58,58,58,58	0
52	MG	DA	3217	1/1	0.96	0.33	62,62,62,62	0
52	MG	DA	3046	1/1	0.96	0.20	28,28,28,28	0
52	MG	BA	3314	1/1	0.96	0.10	56,56,56,56	0
52	MG	BA	3231	1/1	0.96	0.33	52,52,52,52	0
52	MG	DA	3101	1/1	0.96	0.24	43,43,43,43	0
52	MG	BA	3273	1/1	0.96	0.25	58,58,58,58	0
52	MG	BA	3028	1/1	0.96	0.36	28,28,28,28	0
52	MG	BA	3069	1/1	0.96	0.21	18,18,18,18	0
52	MG	BA	3276	1/1	0.96	0.33	55,55,55,55	0
52	MG	DA	3107	1/1	0.96	0.27	38,38,38,38	0
52	MG	CA	1608	1/1	0.96	0.27	51,51,51,51	0
52	MG	BA	3115	1/1	0.96	0.28	49,49,49,49	0
52	MG	BA	3168	1/1	0.96	0.11	43,43,43,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3143	1/1	0.96	0.18	30,30,30,30	0
52	MG	DA	3293	1/1	0.96	0.22	53,53,53,53	0
52	MG	BA	3070	1/1	0.96	0.22	35,35,35,35	0
52	MG	AA	1642	1/1	0.96	0.23	51,51,51,51	0
52	MG	DA	3006	1/1	0.96	0.28	39,39,39,39	0
52	MG	DA	3007	1/1	0.96	0.16	39,39,39,39	0
52	MG	BA	3239	1/1	0.96	0.23	48,48,48,48	0
52	MG	DA	3010	1/1	0.96	0.21	31,31,31,31	0
52	MG	BA	3072	1/1	0.96	0.16	24,24,24,24	0
52	MG	BA	3020	1/1	0.96	0.26	38,38,38,38	0
52	MG	BA	3036	1/1	0.96	0.05	0,0,0,0	0
52	MG	BA	3052	1/1	0.96	0.16	15,15,15,15	0
52	MG	BA	3100	1/1	0.96	0.15	21,21,21,21	0
52	MG	DA	3123	1/1	0.96	0.12	61,61,61,61	0
52	MG	BA	3022	1/1	0.96	0.23	49,49,49,49	0
52	MG	BA	3335	1/1	0.96	0.27	52,52,52,52	0
52	MG	BA	3127	1/1	0.96	0.11	50,50,50,50	0
52	MG	BA	3294	1/1	0.96	0.30	65,65,65,65	0
52	MG	DA	3187	1/1	0.96	0.11	52,52,52,52	0
52	MG	BA	3078	1/1	0.96	0.19	34,34,34,34	0
52	MG	BA	3251	1/1	0.96	0.07	35,35,35,35	0
52	MG	DA	3130	1/1	0.96	0.24	43,43,43,43	0
52	MG	DE	301	1/1	0.96	0.16	40,40,40,40	0
52	MG	BA	3213	1/1	0.96	0.28	32,32,32,32	0
52	MG	B1	101	1/1	0.96	0.13	39,39,39,39	0
52	MG	BA	3299	1/1	0.96	0.34	58,58,58,58	0
52	MG	DA	3256	1/1	0.96	0.12	57,57,57,57	0
52	MG	DU	201	1/1	0.96	0.18	60,60,60,60	0
52	MG	BA	3216	1/1	0.96	0.32	43,43,43,43	0
53	ZN	AD	301	1/1	0.96	0.22	108,108,108,108	0
52	MG	DA	3030	1/1	0.96	0.28	42,42,42,42	0
52	MG	BA	3130	1/1	0.96	0.15	26,26,26,26	0
52	MG	BA	3040	1/1	0.96	0.38	51,51,51,51	0
52	MG	DA	3200	1/1	0.96	0.25	50,50,50,50	0
52	MG	BP	202	1/1	0.97	0.24	58,58,58,58	0
52	MG	DA	3165	1/1	0.97	0.14	52,52,52,52	0
52	MG	BQ	201	1/1	0.97	0.04	32,32,32,32	0
52	MG	DA	3220	1/1	0.97	0.17	62,62,62,62	0
52	MG	DA	3028	1/1	0.97	0.18	39,39,39,39	0
52	MG	BA	3322	1/1	0.97	0.12	20,20,20,20	0
52	MG	BR	201	1/1	0.97	0.10	20,20,20,20	0
52	MG	DA	3170	1/1	0.97	0.22	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3086	1/1	0.97	0.12	18,18,18,18	0
52	MG	BA	3291	1/1	0.97	0.37	54,54,54,54	0
52	MG	BA	3325	1/1	0.97	0.26	43,43,43,43	0
52	MG	BA	3225	1/1	0.97	0.19	33,33,33,33	0
52	MG	BA	3018	1/1	0.97	0.10	26,26,26,26	0
52	MG	AA	1602	1/1	0.97	0.26	37,37,37,37	0
52	MG	BA	3199	1/1	0.97	0.31	49,49,49,49	0
52	MG	BA	3037	1/1	0.97	0.15	14,14,14,14	0
52	MG	BA	3123	1/1	0.97	0.20	22,22,22,22	0
52	MG	DA	3131	1/1	0.97	0.26	47,47,47,47	0
52	MG	BA	3124	1/1	0.97	0.06	42,42,42,42	0
52	MG	DA	3183	1/1	0.97	0.22	44,44,44,44	0
52	MG	BA	3264	1/1	0.97	0.15	35,35,35,35	0
52	MG	BA	3265	1/1	0.97	0.29	63,63,63,63	0
52	MG	BA	3046	1/1	0.97	0.19	37,37,37,37	0
52	MG	BA	3004	1/1	0.97	0.17	23,23,23,23	0
52	MG	BA	3062	1/1	0.97	0.30	44,44,44,44	0
52	MG	BA	3206	1/1	0.97	0.20	29,29,29,29	0
52	MG	BA	3207	1/1	0.97	0.10	23,23,23,23	0
52	MG	DA	3002	1/1	0.97	0.32	38,38,38,38	0
52	MG	DA	3192	1/1	0.97	0.26	55,55,55,55	0
52	MG	DA	3193	1/1	0.97	0.30	50,50,50,50	0
52	MG	DA	3003	1/1	0.97	0.28	56,56,56,56	0
52	MG	BA	3340	1/1	0.97	0.28	62,62,62,62	0
52	MG	BA	3048	1/1	0.97	0.25	30,30,30,30	0
52	MG	DA	3053	1/1	0.97	0.43	51,51,51,51	0
52	MG	AA	1620	1/1	0.97	0.15	73,73,73,73	0
52	MG	BA	3065	1/1	0.97	0.20	32,32,32,32	0
52	MG	BA	3029	1/1	0.97	0.14	26,26,26,26	0
52	MG	BA	3212	1/1	0.97	0.24	30,30,30,30	0
52	MG	DA	3103	1/1	0.97	0.48	70,70,70,70	0
52	MG	B5	101	1/1	0.97	0.09	27,27,27,27	0
52	MG	BA	3243	1/1	0.97	0.10	58,58,58,58	0
52	MG	BA	3169	1/1	0.97	0.23	46,46,46,46	0
52	MG	BA	3042	1/1	0.97	0.17	15,15,15,15	0
52	MG	DA	3063	1/1	0.97	0.19	47,47,47,47	0
52	MG	BB	201	1/1	0.97	0.27	42,42,42,42	0
52	MG	DA	3156	1/1	0.97	0.33	44,44,44,44	0
52	MG	BA	3117	1/1	0.97	0.29	39,39,39,39	0
52	MG	BA	3218	1/1	0.97	0.25	33,33,33,33	0
52	MG	BA	3172	1/1	0.97	0.25	64,64,64,64	0
52	MG	BA	3220	1/1	0.97	0.23	27,27,27,27	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
53	ZN	AN	101	1/1	0.97	0.05	159,159,159,159	0
53	ZN	CD	301	1/1	0.97	0.17	93,93,93,93	0
53	ZN	CN	101	1/1	0.97	0.06	157,157,157,157	0
52	MG	BE	301	1/1	0.97	0.22	29,29,29,29	0
52	MG	BA	3173	1/1	0.97	0.21	24,24,24,24	0
52	MG	BA	3053	1/1	0.97	0.19	15,15,15,15	0
52	MG	DA	3271	1/1	0.97	0.08	46,46,46,46	0
52	MG	BA	3281	1/1	0.98	0.31	46,46,46,46	0
52	MG	BA	3091	1/1	0.98	0.15	9,9,9,9	0
52	MG	DA	3015	1/1	0.98	0.11	23,23,23,23	0
52	MG	DA	3016	1/1	0.98	0.34	56,56,56,56	0
52	MG	BA	3106	1/1	0.98	0.11	12,12,12,12	0
52	MG	BA	3261	1/1	0.98	0.13	38,38,38,38	0
52	MG	BA	3222	1/1	0.98	0.15	23,23,23,23	0
52	MG	BA	3030	1/1	0.98	0.11	17,17,17,17	0
52	MG	DA	3021	1/1	0.98	0.23	47,47,47,47	0
52	MG	DA	3051	1/1	0.98	0.19	26,26,26,26	0
52	MG	BA	3079	1/1	0.98	0.12	0,0,0,0	0
52	MG	B0	101	1/1	0.98	0.16	34,34,34,34	0
52	MG	BA	3290	1/1	0.98	0.24	47,47,47,47	0
52	MG	BA	3032	1/1	0.98	0.20	15,15,15,15	0
52	MG	DA	3180	1/1	0.98	0.24	52,52,52,52	0
52	MG	BA	3012	1/1	0.98	0.13	22,22,22,22	0
52	MG	BA	3061	1/1	0.98	0.06	23,23,23,23	0
52	MG	BA	3247	1/1	0.98	0.03	40,40,40,40	0
52	MG	BA	3318	1/1	0.98	0.28	60,60,60,60	0
52	MG	DA	3060	1/1	0.98	0.04	34,34,34,34	0
52	MG	BA	3248	1/1	0.98	0.05	47,47,47,47	0
52	MG	BA	3193	1/1	0.98	0.19	28,28,28,28	0
52	MG	BA	3035	1/1	0.98	0.11	21,21,21,21	0
52	MG	DA	3253	1/1	0.98	0.25	50,50,50,50	0
52	MG	BA	3099	1/1	0.98	0.15	26,26,26,26	0
52	MG	BA	3147	1/1	0.98	0.04	12,12,12,12	0
52	MG	BA	3021	1/1	0.98	0.14	16,16,16,16	0
52	MG	BA	3016	1/1	0.98	0.12	21,21,21,21	0
52	MG	DA	3008	1/1	0.98	0.41	52,52,52,52	0
52	MG	BA	3075	1/1	0.98	0.17	26,26,26,26	0
52	MG	BA	3002	1/1	0.98	0.20	20,20,20,20	0
52	MG	BA	3056	1/1	0.98	0.07	20,20,20,20	0
52	MG	BB	204	1/1	0.98	0.38	56,56,56,56	0
52	MG	BA	3033	1/1	0.99	0.06	20,20,20,20	0
52	MG	BA	3017	1/1	0.99	0.26	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
52	MG	BA	3215	1/1	0.99	0.18	36,36,36,36	0
52	MG	BA	3266	1/1	0.99	0.21	35,35,35,35	0
52	MG	BA	3131	1/1	0.99	0.11	45,45,45,45	0
52	MG	BA	3286	1/1	0.99	0.03	45,45,45,45	0
52	MG	BA	3055	1/1	0.99	0.19	19,19,19,19	0
52	MG	BA	3260	1/1	0.99	0.17	42,42,42,42	0
52	MG	BA	3083	1/1	0.99	0.06	5,5,5,5	0
52	MG	BP	203	1/1	0.99	0.09	0,0,0,0	0
52	MG	BA	3108	1/1	0.99	0.27	56,56,56,56	0
52	MG	BA	3024	1/1	1.00	0.03	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.