



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 08:47 PM UTC

PDB ID : 4V5E / pdb_00004v5e
Title : Insights into translational termination from the structure of RF2 bound to the ribosome
Authors : Weixlbaumer, A.; Jin, H.; Neubauer, C.; Voorhees, R.M.; Petry, S.; Kelley, A.C.; Ramakrishnan, V.
Deposited on : 2009-04-30
Resolution : 3.45 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

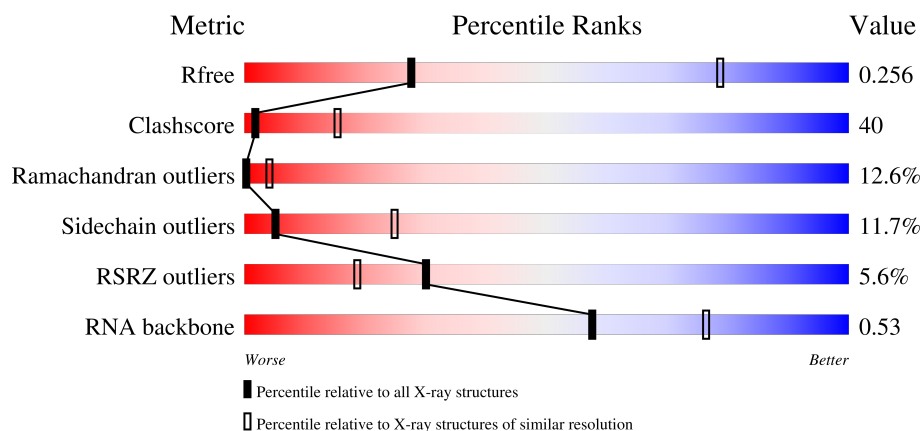
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.45 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	1070 (3.50-3.42)
Clashscore	190562	1128 (3.50-3.42)
Ramachandran outliers	187476	1101 (3.50-3.42)
Sidechain outliers	187428	1102 (3.50-3.42)
RSRZ outliers	180081	1070 (3.50-3.42)
RNA backbone	3983	1186 (3.92-3.00)

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

Mol	Chain	Length	Quality of chain
1	AA	1522	3% 26% 60% 11% ..
1	CA	1522	3% 26% 60% 11% ..
2	AB	256	2% 19% 59% 14% 8%
2	CB	256	4% 20% 57% 15% 8%

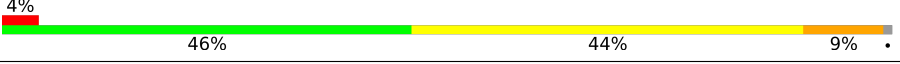
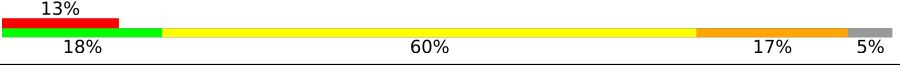
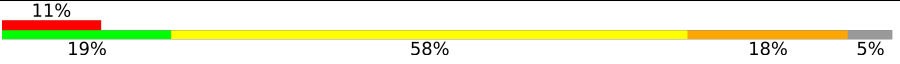
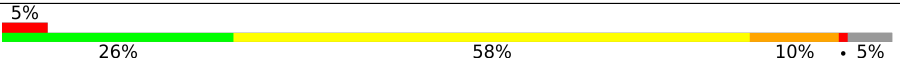
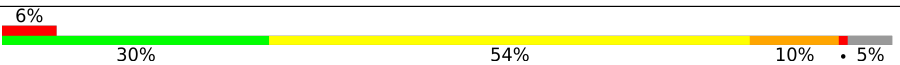
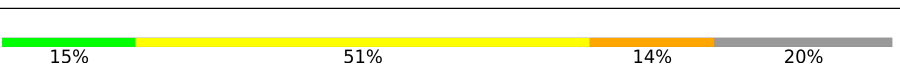
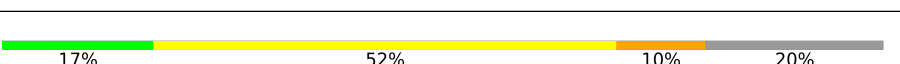
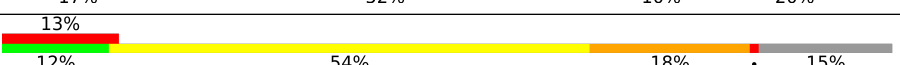
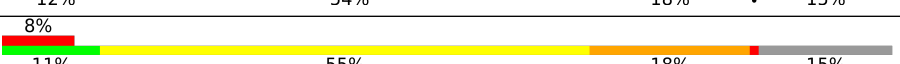
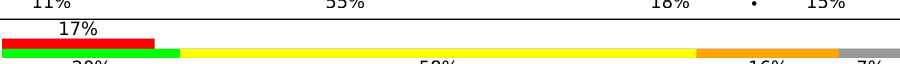
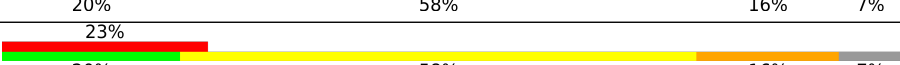
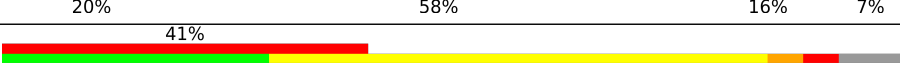
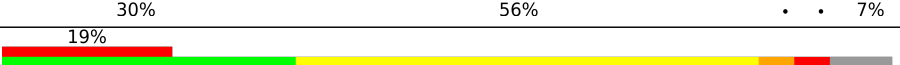
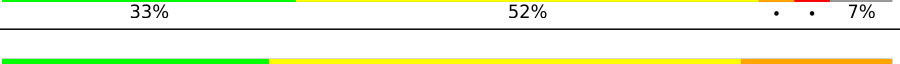
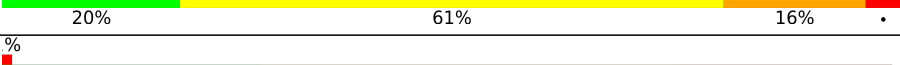
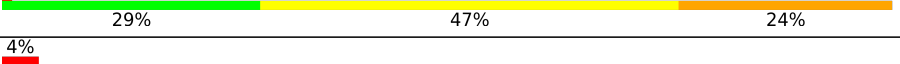
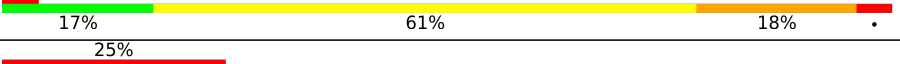
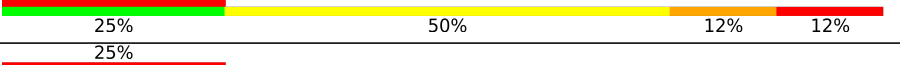
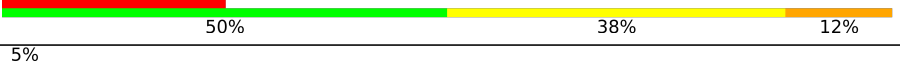
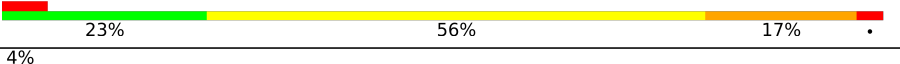
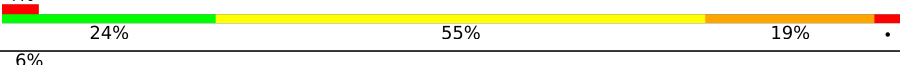
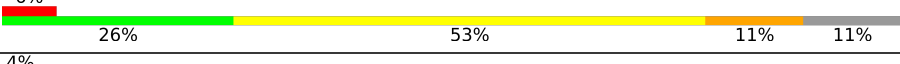
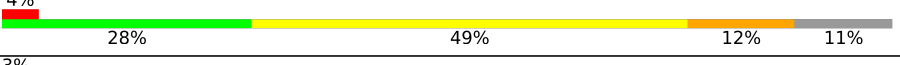
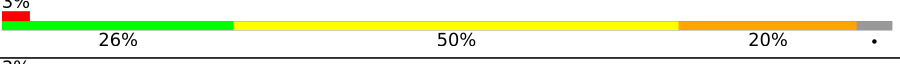
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Mol	Chain	Length	Quality of chain
3	AC	239	
3	CC	239	
4	AD	209	
4	CD	209	
5	AE	162	
5	CE	162	
6	AF	101	
6	CF	101	
7	AG	156	
7	CG	156	
8	AH	138	
8	CH	138	
9	AI	128	
9	CI	128	
10	AJ	105	
10	CJ	105	
11	AK	129	
11	CK	129	
12	AL	132	
12	CL	132	
13	AM	126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

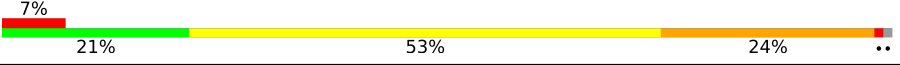
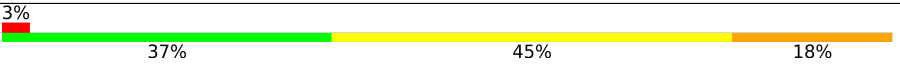
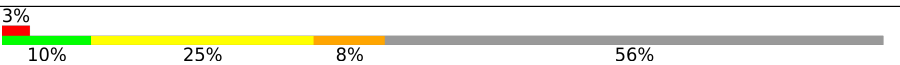
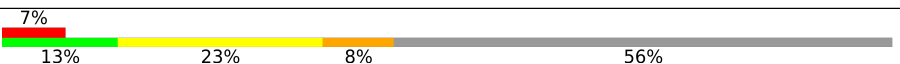
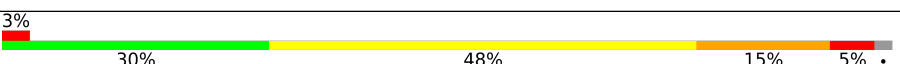
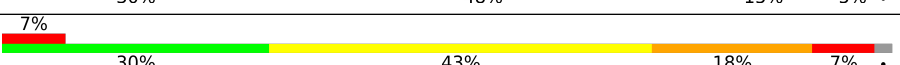
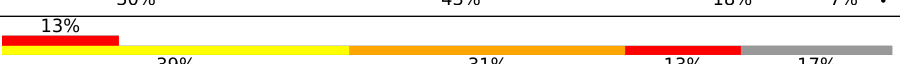
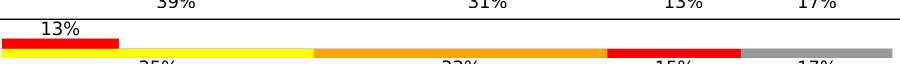
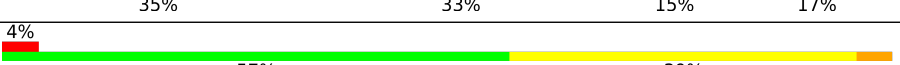
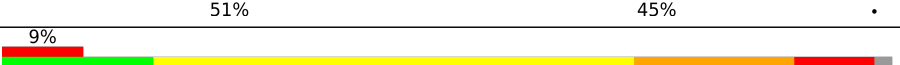
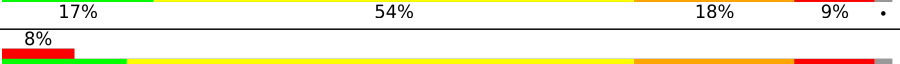
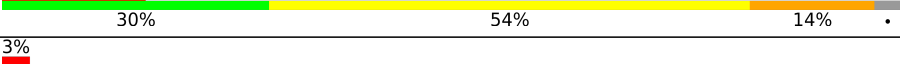
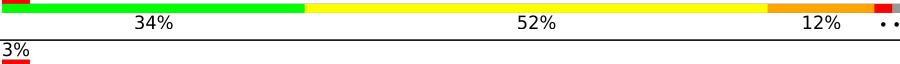
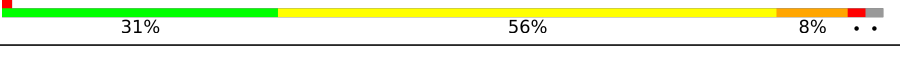
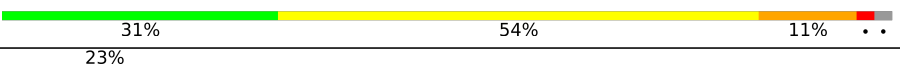
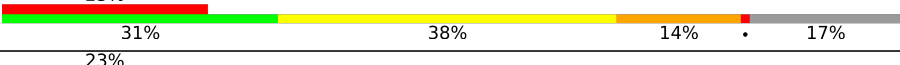
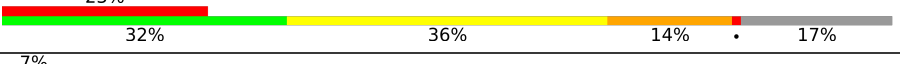
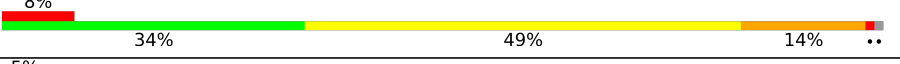
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Mol	Chain	Length	Quality of chain
15	CO	89	
16	AP	88	
16	CP	88	
17	AQ	105	
17	CQ	105	
18	AR	88	
18	CR	88	
19	AS	93	
19	CS	93	
20	AT	106	
20	CT	106	
21	AU	27	
21	CU	27	
22	AV	76	
22	AW	76	
22	CV	76	
22	CW	76	
23	AX	8	
23	CX	8	
24	AY	351	
24	CY	351	
25	B0	85	
25	D0	85	
26	B1	98	
26	D1	98	

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Mol	Chain	Length	Quality of chain
27	B2	72	
27	D2	72	
28	B3	60	
28	D3	60	
29	B4	71	
29	D4	71	
30	B5	60	
30	D5	60	
31	B6	54	
31	D6	54	
32	B7	49	
32	D7	49	
33	B8	65	
33	D8	65	
34	B9	37	
34	D9	37	
35	BA	2901	
35	DA	2901	
36	BB	122	
36	DB	122	
37	BC	229	
37	DC	229	
38	BD	276	
38	DD	276	
39	BE	206	

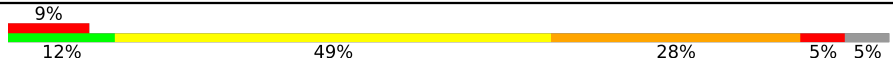
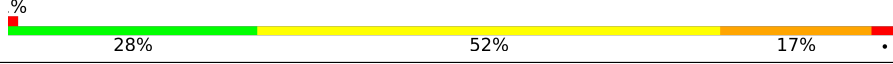
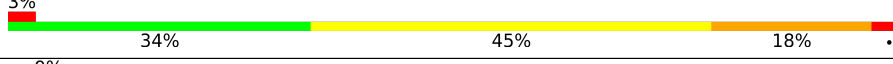
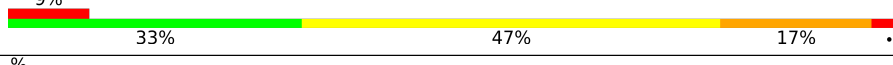
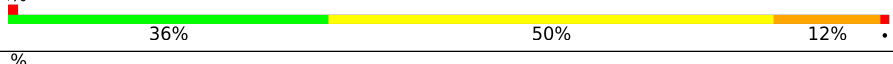
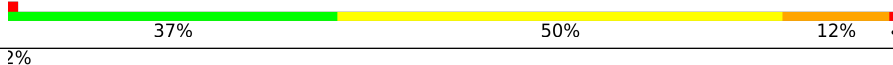
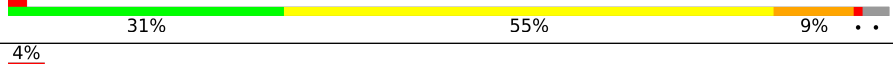
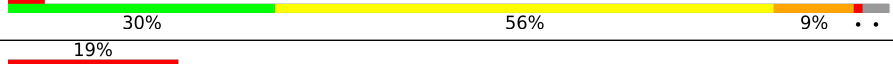
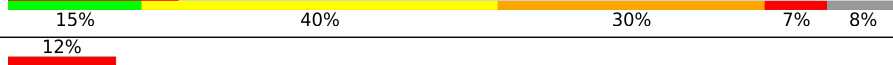
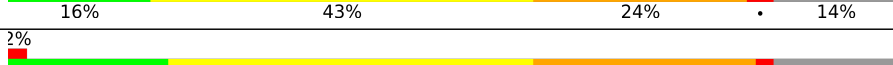
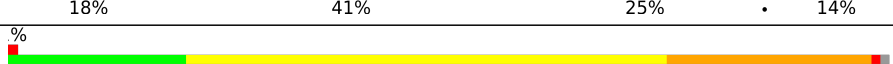
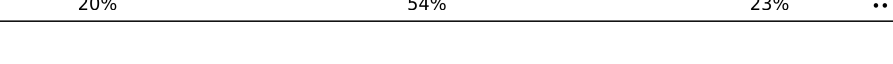
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Mol	Chain	Length	Quality of chain
39	DE	206	
40	BF	210	
40	DF	210	
41	BG	182	
41	DG	182	
42	BH	180	
42	DH	180	
43	BI	148	
44	BJ	130	
44	DJ	130	
45	BK	147	
45	DK	147	
46	BN	140	
46	DN	140	
47	BO	122	
47	DO	122	
48	BP	150	
48	DP	150	
49	BQ	141	
49	DQ	141	
50	BR	118	
50	DR	118	
51	BS	112	
51	DS	112	
52	BT	146	

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Mol	Chain	Length	Quality of chain
52	DT	146	
53	BU	118	
53	DU	118	
54	BV	101	
54	DV	101	
55	BW	113	
55	DW	113	
56	BX	96	
56	DX	96	
57	BY	110	
57	DY	110	
58	BZ	206	
58	DZ	206	
59	DI	148	

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
60	MG	BA	3024	-	-	-	X
60	MG	BA	3102	-	-	-	X
60	MG	BA	3120	-	-	-	X
60	MG	BA	3292	-	-	-	X
60	MG	DA	3078	-	-	-	X
60	MG	DA	3107	-	-	-	X
60	MG	DA	3295	-	-	-	X
60	MG	DA	3303	-	-	-	X
60	MG	DD	301	-	-	-	X

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 304505 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AA	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				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

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

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

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	AL	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			
12	CL	126	Total	C	N	O	S	0	0	1
			976	614	197	164	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	AM	121	Total	C	N	O	S	0	0	1
			956	591	198	165	2			
13	CM	121	Total	C	N	O	S	0	0	1
			956	591	198	165	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

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

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

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

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

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

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

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

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

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

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

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

- Molecule 22 is a RNA chain called E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	AV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	AW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CV	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			
22	CW	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	AX	8	Total	C	N	O	P	0	0	0
			166	76	29	54	7			
23	CX	8	Total	C	N	O	P	0	0	0
			166	76	29	54	7			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	AY	351	Total	C	N	O	S	0	0	0
			2799	1751	503	537	8			
24	CY	351	Total	C	N	O	S	0	0	0
			2799	1751	503	537	8			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AY	303	GLU	ARG	conflict	UNP Q5SM01
CY	303	GLU	ARG	conflict	UNP Q5SM01

- Molecule 25 is a protein called 50S RIBOSOMAL PROTEIN L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	B0	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			
25	D0	76	Total	C	N	O	S	0	0	0
			607	376	128	102	1			

- Molecule 26 is a protein called 50S RIBOSOMAL PROTEIN L28.

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

- Molecule 27 is a protein called 50S RIBOSOMAL PROTEIN L29.

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

- Molecule 28 is a protein called 50S RIBOSOMAL PROTEIN L30.

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

- Molecule 29 is a protein called 50S RIBOSOMAL PROTEIN L31.

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

- Molecule 30 is a protein called 50S RIBOSOMAL PROTEIN L32.

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

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

- Molecule 31 is a protein called 50S RIBOSOMAL PROTEIN L33.

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

- Molecule 32 is a protein called 50S RIBOSOMAL PROTEIN L34.

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

- Molecule 33 is a protein called 50S RIBOSOMAL PROTEIN L35.

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

- Molecule 34 is a protein called 50S RIBOSOMAL PROTEIN L36.

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

- Molecule 35 is a RNA chain called 23S RIBOSOMAL RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	BA	2886	Total	C	N	O	P	0	0	0
			62154	27663	11625	19981	2885			
35	DA	2886	Total	C	N	O	P	0	0	0
			62154	27663	11625	19981	2885			

- Molecule 36 is a RNA chain called 5S RIBOSOMAL RNA.

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

- Molecule 37 is a protein called 50S RIBOSOMAL PROTEIN L1.

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

- Molecule 38 is a protein called 50S RIBOSOMAL PROTEIN L2.

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

- Molecule 39 is a protein called 50S RIBOSOMAL PROTEIN L3.

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

- Molecule 40 is a protein called 50S RIBOSOMAL PROTEIN L4.

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

- Molecule 41 is a protein called 50S RIBOSOMAL PROTEIN L5.

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

- Molecule 42 is a protein called 50S RIBOSOMAL PROTEIN L6.

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

- Molecule 43 is a protein called 50S RIBOSOMAL PROTEIN L9.

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

- Molecule 44 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
44	BJ	130	Total	C	N	O	0	0	0
			651	390	130	131			
44	DJ	130	Total	C	N	O	0	0	0
			651	390	130	131			

- Molecule 45 is a protein called 50S RIBOSOMAL PROTEIN L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
45	BK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			
45	DK	141	Total	C	N	O	S	0	0	1
			1038	661	184	187	6			

- Molecule 46 is a protein called 50S RIBOSOMAL PROTEIN L13.

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

- Molecule 47 is a protein called 50S RIBOSOMAL PROTEIN L14.

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

- Molecule 48 is a protein called 50S RIBOSOMAL PROTEIN L15.

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

- Molecule 49 is a protein called 50S RIBOSOMAL PROTEIN L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
49	BQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			
49	DQ	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 50 is a protein called 50S RIBOSOMAL PROTEIN L17.

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

- Molecule 51 is a protein called 50S RIBOSOMAL PROTEIN L18.

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

- Molecule 52 is a protein called 50S RIBOSOMAL PROTEIN L19.

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

- Molecule 53 is a protein called 50S RIBOSOMAL PROTEIN L20.

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

- Molecule 54 is a protein called 50S RIBOSOMAL PROTEIN L21.

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

- Molecule 55 is a protein called 50S RIBOSOMAL PROTEIN L22.

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

- Molecule 56 is a protein called 50S RIBOSOMAL PROTEIN L23.

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

- Molecule 57 is a protein called 50S RIBOSOMAL PROTEIN L24.

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

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

- Molecule 58 is a protein called 50S RIBOSOMAL PROTEIN L25.

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

- Molecule 59 is a protein called 50S RIBOSOMAL PROTEIN L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
59	DI	146	Total	C	N	O	S	0	0	1
			1133	724	201	207	1			

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	AA	157	Total	Mg	0	0
			157	157		
60	AE	1	Total	Mg	0	0
			1	1		
60	AL	1	Total	Mg	0	0
			1	1		
60	AM	1	Total	Mg	0	0
			1	1		
60	AV	7	Total	Mg	0	0
			7	7		
60	AW	5	Total	Mg	0	0
			5	5		
60	AY	1	Total	Mg	0	0
			1	1		
60	B1	1	Total	Mg	0	0
			1	1		
60	B3	1	Total	Mg	0	0
			1	1		
60	B5	2	Total	Mg	0	0
			2	2		
60	B7	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	BA	354	Total 354	Mg 354	0	0
60	BB	4	Total 4	Mg 4	0	0
60	BC	1	Total 1	Mg 1	0	0
60	BD	2	Total 2	Mg 2	0	0
60	BF	1	Total 1	Mg 1	0	0
60	BH	1	Total 1	Mg 1	0	0
60	BP	1	Total 1	Mg 1	0	0
60	BQ	1	Total 1	Mg 1	0	0
60	BS	1	Total 1	Mg 1	0	0
60	BU	1	Total 1	Mg 1	0	0
60	CA	157	Total 157	Mg 157	0	0
60	CL	1	Total 1	Mg 1	0	0
60	CN	1	Total 1	Mg 1	0	0
60	CV	7	Total 7	Mg 7	0	0
60	CW	5	Total 5	Mg 5	0	0
60	CY	1	Total 1	Mg 1	0	0
60	D1	1	Total 1	Mg 1	0	0
60	D3	1	Total 1	Mg 1	0	0
60	D5	2	Total 2	Mg 2	0	0
60	D7	1	Total 1	Mg 1	0	0
60	DA	353	Total 353	Mg 353	0	0

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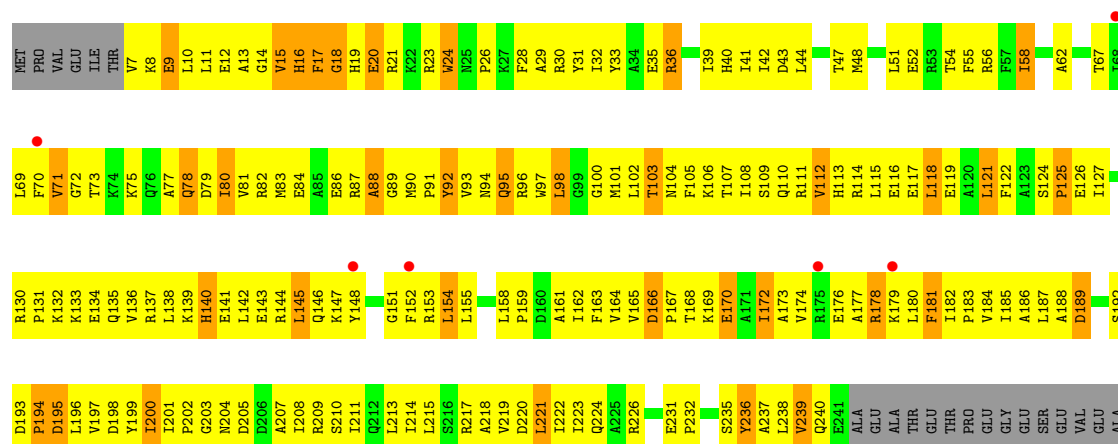
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
60	DB	4	Total 4	Mg 4	0	0
60	DC	1	Total 1	Mg 1	0	0
60	DD	2	Total 2	Mg 2	0	0
60	DF	3	Total 3	Mg 3	0	0
60	DH	1	Total 1	Mg 1	0	0
60	DQ	1	Total 1	Mg 1	0	0
60	DR	1	Total 1	Mg 1	0	0
60	DU	1	Total 1	Mg 1	0	0
60	DX	1	Total 1	Mg 1	0	0
60	DY	1	Total 1	Mg 1	0	0

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn).

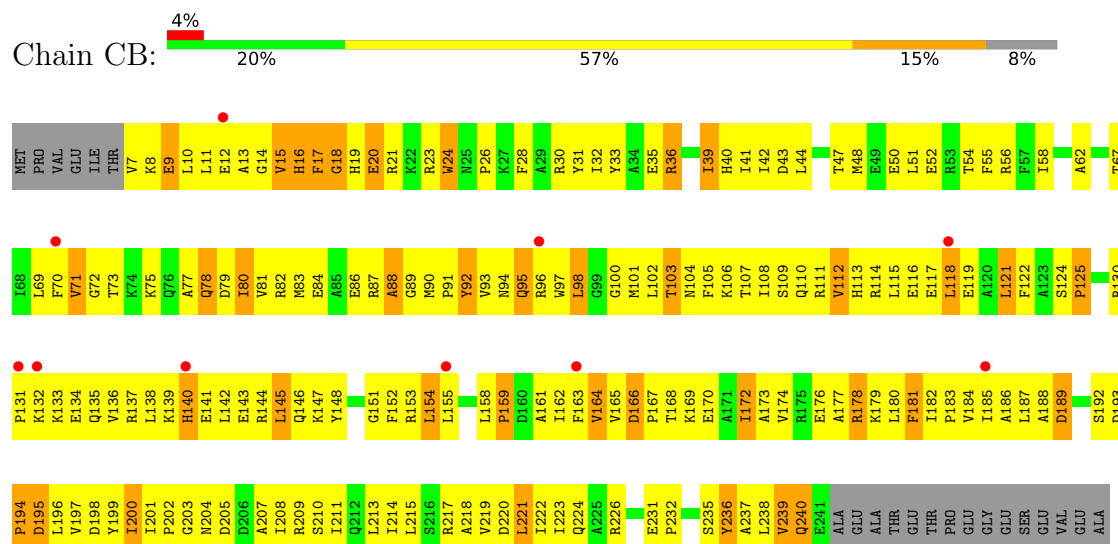
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61	AD	1	Total 1	Zn 1	0	0
61	AN	1	Total 1	Zn 1	0	0
61	B9	1	Total 1	Zn 1	0	0
61	CD	1	Total 1	Zn 1	0	0
61	CN	1	Total 1	Zn 1	0	0
61	D9	1	Total 1	Zn 1	0	0



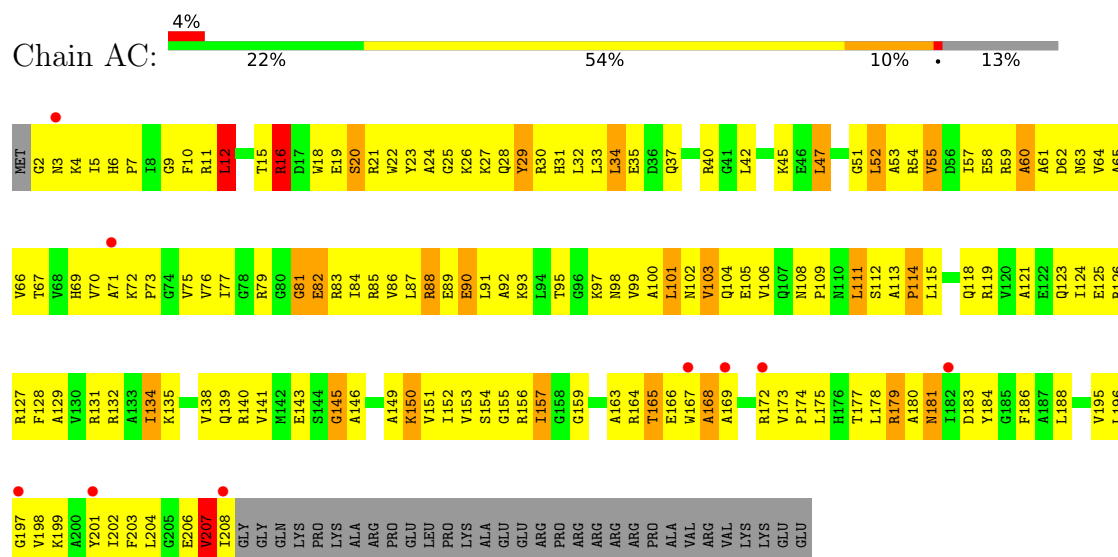




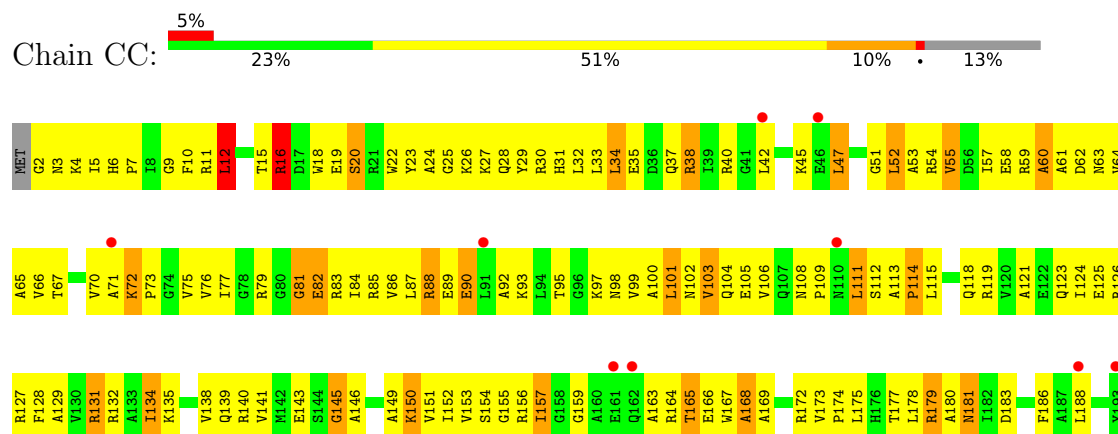
• Molecule 2: 30S RIBOSOMAL PROTEIN S2

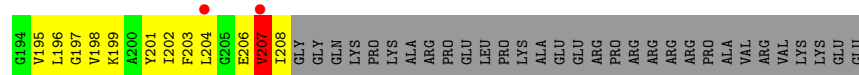


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

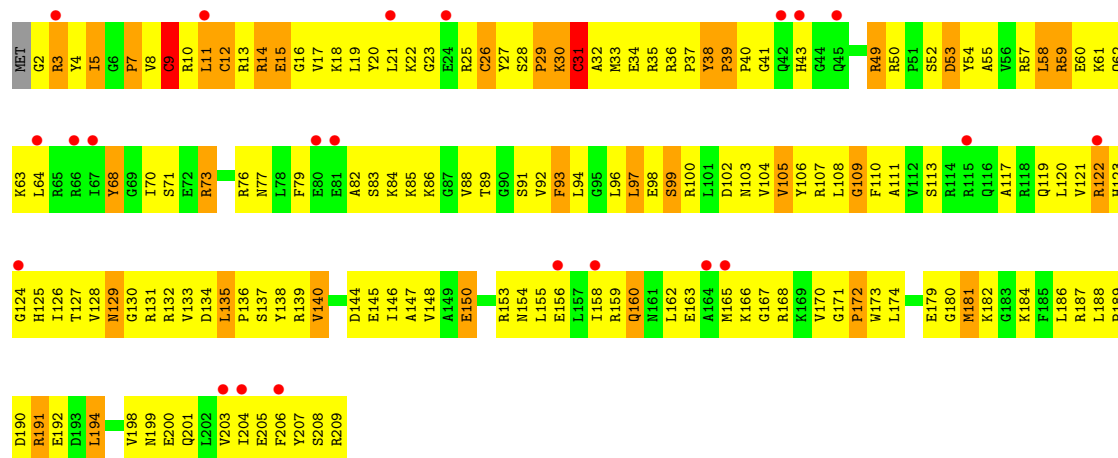


• Molecule 3: 30S RIBOSOMAL PROTEIN S3

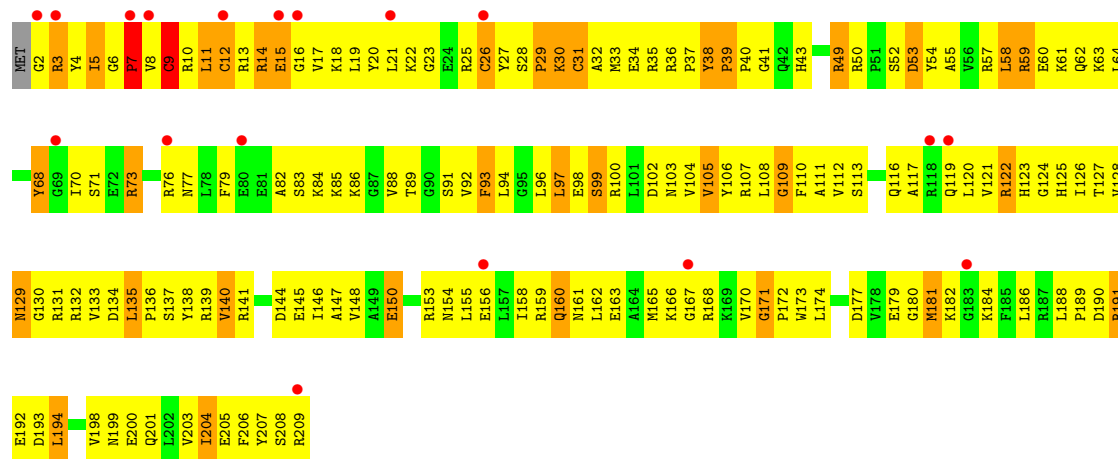




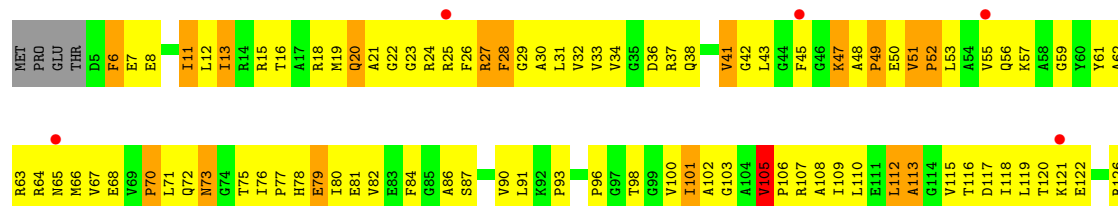
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

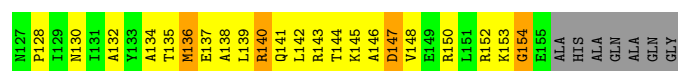


• Molecule 4: 30S RIBOSOMAL PROTEIN S4

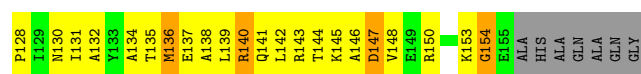
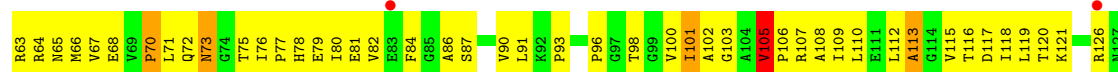
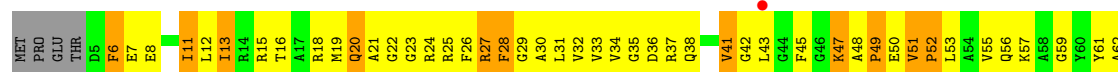


• Molecule 5: 30S RIBOSOMAL PROTEIN S5

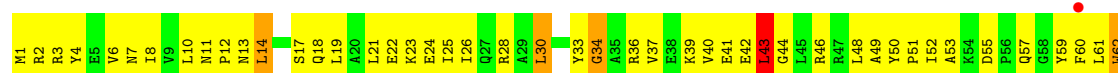




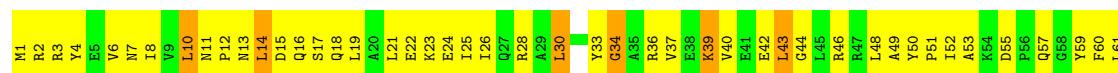
• Molecule 5: 30S RIBOSOMAL PROTEIN S5



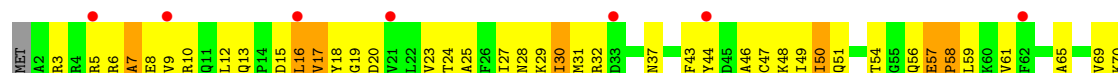
• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 6: 30S RIBOSOMAL PROTEIN S6



• Molecule 7: 30S RIBOSOMAL PROTEIN S7

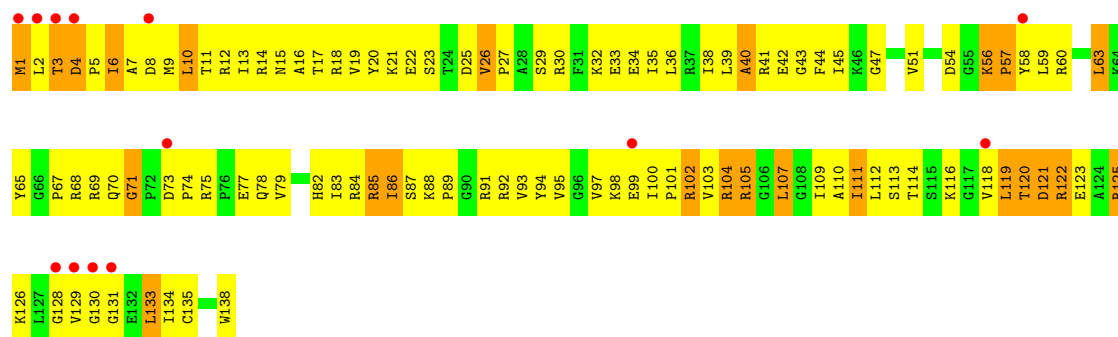




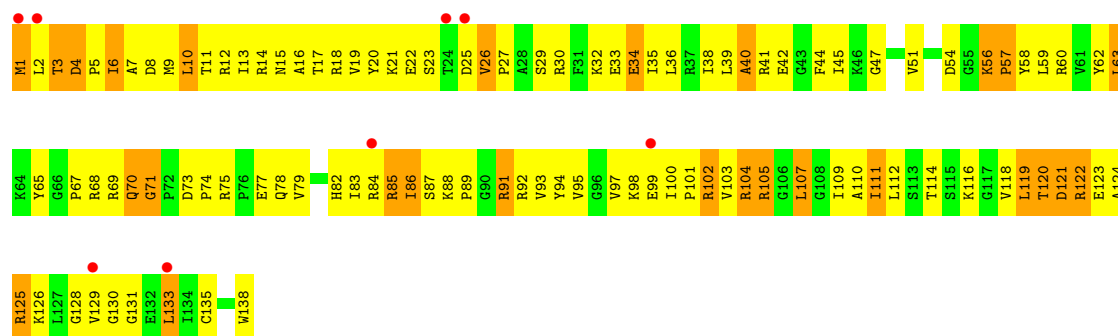
• Molecule 7: 30S RIBOSOMAL PROTEIN S7



• Molecule 8: 30S RIBOSOMAL PROTEIN S8

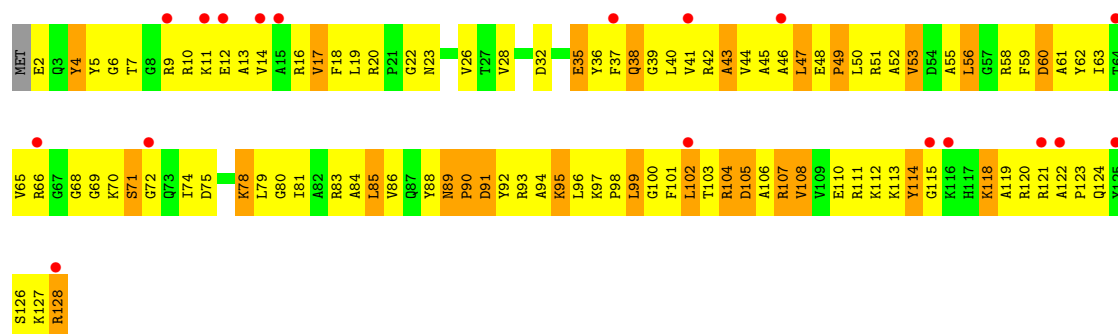


• Molecule 8: 30S RIBOSOMAL PROTEIN S8

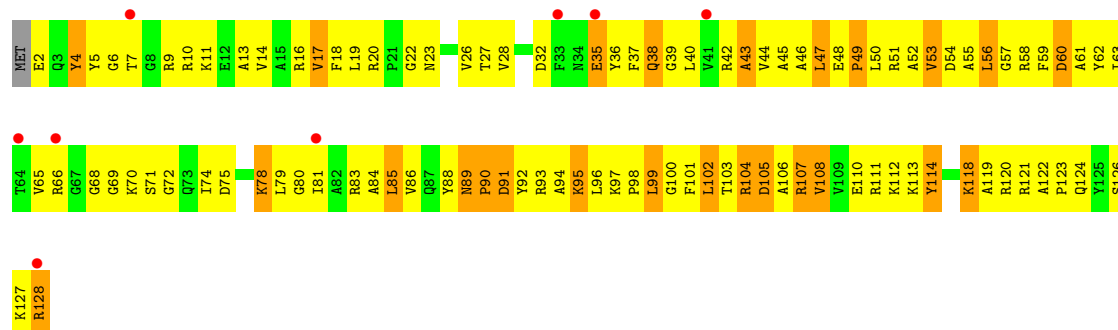


• Molecule 9: 30S RIBOSOMAL PROTEIN S9

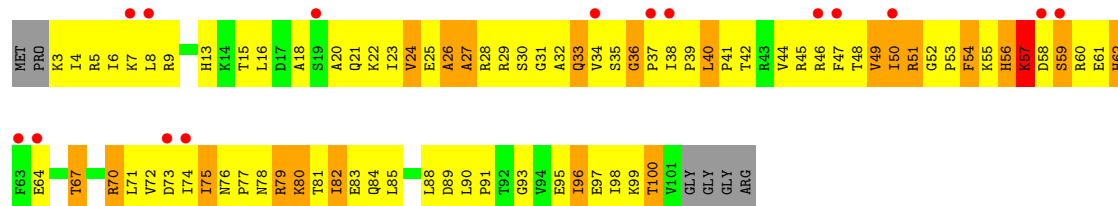
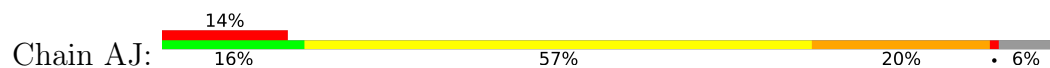




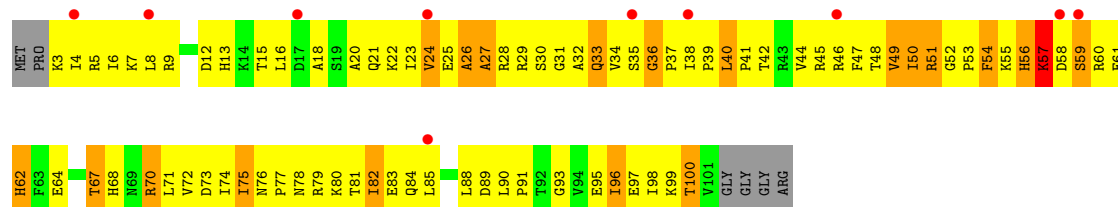
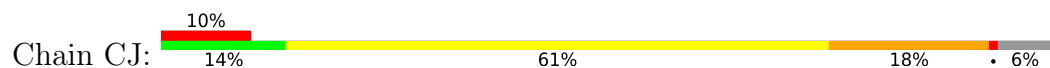
• Molecule 9: 30S RIBOSOMAL PROTEIN S9



• Molecule 10: 30S RIBOSOMAL PROTEIN S10

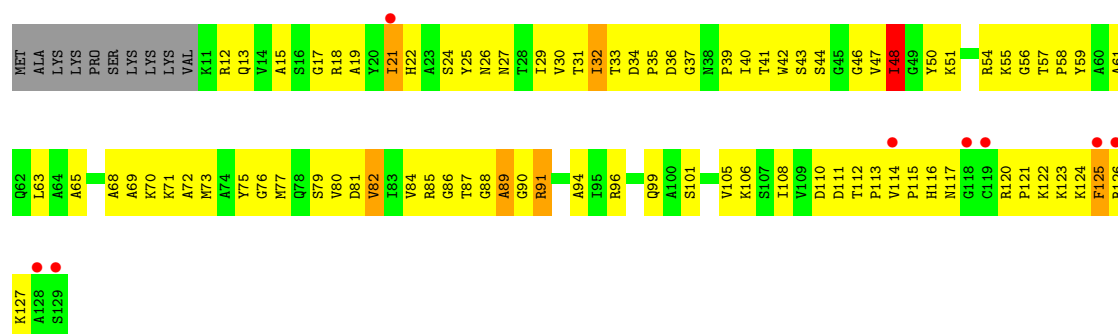


• Molecule 10: 30S RIBOSOMAL PROTEIN S10

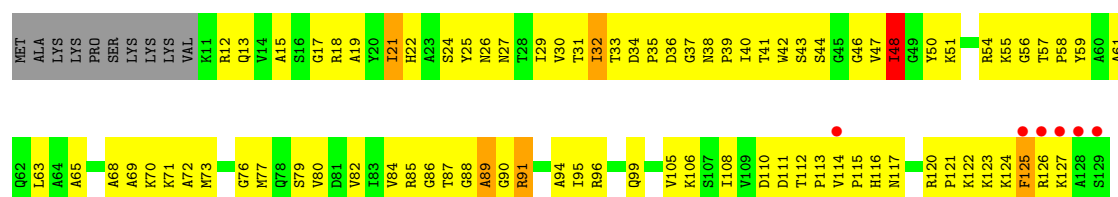


• Molecule 11: 30S RIBOSOMAL PROTEIN S11

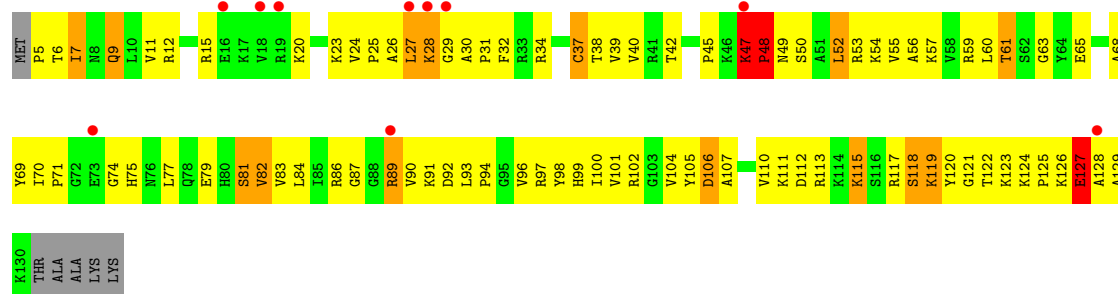




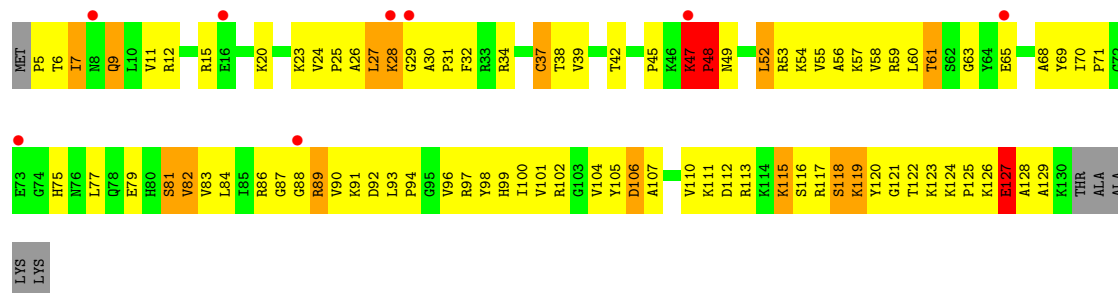
• Molecule 11: 30S RIBOSOMAL PROTEIN S11



• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 12: 30S RIBOSOMAL PROTEIN S12



• Molecule 13: 30S RIBOSOMAL PROTEIN S13



Chain CM:

6% 26% 48% 21%

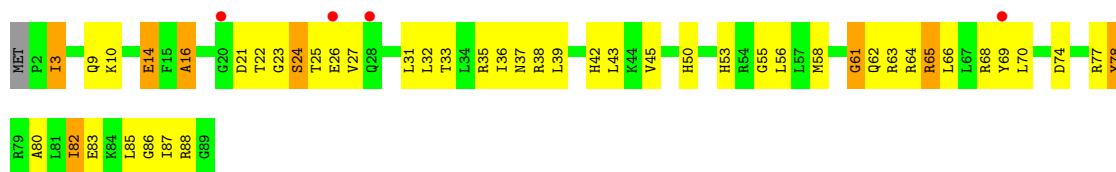
Chain AN:

Chain CN:

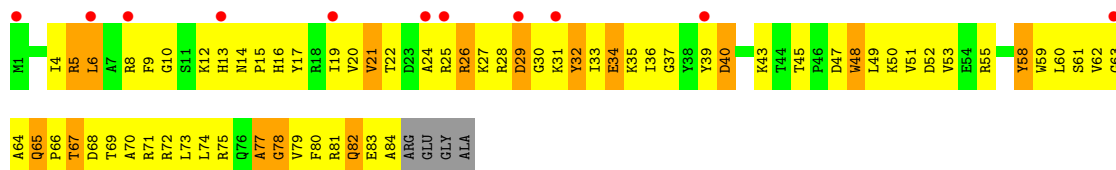
Chain CN	Percentage
A1	1.67%
A2	1.67%
A3	1.67%
A4	1.67%
A5	1.67%
A6	2.22%
A7	2.22%
A8	2.22%
A9	2.22%
A10	2.22%
A11	2.22%
A12	2.22%
A13	2.22%
A14	2.22%
A15	2.22%
A16	2.22%
A17	2.22%
A18	2.22%
A19	2.78%
A20	2.78%
A21	2.78%
A22	2.78%
A23	2.78%
A24	2.78%
A25	2.78%
A26	2.78%
A27	2.78%
A28	2.78%
A29	2.78%
A30	2.78%
A31	2.78%
A32	2.78%
A33	2.78%
A34	2.78%
A35	2.78%
A36	2.78%
A37	2.78%
A38	2.78%
A39	2.78%
A40	2.78%
A41	2.78%
A42	2.78%
A43	2.78%
A44	2.78%
A45	2.78%
A46	2.78%
A47	2.78%
A48	3.33%
A49	3.33%
A50	3.33%
A51	3.33%
A52	3.33%
A53	3.33%
A54	3.33%
A55	3.33%
A56	3.33%
A57	3.33%
A58	3.33%
A59	3.33%

Chain AO:

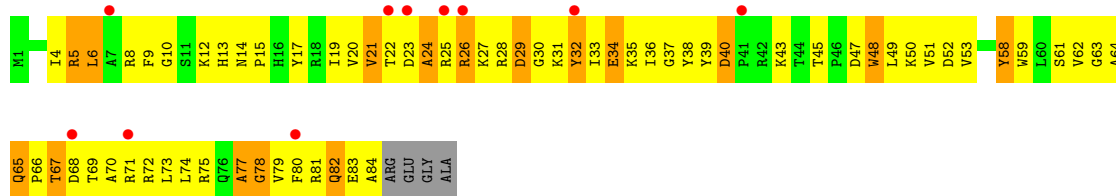
Chain CO: 4% 46% 44% 9%



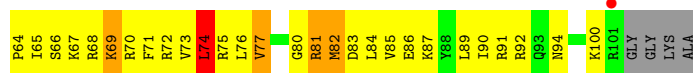
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



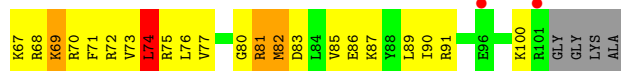
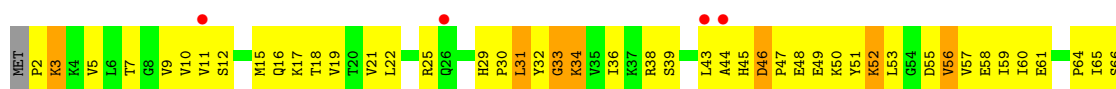
- Molecule 16: 30S RIBOSOMAL PROTEIN S16



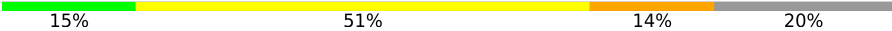
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

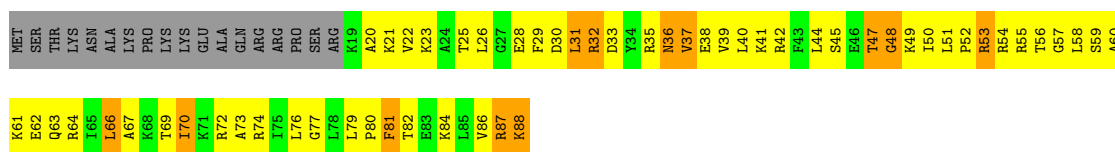


- Molecule 17: 30S RIBOSOMAL PROTEIN S17



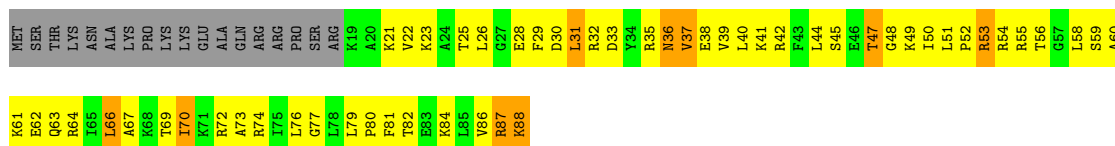
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain AR: 



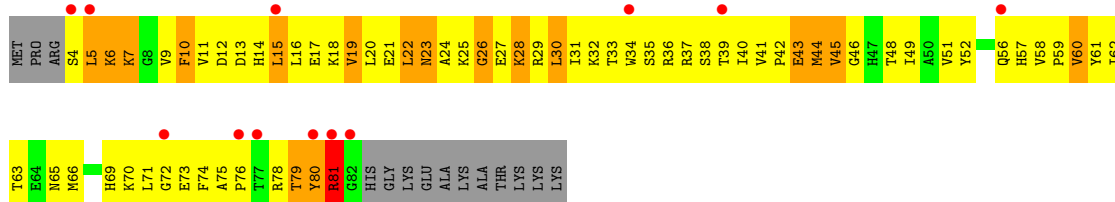
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain CR: 



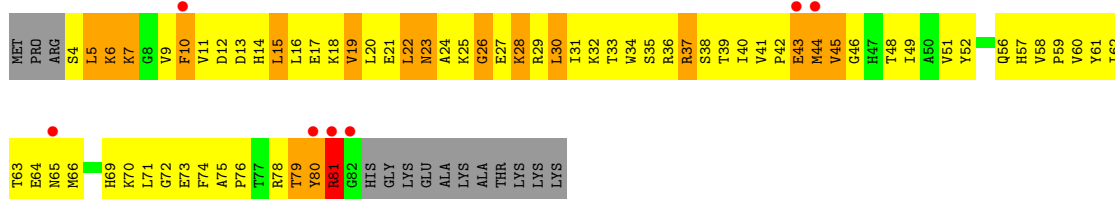
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain AS: 

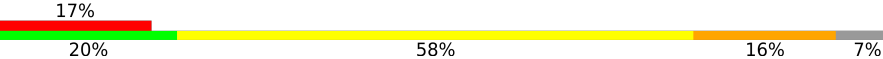


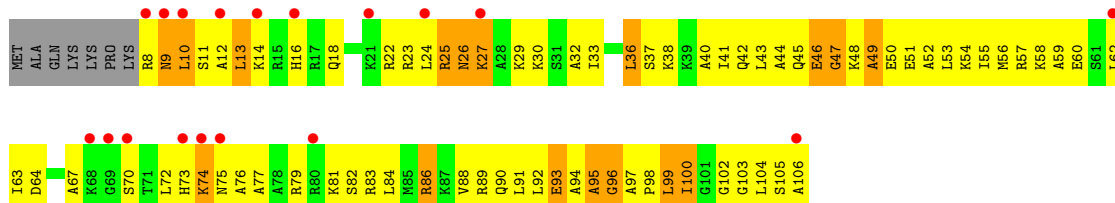
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain CS: 

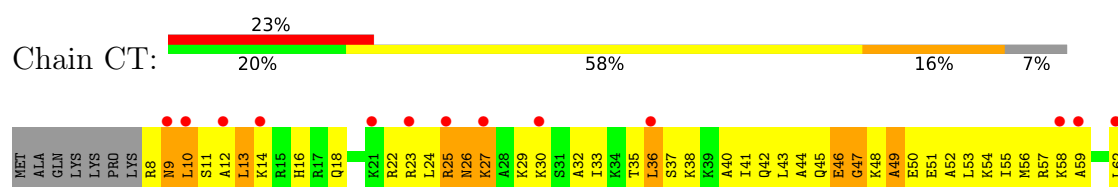


• Molecule 20: 30S RIBOSOMAL PROTEIN S20

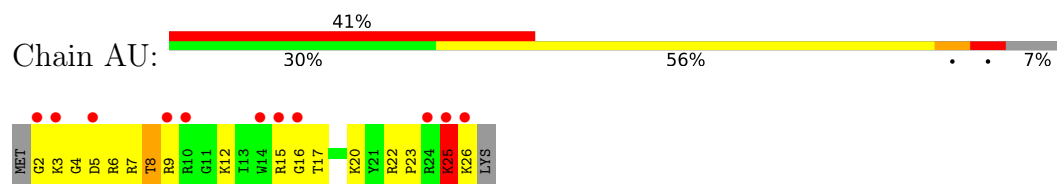
Chain AT: 



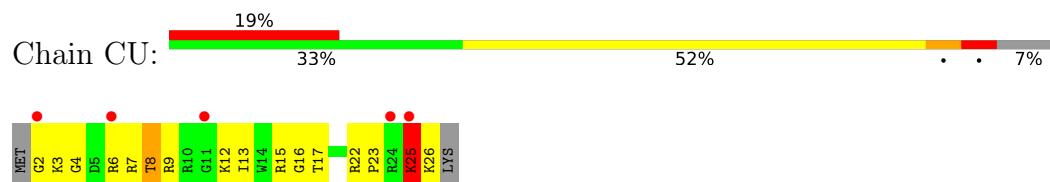
• Molecule 20: 30S RIBOSOMAL PROTEIN S20



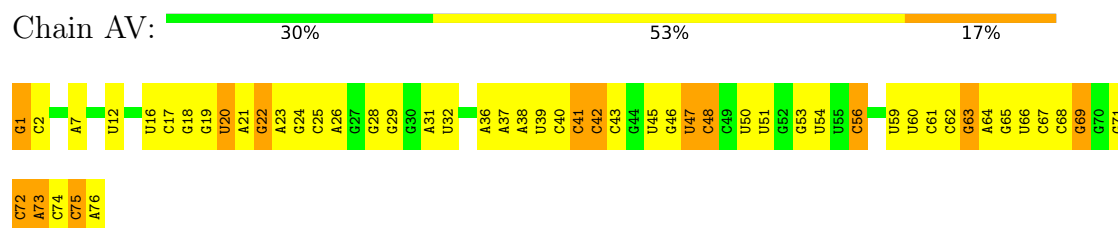
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



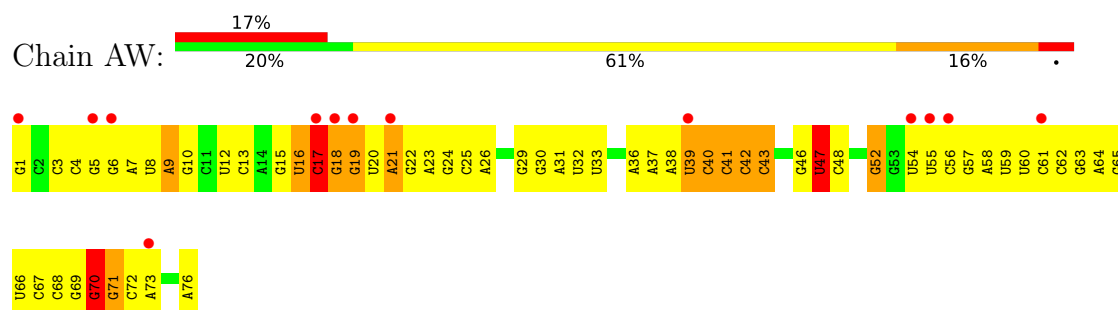
- Molecule 21: 30S RIBOSOMAL PROTEIN THX



- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

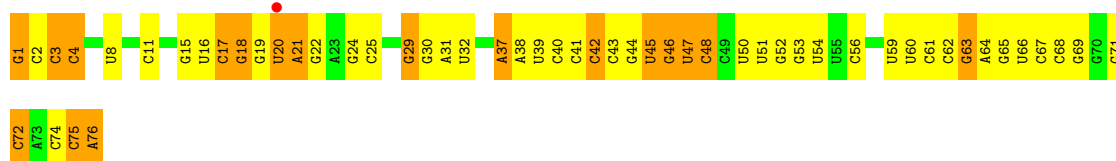


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

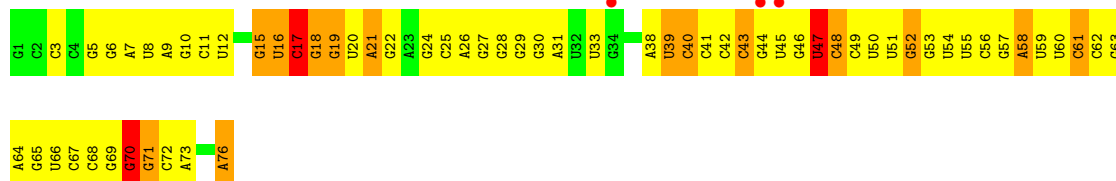


- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)

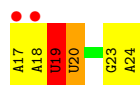




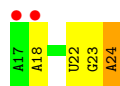
- Molecule 22: E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES)



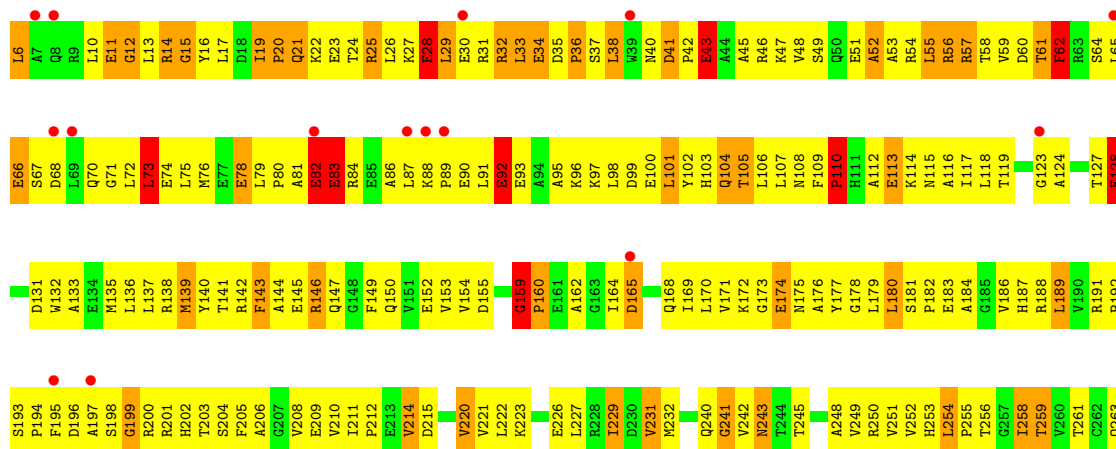
- Molecule 23: MRNA



- Molecule 23: MRNA

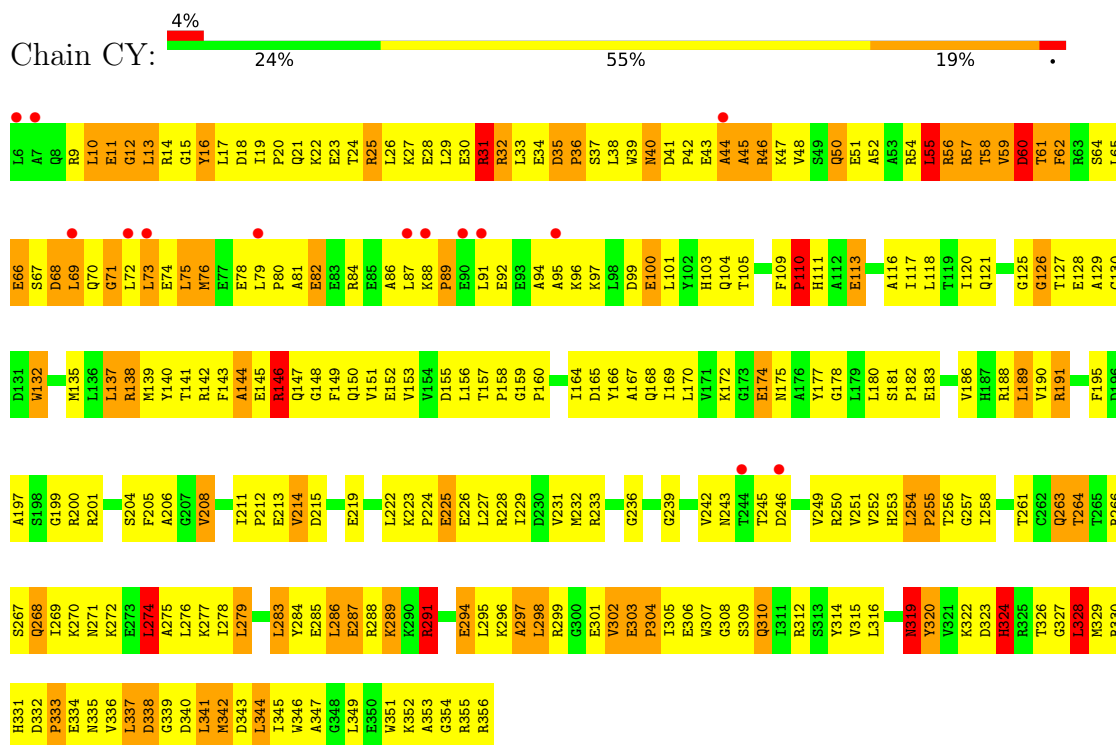


- Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

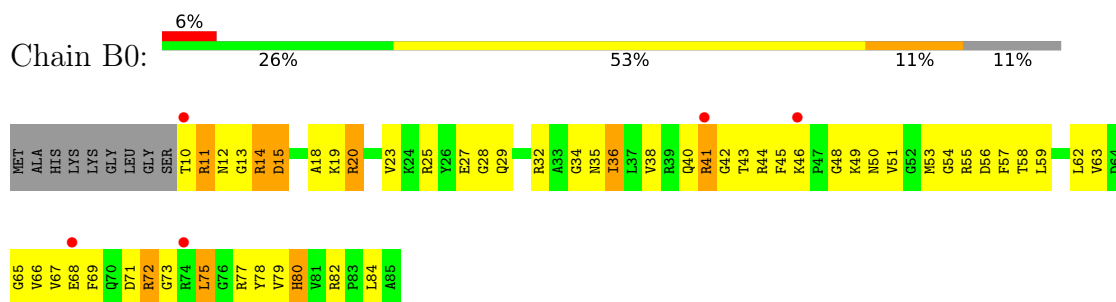




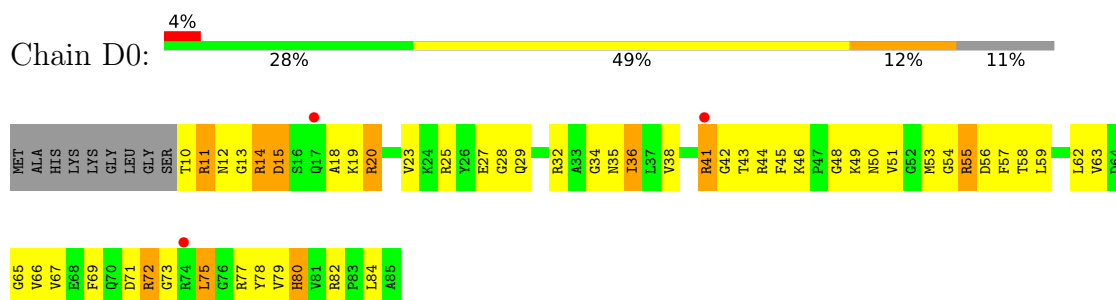
• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2



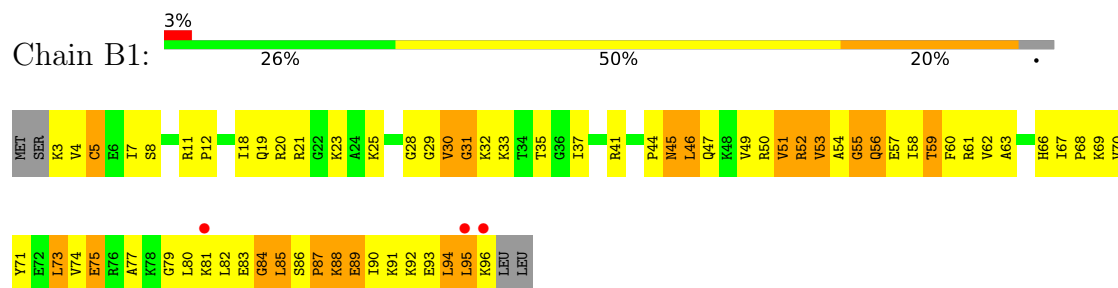
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



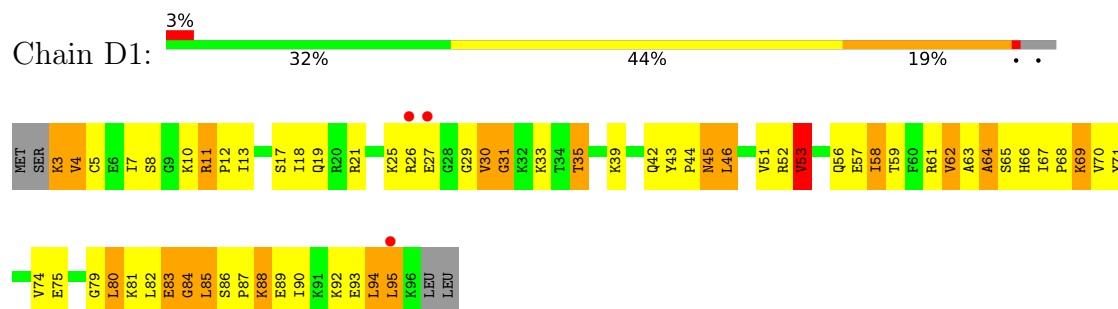
• Molecule 25: 50S RIBOSOMAL PROTEIN L27



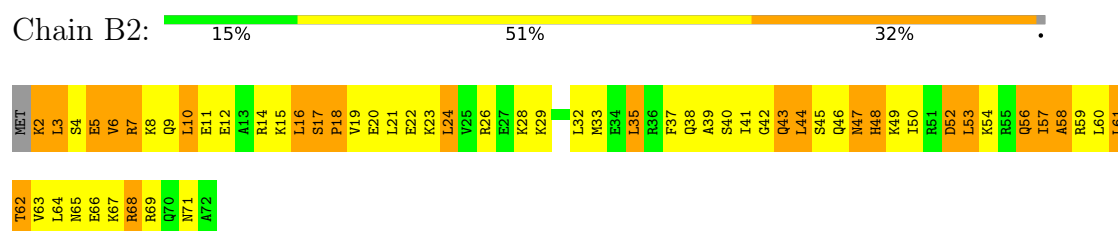
- Molecule 26: 50S RIBOSOMAL PROTEIN L28



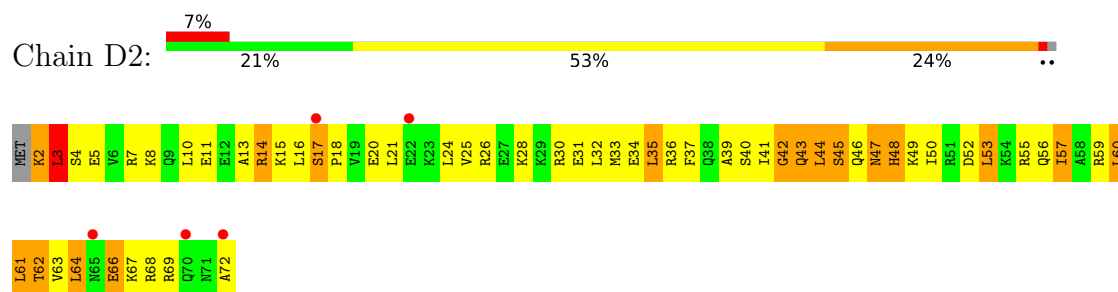
- Molecule 26: 50S RIBOSOMAL PROTEIN L28



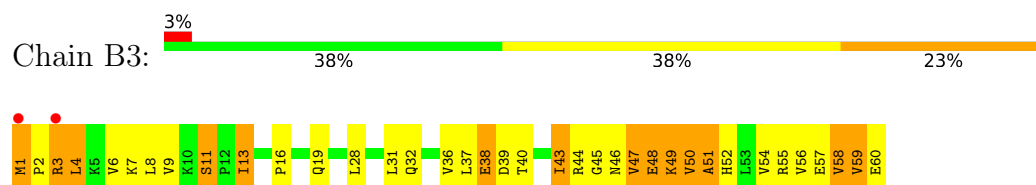
- Molecule 27: 50S RIBOSOMAL PROTEIN L29



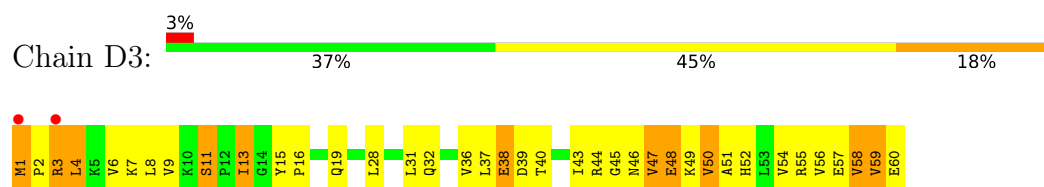
- Molecule 27: 50S RIBOSOMAL PROTEIN L29



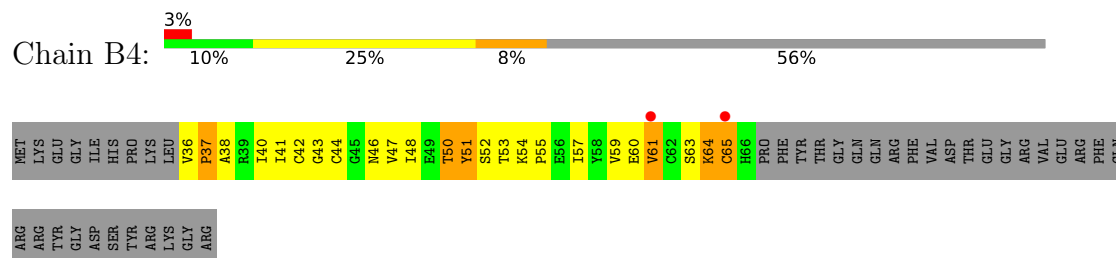
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



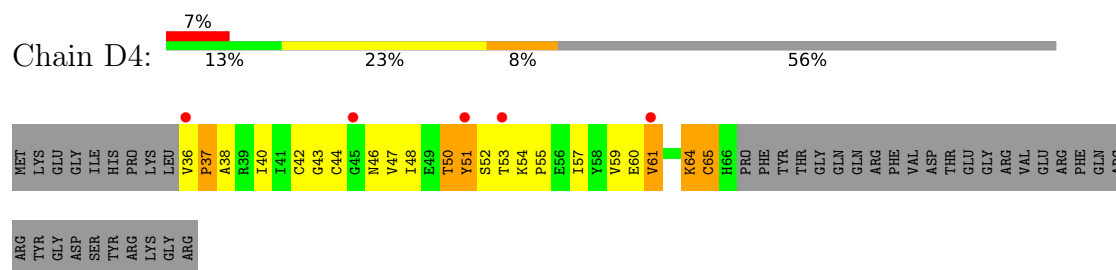
- Molecule 28: 50S RIBOSOMAL PROTEIN L30



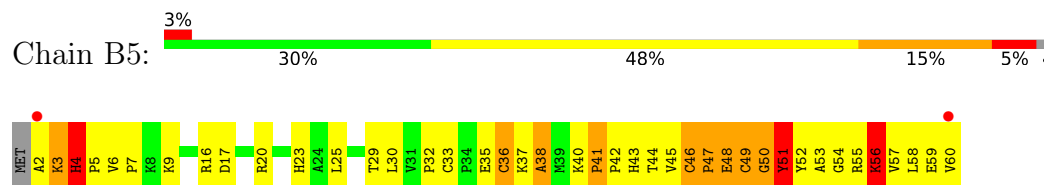
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



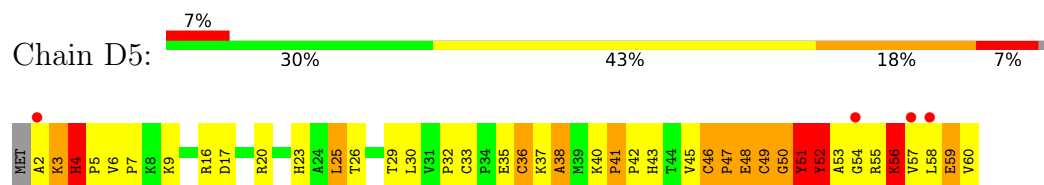
- Molecule 29: 50S RIBOSOMAL PROTEIN L31



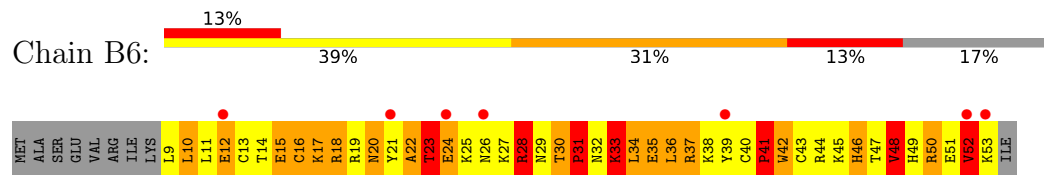
- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 30: 50S RIBOSOMAL PROTEIN L32



- Molecule 31: 50S RIBOSOMAL PROTEIN L33



- Molecule 31: 50S RIBOSOMAL PROTEIN L33





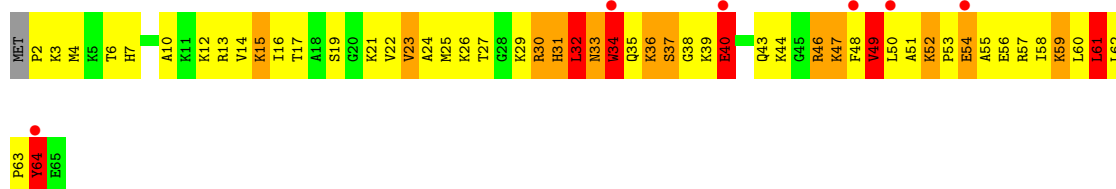
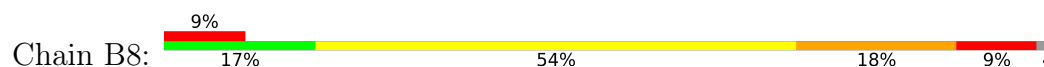
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



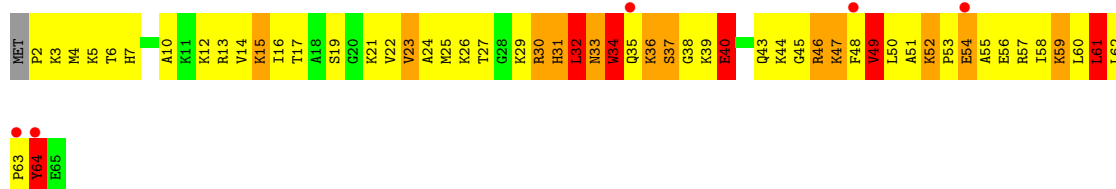
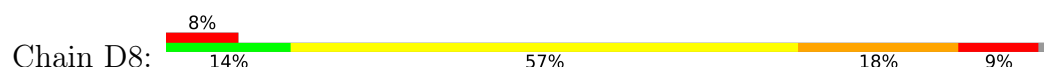
• Molecule 32: 50S RIBOSOMAL PROTEIN L34



• Molecule 33: 50S RIBOSOMAL PROTEIN L35



• Molecule 33: 50S RIBOSOMAL PROTEIN L35

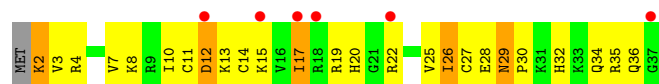


• Molecule 34: 50S RIBOSOMAL PROTEIN L36



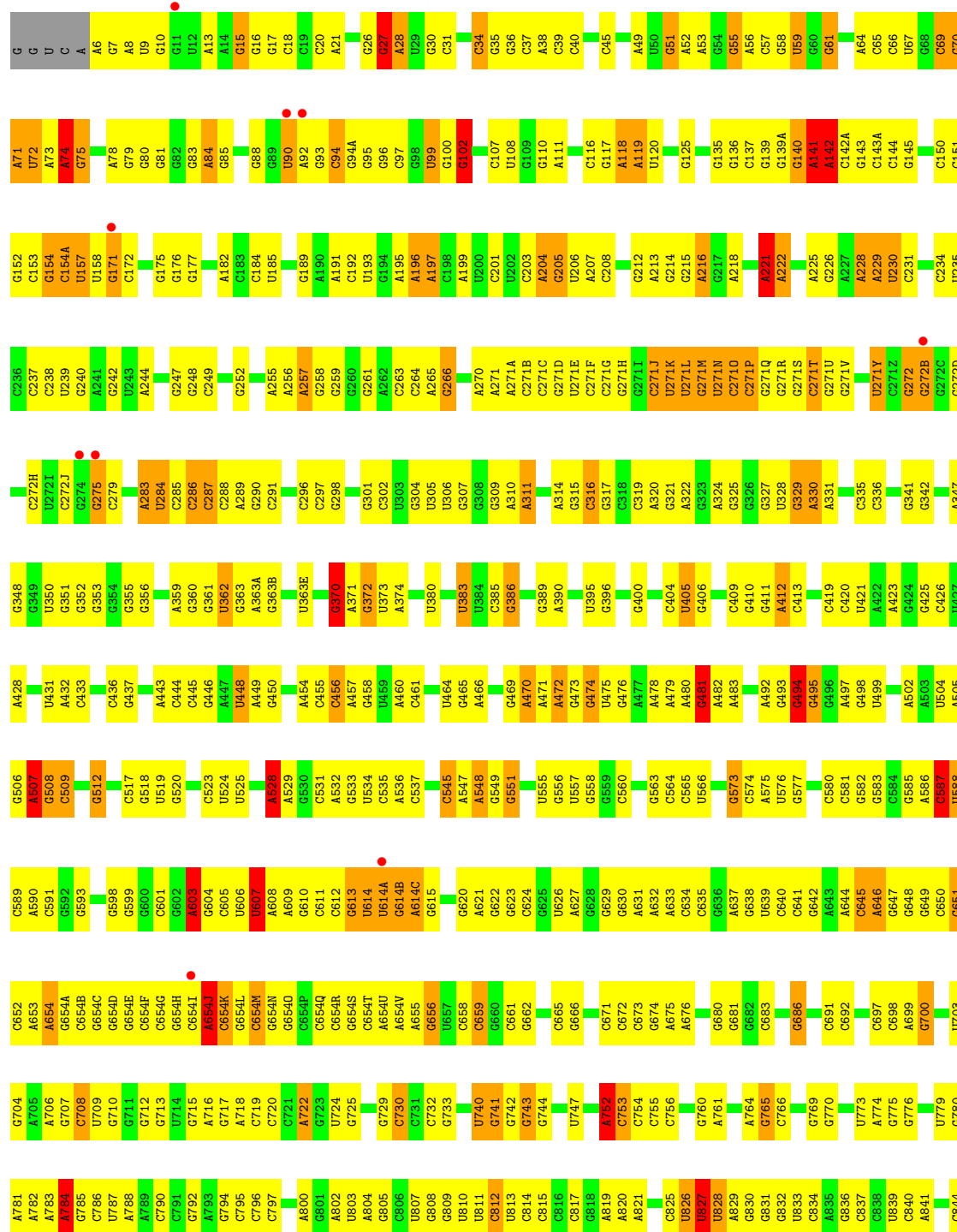
• Molecule 34: 50S RIBOSOMAL PROTEIN L36





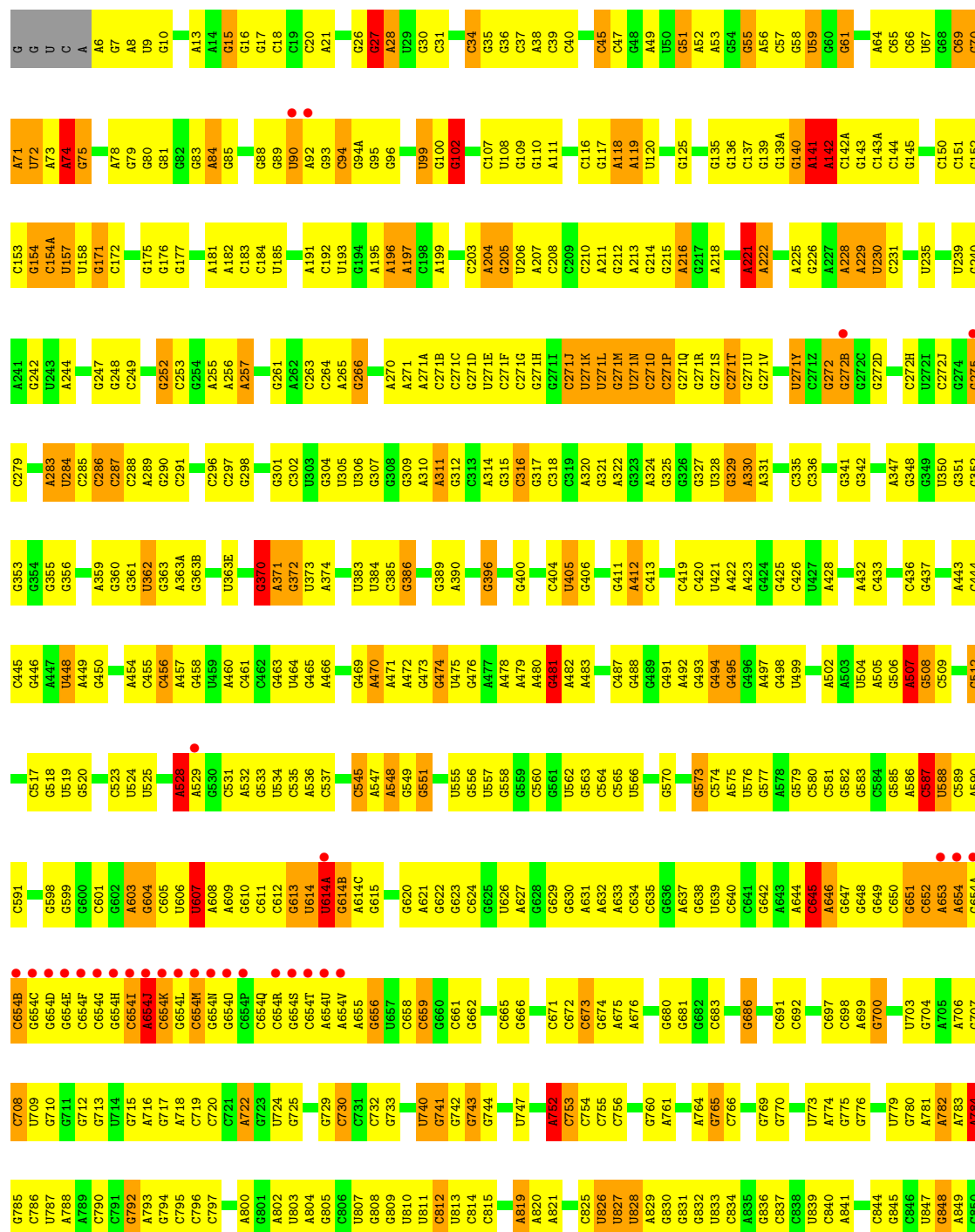
• Molecule 35: 23S RIBOSOMAL RNA

Chain BA: 3% 34% 52% 12% ..



U1820	C1751	A1855	G1573	U1503	G1436	C1363	U1282	U1188	G1125	A1054	C986	C912	G845
G1824	C1752	C1656	C1574	C1504	C1437	G1364	A1286	A1189	A1126	G1055	G987	U913	C846
A1825	G1753	C1657	U1575	C1505	U1438	G1368	A1287	G1190	A1127	A1056	A988	C914	G847
G1826	C1754	U1659	U1577	A1507	A1439	G1369	U1288	G1191	G989	A1057	G988	C915	G848
C1827	A1755	U1578	U1577	A1508	G1440	G1370	U1289	G1192	A1128	G1058	A990	G916	A849
G1828	G1756	A1665	U1579	C1509	G1441	G1371	C1290	A1194	A1129	U1061	C992	A917	C850
A1829	U1757	G1666	A1580	A1509A	G1442	C1375	C1291	G1195	U1130	G1062	G993	A918	U851
	G1758	G1667	U1509B	A1509B	A1445	C1376	C1292	G1196	U1131	G1063	C994	G919	G852
C1832	A1762	A1668	C1584	G1510	C1445A	A1378	C1293	G1197	A1132	C1064	G995	U922	G854
U1833	G1763	A1586	A1587	U1512	C1446	G1379	G1297	G1202	G1133	U1065	A996	C923	G855
G1835	G1764	A1588	C1588	U1514	G1447	G1380	C1298	A1204	C1135	A1066	G997	C924	C856
C1836	C1765	G1589	A1449	U1514	A1449	G1381	G1299	U1205	G1136	A1067	C998	C925	C857
C1837	U1766	U1590	G1450	G1515	G1450	G1382	U1300	U1206	U1140	G1068	U999	A926	U858
C1838	G1767	G1591	U1452	C1516	A1452	A1384	A1301	C1208	U1141	A1069	A1000	C927	G859
G1839	U1768	C1592	U1453	G1517	C1385	C1386	A1302	G1209	U1142	G1070	G1001	G928	G862
U1840	G1769	U1595	U1453	G1518	G1387	G1388	G1309	U1211	A1143	C1072	G1002	G932	A863
U1841		G1595	G1520	G1519	G1389	G1390	G1310	G1212	U1144	C1075	C1005	A933	G864
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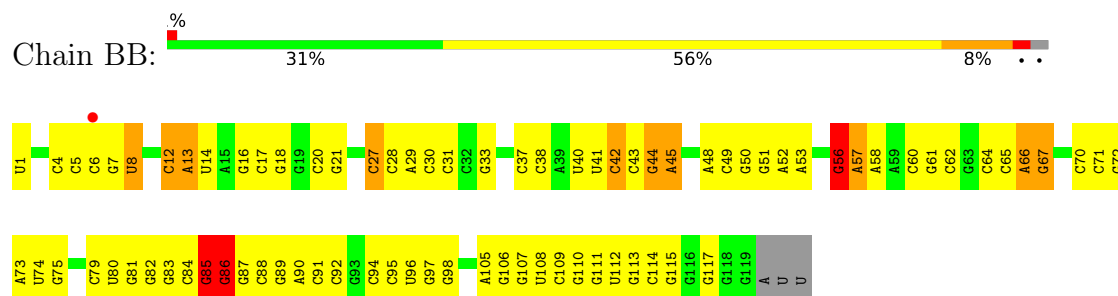
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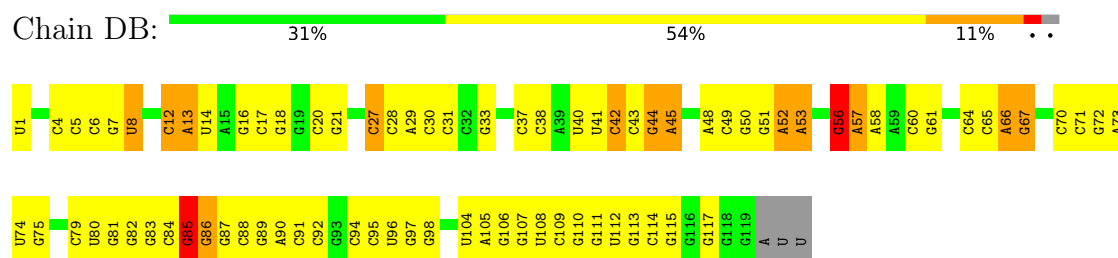
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A1654	A1655	G1656	G1657	G1755	G1756	G1757	G1758	A1665	G1666	G1667	A1668	G1674	G1675	A1676	A1677	G1678	G1681	G1685	G1686	G1687	G1688	G1689	U1693	G1694	G1695	G1696	G1697	A1698	G1699	A1700	A1701	G1708	U1709	G1710	G1711	G1712	G1713	G1714	G1717	G1718	G1719	U1720	G1721	A1722	U1729	G1810	G1811	G1812	A1741	C1744	G1746	G1747	U1819	A1820	G1906		
A1571	A1572	G1573	G1574	G1575	G1576	G1577	G1578	A1579	A1580	G1584	A1586	A1587	G1588	G1589	G1590	G1591	G1595	A1596	A1597	G1598	G1599	G1600	G1601	U1602	A1603	G1607	A1608	A1609	A1610	G1613	A1614	A1615	A1616	G1617	A1618	G1624	G1625	G1626	A1637	G1638	U1639	A1640	A1641	G1642	G1643	C1644	G1647	C1648	G1651	A1652	G1653						
G1501	G1502	G1503	G1504	G1505	G1506	G1507	G1508	A1509A	A1509B	G1510	G1511	U1512	G1513	G1514	G1515	G1516	G1517	G1519	G1520	G1523	G1524	G1525	G1526	G1527	A1528	A1528A	G1529	G1530	G1531	G1532	G1533	G1543	A1544	A1545	C1546	G1547	G1548	G1549	G1550	G1551	A1554	C1557	A1559	G1560	G1561	A1562	G1563	G1564	G1565	A1566	A1567	G1568	A1569	A1570			
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A1127	A1128	U1129	U1130	G1131	A1132	U1133	C1135	G1136	C1140	U1141	A1142A	G1144	G1145	C1146	C1147	A1148	C1149	C1150	G1153	A1155	A1156	G1157	G1158	U1159	G1160	C1161	G1162	G1163	G1164	U1165	C1166	U1167	G1168	G1169	G1170	G1171	G1173	A1174	U1175	G1176	A1177	G1178	C1179	C1180	C1181	G1182	G1183	C1184	C1185	G1186	G1187	U1188	A1189	G1190			
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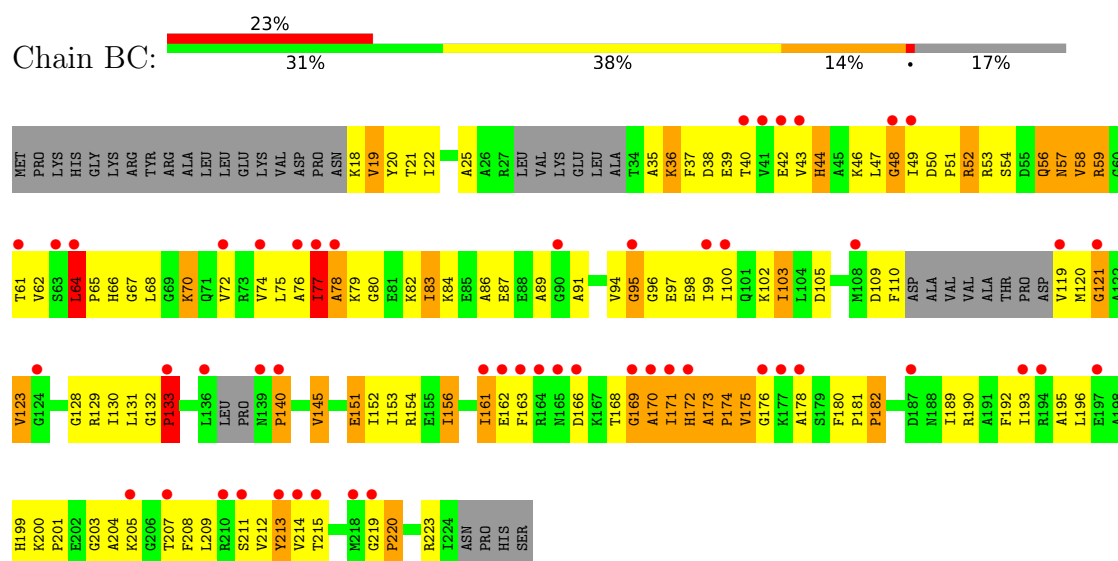
- Molecule 36: 5S RIBOSOMAL RNA



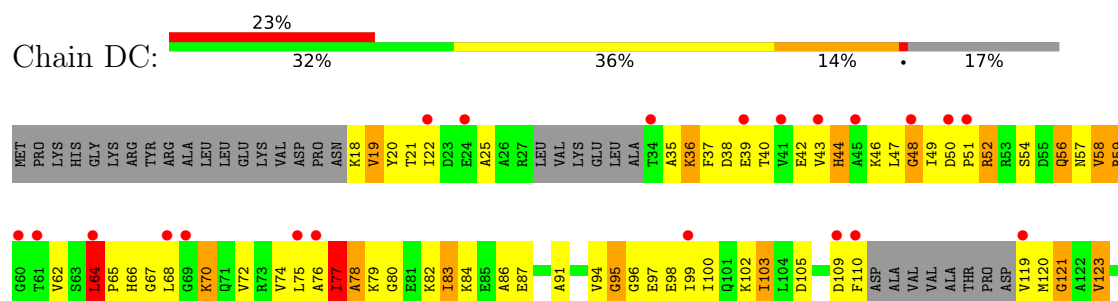
- Molecule 36: 5S RIBOSOMAL RNA

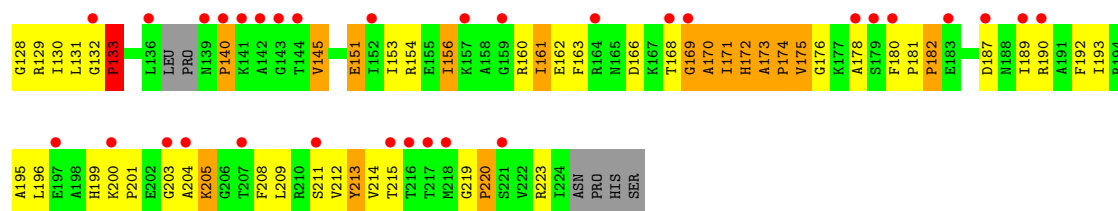


- Molecule 37: 50S RIBOSOMAL PROTEIN L1

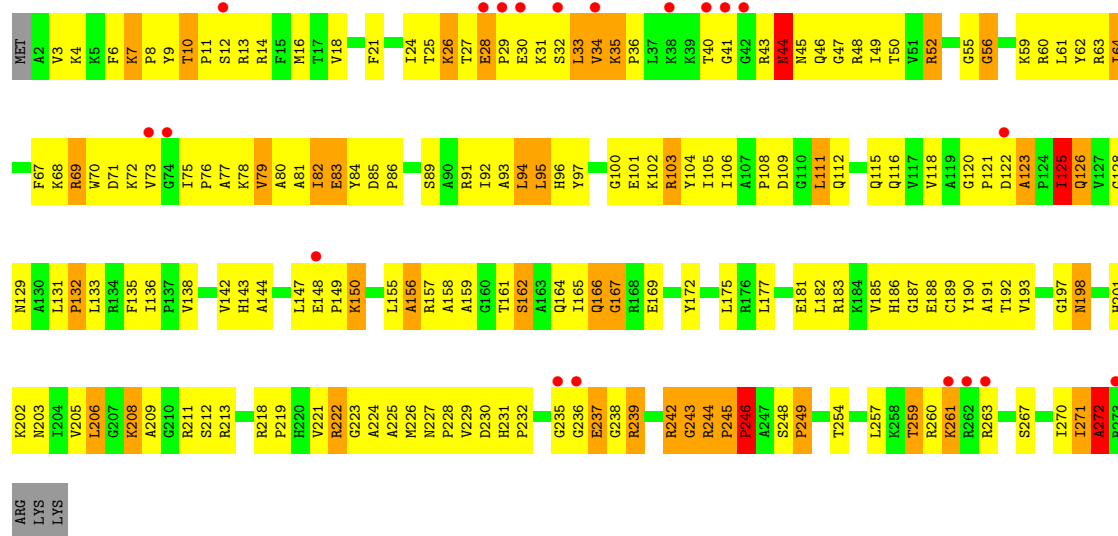


- Molecule 37: 50S RIBOSOMAL PROTEIN L1

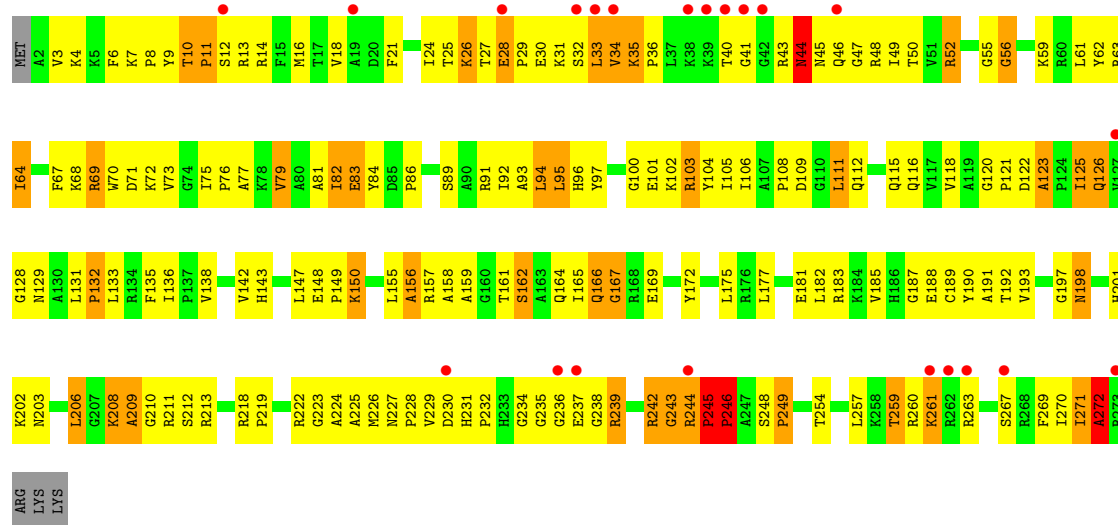




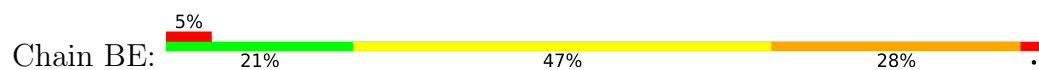
• Molecule 38: 50S RIBOSOMAL PROTEIN L2

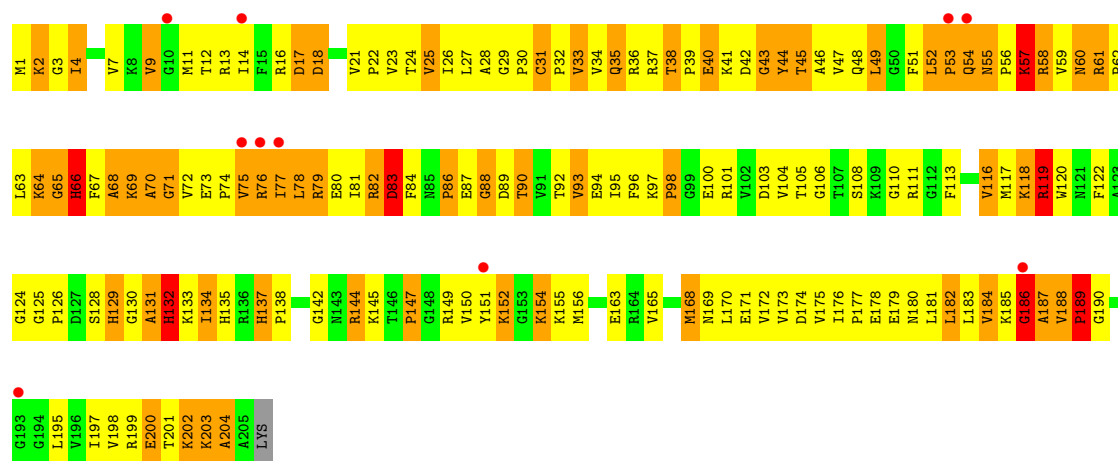


• Molecule 38: 50S RIBOSOMAL PROTEIN L2

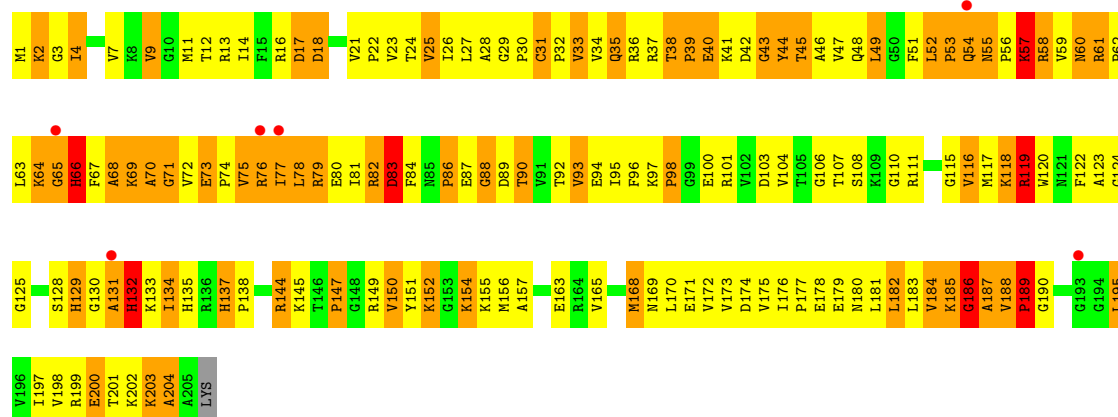
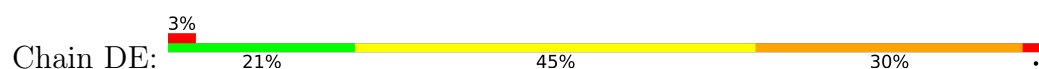


• Molecule 39: 50S RIBOSOMAL PROTEIN L3

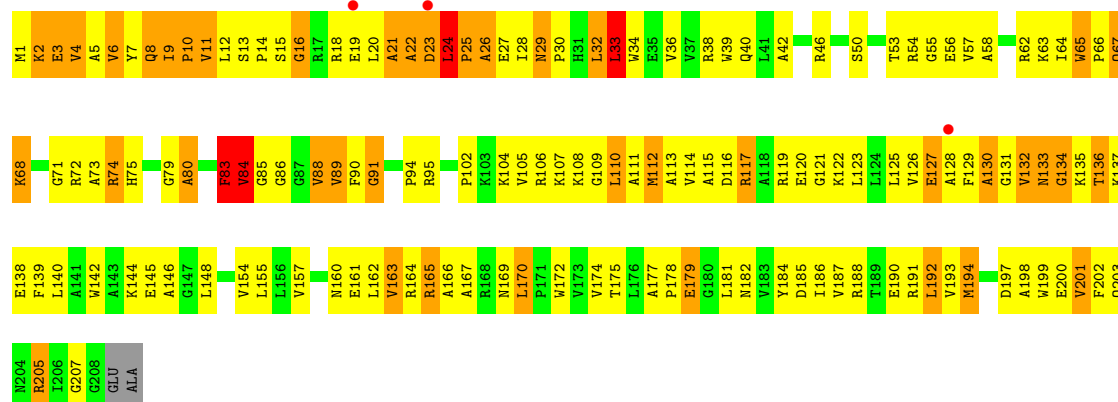




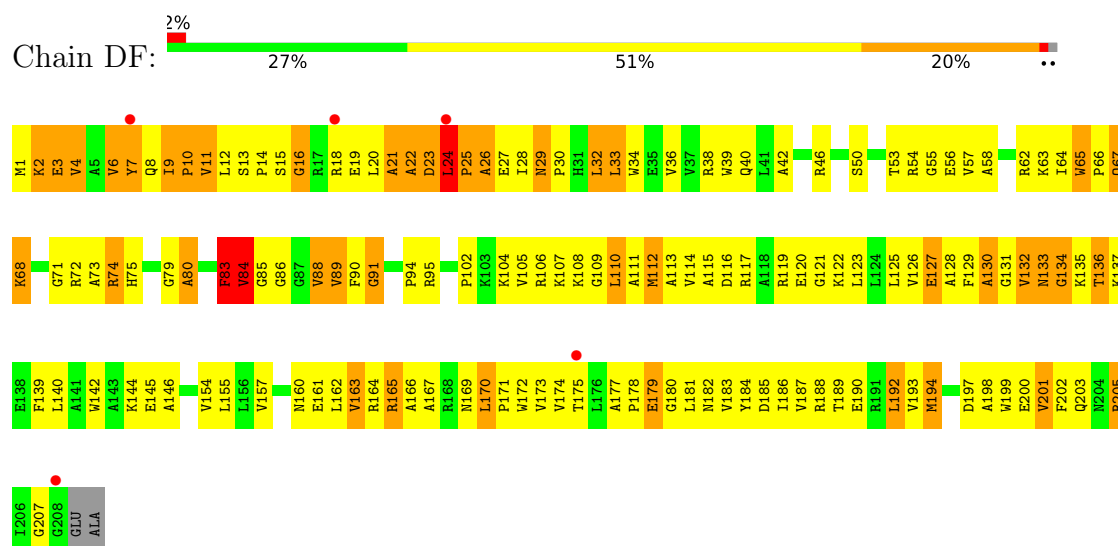
• Molecule 39: 50S RIBOSOMAL PROTEIN L3



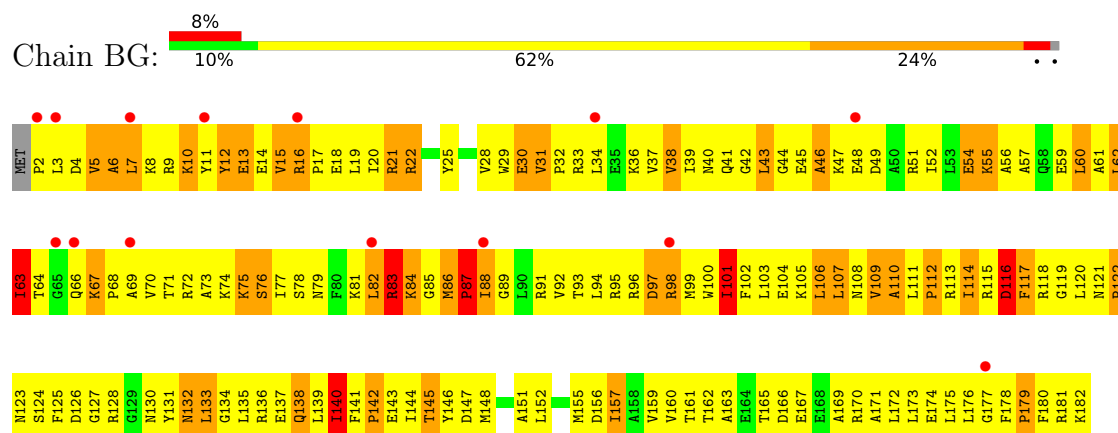
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



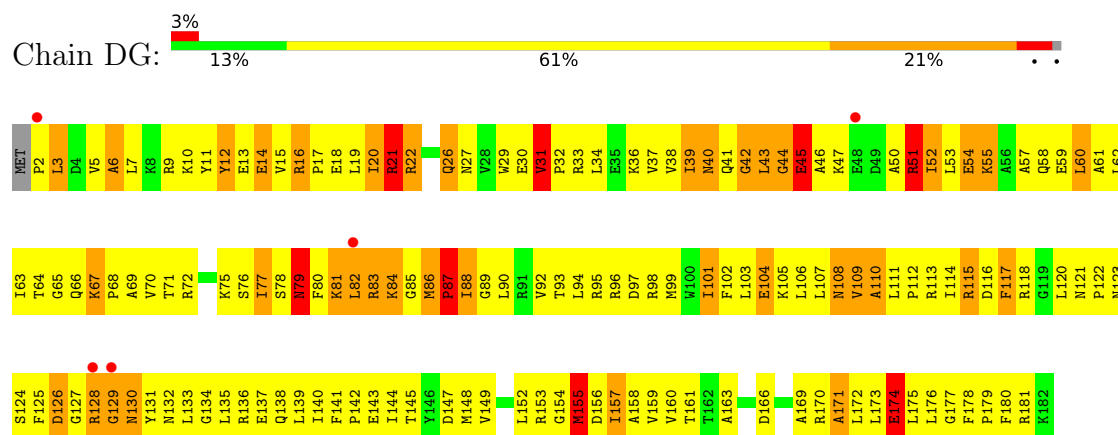
• Molecule 40: 50S RIBOSOMAL PROTEIN L4



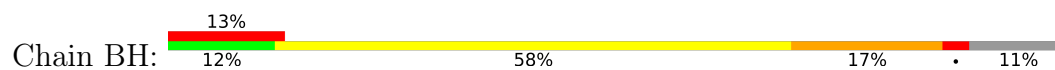
• Molecule 41: 50S RIBOSOMAL PROTEIN L5

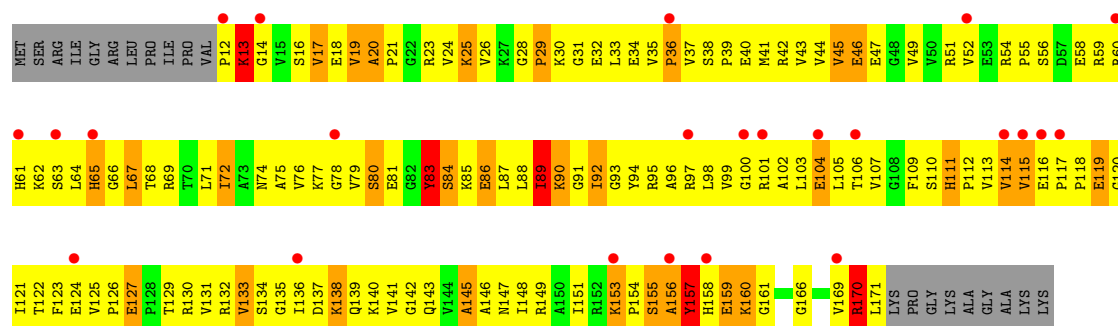


• Molecule 41: 50S RIBOSOMAL PROTEIN L5

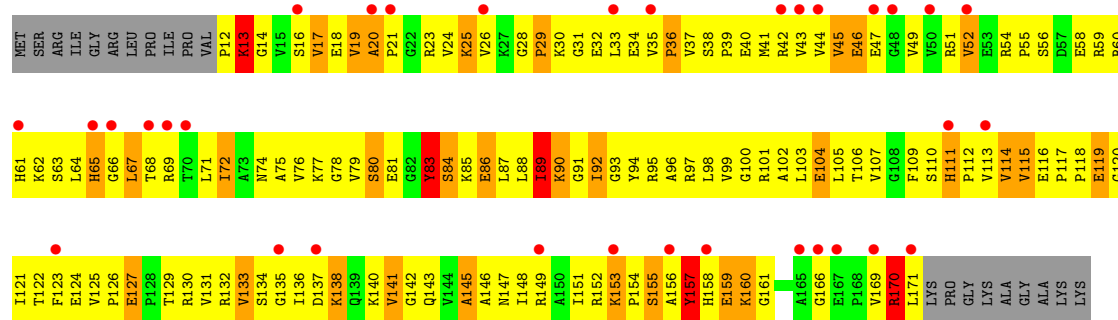
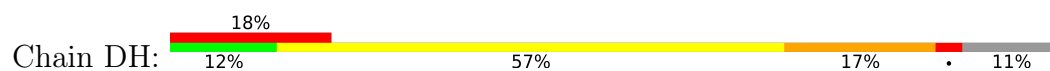


• Molecule 42: 50S RIBOSOMAL PROTEIN L6

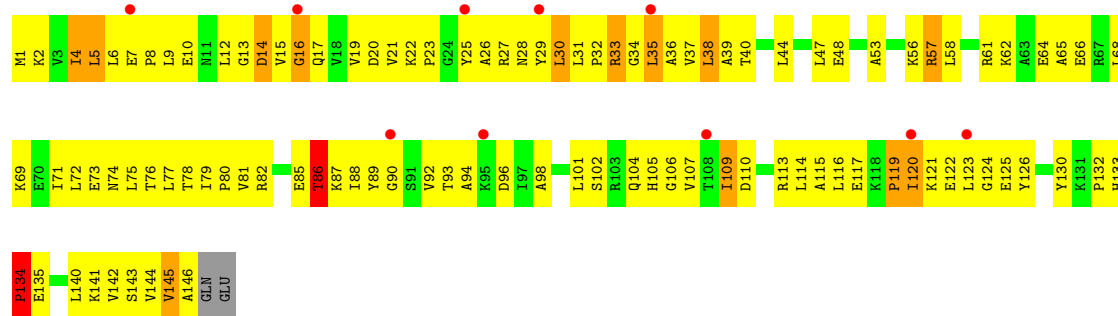




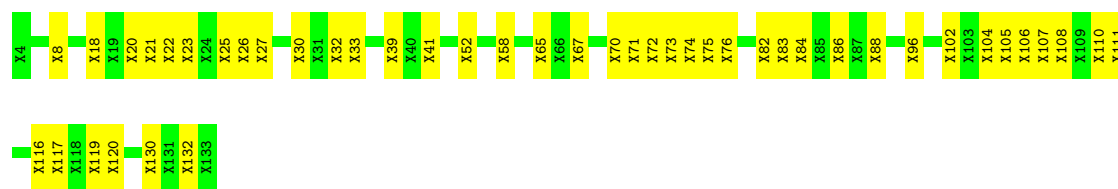
• Molecule 42: 50S RIBOSOMAL PROTEIN L6



• Molecule 43: 50S RIBOSOMAL PROTEIN L9



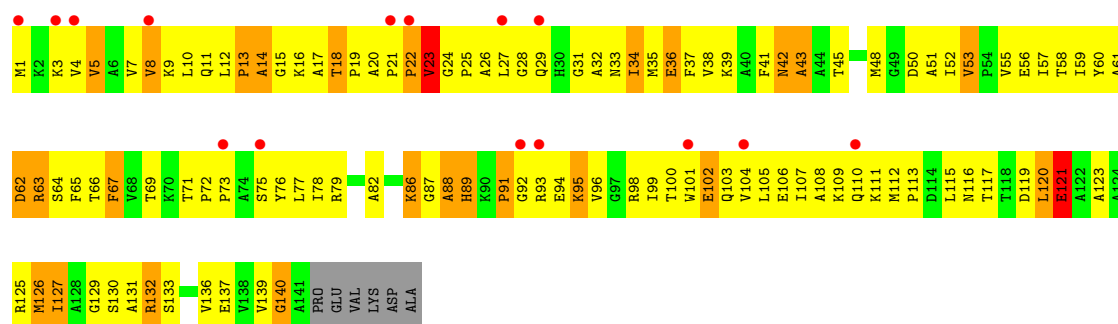
• Molecule 44: 50S RIBOSOMAL PROTEIN L10



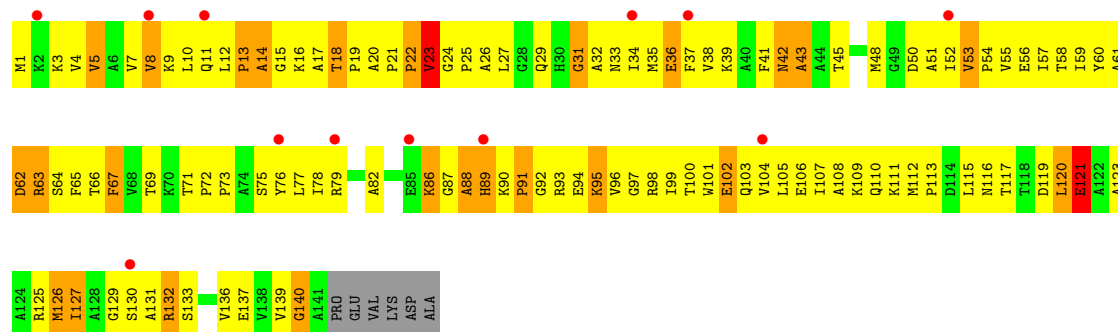
• Molecule 44: 50S RIBOSOMAL PROTEIN L10

[illegible]

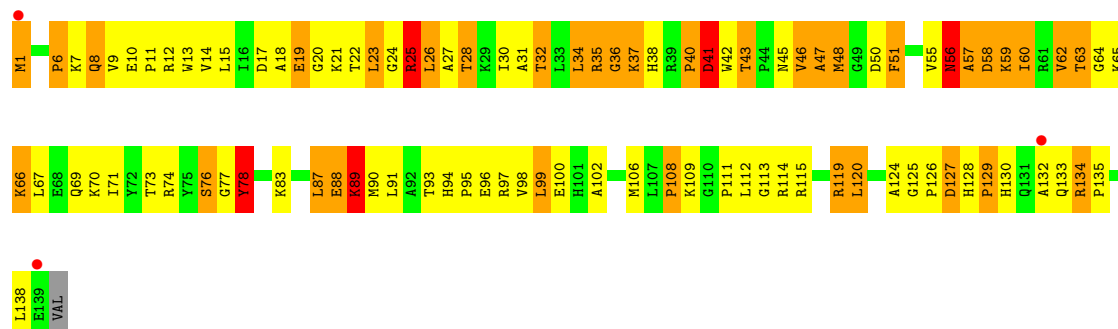
Chain BK:



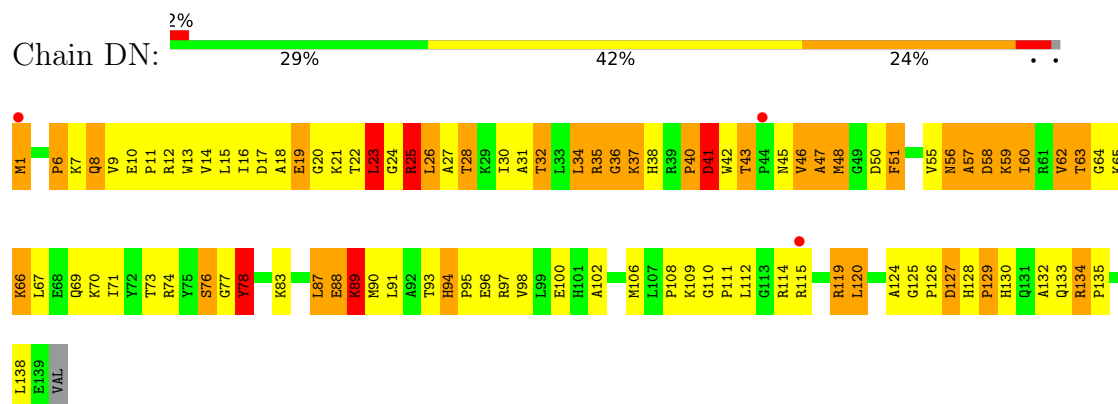
Chain DK:



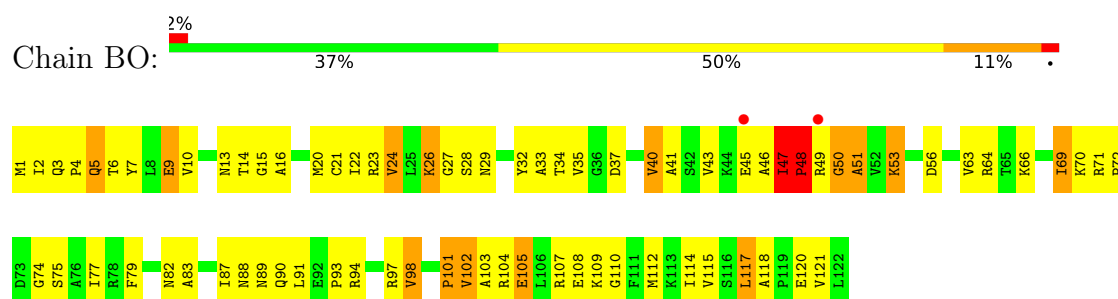
Chain BN:



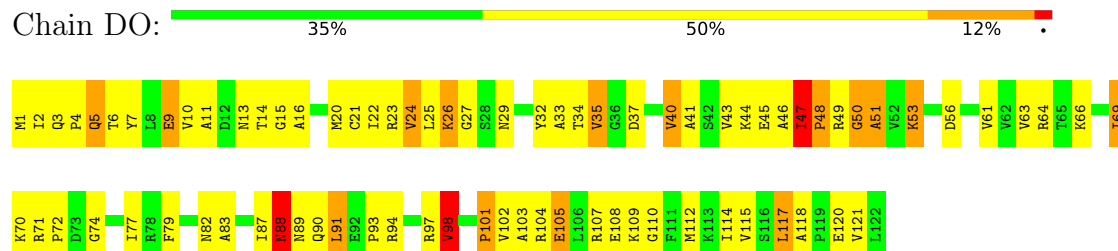
● Molecule 46: 50S RIBOSOMAL PROTEIN L13



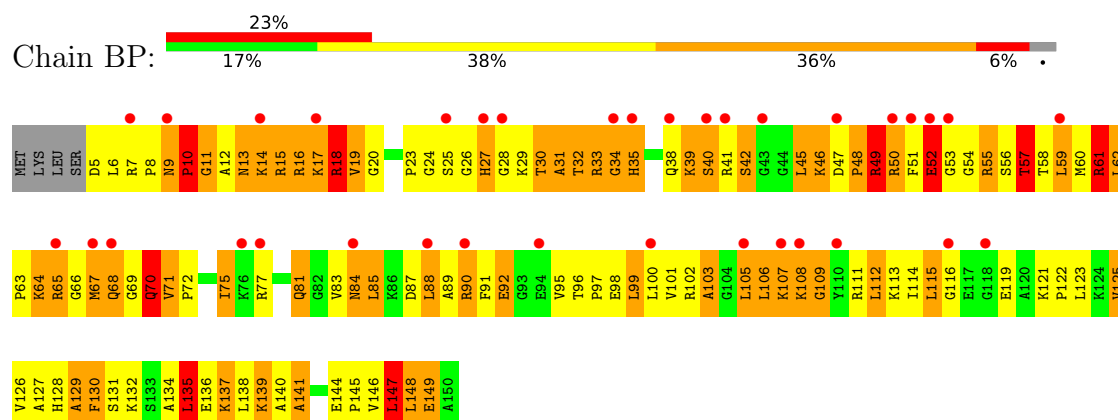
● Molecule 47: 50S RIBOSOMAL PROTEIN L14



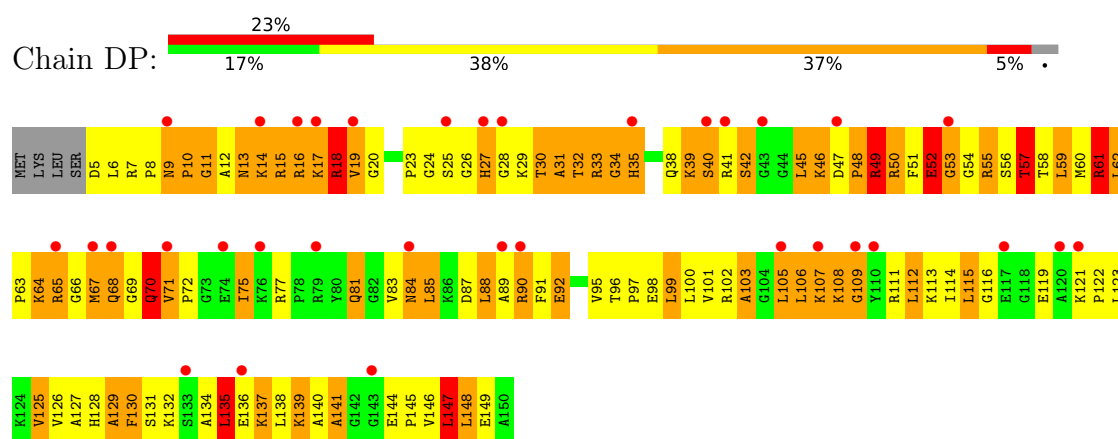
● Molecule 47: 50S RIBOSOMAL PROTEIN L14



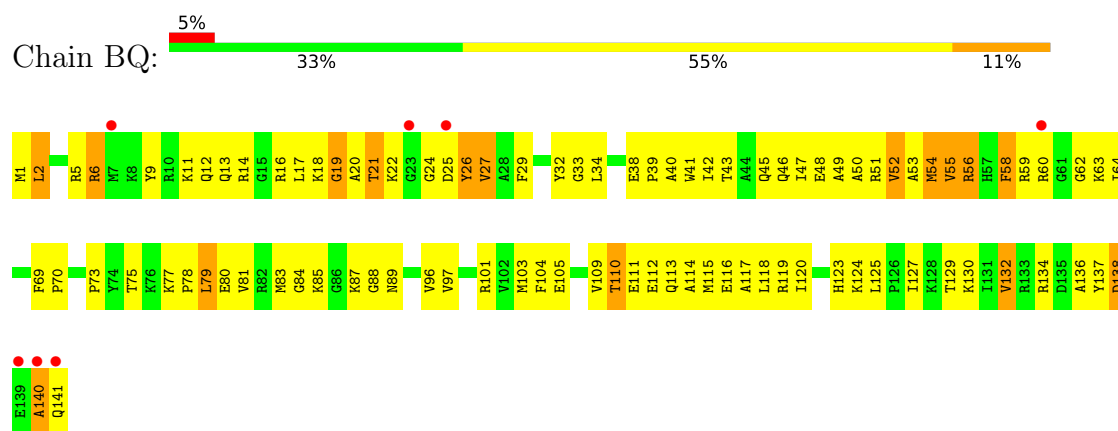
● Molecule 48: 50S RIBOSOMAL PROTEIN L15



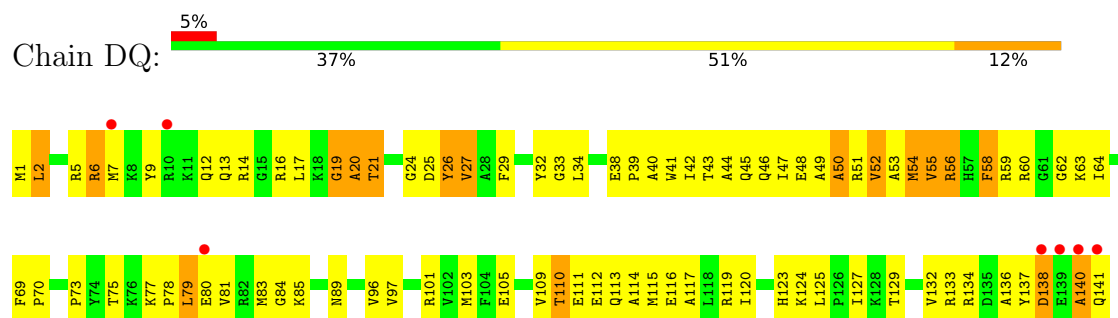
● Molecule 48: 50S RIBOSOMAL PROTEIN L15



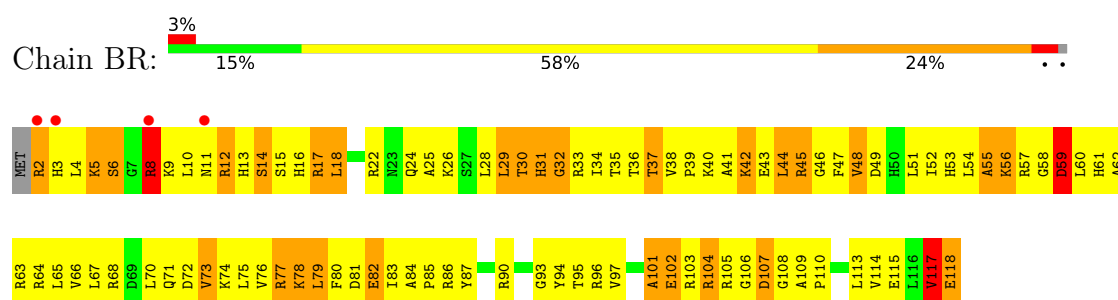
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



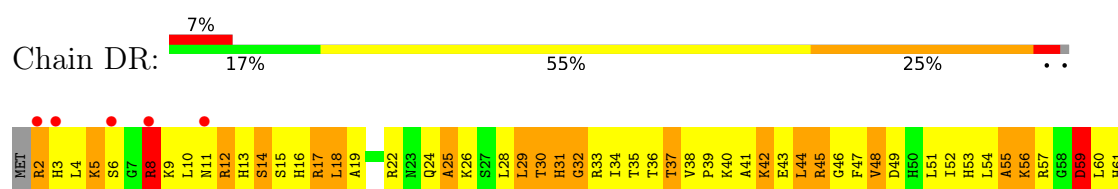
• Molecule 49: 50S RIBOSOMAL PROTEIN L16



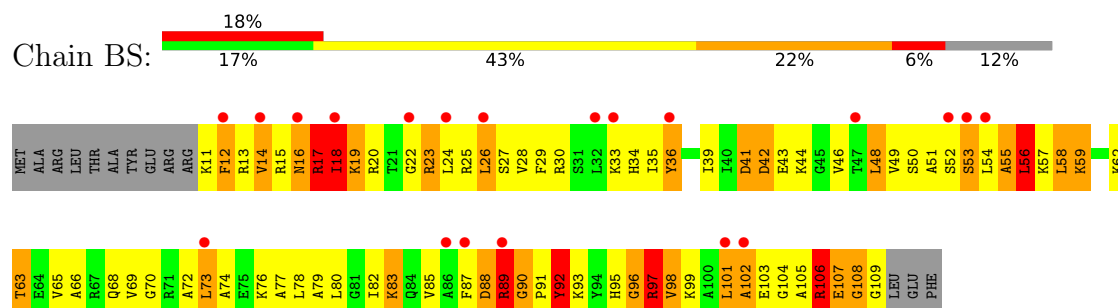
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



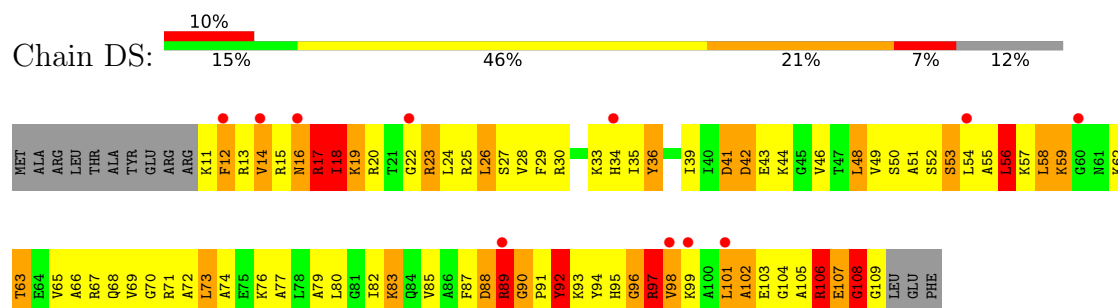
• Molecule 50: 50S RIBOSOMAL PROTEIN L17



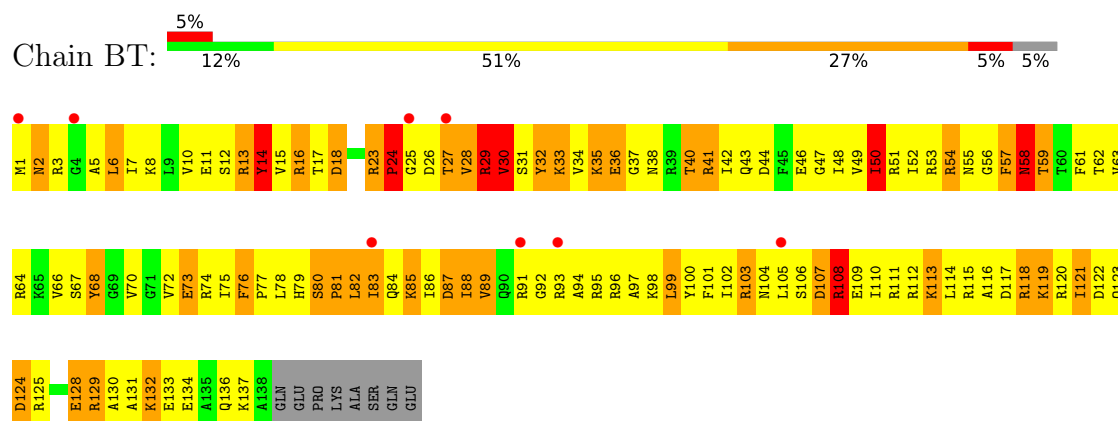
• Molecule 51: 50S RIBOSOMAL PROTEIN L18



• Molecule 51: 50S RIBOSOMAL PROTEIN L18

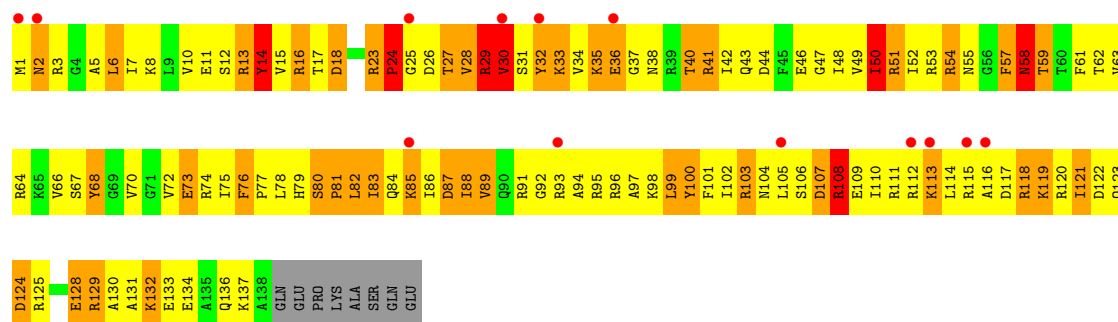


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

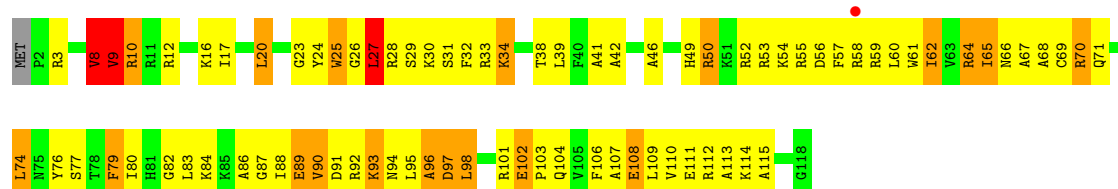


• Molecule 52: 50S RIBOSOMAL PROTEIN L19

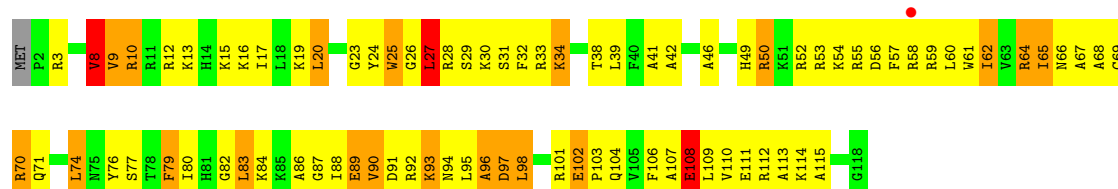




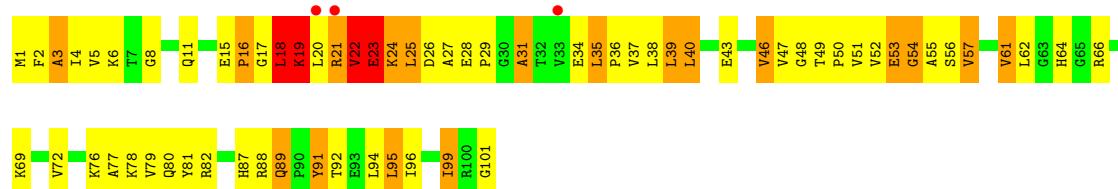
• Molecule 53: 50S RIBOSOMAL PROTEIN L20



• Molecule 53: 50S RIBOSOMAL PROTEIN L20

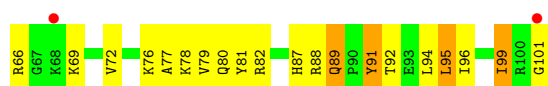


• Molecule 54: 50S RIBOSOMAL PROTEIN L21



• Molecule 54: 50S RIBOSOMAL PROTEIN L21





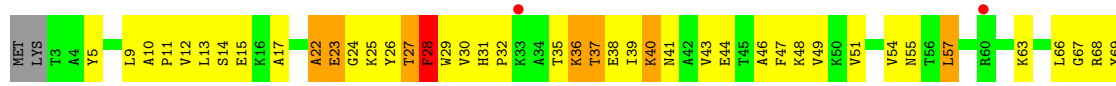
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



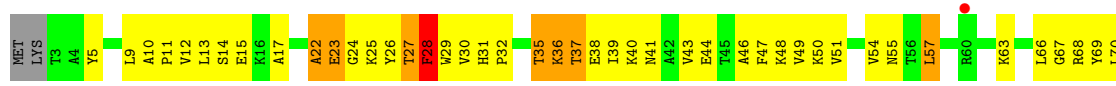
• Molecule 55: 50S RIBOSOMAL PROTEIN L22



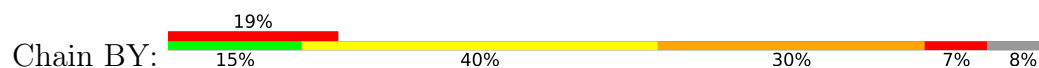
• Molecule 56: 50S RIBOSOMAL PROTEIN L23

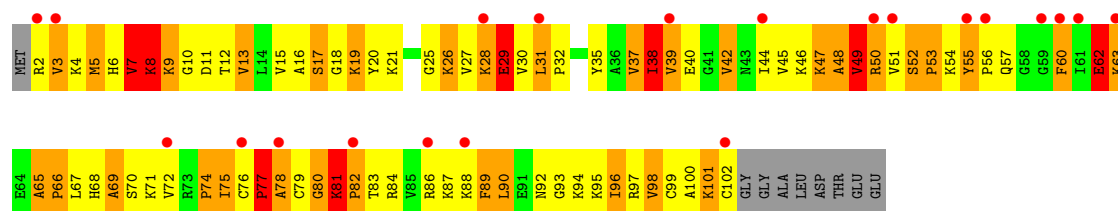


• Molecule 56: 50S RIBOSOMAL PROTEIN L23

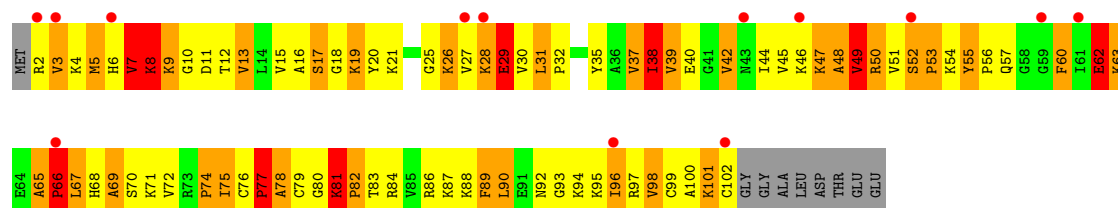
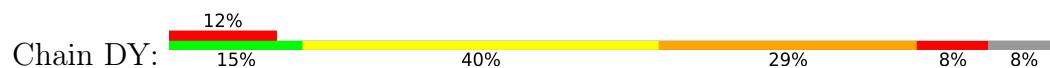


• Molecule 57: 50S RIBOSOMAL PROTEIN L24

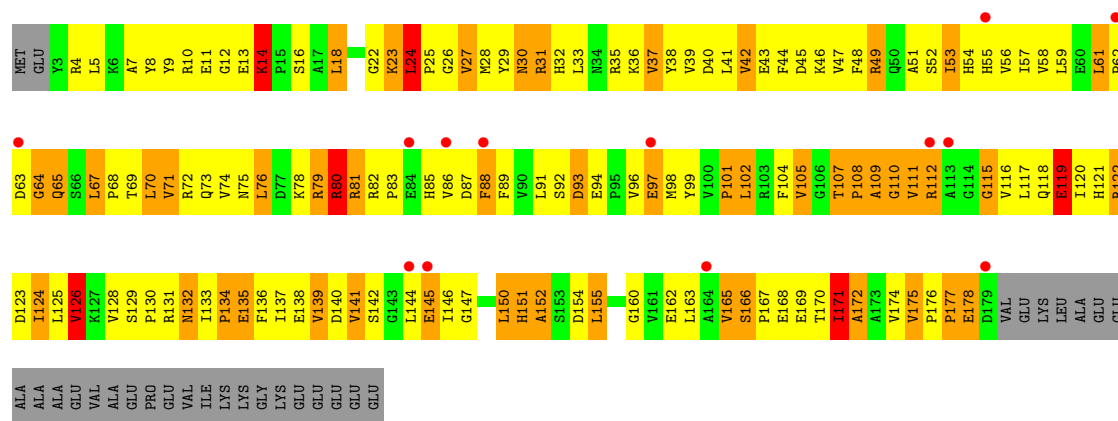
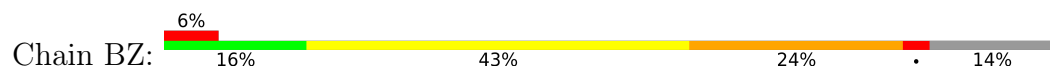




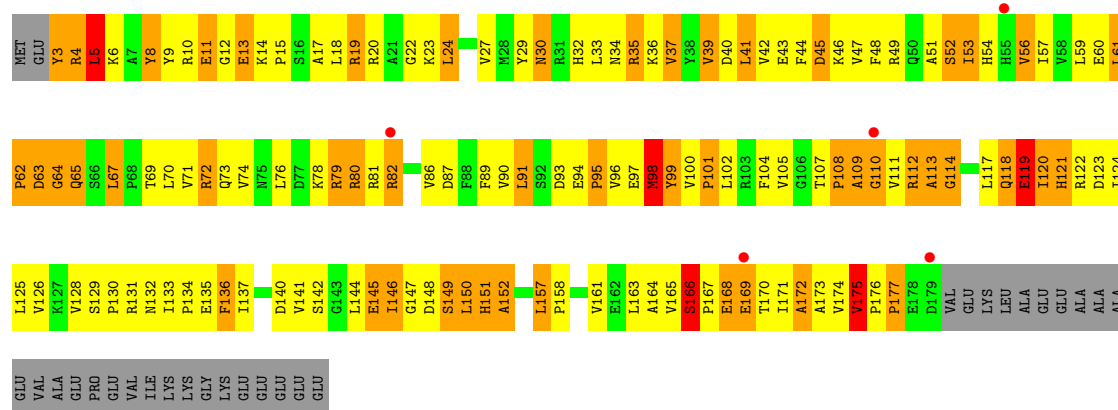
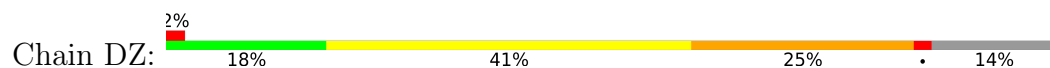
• Molecule 57: 50S RIBOSOMAL PROTEIN L24



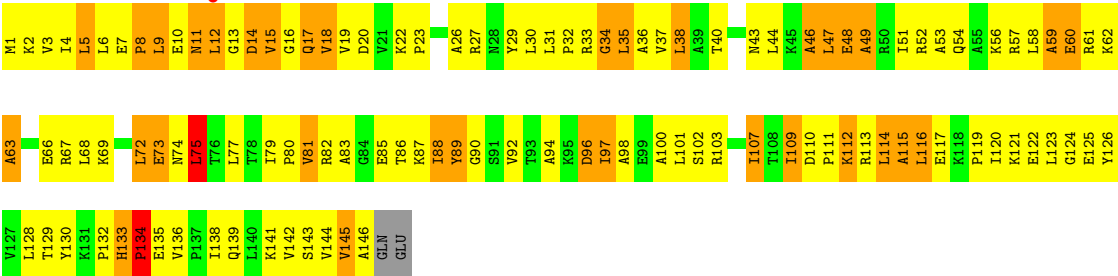
• Molecule 58: 50S RIBOSOMAL PROTEIN L25



• Molecule 58: 50S RIBOSOMAL PROTEIN L25



● Molecule 59: 50S RIBOSOMAL PROTEIN L9



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	211.34Å 450.91Å 614.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.57 – 3.45 49.57 – 3.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.57-3.45) 99.6 (49.57-3.45)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 3.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.210 , 0.257 0.208 , 0.256	Depositor DCC
R_{free} test set	33081 reflections (4.35%)	wwPDB-VP
Wilson B-factor (Å ²)	76.9	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 86.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	304505	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% 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: ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.42	0/36190	0.63	33/56486 (0.1%)
1	CA	0.43	0/36190	0.63	34/56486 (0.1%)
2	AB	0.38	1/1936 (0.1%)	0.95	10/2611 (0.4%)
2	CB	0.39	1/1936 (0.1%)	0.95	9/2611 (0.3%)
3	AC	0.40	1/1637 (0.1%)	0.90	7/2207 (0.3%)
3	CC	0.43	1/1637 (0.1%)	0.90	9/2207 (0.4%)
4	AD	0.39	0/1733	0.96	6/2318 (0.3%)
4	CD	0.41	0/1733	0.97	11/2318 (0.5%)
5	AE	0.44	1/1163 (0.1%)	0.92	2/1566 (0.1%)
5	CE	0.45	1/1163 (0.1%)	0.94	2/1566 (0.1%)
6	AF	0.34	0/856	0.91	1/1154 (0.1%)
6	CF	0.35	0/856	0.90	1/1154 (0.1%)
7	AG	0.35	0/1276	0.91	3/1709 (0.2%)
7	CG	0.40	0/1276	0.93	5/1709 (0.3%)
8	AH	0.41	0/1136	0.97	5/1527 (0.3%)
8	CH	0.42	0/1136	0.97	4/1527 (0.3%)
9	AI	0.34	0/1029	1.00	8/1378 (0.6%)
9	CI	0.37	0/1029	1.00	8/1378 (0.6%)
10	AJ	0.43	1/808 (0.1%)	0.93	4/1087 (0.4%)
10	CJ	0.44	1/808 (0.1%)	0.95	4/1087 (0.4%)
11	AK	0.40	0/900	0.96	1/1213 (0.1%)
11	CK	0.43	0/900	0.96	1/1213 (0.1%)
12	AL	0.51	1/992 (0.1%)	1.14	8/1329 (0.6%)
12	CL	0.52	1/992 (0.1%)	1.14	9/1329 (0.7%)
13	AM	0.42	1/966 (0.1%)	1.00	4/1294 (0.3%)
13	CM	0.46	1/966 (0.1%)	1.01	4/1294 (0.3%)
14	AN	0.38	0/501	0.94	1/664 (0.2%)
14	CN	0.43	0/501	0.97	3/664 (0.5%)
15	AO	0.37	0/745	0.85	2/992 (0.2%)
15	CO	0.40	0/745	0.84	2/992 (0.2%)
16	AP	0.47	1/717 (0.1%)	0.97	2/965 (0.2%)
16	CP	0.46	1/717 (0.1%)	0.97	2/965 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
17	AQ	0.43	1/837 (0.1%)	0.94	2/1119 (0.2%)
17	CQ	0.42	1/837 (0.1%)	0.94	0/1119
18	AR	0.35	0/579	0.97	5/768 (0.7%)
18	CR	0.38	0/579	0.96	2/768 (0.3%)
19	AS	0.45	1/643 (0.2%)	0.92	3/867 (0.3%)
19	CS	0.46	1/643 (0.2%)	0.93	3/867 (0.3%)
20	AT	0.36	0/765	0.91	2/1007 (0.2%)
20	CT	0.35	0/765	0.92	2/1007 (0.2%)
21	AU	0.54	1/213 (0.5%)	0.86	1/279 (0.4%)
21	CU	0.55	1/213 (0.5%)	0.88	1/279 (0.4%)
22	AV	0.43	0/1809	0.73	1/2819 (0.0%)
22	AW	0.47	0/1809	0.70	3/2819 (0.1%)
22	CV	0.45	0/1809	0.75	1/2819 (0.0%)
22	CW	0.42	0/1809	0.67	4/2819 (0.1%)
23	AX	0.47	0/185	0.79	0/286
23	CX	0.50	0/185	0.79	0/286
24	AY	0.42	0/2847	1.11	32/3846 (0.8%)
24	CY	0.45	0/2847	1.18	40/3846 (1.0%)
25	B0	0.50	0/615	1.02	1/819 (0.1%)
25	D0	0.55	0/615	1.04	1/819 (0.1%)
26	B1	0.58	1/739 (0.1%)	1.10	4/983 (0.4%)
26	D1	0.62	1/739 (0.1%)	1.13	5/983 (0.5%)
27	B2	0.49	0/600	1.04	3/793 (0.4%)
27	D2	0.57	0/600	1.07	4/793 (0.5%)
28	B3	0.60	1/473 (0.2%)	1.18	6/636 (0.9%)
28	D3	0.58	1/473 (0.2%)	1.16	5/636 (0.8%)
29	B4	0.51	1/229 (0.4%)	0.82	0/311
29	D4	0.53	1/229 (0.4%)	0.84	0/311
30	B5	0.56	0/473	1.25	4/639 (0.6%)
30	D5	0.57	0/473	1.28	6/639 (0.9%)
31	B6	0.74	1/388 (0.3%)	1.38	5/520 (1.0%)
31	D6	0.81	1/388 (0.3%)	1.42	9/520 (1.7%)
32	B7	0.61	1/427 (0.2%)	1.14	3/563 (0.5%)
32	D7	0.62	1/427 (0.2%)	1.16	4/563 (0.7%)
33	B8	0.80	1/516 (0.2%)	1.26	5/681 (0.7%)
33	D8	0.82	1/516 (0.2%)	1.26	6/681 (0.9%)
34	B9	0.50	0/302	1.22	2/397 (0.5%)
34	D9	0.51	0/302	1.26	2/397 (0.5%)
35	BA	0.45	0/69614	0.71	72/108679 (0.1%)
35	DA	0.46	0/69614	0.71	76/108679 (0.1%)
36	BB	0.45	1/2853 (0.0%)	0.78	5/4451 (0.1%)
36	DB	0.46	1/2853 (0.0%)	0.77	5/4451 (0.1%)
37	BC	0.53	1/1145 (0.1%)	1.02	11/1556 (0.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
37	DC	0.53	1/1145 (0.1%)	1.03	12/1556 (0.8%)
38	BD	0.64	1/2155 (0.0%)	0.98	5/2907 (0.2%)
38	DD	0.67	1/2155 (0.0%)	0.98	5/2907 (0.2%)
39	BE	0.55	1/1597 (0.1%)	1.19	22/2155 (1.0%)
39	DE	0.55	1/1597 (0.1%)	1.19	22/2155 (1.0%)
40	BF	0.61	1/1659 (0.1%)	1.24	17/2246 (0.8%)
40	DF	0.62	1/1659 (0.1%)	1.25	17/2246 (0.8%)
41	BG	0.43	0/1499	1.08	12/2016 (0.6%)
41	DG	0.50	0/1499	1.16	18/2016 (0.9%)
42	BH	0.47	1/1246 (0.1%)	1.09	10/1684 (0.6%)
42	DH	0.48	1/1246 (0.1%)	1.09	11/1684 (0.7%)
43	BI	0.43	1/1147 (0.1%)	0.98	4/1553 (0.3%)
45	BK	0.42	1/1057 (0.1%)	0.99	6/1432 (0.4%)
45	DK	0.41	1/1057 (0.1%)	0.99	6/1432 (0.4%)
46	BN	0.50	1/1132 (0.1%)	1.12	9/1527 (0.6%)
46	DN	0.53	1/1132 (0.1%)	1.12	15/1527 (1.0%)
47	BO	0.52	0/943	1.10	8/1269 (0.6%)
47	DO	0.50	0/943	1.09	10/1269 (0.8%)
48	BP	0.58	0/1131	1.09	9/1504 (0.6%)
48	DP	0.63	0/1131	1.11	8/1504 (0.5%)
49	BQ	0.55	0/1143	1.07	6/1527 (0.4%)
49	DQ	0.55	0/1143	1.08	7/1527 (0.5%)
50	BR	0.45	0/974	1.01	6/1302 (0.5%)
50	DR	0.48	0/974	1.03	6/1302 (0.5%)
51	BS	0.55	1/779 (0.1%)	1.25	8/1038 (0.8%)
51	DS	0.69	1/779 (0.1%)	1.28	7/1038 (0.7%)
52	BT	0.50	1/1156 (0.1%)	1.21	16/1544 (1.0%)
52	DT	0.51	1/1156 (0.1%)	1.22	18/1544 (1.2%)
53	BU	0.58	0/975	1.27	13/1297 (1.0%)
53	DU	0.58	0/975	1.29	14/1297 (1.1%)
54	BV	0.50	0/790	0.96	1/1057 (0.1%)
54	DV	0.56	0/790	0.99	1/1057 (0.1%)
55	BW	0.50	0/907	0.98	3/1216 (0.2%)
55	DW	0.53	0/907	1.01	2/1216 (0.2%)
56	BX	0.52	1/740 (0.1%)	1.06	4/995 (0.4%)
56	DX	0.53	1/740 (0.1%)	1.08	5/995 (0.5%)
57	BY	0.63	1/789 (0.1%)	1.18	10/1053 (0.9%)
57	DY	0.63	1/789 (0.1%)	1.18	10/1053 (0.9%)
58	BZ	0.51	1/1436 (0.1%)	1.19	16/1951 (0.8%)
58	DZ	0.51	0/1436	1.15	16/1951 (0.8%)
59	DI	0.49	1/1148 (0.1%)	1.15	13/1554 (0.8%)
All	All	0.46	59/327803 (0.0%)	0.81	959/489223 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AA	0	9
1	CA	0	10
22	AW	3	0
22	CV	0	2
22	CW	3	0
23	AX	0	1
30	B5	0	1
30	D5	0	2
35	BA	2	40
35	DA	3	46
All	All	11	111

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	DB	86	G	P-OP2	-6.53	1.35	1.49
36	BB	86	G	P-OP1	-6.14	1.36	1.49
29	D4	65	CYS	C-N	-6.03	1.25	1.33
29	B4	65	CYS	C-N	-5.90	1.25	1.33
13	AM	121	LYS	C-N	-5.89	1.25	1.33

The worst 5 of 959 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	BB	85	G	OP1-P-O3'	-17.56	55.33	108.00
51	DS	16	ASN	N-CA-C	-16.48	91.42	111.69
53	BU	97	ASP	N-CA-C	-16.27	93.37	113.38
51	BS	16	ASN	N-CA-C	-16.17	91.80	111.69
53	DU	97	ASP	N-CA-C	-16.07	93.61	113.38

5 of 11 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	AW	17	C	C1'
22	AW	47	U	C1'
22	AW	70	G	C3'
35	BA	1784	A	C3'
35	BA	1799	G	C3'

5 of 111 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	110	C	Sidechain
1	AA	324	G	Sidechain
1	AA	38	G	Sidechain
1	AA	388	G	Sidechain
1	AA	498	U	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AA	32329	0	16318	1298	0
1	CA	32329	0	16318	1284	0
2	AB	1901	0	1951	263	0
2	CB	1901	0	1951	265	0
3	AC	1613	0	1677	205	0
3	CC	1613	0	1677	203	0
4	AD	1703	0	1763	224	0
4	CD	1703	0	1763	226	0
5	AE	1147	0	1207	148	0
5	CE	1147	0	1207	140	0
6	AF	843	0	857	97	0
6	CF	843	0	857	101	0
7	AG	1257	0	1296	123	0
7	CG	1257	0	1296	120	0
8	AH	1116	0	1177	170	0
8	CH	1116	0	1177	164	0
9	AI	1011	0	1043	167	0
9	CI	1011	0	1043	181	0
10	AJ	795	0	840	175	0
10	CJ	795	0	840	169	0
11	AK	885	0	904	102	0
11	CK	885	0	904	108	0
12	AL	976	0	1062	101	0
12	CL	976	0	1062	98	0
13	AM	956	0	1021	109	0
13	CM	956	0	1021	111	0
14	AN	492	0	529	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	CN	492	0	529	61	0
15	AO	734	0	771	58	0
15	CO	734	0	771	53	0
16	AP	701	0	720	104	0
16	CP	701	0	720	109	0
17	AQ	824	0	891	74	0
17	CQ	824	0	891	75	0
18	AR	574	0	644	81	0
18	CR	574	0	644	80	0
19	AS	630	0	652	106	0
19	CS	630	0	652	107	0
20	AT	763	0	861	119	0
20	CT	763	0	861	115	0
21	AU	209	0	221	19	0
21	CU	209	0	221	18	0
22	AV	1619	0	822	76	0
22	AW	1619	0	822	99	0
22	CV	1619	0	822	83	0
22	CW	1619	0	822	92	0
23	AX	166	0	87	17	0
23	CX	166	0	87	7	0
24	AY	2799	0	2809	377	0
24	CY	2799	0	2809	366	0
25	B0	607	0	628	87	0
25	D0	607	0	628	87	0
26	B1	732	0	808	114	0
26	D1	732	0	808	110	0
27	B2	598	0	653	90	0
27	D2	598	0	653	83	0
28	B3	468	0	523	61	3
28	D3	468	0	523	64	0
29	B4	226	0	229	34	0
29	D4	226	0	229	38	0
30	B5	459	0	480	71	0
30	D5	459	0	480	76	0
31	B6	381	0	391	121	0
31	D6	381	0	391	125	0
32	B7	419	0	467	25	0
32	D7	419	0	467	30	0
33	B8	508	0	576	123	0
33	D8	508	0	576	132	0
34	B9	299	0	324	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
34	D9	299	0	324	31	0
35	BA	62154	0	31337	2156	0
35	DA	62154	0	31337	2177	9
36	BB	2551	0	1295	104	6
36	DB	2551	0	1295	103	0
37	BC	1142	0	865	114	0
37	DC	1142	0	865	108	0
38	BD	2105	0	2182	273	0
38	DD	2105	0	2182	265	0
39	BE	1564	0	1629	255	0
39	DE	1564	0	1629	265	0
40	BF	1624	0	1677	237	0
40	DF	1624	0	1677	241	0
41	BG	1474	0	1535	311	0
41	DG	1474	0	1535	268	0
42	BH	1223	0	1282	222	0
42	DH	1223	0	1282	222	0
43	BI	1132	0	1218	126	0
44	BJ	651	0	146	35	0
44	DJ	651	0	146	36	0
45	BK	1038	0	1089	168	0
45	DK	1038	0	1089	197	0
46	BN	1105	0	1180	138	0
46	DN	1105	0	1180	133	0
47	BO	933	0	996	94	0
47	DO	933	0	996	97	0
48	BP	1114	0	1187	278	0
48	DP	1114	0	1187	275	0
49	BQ	1122	0	1179	132	0
49	DQ	1122	0	1179	128	0
50	BR	960	0	1021	140	0
50	DR	960	0	1020	142	0
51	BS	771	0	832	161	0
51	DS	771	0	832	159	0
52	BT	1142	0	1202	239	0
52	DT	1142	0	1202	240	0
53	BU	958	0	1015	144	0
53	DU	958	0	1015	148	0
54	BV	779	0	852	148	0
54	DV	779	0	852	153	0
55	BW	896	0	953	81	0
55	DW	896	0	953	81	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	BX	726	0	778	69	0
56	DX	726	0	778	69	0
57	BY	776	0	870	188	0
57	DY	776	0	870	184	0
58	BZ	1404	0	1432	243	0
58	DZ	1404	0	1432	253	0
59	DI	1133	0	1220	189	0
60	AA	157	0	0	0	0
60	AE	1	0	0	0	0
60	AL	1	0	0	0	0
60	AM	1	0	0	0	0
60	AV	7	0	0	0	0
60	AW	5	0	0	0	0
60	AY	1	0	0	0	0
60	B1	1	0	0	0	0
60	B3	1	0	0	0	0
60	B5	2	0	0	0	0
60	B7	2	0	0	0	0
60	BA	354	0	0	0	0
60	BB	4	0	0	0	0
60	BC	1	0	0	0	0
60	BD	2	0	0	0	0
60	BF	1	0	0	0	0
60	BH	1	0	0	0	0
60	BP	1	0	0	0	0
60	BQ	1	0	0	0	0
60	BS	1	0	0	0	0
60	BU	1	0	0	0	0
60	CA	157	0	0	0	0
60	CL	1	0	0	0	0
60	CN	1	0	0	0	0
60	CV	7	0	0	0	0
60	CW	5	0	0	0	0
60	CY	1	0	0	0	0
60	D1	1	0	0	0	0
60	D3	1	0	0	0	0
60	D5	2	0	0	0	0
60	D7	1	0	0	0	0
60	DA	353	0	0	0	0
60	DB	4	0	0	0	0
60	DC	1	0	0	0	0
60	DD	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	DF	3	0	0	0	0
60	DH	1	0	0	0	0
60	DQ	1	0	0	0	0
60	DR	1	0	0	0	0
60	DU	1	0	0	0	0
60	DX	1	0	0	0	0
60	DY	1	0	0	0	0
61	AD	1	0	0	0	0
61	AN	1	0	0	0	0
61	B9	1	0	0	0	0
61	CD	1	0	0	0	0
61	CN	1	0	0	0	0
61	D9	1	0	0	0	0
All	All	304505	0	207553	20472	9

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 40.

The worst 5 of 20472 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)
26:D1:81:LYS:CE	35:DA:271(H):G:H5'	1.21	1.60
26:B1:81:LYS:HE2	35:BA:271(H):G:C5'	1.23	1.59
26:D1:81:LYS:HE2	35:DA:271(H):G:C5'	1.31	1.54
26:B1:81:LYS:CE	35:BA:271(H):G:H5'	1.10	1.53
35:BA:1887:C:H2'	35:BA:1888:G:H5''	1.22	1.18

The worst 5 of 9 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)
28:B3:48:GLU:O	35:DA:654(L):G:OP2[3_455]	1.99	0.21
36:BB:97:G:N7	35:DA:654(J):A:OP1[3_455]	2.05	0.15
36:BB:97:G:OP2	35:DA:654(I):C:O2'[3_455]	2.06	0.14
36:BB:96:U:C3'	35:DA:654(I):C:O2'[3_455]	2.09	0.11
36:BB:96:U:O2	35:DA:654(K):C:OP1[3_455]	2.10	0.10

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%)	155 (66%)	58 (25%)	20 (9%)	0	7
2	CB	233/256 (91%)	156 (67%)	56 (24%)	21 (9%)	0	7
3	AC	205/239 (86%)	125 (61%)	57 (28%)	23 (11%)	0	5
3	CC	205/239 (86%)	128 (62%)	55 (27%)	22 (11%)	0	5
4	AD	206/209 (99%)	134 (65%)	49 (24%)	23 (11%)	0	5
4	CD	206/209 (99%)	135 (66%)	49 (24%)	22 (11%)	0	5
5	AE	149/162 (92%)	98 (66%)	36 (24%)	15 (10%)	0	6
5	CE	149/162 (92%)	100 (67%)	34 (23%)	15 (10%)	0	6
6	AF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	10
6	CF	99/101 (98%)	75 (76%)	17 (17%)	7 (7%)	1	10
7	AG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	1	9
7	CG	153/156 (98%)	108 (71%)	34 (22%)	11 (7%)	1	9
8	AH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	0	7
8	CH	136/138 (99%)	92 (68%)	32 (24%)	12 (9%)	0	7
9	AI	125/128 (98%)	83 (66%)	30 (24%)	12 (10%)	0	6
9	CI	125/128 (98%)	82 (66%)	31 (25%)	12 (10%)	0	6
10	AJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	0	4
10	CJ	97/105 (92%)	64 (66%)	21 (22%)	12 (12%)	0	4
11	AK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	3	23
11	CK	117/129 (91%)	89 (76%)	24 (20%)	4 (3%)	3	23
12	AL	124/132 (94%)	89 (72%)	26 (21%)	9 (7%)	1	9
12	CL	124/132 (94%)	90 (73%)	25 (20%)	9 (7%)	1	9
13	AM	119/126 (94%)	82 (69%)	23 (19%)	14 (12%)	0	5
13	CM	119/126 (94%)	84 (71%)	21 (18%)	14 (12%)	0	5
14	AN	58/61 (95%)	39 (67%)	12 (21%)	7 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	CN	58/61 (95%)	38 (66%)	12 (21%)	8 (14%)	0	3
15	AO	86/89 (97%)	59 (69%)	23 (27%)	4 (5%)	2	17
15	CO	86/89 (97%)	57 (66%)	25 (29%)	4 (5%)	2	17
16	AP	82/88 (93%)	51 (62%)	22 (27%)	9 (11%)	0	5
16	CP	82/88 (93%)	53 (65%)	20 (24%)	9 (11%)	0	5
17	AQ	98/105 (93%)	68 (69%)	17 (17%)	13 (13%)	0	3
17	CQ	98/105 (93%)	69 (70%)	17 (17%)	12 (12%)	0	4
18	AR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	6
18	CR	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	0	6
19	AS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	3
19	CS	77/93 (83%)	36 (47%)	30 (39%)	11 (14%)	0	3
20	AT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	0	5
20	CT	97/106 (92%)	68 (70%)	18 (19%)	11 (11%)	0	5
21	AU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	0	7
21	CU	23/27 (85%)	18 (78%)	3 (13%)	2 (9%)	0	7
24	AY	349/351 (99%)	246 (70%)	70 (20%)	33 (10%)	0	6
24	CY	349/351 (99%)	256 (73%)	61 (18%)	32 (9%)	0	7
25	B0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	8
25	D0	74/85 (87%)	58 (78%)	10 (14%)	6 (8%)	1	8
26	B1	92/98 (94%)	65 (71%)	15 (16%)	12 (13%)	0	4
26	D1	92/98 (94%)	72 (78%)	12 (13%)	8 (9%)	0	7
27	B2	69/72 (96%)	40 (58%)	17 (25%)	12 (17%)	0	2
27	D2	69/72 (96%)	39 (56%)	20 (29%)	10 (14%)	0	3
28	B3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	6
28	D3	58/60 (97%)	43 (74%)	9 (16%)	6 (10%)	0	6
29	B4	29/71 (41%)	14 (48%)	11 (38%)	4 (14%)	0	3
29	D4	29/71 (41%)	14 (48%)	11 (38%)	4 (14%)	0	3
30	B5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	2
30	D5	57/60 (95%)	40 (70%)	7 (12%)	10 (18%)	0	2
31	B6	43/54 (80%)	17 (40%)	12 (28%)	14 (33%)	0	0
31	D6	43/54 (80%)	17 (40%)	13 (30%)	13 (30%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	B7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
32	D7	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
33	B8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	3
33	D8	62/65 (95%)	38 (61%)	15 (24%)	9 (14%)	0	3
34	B9	34/37 (92%)	23 (68%)	11 (32%)	0	100	100
34	D9	34/37 (92%)	24 (71%)	10 (29%)	0	100	100
37	BC	183/229 (80%)	64 (35%)	71 (39%)	48 (26%)	0	0
37	DC	183/229 (80%)	65 (36%)	72 (39%)	46 (25%)	0	0
38	BD	270/276 (98%)	199 (74%)	39 (14%)	32 (12%)	0	4
38	DD	270/276 (98%)	198 (73%)	40 (15%)	32 (12%)	0	4
39	BE	203/206 (98%)	124 (61%)	45 (22%)	34 (17%)	0	2
39	DE	203/206 (98%)	123 (61%)	44 (22%)	36 (18%)	0	2
40	BF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	0	5
40	DF	206/210 (98%)	149 (72%)	33 (16%)	24 (12%)	0	5
41	BG	179/182 (98%)	92 (51%)	54 (30%)	33 (18%)	0	1
41	DG	179/182 (98%)	107 (60%)	46 (26%)	26 (14%)	0	3
42	BH	158/180 (88%)	90 (57%)	38 (24%)	30 (19%)	0	1
42	DH	158/180 (88%)	91 (58%)	36 (23%)	31 (20%)	0	1
43	BI	144/148 (97%)	100 (69%)	28 (19%)	16 (11%)	0	5
45	BK	139/147 (95%)	88 (63%)	33 (24%)	18 (13%)	0	4
45	DK	139/147 (95%)	87 (63%)	34 (24%)	18 (13%)	0	4
46	BN	137/140 (98%)	97 (71%)	20 (15%)	20 (15%)	0	3
46	DN	137/140 (98%)	99 (72%)	18 (13%)	20 (15%)	0	3
47	BO	120/122 (98%)	97 (81%)	17 (14%)	6 (5%)	1	15
47	DO	120/122 (98%)	98 (82%)	14 (12%)	8 (7%)	1	11
48	BP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
48	DP	144/150 (96%)	68 (47%)	36 (25%)	40 (28%)	0	0
49	BQ	139/141 (99%)	111 (80%)	19 (14%)	9 (6%)	1	11
49	DQ	139/141 (99%)	114 (82%)	16 (12%)	9 (6%)	1	11
50	BR	115/118 (98%)	72 (63%)	29 (25%)	14 (12%)	0	4
50	DR	115/118 (98%)	70 (61%)	31 (27%)	14 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	BS	97/112 (87%)	55 (57%)	22 (23%)	20 (21%)	0	1
51	DS	97/112 (87%)	54 (56%)	22 (23%)	21 (22%)	0	1
52	BT	136/146 (93%)	84 (62%)	23 (17%)	29 (21%)	0	1
52	DT	136/146 (93%)	85 (62%)	22 (16%)	29 (21%)	0	1
53	BU	115/118 (98%)	78 (68%)	27 (24%)	10 (9%)	0	7
53	DU	115/118 (98%)	77 (67%)	28 (24%)	10 (9%)	0	7
54	BV	99/101 (98%)	72 (73%)	13 (13%)	14 (14%)	0	3
54	DV	99/101 (98%)	72 (73%)	14 (14%)	13 (13%)	0	3
55	BW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	1	14
55	DW	111/113 (98%)	83 (75%)	22 (20%)	6 (5%)	1	14
56	BX	91/96 (95%)	75 (82%)	14 (15%)	2 (2%)	5	30
56	DX	91/96 (95%)	74 (81%)	16 (18%)	1 (1%)	11	42
57	BY	99/110 (90%)	46 (46%)	20 (20%)	33 (33%)	0	0
57	DY	99/110 (90%)	47 (48%)	20 (20%)	32 (32%)	0	0
58	BZ	175/206 (85%)	102 (58%)	41 (23%)	32 (18%)	0	1
58	DZ	175/206 (85%)	110 (63%)	36 (21%)	29 (17%)	0	2
59	DI	144/148 (97%)	81 (56%)	42 (29%)	21 (15%)	0	3
All	All	12652/13582 (93%)	8336 (66%)	2725 (22%)	1591 (13%)	0	4

5 of 1591 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	AB	15	VAL
2	AB	20	GLU
2	AB	88	ALA
2	AB	95	GLN
2	AB	195	ASP

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%)	190 (94%)	12 (6%)	18	45
2	CB	202/220 (92%)	189 (94%)	13 (6%)	16	43
3	AC	160/188 (85%)	152 (95%)	8 (5%)	22	49
3	CC	160/188 (85%)	151 (94%)	9 (6%)	19	47
4	AD	180/181 (99%)	160 (89%)	20 (11%)	6	26
4	CD	180/181 (99%)	160 (89%)	20 (11%)	6	26
5	AE	115/123 (94%)	98 (85%)	17 (15%)	3	17
5	CE	115/123 (94%)	99 (86%)	16 (14%)	3	19
6	AF	90/90 (100%)	83 (92%)	7 (8%)	11	37
6	CF	90/90 (100%)	83 (92%)	7 (8%)	11	37
7	AG	126/127 (99%)	117 (93%)	9 (7%)	13	40
7	CG	126/127 (99%)	116 (92%)	10 (8%)	11	37
8	AH	119/119 (100%)	106 (89%)	13 (11%)	6	27
8	CH	119/119 (100%)	106 (89%)	13 (11%)	6	27
9	AI	98/99 (99%)	87 (89%)	11 (11%)	6	26
9	CI	98/99 (99%)	87 (89%)	11 (11%)	6	26
10	AJ	88/92 (96%)	80 (91%)	8 (9%)	9	32
10	CJ	88/92 (96%)	80 (91%)	8 (9%)	9	32
11	AK	90/99 (91%)	84 (93%)	6 (7%)	15	42
11	CK	90/99 (91%)	84 (93%)	6 (7%)	15	42
12	AL	104/109 (95%)	98 (94%)	6 (6%)	18	45
12	CL	104/109 (95%)	98 (94%)	6 (6%)	18	45
13	AM	96/101 (95%)	83 (86%)	13 (14%)	4	20
13	CM	96/101 (95%)	83 (86%)	13 (14%)	4	20
14	AN	49/50 (98%)	46 (94%)	3 (6%)	17	44
14	CN	49/50 (98%)	46 (94%)	3 (6%)	17	44
15	AO	79/80 (99%)	75 (95%)	4 (5%)	21	49
15	CO	79/80 (99%)	75 (95%)	4 (5%)	21	49
16	AP	72/74 (97%)	63 (88%)	9 (12%)	4	22
16	CP	72/74 (97%)	63 (88%)	9 (12%)	4	22
17	AQ	94/97 (97%)	91 (97%)	3 (3%)	34	60
17	CQ	94/97 (97%)	91 (97%)	3 (3%)	34	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	AR	61/77 (79%)	59 (97%)	2 (3%)	33	59
18	CR	61/77 (79%)	59 (97%)	2 (3%)	33	59
19	AS	69/80 (86%)	61 (88%)	8 (12%)	5	25
19	CS	69/80 (86%)	61 (88%)	8 (12%)	5	25
20	AT	76/82 (93%)	70 (92%)	6 (8%)	11	37
20	CT	76/82 (93%)	70 (92%)	6 (8%)	11	37
21	AU	19/22 (86%)	18 (95%)	1 (5%)	20	48
21	CU	19/22 (86%)	18 (95%)	1 (5%)	20	48
24	AY	298/298 (100%)	266 (89%)	32 (11%)	6	27
24	CY	298/298 (100%)	257 (86%)	41 (14%)	3	19
25	B0	61/67 (91%)	57 (93%)	4 (7%)	15	43
25	D0	61/67 (91%)	57 (93%)	4 (7%)	15	43
26	B1	78/83 (94%)	69 (88%)	9 (12%)	5	25
26	D1	78/83 (94%)	66 (85%)	12 (15%)	2	16
27	B2	66/67 (98%)	56 (85%)	10 (15%)	3	16
27	D2	66/67 (98%)	59 (89%)	7 (11%)	6	27
28	B3	51/52 (98%)	46 (90%)	5 (10%)	7	30
28	D3	51/52 (98%)	46 (90%)	5 (10%)	7	30
29	B4	27/63 (43%)	25 (93%)	2 (7%)	13	39
29	D4	27/63 (43%)	25 (93%)	2 (7%)	13	39
30	B5	51/52 (98%)	45 (88%)	6 (12%)	5	24
30	D5	51/52 (98%)	45 (88%)	6 (12%)	5	24
31	B6	43/52 (83%)	32 (74%)	11 (26%)	0	3
31	D6	43/52 (83%)	32 (74%)	11 (26%)	0	3
32	B7	41/42 (98%)	39 (95%)	2 (5%)	22	50
32	D7	41/42 (98%)	39 (95%)	2 (5%)	22	50
33	B8	53/55 (96%)	40 (76%)	13 (24%)	1	4
33	D8	53/55 (96%)	40 (76%)	13 (24%)	1	4
34	B9	33/34 (97%)	28 (85%)	5 (15%)	3	16
34	D9	33/34 (97%)	28 (85%)	5 (15%)	3	16
37	BC	61/181 (34%)	55 (90%)	6 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	DC	61/181 (34%)	55 (90%)	6 (10%)	7	30
38	BD	213/218 (98%)	191 (90%)	22 (10%)	7	28
38	DD	213/218 (98%)	192 (90%)	21 (10%)	7	30
39	BE	165/166 (99%)	134 (81%)	31 (19%)	1	9
39	DE	165/166 (99%)	133 (81%)	32 (19%)	1	8
40	BF	165/166 (99%)	143 (87%)	22 (13%)	4	21
40	DF	165/166 (99%)	144 (87%)	21 (13%)	4	22
41	BG	155/156 (99%)	134 (86%)	21 (14%)	4	20
41	DG	155/156 (99%)	133 (86%)	22 (14%)	3	18
42	BH	132/148 (89%)	122 (92%)	10 (8%)	12	38
42	DH	132/148 (89%)	122 (92%)	10 (8%)	12	38
43	BI	122/124 (98%)	113 (93%)	9 (7%)	13	39
45	BK	106/111 (96%)	98 (92%)	8 (8%)	12	38
45	DK	106/111 (96%)	98 (92%)	8 (8%)	12	38
46	BN	117/119 (98%)	96 (82%)	21 (18%)	2	10
46	DN	117/119 (98%)	98 (84%)	19 (16%)	2	14
47	BO	100/100 (100%)	91 (91%)	9 (9%)	9	33
47	DO	100/100 (100%)	92 (92%)	8 (8%)	11	36
48	BP	112/116 (97%)	83 (74%)	29 (26%)	0	3
48	DP	112/116 (97%)	83 (74%)	29 (26%)	0	3
49	BQ	111/111 (100%)	94 (85%)	17 (15%)	3	16
49	DQ	111/111 (100%)	94 (85%)	17 (15%)	3	16
50	BR	100/101 (99%)	81 (81%)	19 (19%)	1	8
50	DR	100/101 (99%)	81 (81%)	19 (19%)	1	8
51	BS	77/88 (88%)	62 (80%)	15 (20%)	1	8
51	DS	77/88 (88%)	62 (80%)	15 (20%)	1	8
52	BT	120/127 (94%)	101 (84%)	19 (16%)	2	15
52	DT	120/127 (94%)	101 (84%)	19 (16%)	2	15
53	BU	92/94 (98%)	85 (92%)	7 (8%)	12	38
53	DU	92/94 (98%)	85 (92%)	7 (8%)	12	38
54	BV	82/82 (100%)	70 (85%)	12 (15%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	DV	82/82 (100%)	70 (85%)	12 (15%)	3	17
55	BW	91/92 (99%)	78 (86%)	13 (14%)	3	18
55	DW	91/92 (99%)	78 (86%)	13 (14%)	3	18
56	BX	74/78 (95%)	66 (89%)	8 (11%)	6	27
56	DX	74/78 (95%)	66 (89%)	8 (11%)	6	27
57	BY	84/91 (92%)	68 (81%)	16 (19%)	1	8
57	DY	84/91 (92%)	68 (81%)	16 (19%)	1	8
58	BZ	155/179 (87%)	129 (83%)	26 (17%)	2	13
58	DZ	155/179 (87%)	126 (81%)	29 (19%)	1	9
59	DI	122/124 (98%)	113 (93%)	9 (7%)	13	39
All	All	10446/11246 (93%)	9225 (88%)	1221 (12%)	5	25

5 of 1221 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	DE	119	ARG
54	DV	22	VAL
40	DF	127	GLU
39	DE	116	VAL
48	DP	32	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 344 such sidechains are listed below:

Mol	Chain	Res	Type
19	CS	69	HIS
40	DF	31	HIS
24	CY	121	GLN
30	D5	23	HIS
46	DN	94	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	AA	1503/1522 (98%)	223 (14%)	34 (2%)
1	CA	1503/1522 (98%)	218 (14%)	34 (2%)
22	AV	75/76 (98%)	17 (22%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
22	AW	75/76 (98%)	15 (20%)	3 (4%)
22	CV	75/76 (98%)	18 (24%)	0
22	CW	75/76 (98%)	16 (21%)	4 (5%)
23	AX	7/8 (87%)	1 (14%)	1 (14%)
23	CX	7/8 (87%)	1 (14%)	0
35	BA	2885/2901 (99%)	521 (18%)	58 (2%)
35	DA	2885/2901 (99%)	522 (18%)	57 (1%)
36	BB	118/122 (96%)	15 (12%)	3 (2%)
36	DB	118/122 (96%)	14 (11%)	3 (2%)
All	All	9326/9410 (99%)	1581 (16%)	198 (2%)

5 of 1581 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 198 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	CA	508	C
35	DA	221	A
1	CA	687	A
1	CA	1224	G
35	DA	587	C

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 1098 ligands modelled in this entry, 1098 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AA	1504/1522 (98%)	0.21	41 (2%) 56 33	43, 106, 183, 201	0
1	CA	1504/1522 (98%)	0.01	43 (2%) 53 32	35, 87, 183, 201	0
2	AB	235/256 (91%)	0.45	6 (2%) 57 34	76, 137, 191, 201	0
2	CB	235/256 (91%)	0.28	10 (4%) 40 23	51, 117, 180, 201	0
3	AC	207/239 (86%)	0.47	9 (4%) 40 23	71, 130, 177, 201	0
3	CC	207/239 (86%)	0.39	11 (5%) 32 20	48, 96, 159, 200	0
4	AD	208/209 (99%)	0.80	22 (10%) 11 9	53, 116, 168, 199	0
4	CD	208/209 (99%)	0.56	18 (8%) 16 11	41, 95, 158, 183	0
5	AE	151/162 (93%)	0.41	5 (3%) 49 29	48, 102, 156, 179	0
5	CE	151/162 (93%)	0.16	3 (1%) 65 41	29, 86, 145, 193	0
6	AF	101/101 (100%)	0.36	1 (0%) 79 56	75, 120, 170, 189	0
6	CF	101/101 (100%)	0.15	0 100 100	60, 116, 162, 184	0
7	AG	155/156 (99%)	0.62	14 (9%) 15 11	64, 137, 182, 201	0
7	CG	155/156 (99%)	0.23	6 (3%) 43 25	42, 89, 143, 193	0
8	AH	138/138 (100%)	0.57	13 (9%) 14 10	50, 101, 152, 201	0
8	CH	138/138 (100%)	0.31	8 (5%) 29 18	50, 97, 148, 188	0
9	AI	127/128 (99%)	1.09	18 (14%) 6 6	66, 148, 192, 201	0
9	CI	127/128 (99%)	0.57	8 (6%) 26 17	43, 97, 148, 183	0
10	AJ	99/105 (94%)	1.02	15 (15%) 5 5	64, 154, 198, 201	0
10	CJ	99/105 (94%)	0.66	10 (10%) 12 9	44, 122, 197, 201	0
11	AK	119/129 (92%)	0.40	8 (6%) 24 16	52, 100, 155, 172	0
11	CK	119/129 (92%)	0.32	6 (5%) 34 20	49, 89, 165, 183	0
12	AL	126/132 (95%)	0.47	10 (7%) 18 13	42, 81, 146, 193	0
12	CL	126/132 (95%)	0.36	8 (6%) 26 17	37, 75, 148, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	AM	121/126 (96%)	0.80	13 (10%) 11 9	69, 133, 191, 201	0
13	CM	121/126 (96%)	0.35	8 (6%) 24 16	26, 96, 156, 189	0
14	AN	60/61 (98%)	0.94	9 (15%) 5 5	76, 124, 173, 187	0
14	CN	60/61 (98%)	0.23	3 (5%) 34 20	40, 82, 118, 155	0
15	AO	88/89 (98%)	0.23	1 (1%) 78 54	43, 100, 153, 177	0
15	CO	88/89 (98%)	0.27	4 (4%) 38 22	55, 92, 138, 155	0
16	AP	84/88 (95%)	0.88	11 (13%) 7 6	59, 104, 142, 201	0
16	CP	84/88 (95%)	0.94	10 (11%) 9 7	56, 106, 157, 201	0
17	AQ	100/105 (95%)	0.52	5 (5%) 34 20	54, 96, 137, 165	0
17	CQ	100/105 (95%)	0.57	6 (6%) 27 17	53, 99, 152, 162	0
18	AR	70/88 (79%)	0.25	0 100 100	62, 116, 160, 183	0
18	CR	70/88 (79%)	0.06	0 100 100	51, 101, 157, 183	0
19	AS	79/93 (84%)	1.05	12 (15%) 5 5	91, 140, 191, 201	0
19	CS	79/93 (84%)	0.63	7 (8%) 15 11	51, 103, 193, 201	0
20	AT	99/106 (93%)	0.88	18 (18%) 3 4	55, 112, 165, 201	0
20	CT	99/106 (93%)	1.22	24 (24%) 2 2	68, 115, 177, 201	0
21	AU	25/27 (92%)	2.10	11 (44%) 0 1	78, 131, 167, 178	0
21	CU	25/27 (92%)	1.08	5 (20%) 3 3	58, 85, 117, 123	0
22	AV	76/76 (100%)	-0.27	0 100 100	42, 85, 152, 176	0
22	AW	76/76 (100%)	1.13	13 (17%) 4 4	48, 184, 201, 201	0
22	CV	76/76 (100%)	-0.59	1 (1%) 75 51	35, 65, 135, 185	0
22	CW	76/76 (100%)	0.18	3 (3%) 43 25	30, 166, 198, 201	0
23	AX	8/8 (100%)	0.89	2 (25%) 2 2	67, 76, 160, 166	0
23	CX	8/8 (100%)	0.98	2 (25%) 2 2	46, 62, 153, 170	0
24	AY	351/351 (100%)	0.17	16 (4%) 37 21	31, 109, 190, 201	0
24	CY	351/351 (100%)	0.12	14 (3%) 42 25	25, 95, 188, 201	0
25	B0	76/85 (89%)	0.24	5 (6%) 24 16	25, 64, 105, 177	0
25	D0	76/85 (89%)	-0.15	3 (3%) 43 25	10, 43, 103, 179	0
26	B1	94/98 (95%)	-0.02	3 (3%) 50 30	23, 61, 123, 173	0
26	D1	94/98 (95%)	-0.10	3 (3%) 50 30	18, 52, 109, 155	0
27	B2	71/72 (98%)	0.14	0 100 100	36, 85, 156, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
27	D2	71/72 (98%)	0.34	5 (7%) 22 15	27, 76, 144, 186	0
28	B3	60/60 (100%)	0.04	2 (3%) 49 29	19, 56, 131, 197	0
28	D3	60/60 (100%)	-0.09	2 (3%) 49 29	20, 51, 112, 201	0
29	B4	31/71 (43%)	0.74	2 (6%) 25 17	99, 184, 201, 201	0
29	D4	31/71 (43%)	0.96	5 (16%) 4 5	51, 140, 184, 200	0
30	B5	59/60 (98%)	0.25	2 (3%) 48 29	22, 74, 170, 190	0
30	D5	59/60 (98%)	0.24	4 (6%) 23 16	7, 55, 183, 201	0
31	B6	45/54 (83%)	0.91	7 (15%) 5 5	39, 85, 140, 198	0
31	D6	45/54 (83%)	0.90	7 (15%) 5 5	24, 65, 117, 183	0
32	B7	49/49 (100%)	0.22	2 (4%) 41 24	7, 48, 129, 165	0
32	D7	49/49 (100%)	0.14	2 (4%) 41 24	7, 37, 113, 189	0
33	B8	64/65 (98%)	0.44	6 (9%) 14 10	17, 51, 125, 160	0
33	D8	64/65 (98%)	0.31	5 (7%) 19 13	8, 40, 120, 162	0
34	B9	36/37 (97%)	0.42	2 (5%) 30 19	45, 69, 127, 147	0
34	D9	36/37 (97%)	1.01	6 (16%) 4 4	40, 74, 133, 162	0
35	BA	2886/2901 (99%)	-0.30	77 (2%) 56 33	16, 58, 179, 201	0
35	DA	2886/2901 (99%)	-0.34	90 (3%) 51 31	14, 51, 181, 201	0
36	BB	119/122 (97%)	0.24	1 (0%) 82 61	46, 105, 160, 186	0
36	DB	119/122 (97%)	-0.40	0 100 100	34, 65, 99, 129	0
37	BC	191/229 (83%)	1.38	52 (27%) 1 2	91, 174, 201, 201	0
37	DC	191/229 (83%)	1.35	53 (27%) 1 2	104, 177, 201, 201	0
38	BD	272/276 (98%)	0.57	20 (7%) 20 14	27, 71, 122, 165	0
38	DD	272/276 (98%)	0.53	22 (8%) 18 13	25, 66, 108, 168	0
39	BE	205/206 (99%)	0.15	10 (4%) 35 21	22, 69, 152, 201	0
39	DE	205/206 (99%)	0.19	6 (2%) 53 32	16, 67, 144, 197	0
40	BF	208/210 (99%)	0.02	3 (1%) 73 49	9, 52, 134, 194	0
40	DF	208/210 (99%)	0.02	5 (2%) 59 37	9, 48, 140, 179	0
41	BG	181/182 (99%)	0.53	14 (7%) 19 14	64, 118, 173, 200	0
41	DG	181/182 (99%)	-0.02	5 (2%) 55 33	30, 76, 137, 201	0
42	BH	160/180 (88%)	0.83	24 (15%) 5 5	50, 123, 181, 201	0
42	DH	160/180 (88%)	1.08	33 (20%) 2 3	63, 137, 186, 201	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
43	BI	146/148 (98%)	0.64	10 (6%) 23 16	41, 138, 187, 200	0
44	BJ	0/130	-	-	-	-
44	DJ	0/130	-	-	-	-
45	BK	141/147 (95%)	0.73	15 (10%) 11 9	85, 158, 195, 201	0
45	DK	141/147 (95%)	0.69	12 (8%) 16 12	99, 158, 197, 201	0
46	BN	139/140 (99%)	0.08	3 (2%) 62 39	30, 70, 129, 164	0
46	DN	139/140 (99%)	0.14	3 (2%) 62 39	24, 62, 122, 186	0
47	BO	122/122 (100%)	-0.09	2 (1%) 70 46	28, 64, 101, 158	0
47	DO	122/122 (100%)	-0.17	0 100 100	25, 68, 101, 120	0
48	BP	146/150 (97%)	1.32	35 (23%) 2 2	27, 89, 163, 200	0
48	DP	146/150 (97%)	1.25	34 (23%) 2 3	25, 72, 147, 201	0
49	BQ	141/141 (100%)	0.25	7 (4%) 34 20	23, 65, 127, 198	0
49	DQ	141/141 (100%)	0.10	7 (4%) 34 20	14, 53, 105, 196	0
50	BR	117/118 (99%)	0.32	4 (3%) 48 29	33, 72, 126, 156	0
50	DR	117/118 (99%)	0.16	8 (6%) 23 16	26, 68, 122, 150	0
51	BS	99/112 (88%)	1.12	20 (20%) 3 3	60, 104, 165, 188	0
51	DS	99/112 (88%)	0.49	11 (11%) 10 8	25, 61, 120, 171	0
52	BT	138/146 (94%)	0.42	8 (5%) 29 18	44, 87, 164, 201	0
52	DT	138/146 (94%)	0.57	13 (9%) 14 10	39, 87, 172, 199	0
53	BU	117/118 (99%)	-0.02	1 (0%) 81 58	18, 55, 112, 140	0
53	DU	117/118 (99%)	-0.09	1 (0%) 81 58	12, 45, 111, 190	0
54	BV	101/101 (100%)	0.39	3 (2%) 52 31	34, 79, 137, 185	0
54	DV	101/101 (100%)	0.41	9 (8%) 15 11	25, 66, 141, 201	0
55	BW	113/113 (100%)	-0.03	1 (0%) 81 58	25, 57, 114, 201	0
55	DW	113/113 (100%)	-0.18	1 (0%) 81 58	16, 47, 115, 170	0
56	BX	93/96 (96%)	0.39	2 (2%) 62 39	31, 74, 129, 155	0
56	DX	93/96 (96%)	0.06	4 (4%) 40 23	33, 67, 114, 160	0
57	BY	101/110 (91%)	1.19	21 (20%) 2 3	27, 84, 157, 201	0
57	DY	101/110 (91%)	0.87	13 (12%) 7 6	25, 81, 162, 201	0
58	BZ	177/206 (85%)	0.41	13 (7%) 21 15	36, 98, 156, 201	0
58	DZ	177/206 (85%)	0.00	5 (2%) 55 33	30, 83, 130, 192	0
59	DI	146/148 (98%)	0.10	1 (0%) 84 64	28, 109, 155, 183	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	22210/23252 (95%)	0.19	1246 (5%) 30 19	7, 84, 181, 201	0

The worst 5 of 1246 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
49	BQ	140	ALA	12.0
35	DA	654(A)	G	10.9
20	CT	9	ASN	10.0
57	BY	59	GLY	9.7
37	BC	43	VAL	9.5

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
60	MG	DA	3240	1/1	0.33	0.10	55,55,55,55	1
60	MG	CA	1687	1/1	0.51	0.13	58,58,58,58	0
60	MG	CA	1641	1/1	0.53	0.13	55,55,55,55	0
60	MG	DA	3294	1/1	0.58	0.15	49,49,49,49	1
60	MG	BA	3161	1/1	0.59	0.23	47,47,47,47	0
60	MG	CW	101	1/1	0.59	0.12	56,56,56,56	1
60	MG	CA	1652	1/1	0.60	0.37	60,60,60,60	0
60	MG	DA	3219	1/1	0.61	0.25	66,66,66,66	0
60	MG	DA	3327	1/1	0.63	0.33	55,55,55,55	0
60	MG	CA	1719	1/1	0.65	0.09	55,55,55,55	1
60	MG	BA	3105	1/1	0.65	0.39	47,47,47,47	0
60	MG	AA	1688	1/1	0.67	0.35	63,63,63,63	1
60	MG	DA	3193	1/1	0.67	0.14	65,65,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1642	1/1	0.68	0.08	55,55,55,55	0
60	MG	DA	3202	1/1	0.68	0.17	52,52,52,52	1
60	MG	BA	3292	1/1	0.69	0.45	55,55,55,55	0
60	MG	CA	1660	1/1	0.69	0.14	58,58,58,58	0
60	MG	DA	3239	1/1	0.69	0.13	67,67,67,67	1
60	MG	CW	105	1/1	0.70	0.14	53,53,53,53	0
60	MG	AA	1689	1/1	0.70	0.12	59,59,59,59	1
60	MG	DD	301	1/1	0.70	0.48	47,47,47,47	0
60	MG	DA	3265	1/1	0.71	0.40	53,53,53,53	0
60	MG	DA	3106	1/1	0.71	0.38	47,47,47,47	0
60	MG	BA	3102	1/1	0.71	0.57	47,47,47,47	0
60	MG	CA	1679	1/1	0.71	0.12	53,53,53,53	1
60	MG	DA	3295	1/1	0.72	0.56	55,55,55,55	0
60	MG	DA	3181	1/1	0.72	0.25	59,59,59,59	0
60	MG	BA	3153	1/1	0.72	0.39	53,53,53,53	0
60	MG	DA	3252	1/1	0.73	0.14	61,61,61,61	1
60	MG	AA	1698	1/1	0.73	0.09	53,53,53,53	1
60	MG	BA	3082	1/1	0.73	0.29	51,51,51,51	0
60	MG	BA	3024	1/1	0.74	0.41	56,56,56,56	0
60	MG	AA	1720	1/1	0.74	0.09	58,58,58,58	1
60	MG	AA	1739	1/1	0.75	0.10	55,55,55,55	1
60	MG	AA	1628	1/1	0.75	0.23	70,70,70,70	0
60	MG	BA	3307	1/1	0.75	0.28	55,55,55,55	0
60	MG	CA	1605	1/1	0.76	0.40	59,59,59,59	0
60	MG	AA	1716	1/1	0.76	0.22	52,52,52,52	0
60	MG	BA	3248	1/1	0.76	0.10	56,56,56,56	1
60	MG	AA	1718	1/1	0.76	0.14	55,55,55,55	0
60	MG	DA	3099	1/1	0.76	0.27	54,54,54,54	0
60	MG	AA	1648	1/1	0.76	0.14	62,62,62,62	0
60	MG	DA	3225	1/1	0.77	0.26	51,51,51,51	0
60	MG	DA	3098	1/1	0.77	0.28	47,47,47,47	0
60	MG	BA	3106	1/1	0.77	0.38	51,51,51,51	0
60	MG	BA	3120	1/1	0.77	0.41	50,50,50,50	0
60	MG	DA	3107	1/1	0.77	0.47	51,51,51,51	0
60	MG	CA	1729	1/1	0.77	0.15	55,55,55,55	1
60	MG	CA	1670	1/1	0.77	0.20	69,69,69,69	0
60	MG	DA	3300	1/1	0.77	0.10	55,55,55,55	0
60	MG	AA	1668	1/1	0.77	0.23	58,58,58,58	0
60	MG	DA	3009	1/1	0.77	0.30	55,55,55,55	0
60	MG	AA	1655	1/1	0.78	0.22	52,52,52,52	0
60	MG	CW	104	1/1	0.78	0.12	56,56,56,56	0
60	MG	BA	3204	1/1	0.78	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
60	MG	BA	3241	1/1	0.78	0.10	61,61,61,61	1
60	MG	DA	3068	1/1	0.78	0.24	50,50,50,50	0
60	MG	DA	3078	1/1	0.78	0.46	51,51,51,51	0
60	MG	DA	3303	1/1	0.78	0.50	55,55,55,55	0
60	MG	BA	3137	1/1	0.78	0.27	52,52,52,52	0
60	MG	AA	1673	1/1	0.78	0.13	52,52,52,52	0
60	MG	AA	1675	1/1	0.79	0.11	48,48,48,48	0
60	MG	AA	1714	1/1	0.79	0.27	59,59,59,59	0
60	MG	BC	301	1/1	0.79	0.22	52,52,52,52	1
60	MG	CA	1688	1/1	0.79	0.14	48,48,48,48	0
60	MG	CA	1705	1/1	0.79	0.20	49,49,49,49	1
60	MG	BA	3099	1/1	0.79	0.35	55,55,55,55	0
60	MG	BA	3240	1/1	0.79	0.07	58,58,58,58	1
60	MG	CA	1740	1/1	0.79	0.09	55,55,55,55	0
60	MG	CA	1643	1/1	0.79	0.13	49,49,49,49	0
60	MG	AA	1696	1/1	0.79	0.12	62,62,62,62	0
60	MG	BA	3140	1/1	0.79	0.24	56,56,56,56	0
60	MG	DA	3100	1/1	0.80	0.20	55,55,55,55	0
60	MG	AA	1601	1/1	0.80	0.16	56,56,56,56	0
60	MG	BA	3229	1/1	0.80	0.16	49,49,49,49	0
60	MG	DA	3254	1/1	0.80	0.24	54,54,54,54	0
60	MG	DA	3117	1/1	0.80	0.28	47,47,47,47	0
60	MG	DA	3272	1/1	0.80	0.11	59,59,59,59	1
60	MG	BD	301	1/1	0.80	0.53	47,47,47,47	0
60	MG	DA	3073	1/1	0.80	0.29	53,53,53,53	0
60	MG	BA	3264	1/1	0.80	0.33	53,53,53,53	0
60	MG	BA	3186	1/1	0.80	0.33	51,51,51,51	0
60	MG	BA	3301	1/1	0.80	0.15	55,55,55,55	0
60	MG	DA	3229	1/1	0.80	0.18	52,52,52,52	0
60	MG	AA	1694	1/1	0.81	0.12	56,56,56,56	0
60	MG	AA	1666	1/1	0.81	0.11	57,57,57,57	0
60	MG	AA	1686	1/1	0.81	0.17	58,58,58,58	1
60	MG	AA	1637	1/1	0.81	0.14	53,53,53,53	0
60	MG	DA	3134	1/1	0.81	0.18	64,64,64,64	0
60	MG	DA	3177	1/1	0.81	0.14	49,49,49,49	0
60	MG	BA	3108	1/1	0.81	0.44	52,52,52,52	0
60	MG	CA	1613	1/1	0.81	0.16	52,52,52,52	0
60	MG	CA	1698	1/1	0.81	0.08	52,52,52,52	0
60	MG	BA	3265	1/1	0.81	0.33	47,47,47,47	0
60	MG	CA	1642	1/1	0.81	0.20	56,56,56,56	0
60	MG	DA	3337	1/1	0.81	0.10	55,55,55,55	0
60	MG	AA	1616	1/1	0.81	0.13	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AL	201	1/1	0.82	0.35	51,51,51,51	1
60	MG	AA	1693	1/1	0.82	0.14	61,61,61,61	0
60	MG	CA	1744	1/1	0.82	0.20	55,55,55,55	0
60	MG	CA	1756	1/1	0.82	0.19	55,55,55,55	1
60	MG	DA	3260	1/1	0.82	0.25	59,59,59,59	0
60	MG	AA	1647	1/1	0.82	0.09	62,62,62,62	0
60	MG	CA	1684	1/1	0.82	0.23	49,49,49,49	0
60	MG	BA	3183	1/1	0.82	0.32	56,56,56,56	0
60	MG	AA	1653	1/1	0.82	0.25	60,60,60,60	0
60	MG	BA	3188	1/1	0.82	0.35	57,57,57,57	0
60	MG	BA	3135	1/1	0.82	0.21	58,58,58,58	0
60	MG	CA	1712	1/1	0.82	0.21	47,47,47,47	0
60	MG	DA	3082	1/1	0.82	0.39	47,47,47,47	0
60	MG	AA	1743	1/1	0.82	0.24	55,55,55,55	0
60	MG	AA	1608	1/1	0.83	0.25	47,47,47,47	0
60	MG	BA	3237	1/1	0.83	0.17	67,67,67,67	0
60	MG	DA	3136	1/1	0.83	0.34	58,58,58,58	0
60	MG	AA	1692	1/1	0.83	0.31	59,59,59,59	0
60	MG	AA	1747	1/1	0.83	0.14	55,55,55,55	1
60	MG	CA	1753	1/1	0.83	0.21	55,55,55,55	1
60	MG	AA	1645	1/1	0.83	0.11	57,57,57,57	0
60	MG	BA	3253	1/1	0.83	0.32	54,54,54,54	0
60	MG	CW	103	1/1	0.83	0.06	54,54,54,54	1
60	MG	BA	3256	1/1	0.83	0.37	55,55,55,55	0
60	MG	AA	1704	1/1	0.83	0.26	49,49,49,49	1
60	MG	BA	3116	1/1	0.83	0.31	47,47,47,47	0
60	MG	BA	3052	1/1	0.83	0.34	47,47,47,47	0
60	MG	AA	1732	1/1	0.83	0.24	55,55,55,55	0
60	MG	BA	3214	1/1	0.83	0.19	48,48,48,48	0
60	MG	BA	3318	1/1	0.83	0.10	55,55,55,55	0
60	MG	DA	3266	1/1	0.83	0.42	47,47,47,47	0
60	MG	DA	3087	1/1	0.83	0.36	48,48,48,48	0
60	MG	DA	3088	1/1	0.83	0.26	49,49,49,49	0
60	MG	BA	3329	1/1	0.83	0.10	55,55,55,55	1
60	MG	BA	3336	1/1	0.83	0.34	55,55,55,55	0
60	MG	BA	3351	1/1	0.83	0.36	55,55,55,55	0
60	MG	DA	3309	1/1	0.83	0.09	55,55,55,55	1
60	MG	DA	3101	1/1	0.83	0.31	51,51,51,51	0
60	MG	DA	3334	1/1	0.83	0.18	55,55,55,55	0
60	MG	CA	1710	1/1	0.83	0.21	50,50,50,50	0
60	MG	BB	203	1/1	0.83	0.41	55,55,55,55	0
60	MG	BA	3206	1/1	0.84	0.23	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3205	1/1	0.84	0.42	57,57,57,57	0
60	MG	DA	3206	1/1	0.84	0.20	50,50,50,50	0
60	MG	DA	3211	1/1	0.84	0.36	57,57,57,57	0
60	MG	DA	3025	1/1	0.84	0.43	56,56,56,56	0
60	MG	BA	3212	1/1	0.84	0.12	55,55,55,55	0
60	MG	DA	3228	1/1	0.84	0.20	55,55,55,55	0
60	MG	AA	1722	1/1	0.84	0.26	55,55,55,55	0
60	MG	DA	3238	1/1	0.84	0.35	47,47,47,47	0
60	MG	BA	3040	1/1	0.84	0.26	47,47,47,47	0
60	MG	BA	3338	1/1	0.84	0.28	55,55,55,55	0
60	MG	BA	3235	1/1	0.84	0.17	60,60,60,60	0
60	MG	AA	1621	1/1	0.84	0.15	56,56,56,56	0
60	MG	BA	3068	1/1	0.84	0.40	47,47,47,47	0
60	MG	AA	1659	1/1	0.84	0.25	57,57,57,57	0
60	MG	BA	3143	1/1	0.84	0.13	57,57,57,57	0
60	MG	CA	1607	1/1	0.84	0.31	47,47,47,47	0
60	MG	DA	3284	1/1	0.84	0.46	57,57,57,57	0
60	MG	BA	3094	1/1	0.84	0.28	47,47,47,47	0
60	MG	CA	1615	1/1	0.84	0.21	64,64,64,64	0
60	MG	AA	1613	1/1	0.84	0.10	56,56,56,56	0
60	MG	AA	1746	1/1	0.84	0.12	55,55,55,55	1
60	MG	AA	1677	1/1	0.84	0.08	55,55,55,55	1
60	MG	DA	3313	1/1	0.84	0.30	55,55,55,55	0
60	MG	AA	1703	1/1	0.84	0.18	62,62,62,62	0
60	MG	AV	107	1/1	0.84	0.22	54,54,54,54	1
60	MG	DA	3183	1/1	0.84	0.12	53,53,53,53	0
60	MG	DC	301	1/1	0.84	0.09	52,52,52,52	1
60	MG	CA	1668	1/1	0.84	0.35	58,58,58,58	0
60	MG	BA	3187	1/1	0.85	0.22	48,48,48,48	0
60	MG	BA	3148	1/1	0.85	0.20	47,47,47,47	0
60	MG	AA	1697	1/1	0.85	0.10	52,52,52,52	0
60	MG	AW	101	1/1	0.85	0.18	56,56,56,56	1
60	MG	CA	1716	1/1	0.85	0.07	55,55,55,55	0
60	MG	BA	3209	1/1	0.85	0.30	66,66,66,66	0
60	MG	DA	3095	1/1	0.85	0.40	47,47,47,47	0
60	MG	BA	3341	1/1	0.85	0.23	55,55,55,55	0
60	MG	BA	3342	1/1	0.85	0.25	55,55,55,55	0
60	MG	BA	3175	1/1	0.85	0.28	49,49,49,49	1
60	MG	CA	1669	1/1	0.85	0.27	47,47,47,47	0
60	MG	DA	3103	1/1	0.85	0.38	47,47,47,47	0
60	MG	BA	3179	1/1	0.85	0.20	59,59,59,59	0
60	MG	CV	102	1/1	0.85	0.45	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CV	106	1/1	0.85	0.07	57,57,57,57	1
60	MG	DA	3133	1/1	0.85	0.08	57,57,57,57	0
60	MG	CA	1675	1/1	0.85	0.11	48,48,48,48	1
60	MG	B5	101	1/1	0.85	0.25	49,49,49,49	0
60	MG	DA	3159	1/1	0.85	0.59	49,49,49,49	0
60	MG	DA	3172	1/1	0.85	0.27	50,50,50,50	0
60	MG	AM	201	1/1	0.85	0.09	47,47,47,47	0
60	MG	BA	3295	1/1	0.85	0.17	49,49,49,49	0
60	MG	BA	3236	1/1	0.85	0.23	47,47,47,47	0
60	MG	DA	3328	1/1	0.85	0.34	55,55,55,55	1
60	MG	CA	1690	1/1	0.85	0.09	59,59,59,59	0
60	MG	DA	3201	1/1	0.85	0.26	60,60,60,60	0
60	MG	DA	3033	1/1	0.85	0.22	53,53,53,53	0
60	MG	DA	3060	1/1	0.85	0.34	48,48,48,48	0
60	MG	DY	201	1/1	0.85	0.28	55,55,55,55	0
60	MG	CA	1661	1/1	0.86	0.29	52,52,52,52	0
60	MG	DA	3176	1/1	0.86	0.10	58,58,58,58	0
60	MG	AA	1618	1/1	0.86	0.08	51,51,51,51	1
60	MG	DA	3178	1/1	0.86	0.43	48,48,48,48	0
60	MG	BA	3100	1/1	0.86	0.37	51,51,51,51	0
60	MG	BA	3339	1/1	0.86	0.12	55,55,55,55	0
60	MG	CA	1674	1/1	0.86	0.22	50,50,50,50	0
60	MG	BA	3026	1/1	0.86	0.30	47,47,47,47	0
60	MG	AA	1643	1/1	0.86	0.11	56,56,56,56	0
60	MG	BA	3346	1/1	0.86	0.48	55,55,55,55	0
60	MG	BA	3047	1/1	0.86	0.31	47,47,47,47	0
60	MG	DA	3036	1/1	0.86	0.27	55,55,55,55	0
60	MG	DA	3215	1/1	0.86	0.19	48,48,48,48	0
60	MG	DA	3040	1/1	0.86	0.14	68,68,68,68	0
60	MG	DA	3043	1/1	0.86	0.58	47,47,47,47	0
60	MG	DA	3045	1/1	0.86	0.22	56,56,56,56	0
60	MG	AA	1611	1/1	0.86	0.19	48,48,48,48	0
60	MG	DA	3231	1/1	0.86	0.09	54,54,54,54	1
60	MG	AA	1735	1/1	0.86	0.23	55,55,55,55	0
60	MG	CA	1695	1/1	0.86	0.06	56,56,56,56	0
60	MG	AA	1755	1/1	0.86	0.06	55,55,55,55	0
60	MG	DA	3247	1/1	0.86	0.16	55,55,55,55	1
60	MG	BA	3234	1/1	0.86	0.33	52,52,52,52	0
60	MG	DA	3083	1/1	0.86	0.14	51,51,51,51	0
60	MG	BA	3181	1/1	0.86	0.07	53,53,53,53	0
60	MG	CA	1612	1/1	0.86	0.19	56,56,56,56	0
60	MG	DA	3090	1/1	0.86	0.38	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1715	1/1	0.86	0.22	59,59,59,59	0
60	MG	BA	3304	1/1	0.86	0.51	55,55,55,55	0
60	MG	BA	3018	1/1	0.86	0.30	54,54,54,54	0
60	MG	CA	1720	1/1	0.86	0.09	56,56,56,56	0
60	MG	DA	3299	1/1	0.86	0.26	55,55,55,55	0
60	MG	CA	1721	1/1	0.86	0.06	58,58,58,58	0
60	MG	BA	3314	1/1	0.86	0.10	55,55,55,55	0
60	MG	CA	1733	1/1	0.86	0.18	55,55,55,55	0
60	MG	BA	3136	1/1	0.86	0.39	50,50,50,50	0
60	MG	DA	3316	1/1	0.86	0.16	55,55,55,55	0
60	MG	DA	3324	1/1	0.86	0.25	55,55,55,55	0
60	MG	CA	1741	1/1	0.86	0.15	55,55,55,55	0
60	MG	BA	3319	1/1	0.86	0.08	55,55,55,55	0
60	MG	CA	1752	1/1	0.86	0.25	55,55,55,55	1
60	MG	DA	3335	1/1	0.86	0.29	55,55,55,55	0
60	MG	BA	3238	1/1	0.86	0.10	55,55,55,55	1
60	MG	DA	3143	1/1	0.86	0.19	47,47,47,47	1
60	MG	BA	3331	1/1	0.86	0.15	55,55,55,55	0
60	MG	DA	3164	1/1	0.86	0.37	53,53,53,53	0
60	MG	AA	1736	1/1	0.87	0.11	55,55,55,55	0
60	MG	DA	3001	1/1	0.87	0.18	57,57,57,57	0
60	MG	DA	3180	1/1	0.87	0.15	52,52,52,52	0
60	MG	BA	3320	1/1	0.87	0.21	55,55,55,55	0
60	MG	BA	3083	1/1	0.87	0.36	47,47,47,47	0
60	MG	DA	3185	1/1	0.87	0.37	56,56,56,56	0
60	MG	DA	3191	1/1	0.87	0.19	54,54,54,54	0
60	MG	BA	3087	1/1	0.87	0.27	49,49,49,49	0
60	MG	DA	3034	1/1	0.87	0.66	47,47,47,47	0
60	MG	BA	3332	1/1	0.87	0.05	55,55,55,55	0
60	MG	AA	1635	1/1	0.87	0.08	47,47,47,47	0
60	MG	DA	3042	1/1	0.87	0.51	47,47,47,47	0
60	MG	BA	3337	1/1	0.87	0.12	55,55,55,55	0
60	MG	BA	3016	1/1	0.87	0.47	47,47,47,47	0
60	MG	DA	3048	1/1	0.87	0.26	47,47,47,47	0
60	MG	DA	3052	1/1	0.87	0.32	51,51,51,51	0
60	MG	DA	3059	1/1	0.87	0.52	55,55,55,55	0
60	MG	BA	3173	1/1	0.87	0.31	56,56,56,56	0
60	MG	CA	1693	1/1	0.87	0.42	59,59,59,59	0
60	MG	AA	1699	1/1	0.87	0.12	54,54,54,54	1
60	MG	AA	1667	1/1	0.87	0.10	47,47,47,47	0
60	MG	AA	1679	1/1	0.87	0.08	53,53,53,53	0
60	MG	DA	3245	1/1	0.87	0.43	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3251	1/1	0.87	0.09	61,61,61,61	0
60	MG	DA	3084	1/1	0.87	0.30	47,47,47,47	0
60	MG	DA	3085	1/1	0.87	0.35	47,47,47,47	0
60	MG	BA	3029	1/1	0.87	0.25	55,55,55,55	0
60	MG	BA	3034	1/1	0.87	0.21	50,50,50,50	0
60	MG	AA	1724	1/1	0.87	0.37	59,59,59,59	0
60	MG	AA	1683	1/1	0.87	0.14	47,47,47,47	0
60	MG	DA	3274	1/1	0.87	0.15	63,63,63,63	0
60	MG	DA	3276	1/1	0.87	0.45	58,58,58,58	0
60	MG	CA	1606	1/1	0.87	0.19	58,58,58,58	0
60	MG	DA	3292	1/1	0.87	0.40	55,55,55,55	0
60	MG	BA	3273	1/1	0.87	0.18	58,58,58,58	0
60	MG	CA	1725	1/1	0.87	0.36	59,59,59,59	0
60	MG	BA	3280	1/1	0.87	0.23	57,57,57,57	0
60	MG	BA	3289	1/1	0.87	0.27	54,54,54,54	0
60	MG	BA	3189	1/1	0.87	0.13	59,59,59,59	0
60	MG	BA	3200	1/1	0.87	0.17	60,60,60,60	0
60	MG	BA	3300	1/1	0.87	0.19	55,55,55,55	0
60	MG	BA	3133	1/1	0.87	0.14	64,64,64,64	0
60	MG	DA	3321	1/1	0.87	0.22	55,55,55,55	0
60	MG	CA	1651	1/1	0.87	0.27	47,47,47,47	0
60	MG	BA	3048	1/1	0.87	0.48	47,47,47,47	0
60	MG	CA	1655	1/1	0.87	0.31	52,52,52,52	0
60	MG	DA	3154	1/1	0.87	0.29	53,53,53,53	0
60	MG	DA	3156	1/1	0.87	0.28	51,51,51,51	0
60	MG	DA	3336	1/1	0.87	0.22	55,55,55,55	1
60	MG	CA	1659	1/1	0.87	0.15	57,57,57,57	0
60	MG	DA	3348	1/1	0.87	0.32	55,55,55,55	0
60	MG	AA	1733	1/1	0.87	0.22	55,55,55,55	0
60	MG	AA	1715	1/1	0.87	0.11	55,55,55,55	0
60	MG	BA	3138	1/1	0.87	0.12	50,50,50,50	0
60	MG	AA	1713	1/1	0.88	0.06	64,64,64,64	0
60	MG	BA	3170	1/1	0.88	0.29	50,50,50,50	0
60	MG	BA	3328	1/1	0.88	0.27	55,55,55,55	0
60	MG	DA	3005	1/1	0.88	0.27	53,53,53,53	0
60	MG	AA	1700	1/1	0.88	0.10	51,51,51,51	0
60	MG	DA	3017	1/1	0.88	0.43	47,47,47,47	0
60	MG	BA	3103	1/1	0.88	0.37	50,50,50,50	0
60	MG	DA	3026	1/1	0.88	0.30	55,55,55,55	0
60	MG	DA	3188	1/1	0.88	0.21	48,48,48,48	0
60	MG	DA	3027	1/1	0.88	0.41	47,47,47,47	0
60	MG	DA	3028	1/1	0.88	0.26	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3196	1/1	0.88	0.32	52,52,52,52	0
60	MG	BA	3041	1/1	0.88	0.33	47,47,47,47	0
60	MG	BA	3046	1/1	0.88	0.38	47,47,47,47	0
60	MG	CA	1676	1/1	0.88	0.21	58,58,58,58	0
60	MG	BA	3246	1/1	0.88	0.12	55,55,55,55	0
60	MG	AA	1687	1/1	0.88	0.17	48,48,48,48	0
60	MG	BA	3112	1/1	0.88	0.35	48,48,48,48	0
60	MG	DA	3217	1/1	0.88	0.08	49,49,49,49	0
60	MG	AA	1695	1/1	0.88	0.11	62,62,62,62	0
60	MG	AV	101	1/1	0.88	0.21	49,49,49,49	0
60	MG	BA	3057	1/1	0.88	0.34	47,47,47,47	0
60	MG	DA	3053	1/1	0.88	0.33	47,47,47,47	0
60	MG	BA	3349	1/1	0.88	0.21	55,55,55,55	0
60	MG	DA	3234	1/1	0.88	0.41	47,47,47,47	0
60	MG	BA	3025	1/1	0.88	0.34	55,55,55,55	0
60	MG	BA	3203	1/1	0.88	0.29	52,52,52,52	0
60	MG	BA	3278	1/1	0.88	0.21	51,51,51,51	0
60	MG	DA	3244	1/1	0.88	0.24	47,47,47,47	0
60	MG	DA	3075	1/1	0.88	0.29	47,47,47,47	0
60	MG	BA	3072	1/1	0.88	0.28	53,53,53,53	0
60	MG	BD	302	1/1	0.88	0.39	47,47,47,47	0
60	MG	CA	1601	1/1	0.88	0.25	56,56,56,56	0
60	MG	DA	3259	1/1	0.88	0.28	58,58,58,58	0
60	MG	CA	1718	1/1	0.88	0.14	66,66,66,66	0
60	MG	BA	3079	1/1	0.88	0.35	49,49,49,49	0
60	MG	BA	3291	1/1	0.88	0.23	54,54,54,54	0
60	MG	DA	3268	1/1	0.88	0.42	59,59,59,59	0
60	MG	AV	102	1/1	0.88	0.36	54,54,54,54	0
60	MG	CA	1610	1/1	0.88	0.27	48,48,48,48	0
60	MG	DA	3093	1/1	0.88	0.43	50,50,50,50	0
60	MG	DA	3278	1/1	0.88	0.32	51,51,51,51	0
60	MG	DA	3283	1/1	0.88	0.21	65,65,65,65	0
60	MG	BA	3027	1/1	0.88	0.20	50,50,50,50	0
60	MG	BA	3299	1/1	0.88	0.23	55,55,55,55	0
60	MG	CA	1738	1/1	0.88	0.27	55,55,55,55	0
60	MG	AA	1708	1/1	0.88	0.17	65,65,65,65	0
60	MG	CA	1617	1/1	0.88	0.09	51,51,51,51	0
60	MG	DA	3102	1/1	0.88	0.38	47,47,47,47	0
60	MG	CA	1618	1/1	0.88	0.23	49,49,49,49	0
60	MG	DA	3304	1/1	0.88	0.37	55,55,55,55	0
60	MG	CA	1747	1/1	0.88	0.21	55,55,55,55	1
60	MG	BA	3215	1/1	0.88	0.44	60,60,60,60	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3216	1/1	0.88	0.09	49,49,49,49	0
60	MG	DA	3126	1/1	0.88	0.51	47,47,47,47	0
60	MG	BA	3227	1/1	0.88	0.24	55,55,55,55	0
60	MG	CN	101	1/1	0.88	0.19	55,55,55,55	0
60	MG	CV	101	1/1	0.88	0.37	49,49,49,49	0
60	MG	DA	3137	1/1	0.88	0.44	50,50,50,50	0
60	MG	DA	3139	1/1	0.88	0.24	50,50,50,50	0
60	MG	DA	3142	1/1	0.88	0.32	49,49,49,49	0
60	MG	BA	3309	1/1	0.88	0.16	55,55,55,55	0
60	MG	DA	3339	1/1	0.88	0.13	55,55,55,55	0
60	MG	CV	103	1/1	0.88	0.14	54,54,54,54	0
60	MG	DA	3349	1/1	0.88	0.28	55,55,55,55	0
60	MG	DA	3353	1/1	0.88	0.23	55,55,55,55	0
60	MG	BA	3031	1/1	0.88	0.25	50,50,50,50	0
60	MG	BA	3315	1/1	0.88	0.18	55,55,55,55	1
60	MG	BA	3033	1/1	0.88	0.62	47,47,47,47	0
60	MG	AA	1639	1/1	0.89	0.09	53,53,53,53	0
60	MG	B7	101	1/1	0.89	0.26	49,49,49,49	0
60	MG	BA	3064	1/1	0.89	0.42	53,53,53,53	0
60	MG	CA	1730	1/1	0.89	0.06	55,55,55,55	0
60	MG	BA	3303	1/1	0.89	0.21	55,55,55,55	0
60	MG	BA	3013	1/1	0.89	0.33	47,47,47,47	0
60	MG	CA	1626	1/1	0.89	0.12	53,53,53,53	0
60	MG	CA	1627	1/1	0.89	0.17	70,70,70,70	0
60	MG	CA	1635	1/1	0.89	0.35	49,49,49,49	0
60	MG	CA	1639	1/1	0.89	0.22	48,48,48,48	0
60	MG	BA	3220	1/1	0.89	0.26	54,54,54,54	0
60	MG	AA	1644	1/1	0.89	0.18	49,49,49,49	0
60	MG	AA	1745	1/1	0.89	0.46	55,55,55,55	0
60	MG	AA	1705	1/1	0.89	0.20	51,51,51,51	0
60	MG	AA	1640	1/1	0.89	0.31	48,48,48,48	0
60	MG	AA	1748	1/1	0.89	0.17	55,55,55,55	0
60	MG	DA	3257	1/1	0.89	0.33	55,55,55,55	0
60	MG	BA	3168	1/1	0.89	0.33	47,47,47,47	0
60	MG	AA	1709	1/1	0.89	0.32	50,50,50,50	0
60	MG	DA	3261	1/1	0.89	0.25	57,57,57,57	0
60	MG	BA	3239	1/1	0.89	0.09	55,55,55,55	0
60	MG	DA	3116	1/1	0.89	0.26	50,50,50,50	0
60	MG	AA	1757	1/1	0.89	0.20	55,55,55,55	0
60	MG	AA	1727	1/1	0.89	0.23	55,55,55,55	0
60	MG	BA	3242	1/1	0.89	0.20	47,47,47,47	0
60	MG	CY	401	1/1	0.89	0.35	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3101	1/1	0.89	0.40	47,47,47,47	0
60	MG	DA	3282	1/1	0.89	0.24	57,57,57,57	0
60	MG	AA	1729	1/1	0.89	0.17	55,55,55,55	0
60	MG	AA	1711	1/1	0.89	0.17	47,47,47,47	0
60	MG	BA	3185	1/1	0.89	0.43	50,50,50,50	0
60	MG	DA	3018	1/1	0.89	0.36	52,52,52,52	0
60	MG	DA	3144	1/1	0.89	0.24	57,57,57,57	0
60	MG	BA	3036	1/1	0.89	0.21	53,53,53,53	0
60	MG	BA	3263	1/1	0.89	0.14	56,56,56,56	0
60	MG	AA	1670	1/1	0.89	0.16	69,69,69,69	0
60	MG	AV	104	1/1	0.89	0.06	54,54,54,54	0
60	MG	DA	3032	1/1	0.89	0.26	50,50,50,50	0
60	MG	CA	1692	1/1	0.89	0.32	59,59,59,59	0
60	MG	BA	3266	1/1	0.89	0.27	59,59,59,59	0
60	MG	CA	1694	1/1	0.89	0.08	61,61,61,61	0
60	MG	BB	204	1/1	0.89	0.09	55,55,55,55	0
60	MG	CA	1697	1/1	0.89	0.07	62,62,62,62	0
60	MG	DA	3182	1/1	0.89	0.11	56,56,56,56	0
60	MG	DA	3329	1/1	0.89	0.20	55,55,55,55	0
60	MG	BA	3043	1/1	0.89	0.54	47,47,47,47	0
60	MG	AA	1684	1/1	0.89	0.14	49,49,49,49	0
60	MG	BA	3118	1/1	0.89	0.30	49,49,49,49	0
60	MG	DA	3050	1/1	0.89	0.42	47,47,47,47	0
60	MG	BA	3287	1/1	0.89	0.14	51,51,51,51	0
60	MG	AA	1622	1/1	0.89	0.16	48,48,48,48	0
60	MG	BA	3132	1/1	0.89	0.07	57,57,57,57	0
60	MG	BA	3208	1/1	0.89	0.24	51,51,51,51	0
60	MG	DB	201	1/1	0.89	0.20	67,67,67,67	0
60	MG	DA	3065	1/1	0.89	0.45	53,53,53,53	0
60	MG	CA	1608	1/1	0.89	0.22	52,52,52,52	0
60	MG	AW	105	1/1	0.89	0.06	53,53,53,53	0
60	MG	DA	3076	1/1	0.90	0.22	47,47,47,47	0
60	MG	CA	1628	1/1	0.90	0.17	56,56,56,56	0
60	MG	BA	3207	1/1	0.90	0.22	60,60,60,60	0
60	MG	CA	1638	1/1	0.90	0.33	53,53,53,53	0
60	MG	BA	3325	1/1	0.90	0.22	55,55,55,55	0
60	MG	BA	3158	1/1	0.90	0.58	49,49,49,49	0
60	MG	BA	3113	1/1	0.90	0.45	47,47,47,47	0
60	MG	DA	3237	1/1	0.90	0.22	60,60,60,60	0
60	MG	AA	1656	1/1	0.90	0.17	47,47,47,47	0
60	MG	CA	1647	1/1	0.90	0.06	62,62,62,62	0
60	MG	DA	3092	1/1	0.90	0.12	51,51,51,51	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1658	1/1	0.90	0.06	49,49,49,49	0
60	MG	BA	3335	1/1	0.90	0.29	55,55,55,55	0
60	MG	AA	1636	1/1	0.90	0.20	49,49,49,49	0
60	MG	AA	1652	1/1	0.90	0.23	47,47,47,47	0
60	MG	BA	3219	1/1	0.90	0.23	49,49,49,49	0
60	MG	DA	3256	1/1	0.90	0.29	55,55,55,55	0
60	MG	BA	3276	1/1	0.90	0.31	58,58,58,58	0
60	MG	CV	105	1/1	0.90	0.10	50,50,50,50	0
60	MG	CA	1665	1/1	0.90	0.24	50,50,50,50	0
60	MG	BA	3277	1/1	0.90	0.51	57,57,57,57	0
60	MG	BA	3176	1/1	0.90	0.39	48,48,48,48	0
60	MG	BA	3279	1/1	0.90	0.10	55,55,55,55	0
60	MG	CA	1672	1/1	0.90	0.27	53,53,53,53	0
60	MG	DA	3269	1/1	0.90	0.43	52,52,52,52	0
60	MG	BA	3224	1/1	0.90	0.21	51,51,51,51	0
60	MG	BA	3283	1/1	0.90	0.31	65,65,65,65	0
60	MG	DA	3275	1/1	0.90	0.30	59,59,59,59	0
60	MG	AA	1753	1/1	0.90	0.15	55,55,55,55	1
60	MG	DA	3277	1/1	0.90	0.53	57,57,57,57	0
60	MG	AA	1754	1/1	0.90	0.09	55,55,55,55	0
60	MG	DA	3013	1/1	0.90	0.45	49,49,49,49	0
60	MG	DA	3138	1/1	0.90	0.22	52,52,52,52	0
60	MG	BA	3290	1/1	0.90	0.34	57,57,57,57	0
60	MG	DA	3289	1/1	0.90	0.35	54,54,54,54	0
60	MG	BA	3231	1/1	0.90	0.28	51,51,51,51	0
60	MG	DA	3019	1/1	0.90	0.28	54,54,54,54	0
60	MG	BA	3233	1/1	0.90	0.45	47,47,47,47	0
60	MG	BF	301	1/1	0.90	0.35	47,47,47,47	0
60	MG	BS	201	1/1	0.90	0.20	55,55,55,55	0
60	MG	BA	3055	1/1	0.90	0.32	47,47,47,47	0
60	MG	DA	3030	1/1	0.90	0.24	55,55,55,55	0
60	MG	DA	3171	1/1	0.90	0.44	51,51,51,51	0
60	MG	CA	1602	1/1	0.90	0.19	52,52,52,52	0
60	MG	CA	1604	1/1	0.90	0.22	50,50,50,50	0
60	MG	AA	1719	1/1	0.90	0.17	56,56,56,56	0
60	MG	AA	1620	1/1	0.90	0.26	55,55,55,55	0
60	MG	DA	3325	1/1	0.90	0.26	55,55,55,55	0
60	MG	DA	3326	1/1	0.90	0.25	55,55,55,55	0
60	MG	CA	1699	1/1	0.90	0.10	53,53,53,53	1
60	MG	CA	1702	1/1	0.90	0.19	51,51,51,51	0
60	MG	BA	3012	1/1	0.90	0.41	49,49,49,49	0
60	MG	BA	3141	1/1	0.90	0.27	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3070	1/1	0.90	0.37	50,50,50,50	0
60	MG	CA	1713	1/1	0.90	0.09	54,54,54,54	0
60	MG	BA	3305	1/1	0.90	0.35	55,55,55,55	0
60	MG	BA	3192	1/1	0.90	0.13	65,65,65,65	0
60	MG	DA	3058	1/1	0.90	0.41	47,47,47,47	0
60	MG	BA	3144	1/1	0.90	0.34	49,49,49,49	0
60	MG	DA	3351	1/1	0.90	0.19	55,55,55,55	0
60	MG	AA	1681	1/1	0.90	0.15	66,66,66,66	0
60	MG	BA	3149	1/1	0.90	0.32	54,54,54,54	0
60	MG	DB	202	1/1	0.90	0.32	55,55,55,55	0
60	MG	DB	203	1/1	0.90	0.38	55,55,55,55	0
60	MG	CA	1621	1/1	0.90	0.09	48,48,48,48	0
60	MG	AA	1627	1/1	0.90	0.10	53,53,53,53	0
60	MG	BA	3250	1/1	0.90	0.22	52,52,52,52	0
60	MG	CA	1749	1/1	0.91	0.07	55,55,55,55	0
60	MG	DA	3079	1/1	0.91	0.30	56,56,56,56	0
60	MG	CA	1751	1/1	0.91	0.06	55,55,55,55	0
60	MG	CA	1663	1/1	0.91	0.23	51,51,51,51	0
60	MG	B7	102	1/1	0.91	0.14	54,54,54,54	0
60	MG	BA	3311	1/1	0.91	0.18	55,55,55,55	0
60	MG	BA	3092	1/1	0.91	0.38	50,50,50,50	0
60	MG	BA	3093	1/1	0.91	0.29	51,51,51,51	0
60	MG	BA	3134	1/1	0.91	0.09	54,54,54,54	0
60	MG	DA	3091	1/1	0.91	0.28	48,48,48,48	0
60	MG	BA	3178	1/1	0.91	0.12	52,52,52,52	0
60	MG	BA	3002	1/1	0.91	0.17	67,67,67,67	0
60	MG	DA	3094	1/1	0.91	0.29	51,51,51,51	0
60	MG	DA	3248	1/1	0.91	0.11	59,59,59,59	1
60	MG	DA	3250	1/1	0.91	0.20	56,56,56,56	0
60	MG	DA	3251	1/1	0.91	0.14	52,52,52,52	0
60	MG	BA	3324	1/1	0.91	0.11	55,55,55,55	0
60	MG	BA	3032	1/1	0.91	0.15	53,53,53,53	0
60	MG	CA	1681	1/1	0.91	0.13	66,66,66,66	0
60	MG	CA	1611	1/1	0.91	0.14	52,52,52,52	0
60	MG	BA	3326	1/1	0.91	0.33	55,55,55,55	0
60	MG	AA	1669	1/1	0.91	0.21	47,47,47,47	0
60	MG	D1	101	1/1	0.91	0.37	55,55,55,55	0
60	MG	DA	3104	1/1	0.91	0.24	50,50,50,50	0
60	MG	BA	3059	1/1	0.91	0.28	48,48,48,48	0
60	MG	CA	1616	1/1	0.91	0.20	54,54,54,54	0
60	MG	DA	3006	1/1	0.91	0.62	47,47,47,47	0
60	MG	BA	3060	1/1	0.91	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
60	MG	AA	1651	1/1	0.91	0.41	54,54,54,54	0
60	MG	DA	3128	1/1	0.91	0.23	56,56,56,56	0
60	MG	DA	3130	1/1	0.91	0.33	56,56,56,56	0
60	MG	DA	3015	1/1	0.91	0.38	53,53,53,53	0
60	MG	CA	1619	1/1	0.91	0.27	55,55,55,55	0
60	MG	BA	3285	1/1	0.91	0.19	55,55,55,55	0
60	MG	CA	1622	1/1	0.91	0.46	57,57,57,57	0
60	MG	DA	3020	1/1	0.91	0.30	47,47,47,47	0
60	MG	DA	3285	1/1	0.91	0.27	55,55,55,55	0
60	MG	DA	3021	1/1	0.91	0.43	47,47,47,47	0
60	MG	CA	1625	1/1	0.91	0.23	53,53,53,53	0
60	MG	AA	1646	1/1	0.91	0.18	50,50,50,50	0
60	MG	BA	3069	1/1	0.91	0.31	48,48,48,48	0
60	MG	DA	3298	1/1	0.91	0.25	55,55,55,55	0
60	MG	BA	3145	1/1	0.91	0.26	47,47,47,47	0
60	MG	CA	1630	1/1	0.91	0.23	47,47,47,47	0
60	MG	BA	3195	1/1	0.91	0.34	52,52,52,52	0
60	MG	BA	3147	1/1	0.91	0.30	51,51,51,51	0
60	MG	BA	3294	1/1	0.91	0.12	52,52,52,52	0
60	MG	AA	1607	1/1	0.91	0.29	58,58,58,58	0
60	MG	DA	3038	1/1	0.91	0.39	47,47,47,47	0
60	MG	DA	3319	1/1	0.91	0.12	55,55,55,55	0
60	MG	BA	3296	1/1	0.91	0.37	55,55,55,55	0
60	MG	AA	1641	1/1	0.91	0.20	47,47,47,47	0
60	MG	BB	202	1/1	0.91	0.34	55,55,55,55	0
60	MG	CA	1723	1/1	0.91	0.05	55,55,55,55	0
60	MG	DA	3047	1/1	0.91	0.37	47,47,47,47	0
60	MG	CA	1724	1/1	0.91	0.11	57,57,57,57	1
60	MG	CA	1648	1/1	0.91	0.11	53,53,53,53	1
60	MG	CA	1649	1/1	0.91	0.29	47,47,47,47	0
60	MG	DA	3190	1/1	0.91	0.20	59,59,59,59	0
60	MG	BA	3151	1/1	0.91	0.15	47,47,47,47	0
60	MG	BA	3152	1/1	0.91	0.16	50,50,50,50	0
60	MG	DA	3195	1/1	0.91	0.23	53,53,53,53	0
60	MG	DA	3340	1/1	0.91	0.24	55,55,55,55	0
60	MG	CA	1736	1/1	0.91	0.21	55,55,55,55	0
60	MG	DA	3198	1/1	0.91	0.44	58,58,58,58	0
60	MG	AY	401	1/1	0.91	0.39	55,55,55,55	0
60	MG	DA	3064	1/1	0.91	0.34	56,56,56,56	0
60	MG	CA	1658	1/1	0.91	0.07	49,49,49,49	0
60	MG	BA	3114	1/1	0.91	0.20	48,48,48,48	0
60	MG	DA	3207	1/1	0.91	0.27	47,47,47,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1734	1/1	0.91	0.08	55,55,55,55	0
60	MG	AA	1650	1/1	0.91	0.34	47,47,47,47	0
60	MG	CA	1748	1/1	0.91	0.27	55,55,55,55	1
60	MG	DA	3213	1/1	0.92	0.14	55,55,55,55	0
60	MG	DA	3081	1/1	0.92	0.31	52,52,52,52	0
60	MG	DA	3216	1/1	0.92	0.36	60,60,60,60	0
60	MG	AA	1701	1/1	0.92	0.12	51,51,51,51	0
60	MG	CA	1683	1/1	0.92	0.15	47,47,47,47	0
60	MG	DA	3223	1/1	0.92	0.18	49,49,49,49	0
60	MG	DA	3224	1/1	0.92	0.14	52,52,52,52	0
60	MG	CV	107	1/1	0.92	0.19	54,54,54,54	0
60	MG	BA	3316	1/1	0.92	0.17	55,55,55,55	0
60	MG	AA	1624	1/1	0.92	0.08	48,48,48,48	0
60	MG	BA	3254	1/1	0.92	0.38	60,60,60,60	0
60	MG	DA	3233	1/1	0.92	0.35	53,53,53,53	0
60	MG	CA	1614	1/1	0.92	0.41	53,53,53,53	0
60	MG	AA	1630	1/1	0.92	0.37	51,51,51,51	0
60	MG	BA	3322	1/1	0.92	0.35	55,55,55,55	0
60	MG	AA	1632	1/1	0.92	0.22	53,53,53,53	0
60	MG	BA	3023	1/1	0.92	0.46	49,49,49,49	0
60	MG	DA	3241	1/1	0.92	0.06	55,55,55,55	0
60	MG	AA	1706	1/1	0.92	0.08	51,51,51,51	0
60	MG	BA	3327	1/1	0.92	0.23	55,55,55,55	0
60	MG	DA	3011	1/1	0.92	0.24	52,52,52,52	0
60	MG	DA	3012	1/1	0.92	0.23	47,47,47,47	0
60	MG	AV	105	1/1	0.92	0.21	50,50,50,50	1
60	MG	BA	3058	1/1	0.92	0.43	55,55,55,55	0
60	MG	DA	3016	1/1	0.92	0.25	47,47,47,47	0
60	MG	CA	1704	1/1	0.92	0.27	62,62,62,62	0
60	MG	DA	3105	1/1	0.92	0.40	48,48,48,48	0
60	MG	AA	1707	1/1	0.92	0.27	49,49,49,49	0
60	MG	BA	3155	1/1	0.92	0.26	51,51,51,51	0
60	MG	DA	3109	1/1	0.92	0.29	52,52,52,52	0
60	MG	DA	3112	1/1	0.92	0.32	52,52,52,52	0
60	MG	DA	3264	1/1	0.92	0.19	56,56,56,56	0
60	MG	BA	3333	1/1	0.92	0.44	55,55,55,55	0
60	MG	AA	1663	1/1	0.92	0.17	51,51,51,51	0
60	MG	DA	3119	1/1	0.92	0.34	49,49,49,49	0
60	MG	DA	3121	1/1	0.92	0.28	50,50,50,50	0
60	MG	DA	3271	1/1	0.92	0.43	51,51,51,51	0
60	MG	BA	3110	1/1	0.92	0.27	49,49,49,49	0
60	MG	DA	3273	1/1	0.92	0.16	58,58,58,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	CA	1637	1/1	0.92	0.22	52,52,52,52	0
60	MG	BA	3061	1/1	0.92	0.33	48,48,48,48	0
60	MG	AA	1674	1/1	0.92	0.07	50,50,50,50	0
60	MG	BA	3030	1/1	0.92	0.39	47,47,47,47	0
60	MG	AA	1710	1/1	0.92	0.06	55,55,55,55	0
60	MG	DA	3280	1/1	0.92	0.16	57,57,57,57	0
60	MG	CA	1722	1/1	0.92	0.13	55,55,55,55	0
60	MG	BA	3230	1/1	0.92	0.20	54,54,54,54	0
60	MG	DA	3035	1/1	0.92	0.26	50,50,50,50	0
60	MG	DA	3141	1/1	0.92	0.15	56,56,56,56	0
60	MG	DA	3287	1/1	0.92	0.33	51,51,51,51	0
60	MG	DA	3288	1/1	0.92	0.15	66,66,66,66	0
60	MG	CA	1645	1/1	0.92	0.16	50,50,50,50	0
60	MG	DA	3290	1/1	0.92	0.40	57,57,57,57	0
60	MG	DA	3037	1/1	0.92	0.27	53,53,53,53	0
60	MG	AA	1664	1/1	0.92	0.10	60,60,60,60	0
60	MG	DA	3149	1/1	0.92	0.17	47,47,47,47	0
60	MG	DA	3297	1/1	0.92	0.40	55,55,55,55	0
60	MG	BA	3071	1/1	0.92	0.28	47,47,47,47	0
60	MG	BA	3126	1/1	0.92	0.17	52,52,52,52	0
60	MG	DA	3157	1/1	0.92	0.43	48,48,48,48	0
60	MG	BB	201	1/1	0.92	0.10	67,67,67,67	0
60	MG	DA	3162	1/1	0.92	0.16	47,47,47,47	0
60	MG	DA	3044	1/1	0.92	0.39	47,47,47,47	0
60	MG	AA	1604	1/1	0.92	0.20	61,61,61,61	0
60	MG	DA	3046	1/1	0.92	0.44	47,47,47,47	0
60	MG	DA	3317	1/1	0.92	0.14	55,55,55,55	0
60	MG	DA	3173	1/1	0.92	0.26	58,58,58,58	0
60	MG	DA	3175	1/1	0.92	0.35	56,56,56,56	0
60	MG	BA	3077	1/1	0.92	0.24	51,51,51,51	0
60	MG	BA	3184	1/1	0.92	0.28	47,47,47,47	0
60	MG	BA	3298	1/1	0.92	0.27	55,55,55,55	0
60	MG	AA	1649	1/1	0.92	0.13	53,53,53,53	0
60	MG	AE	201	1/1	0.92	0.21	57,57,57,57	0
60	MG	BA	3003	1/1	0.92	0.18	61,61,61,61	0
60	MG	DA	3333	1/1	0.92	0.14	55,55,55,55	0
60	MG	BA	3084	1/1	0.92	0.32	47,47,47,47	0
60	MG	DA	3184	1/1	0.92	0.41	49,49,49,49	0
60	MG	BA	3007	1/1	0.92	0.34	52,52,52,52	0
60	MG	DA	3061	1/1	0.92	0.35	47,47,47,47	0
60	MG	DA	3062	1/1	0.92	0.34	48,48,48,48	0
60	MG	BA	3243	1/1	0.92	0.38	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3343	1/1	0.92	0.10	55,55,55,55	0
60	MG	BA	3245	1/1	0.92	0.11	53,53,53,53	0
60	MG	DA	3067	1/1	0.92	0.50	50,50,50,50	0
60	MG	BA	3091	1/1	0.92	0.14	51,51,51,51	0
60	MG	DA	3071	1/1	0.92	0.28	50,50,50,50	0
60	MG	BA	3042	1/1	0.92	0.54	47,47,47,47	0
60	MG	BA	3312	1/1	0.92	0.27	55,55,55,55	0
60	MG	BA	3198	1/1	0.92	0.28	53,53,53,53	0
60	MG	CA	1609	1/1	0.92	0.20	55,55,55,55	0
60	MG	CV	104	1/1	0.92	0.05	54,54,54,54	0
60	MG	DQ	201	1/1	0.92	0.19	55,55,55,55	0
60	MG	DU	201	1/1	0.92	0.42	48,48,48,48	0
60	MG	DA	3080	1/1	0.92	0.39	49,49,49,49	0
60	MG	BA	3066	1/1	0.93	0.53	50,50,50,50	0
60	MG	CA	1629	1/1	0.93	0.25	51,51,51,51	0
60	MG	DA	3123	1/1	0.93	0.32	64,64,64,64	1
60	MG	CA	1717	1/1	0.93	0.11	52,52,52,52	0
60	MG	DA	3249	1/1	0.93	0.06	56,56,56,56	0
60	MG	DA	3127	1/1	0.93	0.22	52,52,52,52	0
60	MG	BA	3272	1/1	0.93	0.07	59,59,59,59	1
60	MG	BA	3210	1/1	0.93	0.27	57,57,57,57	0
60	MG	DA	3131	1/1	0.93	0.13	48,48,48,48	0
60	MG	BA	3107	1/1	0.93	0.20	51,51,51,51	0
60	MG	BA	3011	1/1	0.93	0.20	47,47,47,47	0
60	MG	BA	3160	1/1	0.93	0.18	47,47,47,47	0
60	MG	CA	1640	1/1	0.93	0.29	47,47,47,47	0
60	MG	BA	3035	1/1	0.93	0.19	55,55,55,55	0
60	MG	DA	3262	1/1	0.93	0.10	52,52,52,52	0
60	MG	DA	3263	1/1	0.93	0.19	63,63,63,63	0
60	MG	BA	3165	1/1	0.93	0.37	47,47,47,47	0
60	MG	BA	3282	1/1	0.93	0.28	57,57,57,57	0
60	MG	AA	1756	1/1	0.93	0.09	55,55,55,55	1
60	MG	BA	3038	1/1	0.93	0.27	51,51,51,51	0
60	MG	CA	1734	1/1	0.93	0.04	55,55,55,55	1
60	MG	DA	3148	1/1	0.93	0.26	51,51,51,51	0
60	MG	BA	3350	1/1	0.93	0.23	55,55,55,55	0
60	MG	DA	3049	1/1	0.93	0.35	47,47,47,47	0
60	MG	BA	3226	1/1	0.93	0.17	56,56,56,56	0
60	MG	CA	1650	1/1	0.93	0.41	54,54,54,54	0
60	MG	BA	3352	1/1	0.93	0.22	55,55,55,55	0
60	MG	AA	1682	1/1	0.93	0.18	53,53,53,53	0
60	MG	BA	3228	1/1	0.93	0.34	52,52,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3279	1/1	0.93	0.11	55,55,55,55	0
60	MG	DA	3169	1/1	0.93	0.29	47,47,47,47	0
60	MG	DA	3281	1/1	0.93	0.13	57,57,57,57	0
60	MG	BA	3015	1/1	0.93	0.32	47,47,47,47	0
60	MG	AW	102	1/1	0.93	0.04	60,60,60,60	1
60	MG	BA	3080	1/1	0.93	0.34	52,52,52,52	0
60	MG	BA	3232	1/1	0.93	0.23	53,53,53,53	0
60	MG	BA	3081	1/1	0.93	0.26	47,47,47,47	0
60	MG	BA	3180	1/1	0.93	0.13	56,56,56,56	0
60	MG	CA	1666	1/1	0.93	0.11	57,57,57,57	0
60	MG	DA	3070	1/1	0.93	0.20	48,48,48,48	0
60	MG	DA	3291	1/1	0.93	0.32	54,54,54,54	0
60	MG	BA	3017	1/1	0.93	0.28	52,52,52,52	0
60	MG	BU	201	1/1	0.93	0.20	48,48,48,48	0
60	MG	BA	3044	1/1	0.93	0.39	56,56,56,56	0
60	MG	AA	1691	1/1	0.93	0.21	59,59,59,59	0
60	MG	CA	1673	1/1	0.93	0.10	52,52,52,52	1
60	MG	DA	3186	1/1	0.93	0.44	50,50,50,50	0
60	MG	CA	1603	1/1	0.93	0.20	61,61,61,61	0
60	MG	BA	3086	1/1	0.93	0.34	48,48,48,48	0
60	MG	AA	1657	1/1	0.93	0.09	54,54,54,54	0
60	MG	CA	1678	1/1	0.93	0.12	49,49,49,49	0
60	MG	BA	3090	1/1	0.93	0.25	48,48,48,48	0
60	MG	B1	101	1/1	0.93	0.39	55,55,55,55	0
60	MG	DA	3197	1/1	0.93	0.39	47,47,47,47	0
60	MG	DA	3318	1/1	0.93	0.07	55,55,55,55	0
60	MG	BA	3049	1/1	0.93	0.35	47,47,47,47	0
60	MG	AA	1728	1/1	0.93	0.14	55,55,55,55	0
60	MG	BA	3193	1/1	0.93	0.15	53,53,53,53	0
60	MG	DA	3204	1/1	0.93	0.29	52,52,52,52	0
60	MG	DA	3003	1/1	0.93	0.10	67,67,67,67	0
60	MG	B5	102	1/1	0.93	0.24	53,53,53,53	0
60	MG	BA	3247	1/1	0.93	0.07	59,59,59,59	0
60	MG	BA	3095	1/1	0.93	0.42	60,60,60,60	0
60	MG	DA	3331	1/1	0.93	0.05	55,55,55,55	1
60	MG	DA	3010	1/1	0.93	0.48	47,47,47,47	0
60	MG	DA	3214	1/1	0.93	0.26	58,58,58,58	0
60	MG	BA	3249	1/1	0.93	0.22	56,56,56,56	0
60	MG	AA	1750	1/1	0.93	0.11	55,55,55,55	0
60	MG	BA	3202	1/1	0.93	0.35	47,47,47,47	0
60	MG	DA	3338	1/1	0.93	0.38	55,55,55,55	0
60	MG	AA	1606	1/1	0.93	0.14	59,59,59,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1741	1/1	0.93	0.42	55,55,55,55	0
60	MG	BA	3205	1/1	0.93	0.08	50,50,50,50	0
60	MG	CA	1620	1/1	0.93	0.12	56,56,56,56	0
60	MG	BA	3259	1/1	0.93	0.18	59,59,59,59	0
60	MG	DA	3350	1/1	0.93	0.33	55,55,55,55	0
60	MG	BA	3260	1/1	0.93	0.21	57,57,57,57	0
60	MG	DA	3230	1/1	0.93	0.08	49,49,49,49	0
60	MG	CA	1707	1/1	0.93	0.30	51,51,51,51	0
60	MG	DA	3023	1/1	0.93	0.45	47,47,47,47	0
60	MG	CA	1709	1/1	0.93	0.13	65,65,65,65	0
60	MG	AA	1721	1/1	0.93	0.15	55,55,55,55	1
60	MG	DA	3115	1/1	0.93	0.19	48,48,48,48	0
60	MG	BA	3004	1/1	0.93	0.18	53,53,53,53	0
60	MG	AV	106	1/1	0.93	0.13	57,57,57,57	0
60	MG	DA	3118	1/1	0.93	0.28	52,52,52,52	0
60	MG	BA	3271	1/1	0.94	0.45	51,51,51,51	0
60	MG	BA	3321	1/1	0.94	0.19	55,55,55,55	0
60	MG	DA	3140	1/1	0.94	0.12	50,50,50,50	1
60	MG	AA	1752	1/1	0.94	0.06	55,55,55,55	0
60	MG	DA	3255	1/1	0.94	0.32	60,60,60,60	0
60	MG	BA	3150	1/1	0.94	0.33	51,51,51,51	0
60	MG	AA	1680	1/1	0.94	0.15	49,49,49,49	0
60	MG	BA	3050	1/1	0.94	0.33	47,47,47,47	0
60	MG	DA	3146	1/1	0.94	0.39	47,47,47,47	0
60	MG	DA	3054	1/1	0.94	0.20	51,51,51,51	0
60	MG	DA	3056	1/1	0.94	0.30	47,47,47,47	0
60	MG	DA	3153	1/1	0.94	0.14	50,50,50,50	0
60	MG	DA	3057	1/1	0.94	0.42	47,47,47,47	0
60	MG	CA	1677	1/1	0.94	0.46	55,55,55,55	1
60	MG	BA	3074	1/1	0.94	0.24	47,47,47,47	0
60	MG	DA	3267	1/1	0.94	0.33	54,54,54,54	0
60	MG	BA	3097	1/1	0.94	0.28	47,47,47,47	0
60	MG	DA	3161	1/1	0.94	0.15	47,47,47,47	0
60	MG	BA	3194	1/1	0.94	0.29	53,53,53,53	0
60	MG	BA	3129	1/1	0.94	0.25	56,56,56,56	0
60	MG	DA	3167	1/1	0.94	0.16	47,47,47,47	0
60	MG	BA	3196	1/1	0.94	0.32	47,47,47,47	0
60	MG	CA	1686	1/1	0.94	0.14	57,57,57,57	0
60	MG	BA	3021	1/1	0.94	0.30	47,47,47,47	0
60	MG	AA	1726	1/1	0.94	0.10	56,56,56,56	0
60	MG	DA	3069	1/1	0.94	0.25	47,47,47,47	0
60	MG	BA	3162	1/1	0.94	0.39	50,50,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	BA	3163	1/1	0.94	0.26	53,53,53,53	0
60	MG	BA	3037	1/1	0.94	0.30	47,47,47,47	0
60	MG	DA	3074	1/1	0.94	0.27	52,52,52,52	0
60	MG	BA	3166	1/1	0.94	0.10	47,47,47,47	0
60	MG	BA	3340	1/1	0.94	0.24	55,55,55,55	0
60	MG	AA	1615	1/1	0.94	0.43	53,53,53,53	0
60	MG	D3	101	1/1	0.94	0.35	58,58,58,58	0
60	MG	D5	101	1/1	0.94	0.15	49,49,49,49	0
60	MG	BA	3169	1/1	0.94	0.36	51,51,51,51	0
60	MG	DA	3187	1/1	0.94	0.20	51,51,51,51	0
60	MG	BA	3344	1/1	0.94	0.26	55,55,55,55	0
60	MG	DA	3189	1/1	0.94	0.26	57,57,57,57	0
60	MG	DA	3293	1/1	0.94	0.17	52,52,52,52	0
60	MG	DA	3004	1/1	0.94	0.18	61,61,61,61	0
60	MG	AA	1690	1/1	0.94	0.42	52,52,52,52	0
60	MG	DA	3192	1/1	0.94	0.06	61,61,61,61	1
60	MG	BA	3348	1/1	0.94	0.40	55,55,55,55	0
60	MG	DA	3194	1/1	0.94	0.24	53,53,53,53	0
60	MG	DA	3008	1/1	0.94	0.24	52,52,52,52	0
60	MG	DA	3301	1/1	0.94	0.24	55,55,55,55	0
60	MG	BA	3297	1/1	0.94	0.24	55,55,55,55	0
60	MG	BA	3104	1/1	0.94	0.41	48,48,48,48	0
60	MG	DA	3306	1/1	0.94	0.14	55,55,55,55	0
60	MG	CA	1708	1/1	0.94	0.19	49,49,49,49	0
60	MG	DA	3311	1/1	0.94	0.27	55,55,55,55	0
60	MG	DA	3200	1/1	0.94	0.41	58,58,58,58	0
60	MG	DA	3314	1/1	0.94	0.19	55,55,55,55	1
60	MG	AA	1631	1/1	0.94	0.18	47,47,47,47	0
60	MG	BA	3139	1/1	0.94	0.06	50,50,50,50	0
60	MG	CA	1711	1/1	0.94	0.05	55,55,55,55	0
60	MG	BA	3353	1/1	0.94	0.28	55,55,55,55	0
60	MG	BA	3354	1/1	0.94	0.09	55,55,55,55	0
60	MG	DA	3323	1/1	0.94	0.17	55,55,55,55	0
60	MG	BA	3213	1/1	0.94	0.15	58,58,58,58	0
60	MG	BA	3302	1/1	0.94	0.22	55,55,55,55	0
60	MG	AA	1660	1/1	0.94	0.09	58,58,58,58	0
60	MG	AA	1676	1/1	0.94	0.16	58,58,58,58	0
60	MG	AA	1614	1/1	0.94	0.11	52,52,52,52	0
60	MG	DA	3024	1/1	0.94	0.57	49,49,49,49	0
60	MG	BA	3089	1/1	0.94	0.33	48,48,48,48	0
60	MG	BA	3257	1/1	0.94	0.09	51,51,51,51	0
60	MG	DA	3220	1/1	0.94	0.29	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3221	1/1	0.94	0.26	54,54,54,54	0
60	MG	BA	3182	1/1	0.94	0.33	49,49,49,49	0
60	MG	BP	201	1/1	0.94	0.16	49,49,49,49	0
60	MG	DA	3029	1/1	0.94	0.23	52,52,52,52	0
60	MG	CA	1656	1/1	0.94	0.36	47,47,47,47	0
60	MG	DA	3031	1/1	0.94	0.52	47,47,47,47	0
60	MG	BQ	201	1/1	0.94	0.29	55,55,55,55	0
60	MG	DA	3344	1/1	0.94	0.57	55,55,55,55	0
60	MG	DA	3346	1/1	0.94	0.54	55,55,55,55	0
60	MG	DA	3347	1/1	0.94	0.12	55,55,55,55	0
60	MG	BA	3222	1/1	0.94	0.18	49,49,49,49	0
60	MG	BA	3313	1/1	0.94	0.18	55,55,55,55	0
60	MG	CA	1731	1/1	0.94	0.16	55,55,55,55	0
60	MG	BA	3223	1/1	0.94	0.09	52,52,52,52	0
60	MG	CA	1662	1/1	0.94	0.26	52,52,52,52	0
60	MG	BA	3111	1/1	0.94	0.21	52,52,52,52	0
60	MG	CA	1737	1/1	0.94	0.12	55,55,55,55	1
60	MG	DA	3041	1/1	0.94	0.18	47,47,47,47	0
60	MG	AA	1749	1/1	0.94	0.24	55,55,55,55	0
60	MG	BA	3317	1/1	0.94	0.18	55,55,55,55	0
60	MG	DF	302	1/1	0.94	0.07	53,53,53,53	0
60	MG	AA	1623	1/1	0.94	0.15	57,57,57,57	0
60	MG	CA	1742	1/1	0.94	0.49	55,55,55,55	0
60	MG	BA	3268	1/1	0.94	0.42	59,59,59,59	0
60	MG	BA	3130	1/1	0.95	0.12	48,48,48,48	0
60	MG	BA	3201	1/1	0.95	0.12	52,52,52,52	0
60	MG	DA	3174	1/1	0.95	0.22	52,52,52,52	0
60	MG	AA	1702	1/1	0.95	0.22	47,47,47,47	0
60	MG	BA	3281	1/1	0.95	0.16	57,57,57,57	0
60	MG	AA	1730	1/1	0.95	0.29	55,55,55,55	0
60	MG	DA	3086	1/1	0.95	0.13	47,47,47,47	0
60	MG	DA	3179	1/1	0.95	0.38	47,47,47,47	0
60	MG	CA	1664	1/1	0.95	0.21	60,60,60,60	0
60	MG	BA	3167	1/1	0.95	0.22	53,53,53,53	0
60	MG	DA	3089	1/1	0.95	0.51	48,48,48,48	0
60	MG	CA	1728	1/1	0.95	0.23	55,55,55,55	0
60	MG	AA	1626	1/1	0.95	0.20	53,53,53,53	0
60	MG	BA	3098	1/1	0.95	0.18	54,54,54,54	0
60	MG	BA	3288	1/1	0.95	0.14	66,66,66,66	0
60	MG	BA	3334	1/1	0.95	0.19	55,55,55,55	0
60	MG	AA	1633	1/1	0.95	0.06	55,55,55,55	0
60	MG	CA	1735	1/1	0.95	0.06	55,55,55,55	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AW	104	1/1	0.95	0.04	56,56,56,56	0
60	MG	AA	1672	1/1	0.95	0.14	53,53,53,53	0
60	MG	AA	1634	1/1	0.95	0.30	52,52,52,52	0
60	MG	DA	3286	1/1	0.95	0.30	60,60,60,60	0
60	MG	CA	1739	1/1	0.95	0.10	55,55,55,55	0
60	MG	BA	3211	1/1	0.95	0.14	59,59,59,59	1
60	MG	BA	3075	1/1	0.95	0.20	47,47,47,47	0
60	MG	AA	1662	1/1	0.95	0.14	52,52,52,52	0
60	MG	B3	101	1/1	0.95	0.41	58,58,58,58	0
60	MG	CA	1745	1/1	0.95	0.14	55,55,55,55	0
60	MG	DA	3199	1/1	0.95	0.28	53,53,53,53	0
60	MG	CA	1680	1/1	0.95	0.15	49,49,49,49	0
60	MG	BA	3343	1/1	0.95	0.27	55,55,55,55	0
60	MG	DA	3114	1/1	0.95	0.28	47,47,47,47	0
60	MG	CA	1624	1/1	0.95	0.22	51,51,51,51	0
60	MG	CA	1750	1/1	0.95	0.20	55,55,55,55	0
60	MG	AA	1603	1/1	0.95	0.09	57,57,57,57	0
60	MG	CA	1685	1/1	0.95	0.15	47,47,47,47	0
60	MG	DA	3209	1/1	0.95	0.20	51,51,51,51	0
60	MG	BA	3252	1/1	0.95	0.29	49,49,49,49	0
60	MG	DA	3120	1/1	0.95	0.44	49,49,49,49	0
60	MG	CA	1754	1/1	0.95	0.10	55,55,55,55	0
60	MG	DA	3310	1/1	0.95	0.15	55,55,55,55	0
60	MG	DA	3122	1/1	0.95	0.12	50,50,50,50	0
60	MG	CA	1755	1/1	0.95	0.16	55,55,55,55	0
60	MG	AA	1740	1/1	0.95	0.09	55,55,55,55	0
60	MG	BA	3217	1/1	0.95	0.30	51,51,51,51	0
60	MG	AA	1617	1/1	0.95	0.04	54,54,54,54	0
60	MG	DA	3129	1/1	0.95	0.14	50,50,50,50	0
60	MG	AA	1629	1/1	0.95	0.07	56,56,56,56	0
60	MG	DA	3051	1/1	0.95	0.23	47,47,47,47	0
60	MG	BA	3258	1/1	0.95	0.21	58,58,58,58	0
60	MG	DA	3226	1/1	0.95	0.14	51,51,51,51	0
60	MG	BA	3028	1/1	0.95	0.25	52,52,52,52	0
60	MG	BA	3085	1/1	0.95	0.15	47,47,47,47	0
60	MG	BA	3261	1/1	0.95	0.29	52,52,52,52	0
60	MG	BA	3310	1/1	0.95	0.14	55,55,55,55	0
60	MG	BA	3262	1/1	0.95	0.12	63,63,63,63	1
60	MG	CW	102	1/1	0.95	0.04	60,60,60,60	0
60	MG	DA	3332	1/1	0.95	0.33	55,55,55,55	0
60	MG	DA	3236	1/1	0.95	0.41	52,52,52,52	0
60	MG	CA	1701	1/1	0.95	0.12	51,51,51,51	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1725	1/1	0.95	0.38	54,54,54,54	0
60	MG	AA	1602	1/1	0.95	0.22	52,52,52,52	0
60	MG	AA	1712	1/1	0.95	0.14	54,54,54,54	0
60	MG	CA	1706	1/1	0.95	0.13	51,51,51,51	0
60	MG	DA	3243	1/1	0.95	0.07	61,61,61,61	1
60	MG	BA	3190	1/1	0.95	0.27	54,54,54,54	0
60	MG	BA	3154	1/1	0.95	0.21	48,48,48,48	0
60	MG	DA	3150	1/1	0.95	0.45	54,54,54,54	0
60	MG	D5	102	1/1	0.95	0.24	53,53,53,53	0
60	MG	BA	3269	1/1	0.95	0.25	52,52,52,52	0
60	MG	BA	3117	1/1	0.95	0.21	52,52,52,52	0
60	MG	DA	3072	1/1	0.95	0.21	47,47,47,47	0
60	MG	AA	1612	1/1	0.95	0.09	52,52,52,52	0
60	MG	DA	3253	1/1	0.95	0.26	49,49,49,49	0
60	MG	BA	3008	1/1	0.95	0.34	55,55,55,55	0
60	MG	CA	1654	1/1	0.95	0.26	57,57,57,57	0
60	MG	BA	3009	1/1	0.95	0.46	47,47,47,47	0
60	MG	DA	3165	1/1	0.95	0.22	47,47,47,47	0
60	MG	DA	3258	1/1	0.95	0.17	51,51,51,51	1
60	MG	DA	3166	1/1	0.95	0.35	47,47,47,47	0
60	MG	BA	3010	1/1	0.95	0.24	52,52,52,52	0
60	MG	DA	3168	1/1	0.95	0.22	53,53,53,53	0
60	MG	DR	201	1/1	0.95	0.25	47,47,47,47	0
60	MG	CA	1657	1/1	0.95	0.20	54,54,54,54	0
60	MG	DX	101	1/1	0.95	0.09	55,55,55,55	0
60	MG	BA	3323	1/1	0.95	0.47	55,55,55,55	0
60	MG	CA	1732	1/1	0.96	0.19	55,55,55,55	0
60	MG	CA	1634	1/1	0.96	0.20	47,47,47,47	0
60	MG	BA	3156	1/1	0.96	0.39	48,48,48,48	0
60	MG	AA	1717	1/1	0.96	0.15	66,66,66,66	0
60	MG	BA	3159	1/1	0.96	0.31	55,55,55,55	0
60	MG	DA	3014	1/1	0.96	0.28	47,47,47,47	0
60	MG	DA	3135	1/1	0.96	0.33	54,54,54,54	0
60	MG	BA	3218	1/1	0.96	0.25	66,66,66,66	0
60	MG	AA	1671	1/1	0.96	0.19	47,47,47,47	0
60	MG	DA	3210	1/1	0.96	0.25	66,66,66,66	0
60	MG	BA	3286	1/1	0.96	0.26	60,60,60,60	0
60	MG	AA	1723	1/1	0.96	0.07	57,57,57,57	0
60	MG	CA	1691	1/1	0.96	0.42	52,52,52,52	0
60	MG	DA	3077	1/1	0.96	0.26	48,48,48,48	0
60	MG	BA	3221	1/1	0.96	0.31	53,53,53,53	0
60	MG	CA	1743	1/1	0.96	0.10	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1685	1/1	0.96	0.09	57,57,57,57	0
60	MG	AW	103	1/1	0.96	0.04	54,54,54,54	0
60	MG	CA	1746	1/1	0.96	0.23	55,55,55,55	0
60	MG	DA	3222	1/1	0.96	0.31	53,53,53,53	0
60	MG	BA	3255	1/1	0.96	0.21	55,55,55,55	0
60	MG	BA	3330	1/1	0.96	0.10	55,55,55,55	0
60	MG	DA	3151	1/1	0.96	0.35	51,51,51,51	0
60	MG	DA	3302	1/1	0.96	0.24	55,55,55,55	0
60	MG	DA	3152	1/1	0.96	0.23	47,47,47,47	0
60	MG	DA	3227	1/1	0.96	0.14	56,56,56,56	0
60	MG	DA	3305	1/1	0.96	0.22	55,55,55,55	0
60	MG	BA	3067	1/1	0.96	0.17	50,50,50,50	0
60	MG	DA	3308	1/1	0.96	0.20	55,55,55,55	0
60	MG	BA	3293	1/1	0.96	0.14	55,55,55,55	1
60	MG	DA	3155	1/1	0.96	0.25	48,48,48,48	0
60	MG	CA	1700	1/1	0.96	0.09	54,54,54,54	0
60	MG	DA	3232	1/1	0.96	0.04	51,51,51,51	0
60	MG	BA	3088	1/1	0.96	0.54	48,48,48,48	0
60	MG	DA	3158	1/1	0.96	0.18	53,53,53,53	0
60	MG	DA	3235	1/1	0.96	0.23	49,49,49,49	0
60	MG	BA	3109	1/1	0.96	0.31	48,48,48,48	0
60	MG	CA	1703	1/1	0.96	0.20	47,47,47,47	0
60	MG	BA	3045	1/1	0.96	0.44	47,47,47,47	0
60	MG	DA	3322	1/1	0.96	0.42	55,55,55,55	0
60	MG	DA	3163	1/1	0.96	0.31	50,50,50,50	0
60	MG	BA	3199	1/1	0.96	0.34	58,58,58,58	0
60	MG	CA	1757	1/1	0.96	0.09	55,55,55,55	0
60	MG	AA	1744	1/1	0.96	0.19	55,55,55,55	0
60	MG	AA	1665	1/1	0.96	0.27	50,50,50,50	0
60	MG	DA	3096	1/1	0.96	0.33	60,60,60,60	0
60	MG	DA	3246	1/1	0.96	0.23	60,60,60,60	0
60	MG	DA	3097	1/1	0.96	0.24	56,56,56,56	0
60	MG	DA	3170	1/1	0.96	0.27	49,49,49,49	1
60	MG	DA	3039	1/1	0.96	0.43	51,51,51,51	0
60	MG	BA	3005	1/1	0.96	0.56	47,47,47,47	0
60	MG	BA	3174	1/1	0.96	0.20	58,58,58,58	0
60	MG	BA	3019	1/1	0.96	0.38	47,47,47,47	0
60	MG	BA	3006	1/1	0.96	0.34	53,53,53,53	0
60	MG	BA	3267	1/1	0.96	0.25	54,54,54,54	0
60	MG	BA	3177	1/1	0.96	0.39	47,47,47,47	0
60	MG	BA	3345	1/1	0.96	0.08	55,55,55,55	0
60	MG	DA	3342	1/1	0.96	0.09	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AV	103	1/1	0.96	0.14	54,54,54,54	1
60	MG	BA	3270	1/1	0.96	0.33	67,67,67,67	0
60	MG	DA	3108	1/1	0.96	0.17	51,51,51,51	0
60	MG	BA	3076	1/1	0.96	0.15	48,48,48,48	0
60	MG	DA	3110	1/1	0.96	0.35	48,48,48,48	0
60	MG	DA	3111	1/1	0.96	0.20	49,49,49,49	0
60	MG	BA	3053	1/1	0.96	0.09	51,51,51,51	0
60	MG	DA	3113	1/1	0.96	0.21	48,48,48,48	0
60	MG	DA	3352	1/1	0.96	0.14	55,55,55,55	0
60	MG	CA	1671	1/1	0.96	0.13	47,47,47,47	0
60	MG	CA	1623	1/1	0.96	0.18	48,48,48,48	0
60	MG	BA	3124	1/1	0.96	0.20	49,49,49,49	0
60	MG	BA	3274	1/1	0.96	0.21	63,63,63,63	0
60	MG	DB	204	1/1	0.96	0.13	55,55,55,55	0
60	MG	BA	3275	1/1	0.96	0.17	59,59,59,59	0
60	MG	AA	1737	1/1	0.96	0.16	55,55,55,55	0
60	MG	DD	302	1/1	0.96	0.33	47,47,47,47	0
60	MG	DF	301	1/1	0.96	0.28	47,47,47,47	0
60	MG	DA	3002	1/1	0.96	0.39	54,54,54,54	1
60	MG	DF	303	1/1	0.96	0.38	59,59,59,59	0
60	MG	CA	1726	1/1	0.96	0.30	54,54,54,54	0
60	MG	AA	1738	1/1	0.96	0.10	55,55,55,55	0
60	MG	BA	3039	1/1	0.96	0.10	68,68,68,68	0
60	MG	BA	3131	1/1	0.96	0.27	59,59,59,59	0
60	MG	CA	1631	1/1	0.96	0.37	53,53,53,53	0
60	MG	DA	3063	1/1	0.97	0.37	47,47,47,47	0
60	MG	DA	3312	1/1	0.97	0.17	55,55,55,55	0
60	MG	CA	1714	1/1	0.97	0.09	64,64,64,64	0
60	MG	AA	1731	1/1	0.97	0.24	55,55,55,55	0
60	MG	DA	3208	1/1	0.97	0.15	60,60,60,60	0
60	MG	DA	3160	1/1	0.97	0.24	55,55,55,55	0
60	MG	DA	3022	1/1	0.97	0.16	47,47,47,47	0
60	MG	AA	1742	1/1	0.97	0.06	55,55,55,55	0
60	MG	DA	3212	1/1	0.97	0.08	59,59,59,59	0
60	MG	BA	3078	1/1	0.97	0.37	56,56,56,56	0
60	MG	CL	201	1/1	0.97	0.20	51,51,51,51	1
60	MG	BA	3014	1/1	0.97	0.42	53,53,53,53	0
60	MG	BA	3096	1/1	0.97	0.24	56,56,56,56	0
60	MG	BA	3306	1/1	0.97	0.17	55,55,55,55	0
60	MG	DA	3218	1/1	0.97	0.34	51,51,51,51	0
60	MG	BA	3063	1/1	0.97	0.22	56,56,56,56	0
60	MG	BA	3308	1/1	0.97	0.33	55,55,55,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	DA	3330	1/1	0.97	0.09	55,55,55,55	0
60	MG	CA	1644	1/1	0.97	0.05	57,57,57,57	0
60	MG	BA	3164	1/1	0.97	0.20	47,47,47,47	0
60	MG	CA	1646	1/1	0.97	0.26	62,62,62,62	0
60	MG	BA	3191	1/1	0.97	0.10	61,61,61,61	0
60	MG	DA	3125	1/1	0.97	0.20	49,49,49,49	0
60	MG	CA	1727	1/1	0.97	0.07	56,56,56,56	0
60	MG	AA	1609	1/1	0.97	0.07	52,52,52,52	0
60	MG	BA	3065	1/1	0.97	0.07	52,52,52,52	0
60	MG	CA	1689	1/1	0.97	0.13	63,63,63,63	1
60	MG	BA	3142	1/1	0.97	0.09	47,47,47,47	0
60	MG	DA	3341	1/1	0.97	0.23	55,55,55,55	0
60	MG	AA	1610	1/1	0.97	0.05	55,55,55,55	0
60	MG	BA	3347	1/1	0.97	0.29	55,55,55,55	0
60	MG	AA	1751	1/1	0.97	0.05	55,55,55,55	0
60	MG	DA	3345	1/1	0.97	0.36	55,55,55,55	0
60	MG	BA	3284	1/1	0.97	0.26	57,57,57,57	0
60	MG	BA	3225	1/1	0.97	0.07	51,51,51,51	0
60	MG	BA	3197	1/1	0.97	0.29	58,58,58,58	0
60	MG	BA	3122	1/1	0.97	0.25	64,64,64,64	1
60	MG	BA	3171	1/1	0.97	0.20	58,58,58,58	0
60	MG	BA	3172	1/1	0.97	0.24	52,52,52,52	0
60	MG	BA	3146	1/1	0.97	0.39	47,47,47,47	0
60	MG	BA	3051	1/1	0.97	0.20	51,51,51,51	0
60	MG	BA	3125	1/1	0.97	0.47	47,47,47,47	0
60	MG	DA	3296	1/1	0.97	0.23	55,55,55,55	0
60	MG	BA	3001	1/1	0.97	0.09	54,54,54,54	0
60	MG	DA	3145	1/1	0.97	0.42	49,49,49,49	0
60	MG	BA	3127	1/1	0.97	0.10	56,56,56,56	0
60	MG	BA	3128	1/1	0.97	0.11	50,50,50,50	0
60	MG	DA	3055	1/1	0.97	0.26	47,47,47,47	0
60	MG	CA	1667	1/1	0.97	0.23	47,47,47,47	0
60	MG	AA	1625	1/1	0.97	0.16	51,51,51,51	0
60	MG	BA	3020	1/1	0.97	0.38	47,47,47,47	0
60	MG	BA	3056	1/1	0.97	0.39	47,47,47,47	0
60	MG	AA	1619	1/1	0.97	0.39	49,49,49,49	0
60	MG	CA	1633	1/1	0.97	0.49	52,52,52,52	0
60	MG	DA	3203	1/1	0.97	0.38	47,47,47,47	0
60	MG	BA	3022	1/1	0.97	0.40	47,47,47,47	0
60	MG	BA	3062	1/1	0.98	0.40	47,47,47,47	0
60	MG	BA	3119	1/1	0.98	0.46	49,49,49,49	0
60	MG	DA	3007	1/1	0.98	0.31	53,53,53,53	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
60	MG	AA	1605	1/1	0.98	0.07	50,50,50,50	0
60	MG	CA	1632	1/1	0.98	0.03	55,55,55,55	0
60	MG	AA	1661	1/1	0.98	0.16	52,52,52,52	0
60	MG	BA	3123	1/1	0.98	0.23	53,53,53,53	0
60	MG	DA	3242	1/1	0.98	0.03	58,58,58,58	1
60	MG	DA	3147	1/1	0.98	0.35	47,47,47,47	0
60	MG	BA	3054	1/1	0.98	0.34	47,47,47,47	0
60	MG	DA	3307	1/1	0.98	0.29	55,55,55,55	0
60	MG	BH	201	1/1	0.98	0.24	50,50,50,50	0
60	MG	AA	1638	1/1	0.98	0.12	52,52,52,52	0
60	MG	DA	3132	1/1	0.98	0.23	59,59,59,59	0
60	MG	CA	1653	1/1	0.98	0.03	53,53,53,53	0
60	MG	BA	3244	1/1	0.98	0.23	60,60,60,60	0
60	MG	DA	3270	1/1	0.98	0.37	67,67,67,67	0
60	MG	BA	3115	1/1	0.98	0.22	50,50,50,50	0
60	MG	DA	3315	1/1	0.98	0.09	55,55,55,55	0
60	MG	DH	201	1/1	0.98	0.17	50,50,50,50	0
60	MG	DA	3066	1/1	0.98	0.28	52,52,52,52	0
60	MG	BA	3157	1/1	0.98	0.11	53,53,53,53	0
60	MG	BA	3073	1/1	0.98	0.21	52,52,52,52	0
60	MG	AA	1678	1/1	0.98	0.04	49,49,49,49	0
60	MG	DA	3320	1/1	0.98	0.10	55,55,55,55	0
60	MG	BA	3121	1/1	0.99	0.14	50,50,50,50	0
60	MG	CA	1696	1/1	0.99	0.07	62,62,62,62	0
60	MG	D7	101	1/1	0.99	0.15	54,54,54,54	0
60	MG	AA	1654	1/1	0.99	0.06	53,53,53,53	0
60	MG	CA	1636	1/1	0.99	0.23	53,53,53,53	0
60	MG	CA	1682	1/1	0.99	0.05	53,53,53,53	0
60	MG	DA	3124	1/1	0.99	0.17	53,53,53,53	0
61	ZN	AD	301	1/1	0.99	0.09	52,52,52,52	0
61	ZN	AN	101	1/1	0.99	0.02	60,60,60,60	1
61	ZN	B9	101	1/1	0.99	0.02	55,55,55,55	0
61	ZN	CD	301	1/1	0.99	0.17	52,52,52,52	0
61	ZN	D9	101	1/1	0.99	0.06	55,55,55,55	1
61	ZN	CN	102	1/1	1.00	0.02	60,60,60,60	0

6.5 Other polymers

There are no such residues in this entry.